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Translation of a Physiologically Based Pharmacokinetic Model Used to Develop Health Protective Levels for Trichloroethylene



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1.0 SUMMARY

Trichloroethylene (TCE) was commonly used as a solvent by the Department of Defense, as well as at private sector facilities. Releases to the environment from its past use make TCE one of the most common contaminants encountered at hazardous waste sites. The Air Force Research Laboratory previously worked with the U.S. Environmental Protection Agency (EPA) to develop a harmonized physiologically-based pharmacokinetic model for TCE; the model was updated by the EPA for their use in their toxicological review.

A request was made for technical support from the Air Force Civil Engineer Center and Mr. John Seibert at the Environment, Safety and Occupational Health Directorate in the Office of the Assistant Secretary of Defense (Energy, Installations and Environment) to participate in developing Department of Defense health protective levels for TCE by participating in a joint effort through the TriService Toxicology Consortium. In a previous effort, work was done to: 1) obtain the physiologically-based pharmacokinetic model EPA used in its *Toxicological Review of Trichloroethylene* dated September 2011 [1] and make initial efforts to validate the model; 2) perform a sensitivity analysis and evaluate the EPA's Bayesian method for prior validation and impact of their use of the method (see Appendix A of the Toxicological Review); and 3) develop a report describing the work completed. Follow-on funding was later obtained to address some of the issues noted in the previous work and to provide modeling support in the completion of a risk assessment for TCE. This new work involved the following tasks: 1) adding code to the model to ensure mass balance in tissue blood flows and volumes; 2) modify/edit the code to resolve instability in the model; 3) regenerate the validation figures and re-run the sensitivity analysis; 4) use the model to predict dose metrics for relevant endpoints for occupational exposure limit determination for specific predetermined oral and inhalation studies; and 5) develop deliverables describing the methods used and the outcomes of each of these tasks. The methods used to complete these tasks and the resulting findings are presented below.

The issues previously noted [2] with the model have been resolved with this work and any perceived barriers to using the model have been eliminated. The validation figures, for the most part, appear to duplicate those in USEPA [1], indicating that the acslX model accurately represents the MCSim model presented in USEPA [1]. This work also demonstrated that, with very few exceptions, the model is not extremely sensitive to any of the model parameters. The model was then used to generate mouse and rat internal dosimetrics corresponding to selected studies and the resulting human equivalent concentrations for both continuous and occupational inhalation exposure.

2.0 INTRODUCTION

Trichloroethylene (TCE) was commonly used as a solvent by the Department of Defense (DoD), as well as at private sector facilities. Releases to the environment from its past use make TCE one of the most common contaminants encountered at hazardous waste sites. In 2011 the U.S. Environmental Protection Agency (EPA) Integrated Risk Information System (IRIS) program finalized their toxicological review for TCE [1]. The study used for dose response for the developmental endpoint reference concentration (RfC) is controversial; the EPA used Johnson *et al.* [3], a rat ingestion study, to develop the RfC for inhaled exposures. There is value, however, in better understanding the physiologically-based pharmacokinetic (PBPK)

model used for route-to-route and inter- and intra-species extrapolation and the parameters to which the model is sensitive. Air Force Research Laboratory (AFRL) previously worked with EPA to develop a harmonized PBPK model for TCE [4, 5] but it was updated by EPA for their use in their toxicological review [1]. A more mechanistic understanding of the PBPK model will provide insight into the uncertainty associated with its use by USEPA [1] to derive a human RfC. This understanding will enhance risk communication efforts to the public and DoD personnel that may be exposed to TCE via the inhalation pathway. It will also be useful to those that may use Johnson *et al.* [3] to determine values protective of occupational health and enable estimation of the impact that a repeat of this study may have on the RfC.

A request was made for technical support from the Air Force Civil Engineer Center (AFCEC) and Mr. John Seibert at the Environment, Safety and Occupational Health Directorate in the Office of the Assistant Secretary of Defense (Energy, Installations and Environment) (OASD EI&E) to participate in developing DoD health protective levels for TCE by participating in a joint effort through the TriService Toxicology Consortium (TSTC). In a previous effort [2], work was done to: 1) obtain the PBPK model EPA used in its *Toxicological Review of Trichloroethylene* dated September 2011 [1] and make initial efforts to validate the model; 2) perform a sensitivity analysis and evaluate the EPA's Bayesian method for prior validation and impact of their use of the method (see Appendix A of the Toxicological Review); and 3) develop a report describing the work completed. Follow on funding was later obtained to address some of the issues noted in the previous work and to provide modeling support in the completion of a risk assessment for TCE. This new work involved the following tasks: 1) adding code to the model to ensure mass balance in tissue blood flows and volumes; 2) modify/edit the code to resolve instability in the model and make sure there are no additional issues; 3) regenerate the validation figures and re-run the sensitivity analysis; 4) use the model to predict dose metrics for relevant endpoints for operational exposure limit (OEL) determination for specific oral and inhalation studies; and 5) develop deliverables describing the methods used and the outcomes of each of these tasks. The methods used to complete these tasks and the resulting findings are presented below.

This effort will assist in developing DoD health protective levels for TCE. It will also identify data gaps that will reduce uncertainty in current and future protective levels.

3.0 TASK 1: ADD CODE TO ENSURE MASS BALANCE FOR TISSUE BLOOD FLOWS AND VOLUMES

3.1 Methods

Previously, the MCSim [6] code for the model listed in Appendix A of USEPA [1] was translated/reformatted for use in acslX (AEgis Technologies, Orlando FL, production discontinued). This reformatting involved the deletion of unnecessary lines of code (*e.g.*, lines defining input, output and state variables in MCSim that are not used in acslX) and some recoding to account for differences between how MCSim completes some tasks and how acslX completes them (*e.g.*, integration, code for dosing). Some variables were also renamed slightly for consistency (*e.g.*, RUrnTCA was renamed to RAUrnTCA) or to be shorter (*e.g.*, "Collect" in the variable name changed to "Coll"). Units for the constants were updated in the comments if appropriate and were added, when known, if missing in the comments. Variables calculated in

the MCSim code but not used as an output or in another calculation were deleted to decrease computational memory required [2].

Original coding in the MCSim model calculated the blood flow to the rapidly perfused tissues as the total cardiac output minus all of the other tissue blood flows, and the volume of the slowly perfused tissues as a total perfused volume of the body minus all of the other tissue volumes [6].

$Q_{Tiss} = Q_{TissC} * QC$, where *Tiss* equals *Fat*, *Gut*, *Kid*, *Liv* or *Slw*, and *TissC* is the fractional blood flow to the tissue.

$$Q_{Rap} = QC - Q_{Fat} - Q_{Gut} - Q_{Kid} - Q_{Liv} - Q_{Slw}$$

$V_{Tiss} = V_{TissC} * BW$, where *Tiss* equals *Bld*, *Fat*, *Gut*, *Kid*, *Liv*, *Rap* or *Resp*, and *TissC* is the fractional volume of the tissue.

$V_{Slw} = (V_{PerfC} * BW) - V_{Bld} - V_{Fat} - V_{Gut} - V_{Kid} - V_{Liv} - V_{Rap} - V_{Resp}$, where *PerfC* is the fractional volume of the perfused portion of the body.

While unlikely, if the upper bounds (as given in the distribution definitions in the MCSim input files in the supplemental material) for all of the fractional blood flows were selected for an iteration, the sum of these fractional blood flows (Q_{FatC} , Q_{GutC} , Q_{KidC} , Q_{LivC} and Q_{SlwC}) would sum to more than 1.0. This alone would cause issues with mass balance for the flows; however, the rapidly perfused blood flow (Q_{Rap}) would be negative. The potential for negative values also exists for the fractional tissue volumes. Issues could also arise if fractional values were incorrectly entered. To avoid the potential for mass balance issues, the code was modified for the current project to adjust the individual parameters based on the sum of the fractional values.

$$Q_{Adjus} = Q_{FatC} + Q_{GutC} + Q_{KidC} + Q_{LivC} + Q_{RapC} + Q_{SlwC}$$

$$Q_{Tiss} = \frac{Q_{TissC}}{Q_{Adjus}} * QC$$

$$QC = Q_{Fat} + Q_{Gut} + Q_{Kid} + Q_{Liv} + Q_{Rap} + Q_{Slw}$$

$$V_{TotC} = V_{BldC} + V_{FatC} + V_{GutC} + V_{KidC} + V_{LivC} + V_{RapC} + V_{RespC} + V_{SlwC}$$

$$V_{Adjus} = \frac{V_{PerfC}}{V_{TotC}}$$

$$V_{Tiss} = (V_{TissC} * V_{Adjus}) * BW$$

This coding also required setting values for Q_{RapC} and V_{SlwC} rather than calculating them as in the MCSim code listing. These values were manually calculated.

3.2 Results

The completed reformatting of the model code compiled in acslX with no errors.

4.0 TASK 2: MODIFY/EDIT THE CODE TO RESOLVE MODEL INSTABILITY

4.1 Methods

There were issues with the acslX version of the MCSim model code predicting negative values for parameters and exhibiting instability for some of the runs. In particular, for non-inhalation dosing, the code results in negative values for the concentration in the inhalation respiratory tract lumen ($C_{InhResp}$) and the respiratory tract tissue (C_{Resp}) which, in turn, results in negative values for concentration in arterial blood (C_{Art}) and the exhalation respiratory tract lumen ($C_{ExhResp}$). For some of the inhalation dosing simulations, the model also predicted unexpected drops in venous blood concentration (C_{Ven}), indicating it may also not be working as intended for inhalation dosing. It was also noted that the MCSim model code contains numerous statements that essentially reset variable values to zero if the variable value was less than 0 or a variable used in its calculation was less than 0 (e.g., if A_{BodTCA} is less than zero, the model sets C_{BodTCA} to zero rather than A_{BodTCA}/V_{Bod}). These statements, however, did not eliminate the issue of some model instability in the acslX version of the code.

In order to address the instability and prediction of negative values, the formatting of the acslX code was modified and/or edited.

- Statements resetting values to zero if the value was less than 0 were removed as it was felt that these should not be needed in the acslX code if the model maintained mass balance and was stable.
- Equations defining state variables with the rate equations embedded were separated into separate rate equations and state variable definition equations.
- Some parameters within the model were renamed for consistency.
- Coding to calculate $AExhExp$ was altered to better duplicate the coding in the MCSim model code.
- Equations in the MCSim code for C_{Art} and C_{Art_Tmp} were combined as it was felt that having them separate would not make any difference in the acslX code.
- Predictions for $AUrnTCA\_Sat$ when $TCAUrnSat$ is 1 are the same as for $AUrnTCA\_Coll$ when $TCAUrnSat$ is 0 (same for $AUrnTCOG\_Sat$ and $AUrnTCOG\_Coll$) so $TCAUrnSat$ and $TCOGUrnSat$ were deleted and $AUrnTCA\_Sat$ and $AUrnTCA\_Coll$ were replaced with $AUrnTCA\_SatColl$ and $AUrnTCOG\_Sat$ and $AUrnTCOG\_Coll$ were replaced with $AUrnTCOG\_SatColl$.
- Code for changing the inhaled concentration during exposure was added to the model code itself rather than changing it within the script file to more efficiently change the concentration during a simulation.
- Additional equations were added to calculate additional dose metric values not originally in the MCSim model code.

In addition to the changes to the acslX model code, error tolerances were altered separately for the mouse, rat and human simulations such that any negative values predicted for the validation figures were smaller than approximately $-2e-7$ with most being smaller than $-1.0e-10$. Some values of $ExhFac\_Den$, $ExhFactor$ and $AExhPost$ were an exception, but as these were

only used for output variables and, thus, did not affect any other variables, no additional changes were made.

4.2 Results

The modified/edited acslX version of the model code compiled in acslX with no errors and runs without displaying any instability. Any predicted negative values are now within an acceptable tolerance. The model code is given in Appendix A.

5.0 TASK 3A: REGENERATE THE VALIDATION FIGURES

5.1 Methods

As noted in the previous work [2], while some of the reproduced figures appeared to match the figures in Appendix A of USEPA [1] quite well, others did not match and some deviated greatly. However, the shape of the curves was similar suggesting that some of the discrepancies were due to parameterization issues. Also, the reproduced figures used the population posterior means as the posterior subject-specific parameters were not given in USEPA [1]. An additional issue in creating the script files to reproduce the figures was the truncation of some of the data lines in the PDF of the MCSim files. Following the completion of the previous work, the original text versions of the MCSim input and output files were obtained through personal communication with Dr. Weihsueh Chiu (Appendices B, C and D). Thus the data in the previously developed script files were updated with the data from the MCSim input files and the subject-specific parameters were used from the MCSim output files.

As mentioned above, the subject-specific parameters were not necessarily the parameters needed for input into the model. For example, $\ln QCC$, the natural log of the change in QCC from the baseline value is in the output file but the model expects QCC . Also, not all of the parameter values were included in the MCSim output file (*e.g.*, parameters that were set in the MCSim input file and not varied). Therefore, spreadsheets were created for mouse, rat and human to convert the values, as necessary, for use in the acslX model code. These calculations were made using values from the MCSim model definition file as the baseline values, and the MCSim input files were checked to see which values were directly set rather than being defined with distributions so that they could be set accordingly in the script files for the figures. Study- and individual-specific parameter values and dose-specific parameter values are included in the M files in Appendix E.

There were also some discrepancies, noted in Covington *et al.* [2], with trying to align the reproduced figures for human data from Kimmerle and Eben [7] with those in Appendix A of USEPA [1]. These discrepancies were eliminated by having the MCSim input file and being able to see the data and parameter settings for the figures in question.

5.2 Results

Reproduced figures for the mouse, rat and human are shown in the attached Appendices F, G and H, respectively. M files to generate these figures for mouse, rat and human are given in Appendices I, J and K, respectively, with the corresponding data presented in Appendices L, M and N. With few exceptions, the reproduced figures appear to match the figures in Appendix A

of USEPA [1]. The figures for the Chiu *et al.* [8] human study seem a little off, particularly for those labeled for Human #37 and #39. These differences and any others not perceptible upon visual comparison could simply be due to differences in the way MCSim and acslX solve the system of equations and the manner in which some of the code for dosing differs between the two modeling platforms.

The figures for the Muller *et al.* [9] human study show that the acslX version of the model consistently under-predicts the data. Given that mouse and rat data for oral TCA dosing are both well predicted by the model, it is felt that the issue for the human data is not due to coding issues. There were no other data for oral TCOH dosing with which to compare to validate the coding for TCOH dosing. The shape of the curves for predictions of the Muller *et al.* [9] data also match the shape of the data well. Thus it is thought that the under-predictions may be due to issues in parameterization for this study; however, upon closer inspection, no discrepancies were found between the parameters used here and those provided by Dr. Chiu via MCSim input and output files. Given that the purpose of the model here is for simulating dosing with TCE only, this issue should not impact any predictions for animal internal dose metrics or corresponding predictions for human equivalent concentrations (HECs).

It is important to note that these reproduced figures will differ from the ones in USEPA [1] in that the lines for the simulations will be smoother for the reproductions. USEPA [1] simulations using MCSim outputs the endpoint values at discrete time points that match the data collection time points. Output from the acslX runs to validate the model were continuous time-courses for the simulation period; thus, more points are plotted on the simulation lines in the reproduced figures. The reproduced figures use approximately the same axis-scale limits as USEPA [1] figures to the extent possible. The figures here are in the same order as those they reproduce from USEPA [1].

6.0 TASK 3B: RE-RUN THE SENSITIVITY ANALYSIS

6.1 Methods

Sensitivity analyses were re-run for the mouse, rat and human at the same TCE doses and exposure scenarios as used by USEPA [1] for their sensitivity analyses. In Covington *et al.* [2], only three of the dosemetrics used by USEPA [1] for their sensitivity analyses were included in the sensitivity analyses as the additional endpoints included in the analyses were not calculated in the MCSim model definition file. The calculations for the additional endpoints were obtained from Dr. Chiu along with the MCSim input and output files. Mouse and rat runs simulated inhalation (100 and 600 ppm) exposure for 7 hours per day, 5 days per week or oral gavage (300 and 1000 mg/kg/day) exposure 5 days per week for 10 weeks. Separate human simulations were run for male and females; simulations for both were run for continuous exposure to 0.001 ppm or 0.001 mg/kg/day. All human simulations were run for 100 weeks. The mean posterior values in Tables 1 through 4 were used for the simulations. As with the study- and individual-specific values in the M files in the appendices, these values were obtained from the MCSim model definition file from USEPA [1] and from the MCSim input and output files from Dr. Chiu.

Table 1. Mean Mouse Posterior Parameters

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
BW	0.03			0.03
QCC	11.6		1.228	14.24
VPR	2.5		0.8074	2.019
DRespC		1.221		1.221
QFatC	0.07		1.033	0.07231
QGutC	0.141		1.178	0.1661
QKidC	0.091		0.9933	0.09039
QLivC	0.02		1.033	0.02066
QRapC				0.4370 ^a
QSlwC	0.217		0.9842	0.2136
VBldC	0.049		0.9921	0.04861
VFatC	0.07		1.328	0.09296
VGutC	0.049		0.9869	0.04836
VKidC	0.017		1.0	0.0170
VLivC	0.055		0.8080	0.04444
VPerfC	0.8897			0.8897
VRapC	0.1		0.9968	0.09968
VRespC	0.0007		1.0	0.0007
VRespLumC	0.004667		1.0	0.004667
VSlwC				0.5379 ^b
FracPlas	0.52		0.8718	0.4533
PB	15		0.9297	13.95
PFat	36		0.9880	35.57
PGut	1.9		0.8075	1.534
PKid	2.1		1.266	2.658
PLiv	1.7		1.283	2.182
PRap	1.9		0.9555	1.815
PResp	2.6		0.9947	2.586
PSlw	2.4		0.9258	2.222
PRBCPlasTCA	0.5		2.470	1.235
PBodTCAC	0.88		0.8875	0.7810
PLivTCAC	1.18		0.8034	0.9480
PBodTCOH	1.11		0.8040	0.8924
PLivTCOH	1.3		1.497	1.946
PBodTCOG	1.11		0.420	0.4662
PLivTCOG	1.3		1.015	1.319
PEffDCVG		0.9871		0.9871
BMaxkDC	0.88		1.241	1.092
kDissoc	107		1.178	126.0
kAS		1.798		1.798
kTSD		5.259		5.259

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
kAD		0.2677		0.2677
kTD	0.0 ^c			0.0 ^c
kASTCA		3.975		3.975
kASTCOH		0.730		0.730
VMaxC	2700		0.6707	1811
KMC	36		0.07288	2.624
Cl	na			na
FracTCAC	0.32		0.4870	0.1559
FracOtherC		0.02371		0.02371
VMaxDCVGC	300		2.621	786.4
KMDCVGC	na			na
ClDCVG	1.53		0.3588	0.5490
VMaxKidDCVGC	60		2.573	154.4
KMKidDCVGC	na			na
ClKidDCVG	0.34		1.216	0.4134
VMaxLungLiv	0.0701021		2.782	0.1950
KMClara		0.01195		0.01195
FracLungSysC		4.384		4.384
VMaxTCOHC		1.643		1.643
KMTCOH		0.9326		0.9326
ClTCOH	na			na
VMaxGlucC		69.55		69.55
KMGluc		30.45		30.45
ClGluc	na			na
kMetTCOHC		3.367		3.367
kUrnTCAC	0.6		0.1096	0.06575
kMetTCAC		0.6127		0.6127
kBileC		1.014		1.014
kEHRC		0.01208		0.01208
kUrnTCOGC	0.6		8.593	5.156
kDCVGC		0.1890		0.1890
FracKidDCVCC		1.537		1.537
kNATC		0.1165		0.1165
kKidBioactC		0.08786		0.08786

Notes: Baseline values are from MCSim model code. Absolute values and fractional increases are from the MCSim output file from Dr. Chiu. Calculated posteriors of “na” are parameters not used for the mouse.

^aCalculated as 1.0 minus the sum of the other fractional tissue blood flows.

^bCalculated as VPerfC minus the sum of the fractional volumes for blood, fat, gut, kidney, liver, rapid and respiratory tissue.

^cSet to zero in the model definition file in the appendix of USEPA [1].

Table 2. Mean Rat Posterior Parameters

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
BW	0.3			0.3
QCC	13.3		1.192	15.85
VPR	1.9		0.6229	1.184
DRespC		2.553		2.553
QFatC	0.07		1.187	0.08309
QGutC	0.153		1.147	0.1755
QKidC	0.141		1.002	0.1413
QLivC	0.021		1.032	0.02167
QRapC				0.2751 ^a
QSlwC	0.336		0.9028	0.3033
VBldC	0.074		1.002	0.07415
VFatC	0.07		0.9720	0.06804
VGutC	0.032		0.9892	0.03165
VKidC	0.007		0.9927	0.006949
VLivC	0.034		0.9844	0.03347
VPerfC	0.8995			0.8995
VRapC	0.088		0.9931	0.08739
VRespC	0.0005		0.9917	0.0004959
VRespLumC	0.004667		1.005	0.004690
VSlwC				0.5974 ^b
FracPlas	0.53		1.042	0.5523
PB	22		0.8544	18.80
PFat	27		1.130	30.50
PGut	1.4		0.8654	1.212
PKid	1.3		0.9398	1.222
PLiv	1.5		1.042	1.564
PRap	1.3		1.079	1.403
PResp	1		0.9555	0.9555
PSlw	0.58		1.292	0.7493
PRBCPlasTCA	0.5		0.9624	0.4812
PBodTCAC	0.88		1.117	0.9826
PLivTCAC	1.18		1.282	1.513
PBodTCOH	1.11		0.9510	1.056
PLivTCOH	1.3		0.9601	1.248
PBodTCOG	1.11		1.240	1.376
PLivTCOG	1.3		8.585	11.16
PEffDCVG	na			na
BMaxkDC	1.22		0.9516	1.161
kDissoc	275		0.9762	268.5
kAS		2.721		2.721
kTSD		4.166		4.166
kAD		0.1810		0.1810

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
kTD	0.0 ^c			0.0 ^c
kASTCA		1.488		1.488
kASTCOH		0.6880		0.6880
VMaxC	600		0.9528	571.7
KMC	21		0.03515	0.7382
Cl	na			na
FracTCAC	0.32		0.2488	0.07962
FracOtherC		0.3097		0.3097
VMaxDCVGC	66		11.98	790.5
KMDCVGC	na			na
ClDCVG	0.25		0.3721	0.09302
VMaxKidDCVGC	6		0.2108	1.265
KMKidDCVGC	na			na
ClKidDCVG	0.026		181.8	4.727
VMaxLungLiv	0.01435		3.323	0.04768
KMClara		0.02078		0.02078
FracLungSysC		1.981		1.981
VMaxTCOHC		2.018		2.018
KMTCOH		22.42		22.42
CITCOH	na			na
VMaxGlucC		27.17		27.17
KMGluc		5.877		5.877
ClGluc	na			na
kMetTCOHC		1.976		1.976
kUrnTCAC	0.522		0.07186	0.03751
kMetTCAC		0.3253		0.3253
kBileC		7.553		7.553
kEHRC		1.468		1.468
kUrnTCOGC	0.522		20.51	10.71
kDCVGC		22026 ^d		22026 ^d
FracKidDCVCC		22026 ^d		22026 ^d
kNATC		0.002089		0.002089
kKidBioactC		0.006902		0.006902

Notes: Baseline values are from MCSim model code. Absolute values and fractional increases are from the MCSim output file from Dr. Chiu. Calculated posteriors of “na” are parameters not used for the rat.

^aCalculated as 1.0 minus the sum of the other fractional tissue blood flows.

^bCalculated as VPerfC minus the sum of the fractional volumes for blood, fat, gut, kidney, liver, rapid and respiratory tissue.

^cSet to zero in the model definition file in the appendix of USEPA [1].

^dValue is set in MCSim input file for the rat from Dr. Chiu.

Table 3. Mean Human Female Posterior Parameters

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
BW	60			60
QCC	16		0.8353	13.36
VPR	0.96		1.526	1.465
DRespC		0.6080		0.6080
QFatC	0.085		0.7783	0.06616
QGutC	0.21		0.7914	0.1662
QKidC	0.17		1.008	0.1714
QLivC	0.065		0.5071	0.03296
QRapC				0.4410 ^a
QSlwC	0.17		0.7196	0.1223
VBldC	0.068		1.012	0.06882
VFatC	0.317		0.7823	0.2480
VGutC	0.022		1.001	0.02202
VKidC	0.0046		0.9969	0.004586
VLivC	0.023		1.044	0.02401
VPerfC	0.85778			0.85778
VRapC	0.093		0.9959	0.09262
VRespC	0.00018		0.9999	0.000180
VRespLumC	0.002386		1.003	0.002393
VSlwC				0.3976 ^b
FracPlas	0.615		1.001	0.6156
PB	9.5		0.9699	9.214
PFat	67		0.8515	57.05
PGut	2.6		1.090	2.834
PKid	1.6		0.9996	1.599
PLiv	4.1		0.9890	4.055
PRap	2.6		0.9256	2.407
PResp	1.3		1.011	1.314
PSlw	2.1		1.160	2.435
PRBCPlasTCA	0.5		0.2888	0.1444
PBodTCAC	0.52		1.189	0.6182
PLivTCAC	0.66		1.193	0.7873
PBodTCOH	0.91		1.718	1.564
PLivTCOH	0.59		1.067	0.6294
PBodTCOG	0.91		0.6819	0.6206
PLivTCOG	0.59		6.514	3.843
PEffDCVG		0.01028		0.01028
BMaxkDC	4.62		0.8813	4.071
kDissoc	182		0.9933	180.8
kAS	na ^c			na ^c
kTSD	na ^c			na ^c
kAD	na ^c			na ^c

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
kTD	0.0 ^d			0.0 ^d
kASTCA		5.270		5.270
kASTCOH		7.301		7.301
VMaxC	255		0.3714	94.70
KMC	na			na
Cl	66		13.05	861.5
FracTCAC	0.32		0.1278	0.04091
FracOtherC		0.1072		0.1072
VMaxDCVGC	na			na
KMDCVGC	2.9		1.247	3.618
ClDCVG	19		2.779	52.80
VMaxKidDCVGC	na			na
KMKidDCVGC	2.7		0.3097	0.8363
ClKidDCVG	230		0.03453	7.941
VMaxLungLiv	0.02727		3.466	0.09453
KMClara		0.2434		0.2434
FracLungSysC		23.57		23.57
VMaxTCOHC	na			na
KMTCOH		2.271		2.271
CITCOH		0.1766		0.1766
VMaxGlucC	na			na
KMGluc		129.3		129.3
ClGluc		0.2811		0.2811
kMetTCOHC		0.6991		0.6991
kUrnTCAC	0.108		0.04537	0.004899
kMetTCAC		0.2755		0.2755
kBileC		7.243		7.243
kEHRC		0.1561		0.1561
kUrnTCOGC	0.108		16.93	1.828
kDCVGC		7.171		7.171
FracKidDCVCC		22026 ^e		22026 ^e
kNATC		0.0003495		0.0003495
kKidBioactC		0.06279		0.06279

Notes: Baseline values are from MCSim model code. Absolute values and fractional increases are from the MCSim output file from Dr. Chiu. Calculated posteriors of “na” are parameters not used for the human females.

^aCalculated as 1.0 minus the sum of the other fractional tissue blood flows.

^bCalculated as VPerfC minus the sum of the fractional volumes for blood, fat, gut, kidney, liver, rapid and respiratory tissue.

^cNot included in posterior estimations. No TCE oral dosing data so set to zero.

^dSet to zero in the model definition file in the appendix of USEPA [1].

^eValue is set in MCSim input file for the rat from Dr. Chiu.

Table 4. Mean Human Male Posterior Parameters

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
BW	70			70
QCC	16		0.8353	13.36
VPR	0.96		1.526	1.465
DRespC		0.6080		0.6080
QFatC	0.05		0.7783	0.03892
QGutC	0.19		0.7914	0.1504
QKidC	0.19		1.008	0.1915
QLivC	0.065		0.5071	0.03296
QRapC				0.4279 ^a
QSlwC	0.22		0.7196	0.1583
VBldC	0.077		1.012	0.07792
VFatC	0.199		0.7823	0.1557
VGutC	0.02		1.001	0.02002
VKidC	0.0043		0.9969	0.004287
VLivC	0.025		1.044	0.02610
VPerfC	0.856			0.8560
VRapC	0.088		0.9959	0.08764
VRespC	0.00018		0.9999	0.000180
VRespLumC	0.002386		1.003	0.002393
VSlwC				0.4842 ^b
FracPlas	0.567		1.001	0.5676
PB	9.5		0.9699	9.214
PFat	67		0.8515	57.05
PGut	2.6		1.090	2.834
PKid	1.6		0.9996	1.599
PLiv	4.1		0.9890	4.055
PRap	2.6		0.9256	2.407
PResp	1.3		1.011	1.314
PSlw	2.1		1.160	2.435
PRBCPlasTCA	0.5		0.2888	0.1444
PBodTCAC	0.52		1.189	0.6182
PLivTCAC	0.66		1.193	0.7873
PBodTCOH	0.91		1.718	1.564
PLivTCOH	0.59		1.067	0.6294
PBodTCOG	0.91		0.6819	0.6206
PLivTCOG	0.59		6.514	3.843
PEffDCVG		0.01028		0.01028
BMaxkDC	4.62		0.8813	4.071
kDissoc	182		0.9933	180.8
kAS	0.0 ^c			0.0 ^c
kTSD	0.0 ^c			0.0 ^c
kAD	0.0 ^c			0.0 ^c

Parameter	Baseline	Absolute Value	Fractional Increase	Final Value
kTD	0.0 ^d			0.0 ^d
kASTCA		5.270		5.270
kASTCOH		7.301		7.301
VMaxC	255		0.3714	94.70
KMC	na			na
Cl	66		13.05	861.5
FracTCAC	0.32		0.1278	0.04091
FracOtherC		0.1072		0.1072
VMaxDCVGC	na			na
KMDCVGC	2.9		1.247	3.618
ClDCVG	19		2.779	52.80
VMaxKidDCVGC	na			na
KMKidDCVGC	2.7		0.3097	0.8363
ClKidDCVG	230		0.03453	7.941
VMaxLungLiv	0.02525		3.466	0.08753
KMClara		0.2434		0.2434
FracLungSysC		23.57		23.57
VMaxTCOHC	na			na
KMTCOH		2.271		2.271
CITCOH		0.1766		0.1766
VMaxGlucC	na			na
KMGluc		129.3		129.3
ClGluc		0.2811		0.2811
kMetTCOHC		0.6991		0.6991
kUrnTCAC	0.108		0.04537	0.004899
kMetTCAC		0.2755		0.2755
kBileC		7.243		7.243
kEHRC		0.1561		0.1561
kUrnTCOGC	0.108		16.93	1.828
kDCVGC		7.171		7.171
FracKidDCVCC		22026 ^e		22026 ^e
kNATC		0.0003495		0.0003495
kKidBioactC		0.06279		0.06279

Notes: Baseline values are from MCSim model code. Absolute values and fractional increases are from the MCSim output file from Dr. Chiu. Calculated posteriors of “na” are parameters not used for the human males.

^a Calculated as 1.0 minus the sum of the other fractional tissue blood flows.

^b Calculated as VPerfC minus the sum of the fractional volumes for blood, fat, gut, kidney, liver, rapid and respiratory tissue.

^c Not included in posterior estimations. No TCE oral dosing data so set to zero.

^d Set to zero in the model definition file in the appendix of USEPA [1].

^e Value is set in MCSim input file for the rat from Dr. Chiu.

Calculations for the sensitivity analysis used the central difference method with increases and decreases for the posterior parameter values of 5 percent (*i.e.*, overall change in input parameter of 10 percent). The equation used to calculate the sensitivity coefficients (SC) in USEPA [1] is given below. It normalizes the SC to both the output and input parameters so that it is unitless [10].

$$SC = \frac{(f(\theta_+) - f(\theta_-))}{f(\theta_-)} \div \frac{(\theta_+ - \theta_-)}{\theta_-} = \frac{(f(\theta_+) - f(\theta_-))}{f(\theta_-)} * \frac{\theta_-}{(\theta_+ - \theta_-)}$$

where θ_- is the baseline value minus 5 percent, θ_+ is the baseline value plus 5 percent, $f(\theta_-)$ is the response variable value resulting from an input parameter value of θ_- , and $f(\theta_+)$ is the response variable resulting from an input parameter value of θ_+ . USEPA [1] used a variation of this equation to calculate their SCs. Since the fractional change in the input parameter is always 10 percent, that term in the equation was replaced with 10 percent or 0.1.

$$SC = \frac{(f(\theta_+) - f(\theta_-))}{f(\theta_-)} \div 0.1 = \frac{(f(\theta_+) - f(\theta_-))}{f(\theta_-)} * 10$$

Next, $f(\theta_-)$ in the denominator was replaced with $(\frac{1}{2} * \{f(\theta_+) + f(\theta_-)\})$. So the USEPA [1] equation becomes:

$$SC = \frac{(f(\theta_+) - f(\theta_-))}{f(\theta_-)} * 10 = 10 * \frac{(f(\theta_+) - f(\theta_-))}{\left(\frac{1}{2} * (f(\theta_+) + f(\theta_-))\right)}$$

Given the slight difference in equations, SCs were calculated using both equations for comparison.

6.2 Results

That problems that were seen in the previous work [2] in trying to run the sensitivity analyses were not seen (*e.g.*, problems with runs not completing, numerical instability in predictions) with the modified/edited acslX version. The plots of the SCs (Figures 1 - 12) look very similar to those from USEPA [1], but do appear to differ somewhat. These differences could be due to the platforms used for the modeling and/or the manner in which the SCs were calculated (*i.e.*, during the simulation or outside of the simulation where the precision of the numbers used could vary). Another very likely cause of some differences could be that USEPA [1] conducted the sensitivity analyses on the scaling parameters (*e.g.*, the fractional change in the baseline value for the parameters), whereas the analyses here were conducted by changing the actual parameters themselves. Without the actual numerical values for the SCs, it is difficult to compare how much they differ. It should be noted that some of the axes limits in the figures here differ from those used by USEPA [1] to ensure that none of the bars are truncated.

With the modified/edited acslX version of the model, calculating the SCs using the equation in USEPA [1] as opposed to calculating them as the fractional change in output per fractional change in input made little difference. The SCs using the two different methods were

almost all within 10 percent of each other. M files to generate the output for these figures for mouse, rat and human are given in Appendix O.

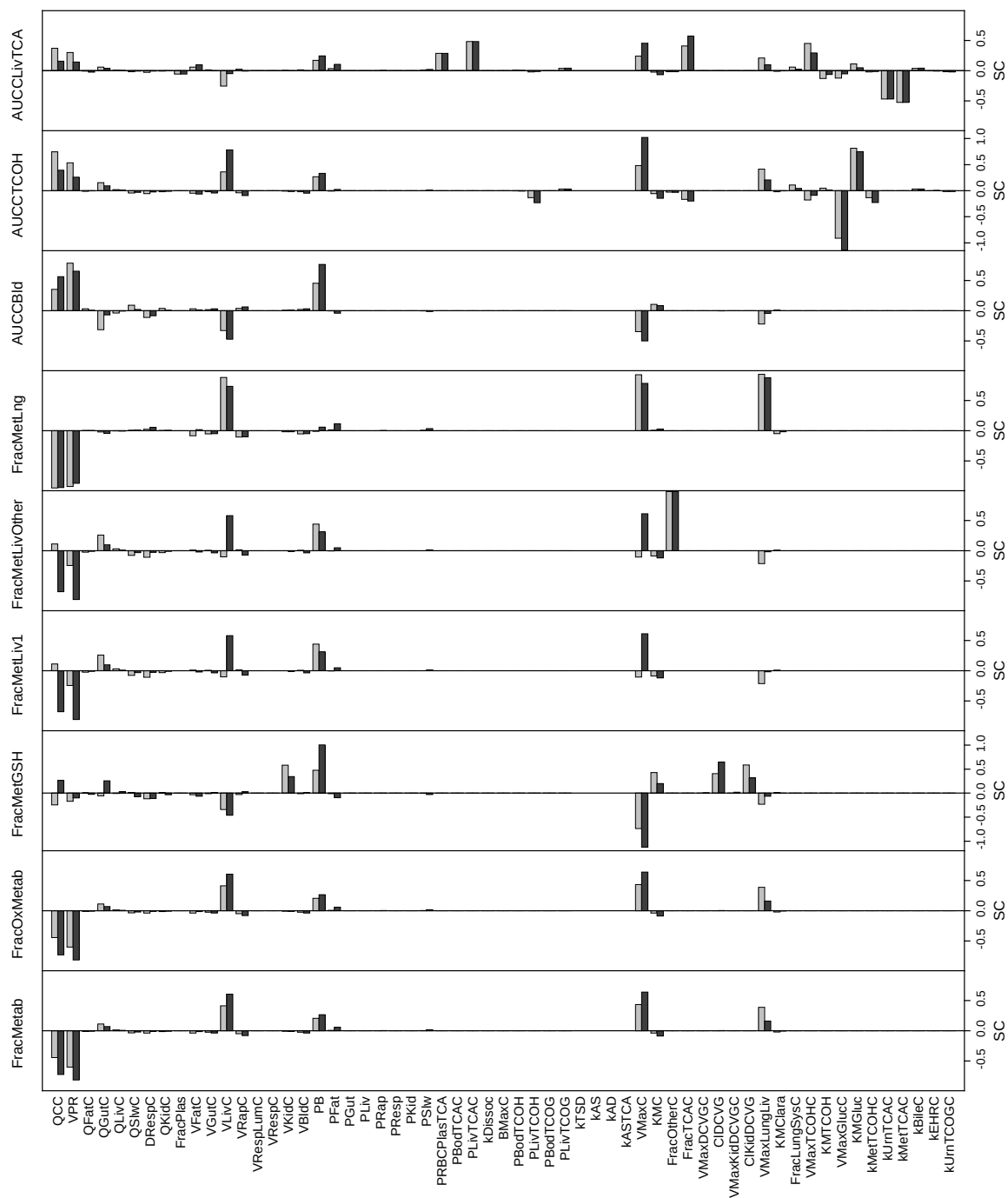


Figure 1. Sensitivity Coefficients Using USEPA [1] Equation for Mouse Following Inhalation Exposure. Exposure was 100 (light bars) or 600 ppm (dark bars) for 7 hours/day, 5 days/week for 10 weeks. SCs were calculated using equation in USEPA [1].

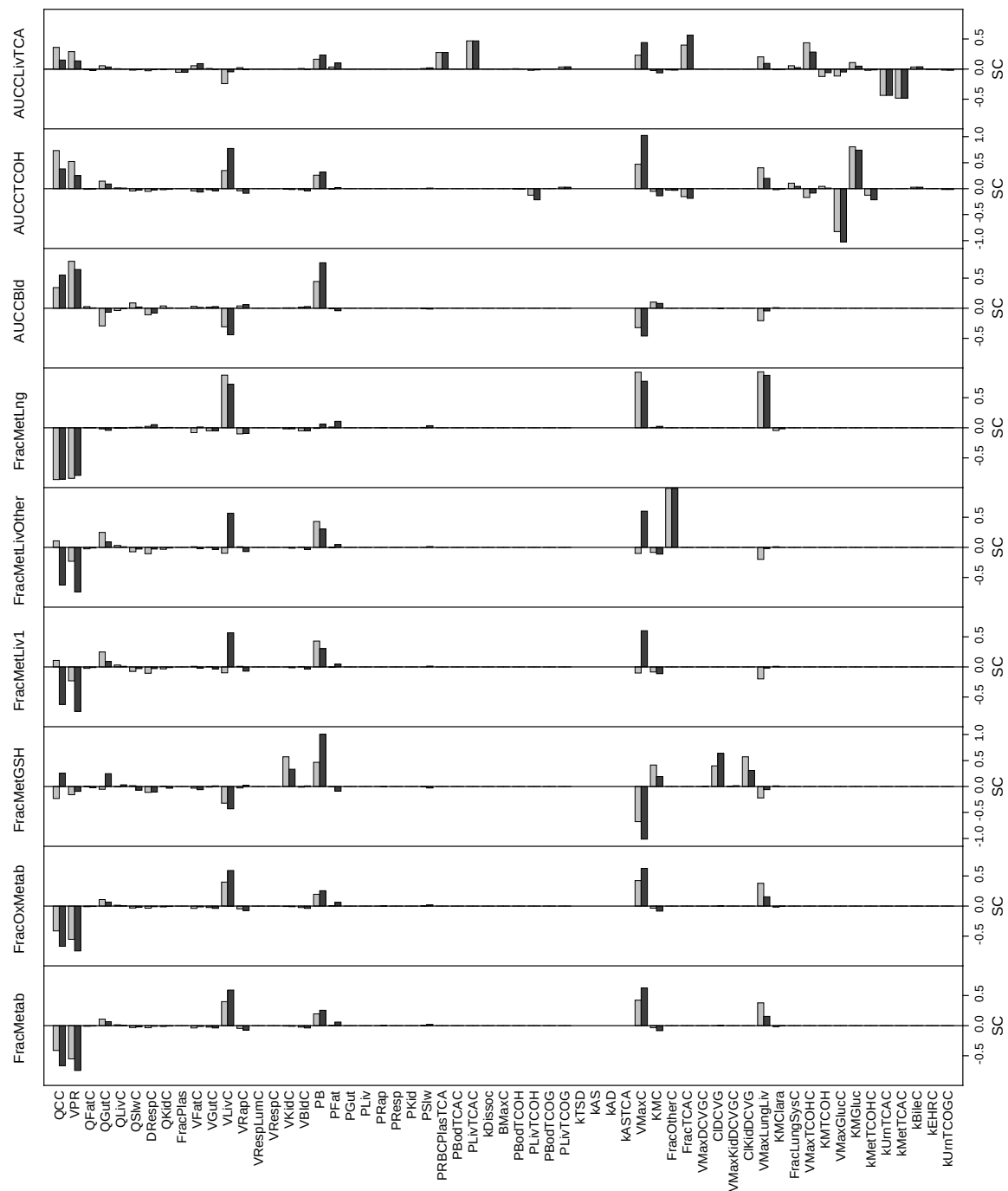
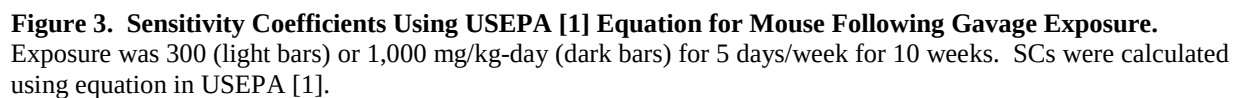


Figure 2. Sensitivity Coefficients Using Fractional Change Equation for Mouse Following Inhalation Exposure. Exposure was 100 (light bars) or 600 ppm (dark bars) for 7 hours/day, 5 days/week for 10 weeks. SCs were calculated as fractional change in output per fractional change in input.



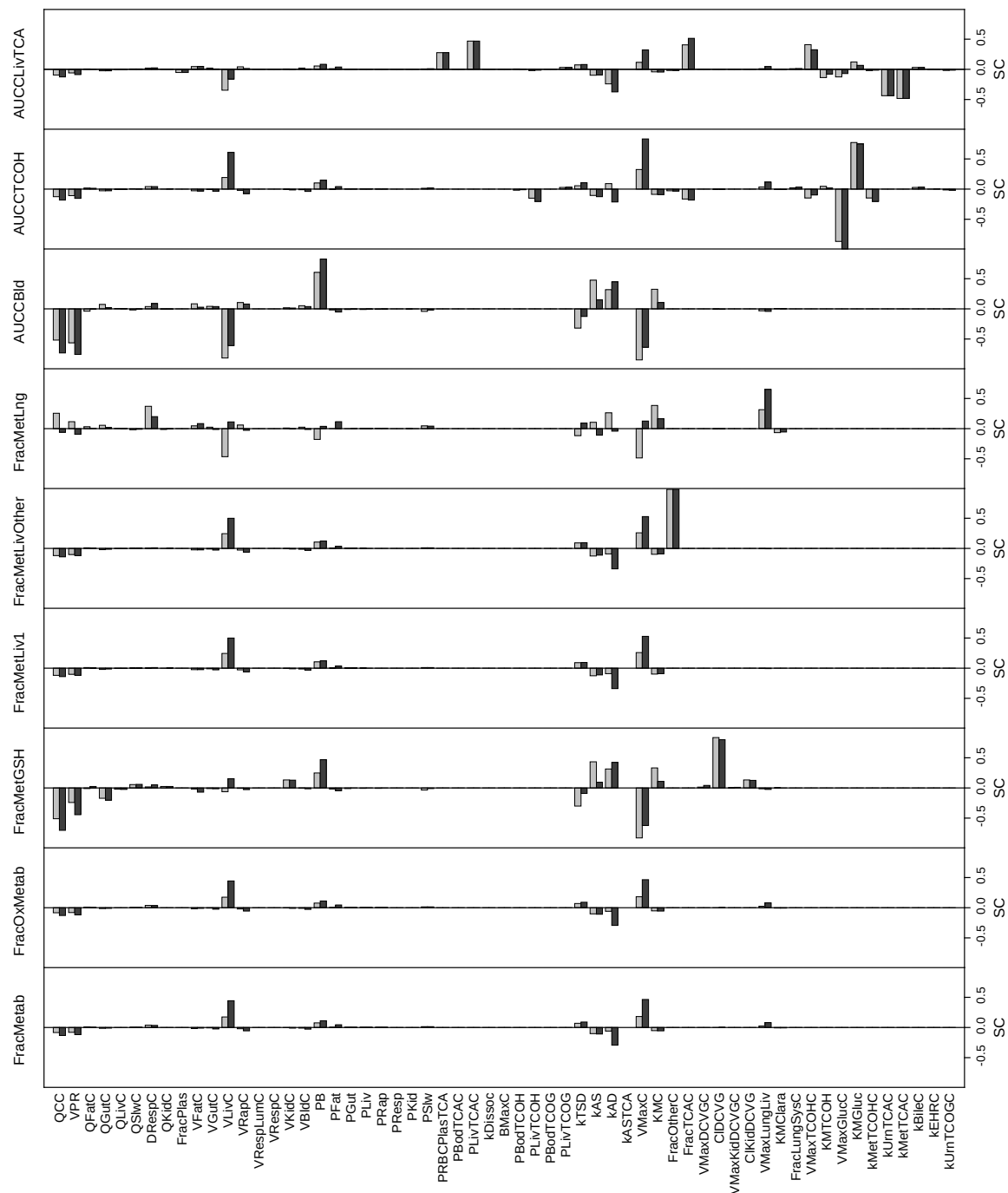


Figure 4. Sensitivity Coefficients Using Fractional Change Equation for Mouse Following Gavage Exposure. Exposure was 300 (light bars) or 1,000 mg/kg-day (dark bars) for 5 days/week for 10 weeks. SCs were calculated as fractional change in output per fractional change in input.

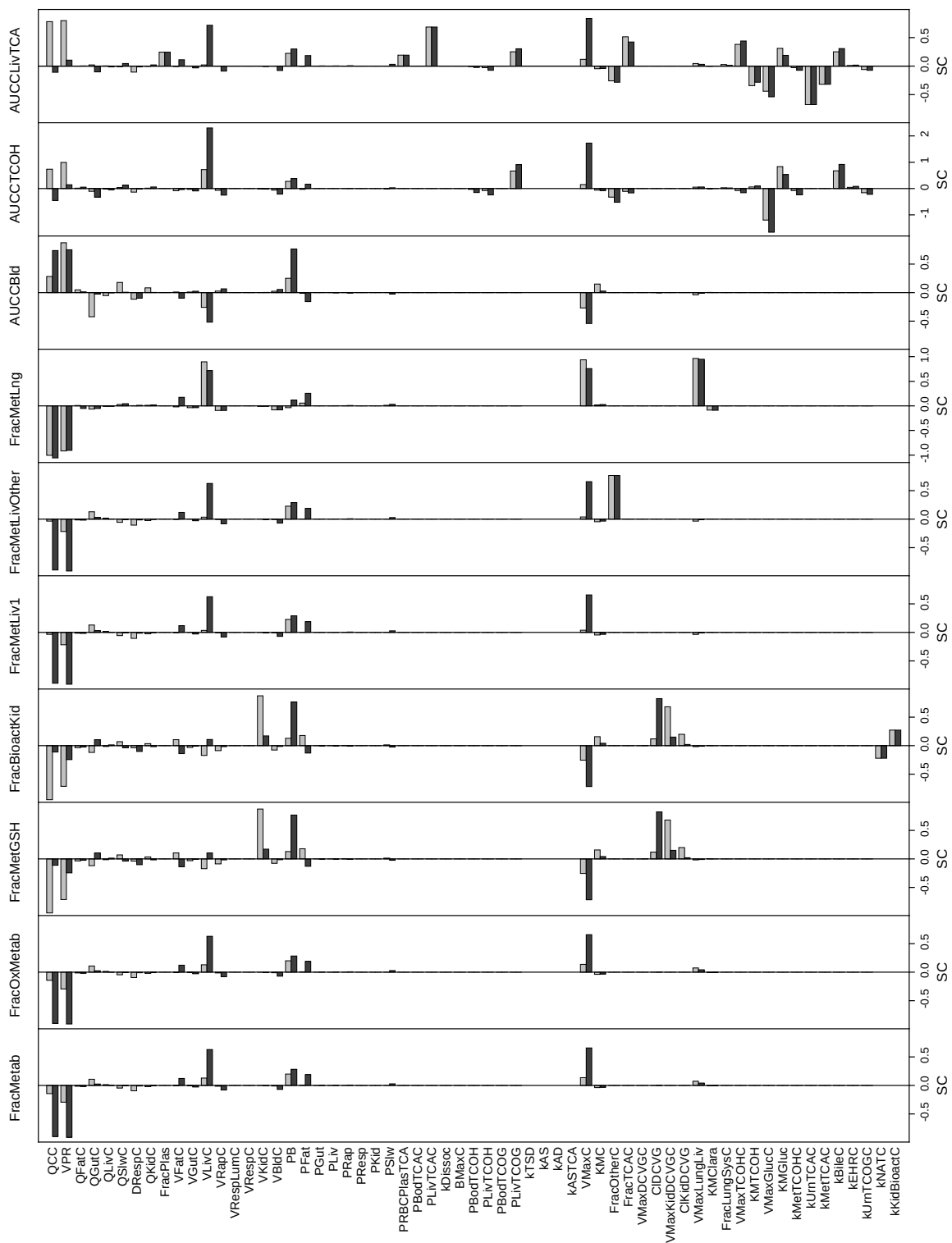


Figure 5. Sensitivity Coefficients Using USEPA [1] Equation for Rat Following Inhalation Exposure. Exposure was 100 (light bars) or 600 ppm (dark bars) for 7 hours/day, 5 days/week for 10 weeks. SCs were calculated using equation in USEPA [1].

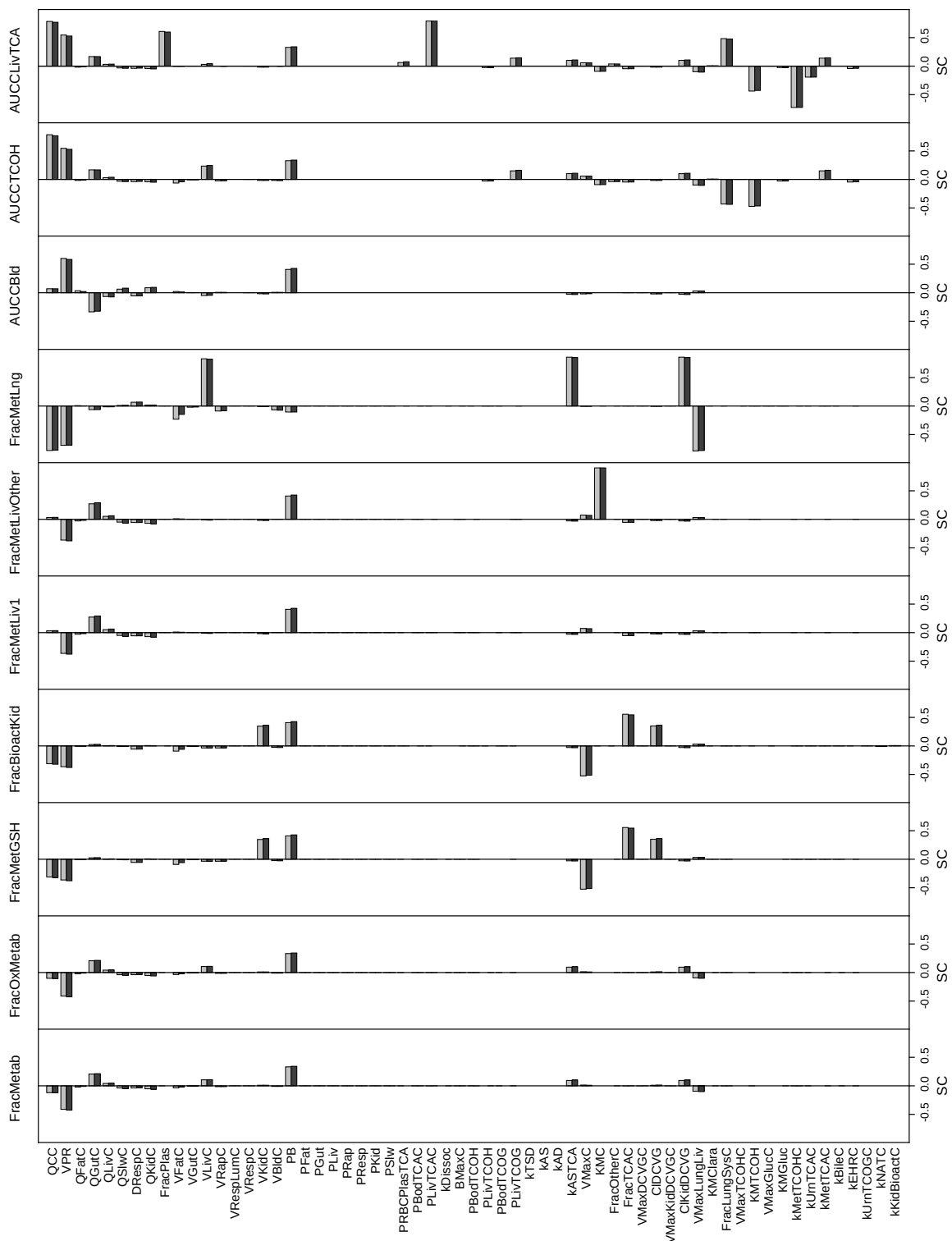


Figure 10. Sensitivity Coefficients Using Fractional Change Equation for Human Following Inhalation Exposure. Exposure was continuous 0.001 ppm to females (light bars) or males (dark bars) for 100 weeks. SCs were calculated as fractional change in output per fractional change in input.

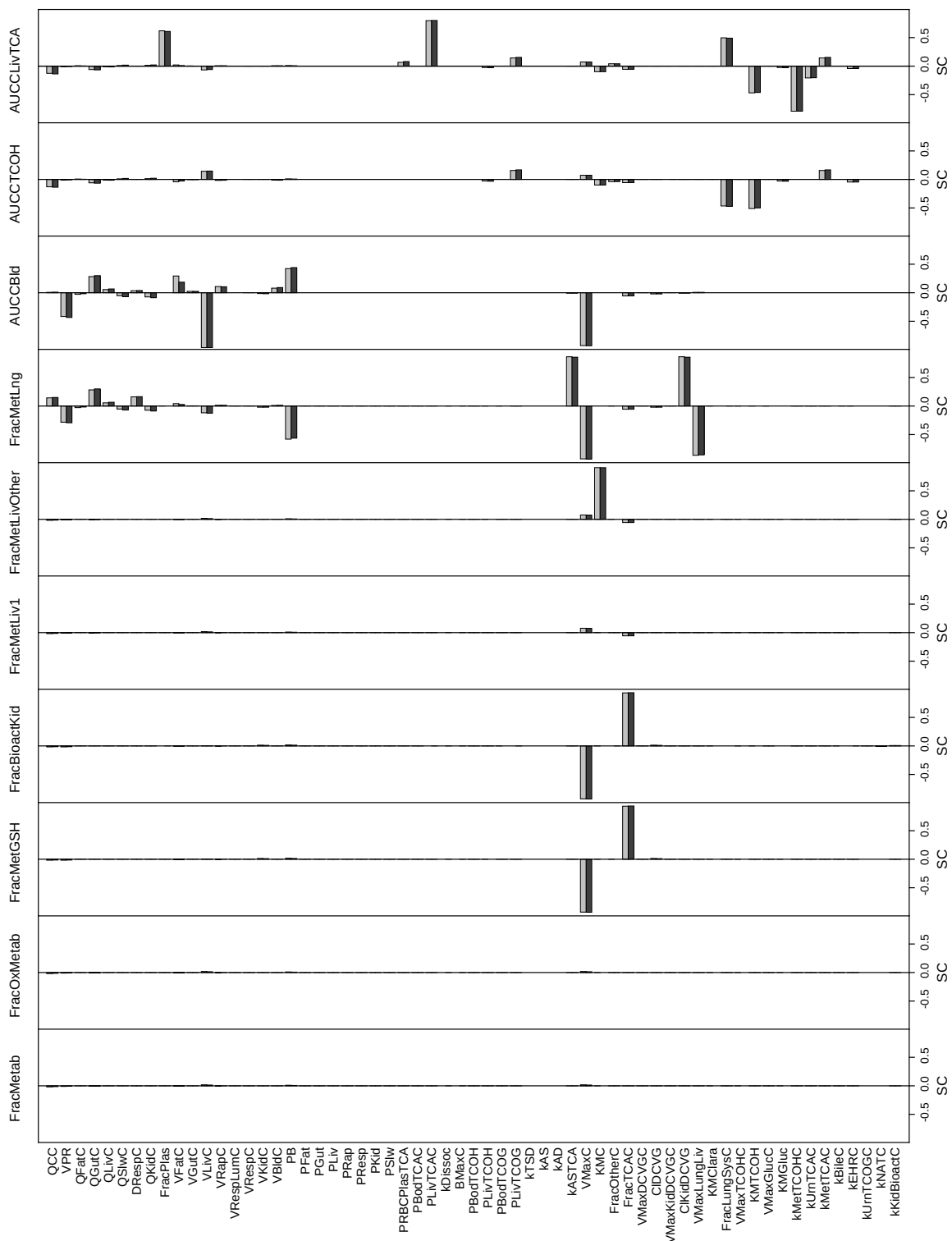


Figure 11. Sensitivity Coefficients Using USEPA [1] Equation for Human Following Oral Exposure. Exposure was continuous 0.001 mg/kg-day to females (light bars) or males (dark bars) for 100 weeks. SCs were calculated using equation in USEPA [1].

7.0 TASK 4: PREDICT DOSE METRICS FOR OEL DETERMINATION

7.1 Methods

A spreadsheet of points of departure for animal studies for which internal dose metrics needed to be simulated were sent by Dr. Thomas Sussan along with the published studies. Script files (Appendices P and Q) were then created for these simulations using the mean posterior animal parameters (Tables 1 and 2) and the study-specific parameter settings (*e.g.*, body weights, dose, exposure scenario). For some studies, the body weights were not reported. In these cases, internet searches were conducted to find an appropriate body weight given the particular animal strain and age (if reported). For longer term exposures, the model was run until steady-state or periodicity was reached rather than for the entire length of the study in order to decrease computational time. Details of settings for the simulations are given in Table 5. For daily exposures, the dose metrics are the values for last day of exposure; for exposures that were not daily (*i.e.*, 6 hours/day for 5 days/week), the values are for the last week and are then divided by 7 to get an average daily value. All simulations were checked to ensure that any predicted negative values were within an acceptable tolerance. The dose metrics output and the corresponding units were:

- Peak concentration of TCE in the blood (mg/L)
- Area under the curve (AUC) for TCE in the blood (mg-h/L/d)
- Total amount of TCE metabolized scaled by body weight (mg/kg^{0.75}/d)
- Total amount of TCE metabolized by oxidation scaled by body weight (mg/kg^{0.75}/d)
- Peak concentration of TCE in the liver (mg/L)
- AUC for TCE in the liver (mg-h/L/d)
- Amount of TCE metabolized in the liver scaled by body weight (mg/kg^{0.75}/d)
- Peak concentration of TCE in the kidney (mg/L)
- AUC for TCE in the kidney (mg-h/L/d)
- Amount of TCE metabolized in the kidney scaled by body weight (mg/kg^{0.75}/d)

Table 5. Summary of Settings for Animal Study Simulations

Study Name	Route	Species	Sex	Domain	Body Weight (kg)	Dose or Concentration	Simulation
Adams <i>et al.</i> , [11]	Inhalation	Rat	Female & Male	Kidney & Liver	0.207 & 0.349	200 ppm	7 hours/day, 5 days/week for 6 weeks (until periodicity)
Albee <i>et al.</i> [12]	Inhalation	Rat	Female & Male	Neuro	0.2 & 0.4	800 ppm	6 hours/day, 5 days/week for 13 weeks
Arito <i>et al.</i> [13]	Inhalation	Rat	Male	Neuro	0.375	18.4 ppm	8 hours/day, 5 days/week for 6 weeks
Bushnell [14] ^a	Inhalation	Rat	Male	Neuro	0.35	1366 ppm	1 hour for 1 day OR 1 hour/day for days 2, 3 and 4 of the week for 2 weeks
Carney <i>et al.</i> [15]	Inhalation	Rat	Female	Develop	0.225	600 ppm	6 hours/day, 7 days/week for 15 days
Cosby & Dukelow [16]	Gavage	Mouse	Female	Develop	0.022	240.2 mg/kg	Once per day for 5 days
Crofton & Zhao [17]	Inhalation	Rat	Male	Neuro	0.7	1367 ppm	6 hours/day, 5 days/week for 13 weeks
Fisher <i>et al.</i> [18]	Gavage	Rat	Female	Develop	0.25	500 mg/kg	Once per day for 10 days
George <i>et al.</i> [19]	Diet	Mouse	Male	Repro	0.038	750 mg/kg	10 hours/day, 7 days/week for 6 weeks (until periodicity)
Griffin <i>et al.</i> [20]	Drinking water	Mouse	MRL female	Immuno	0.043	13.4 mg/kg/d	12 days (until steady state)
Healy <i>et al.</i> [21]	Inhalation	Rat	Female	Develop	0.3	100 ppm	4 hours/day, 7 days/week for 14 days
Jaspers <i>et al.</i> [22]	Inhalation	Rat	Male	Neuro	0.24	1500 ppm	18 hours/day, 5 days/week for 3 weeks
Kaneko <i>et al.</i> [23]	Inhalation	Mouse	MRL male	Immuno	0.047	500 ppm	4 hours/day, 6 days/week for 5 weeks (until periodicity)
Kjellstrand <i>et al.</i> [24]	Inhalation	Mouse	Female & Male	Liver	0.035 & 0.0362	37 ppm	Continuous for 30 days
Kumar <i>et al.</i> [25, 26]	Inhalation	Rat	Male	Liver & Repro	0.5	376 ppm	4 hours/day, 5 days/week for 7 weeks (until periodicity)
Land <i>et al.</i> [27]	Inhalation	Mouse	Male	Repro	0.026	575 ppm	4 hours/day, 5 days/week for 5 days
Maltoni <i>et al.</i> [28]	Inhalation	Rat	Male	Kidney	0.85	221 ppm	7 hours/day, 5 days/week for 5 weeks (until periodicity)
Manson <i>et al.</i> [29]	Gavage	Rat	Female	Develop	0.405	100 mg/kg	7 days/week for 3 weeks (until periodicity)
Narotsky <i>et al.</i> [30]	Gavage	Rat	Female	Develop	0.175	36 mg/kg	Once per day for 10 days

Study Name	Route	Species	Sex	Domain	Body Weight (kg)	Dose or Concentration	Simulation
Ramadhan <i>et al.</i> [31]	Inhalation	Mouse	Male	Liver	0.025	546 ppm	8 hours/day for 7 days
Sanders <i>et al.</i> [32]	Drinking water	Mouse	Female & Male	Immuno	0.04 & 0.049	18.4 mg/kg/d	Daily for 13 days (until steady state)
Schwetz <i>et al.</i> [33]	Inhalation	Mouse & Rat	Female	Develop	0.054 & 0.37	306 ppm	7 hours/day for 10 days
Woolhiser <i>et al.</i> [34]	Inhalation	Rat	Female	Immuno, Kidney & Liver	0.2146	243 ppm, 90 ppm & 108 ppm	6 hours/day, 5 days/weeks for 4 weeks
Wu & Berger [35]	Drinking water	Rat	Female	Repro	0.2	66 mg/kg/d	Daily for 2 weeks

^aIn the study, all animals were exposed to air, then 3 different concentrations on 4 consecutive days of a week (0 ppm on day 1). The following week, the same rats are exposed in the same manner only to different concentrations (still 0 ppm on day 1). For dose metric simulations, the same dose (the point of departure) was used for all exposed days.

Script files (Appendix R) were then created to fit the external inhalation dose (HEC) necessary in the human to match the internal dose metrics predicted from the animal studies. The HECs were estimated for both male and female using average posterior parameter values (Tables 3 and 4). These simulations were for either continuous inhalation exposure or occupational exposure (*i.e.*, 8 hours/day, 5 days/week) and all simulations were run long enough to reach steady-state or periodicity. As with the animal predictions, all simulations were checked to ensure that any predicted negative values were within an acceptable tolerance.

7.2 Results

The predicted internal animal dose metrics are shown in Table 6, and the estimated HECs are presented in Tables 7, 8, 9 and 10.

Table 6. Animal Internal Dose Metric Values

Study Name	Species	Route	Sex	Domain	Peak TCE in Blood (mg/L)	TCE AUC in Blood (mg-h/L/d)	Total Metabolized (mg/kg ^{0.75} /d)	Total Amount Metabolized by Oxidation (mg/kg ^{0.75} /d)	Peak TCE in Liver (mg/L)	TCE AUC in Liver (mg-h/L/d)	TCE Metabolized in Liver (mg/kg ^{0.75} /d)	Peak TCE in Kidney (mg/L)	TCE AUC in Kidney (mg-h/L/d)	TCE Metabolized in Kidney (mg/kg ^{0.75} /d)
Adams <i>et al.</i> [11] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	6.034 & 5.360	28.36 & 25.73	56.65 & 58.92	56.59 & 58.85	4.331 & 3.042	17.77 & 12.76	53.07 & 54.86	7.369 & 6.545	34.62 & 31.41	0.04146 & 0.04805
Albee <i>et al.</i> [12]	Rat	Inhalation	Female & Male	Neuro	55.80 & 50.59	222.8 & 200.4	95.52 & 112.9	95.07 & 112.5						
Arito <i>et al.</i> [13]	Rat	Inhalation	Male	Neuro	0.3464	1.979	8.287	8.262						
Bushnell [14] ^b	Rat	Inhalation	Male	Neuro	50.88 & 50.88	65.22 & 27.95	56.55 & 24.24	56.39 & 24.17						
Carney <i>et al.</i> [15]	Rat	Inhalation	Female	Develop	37.54	203.5	124.0	123.5						
Cosby & Dukelow [16]	Mouse	Gavage	Female	Develop	14.38	10.04	79.98	79.79						
Crofton & Zhao [17]	Rat	Inhalation	Male	Neuro	91.63	386.8	158.6	157.6						
Fisher <i>et al.</i> [18]	Rat	Gavage	Female	Develop	124.1	250.1	170.2	169.4						
George <i>et al.</i> [19]	Mouse	Diet	Male	Repro	3.205	26.28	300.7	300.1						
Griffin <i>et al.</i> [20]	Mouse	Drinking water	MRL female	Immuno	0.009553	0.2293	5.840	5.834						
Healy <i>et al.</i> [21]	Rat	Inhalation	Female	Develop	2.200	8.918	25.39	25.35						
Jaspers <i>et al.</i> [22]	Rat	Inhalation	Male	Neuro	132.5	1635	241.2	237.7						
Kaneko <i>et al.</i> [23]	Mouse	Inhalation	MRL male	Immuno	17.91	60.62	135.1	134.7						
Kjellstrand <i>et al.</i> [24]	Mouse	Inhalation	Female & Male	Liver	0.7902 & 0.7885	18.96 & 18.92	146.4 & 146.7	146.3 & 146.6	0.3001 & 0.2973	7.202 & 7.134	41.62 & 41.60			
Kumar <i>et al.</i> [25, 26]	Rat	Inhalation	Male	Liver & Repro	13.25	34.88	57.29	57.20	13.26	27.56	53.85			
Land <i>et al.</i> [27]	Mouse	Inhalation	Male	Repro	23.90	92.08	157.6	156.9						
Maltoni <i>et al.</i> [28]	Rat	Inhalation	Male	Kidney	5.308	26.00	67.33	67.24				6.480	31.73	0.06425

Study Name	Species	Route	Sex	Domain	Peak TCE in Blood (mg/L)	TCE AUC in Blood (mg-h/L/d)	Total Metabolized (mg/kg ^{0.75} /d)	Total Amount Metabolized by Oxidation (mg/kg ^{0.75} /d)	Peak TCE in Liver (mg/L)	TCE AUC in Liver (mg-h/L/d)	TCE Metabolized in Liver (mg/kg ^{0.75} /d)	Peak TCE in Kidney (mg/L)	TCE AUC in Kidney (mg-h/L/d)	TCE Metabolized in Kidney (mg/kg ^{0.75} /d)
Manson <i>et al.</i> [29]	Rat	Gavage	Female	Develop	23.13	20.12	66.10	65.98						
Narotsky <i>et al.</i> [30]	Rat	Gavage	Female	Develop	5.966	3.550	21.02	20.99						
Ramdhan <i>et al.</i> [31]	Mouse	Inhalation	Male	Liver	23.50	179.9	287.6	286.2	29.21	204.7	228.0			
Sanders <i>et al.</i> [32]	Mouse	Drinking water	Female & Male	Immuno	0.01313 & 0.01318	0.3151 & 0.3163	7.868 & 8.295	7.861 & 8.288						
Schwetz <i>et al.</i> [33]	Mouse & Rat	Inhalation	Female	Develop	9.794 & 11.35	67.89 & 71.04	193.4 & 112.9	193.0 & 112.7						
Woolhiser <i>et al.</i> [34]	Rat	Inhalation	Female	Immuno, Kidney & Liver	8.387, 2.057 & 2.539	32.73, 8.757 & 10.76	56.36, 24.32 & 28.70	56.29, 24.28 & 28.66	0.9786 ^c	3.879 ^c	25.88 ^c	2.510 ^d	10.68 ^d	0.03028 ^d
Wu & Berger [35]	Rat	Drinking water	Female	Repro	0.09164	2.199	42.90	42.85						

^aFirst number is the value for the female rats and the second is for male rats.

^bFirst number is the value for the single dose scenario and the second is for the 2 week scenario.

^cValue is for liver effects. Rat internal dose metric was from simulating inhalation exposure at 108.0 ppm.

^dValue is for kidney effects. Rat internal dose metric was from simulating inhalation exposure at 90.0 ppm.

Table 7. Estimated HECs for Human Male Continuous Inhalation

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Adams <i>et al.</i> , [11] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	241.9 & 219.4	54.86 & 49.90	41.38 & 43.11	45.43 & 47.37	209.0 & 182.5	103.4 & 87.80	48.02 & 49.69	194.3 & 175.7	42.92 & 39.06	0.8958 & 1.041
Albee <i>et al.</i> , [12]	Rat	Inhalation	Female & Male	Neuro	1349 & 1243	340.5 & 313.7	71.61 & 85.54	80.60 & 98.76						
Arito <i>et al.</i> , [13]	Rat	Inhalation	Male	Neuro	16.46	3.960	5.778	6.257						
Bushnell [14] ^b	Rat	Inhalation	Male	Neuro	1249 & 1249	121.4 & 54.09	41.30 & 17.21	45.25 & 18.66						
Carney <i>et al.</i> , [15]	Rat	Inhalation	Female	Develop	974.3	317.4	94.57	111.6						
Cosby & Dukelow [16]	Mouse	Gavage	Female	Develop	472.6	19.82	59.38	66.04						
Crofton & Zhao [17]	Rat	Inhalation	Male	Neuro	2077	513.8	123.7	171.8						
Fisher <i>et al.</i> , [18]	Rat	Gavage	Female	Develop	2735	371.9	133.8	220.8						
George <i>et al.</i> , [19]	Mouse	Diet	Male	Repro	141.0	50.94	269.3	-- ^c						
Griffin <i>et al.</i> , [20]	Mouse	Drinking water	MRL female	Immuno	0.4604	0.4605	4.060	4.404						
Healy <i>et al.</i> , [21]	Rat	Inhalation	Female	Develop	99.69	17.64	18.05	19.60						
Jaspers <i>et al.</i> , [22]	Rat	Inhalation	Male	Neuro	2905	1600	201.9	-- ^c						
Kaneko <i>et al.</i> , [23]	Mouse	Inhalation	MRL male	Immuno	555.1	113.4	103.7	126.6						
Kjellstrand <i>et al.</i> , [24]	Mouse	Inhalation	Female & Male	Liver	37.04 & 36.96	37.03 & 36.95	113.2 & 113.5	145.7 & 146.3	63.15 & 62.78	63.15 & 62.77	37.48 & 37.46			
Kumar <i>et al.</i> , [25, 26]	Rat	Inhalation	Male	Liver & Repro	444.9	67.05	41.87	45.95	329.2	125.3	48.75			
Land <i>et al.</i> , [27]	Mouse	Inhalation	Male	Repro	687.3	165.2	122.8	169.8						
Maltoni <i>et al.</i> , [28]	Rat	Inhalation	Male	Kidney	217.7	50.41	49.56	54.71				174.2	39.44	1.403
Manson <i>et al.</i> , [29]	Rat	Gavage	Female	Develop	670.7	39.25	48.61	53.59						
Narotsky <i>et al.</i> , [30]	Rat	Gavage	Female	Develop	239.7	7.082	14.87	16.15						
Ramdhan <i>et al.</i> , [31]	Mouse	Inhalation	Male	Liver	678.7	288.1	253.4	-- ^c	463.2	274.1	-- ^c			

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Sanders <i>et al.</i> [32]	Mouse	Drinking water	Female & Male	Immuno	0.6327 & 0.6351	0.6327 & 0.6351	5.483 & 5.784	5.950 & 6.276						
Schwetz <i>et al.</i> [33]	Mouse & Rat	Inhalation	Female	Develop	354.8 & 396.6	125.9 & 131.2	154.9 & 85.54	-- ^c & 98.98						
Woolhiser <i>et al.</i> [34]	Rat	Inhalation	Female	Immuno, Kidney & Liver	314.7, 93.55 & 114.0	63.04, 17.32 & 21.22	41.16, 17.27 & 20.47	45.17, 18.75 & 22.25	117.1 ^d	41.18 ^d	23.22 ^d	73.14 ^e	13.63 ^e	0.6508 ^e
Wu & Berger [35]	Rat	Drinking water	Female	Repro	4.399	4.398	30.99	33.83						

^aFirst number is the value based on female rats and the second is for male rats.

^bFirst number is the HEC for the single dose scenario and the second is for the 2 week scenario.

^cDue to saturation of metabolism, the HEC could not be estimated.

^dHEC is for liver effects. HEC is from simulating inhalation exposure at 114.0 ppm.

^eHEC is for kidney effects. HEC is from simulating inhalation exposure at 93.55 ppm.

Table 8. Estimated HECs for Human Male Occupational Inhalation

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Adams <i>et al.</i> , [11] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	268.3 & 242.7	214.6 & 196.8	189.1 & 197.8	292.5 & 319.9	231.1 & 201.2	220.2 & 192.7	292.8 & 315.4	214.3 & 193.3	170.1 & 155.6	3.914 & 4.581
Albee <i>et al.</i> [12]	Rat	Inhalation	Female & Male	Neuro	1625 & 1493	1157 & 1062	352.6 & 439.9	919.4 & 1314						
Arito <i>et al.</i> [13]	Rat	Inhalation	Male	Neuro	17.91	16.49	24.86	27.01						
Bushnell [14] ^b	Rat	Inhalation	Male	Neuro	1500 & 1500	434.7 & 211.9	188.8 & 75.85	290.2 & 84.37						
Carney <i>et al.</i> [15]	Rat	Inhalation	Female	Develop	1159	1075	502.3	1613						
Cosby & Dukelow [16]	Mouse	Gavage	Female	Develop	540.2	81.25	282.9	634.2						
Crofton & Zhao [17]	Rat	Inhalation	Male	Neuro	2529	1829	742.1	3079						
Fisher <i>et al.</i> [18]	Rat	Gavage	Female	Develop	3344	1271	840.8	4221						
George <i>et al.</i> [19]	Mouse	Diet	Male	Repro	154.5	200.6	2696	-- ^c						
Griffin <i>et al.</i> [20]	Mouse	Drinking water	MRL female	Immuno	0.5008	1.932	17.37	18.87						
Healy <i>et al.</i> [21]	Rat	Inhalation	Female	Develop	108.9	72.42	79.64	88.97						
Jaspers <i>et al.</i> [22]	Rat	Inhalation	Male	Neuro	3554	6553	1669	-- ^c						
Kaneko <i>et al.</i> [23]	Mouse	Inhalation	MRL male	Immuno	640.7	409.6	571.1	1974						
Kjellstrand <i>et al.</i> [24]	Mouse	Inhalation	Female & Male	Liver	40.34 & 40.25	149.0 & 148.7	648.7 & 650.9	2443 & 2457	68.87 & 68.46	152.1 & 151.5	183.6 & 183.5			
Kumar <i>et al.</i> [25, 26]	Rat	Inhalation	Male	Liver & Repro	506.8	257.2	191.6	299.7	369.8	263.4	302.5			
Land <i>et al.</i> [27]	Mouse	Inhalation	Male	Repro	803.6	573.0	734.1	3031						
Maltoni <i>et al.</i> [28]	Rat	Inhalation	Male	Kidney	240.7	198.7	230.6	434.9				191.7	157.1	6.274
Manson <i>et al.</i> [29]	Rat	Gavage	Female	Develop	783.0	157.4	225.7	416.6						
Narotsky <i>et al.</i> [30]	Rat	Gavage	Female	Develop	265.8	29.37	65.32	72.25						
Ramdhan <i>et al.</i> [31]	Mouse	Inhalation	Male	Liver	792.9	973.4	2439	-- ^c	529.9	649.4	-- ^c			

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Sanders <i>et al.</i> [32]	Mouse	Drinking water	Female & Male	Immuno	0.6881 & 0.6908	2.653 & 2.663	23.57 & 24.89	25.65 & 27.10						
Schwetz <i>et al.</i> [33]	Mouse & Rat	Inhalation	Female	Develop	399.3 & 448.8	449.1 & 465.9	1068 & 439.9	-- ^c & 1319						
Woolhiser <i>et al.</i> [34]	Rat	Inhalation	Female	Immuno, Kidney & Liver	352.3, 102.1 & 124.6	243.4, 71.15 & 86.89	188.1, 76.12 & 90.61	289.1, 84.79 & 102.3	128.2 ^d	113.6 ^d	100.7 ^d	79.77 ^e	55.69 ^e	2.813 ^e
Wu & Berger [35]	Rat	Drinking water	Female	Repro	4.785	18.31	139.1	172.0						

^aFirst number is the value based on female rats and the second is for male rats.

^bFirst number is the HEC for the single dose scenario and the second is for the 2 week scenario.

^cDue to saturation of metabolism, the HEC could not be estimated.

^dHEC is for liver effects. HEC is from simulating inhalation exposure at 124.6 ppm.

^eHEC is for kidney effects. HEC is from simulating inhalation exposure at 102.1 ppm.

Table 9. Estimated HECs for Human Female Continuous Inhalation

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Adams <i>et al.</i> , [11] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	237.8 & 216.6	56.81 & 51.71	40.39 & 42.08	44.56 & 46.48	182.0 & 158.4	89.03 & 75.54	46.79 & 48.44	192.9 & 175.3	44.64 & 40.65	0.9104 & 1.058
Albee <i>et al.</i> , [12]	Rat	Inhalation	Female & Male	Neuro	1324 & 1218	330.5 & 305.3	69.99 & 83.74	80.14 & 99.89						
Arito <i>et al.</i> , [13]	Rat	Inhalation	Male	Neuro	17.12	4.122	5.654	6.122						
Bushnell [14] ^b	Rat	Inhalation	Male	Neuro	1224 & 1224	123.2 & 56.01	40.32 & 16.82	44.39 & 18.26						
Carney <i>et al.</i> , [15]	Rat	Inhalation	Female	Develop	950.5	308.8	92.72	115.2						
Cosby & Dukelow [16]	Mouse	Gavage	Female	Develop	456.1	20.61	57.99	65.16						
Crofton & Zhao [17]	Rat	Inhalation	Male	Neuro	2052	495.9	122.2	264.4						
Fisher <i>et al.</i> , [18]	Rat	Gavage	Female	Develop	2709	360.1	132.6	-- ^c						
George <i>et al.</i> , [19]	Mouse	Diet	Male	Repro	142.1	52.78	282.7	-- ^c						
Griffin <i>et al.</i> , [20]	Mouse	Drinking water	MRL female	Immuno	0.4793	0.4794	3.973	4.310						
Healy <i>et al.</i> , [21]	Rat	Inhalation	Female	Develop	102.0	18.34	17.63	19.18						
Jaspers <i>et al.</i> , [22]	Rat	Inhalation	Male	Neuro	2879	1575	205.3	-- ^c						
Kaneko <i>et al.</i> , [23]	Mouse	Inhalation	MRL male	Immuno	536.0	115.5	101.9	135.9						
Kjellstrand <i>et al.</i> , [24]	Mouse	Inhalation	Female & Male	Liver	38.45 & 38.37	38.44 & 38.36	111.5 & 111.8	171.2 & 172.5	54.27 & 53.94	54.26 & 53.94	36.42 & 36.40			
Kumar <i>et al.</i> , [25, 26]	Rat	Inhalation	Male	Liver & Repro	429.6	69.26	40.87	45.08	291.3	108.0	47.51			
Land <i>et al.</i> , [27]	Mouse	Inhalation	Male	Repro	665.8	165.2	121.3	253.4						
Maltoni <i>et al.</i> , [28]	Rat	Inhalation	Male	Kidney	214.9	52.24	48.39	53.77				173.8	41.05	1.426
Manson <i>et al.</i> , [29]	Rat	Gavage	Female	Develop	649.4	40.73	47.46	52.66						
Narotsky <i>et al.</i> , [30]	Rat	Gavage	Female	Develop	235.7	7.370	14.54	15.80						
Ramdhan <i>et al.</i> , [31]	Mouse	Inhalation	Male	Liver	657.2	281.3	263.7	-- ^c	417.4	240.7	-- ^c			

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Sanders <i>et al.</i> [32]	Mouse	Drinking water	Female & Male	Immuno	0.6587 & 0.6612	0.6586 & 0.6611	5.365 & 5.659	5.822 & 6.141						
Schwetz <i>et al.</i> [33]	Mouse & Rat	Inhalation	Female	Develop	344.0 & 383.5	127.6 & 132.7	154.6 & 83.74	-- ^c & 100.1						
Woolhiser <i>et al.</i> [34]	Rat	Inhalation	Female	Immuno, Kidney & Liver	306.3, 95.93 & 116.0	65.18, 18.02 & 22.07	40.18, 16.87 & 20.00	44.30, 18.35 & 21.77	101.0 ^d	35.35 ^d	22.51 ^d	75.59 ^e	14.24 ^e	0.6615 ^e
Wu & Berger [35]	Rat	Drinking water	Female	Repro	4.578	4.578	30.26	33.13						

^aFirst number is the value based on female rats and the second is for male rats.

^bFirst number is the HEC for the single dose scenario and the second is for the 2 week scenario.

^cDue to saturation of metabolism, the HEC could not be estimated.

^dHEC is for liver effects. HEC is from simulating inhalation exposure at 116.0 ppm.

^eHEC is for kidney effects. HEC is from simulating inhalation exposure at 95.93 ppm.

Table 10. Estimated HECs for Human Female Occupational Inhalation

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Adams <i>et al.</i> , [11] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	276.6 & 250.9	216.9 & 199.4	186.5 & 195.2	307.2 & 333.7	209.6 & 181.6	195.8 & 170.7	307.0 & 328.9	222.5 & 201.5	173.5 & 159.3	3.962 & 4.633
Albee <i>et al.</i> [12]	Rat	Inhalation	Female & Male	Neuro	1700 & 1559	1158 & 1061	354.2 & 445.4	839.8 & 1162						
Arito <i>et al.</i> [13]	Rat	Inhalation	Male	Neuro	19.29	17.17	24.28	26.40						
Bushnell [14] ^b	Rat	Inhalation	Male	Neuro	1567 & 1567	432.2 & 214.2	186.1 & 73.97	304.9 & 82.84						
Carney <i>et al.</i> [15]	Rat	Inhalation	Female	Develop	1204	1074	510.7	1420						
Cosby & Dukelow [16]	Mouse	Gavage	Female	Develop	551.9	84.16	282.1	607.1						
Crofton & Zhao [17]	Rat	Inhalation	Male	Neuro	2662	1839	756.0	3901						
Fisher <i>et al.</i> [18]	Rat	Gavage	Female	Develop	3530	1274	853.1	-- ^c						
George <i>et al.</i> [19]	Mouse	Diet	Male	Repro	162.2	203.1	2546	-- ^c						
Griffin <i>et al.</i> [20]	Mouse	Drinking water	MRL female	Immuno	0.5397	2.011	16.97	18.45						
Healy <i>et al.</i> [21]	Rat	Inhalation	Female	Develop	115.7	75.09	77.66	87.45						
Jaspers <i>et al.</i> [22]	Rat	Inhalation	Male	Neuro	3753	6536	1617	-- ^c						
Kaneko <i>et al.</i> [23]	Mouse	Inhalation	MRL male	Immuno	656.1	407.6	582.2	1772						
Kjellstrand <i>et al.</i> [24]	Mouse	Inhalation	Female & Male	Liver	43.38 & 43.28	152.4 & 152.1	661.9 & 664.1	2365 & 2386	61.30 & 60.94	134.0 & 133.4	189.1 & 189.0			
Kumar <i>et al.</i> [25, 26]	Rat	Inhalation	Male	Liver & Repro	517.6	258.6	188.9	314.3	342.6	235.6	316.5			
Land <i>et al.</i> [27]	Mouse	Inhalation	Male	Repro	826.9	568.7	747.9	3715						
Maltoni <i>et al.</i> [28]	Rat	Inhalation	Male	Kidney	248.9	201.3	228.5	437.9				199.8	160.7	6.332
Manson <i>et al.</i> [29]	Rat	Gavage	Female	Develop	805.2	160.7	223.6	421.7						
Narotsky <i>et al.</i> [30]	Rat	Gavage	Female	Develop	274.1	30.55	63.69	70.80						
Ramdhan <i>et al.</i> [31]	Mouse	Inhalation	Male	Liver	815.7	971.5	2310	-- ^c	502.5	610.1	-- ^c			

Study Name	Species	Route	Sex	Domain	Endpoint									
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver	Peak TCE in Kidney	TCE AUC in Kidney	TCE Metabolized in Kidney
Sanders <i>et al.</i> [32]	Mouse	Drinking water	Female & Male	Immuno	0.7416 & 0.7444	2.762 & 2.772	23.02 & 24.30	25.08 & 26.49						
Schwetz <i>et al.</i> [33]	Mouse & Rat	Inhalation	Female	Develop	408.2 & 458.4	446.3 & 462.8	1070 & 445.4	-- ^c & 1166						
Woolhiser <i>et al.</i> [34]	Rat	Inhalation	Female	Immuno, Kidney & Liver	360.9, 108.8 & 131.9	245.1, 73.78 & 89.93	185.4, 74.22 & 88.40	303.8, 83.27 & 100.9	114.6 ^d	99.50 ^d	98.76 ^d	85.51 ^e	58.04 ^e	2.851 ^e
Wu & Berger [35]	Rat	Drinking water	Female	Repro	5.156	19.05	136.3	176.4						

^aFirst number is the value based on female rats and the second is for male rats.

^bFirst number is the HEC for the single dose scenario and the second is for the 2 week scenario.

^cDue to saturation of metabolism, the HEC could not be estimated.

^dHEC is for liver effects. HEC is from simulating inhalation exposure at 131.9 ppm.

^eHEC is for kidney effects. HEC is from simulating inhalation exposure at 131.9 ppm.

8.0 TASK 5: DEVELOP DELIVERABLES DESCRIBING METHODS USED AND OUTCOMES OF TASKS

This report fulfills the requirements for Task 5.

9.0 CONCLUSIONS

While there were previously some issues with the acslX version of the USEPA [1] model code [2], these issues have been resolved with subsequent modifications and additional restrictions placed on the error tolerances. Any negative values predicted now were less than $2e-7$ in absolute value with most being less than $1e-10$ in absolute value. Values for *ExhFac_Den*, *ExhFactor* and *AExhPost* are not included in this assessment as they were only used for output variables having no effect any other variables and were not always applicable for a given simulation's dose route. For the most part, the validation figures appear to duplicate those in USEPA [1] with the primary exception being those for the data from Muller *et al.* [9] where the acslX version consistently under-predicts the data. Given that the model performs well at predicting oral TCA dosing for the mouse and rat, the issues for human with the Muller *et al.*, [9] data are more likely due to parameterization issues than coding issues. As there were no other data for oral TCOH dosing for comparison, the issues for simulations of oral TCOH dosing are more uncertain. No discrepancies, however, were found between the parameters used here and those provided by Dr. Chiu via the MCSim input and output files. Given that the purpose of the model here is for simulating dosing with TCE only, this issue should not impact any predictions for animal internal dose metrics or corresponding predictions for HECs.

As with the validation figures, issues previously seen in conducting the sensitivity analyses [2] have been resolved with the subsequent model coding modifications. The sensitivity analyses conducted with the acslX version of the USEPA [1] model seem to result in predicted SCs that are now very similar to those in USEPA [1]. Without the actual numerical values for the SCs, it is difficult to determine exactly how well they compare. Any differences, however, appear to be small and could well be due to differences in the modeling platforms used (*i.e.*, numerical precision and algorithm used for solving the ordinary differential equations), the manner in which the SCs were calculated (*i.e.*, during the simulation or outside of the simulation where the precision of the numbers used could vary), and conducting the analyses on the scaling parameters (*e.g.*, the fractional change in the baseline value for the parameters) by USEPA [1], as opposed to changing the actual parameters themselves as was done here.

With the coding modifications to the acslX version of the USEPA [1] model and the additional restrictions placed on the error tolerances, the acslX version of the model now seems to give results true to the MCSim version of the USEPA [1] model. The acslX model was, thus, used to predict mouse and rat internal dose metrics and the subsequent HECs for continuous or occupational inhalation exposure. The model appears to have behaved well (*i.e.*, values within acceptable limits and no unexpected behaviors in predicted blood concentrations) and the only issues in predicting the HECs were the inability to predict an HEC for some of the metabolism dose metrics. However, it is felt that this was due to the predicted saturation of the metabolic system such that regardless of an increase in dose, an increase in the dose metric could not be achieved.

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APPENDIX A

acslX Model Code for USEPA [1] Model

```

PROGRAM EPA_2011_TCE_REV.csl
! revised acslX version of model from Appendix A of EPA Toxicological Review of TCE
! (September 2011)

! --- HISTORY OF HACK ET AL. (2006) MODEL
! Model code to correspond to the block diagram version of the harmonized model edited by Deborah
! Keys to incorporate Lapare et al. 1995 data -- Last edited: August 6, 2004
! Translated into MCSim from acslXtreme CSL file by Eric Hack, completed September 15, 2004
! Removed non-essential differential equations (i.e., AUCCBld) for MCMC runs
! Changed QRap and QSlw calculations and added QTot to scale fractional flows back to 1.0 after
! sampling
! Changed QSlw calculation and removed QTot (September 21, 2004)
! Removed diffusion-limited fat uptake (September 24, 2004)

! --- HISTORY OF U.S. EPA (2009) MODEL (Chiu et al., 2009)
! Extensively revised by U.S. EPA June 2007 - June 2008
! Version 1
! Fixed hepatic plasma flow for TCA-submodel to include portal vein (i.e., QGutLivPlas -
! originally was just QLivPlas, which was only hepatic artery)
! Clearer coding and in-line documentation
! Single model for 3 species
! Revised physiological parameters, with discussion of uncertainty and variability
! In vitro data used for default metabolism parameters, with discussion of uncertainty and
! variability
! Added
! TCE blood compartment
! TCE kidney compartment, with GSH metabolism
! DCVG compartment
! Additional outputs available from in vivo data
! IA and PV dosing (for rats)
! Removed DCA compartment
!
! Version 1.1 -- fixed urinary parameter scaling
! Fixed VBod in KurnTCOG (should be VBodTCOH)
!
! Version 1.1.1 -- changed some truncation limits (in comments only)
! Version 1.2
! Removed TB compartment as currently coded
! Added respiratory oxidative metabolism: 3 states: AInhResp, AResp, AExhResp
! Removed clearance from respiratory metabolism
!
! Version 1.2.1 -- changed oral dosing to be similar to IV
! Version 1.2.2 -- fixed default lung metabolism (additional scaling by lung/liver weight ratio)
! Version 1.2.3 -- fixed FracKidDCVC scaling

! --- Changes made in converting EPA model from MCSim to acslX
! Terms in some equations were rearranged for better readability
! Model changed to not use the parameter "Male" -- calculations didn't differ, only baseline
! values for parameters -- male and female specific M files created and those should be used
! Model changed to use absolute value rather than the baseline value times the fractional
! increase -- values in M files set accordingly (i.e., changed
! PLivTCA=TCAPlas*exp(lnPLivTCAC)*(baseline values) to PLivTCA=TCAPlas*PLivTCAC)
! Replaced "exp(ln*)" with "***" where "***" is the parameter name (i.e., replaced "exp(lnPBodTCAC)"
! with "PBodTCAC") -- "ln" removed from parameter names as appropriate
! Changed code to set measured values for BW, QP, VFatC, PB or Hematocrit in M file rather than
! having separate parameter for it and using IF statements to set
! if Hematocrit measured, in the M file set FracPlas to (1-HematocritMeas) where
! HematocritMeas is the measured value
! if QP is measured, in the M file set QCC to (QPMeas/VPR)/(BW^0.75) where QPMeas is the
! measured value -- not used in any of the M files
! QC used instead of QCNow since code was changed in how it uses measured QP values
! No fractional increase for QSlw since it is calculated in model but it does use a baseline
! value for total volume of perfused tissues so parameter VPerfC defined to be the baseline
! value

```

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! New parameter defined for initial value for ACh called ACh0 since acslX handles initial values
!   for state parameters differently than MCSim
! Use of "CC" for inhalation concentration for closed chamber changed to be used as a flag to
!   denote closed chamber and concentration set with "CONC"
! AurnTCA_sat, zAurnTCA_sat, AurnTCOG_sat and AurnTCOGTCOH_sat are not used in any of the M files
!   so these were removed since it was unclear what they should represent and how to recode them
!   for acslX

! Parameter "ConcOn" defined to turn inhalation dosing on and off -- used for acslX
!   implementation of inhalation dosing but not needed for MCSim
! Equation for CInhPPM changed from "ACh/VCh*24450.0/MWTCE" to "(CInh*24450.0)/MWTCE" which would
!   be the same results for closed chamber inhalation it uses CInh which is calculated as
!   separately for open and closed chamber and, by changing the equation this way allows it
!   to work for either closed or open chamber
! Changed equation for AExhExp -- instead of "AExhExp=INTEG(RAExh, 0.0)" used "AExhExp=AExh"
! Code for calculating AurnTCA_Coll changed to work better in acslX
! Added code for weekly and daily average dosemetrics
! Added parameters Days and TMax for repeated dosing

! Q*Ctmp renamed to Q*C where * is for the tissue (Fat, Gut, Kid, Liv, or Slw)
! DResptmp renamed DRespC
! VRespEffC renamed VRespC
! VRespEfftmp renamed VResp
! ClC renamed Cl (became ClC after removing "exp(ln" from equations)
! ClDCVGC renamed ClDCVG (became ClDCVGC after removing "exp(ln" from equations)
! ClKidDCVGC renamed ClKidDCVG (became ClKidDCVGC after removing "exp(ln" from equations)
! VMaxLungLivC renamed VMaxLungLiv (became VMaxLungLivC after removing "exp(ln" from equations)
! ClTCOHC renamed ClTCOH (became ClTCOHC after removing "exp(ln" from equations)
! ClGlucC renamed ClGluc (became ClGlucC after removing "exp(ln" from equations)
! ExhFactor_Den renamed ExhFac_Den
! CPlasTCAMole and CPlasTCAFreeMole renamed CPlasTCA_uMole and CPlasTCAFree_uMole, respectively,
!   since the units are actually umoles
! RurnTCA renamed RAurnTCA
! RurnTCOG renamed RAurnTCOG
! RAMetDCVGmole renamed RAMetDCVG_Mole
! ADCVGmol renamed ADCVG_Mole
! CDCVGmol renamed CDCVG_Mole
! AMetDCVG renamed AMetDCVG_Mole
! CVenMole renamed CVen_Mole
! AurnTCA_collect and zAurnTCA_collect renamed AurnTCA_Coll and zAurnTCA_Coll, respectively
! AurnTCOGTCOH_collect renamed AurnTCOGTCOH_Coll

! AurnTCTotMole renamed AurnTCTot_Mole
! AurnNDCVCequiv renamed AurnNDCVC_Eq

! These parameters weren't used so they are not included in the acslX code (in alphabetical
order):
!   AurnTCA_sat, AurnTCOG_sat, AurnTCOGTCOH_sat, CDCVGmolLD, CDCVG_NDtmp, CDCVG_ND, MWChlor,
!   QRapC, RurnNDCVC, RurnTCOGTCOH, StochChlorTCE, StochTCEGluc, StochDCATCE, TCAurnSat,
!   TCOGurnSat, VBldCtmp, VBodCtmp, VBodTCOHCtmp, VFatCtmp, VGutCtmp, VKidCtmp, VlivCtmp,
!   VRapCtmp, VRespEffCtmp, VRespLumCtmp, VslwCtmp, VPlasCtmp, zAurnTCA_sat

! Combined the equations for CART and CART_Tmp
! Plot for AurnTCA_Sat when TCAurnSat is 1 is the same as the plot for AurtTCA_Coll when
!   TCAurnSat is 0 -- same for AurnTCOG_Sat and AurnTCOG_Coll
! TCAurnSat and TCOGurnSat only set in lines that are commented out so got rid of TCAurnSat,
!   TCOGurnSat, AurnTCA_Sat and AurnTCOG_Sat
! Added additional code for additional weekly and daily average dosemetrics

! Model runs in mg, L, hrs

INITIAL
  LOGICAL CC
  INTEGER I, J, Species
  DIMENSION ConclList(150), StrtNextList(150), UrnMissList(10)

  CONSTANT BW = 0.0 ! Body weight (kg)
  CONSTANT QCC = 1.0 ! Cardiac output (L/hr/kg^0.75)
  CONSTANT VPR = 1.0 ! Alveolar ventilation-perfusion ratio (unitless)
  CONSTANT DRespC = 1.0 ! Respiratory lumen/tissue diffusive clearance rate (fraction of QP)

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! Fractional Blood Flows to Tissues (fraction of cardiac output)
CONSTANT    QFatC = 1.0    ! Fat
CONSTANT    QGutC = 1.0    ! Gut
CONSTANT    QKidC = 1.0    ! Kidney
CONSTANT    QLivC = 1.0    ! Liver
CONSTANT    QRapC = 1.0    ! Rapidly perfused tissues
CONSTANT    QSlwC = 1.0    ! Slowly perfused tissues

! Tissue Volumes (fraction of body weight)
! (Respiratory tissue represents the tracheobronchial region = trachea + bronchial basal +
!   bronchial secretory + bronchiolar)
CONSTANT    VBldC = 1.0    ! Blood
CONSTANT    VFatC = 1.0    ! Fat
CONSTANT    VGutC = 1.0    ! Gut
CONSTANT    VKidC = 1.0    ! Kidney
CONSTANT    VLivC = 1.0    ! Liver
CONSTANT    VPerfC = 1.0    ! Body that is blood perfused
CONSTANT    VRapC = 1.0    ! Rapidly perfused tissues
CONSTANT    VRespC = 1.0    ! Respiratory tissue
CONSTANT    VResplumC = 1.0    ! Respiratory lumen air volume
CONSTANT    VSlwC = 1.0    ! Slowly perfused tissues
CONSTANT    FracPlas = 1.0    ! Fraction of blood that is plasma (1.0 - hematocrit) (unitless)

! Molecular Weights (g/mole = mg/m mole)
CONSTANT    MWTCE = 131.39    ! TCE
CONSTANT    MWDCVC = 216.1    ! DCVC
CONSTANT    MWTCA = 163.5    ! TCA
CONSTANT    MWTCOH = 149.5    ! TCOH
CONSTANT    MWTCOHGluc = 325.53    ! TCOH-Gluc
CONSTANT    MWNADCVC = 258.8    ! N Acetyl DCVC

! Partition Coefficients for TCE (unitless)
CONSTANT    PB = 1.0    ! Blood/air
CONSTANT    PFat = 1.0    ! Fat/blood
CONSTANT    PGut = 1.0    ! Gut/blood
CONSTANT    PKid = 1.0    ! Kidney/blood
CONSTANT    PLiv = 1.0    ! Liver/blood
CONSTANT    PRap = 1.0    ! Rapidly perfused/blood
CONSTANT    PResp = 1.0    ! Respiratory tissue/air
CONSTANT    PSlw = 1.0    ! Slowly perfused/blood

! Partition Coefficients for TCA (unitless)
CONSTANT    PRBCPlasTCA = 1.0    ! Scaled to species-specific central estimates
CONSTANT    PBodTCAC = 1.0    ! Free body/blood plasma
CONSTANT    PLivTCAC = 1.0    ! Free liver/blood plasma

! Partition Coefficients for TCOH (unitless)
CONSTANT    PBodTCOH = 1.0    ! Body/blood
CONSTANT    PLivTCOH = 1.0    ! Liver/blood

! Partition Coefficients for TCOG (unitless)
CONSTANT    PBodTCOG = 1.0    ! Body/blood
CONSTANT    PLivTCOG = 1.0    ! Liver/blood

! Partition Coefficient for DCVG (unitless)
CONSTANT    PEffDCVG = 1.0    ! Effective PC for the "body" (non-blood) compartment

! Binding Parameters for TCA
CONSTANT    BMaxkDC = 1.0    ! Ratio of max binding conc. to dissociation constant (unitless)
CONSTANT    kDissoc = 1.0    ! Protein/TCA dissociation constant (umole/L)

! Oral Uptake Constants (/hr)
CONSTANT    kAS = 1.4    ! TCE stomach absorption coefficient
CONSTANT    kTSD = 1.4    ! TCE stomach to duodenum transfer coefficient
CONSTANT    kAD = 0.75    ! TCE duodenum absorption coefficient
CONSTANT    kTD = 0.1    ! TCE duodenum-feces transfer coefficient
CONSTANT    kASTCA = 0.75    ! TCA stomach absorption coefficient
CONSTANT    kASTCOH = 0.75    ! TCOH stomach absorption coefficient

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! TCE Metabolism Constants
CONSTANT      VMaxC = 1.0      ! Capacity for hepatic TCE oxidation (mg/hr/kg liver)
CONSTANT      KMC = 1.0       ! Affinity for hepatic TCE oxidation (mg/L)
CONSTANT      Cl = 1.0        ! Ratio of capacity to affinity per kg liver for TCE hepatic
!                               oxidation (L/hr/kg liver)
CONSTANT      FracTCAC = 1.0   ! Fraction of hepatic TCE oxidation to TCA (unitless)
CONSTANT      FracOtherC = 1.0 ! Fraction of hepatic TCE oxidation not to TCA and TCOH
!                               (unitless)
CONSTANT      VMaxDCVGC = 1.0  ! Capacity for hepatic TCE GSH conjugation (mg/hr/kg liver)
CONSTANT      KMDCVGC = 1.0    ! Affinity for hepatic TCE GSH conjugation (mg/L)
CONSTANT      ClDCVG = 1.0     ! Ratio of capacity to affinity per kg liver for TCE GSH
!                               conjugation (L/hr/kg liver)
CONSTANT      VMaxKidDCVGC = 1.0 ! Capacity for renal TCE GSH conjugation (mg/hr/kg kidney)
CONSTANT      KMKidDCVGC = 1.0  ! Affinity for renal TCE GSH conjugation (mg/L)
CONSTANT      ClKidDCVG = 1.0   ! Ratio of capacity to affinity per kg kidney for TCE GSH
!                               conjugation (L/hr/kg kidney)

! TCE Metabolism Constants for Chloral Kinetics in Clara Cells in Lung
CONSTANT      VMaxLungLiv = 1.0 ! Ratio of capacities for lung to liver, scaled central
!                               estimates (unitless)
CONSTANT      KMClara = 1.0     ! Affinity for tracheo-bronchial TCE oxidation but in units of
!                               air concentration (mg/L)
CONSTANT      FracLungSysC = 1.0 ! Fraction of respiratory oxidative metabolism that enters
!                               systemic circulation (unitless)

! TCOH Metabolism Constants
CONSTANT      VMaxTCOHC = 1.0   ! Capacity for hepatic clearance of TCOH to TCA (mg/hr/kg^0.75)
CONSTANT      KMTCOH = 1.0     ! Affinity for hepatic clearance of TCOH to TCA (mg/L)
CONSTANT      ClTCOH = 1.0     ! (scaled by BW^0.75)
CONSTANT      VMaxGlucC = 1.0   ! Capacity for hepatic glucuronidation of TCOH to TCOG
!                               (mg/hr/kg^0.75)
CONSTANT      KMGluc = 1.0     ! Affinity for hepatic glucuronidation of TCOH to TCOG (mg/L)
CONSTANT      ClGluc = 1.0     ! (scaled by BW^0.75)
CONSTANT      kMetTCOHC = 1.0   ! Rate constant for hepatic clearance of TCOH to other
!                               (kg^0.25/hr)

! TCA Metabolism and Clearance Rates
CONSTANT      kUrntCAC = 1.0    ! Rate constant for urinary clearance of TCA in plasma to urine
!                               (L/hr/kg)
CONSTANT      kMetTCAC = 1.0    ! Rate constant for hepatic clearance of TCA to other (kg^0.25/hr)

! TCOG Metabolism and Clearance Rates
CONSTANT      kBileC = 1.0     ! Rate constant for excretion of TCOG in liver to bile (kg^0.25/hr)
CONSTANT      KEHRC = 1.0     ! Lumped rate constant for TCOG in bile to TCOH in liver
!                               (kg^0.25/hr)
CONSTANT      kUrntCOGC = 1.0  ! Rate constant for excretion of TCOG in urine (L/hr/kg)

! DCVG Metabolism Rates
CONSTANT      kDCVGC = 1.0     ! Rate constant for hepatic clearance of DCVG to DCVC
!                               (kg^0.25/hr)
CONSTANT      FracKidDCVCC = 1.0 ! Fraction of renal TCE GSH conjugation "directly" to DCVC
!                               (i.e., via first pass) (unitless)

! DCVC Metabolism and Clearance Rates (kg^0.25/hr)
CONSTANT      kNATC = 1.0     ! Lumped rate constant for DCVC clearance to urinary NAcDCVC
!                               (kg^0.25/hr)
CONSTANT      kKidBioactC = 1.0 ! Rate constant for other bioactivation of DCVC (kg^0.25/hr)

! Closed Chamber Parameters
CONSTANT      CC = .FALSE.    ! Default to open chamber
CONSTANT      NRodents = 1.0  ! Number of rodents in the chamber
CONSTANT      kLossC = 1.0    ! Rate constant for closed chamber air loss (/hr)
CONSTANT      VChC = 1.0     ! Volume of the chamber without animals (L)

! TCE Dosing Parameters
CONSTANT      ConcList = 150*0.0 ! Inhalation exposure concentrations (ppm)
CONSTANT      StrtNextList = 150*0.0 ! Start times for inhalation exposures (hrs)
CONSTANT      TStrt = 1000.0    ! Time to start first inhalation exposure (hrs)
CONSTANT      IVDose = 0.0     ! IV dose (mg/kg/day)
CONSTANT      TChng = 0.003    ! IV infusion duration (hrs)
CONSTANT      Days = 1.0       ! Days of exposure each week

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CONSTANT      TMax = 24.0      ! Maximum length of multiple exposures (hrs)
CONSTANT      PDose = 0.0      ! Oral dose (mg/kg/day)
CONSTANT      Drink = 0.0      ! Drinking water dose (mg/kg/day)
CONSTANT      IADose = 0.0     ! Intraarterial dose (mg/kg)
CONSTANT      PVDose = 0.0     ! Portal vein dose (mg/kg)

! TCA Dosing Parameters
CONSTANT      IVDoseTCA = 0.0  ! IV dose of TCA (mg/kg/day)
CONSTANT      PODoseTCA = 0.0  ! Oral dose of TCA (mg/kg/day)

! TCOH Dosing Parameters
CONSTANT      IVDoseTCOH = 0.0 ! IV dose of TCOH (mg/kg/day)
CONSTANT      PODoseTCOH = 0.0 ! Oral dose of TCOH (mg/kg/day)

! Flags for Species and Urine Collection
CONSTANT      Species = 1      ! 1=human, 2=rat, 3=mouse
CONSTANT      UrnMissList = 10*1000.0 ! Start times for urine collection (hrs)
CONSTANT      Turn = 0.0       ! Time to start first collection (hrs)

! Simulation Control Parameters
CONSTANT      TStp = 24.0      ! Time to stop simulation (hrs)
CINTERVAL     CINT = 0.01

! Scaled Flow Rates (L/hr)
QC = QCC * (BW**0.75)
QP = QC * VPR
QM = QP / 0.7              ! Minute-volume
DResp = DRespC * QP

! Blood Flows to Tissues (L/hr)
QAdjus = QFatC + QGutC + QKidC + QLivC + QRapC + QSlwC
QFat = (QFatC / QAdjus) * QC
QGut = (QGutC / QAdjus) * QC
QKid = (QKidC / QAdjus) * QC
QLiv = (QLivC / QAdjus) * QC
QRap = (QRapC / QAdjus) * QC
QSlw = (QSlwC / QAdjus) * QC
QC = QFat + QGut + QKid + QLiv + QRap + QSlw
QGutLiv = QGut + QLiv
QBod = QC - QGutLiv

! Plasma Flows to Tissues (L/hr)
QCPlas = FracPlas * QC
QBodPlas = FracPlas * QBod
QGutLivPlas = FracPlas * QGutLiv

! Tissue Volumes (L)
VTotC = VBldC + VFatC + VGutC + VKidC + VLivC + VRapC + VRespC + VSlwC
VAdjus = VPerfC / VTotC
VBld = (VBldC * VAdjus) * BW
VFat = (VFatC * VAdjus) * BW
VGut = (VGutC * VAdjus) * BW
VKid = (VKidC * VAdjus) * BW
VLiv = (VLivC * VAdjus) * BW
VRap = (VRapC * VAdjus) * BW
VResp = (VRespC * VAdjus) * BW
VSlw = (VSlwC * VAdjus) * BW
VPlas = FracPlas * VBld
VBod = VFat + VGut + VKid + VRap + VResp + VSlw
VBodTCOH = VBod + VBld
VDCVG = VBld + PEffDCVG * (VBod + VLiv)

! Respiratory Tract Air Volumes (L of air)
! (VRespEff is the effective respiratory tissue air volume = V(tissue) * Resp:Air partition
! coefficient
VResplum = VResplumC * BW
VRespEff = VResp * PResp * PB

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! Stoichiometry
  StochTCATCE = MWTCA / MWTCE
  StochTCATCOH = MWTCA / MWTCOH
  StochTCOHTCE = MWTCOH / MWTCE
  StochGlucTCOH = MWTCOHGluc / MWTCOH
  StochTCOHGluc = MWTCOH / MWTCOHGluc
  StochDCVCTCE = MWDCVC / MWTCE
  StochN = MWNADCVC / MWDCVC

! Partition Coefficients for TCA (unitless)
  TCAPlas = FracPlas + (1.0 - FracPlas) * PRBCPlasTCA
  PBodTCA = TCAPlas * PBodTCAC
  PLivTCA = TCAPlas * PLivTCAC

! Maximum Binding Concentration for TCA (umole/L)
  BMax = kDissoc * BMaxkDC

! TCE Metabolism Constants (scale some parameters differently for humans than for mice and rats)
  VMax = VMaxC * VLiv ! (mg/hr)
  FracOther = FracOtherC / (1.0 + FracOtherC) ! (fraction)
  FracTCA = FracTCAC * (1.0 - FracOther) / (1.0 + FracTCAC) ! (fraction)

IF (Species .EQ. 1) THEN
  KM = VMax / (VLiv * Cl) ! (mg/L)
  VMaxDCVG = VLiv * ClDCVG * KMDCVGC ! (mg/hr)
  KMDCVG = KMDCVGC ! (mg/L)
  VMaxKidDCVG = VKid * ClKidDCVG * KMKidDCVGC ! (mg/hr)
  KMKidDCVG = KMKidDCVGC ! (mg/L)
ELSE
  KM = KMC ! (mg/L)
  VMaxDCVG = VMaxDCVGC * VLiv ! (mg/hr)
  KMDCVG = VMaxDCVG / (VLiv * ClDCVG) ! (mg/L)
  VMaxKidDCVG = VMaxKidDCVGC * VKid ! (mg/hr)
  KMKidDCVG = VMaxKidDCVG / (VKid * ClKidDCVG) ! (mg/L)
ENDIF

! TCE Metabolism Constants for Chloral Kinetics in Lung
  VMaxClara = VMaxLungLiv * VMax ! (mg/hr)
  FracLungSys = FracLungSysC / (1.0 + FracLungSysC) ! (fraction)

! TCOH Metabolism Constants (scale some parameters differently for humans than for mice and rats)
  kMetTCOH = kMetTCOHC / (BW**0.25) ! (/hr)

IF (Species .EQ. 1) THEN
  VMaxTCOH = ClTCOH * KMTCOH * (BW**0.75) ! (mg/hr)
  VMaxGluc = ClGluc * KMGluc * (BW**0.75) ! (mg/hr)
ELSE
  VMaxTCOH = VMaxTCOHC * (BW**0.75) ! (mg/hr)
  VMaxGluc = VMaxGlucC * (BW**0.75) ! (mg/hr)
ENDIF

! TCA Metabolism and Clearance Rates
  kUrnTCA = (kUrnTCAC * BW) / VPlas ! (L/hr)
  kMetTCA = kMetTCAC / (BW**0.25) ! (/hr)

! TCOG Metabolism and Clearance Rates
  kBile = kBileC / (BW**0.25) ! (/hr)
  kEHR = kEHRC / (BW**0.25) ! (/hr)
  kUrnTCOG = kUrnTCOGC * BW / (VBodTCOH * PBodTCOG) ! (L/hr)

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! DCVG Metabolism Rates
      kDCVG = kDCVGC / (BW**0.25)                ! (/hr)
      FracKidDCVC = FracKidDCVCC / (1.0 + FracKidDCVCC)    ! (fraction)

! DCVC Metabolism and Clearance Rates
      kNAT = kNATC / (BW**0.25)                ! (/hr)
      kKidBioact = kKidBioactC / (BW**0.25)      ! (/hr)

! Exposure definition
  IF (CC) THEN
    Rodents = NRodents                ! Closed chamber simulation
    kLoss = kLossC                    ! (/hr)
    VCh = VChC - (Rodents * BW)      ! Calculate net chamber volume (L)
  ELSE
    Rodents = 0.0                    ! Open chamber simulation
    kLoss = 0.0                      ! Turn off chamber losses so concentration is constant (/hr)
    VCh = 1.0                        ! So that VCh drops out of equations (L)
  ENDIF

! Initialize starting value
  UrnMissing = 0.0                    ! Indicator for missing urine collection times
  I = 1
  J = 1
  ACh0 = (ConcList(1) * VCh * MWTCE) / 24450.0    ! Initial amount in chamber (mg)
  Day = 0.5
  Conc = 0.0
  CInh = 0.0
  kDrink = (Drink * BW) / 24.0        ! Ingestion rate via drinking water (mg/hr)
  kIA = 0.0
  kIV = 0.0
  kIVTCA = 0.0
  kIVTCOH = 0.0
  kPV = 0.0
  kStom = 0.0
  kStomTCA = 0.0
  kStomTCOH = 0.0
  AExhExp = 0.0
  AExhPost = 0.0
  ExhFactor = 1.0
  ExhFac_Den = 0.0
  TotDoseBW34 = 0.0
  FracMetab = 0.0
  FracOxMetab = 0.0
  FracMetLiv1 = 0.0
  FracMetLivOther = 0.0
  FracMetGSH = 0.0
  FracBioactKid = 0.0
  FracMetLng = 0.0

! Initialize values for AUC dosemetrics
  PAUCCBld = 0.0
  AUCCBldDM = 0.0
  PAUCCPlasTCA = 0.0
  AUCCPlasTCADM = 0.0
  PAUCCPlasTCAFree = 0.0
  AUCCPlasTCAFreeDM = 0.0
  PAUCCTCOH = 0.0
  AUCCTCOHDM = 0.0
  PAUCCTCOG = 0.0
  AUCCTCOGDM = 0.0
  PAUCTotCTCOH = 0.0
  AUCTotCTCOHDM = 0.0
  PAUCLiv = 0.0
  AUCLivDM = 0.0
  PAUCLivTCA = 0.0
  AUCLivTCADM = 0.0
  PAUCLivTCOH = 0.0

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    AUCCLivTCOHDM = 0.0
    PAUCCLivTCOG = 0.0
    AUCCLivTCOGDM = 0.0
    PAUCCKid = 0.0
    AUCCKidDM = 0.0
    PAUCCDCVG_mMole = 0.0
    AUCCDCVG_mMoleDM = 0.0

! Initialize values for metabolism dosemetrics
    PTotMetabBW34 = 0.0
    TotMetabBW34DM = 0.0
    PTotOxMetBW34 = 0.0
    TotOxMetBW34DM = 0.0
    PAMetLiv1VLiv = 0.0
    AMetLiv1VLivDM = 0.0
    PAMetLiv1BW34 = 0.0
    AMetLiv1BW34DM = 0.0
    PAMetLiv1TCAVLiv = 0.0
    AMetLiv1TCAVLivDM = 0.0
    PAMetLiv1TCABW34 = 0.0
    AMetLiv1TCABW34DM = 0.0
    PAMetLiv1TCOHVLiv = 0.0
    AMetLiv1TCOHVLivDM = 0.0
    PAMetLiv1TCOHBW34 = 0.0
    AMetLiv1TCOHBW34DM = 0.0
    PAMetLiv2VLiv = 0.0
    AMetLiv2VLivDM = 0.0
    PAMetLiv2BW34 = 0.0
    AMetLiv2BW34DM = 0.0
    PAMetLivOtherVLiv = 0.0
    AMetLivOtherVLivDM = 0.0
    PAMetLivOtherBW34 = 0.0
    AMetLivOtherBW34DM = 0.0
    PAMetTCAVLiv = 0.0
    AMetTCAVLivDM = 0.0
    PAMetTCABW34 = 0.0
    AMetTCABW34DM = 0.0
    PAMetTCOHTCAVLiv = 0.0
    AMetTCOHTCAVLivDM = 0.0
    PAMetTCOHTCABW34 = 0.0
    AMetTCOHTCABW34DM = 0.0
    PAMetTCOHGlucVLiv = 0.0
    AMetTCOHGlucVLivDM = 0.0
    PAMetTCOHGlucBW34 = 0.0
    AMetTCOHGlucBW34DM = 0.0
    PAMetTCOHOtherVLiv = 0.0
    AMetTCOHOtherVLivDM = 0.0
    PAMetTCOHOtherBW34 = 0.0
    AMetTCOHOtherBW34DM = 0.0
    PAMetKid = 0.0
    AMetKidDM = 0.0
    PAMetKidVKid = 0.0
    AMetKidVKidDM = 0.0
    PAMetKidBW34 = 0.0
    AMetKidBW34DM = 0.0
    PAMetDCVG_mMole = 0.0
    AMetDCVG_mMoleDM = 0.0
    PAMetDCVG_mMoleVKid = 0.0
    AMetDCVG_mMoleVKidDM = 0.0
    PAMetDCVG_mMoleBW34 = 0.0
    AMetDCVG_mMoleBW34DM = 0.0

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SCHEDULE ConcOn .AT. Tstrt
SCHEDULE UrnMissOn .AT. TUrN

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END

DYNAMIC

ALGORITHM IALG = 2

DISCRETE DoseOn

INTERVAL DoseInt = 10000.0

! Dosing interval (hrs)

SCHEDULE DoseOff .AT. T + TChng

IF ((T .LT. TMax) .AND. (Day .LE. Days)) THEN

kIA = (IADose * BW) / TChng ! IA infusion rate (mg/hr)

kIV = (IVDose * BW) / TChng ! TCE IV infusion rate (mg/hr)

kPV = (PVDose * BW) / TChng ! PV infusion rate (mg/hr)

kIVTCA = (IVDoseTCA * BW) / TChng ! TCA IV infusion rate (mg/hr)

kIVTCOH = (IVDoseTCOH * BW) / TChng ! TCOH IV infusion rate (mg/hr)

kStom = (PDose * BW) / TChng ! PO dose rate (into stomach) (mg/hr)

kStomTCA = (PODoseTCA * BW) / TChng ! TCA PO dose rate into stomach (mg/hr)

kStomTCOH = (PODoseTCOH * BW) / TChng ! TCOH PO dose rate into stomach (mg/hr)

ENDIF

IF (Days .GT. 1.0) THEN

Day = Day + 1.0

IF (Day .GT. 7.0) Day = 0.5

ENDIF

END

DISCRETE ConcOn ! Start inhalation

SCHEDULE ConcOn .AT. T + StrtNextList(I)

Conc = ConcList(I)

I = I + 1

END

DISCRETE DoseOff

kIA = 0.0

kIV = 0.0

kPV = 0.0

kIVTCA = 0.0

kIVTCOH = 0.0

kStom = 0.0

kStomTCA = 0.0

kStomTCOH = 0.0

END

DISCRETE UrnMissOn

SCHEDULE UrnMissOff .AT. T + UrnMissList(J)

UrnMissing = 1.0

J = J + 1

END

DISCRETE UrnMissOff

SCHEDULE UrnMissOn .AT. T + UrnMissList(J)

UrnMissing = 0.0

J = J + 1

END

DISCRETE Calc

! Save previous value for calculating daily or weekly dosemetrics

INTERVAL DMInt = 10000.0

! Interval for calculating dose metrics (hrs)

! Calculate daily or weekly AUC dosemetrics

AUCCBldDM = AUCCBld - PAUCCBld

AUCCPlastTCADM = AUCCPlastTCA - PAUCCPlastTCA

AUCCPlastTCAFreeDM = AUCCPlastTCAFree - PAUCCPlastTCAFree

AUCCTCOHDM = AUCCTCOH - PAUCCTCOH

AUCCTCOGDM = AUCCTCOG - PAUCCTCOG

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AUCTotCTCOHDM = AUCTotCTCOH - PAUCTotCTCOH
AUCCLivDM = AUCCLiv - PAUCCLiv
AUCCLivTCADM = AUCCLivTCA - PAUCCLivTCA
AUCCLivTCOHDM = AUCCLivTCOH - PAUCCLivTCOH
AUCCLivTCOGDM = AUCCLivTCOG - PAUCCLivTCOG
AUCCKidDM = AUCCKid - PAUCCKid
AUCCDCVG_mMoleDM = AUCCDCVG_mMole - PAUCCDCVG_mMole

! Calculate daily or weekly metabolism dosemetrics
TotMetabBW34DM = TotMetabBW34 - PTotMetabBW34
TotOxMetBW34DM = TotOxMetBW34 - PTotOxMetBW34
AMetLiv1VLivDM = AMetLiv1VLiv - PAMetLiv1VLiv
AMetLiv1BW34DM = AMetLiv1BW34 - PAMetLiv1BW34
AMetLiv1TCAVLivDM = AMetLiv1TCAVLiv - PAMetLiv1TCAVLiv
AMetLiv1TCABW34DM = AMetLiv1TCABW34 - PAMetLiv1TCABW34
AMetLiv1TCOHVLivDM = AMetLiv1TCOHVLiv - PAMetLiv1TCOHVLiv
AMetLiv1TCOHBW34DM = AMetLiv1TCOHBW34 - PAMetLiv1TCOHBW34
AMetLiv2VLivDM = AMetLiv2VLiv - PAMetLiv2VLiv
AMetLiv2BW34DM = AMetLiv2BW34 - PAMetLiv2BW34
AMetLivOtherVLivDM = AMetLivOtherVLiv - PAMetLivOtherVLiv
AMetLivOtherBW34DM = AMetLivOtherBW34 - PAMetLivOtherBW34
AMetTCAVLivDM = AMetTCAVLiv - PAMetTCAVLiv
AMetTCABW34DM = AMetTCABW34 - PAMetTCABW34
AMetTCOHTCAVLivDM = AMetTCOHTCAVLiv - PAMetTCOHTCAVLiv
AMetTCOHTCABW34DM = AMetTCOHTCABW34 - PAMetTCOHTCABW34
AMetTCOHGlucVLivDM = AMetTCOHGlucVLiv - PAMetTCOHGlucVLiv
AMetTCOHGlucBW34DM = AMetTCOHGlucBW34 - PAMetTCOHGlucBW34
AMetTCOHOtherVLivDM = AMetTCOHOtherVLiv - PAMetTCOHOtherVLiv
AMetTCOHOtherBW34DM = AMetTCOHOtherBW34 - PAMetTCOHOtherBW34
AMetKidDM = AMetKid - PAMetKid
AMetKidVKidDM = AMetKidVKid - PAMetKidVKid
AMetKidBW34DM = AMetKidBW34 - PAMetKidBW34
AMetDCVG_mMoleDM = AMetDCVG_mMole - PAMetDCVG_mMole
AMetDCVG_mMoleVKidDM = AMetDCVG_mMoleVKid - PAMetDCVG_mMoleVKid
AMetDCVG_mMoleBW34DM = AMetDCVG_mMoleBW34 - PAMetDCVG_mMoleBW34

PAUCCBld = AUCCBld
PAUCCPlasTCA = AUCCPlasTCA
PAUCCPlasTCAFree = AUCCPlasTCAFree
PAUCCTCOH = AUCCTCOH
PAUCCTCOG = AUCCTCOG
PAUCTotCTCOH = AUCTotCTCOH
PAUCCLiv = AUCCLiv
PAUCCLivTCA = AUCCLivTCA
PAUCCLivTCOH = AUCCLivTCOH
PAUCCLivTCOG = AUCCLivTCOG
PAUCCKid = AUCCKid
PAUCCDCVG_mMole = AUCCDCVG_mMole

PTotMetabBW34 = TotMetabBW34
PTotOxMetBW34 = TotOxMetBW34
PAMetLiv1VLiv = AMetLiv1VLiv
PAMetLiv1BW34 = AMetLiv1BW34
PAMetLiv1TCAVLiv = AMetLiv1TCAVLiv
PAMetLiv1TCABW34 = AMetLiv1TCABW34
PAMetLiv1TCOHVLiv = AMetLiv1TCOHVLiv
PAMetLiv1TCOHBW34 = AMetLiv1TCOHBW34
PAMetLiv2VLiv = AMetLiv2VLiv
PAMetLiv2BW34 = AMetLiv2BW34
PAMetLivOtherVLiv = AMetLivOtherVLiv
PAMetLivOtherBW34 = AMetLivOtherBW34
PAMetTCAVLiv = AMetTCAVLiv
PAMetTCABW34 = AMetTCABW34
PAMetTCOHTCAVLiv = AMetTCOHTCAVLiv
PAMetTCOHTCABW34 = AMetTCOHTCABW34
PAMetTCOHGlucVLiv = AMetTCOHGlucVLiv
PAMetTCOHGlucBW34 = AMetTCOHGlucBW34
PAMetTCOHOtherVLiv = AMetTCOHOtherVLiv
PAMetTCOHOtherBW34 = AMetTCOHOtherBW34
PAMetKid = AMetKid
PAMetKidVKid = AMetKidVKid

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PAMetKidBW34 = AMetKidBW34
PAMetDCVG_mMole = AMetDCVG_mMole
PAMetDCVG_mMoleVKid = AMetDCVG_mMoleVKid
PAMetDCVG_mMoleBW34 = AMetDCVG_mMoleBW34

END

DERIVATIVE

      Hours = T

      TERMT(T.GE.TStp, 'Simulation Finished')

! -----
! ----- TCE Model -----
! -----
! Amount of TCE in inhaled air
      RACH = (Rodents * (QM * CExhResp - QM * ACh / VCh)) - (kLoss * ACh) ! (mg/hr)
      ACh = INTEG(RACH, ACh0) ! (mg)
      CInhPPM = (CInh * 24450.0) / MWTCE ! (ppm)

      PROCEDURAL (CInh = CC, ACh, VCh, Conc, MWTCE)
        CInh = Conc * MWTCE / 24450.0 ! (mg/L)
        IF (CC) CInh = ACh / VCh ! (mg/L)
      END

! Amount of TCE in inhalation respiratory lumen
      RAIInhResp = (QM * CInh + DResp * (CResp - CInhResp) - QM * CInhResp) ! (mg/hr)
      AInhResp = INTEG(RAIInhResp, 0.0) ! (mg)
      CInhResp = AInhResp / VRespLum ! (mg/L)

! Amount of TCE in exhalation respiratory lumen
      RAEhResp = (QM * (CInhResp - CExhResp) + QP * (CART / PB - CInhResp) &
&      + DResp * (CResp - CExhResp)) ! (mg/hr)
      AEhResp = INTEG(RAEhResp, 0.0) ! (mg)
      CEhResp = AEhResp / VRespLum ! (mg/L)

! Amount of TCE in the effective respiratory tissue
      RAResp = DResp * (CInhResp + CExhResp - 2.0 * CResp) - RAMetLng ! (mg/hr)
      AResp = INTEG(RAResp, 0.0) ! (mg)
      CResp = AResp / VRespEff ! (mg/L)

! Amount of TCE metabolized in the effective respiratory tissue
      RAMetLng = VMaxClara * CResp / (KMClara + CResp) ! (mg/hr)
      AMetLng = INTEG(RAMetLng, 0.0) ! (mg)
      AMetLngBW34 = AMetLng / (BW**0.75) ! (mg/kg^0.75)
      IF (TotDoseBW34. GT. 0.0) FracMetLng = AMetLngBW34 / TotDoseBW34 ! (unitless)
      AMetLngVResp = AMetLng / VResp ! (mg/L)

! Concentration of TCE in arterial blood
      CART = (QC * CVen + QP * CInhResp + kIA) / (QC + (QP / PB)) ! (mg/L)
      AUCCBld = INTEG(CART, 0.0) ! (mg-hr/L)

! Concentration of TCE in alveolar air
      ExhFac_Den = (QP * CART / PB + (QM - QP) * CInhResp) ! (mg)
      CALv = CART / PB * ExhFactor ! (unitless)
      CALvPPM = CALv * (24450.0 / MWTCE) ! (ppm)

      PROCEDURAL (ExhFactor = QM, CExhResp, ExhFac_Den)
        ExhFactor = 1.0 ! (unitless)
        IF (ExhFac_Den .GT. 0.0) ExhFactor = (QM * CExhResp) / ExhFac_Den ! (unitless)
      END

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! Amount of TCE exhaled
  RAExh = QM * CExhResp                                ! (mg/hr)
  AExh = INTEG(RAExh, 0.0)                              ! (mg)
  AExhPost = AExh - AExhExp                             ! (mg)
  IF (Conc .GT. 0.0) AExhExp = AExh                    ! (mg)

! Amount of TCE in fat tissue
  RAFat = QFat * (CArt - CVFat)                         ! (mg/hr)
  AFat = INTEG(RAFat, 0.0)                              ! (mg)
  CFat = AFat / VFat                                    ! (mg/L)
  CVFat = CFat / PFat                                   ! (mg/L)

! Amount of TCE in stomach -- for oral dosing only
  RAStom = kStom - (kAS + kTSD) * AStom                 ! (mg/hr)
  AStom = INTEG(RAStom, 0.0)                           ! (mg)

! Amount of TCE in duodenum -- for oral dosing only
  RADuod = (kTSD * AStom) - (kAD + kTD) * ADuod        ! (mg/hr)
  ADuod = INTEG(RADuod, 0.0)                           ! (mg)

! Amount of TCE excreted in feces
  RAExc = kTD * ADuod                                   ! (mg/hr)
  AExc = INTEG(RAExc, 0.0)                             ! (mg)

! Rate TCE absorbtion
  RAO = (kAS * AStom) + (kAD * ADuod)                  ! (mg/hr)

! Amount of TCE in gut compartment
  RAGut = (QGut * (CArt - CVGut)) + kDrink + RAO       ! (mg/hr)
  AGut = INTEG(RAGut, 0.0)                             ! (mg)
  CGut = AGut / VGut                                    ! (mg/L)
  CVGut = CGut / PGut                                  ! (mg/L)

! Amount of TCE in kidneys
  RAKid = (QKid * (CArt - CVKid)) - RAMetKid            ! (mg/hr)
  AKid = INTEG(RAKid, 0.0)                              ! (mg)
  CKid = AKid / VKid                                    ! (mg/L)
  CVKid = CKid / PKid                                   ! (mg/L)
  AUCCKid = INTEG(CKid, 0.0)                           ! (mg-hr/L)

! Amount of TCE metabolized to DCVG in kidneys
  RAMetKid = (VMaxKidDCVG * CVKid) / (KMKidDCVG + CVKid) ! (mg/hr)
  AMetKid = INTEG(RAMetKid, 0.0)                       ! (mg)
  AMetKidVKid = AMetKid / VKid                         ! (mg/kg)
  AMetKidBW34 = AMetKid / (BW**0.75)                  ! (mg/kg^0.75)

! Amount of TCE in liver
  RALiv = (QLiv * (CArt - CVLiv)) + (QGut * (CVGut - CVLiv)) + kPV - RAMetLiv1 - RAMetLiv2 ! (mg/hr)
  ALiv = INTEG(RALiv, 0.0)                             ! (mg)
  CLiv = ALiv / VLiv                                    ! (mg/L)
  CVLiv = CLiv / PLiv                                   ! (mg/L)
  AUCCLiv = INTEG(CLiv, 0.0)                           ! (mg-hr/L)

! Amount of TCE metabolized to TCA, DCA and TCOH in liver
  RAMetLiv1 = (VMax * CVLiv) / (KM + CVLiv)            ! (mg/hr)
  AMetLiv1 = INTEG(RAMetLiv1, 0.0)                    ! (mg)
  AMetLiv1VLiv = AMetLiv1 / VLiv                      ! (mg/kg)
  AMetLiv1BW34 = AMetLiv1 / (BW**0.75)               ! (mg/kg^0.75)
  IF (TotDoseBW34 .GT. 0.0) FracMetLiv1 = AMetLiv1BW34 / TotDoseBW34 ! (unitless)
  AMetLiv1TCA = FracTCA * AMetLiv1                   ! (mg TCE)
  AMetLiv1TCAVLiv = AMetLiv1TCA / VLiv               ! (mg TCE/kg)

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AMetLiv1TCABW34 = AMetLiv1TCA / (BW**0.75) ! (mg TCE/kg^0.75)
AMetLiv1TCOH = (1.0 - FracOther - FracTCA) * AMetLiv1 ! (mg TCE)
AMetLiv1TCOHVLiv = AMetLiv1TCOH / VLiv ! (mg TCE/kg)
AMetLiv1TCOHBW34 = AMetLiv1TCOH / (BW**0.75) ! (mg TCE/kg^0.75)
AMetLivOther = FracOther * AMetLiv1 ! (mg)
AMetLivOtherVLiv = AMetLivOther / VLiv ! (mg/kg)
AMetLivOtherBW34 = AMetLivOther / (BW**0.75) ! (mg/kg^0.75)
IF (TotDoseBW34 .GT. 0.0) FracMetLivOther = AMetLivOtherBW34 / TotDoseBW34 ! (unitless)

! Amount of TCE metabolized to DCVG in liver
RAMetLiv2 = (VMaxDCVG * CVLiv) / (KMDCVG + CVLiv) ! (mg/hr)
AMetLiv2 = INTEG(RAMetLiv2, 0.0) ! (mg)
AMetLiv2VLiv = AMetLiv2 / VLiv ! (mg/kg)
AMetLiv2BW34 = AMetLiv2 / (BW**0.75) ! (mg/kg^0.75)
AMetGSH = AMetLiv2 + AMetKid ! (mg)
AMetGSHBW34 = AMetGSH / (BW**0.75) ! (mg/kg^0.75)
IF (TotDoseBW34 .GT. 0.0) FracMetGSH = AMetGSHBW34 / TotDoseBW34 ! (unitless)

! Amount of TCE in rapidly perfused tissues
RARap = QRap * (CART - CVRap) ! (mg/hr)
ARap = INTEG(RARap, 0.0) ! (mg)
CRap = ARap / VRap ! (mg/L)
CVRap = CRap / PRap ! (mg/L)
AUCCRap = INTEG(CRap, 0.0) ! (mg-hr/L)
CHrt = CRap ! (mg/L)
CLung = CRap ! (mg/L)
CSpl = CRap ! (mg/L)
CBrn = CRap ! (mg/L)

! Amount of TCE in slowly perfused tissues
RASlw = QSlw * (CART - CVSlw) ! (mg/hr)
ASlw = INTEG(RASlw, 0.0) ! (mg)
CSlw = ASlw / VSlw ! (mg/L)
CVSlw = CSlw / PSlw ! (mg/L)
CMus = CSlw ! (mg/L)

! Concentration of TCE in mixed venous blood (mg/L)
RABld = (QFat*CVFat + QKid*CVKid + QGutLiv*CVLiv + QRap*CVRap + QSlw*CVSlw + kIV) &
& - QC * CVen ! (mg/hr)
ABld = INTEG(RABld, 0.0) ! (mg)
CVen = ABld / VBld ! (mg/L)
CVen_mMole = CVen / MWTCe ! (mmoles/hr)
CBldMix = (CART + CVen) / 2.0 ! (mg/L)

! Total intake of TCE from inhalation
RInhDose = QM * CInh ! (mg/hr)
RetDose = INTEG(RInhDose, 0.0) - AExhExp ! (mg)
IF (ConcList(1) .EQ. 0.0) RetDose = 0.0

! Total intake of TCE from all routes
TotDose = INTEG((kDrink + kIA + kIV + kPV + kStom + RInhDose), 0.0) ! (mg)

! Mass Balance (mg)
TotTissue = AInhResp + AExhResp + AResp + ABld + AFat + AStom + ADuod + AGut + AKid &
& + ALiv + ARap + ASlw
TotMetab = AMetLng + AMetKid + AMetLiv1 + AMetLiv2
MassBalTCE = TotDose - TotTissue - TotMetab - AExc - AExh
TotDoseBW34 = TotDose / (BW**0.75) ! (mg/kg^0.75)
TotMetabBW34 = TotMetab / (BW**0.75) ! (mg/kg^0.75)
IF (TotDoseBW34 .GT. 0.0) FracMetab = TotMetabBW34 / TotDoseBW34 ! (unitless)
TotOxMetBW34 = (AMetLng + AMetLiv1) / (BW**0.75) ! (mg/kg^0.75)
IF (TotDoseBW34 .GT. 0.0) FracOxMetab = TotOxMetBW34 / TotDoseBW34 ! (unitless)

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! ----- TCA Sub-Model -----
!
! Amount of TCA in plasma
RAPlasTCA = (QBodPlas * CVBodTCA) + (QGutLivPlas * CVLivTCA) + kIVTCA &
&      - (QCPlas * CPlasTCA) - RAUrnTCA      ! (mg/hr)
      APlasTCA = INTEG(RAPlasTCA, 0.0)      ! (mg)
      CPlasTCA = APlasTCA / VPlas            ! (mg/L)
      CBldTCA = CPlasTCA * TCAPlas          ! (mg/L)
      AUCCPlasTCA = INTEG(CPlasTCA, 0.0)    ! (mg-hr/L)

! Amount of free TCA in plasma
APlasTCAFree = CPlasTCAFree * VPlas      ! (mg)
AUCCPlasTCAFree = INTEG(CPlasTCAFree, 0.0) ! (mg-hr/L)

      A = kDissoc + BMax - ((CPlasTCA / MWTCA) * 1000.0) ! (umoles/L)
      B = 4.0 * kDissoc * ((CPlasTCA / MWTCA) * 1000.0) ! (umoles/L)
PROCEDURAL (CPlasTCAFree = A, B, MWTCA)
  IF (B .LT. (0.01 * (A**2.0))) THEN
    CPlasTCAFree = (0.5 * (B / 2.0 / A)) * MWTCA / 1000.0 ! (mg/L)
  ELSE
    CPlasTCAFree = (0.5 * (SQRT((A**2.0) + B) - A)) * MWTCA / 1000.0 ! (mg/L)
  ENDIF
END

! Concentration of bound TCA in plasma
CPlasTCABnd = CPlasTCA - CPlasTCAFree    ! (mg/L)

! Amount of TCA in the body
RABodTCA = QBodPlas * (CPlasTCAFree - CVBodTCAFree) ! (mg/hr)
ABodTCA = INTEG(RABodTCA, 0.0)              ! (mg)
CBodTCA = ABodTCA / VBod                    ! (mg/L)
CVBodTCA = CPlasTCABnd + CVBodTCAFree       ! (mg/L)
CVBodTCAFree = CBodTCA / PBodTCA            ! (mg/L)
CKidTCA = CBodTCA                          ! (mg/L)
CLungTCA = CBodTCA                         ! (mg/L)

! Amount of TCA in stomach -- for oral dosing only
RAStomTCA = kStomTCA - kASTCA * AStomTCA    ! (mg/hr)
AStomTCA = INTEG(RAStomTCA, 0.0)           ! (mg)

! Amount of TCA in the liver
RALivTCA = (QGutLivPlas * (CPlasTCAFree - CVLivTCAFree)) + (kASTCA * AStomTCA) &
&      + (StochTCATCOH * RAMetTCOHTCA) &
&      + (FracTCA * StochTCATCE * (RAMetLiv1 + FracLungSys * RAMetLng)) &
&      - RAMetTCA      ! (mg/hr)
      ALivTCA = INTEG(RALivTCA, 0.0)      ! (mg)
      CLivTCA = ALivTCA / VLiv            ! (mg/L)
      CVLivTCA = CPlasTCABnd + CVLivTCAFree ! (mg/L)
      CVLivTCAFree = CLivTCA / PLivTCA    ! (mg/L)
      AUCCLivTCA = INTEG(CLivTCA, 0.0)    ! (mg-hr/L)

! Amount of TCA metabolized in liver
RAMetTCA = kMetTCA * ALivTCA              ! (mg/hr)
AMetTCA = INTEG(RAMetTCA, 0.0)            ! (mg)
AMetTCAVLiv = AMetTCA / VLiv              ! (mg TCA/kg)
AMetTCABW34 = AMetTCA / (BW**0.75)       ! (mg TCA/kg^0.75)

! Amount of TCA in urine
RAUrnTCA = kUrnTCA * APlasTCAFree         ! (mg/hr)
AUrnTCA = INTEG(RAUrnTCA, 0.0)            ! (mg)
RAUrnTCA_Coll = (1.0 - UrnMissing) * RAUrnTCA ! (mg/hr)
AUrnTCA_Coll = INTEG(RAUrnTCA_Coll, 0.0)  ! (mg)

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! Total intake of TCA from all routes
AOTCA = INTEG((kIVTCA + (kASTCA * ASomTCA)), 0.0) ! (mg)

! Mass Balance (mg)
TotTCAIn = AOTCA + (FracTCA * StochTCATCE * (AMetLiv1 + FracLungSys * AMetLng)) &
& + (StochTCATCOH * AMetTCOHTCA)
TotTissueTCA = APlasTCA + ABodTCA + ALivTCA
MassBalTCA = TotTCAIn - TotTissueTCA - AMetTCA - AURNtCA
TotTCAInBW = TotTCAIn / BW

! -----
! ----- TCOH Sub-Model -----
! -----

! Concentration of TCOH in blood
CTCOH = (QBod * CVBodTCOH + QGutLiv * CVLivTCOH + kIVTCOH) / QC ! (mg/L)
AUCCTCOH = INTEG(CTCOH, 0.0) ! (mg-hr/L)

! Amount of TCOH in the body
RABodTCOH = QBod * (CTCOH - CVBodTCOH) ! (mg/hr)
ABodTCOH = INTEG(RABodTCOH, 0.0) ! (mg)
CBodTCOH = ABodTCOH / VBodTCOH ! (mg/L)
CVBodTCOH = ABodTCOH / VBodTCOH / PBodTCOH ! (mg/L)
AUCCBodTCOH = INTEG((ABodTCOH / VBodTCOH), 0.0) ! (mg-hr/L)
CKidTCOH = CBodTCOH ! (mg/L)
CLungTCOH = CBodTCOH ! (mg/L)

! Concentration of TCOH-Gluc in the body
CBodTCOGTCOH = StochTCOHGluc * (ABodTCOG / VBodTCOH) ! (mg/L)
CKidTCOGTCOH = CBodTCOGTCOH ! (mg/L)
CLungTCOGTCOH = CBodTCOGTCOH ! (mg/L)

! Amount of TCOH in stomach -- for oral dosing only
RAStomTCOH = kStomTCOH - kASTCOH * ASomTCOH ! (mg/hr)
ASomTCOH = INTEG(RAStomTCOH, 0.0) ! (mg)

! Amount of TCOH in liver
RALivTCOH = (QGutLiv * (CTCOH - CVLivTCOH)) + (kASTCOH * ASomTCOH) &
& + (StochTCOHGluc * RARECircTCOG) &
& + ((1.0-FracOther-FracTCA) * StochTCOHTCE * (RAMetLiv1 + FracLungSys * RAMetLng)) &
& - RAMetTCOHTCA - RAMetTCOHGluc - RAMetTCOHOther ! (mg/hr)
ALivTCOH = INTEG(RALivTCOH, 0.0) ! (mg)
CLivTCOH = ALivTCOH / VLiv ! (mg/L)
CVLivTCOH = ALivTCOH / VLiv / PLivTCOH ! (mg/L)
AUCCLivTCOH = INTEG((ALivTCOH / VLiv), 0.0) ! (ug-hr/L)

! Concentration of TCOH-Gluc in liver
CLivTCOGTCOH = StochTCOHGluc * (ALivTCOG / VLiv) ! (mg/L)

! Rate of TCOH oxidation to TCA
RAMetTCOHTCA = (VMaxTCOH * CVLivTCOH) / (KMTCOH + CVLivTCOH) ! (mg/hr)
AMetTCOHTCA = INTEG(RAMetTCOHTCA, 0.0) ! (mg)
AMetTCOHTCAVLiv = AMetTCOHTCA / VLiv ! (mg TCOH/kg)
AMetTCOHTCABW34 = AMetTCOHTCA / (BW**0.75) ! (mg TCOH/kg^0.75)

! Amount of TCOH glucuronidation to TCOG
RAMetTCOHGluc = (VMaxGluc * CVLivTCOH) / (KMGluc + CVLivTCOH) ! (mg/hr)
AMetTCOHGluc = INTEG(RAMetTCOHGluc, 0.0) ! (mg)
AMetTCOHGlucVLiv = AMetTCOHGluc / VLiv ! (mg TCOH/kg)
AMetTCOHGlucBW34 = AMetTCOHGluc / (BW**0.75) ! (mg TCOH/kg^0.75)

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! Amount of TCOH metabolized by other routes in liver
RAMetTCOHOther = kMetTCOH * ALivTCOH                                ! (mg/hr)
AMetTCOHOther = INTEG(RAMetTCOHOther, 0.0)                          ! (mg)
AMetTCOHOtherVLiv = AMetTCOHOther / VLiv                            ! (mg TCOH/kg)
AMetTCOHOtherBW34 = AMetTCOHOther / (BW**0.75)                     ! (mg TCOH/kg^0.75)

! Total intake of TCOH from all routes
AOTCOH = INTEG((kIVTCOH + (kASTCOH * ASomTCOH)), 0.0)              ! (mg)

! Mass Balance (mg)
TotTCOHIn = AOTCOH + (StochTCOHGluc * ARecircTCOG) &
& + ((1.0-FracOther-FracTCA) * StochTCOHTCE * (AMetLiv1 + FracLungSys * AMetLng))
TotTissueTCOH = ABodTCOH + ALivTCOH
TotMetabTCOH = AMetTCOHTCA + AMetTCOHGluc + AMetTCOHOther
MassBalTCOH = TotTCOHIn - TotTissueTCOH - TotMetabTCOH
TotTCOHDose = TotTCOHIn - (StochTCOHGluc * ARecircTCOG)

! -----
! ----- TCOG Sub-Model -----
! -----

! Concentration of TCOH-Gluc in blood
CTCOG = (QBod * CVBodTCOG + QGutLiv * CVLivTCOG) / QC              ! (mg/L)
AUCCTCOG = INTEG(CTCOG, 0.0)                                       ! (mg-hr/L)
CTCOGTCOH = (StochTCOHGluc * CTCOG)                                ! (mg/L)

! Amount of TCOH-Gluc in the body
RABodTCOG = QBod * (CTCOG - CVBodTCOG) - RAUrntTCOG               ! (mg/hr)
ABodTCOG = INTEG(RABodTCOG, 0.0)                                    ! (mg)
CVBodTCOG = ABodTCOG / VBodTCOH / PBodTCOG                        ! (mg/L)

! Amount of TCOH-Gluc in liver
RALivTCOG = QGutLiv * (CTCOG - CVLivTCOG) + (StochGlucTCOH * RAMetTCOHGluc) &
& - (kBile * ALivTCOG)                                             ! (mg/hr)
ALivTCOG = INTEG(RALivTCOG, 0.0)                                    ! (mg)
CLivTCOG = ALivTCOG / VLiv                                         ! (mg/L)
CVLivTCOG = ALivTCOG / VLiv / PLivTCOG                             ! (mg/L)
AUCCLivTCOG = INTEG((ALivTCOG / VLiv), 0.0)                       ! (mg-hr/L)

! Amount of TCOH-Gluc excreted into bile
RABileTCOG = (kBile * ALivTCOG) - RAREcircTCOG                    ! (mg/hr)
ABileTCOG = INTEG(RABileTCOG, 0.0)                                  ! (mg)

! Amount of TCOH-Gluc recirculated
RAREcircTCOG = KEHR * ABileTCOG                                    ! (mg/hr)
AREcircTCOG = INTEG(RAREcircTCOG, 0.0)                             ! (mg)

! Amount of TCOH-Gluc excreted in urine
RAUrntTCOG = kUrntTCOG * ABodTCOG                                  ! (mg/hr)
AUrntTCOG = INTEG(RAUrntTCOG, 0.0)                                 ! (mg)
AUrntTCOGTCOH = StochTCOHGluc * AUrntTCOG                         ! (mg)
RAUrntTCOG_Coll = (1.0 - UrnMissing) * RAUrntTCOG                 ! (mg/hr)
AUrntTCOG_Coll = INTEG(RAUrntTCOG_Coll, 0.0)                     ! (mg)
AUrntTCOGTCOH_Coll = StochTCOHGluc * AUrntTCOG_Coll              ! (mg)

! Total amount of TCA and TCOG in urine
AUrntCTot_mMole = (AUrntTCA / MWTCA) + (AUrntTCOGTCOH / MWTCOH)  ! (mmoles)

! Total amount of TCOH-Gluc in tissues
ATCOG = ABodTCOG + ALivTCOG                                       ! (mg)

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! Total concentration of TCOH and TCOH-Gluc
  TotCTCOH = CTCOH + (StochTCOHGluc * CTCOG)          ! (mg/L)
  AUCTotCTCOH = INTEG(TotCTCOH, 0.0)                  ! (mg-hr/L)

! Mass Balance (mg)
  TotTCOGIn = StochGlucTCOH * AMetTCOHGluc
  TotTissueTCOG = ABodTCOG + ALivTCOG + ABileTCOG
  MassBalTCOG = TotTCOGIn - TotTissueTCOG - ARecircTCOG - AUrnTCOG

! ----- DCVC Sub-Model -----
! Amount of DCVC in kidney
  RADCVC = FracKidDCVC * StochDCVCTCE * RAMetKid + RAMetDCVG_mMole * MWDCVC &
&      - ((kNat + kKidBioact) * ADCVC)                ! (mg/hr)
  ADCVC = INTEG(RADCVC, 0.0)                          ! (mg)
  RABioactDCVC = kKidBioact * ADCVC                   ! (mg/hr)
  ABioactDCVC = INTEG(RABioactDCVC, 0.0)              ! (mg)
  ABioactDCVCVKid = ABioactDCVC / VKid                ! (mg/L)
  ABioactDCVCBW34 = ABioactDCVC / (BW**0.75)         ! (mg/kg^0.75)
  IF (TotDoseBW34 .GT. 0.0) FracBioactKid = ABioactDCVCBW34 / TotDoseBW34 ! (unitless)

! Amount of DCVC excreted into urine
  RAUrDCVC = kNAT * ADCVC                             ! (mg/hr)
  AUrnDCVC = INTEG(RAUrnDCVC, 0.0)                   ! (mg)

! Amount of N Acetyl DCVC excreted
  AUrnNDCVC_Eq = AUrnNDCVC / StochN                  ! (mg)

! Amount of N Acetyl DCVC excreted
  AUrnNDCVC = StochN * AUrnDCVC                      ! (mg)

! Mass Balance (mg)
  ADCVCIn = (FracKidDCVC * StochDCVCTCE * AMetKid) + (AMetDCVG_mMole * MWDCVC)
  MassBalDCVC = ADCVCIn - ADCVC - ABioactDCVC - AUrnNDCVC_Eq

! ----- DCVG Sub-Model -----
! Amount of DCVG in kidney
  RADCVG_mMole = ((RAMetLiv2 + (1.0 - FracKidDCVC) * RAMetKid) / MWTCE) - RAMetDCVG_mMole
!      (mMole/hr)
  ADCVG_mMole = INTEG(RADCVG_mMole, 0.0)              ! (mMole)
  CDCVG_mMole = ADCVG_mMole / VDCVG                  ! (mMole/L)
  AUCCDCVG_mMole = INTEG(CDCVG_mMole, 0.0)           ! (mMole-hr/L)

! Amount of DCVG metabolized
  RAMetDCVG_mMole = kDCVG * ADCVG_mMole              ! (mMole/hr)
  AMetDCVG_mMole = INTEG(RAMetDCVG_mMole, 0.0)       ! (mMole)
  AMetDCVG_mMoleVKid = AMetDCVG_mMole / VDCVG        ! (mMole/kg)
  AMetDCVG_mMoleBW34 = AMetDCVG_mMole / (BW**0.75)  ! (mMole/kg^0.75)

! Mass Balance (mg)
  ADCVGIn = (AMetLiv2 + ((1.0 - FracKidDCVC) * AMetKid)) / MWTCE
  MassBalDCVG = ADCVGIn - ADCVG_mMole - AMetDCVG_mMole

END      ! of Derivative
END      ! of Dynamic

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TERMINAL

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! Convert daily or weekly AUC dosemetrics to daily
AUCCBldDM = AUCCBldDM / (DMInt / 24.0)
AUCCPlasTCADM = AUCCPlasTCADM / (DMInt / 24.0)
AUCCPlasTCAFreeDM = AUCCPlasTCAFreeDM / (DMInt / 24.0)
AUCCTCOHDM = AUCCTCOHDM / (DMInt / 24.0)
AUCCTCOGDM = AUCCTCOGDM / (DMInt / 24.0)
AUCTotCTCOHDM = AUCTotCTCOHDM / (DMInt / 24.0)
AUCCLivDM = AUCCLivDM / (DMInt / 24.0)
AUCCLivTCADM = AUCCLivTCADM / (DMInt / 24.0)
AUCCLivTCOHDM = AUCCLivTCOHDM / (DMInt / 24.0)
AUCCLivTCOGDM = AUCCLivTCOGDM / (DMInt / 24.0)
AUCCKidDM = AUCCKidDM / (DMInt / 24.0)
AUCCDCVG_mMoleDM = AUCCDCVG_mMoleDM / (DMInt / 24.0)

! Convert daily or weekly metabolism dosemetrics to daily
TotMetabBW34DM = TotMetabBW34DM / (DMInt / 24.0)
TotOxMetBW34DM = TotOxMetBW34DM / (DMInt / 24.0)
AMetLiv1VLivDM = AMetLiv1VLivDM / (DMInt / 24.0)
AMetLiv1BW34DM = AMetLiv1BW34DM / (DMInt / 24.0)
AMetLiv1TCAVLivDM = AMetLiv1TCAVLivDM / (DMInt / 24.0)
AMetLiv1TCABW34DM = AMetLiv1TCABW34DM / (DMInt / 24.0)
AMetLiv1TCOHVLivDM = AMetLiv1TCOHVLivDM / (DMInt / 24.0)
AMetLiv1TCOHBW34DM = AMetLiv1TCOHBW34DM / (DMInt / 24.0)
AMetLiv2VLivDM = AMetLiv2VLivDM / (DMInt / 24.0)
AMetLiv2BW34DM = AMetLiv2BW34DM / (DMInt / 24.0)
AMetLivOtherVLivDM = AMetLivOtherVLivDM / (DMInt / 24.0)
AMetLivOtherBW34DM = AMetLivOtherBW34DM / (DMInt / 24.0)
AMetTCAVLivDM = AMetTCAVLivDM / (DMInt / 24.0)
AMetTCABW34DM = AMetTCABW34DM / (DMInt / 24.0)
AMetTCOHTCAVLivDM = AMetTCOHTCAVLivDM / (DMInt / 24.0)
AMetTCOHTCABW34DM = AMetTCOHTCABW34DM / (DMInt / 24.0)
AMetTCOHGlucVLivDM = AMetTCOHGlucVLivDM / (DMInt / 24.0)
AMetTCOHGlucBW34DM = AMetTCOHGlucBW34DM / (DMInt / 24.0)
AMetTCOHOtherVLivDM = AMetTCOHOtherVLivDM / (DMInt / 24.0)
AMetTCOHOtherBW34DM = AMetTCOHOtherBW34DM / (DMInt / 24.0)
AMetKidDM = AMetKidDM / (DMInt / 24.0)
AMetKidVKidDM = AMetKidVKidDM / (DMInt / 24.0)
AMetKidBW34DM = AMetKidBW34DM / (DMInt / 24.0)
AMetDCVG_mMoleDM = AMetDCVG_mMoleDM / (DMInt / 24.0)
AMetDCVG_mMoleVKidDM = AMetDCVG_mMoleVKidDM / (DMInt / 24.0)
AMetDCVG_mMoleBW34DM = AMetDCVG_mMoleBW34DM / (DMInt / 24.0)

END          ! End of Terminal
END          ! of Program

```


APPENDIX B

Mouse MCSim Input and Output Files from Dr. Chiu

This is the MCSim input file for the mouse provided by Dr. Weihsueh Chiu. It has been reformatted for better readability and some lines are now continued on additional lines due to the line length constriction in Word. While the output file is more easily read as an Excel file, it is included here for completeness.

TCE.1.2.3.3.Mouse.pop.1.5.in

USEPA TCE MODEL VERSION 1.2.3

Integrate(Lsodes, 1.0e-5, 0.3e-8, 1);

MCMC ("TCE.1.2.3.3.Mouse.pop.1.5.out", "TCE.1.2.3.3.Mouse.pop.1.4.restart.out", "", 80000, 0, 20, 80000, 46.4564);

Level { #Population level

#Error distributions

```
# Distrib( Ve_RetDose , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CALv , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CALvPPM , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CInhPPM , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CInh , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CMixExh , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CArt , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CVen , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CBldMix , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CFat , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CGut , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CRap , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CSlw , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CHrt , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CKid , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CLiv , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLung , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CMus , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CSpl , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CBrn , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAExh , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zAExhpost , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CKidTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CLivTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLungTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CPlastTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CBldTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CBodTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CKidTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CLivTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLungTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zAUrnTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAUrnTCA_collect , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAUrnTCA_sat , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zABileTCOG , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CTCOG , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CTCOGTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CKidTCOGTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CLivTCOGTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLungTCOGTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_AurnTCOGTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_AurnTCOGTCOH_collect , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_AurnTCOGTCOH_sat , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CDCVGmol , LogUniform , 0.1 , 3.3 );
# Distrib( Ve_zAUrnNDCVC , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_AurnTCTotMole , LogUniform , 0.01 , 3.3 );
Distrib( Ve_TotCTCOH , LogUniform , 0.01 , 3.3 );
```

```

#   Distrib( Ve_QPsamp , LogUniform , 0.01 , 3.3 );

##### POPULATION MEANS
Distrib( M_lnQCC TruncNormal 0.0 0.2 -0.8 0.8 );
Distrib( M_lnVPRC TruncNormal 0.0 0.2 -0.8 0.8 );
Distrib( M_QFatC TruncNormal 1.0 0.46 0.08 1.92 );
Distrib( M_QGutC TruncNormal 1.0 0.17 0.66 1.34 );
Distrib( M_QLivC TruncNormal 1.0 0.17 0.66 1.34 );
Distrib( M_QSlwC TruncNormal 1.0 0.29 0.42 1.58 );
Distrib( M_lnDRespC Uniform -11.513 2.303 );
Distrib( M_QKidC TruncNormal 1.0 0.32 0.36 1.64 );
Distrib( M_FracPlasC TruncNormal 1.0 0.2 0.4 1.6 );
Distrib( M_VFatC TruncNormal 1.0 0.45 0.1 1.9 );
Distrib( M_VGutC TruncNormal 1.0 0.13 0.74 1.26 );
Distrib( M_VLivC TruncNormal 1.0 0.24 0.52 1.48 );
Distrib( M_VRapC TruncNormal 1.0 0.1 0.8 1.2 );
Distrib( M_VRespLumC TruncNormal 1.0 0.11 0.78 1.22 );
Distrib( M_VRespEffC TruncNormal 1.0 0.11 0.78 1.22 );
Distrib( M_VKidC TruncNormal 1.0 0.1 0.8 1.2 );
Distrib( M_VBldC TruncNormal 1.0 0.12 0.76 1.24 );
Distrib( M_lnPBC TruncNormal 0.0 0.25 -0.75 0.75 );
Distrib( M_lnPFatC TruncNormal 0.0 0.3 -0.9 0.9 );
Distrib( M_lnPGutC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPLivC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPRapC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPRespC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPKidC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPSlwC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPRBCPlasTCAC Uniform -4.605 4.605 );
Distrib( M_lnPBodTCAC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnPLivTCAC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnkDissoC TruncNormal 0.0 1.191 -3.573 3.573 );
Distrib( M_lnBMaxkDC TruncNormal 0.0 0.495 -1.485 1.485 );
Distrib( M_lnPBodTCOHC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnPLivTCOHC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnPBodTCOGC Uniform -4.605 4.605 );
Distrib( M_lnPLivTCOGC Uniform -4.605 4.605 );
Distrib( M_lnPeffDCVG Uniform -6.908 6.908 );
Distrib( M_lnkTSD Uniform -4.269 4.942 );
Distrib( M_lnkAS Uniform -6.571 7.244 );
Distrib( M_lnkTD Uniform -4.605 0 );
Distrib( M_lnkAD Uniform -7.195 6.62 );
Distrib( M_lnkASTCA Uniform -7.195 6.62 );
Distrib( M_lnkASTCOH Uniform -7.195 6.62 );
Distrib( M_lnVMaxC TruncNormal 0.0 0.693 -2.079 2.079 );
Distrib( M_lnkMC TruncNormal 0.0 1.386 -4.158 4.158 );
#   Distrib( M_lnClC Normal 0 1 );
Distrib( M_lnFracOtherC Uniform -6.908 6.908 );
Distrib( M_lnFracTCAC TruncNormal 0.0 1.163 -3.489 3.489 );
Distrib( M_lnVMaxDCVGC Uniform -4.605 9.21 );
Distrib( M_lnClDCVGC Uniform -4.605 9.21 );
#   Distrib( M_lnkMDCVGC Normal 0 1 );
Distrib( M_lnVMaxKidDCVGC Uniform -4.605 9.21 );
Distrib( M_lnClKidDCVGC Uniform -4.605 9.21 );
#   Distrib( M_lnkMKidDCVGC Normal 0 1 );
Distrib( M_lnVMaxLungLivC TruncNormal 0.0 1.099 -3.297 3.297 );
Distrib( M_lnkMClara Uniform -6.908 6.908 );
Distrib( M_lnFracLungSysC Uniform -6.908 6.908 );
Distrib( M_lnVMaxTCOHC Uniform -9.21 9.21 );
#   Distrib( M_lnClTCOHC Normal 0 1 );
Distrib( M_lnkMTCOH Uniform -9.21 9.21 );
Distrib( M_lnVMaxGlucC Uniform -9.21 9.21 );
#   Distrib( M_lnClGlucC Normal 0 1 );
Distrib( M_lnkMGluc Uniform -6.908 6.908 );
Distrib( M_lnkMetTCOHC Uniform -11.513 6.908 );
Distrib( M_lnkUrntCAC Uniform -4.605 4.605 );
Distrib( M_lnkMetTCAC Uniform -9.21 4.605 );
Distrib( M_lnkBileC Uniform -9.21 4.605 );
Distrib( M_lnkEHRC Uniform -9.21 4.605 );
Distrib( M_lnkUrntCOGC Uniform -6.908 6.908 );

```

```

Distrib( M_lnFracKidDCVCC Uniform -6.908 6.908 );
Distrib( M_lnkDCVGC Uniform -9.21 4.605 );
Distrib( M_lnkNATC Uniform -9.21 4.605 );
Distrib( M_lnkKidBioactC Uniform -9.21 4.605 );

##### POPULATION VARIANCES
Distrib( V_lnQCC InvGamma 2.25 0.0500 );
Distrib( V_lnVPRC InvGamma 2.25 0.0500 );
Distrib( V_QFatC InvGamma 6 1.0580 );
Distrib( V_QGutC InvGamma 6 0.1445 );
Distrib( V_QLivC InvGamma 6 0.1445 );
Distrib( V_QSlwC InvGamma 6 0.4205 );
Distrib( V_lnDRespC InvGamma 6 0.2000 );
Distrib( V_QKidC InvGamma 6 0.5120 );
Distrib( V_FracPlasC InvGamma 6 0.2000 );
Distrib( V_VFatC InvGamma 6 1.0125 );
Distrib( V_VGutC InvGamma 6 0.0845 );
Distrib( V_VLivC InvGamma 6 0.2880 );
Distrib( V_VRapC InvGamma 6 0.0500 );
Distrib( V_VRespLumC InvGamma 6 0.0605 );
Distrib( V_VRespEffC InvGamma 6 0.0605 );
Distrib( V_VKidC InvGamma 6 0.0500 );
Distrib( V_VBldC InvGamma 6 0.0720 );
Distrib( V_lnPBC InvGamma 2.25 0.0781 );
Distrib( V_lnPFatC InvGamma 2.25 0.1125 );
Distrib( V_lnPGutC InvGamma 2.25 0.2000 );
Distrib( V_lnPLivC InvGamma 2.25 0.2000 );
Distrib( V_lnPRapC InvGamma 2.25 0.2000 );
Distrib( V_lnPRespC InvGamma 2.25 0.2000 );
Distrib( V_lnPKidC InvGamma 2.25 0.2000 );
Distrib( V_lnPSlwC InvGamma 2.25 0.2000 );
Distrib( V_lnPRBCPlasTCAC InvGamma 2.25 0.1411 );
Distrib( V_lnPBodTCAC InvGamma 2.25 0.1411 );
Distrib( V_lnPLivTCAC InvGamma 2.25 0.1411 );
Distrib( V_lnkDissocC InvGamma 2.25 1.7731 );
Distrib( V_lnBMaxkDC InvGamma 2.25 0.3063 );
Distrib( V_lnPBodTCOHC InvGamma 2.25 0.1411 );
Distrib( V_lnPLivTCOHC InvGamma 2.25 0.1411 );
Distrib( V_lnPBodTCOGC InvGamma 2.25 0.2000 );
Distrib( V_lnPLivTCOGC InvGamma 2.25 0.2000 );
Distrib( V_lnPeffDCVG InvGamma 2.25 0.2000 );
Distrib( V_lnkTSD InvGamma 2.25 5.0000 );
Distrib( V_lnkAS InvGamma 2.25 5.0000 );
Distrib( V_lnkTD InvGamma 2.25 5.0000 );
Distrib( V_lnkAD InvGamma 2.25 5.0000 );
Distrib( V_lnkASTCA InvGamma 2.25 5.0000 );
Distrib( V_lnkASTCOH InvGamma 2.25 5.0000 );
Distrib( V_lnVMaxC InvGamma 3 1.3585 );
Distrib( V_lnKMC InvGamma 3 0.1458 );
# Distrib( V_lnClC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnFracOtherC InvGamma 2.25 0.3125 );
Distrib( V_lnFracTCAC InvGamma 2.25 0.3125 );
Distrib( V_lnVMaxDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnClDCVGC InvGamma 2.25 0.3125 );
# Distrib( V_lnKMDCVGC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnVMaxKidDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnClKidDCVGC InvGamma 2.25 0.3125 );
# Distrib( V_lnKMKidDCVGC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnVMaxLungLivC InvGamma 2.25 0.3125 );
Distrib( V_lnKMClara InvGamma 2.25 0.3125 );
Distrib( V_lnFracLungSysC InvGamma 2.25 0.3125 );
Distrib( V_lnVMaxTCOHC InvGamma 2.25 0.3125 );
# Distrib( V_lnClTCOHC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnKMTCOH InvGamma 2.25 0.3125 );
Distrib( V_lnVMaxGlucC InvGamma 2.25 0.3125 );
# Distrib( V_lnClGlucC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnKMGluc InvGamma 2.25 0.3125 );
Distrib( V_lnkMetTCOHC InvGamma 2.25 0.3125 );
Distrib( V_lnkUrnTCAC InvGamma 2.25 0.3125 );
Distrib( V_lnkMetTCAC InvGamma 2.25 0.3125 );
Distrib( V_lnkBileC InvGamma 2.25 0.3125 );

```

```

Distrib( V_lnkEHRC InvGamma 2.25 0.3125 );
Distrib( V_lnkUrntCOGC InvGamma 2.25 0.3125 );
Distrib( V_lnFracKidDCVCC InvGamma 2.25 0.3125 );
Distrib( V_lnkDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnkNATC InvGamma 2.25 0.3125 );
Distrib( V_lnkKidBioactC InvGamma 2.25 0.3125 );

#Likelihoods
# Likelihood( RetDose , LogNormal_v , Prediction( RetDose ) , Ve_RetDose );
# Likelihood( CALv , LogNormal_v , Prediction( CALv ) , Ve_CALv );
# Likelihood( CALvPPM , LogNormal_v , Prediction( CALvPPM ) , Ve_CALvPPM );
Likelihood( CInhPPM , LogNormal_v , Prediction( CInhPPM ) , Ve_CInhPPM );
# Likelihood( CInh , LogNormal_v , Prediction( CInh ) , Ve_CInh );
# Likelihood( CMixExh , LogNormal_v , Prediction( CMixExh ) , Ve_CMixExh );
# Likelihood( Cart , LogNormal_v , Prediction( Cart ) , Ve_Cart );
Likelihood( Cven , LogNormal_v , Prediction( Cven ) , Ve_Cven );
Likelihood( CBldMix , LogNormal_v , Prediction( CBldMix ) , Ve_CBldMix );
Likelihood( CFat , LogNormal_v , Prediction( CFat ) , Ve_CFat );
# Likelihood( CGut , LogNormal_v , Prediction( CGut ) , Ve_CGut );
# Likelihood( CRap , LogNormal_v , Prediction( CRap ) , Ve_CRap );
# Likelihood( CSLw , LogNormal_v , Prediction( CSLw ) , Ve_CSLw );
# Likelihood( CHrt , LogNormal_v , Prediction( CHrt ) , Ve_CHrt );
Likelihood( CKid , LogNormal_v , Prediction( CKid ) , Ve_CKid );
Likelihood( CLiv , LogNormal_v , Prediction( CLiv ) , Ve_CLiv );
# Likelihood( CLung , LogNormal_v , Prediction( CLung ) , Ve_CLung );
# Likelihood( CMus , LogNormal_v , Prediction( CMus ) , Ve_CMus );
# Likelihood( CSpl , LogNormal_v , Prediction( CSpl ) , Ve_CSpl );
# Likelihood( CBrn , LogNormal_v , Prediction( CBrn ) , Ve_CBrn );
# Likelihood( zAExh , LogNormal_v , Prediction( zAExh ) , Ve_zAExh );
Likelihood( zAExhpost , LogNormal_v , Prediction( zAExhpost ) , Ve_zAExhpost );
Likelihood( CTCOH , LogNormal_v , Prediction( CTCOH ) , Ve_CTCOH );
# Likelihood( CKidTCOH , LogNormal_v , Prediction( CKidTCOH ) , Ve_CKidTCOH );
Likelihood( CLivTCOH , LogNormal_v , Prediction( CLivTCOH ) , Ve_CLivTCOH );
# Likelihood( CLungTCOH , LogNormal_v , Prediction( CLungTCOH ) , Ve_CLungTCOH );
Likelihood( CPlasTCA , LogNormal_v , Prediction( CPlasTCA ) , Ve_CPlasTCA );
Likelihood( CBldTCA , LogNormal_v , Prediction( CBldTCA ) , Ve_CBldTCA );
# Likelihood( CBodTCA , LogNormal_v , Prediction( CBodTCA ) , Ve_CBodTCA );
# Likelihood( CKidTCA , LogNormal_v , Prediction( CKidTCA ) , Ve_CKidTCA );
Likelihood( CLivTCA , LogNormal_v , Prediction( CLivTCA ) , Ve_CLivTCA );
# Likelihood( CLungTCA , LogNormal_v , Prediction( CLungTCA ) , Ve_CLungTCA );
Likelihood( zAUrnTCA , LogNormal_v , Prediction( zAUrnTCA ) , Ve_zAUrnTCA );
# Likelihood( zAUrnTCA_collect, LogNormal_v, Prediction(zAUrnTCA_collect), Ve_zAUrnTCA_collect );
# Likelihood( zAUrnTCA_sat , LogNormal_v , Prediction( zAUrnTCA_sat ) , Ve_zAUrnTCA_sat );
# Likelihood( zABileTCOG , LogNormal_v , Prediction( zABileTCOG ) , Ve_zABileTCOG );
# Likelihood( CTCOG , LogNormal_v , Prediction( CTCOG ) , Ve_CTCOG );
Likelihood( CTCOGTCOH , LogNormal_v , Prediction( CTCOGTCOH ) , Ve_CTCOGTCOH );
# Likelihood( CKidTCOGTCOH , LogNormal_v , Prediction( CKidTCOGTCOH ) , Ve_CKidTCOGTCOH );
Likelihood( CLivTCOGTCOH , LogNormal_v , Prediction( CLivTCOGTCOH ) , Ve_CLivTCOGTCOH );
# Likelihood( CLungTCOGTCOH , LogNormal_v , Prediction( CLungTCOGTCOH ) , Ve_CLungTCOGTCOH );
Likelihood( AUrnTCOGTCOH , LogNormal_v , Prediction( AUrnTCOGTCOH ) , Ve_AUrnTCOGTCOH );
# Likelihood( AUrnTCOGTCOH_collect , LogNormal_v , Prediction( AUrnTCOGTCOH_collect ) ,
# Ve_AUrnTCOGTCOH_collect );
# Likelihood( AUrnTCOGTCOH_sat , LogNormal_v , Prediction( AUrnTCOGTCOH_sat ) ,
# Ve_AUrnTCOGTCOH_sat );
# Likelihood( CDCVGmol , LogNormal_v , Prediction( CDCVGmol ) , Ve_CDCVGmol );
# Likelihood( zAUrnNDCVC , LogNormal_v , Prediction( zAUrnNDCVC ) , Ve_zAUrnNDCVC );
# Likelihood( AUrnTCTotMole , LogNormal_v , Prediction( AUrnTCTotMole ) , Ve_AUrnTCTotMole );
Likelihood( TotCTCOH , LogNormal_v , Prediction( TotCTCOH ) , Ve_TotCTCOH );
# Likelihood( QPsamp , LogNormal_v , Prediction( QPsamp ) , Ve_QPsamp );

Level { #Subject/group level
  Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
  Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );
  Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
  Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.66 1.34 );
  Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.66 1.34 );
  Distrib( QSlwC TruncNormal_v M_QSlwC V_QSlwC 0.42 1.58 );
  Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
  Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.36 1.64 );
  Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.4 1.6 );

```

```

Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.74 1.26 );
Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.52 1.48 );
Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.8 1.2 );
Distrib( VRespLumC TruncNormal_v M_VRespLumC V_VRespLumC 0.78 1.22 );
Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.78 1.22 );
Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.8 1.2 );
Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.75 0.75 );
Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.9 0.9 );
Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -1.2 1.2 );
Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -1.2 1.2 );
Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
Distrib( lnkDissocC TruncNormal_v M_lnkdissocC V_lnkdissocC -3.573 3.573 );
Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -1.485 1.485 );
Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );
Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
Distrib( lnkTSD TruncNormal_v M_lnktSD V_lnktSD -4.269 4.942 );
Distrib( lnKAS TruncNormal_v M_lnKAS V_lnKAS -6.571 7.244 );
Distrib( lnkTD TruncNormal_v M_lnktD V_lnktD -4.605 0 );
Distrib( lnKAD TruncNormal_v M_lnKAD V_lnKAD -7.195 6.62 );
Distrib( lnkASTCA TruncNormal_v M_lnKASTCA V_lnKASTCA -7.195 6.62 );
Distrib( lnkASTCOH TruncNormal_v M_lnKASTCOH V_lnKASTCOH -7.195 6.62 );
Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC -4.158 4.158 );
# Distrib( lnClC TruncNormal_v M_lnClC V_lnClC 0 1 );
Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC -4.605 9.21 );
Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -4.605 9.21 );
# Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC 0 1 );
Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC -4.605 9.21 );
Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -4.605 9.21 );
# Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC 0 1 );
Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC -9.21 9.21 );
# Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC 0 1 );
Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC -9.21 9.21 );
# Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC 0 1 );
Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
Distrib( lnkUrnTCAC TruncNormal_v M_lnkUrnTCAC V_lnkUrnTCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
Distrib( lnKEHRC TruncNormal_v M_lnKEHRC V_lnKEHRC -9.21 4.605 );
Distrib( lnkUrnTCOGC TruncNormal_v M_lnkUrnTCOGC V_lnkUrnTCOGC -6.908 6.908 );
Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );
Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
Distrib( lnkNATC TruncNormal_v M_lnkNATC V_lnkNATC -9.21 4.605 );
Distrib( lnkKidBioactC TruncNormal_v M_lnkKidBioactC V_lnKkidBioactC -9.21 4.605 );

Species = 3;

```

```

##### DATA USED IN CALIBRATION #####
#####

##### BEGIN GROUP 1
Level {
#### BEGIN Abbas97a
Experiment { # Begin Abbas97a TCEmceB6aMorloil12e
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0275 ;

# Exposure/Dosing
  PDose = NDoses(2, 1200 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 24, 48, 72, 96, 120, 144 );
  Data( AUrnTCOGTCOH , 8.23, 11.263, 12.195, 12.409, 12.641, 12.709 );
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 16, 24, 30, 40 );
  Data( CBldTCA , 16.5, 23.1, 29.2, 36.1, 41.8, 59.1, 64, 70.2, 94.1, 90.8, 65.2,
    43.86, 41.48, 9.15 );
  Print( CFat , 0.083, 0.17, 0.25, 0.5, 0.75, 1.5, 2, 3, 4, 6, 8, 16, 24 );
  Data( CFat , 61.53, 156.7, 567.2, 826, 865.3, 1199.9, 1050.5, 550.2, 485, 219.2,
    293.7, 4.4, 1.446 );
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0.083, 0.17, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 6, 8, 16, 24 );
  Data( CKid , 144.9, 171.3, 265.6, 282.6, 1095.6, 690.1, 303.8, 109.8, 32.4, 40.2,
    17.3, 3.6, 2.2 );
  Print( CLiv , 0.083, 0.17, 0.25, 0.5, 0.75, 1, 1.5, 2, 4, 6, 8, 16, 24 );
  Data( CLiv , 522.6, 585.3, 499.4, 408, 289.8, 228.8, 63.04, 38.97, 26.5, 15.37,
    14.97, 12.86, 1.79 );
  Print( CLivTCA , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 16, 24, 30, 40 );
  Data( CLivTCA , 11.09, 16.95, 20.09, 26.02, 29.44, 35.65, 37.76, 42.07, 43.92, 57.83,
    27.71, 18.801, 22.67, 6.34 );
  Print( CLivTCOGTCOH , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8 );
  Data( CLivTCOGTCOH , 23.67, 23.3, 19.03, 34.89, 54.87, 62.31, 74.66, 76.92, 26.66,
    55.43 );
  Print( CLivTCOH , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 16 );
  Data( CLivTCOH , 65.35, 75.33, 98.28, 105.3, 88.25, 92.24, 55.03, 57.64, 35.96,
    37.45, 10.12 );
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 16 );
  Data( CTCOGTCOH , 62.12, 63.13, 67.59, 50.86, 64.31, 95.02, 41.5, 46.7, 51.86, 40.88,
    10.11 );
  Print( CTCOH , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 12 );
  Data( CTCOH , 18.83, 27.73, 31.36, 35.42, 28.26, 41.86, 21.54, 24.64, 4.589, 4.487 );
  Print( CVen , 0.083, 0.17, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 8, 12, 16, 24 );
  Data( CVen , 165.87, 191.31, 123.52, 86.9, 70.9, 43.08, 35.17, 20.36, 8.97, 7.5,
    1.64, 0.72, 0.47, 0.52 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 24, 48, 72, 96, 120, 144 );
  Data( zAUrnTCA , 2.294, 3.731, 4.579, 4.796, 4.848, 4.87 );
} # End Abbas97a TCEmceB6aMorloil12e

Experiment { # Begin Abbas97a TCEmceB6aMorloil2e3
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0275 ;

```

```

# Exposure/Dosing
  PDose = NDoses(2, 2000 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AurnTCOGTCOH , 24, 48, 72, 96, 120, 144, 168, 192 );
  Data( AurnTCOGTCOH , 15.28, 21.19, 23.92, 24.79, 25.51, 25.94, 25.95, 25.98 );
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0.25, 0.5, 1, 2, 4, 16, 24, 30, 48 );
  Data( CBldTCA , 11.22, 20.57, 30.34, 43.51, 63.43, 131.85, 51.38, 54.57, 8.74 );
  Print( CFat , 0.25, 0.5, 1, 2, 4, 8, 16, 24 );
  Data( CFat , 1152, 1993, 4279, 2015, 1991, 1503, 75.5, 7.4 );
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0.25, 0.5, 1, 2, 8, 16, 24 );
  Data( CKid , 636, 652, 542, 176, 139.4, 55, 1.3 );
  Print( CLiv , 0.25, 0.5, 1, 2, 4, 8, 16, 24 );
  Data( CLiv , 1498, 335, 379.7, 116.2, 114.5, 105.1, 9.2, 2 );
  Print( CLivTCA , 0.25, 0.5, 1, 2, 4, 8, 16, 24, 30, 48 );
  Data( CLivTCA , 15.18, 27.58, 37.49, 49.46, 65.32, 105.65, 59, 44.6, 36.35, 9.98 );
  Print( CLivTCOGTCOH , 0.25, 0.5, 4, 8, 16 );
  Data( CLivTCOGTCOH , 17.3, 14.47, 66.23, 23.04, 13.08 );
  Print( CLivTCOH , 0.25, 0.5, 1, 2, 4, 8, 16 );
  Data( CLivTCOH , 64.69, 73.45, 205.3, 237.98, 114.88, 73.96, 30.8 );
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0.25, 0.5, 1, 2, 4, 8, 16 );
  Data( CTCOGTCOH , 16.2, 22.88, 26.1, 30.21, 61.1, 40.88, 21.68 );
  Print( CTCOH , 0.25, 0.5, 1, 2, 4, 16 );
  Data( CTCOH , 21.41, 32.94, 41.84, 36.4, 29.14, 4.21 );
  Print( CVen , 0.25, 0.5, 1, 2, 4, 8, 16 );
  Data( CVen , 208.3, 162, 140.1, 64.8, 48.6, 17.48, 1.15 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAurnTCA , 24, 48, 72, 96, 120, 144, 168, 192 );
  Data( zAurnTCA , 1.423, 2.486, 3.122, 3.294, 3.395, 3.426, 3.438, 3.45 );
} # End Abbas97a TCEmceB6aMorloil2e3

Experiment { # Begin Abbas97a TCEmceB6aMorloil300
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0275 ;

# Exposure/Dosing
  PDose = NDoses(2, 300 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AurnTCOGTCOH , 24, 48, 72, 96, 120, 144 );
  Data( AurnTCOGTCOH , 1.912, 3.555, 3.76, 3.803, 3.84, 3.855 );
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0.25, 0.5, 2, 4, 8, 16, 24, 30 );
  Data( CBldTCA , 26.7, 20.4, 42.6, 53.4, 47.6, 43.2, 35.9, 25 );
  Print( CFat , 0.25, 0.5, 1, 2, 4, 8, 16, 24 );
  Data( CFat , 60.13, 125.4, 189.9, 72.58, 40.32, 18.12, 31.3, 0.65 );
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0.25, 0.5, 1, 2, 4, 8, 16, 24 );
  Data( CKid , 90.4, 21.4, 25.8, 7.92, 6.69, 3.4, 6.7, 3.26 );
  Print( CLiv , 0.25, 0.5, 1, 2, 4, 8, 16 );
  Data( CLiv , 70, 42.1, 16.98, 8.81, 4.17, 1.89, 0.945 );
  Print( CLivTCA , 0.25, 2, 4, 8, 16, 24, 30, 48 );
  Data( CLivTCA , 18.9, 35.8, 45.6, 48, 35.3, 8.16, 10.4, 1.229 );
  Print( CLivTCOGTCOH , 0.25 );
  Data( CLivTCOGTCOH , -1 ); ## Zero replaced by no data

```

```

Print( CLivTCOH , 0.25, 0.5, 1, 2, 4, 8, 16 );
Data( CLivTCOH , 39.8, 66.2, 41.52, 18.82, 20.69, 14.68, 5.06 );
Print( CPlasTCA , 0);
Data( CPlasTCA , -1);
Print( CTCOGTCOH , 0.25, 0.5, 1, 2, 4, 8, 16 );
Data( CTCOGTCOH , 15.92, 21.31, 31.27, 10.58, 13.57, 9.51, 1.82 );
Print( CTCOH , 0.25, 0.5, 1, 2, 4, 8, 16 );
Data( CTCOH , 14.54, 19.66, 37.54, 9.85, 4.78, 2.23, 1.48 );
Print( CVen , 0.25, 0.5, 1, 2, 4 );
Data( CVen , 26.11, 12.99, 6.67, 0.68, 0.61 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 24, 48, 72, 96, 120, 144 );
Data( zAUrnTCA , 0.707, 1.176, 1.292, 1.304, 1.307, 1.308 );
} # End Abbas97a TCEmceB6aMorloil300

Experiment { # Begin Abbas97a TCEmceB6aMorloil600
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0275 ;

# Exposure/Dosing
  PDose = NDoses(2, 600 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 24, 48, 72, 96, 120, 144 );
  Data( AUrnTCOGTCOH , 6.892, 9.072, 9.593, 9.716, 9.829, 9.895 );
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0.25, 0.5, 2, 4, 8, 16, 24, 40 );
  Data( CBldTCA , 11.18, 14.26, 26.98, 31.73, 31.87, 29.48, 24.81, 21.1 );
  Print( CFat , 0.25, 0.5, 2, 4, 8, 16, 24 );
  Data( CFat , 278.5, 659, 468.91, 46.76, 9.48, 0.71, 0.32 );
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0.25, 0.5, 2, 4, 8, 24 );
  Data( CKid , 83.08, 135.5, 15.98, 10.89, 5.4, 0.42 );
  Print( CLiv , 0.25, 0.5, 2, 4, 8, 24 );
  Data( CLiv , 213.5, 163.8, 19.43, 10.63, 0.71, 0.339 );
  Print( CLivTCA , 0.25, 0.5, 2, 4, 8, 16, 24, 30, 40 );
  Data( CLivTCA , 11.2, 22.9, 33.5, 39.9, 54.99, 39.06, 28.2, 15.2, 7.6 );
  Print( CLivTCOGTCOH , 0.25, 0.5, 2, 4, 8 );
  Data( CLivTCOGTCOH , 18.45, 20.07, 39.44, 19.59, 46.06 );
  Print( CLivTCOH , 0.25, 0.5, 2, 4, 8, 12 );
  Data( CLivTCOH , 50.25, 46.83, 36.29, 21.06, 11.24, 4.29 );
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0.25, 0.5, 2, 4, 8, 12 );
  Data( CTCOGTCOH , 10.51, 39.66, 27.01, 23.55, 14.76, 6.89 );
  Print( CTCOH , 0.25, 0.5, 2, 4, 8, 12 );
  Data( CTCOH , 18.8, 26.76, 24.01, 8.23, 2.16, 1.02 );
  Print( CVen , 0.25, 0.5, 2, 4, 8 );
  Data( CVen , 81.9, 71.3, 5.71, 1.94, 0.965 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 24, 48, 72, 96, 120, 144 );
  Data( zAUrnTCA , 0.762, 1.683, 1.867, 1.904, 1.927, 1.941 );
} # End Abbas97a TCEmceB6aMorloil600
#### END Abbas97a

#### BEGIN Abbas97b
Experiment { # Begin Abbas97b TCAmceB6aM_iv_aq100
  Species = 3 ;
  Male = 1 ;

```



```

# Measured Covariates (if any)
  BWmeas = 0.035 ;

# Exposure/Dosing
  IVDoseTCA = NDoses(2, 100 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AurnTCOGTCOH , 0);
  Data( AurnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0.1, 0.15, 0.35, 0.65, 1, 2, 4, 8, 24, 30 );
  Data( CBldTCA , 281.9, 380.3, 374.4, 207, 204.6, 94.3, 83.1, 48.97, 9.37, 3.91 );
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAurnTCA , 24, 48, 72, 96, 120, 144, 168 );
  Data( zAurnTCA , 0.937, 1.744, 1.801, 1.828, 1.843, 1.849, 1.853 );
} # End Abbas97b TCAmceB6aM_iv_aq100

Experiment { # Begin Abbas97b TCHmceB6aM_iv_aq100
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.035 ;

# Exposure/Dosing
  IVDoseTCOH = NDoses(2, 100 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AurnTCOGTCOH , 24, 48, 72, 96, 120, 144, 168 );
  Data( AurnTCOGTCOH , 1.093, 1.859, 1.986, 2.097, 2.061, 2.071, 2.1 );
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0.05, 0.1, 0.5, 1, 2 );
  Data( CBldTCA , 0.83, 2.05, 2.21, 7.45, 21.1 );
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);

```

```

Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 0);
Data( CPlasTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0.05, 0.1, 0.5, 1, 2 );
Data( CTCOH , 77.34, 44.75, 19.11, 7.17, 0.163 );
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Abbas97b TCHmceB6aM_iv_aq100
#### END Abbas97b
##### END GROUP 1
}

##### BEGIN GROUP 2
Level {
#### BEGIN Fisher91
Experiment { # Begin Fisher91 TCEmceB6aFinh004042
Species = 3 ;
Male = 0 ;

# Measured Covariates (if any)
BWmeas = 0.025 ;

# Exposure/Dosing
Conc = NDoses(2, 42 0 , 0 4 );

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 2, 3.83, 4.167, 4.333, 4.5, 4.67, 6, 9 );
Data( CPlasTCA , 17.69, 23.94, 29.92, 35.03, 24.33, 29.72, 25.18, 7.86 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 2, 3.83 );
Data( CVen , 0.306666667, 0.34 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);

```

```

        Print( zAUrnTCA , 0);
        Data( zAUrnTCA , -1);
    } # End Fisher91 TCEmceB6aFinh004042

    Experiment { # Begin Fisher91 TCEmceB6aFinh004236
        Species = 3 ;
        Male = 0 ;

    # Measured Covariates (if any)
        BWmeas = 0.023 ;

    # Exposure/Dosing
        Conc = NDoses(2, 236 0 , 0 4 );

    # Data
        Print( AUrnTCOGTCOH , 0);
        Data( AUrnTCOGTCOH , -1);
        Print( CBldMix , 0);
        Data( CBldMix , -1);
        Print( CBldTCA , 0);
        Data( CBldTCA , -1);
        Print( CFat , 0);
        Data( CFat , -1);
        Print( CInhPPM , 0);
        Data( CInhPPM , -1);
        Print( CKid , 0);
        Data( CKid , -1);
        Print( CLiv , 0);
        Data( CLiv , -1);
        Print( CLivTCA , 0);
        Data( CLivTCA , -1);
        Print( CLivTCOGTCOH , 0);
        Data( CLivTCOGTCOH , -1);
        Print( CLivTCOH , 0);
        Data( CLivTCOH , -1);
        Print( CPlasTCA , 2, 3.83, 5, 6, 7, 9 );
        Data( CPlasTCA , 50.8, 57.2, 58.4, 43.2, 24, 14.4 );
        Print( CTCOGTCOH , 0);
        Data( CTCOGTCOH , -1);
        Print( CTCOH , 0);
        Data( CTCOH , -1);
        Print( CVen , 2, 3.83, 4.5, 5 );
        Data( CVen , 4.58, 4.95, 0.88, 0.45 );
        Print( TotCTCOH , 0);
        Data( TotCTCOH , -1);
        Print( zAExhpost , 0);
        Data( zAExhpost , -1);
        Print( zAUrnTCA , 0);
        Data( zAUrnTCA , -1);
    } # End Fisher91 TCEmceB6aFinh004236

    Experiment { # Begin Fisher91 TCEmceB6aFinh004368
        Species = 3 ;
        Male = 0 ;

    # Measured Covariates (if any)
        BWmeas = 0.024 ;

    # Exposure/Dosing
        Conc = NDoses(2, 368 0 , 0 4 );

    # Data
        Print( AUrnTCOGTCOH , 0);
        Data( AUrnTCOGTCOH , -1);
        Print( CBldMix , 0);
        Data( CBldMix , -1);
        Print( CBldTCA , 0);
        Data( CBldTCA , -1);
        Print( CFat , 0);
        Data( CFat , -1);
        Print( CInhPPM , 0);

```

```

Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 2, 3.83, 4.33, 4.67, 5, 5.33, 7, 10, 30 );
Data( CPlasTCA , 58.5, 59.8, 61.7, 69.9, 59.7, 57.7, 35.9, 24.5, 0.32 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 2, 3.83, 4.33, 4.67, 5 );
Data( CVen , 5.9, 6.3, 1.03, 0.8, 0.22 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6aFinh004368

Experiment { # Begin Fisher91 TCEmceB6aFinh004889
  Species = 3 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.03 ;

# Exposure/Dosing
  Conc = NDoses(2, 889 0 , 0 4 );

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 2, 3.83, 4.167, 4.333, 4.5, 5, 6, 8, 26 );
  Data( CPlasTCA , 51.1, 83.2, 90.9, 92.3, 94.1, 94.3, 76.7, 28.6, 0.46 );
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 2, 3.83, 4.167, 4.333, 4.5, 5 );
  Data( CVen , 3.9, 3.6, 2, 1.4, 0.72, 0.55 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);

```

```

        Data( zAurnTCA , -1);
} # End Fisher91 TCEmceB6aFinh004889

Experiment { # Begin Fisher91 TCEmceB6fFinhc9111e
  Species = 3 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.022 ;

# Exposure/Dosing
  CC = 1100 ;
  NROdents = 14 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

# Data
  Print( AurnTCOGTCOH , 0);
  Data( AurnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0.05, 0.15, 0.29, 0.47, 0.66, 0.82, 0.97, 1.14, 1.32, 1.49, 1.65, 1.81,
        1.98, 2.14, 2.32, 2.5, 2.67, 2.83, 2.98, 3.17, 3.32, 3.49, 3.65, 3.83 );
  Data( CInhPPM , 975.3949772, 816.6746575, 603.8070776, 479.8824201, 395.4052511,
        325.6278539, 277.8070776, 250.2682648, 206.1689498, 160.9531963, 144.9509132,
        119.2728311, 101.9680365, 88.57077626, 72.94063927, 60.10159817, 51.35616438,
        42.23858447, 35.35388128, 28.65525114, 22.32876712, 19.72374429, 16.37442922,
        13.39726027 );
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlastTCA , 0);
  Data( CPlastTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAurnTCA , 0);
  Data( zAurnTCA , -1);
} # End Fisher91 TCEmceB6fFinhc9111e

Experiment { # Begin Fisher91 TCEmceB6fFinhc91300
  Species = 3 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.024 ;

# Exposure/Dosing
  CC = 300 ;
  NROdents = 14 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

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```

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CinhPPM , 0.05, 0.5, 0.64, 0.84, 1, 1.2, 1.3, 1.5, 1.7, 1.8, 2 );
Data( CinhPPM , 228.4977169, 101.0376712, 72.01027397, 53.21689498, 37.95890411,
      28.65525114, 21.956621, 17.11872146, 12.28082192, 9.489726027, 7.070776256 );
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fFinhc91300

Experiment { # Begin Fisher91 TCEmceB6fFinhc9137e
  Species = 3 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.022 ;

# Exposure/Dosing
  CC = 3700 ;
  NRodents = 14 ;
  VChC = 9.1 ;
  lnLossC = -3.912 ;

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CinhPPM , 0.04, 0.12, 0.3, 0.47, 0.63, 0.81, 0.95, 1.14, 1.29, 1.49, 1.63, 1.8,
      1.98, 2.14, 2.32, 2.48, 2.65, 2.98, 3.14, 3.32, 3.48, 3.65, 3.82, 4, 4.14, 4.32,
      4.48, 4.65, 4.82, 5, 5.14, 5.33, 5.48, 5.64, 5.99 );
Data( CinhPPM , 3673.082192, 2913.90411, 2316.609589, 1907.248858, 1570.456621,
      1317.39726, 1250.410959, 1168.538813, 1110.856164, 1001.073059, 950.8333333,
      971.3013699, 891.2899543, 876.4041096, 848.4931507, 835.4680365, 794.5319635,
      744.2922374, 720.1027397, 697.7739726, 686.609589, 664.2808219, 619.6232877,
      612.1803653, 580.5479452, 552.6369863, 524.7260274, 507.9794521, 474.4863014,
      442.8538813, 435.4109589, 400.0570776, 366.5639269, 347.956621, 288.413242 );

```

```

Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 0);
Data( CPlasTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fFinhc9137e

Experiment { # Begin Fisher91 TCEmceB6fFinhc91700
  Species = 3 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.021 ;

# Exposure/Dosing
  CC = 700 ;
  NRodents = 14 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0.03, 0.14, 0.31, 0.49, 0.64, 0.83, 0.97, 1.13, 1.32, 1.49, 1.65, 1.83,
    1.97, 2.2, 2.33, 2.48, 2.69 );
  Data( CInhPPM , 645.673516, 503.3276256, 379.0308219, 261.0605023, 182.9098174,
    137.880137, 111.4577626, 86.89611872, 65.49771689, 52.10045662, 41.30821918,
    33.49315068, 28.46917808, 21.58447489, 16.18835616, 14.32762557, 11.72260274 );
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);

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```

Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fFinhc91700

Experiment { # Begin Fisher91 TCEmceB6fFinhc917e3
  Species = 3 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.022 ;

# Exposure/Dosing
  CC = 7000 ;
  NRODENTS = 14 ;
  VChC = 9.1 ;
  lnLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0.03, 0.12, 0.29, 0.46, 0.62, 0.79, 0.97, 1.14, 1.3, 1.46, 1.63, 1.79,
    1.96, 2.14, 2.3, 2.47, 2.64, 2.8, 2.95, 3.12, 3.3, 3.49, 3.64, 3.83, 3.95, 4.15,
    4.3, 4.46, 4.98, 5.15, 5.33, 5.48, 5.63, 5.81, 5.97 );
  Data( CInhPPM , 6514.417808, 5455.6621, 4182.922374, 3323.26484, 2887.853881,
    2744.577626, 2472.910959, 2309.166667, 2232.876712, 2123.093607, 2091.461187,
    2022.614155, 1994.703196, 2000.285388, 1970.513699, 1907.248858, 1845.844749,
    1817.93379, 1790.022831, 1732.340183, 1737.922374, 1713.732877, 1657.910959,
    1693.26484, 1607.671233, 1585.342466, 1561.152968, 1536.96347, 1551.849315,
    1529.520548, 1453.230594, 1380.6621, 1360.194064, 1317.39726, 1274.600457 );
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);
  Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fFinhc917e3
#### END Fisher91
##### END GROUP 2
}

```



```

##### BEGIN GROUP 3
Level {
#### BEGIN Fisher91
Experiment { # Begin Fisher91 TCEmceB6aMinh004110
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.031 ;

# Exposure/Dosing
Conc = NDoses(2, 110 0 , 0 4 );

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 2, 3.75, 3.9, 4.2, 5, 6, 8, 21 );
Data( CPlastTCA , 17.76, 46.18, 49.81, 38.99, 70.53, 54.29, 41.02, 7.06 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 2, 3.9, 4.2, 4.4 );
Data( CVen , 1.5, 1.51, 0.38, 0.38 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6aMinh004110

Experiment { # Begin Fisher91 TCEmceB6aMinh004297
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.031 ;

# Exposure/Dosing
Conc = NDoses(2, 297 0 , 0 4 );

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);

```

```

Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 2.5, 4.2, 4.4, 4.8, 4.9, 5.3, 5.5, 6.3, 24 );
Data( CPlasTCA , 58, 101.7, 88.5, 109.6, 114.7, 85.8, 80.6, 83, 5.7 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 2, 3.9, 4.2, 4.4 );
Data( CVen , 1.48, 1.2, 0.88, 0.37 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6aMinh004297

Experiment { # Begin Fisher91 TCEmceB6aMinh004368
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.031 ;

# Exposure/Dosing
  Conc = NDoses(2, 368 0 , 0 4 );

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 2, 3.9, 4.2, 4.4, 4.75, 5, 5.5, 6.5, 24 );
  Data( CPlasTCA , 61.8, 94.2, 103.1, 103, 97, 101.4, 71.6, 58.8, 9.8 );
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 2, 3.9, 4.2, 4.4, 4.75 );
  Data( CVen , 3.82, 3.72, 1.24, 0.51, 0.22 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);
  Data( zAUrnTCA , -1);

```

```

} # End Fisher91 TCEmceB6aMinh004368

Experiment { # Begin Fisher91 TCEmceB6aMinh004748
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.031 ;

# Exposure/Dosing
  Conc = NDoses(2, 748 0 , 0 4 );

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlastTCA , 2, 3.9, 4.2, 4.5, 4.75, 5, 7.75, 9, 24 );
  Data( CPlastTCA , 88.6, 127.4, 123.6, 123.6, 125.5, 106.2, 82.1, 58, 9.4 );
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 2, 3.9, 4.2, 4.4, 4.5 );
  Data( CVen , 7.18, 7.2, 1.5, 0.88, 0.49 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);
  Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6aMinh004748

Experiment { # Begin Fisher91 TCEmceB6fMinhc9118e
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.026 ;

# Exposure/Dosing
  CC = 1800 ;
  NRodents = 14 ;
  VChC = 9.1 ;
  lnLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);

```

```

Print( CInhPPM , 0.16, 0.25, 0.33, 0.48, 0.67, 0.83, 1, 1.16, 1.33, 1.49, 1.67, 1.84,
      2.01, 2.17, 2.33, 2.5, 2.68, 2.83 );
Data( CInhPPM , 1352.937215, 1113.833333, 950.0890411, 716.0091324, 600.0856164,
      494.2100457, 399.8710046, 312.2305936, 243.7557078, 187.0034247, 128.9486301,
      93.78082192, 62.52054795, 40.19178082, 27.16666667, 16.9326484, 11.9086758,
      8.373287671 );
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fMinhc9118e

Experiment { # Begin Fisher91 TCEmceB6fMinhc911e3
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.03 ;

# Exposure/Dosing
  CC = 1020 ;
  NRodents = 14 ;
  VChC = 9.1 ;
  lnLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0.07, 0.16, 0.33, 0.5, 0.66, 0.84, 1, 1.18, 1.33, 1.51, 1.69, 1.85, 2,
      2.16, 2.32 );
  Data( CInhPPM , 838.4452055, 609.7614155, 384.9851598, 222.543379, 156.3013699,
      100.293379, 64.5673516, 41.49429224, 28.09703196, 18.42123288, 12.65296804,
      8.559360731, 6.512557078, 5.023972603, 4.465753425 );
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlastTCA , 0);
  Data( CPlastTCA , -1);

```

```

Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fMinhc911e3

Experiment { # Begin Fisher91 TCEmceB6fMinhc911e4
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.026 ;

# Exposure/Dosing
  CC = 10000 ;
  NRodents = 14 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0.08, 0.15, 0.31, 0.47, 0.66, 0.82, 0.97, 1.16, 1.33, 1.5, 1.67, 1.82,
    2.01, 2.15, 2.34, 2.51, 2.65, 2.82, 3.01 );
  Data( CInhPPM , 8384.452055, 7279.178082, 5889.212329, 5204.46347, 4683.458904,
    4443.424658, 4069.417808, 3861.015982, 3600.513699, 3475.844749, 3299.075342,
    3185.570776, 3131.609589, 2969.726027, 2869.246575, 2820.86758, 2724.109589,
    2725.97032, 2631.073059 );
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);
  Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fMinhc911e4

Experiment { # Begin Fisher91 TCEmceB6fMinhc9138e
  Species = 3 ;
  Male = 1 ;

```

```

# Measured Covariates (if any)
  BWmeas = 0.03 ;

# Exposure/Dosing
  CC = 3800 ;
  NRodents = 14 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0.14, 0.32, 0.51, 0.69, 0.83, 1, 1.19, 1.35, 1.49, 1.66, 1.85, 2.01,
    2.15, 2.34, 2.52, 2.68, 2.81, 2.99, 3.17, 3.33, 3.49, 3.67, 3.8, 3.98, 4.16,
    4.31, 4.5, 4.65, 4.82, 5.01, 5.15 );
  Data( CInhPPM , 2471.050228, 1862.591324, 1507.191781, 1356.472603, 1220.639269,
    1116.438356, 1023.401826, 952.6940639, 904.3150685, 857.7968037, 785.2283105,
    733.1278539, 682.8881279, 614.0410959, 573.1050228, 534.0296804, 480.0684932,
    455.8789954, 403.7785388, 349.8173516, 303.2990868, 249.3378995, 206.5410959,
    160.0228311, 117.2260274, 87.4543379, 63.26484018, 48.37899543, 33.49315068,
    22.32876712, 16.74657534 );
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlastTCA , 0);
  Data( CPlastTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);
  Data( zAUrnTCA , -1);
} # End Fisher91 TCEmceB6fMinhc9138e

Experiment { # Begin Fisher91 TCEmceB6fMinhc9156e
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.028 ;

# Exposure/Dosing
  CC = 5600 ;
  NRodents = 14 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);

```

```

Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0.07, 0.16, 0.33, 0.48, 0.68, 0.84, 0.97, 1.18, 1.32, 1.51, 1.68, 1.83,
      2, 2.15, 2.33, 2.48, 2.65, 2.75, 2.92, 3.08, 3.26, 3.42, 3.58, 3.76, 3.9, 4.08,
      4.24, 4.41, 4.56, 4.75, 4.87, 5.04, 5.23 );

Data( CInhPPM , 5384.954338, 4434.121005, 3224.646119, 2608.744292, 2186.358447,
      1933.299087, 1769.554795, 1620.696347, 1510.913242, 1434.623288, 1384.383562,
      1313.675799, 1246.689498, 1183.424658, 1142.488584, 1103.413242, 1047.591324,
      1028.984018, 975.0228311, 943.390411, 909.8972603, 863.3789954, 833.6073059,
      790.8105023, 777.7853881, 738.7100457, 712.6598174, 677.3059361, 653.1164384,
      630.7876712, 599.1552511, 558.2191781, 530.3082192 );
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAurnTCA , 0);
Data( zAurnTCA , -1);
} # End Fisher91 TCEmceB6fMinhc9156e
#### END Fisher91
##### END GROUP 3
}

##### BEGIN GROUP 4
Level {
#### BEGIN Fisher93
Experiment { # Begin Fisher93 TCEmceB6aForloil2e3
Species = 3 ;
Male = 0 ;

# Measured Covariates (if any)
BWmeas = 0.0257 ;

# Exposure/Dosing
PDose = NDoses(2, 1947 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);

```

```

Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 0.033, 0.083, 0.17, 0.25, 0.5, 1, 2, 4, 6, 24, 30 );
Data( CPlasTCA , 2, 5.1, 16.3, 15.2, 28.6, 33, 54.1, 89.3, 86, 14.6, 4 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0.033, 0.083, 0.17, 0.25, 0.5, 1, 2, 3, 4, 6, 8, 9 );
Data( CVen , 14.3, 38.6, 48.9, 42.5, 50, 27.9, 136, 167.5, 119.8, 48.6, 2.233333333,
      10.37333333 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher93 TCEmceB6aForloil2e3

Experiment { # Begin Fisher93 TCEmceB6aForloil487
  Species = 3 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.0273 ;

# Exposure/Dosing
  PDose = NDoses(2, 487 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0.083, 0.17, 0.5, 1, 2, 4, 7, 24 );
  Data( CPlasTCA , 3.066666667, 5.466666667, 14.8, 25.4, 33.8, 55.63333333, 56.56666667,
      2.2 );
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0.083, 0.17, 0.5, 1, 2 );
  Data( CVen , 38.5, 24.33333333, 12.9, 6.233333333, 2.8 );
  Print( TotCTCOH , 0);

```



```

        Data( TotCTCOH , -1);
        Print( zAExhpost , 0);
        Data( zAExhpost , -1);
        Print( zAUrnTCA , 0);
        Data( zAUrnTCA , -1);
    } # End Fisher93 TCEmceB6aForloil487

    Experiment { # Begin Fisher93 TCEmceB6aForloil973
        Species = 3 ;
        Male = 0 ;

# Measured Covariates (if any)
        BWmeas = 0.0238 ;

# Exposure/Dosing
        PDose = NDoses(2, 973 0 , 0 0.05 );
        TChng = 0.05 ;

# Data
        Print( AUrnTCOGTCOH , 0);
        Data( AUrnTCOGTCOH , -1);
        Print( CBldMix , 0);
        Data( CBldMix , -1);
        Print( CBldTCA , 0);
        Data( CBldTCA , -1);
        Print( CFat , 0);
        Data( CFat , -1);
        Print( CInhPPM , 0);
        Data( CInhPPM , -1);
        Print( CKid , 0);
        Data( CKid , -1);
        Print( CLiv , 0);
        Data( CLiv , -1);
        Print( CLivTCA , 0);
        Data( CLivTCA , -1);
        Print( CLivTCOGTCOH , 0);
        Data( CLivTCOGTCOH , -1);
        Print( CLivTCOH , 0);
        Data( CLivTCOH , -1);
        Print( CPlastTCA , 0.083, 0.17, 0.25, 0.5, 1, 2, 3, 7, 27 );
        Data( CPlastTCA , 5.39, 6.6, 7, 12, 20.16666667, 41.1, 41.2, 43.7, 5.46666667 );
        Print( CTCOGTCOH , 0);
        Data( CTCOGTCOH , -1);
        Print( CTCOH , 0);
        Data( CTCOH , -1);
        Print( CVen , 0.083, 0.17, 0.25, 0.5, 1, 2, 4 );
        Data( CVen , 22.1, 16.3, 35.8, 12.5, 17.88666667, 21.4, 13.70666667 );
        Print( TotCTCOH , 0);
        Data( TotCTCOH , -1);
        Print( zAExhpost , 0);
        Data( zAExhpost , -1);
        Print( zAUrnTCA , 0);
        Data( zAUrnTCA , -1);
    } # End Fisher93 TCEmceB6aForloil973
#### END Fisher93
##### END GROUP 4
}

##### BEGIN GROUP 5
Level {
#### BEGIN Fisher93
    Experiment { # Begin Fisher93 TCEmceB6aMorloil2e3
        Species = 3 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.0306 ;

# Exposure/Dosing
        PDose = NDoses(2, 1947 0 , 0 0.05 );
        TChng = 0.05 ;

```

```

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0.033, 0.083, 0.17, 0.25, 0.5, 1, 2, 3, 4, 5, 6, 7, 24, 30, 48, 72 );
Data( CPlastTCA , 1.2, 3.9, 11.9, 16.3, 32.7, 61.6, 41.3, 56.1, 54.9, 61.1, 91, 94.4,
      47.5, 29.4, 28.5, 1.9 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0.033, 0.083, 0.17, 0.25, 0.5, 1, 2, 3, 4, 5, 6, 7 );
Data( CVen , 20, 30.7, 45.1, 64.7, 71.7, 127.3, 33.26666667, 106.7, 75.7, 103.4, 47.9,
      23.9 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher93 TCEmceB6aMorloil2e3

Experiment { # Begin Fisher93 TCEmceB6aMorloil487
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0338 ;

# Exposure/Dosing
  PDose = NDoses(2, 487 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);

```

```

Data( CLivTCOH , -1);
Print( CPlasTCA , 0.083, 0.17, 0.5, 1, 2, 7, 24, 30 );
Data( CPlasTCA , 5.8, 6.9, 17.9, 32, 54.9, 82.2, 13.8, 4.1 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0.083, 0.17, 1, 2 );
Data( CVen , 50.9, 39, 6.9, 1.5 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Fisher93 TCEmceB6aMorloil487

Experiment { # Begin Fisher93 TCEmceB6aMorloil973
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0306 ;

# Exposure/Dosing
  PDose = NDoses(2, 973 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0.033, 0.083, 0.17, 0.25, 0.5, 1, 2, 3, 4, 5, 6, 7, 30, 48 );
  Data( CPlasTCA , 8.933333333, 12.1, 11.8, 17.9, 27.4, 49.2, 76.6, 85.3, 48.6, 80.9,
      86.4, 91.4, 12.56666667, 2 );
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0.033, 0.083, 0.17, 0.25, 0.5, 1, 2, 3, 4, 7 );
  Data( CVen , 9.7, 29.9, 50.9, 69.3, 66.4, 48.2, 12.68666667, 4.8, 16.86666667, 5.9 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);
  Data( zAUrnTCA , -1);
} # End Fisher93 TCEmceB6aMorloil973
#### END Fisher93
##### END GROUP 5
}

```

```

##### BEGIN GROUP 6
Level {
#### BEGIN Green85
Experiment { # Begin Green85 TCEmceB6aMorloil010
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.0285 ;

# Exposure/Dosing
PDose = NDoses(2, 10 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 24 );
Data( AUrnTCOGTCOH , 0.151246897 );
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 24, 72 );
Data( zAExhpost , 0.011115, 0.011115 );
Print( zAUrnTCA , 24 );
Data( zAUrnTCA , 0.023867144 );
} # End Green85 TCEmceB6aMorloil010

Experiment { # Begin Green85 TCEmceB6aMorloil1e3
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.0285 ;

# Exposure/Dosing
PDose = NDoses(2, 1000 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 24 );
Data( AUrnTCOGTCOH , 11.99527586 );
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);

```

```

Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 0);
Data( CPlasTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 24, 72 );
Data( zAExhpost , 4.9875, 4.9875 );
Print( zAUrnTCA , 24 );
Data( zAUrnTCA , 1.036993105 );
} # End Green85 TCEmceB6aMorloil1e3

Experiment { # Begin Green85 TCEmceB6aMorloil2e3
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0285 ;

# Exposure/Dosing
  PDose = NDoses(2, 2000 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 24 );
  Data( AUrnTCOGTCOH , 27.90858197 );
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 24, 72 );

```

```

    Data( zAExhpost , 7.752, 7.752 );
    Print( zAurnTCA , 24 );
    Data( zAurnTCA , 2.230208548 );
} # End Green85 TCEmceB6aMorloil2e3

Experiment { # Begin Green85 TCEmceB6aMorloil500
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0285 ;

# Exposure/Dosing
  PDose = NDoses(2, 500 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AurnTCOGTCOH , 24 );
  Data( AurnTCOGTCOH , 8.743811279 );
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 0);
  Data( CBldTCA , -1);
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlastTCA , 0);
  Data( CPlastTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0);
  Data( CTCOH , -1);
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 24, 72 );
  Data( zAExhpost , 0.855, 0.855 );
  Print( zAurnTCA , 24 );
  Data( zAurnTCA , 0.755310904 );
} # End Green85 TCEmceB6aMorloil500
##### END Green85

##### BEGIN Prout85
  Experiment { # Begin Prout85 TCEmceB6iMorloil1e3
    Species = 3 ;
    Male = 1 ;

# Measured Covariates (if any)
    BWmeas = 0.0295 ;

# Exposure/Dosing
    PDose = NDoses(2, 1000 0 , 0 0.05 );
    TChng = 0.05 ;

# Data
    Print( AurnTCOGTCOH , 0);
    Data( AurnTCOGTCOH , -1);
    Print( CBldMix , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5 );
    Data( CBldMix , 10.3, 18, 13.6, 8, 10.5, 6.2, 6.3, 1.5, 1.7, 1.8, 2.2, 2.3, 2.9, 3.3,

```

```

    4.3, 1.9 );
Print( CBldTCA , 0.75, 1, 2, 2.5, 3, 4, 4.5, 5, 5.5, 6, 7, 7.5, 8, 9, 10, 11, 12, 13,
    14, 15, 16, 17, 18, 19, 20, 21, 22, 24, 25, 27, 28, 29, 30, 32, 34, 35, 37, 39,
    41, 45 );
Data( CBldTCA , 39, 106, 69, 146, 121, 157, 133, 149, 101, 121, 162, 196, 211, 201, 190,
    189, 170, 260, 242, 216, 179, 118, 59, 124, 197, 170, 146, 238, 224, 158, 150,
    267, 285, 70, 56, 29, 40, 29, 20, 7 );
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH,0.3, 0.5, 0.75, 1, 1.5, 2, 2.5, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8);
Data( TotCTCOH , 9.6, 21.7, 29.4, 27.8, 30.6, 27.6, 20.3, 9.5, 10.7, 14.3, 2.8, 7.4,
    6.6, 5.5, 2.6, 1.5, 0.7 );
Print( zAExhpost , 0.5, 1, 1.5, 2, 2.5, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8, 8.5, 9);
Data( zAExhpost , 0.74, 1.34, 1.78, 2.18, 2.59, 2.88, 3.04, 3.09, 3.1, 3.15, 3.17, 3.19,
    3.17, 3.24, 3.24, 3.25, 3.27 );
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Prout85 TCEmceB6iMorloille3
#### END Prout85
##### END GROUP 6
}

##### BEGIN GROUP 7
Level {
#### BEGIN Greenberg99
    Experiment { # Begin Greenberg99 TCEmceB6aMinh004100
        Species = 3 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.03 ;

# Exposure/Dosing
        Conc = NDoses(2, 100 0 , 0 4 );

# Data
        Print( AUrnTCOGTCOH , 0);
        Data( AUrnTCOGTCOH , -1);
        Print( CBldMix , 0);
        Data( CBldMix , -1);
        Print( CBldTCA , 2, 4, 4.25, 4.5, 4.75, 6, 12, 18, 28 );
        Data( CBldTCA , 18.23, 29.86, 33.72, 25.03, 31.63, 27.06, 6.798, 3.992, 1.908 );
        Print( CFat , 2, 4, 4.5 );
        Data( CFat , 19.35, 44.46, 27.68 );
        Print( CInhPPM , 0);
        Data( CInhPPM , -1);
        Print( CKid , 2, 4, 4.5 );
        Data( CKid , 3.473, 4.91, 0.1341 );
        Print( CLiv , 2, 4, 4.25, 4.5 );
        Data( CLiv , 0.5719, 0.7577, 0.1673, 0.051 );
        Print( CLivTCA , 2, 4, 4.25, 4.5, 4.75, 6, 12, 18, 28 );

```

```

Data( CLivTCA , 12.84, 21.17, 21.81, 16.32, 20.74, 17.04, 5.15, 2.732, 1.404 );
Print( CLivTCOGTCOH , 2, 4, 4.25, 4.5, 4.75, 6 );
Data( CLivTCOGTCOH , 18.52, 22.91, 13.73, 5.328, 6.365, 0.8768 );
Print( CLivTCOH , 2, 4, 4.25, 4.5, 4.75, 6 );
Data( CLivTCOH , 4.134, 4.446, 1.162, 5.099, 0.5918, 0.4164 );
Print( CPlasTCA , 0);
Data( CPlasTCA , -1);
Print( CTCOGTCOH , 2, 4, 4.25, 4.5, 4.75, 6 );
Data( CTCOGTCOH , 4.51, 6.222, 2.733, 1.97, 2.09, 0.1985 );
Print( CTCOH , 2, 4, 4.25, 4.5, 4.75, 6 );
Data( CTCOH , 2.041, 1.847, 1.778, 0.7934, 0.3029, 0.0899 );
Print( CVen , 2, 4, 4.25, 4.5 );
Data( CVen , 0.6651, 0.8605, 0.1387, 0.1497 );
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Greenberg99 TCEmceB6aMinh004100

Experiment { # Begin Greenberg99 TCEmceB6aMinh004600
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.03 ;

# Exposure/Dosing
  Conc = NDoses(2, 600 0 , 0 4 );

# Data
  Print( AUrnTCOGTCOH , 0);
  Data( AUrnTCOGTCOH , -1);
  Print( CBldMix , 0);
  Data( CBldMix , -1);
  Print( CBldTCA , 2, 4, 4.25, 4.5, 4.75, 6, 12, 18, 28, 47 );
  Data( CBldTCA , 56.1, 96.66, 74.62, 99.03, 77.74, 107.67, 25.82, 13.34, 7.191, 0.8069 );
  Print( CFat , 2, 4, 4.25, 4.5, 4.75, 6 );
  Data( CFat , 244.48, 233.7, 198.4, 167.5, 142.2, 104.1 );
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 2, 4, 4.25, 4.5, 4.75, 6 );
  Data( CKid , 22.85, 22.04, 6.167, 4.714, 2.855, 0.6404 );
  Print( CLiv , 2, 4, 4.25, 4.5, 4.75, 6 );
  Data( CLiv , 10.19, 12.62, 3.013, 1.074, 0.6447, 0.2754 );
  Print( CLivTCA , 2, 4, 4.25, 4.5, 4.75, 6, 12, 18, 28, 47 );
  Data( CLivTCA , 33.72, 52.12, 45.67, 54.97, 48.54, 48.74, 13.01, 7.952, 4.405, 0.7298 );
  Print( CLivTCOGTCOH , 2, 4, 4.25, 4.5, 4.75, 6, 28, 47 );
  Data( CLivTCOGTCOH , 36.6, 62.08, 49.31, 19.37, 30.51, 4.313, 0.1568, 0.1025 );
  Print( CLivTCOH , 2, 4, 4.25, 4.5, 4.75, 6 );
  Data( CLivTCOH , 28.93, 24.7, 17.65, 5.476, 6.282, 2.647 );
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 2, 4, 4.25, 4.5, 4.75, 6, 12 );
  Data( CTCOGTCOH , 16.17, 25.1, 17.87, 6.746, 8.252, 2.028, 0.3544 );
  Print( CTCOH , 2, 4, 4.25, 4.5, 4.75, 6 );
  Data( CTCOH , 16.53, 13.37, 10.89, 3.979, 3.201, 1.007 );
  Print( CVen , 2, 4, 4.25, 4.5, 4.75, 6 );
  Data( CVen , 6.851, 7.325, 1.534, 0.5987, 0.4649, 0.1699 );
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);
  Data( zAExhpost , -1);
  Print( zAUrnTCA , 0);
  Data( zAUrnTCA , -1);
} # End Greenberg99 TCEmceB6aMinh004600
##### END Greenberg99
##### END GROUP 7
}

```



```

##### BEGIN GROUP 8
Level {
#### BEGIN Larson92a
Experiment { # Begin Larson92a TCEmceB6aMorl_aq197
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.0264 ;

# Exposure/Dosing
PDose = NDoses(2, 197.25 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0.25, 0.75 ); # , 2 );
Data( CBldMix , 44.8074, 20.8926 ); # , 0 ); ## removed zero
Print( CBldTCA , 0.25, 0.75, 2, 8, 24 );
Data( CBldTCA , 22.876, 35.131, 24.3466, 20.5884, 2.451 );
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0.25, 0.75 ); # , 2 );
Data( CTCOH , 28.24055, 19.4051); # , 0 ); ## removed zero
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Larson92a TCEmceB6aMorl_aq197

Experiment { # Begin Larson92a TCEmceB6aMorl_aq2e3
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.0264 ;

# Exposure/Dosing
PDose = NDoses(2, 1972.5 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0.25, 0.75, 2, 8 );
Data( CBldMix , 436.3794, 292.8906, 154.9206, 4.0734 );
Print( CBldTCA , 0.25, 0.75, 2, 8, 24, 48 );
Data( CBldTCA , 22.876, 42.9742, 68.4646, 122.3866, 28.2682, 4.7386 );
Print( CFat , 0);
Data( CFat , -1);

```

```

Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 0);
Data( CPlasTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0.25, 0.75, 2, 8 );
Data( CTCOH , 38.3617, 34.8634, 59.8897, 17.98485 );
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAurnTCA , 0);
Data( zAurnTCA , -1);
} # End Larson92a TCEmceB6aMorl_aq2e3

Experiment { # Begin Larson92a TCEmceB6aMorl_aq592
  Species = 3 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.0264 ;

# Exposure/Dosing
  PDose = NDoses(2, 591.75 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AurnTCOGTCOH , 0);
  Data( AurnTCOGTCOH , -1);
  Print( CBldMix , 0.25, 0.75, 2 );
  Data( CBldMix , 151.11, 74.03076, 30.11688 );
  Print( CBldTCA , 0.25, 0.75, 2, 8, 24 );
  Data( CBldTCA , 14.0524, 36.4382, 63.0724, 100.8178, 6.6994 );
  Print( CFat , 0);
  Data( CFat , -1);
  Print( CInhPPM , 0);
  Data( CInhPPM , -1);
  Print( CKid , 0);
  Data( CKid , -1);
  Print( CLiv , 0);
  Data( CLiv , -1);
  Print( CLivTCA , 0);
  Data( CLivTCA , -1);
  Print( CLivTCOGTCOH , 0);
  Data( CLivTCOGTCOH , -1);
  Print( CLivTCOH , 0);
  Data( CLivTCOH , -1);
  Print( CPlasTCA , 0);
  Data( CPlasTCA , -1);
  Print( CTCOGTCOH , 0);
  Data( CTCOGTCOH , -1);
  Print( CTCOH , 0.25, 0.75, 2 );
  Data( CTCOH , 25.415, 32.89, 37.375 );
  Print( CVen , 0);
  Data( CVen , -1);
  Print( TotCTCOH , 0);
  Data( TotCTCOH , -1);
  Print( zAExhpost , 0);

```

```

        Data( zAExhpost , -1);
        Print( zAUrnTCA , 0);
        Data( zAUrnTCA , -1);
    } # End Larson92a TCemceB6aMorl_aq592
#### END Larson92a

#### BEGIN Larson92b
    Experiment { # Begin Larson92b TCAmceB6aMorl_aq020
        Species = 3 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.0264 ;

# Exposure/Dosing
        PODoseTCA = NDoses(2, 20 0 , 0 0.05 );
        TChng = 0.05 ;

# Data
        Print( AUrnTCOGTCOH , 0);
        Data( AUrnTCOGTCOH , -1);
        Print( CBldMix , 0);
        Data( CBldMix , -1);
        Print( CBldTCA , 0);
        Data( CBldTCA , -1);
        Print( CFat , 0);
        Data( CFat , -1);
        Print( CInhPPM , 0);
        Data( CInhPPM , -1);
        Print( CKid , 0);
        Data( CKid , -1);
        Print( CLiv , 0);
        Data( CLiv , -1);
        Print( CLivTCA , 0);
        Data( CLivTCA , -1);
        Print( CLivTCOGTCOH , 0);
        Data( CLivTCOGTCOH , -1);
        Print( CLivTCOH , 0);
        Data( CLivTCOH , -1);
        Print( CPlastTCA , 0.25, 1, 3, 5, 10, 16 );
        Data( CPlastTCA , 35.131, 33.6604, 33.6604, 23.5296, 9.1504, 4.085 );
        Print( CTCOGTCOH , 0);
        Data( CTCOGTCOH , -1);
        Print( CTCOH , 0);
        Data( CTCOH , -1);
        Print( CVen , 0);
        Data( CVen , -1);
        Print( TotCTCOH , 0);
        Data( TotCTCOH , -1);
        Print( zAExhpost , 0);
        Data( zAExhpost , -1);
        Print( zAUrnTCA , 0);
        Data( zAUrnTCA , -1);
    } # End Larson92b TCAmceB6aMorl_aq020

    Experiment { # Begin Larson92b TCAmceB6aMorl_aq100
        Species = 3 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.0264 ;

# Exposure/Dosing
        PODoseTCA = NDoses(2, 100 0 , 0 0.05 );
        TChng = 0.05 ;

# Data
        Print( AUrnTCOGTCOH , 0);
        Data( AUrnTCOGTCOH , -1);
        Print( CBldMix , 0);
        Data( CBldMix , -1);

```

```

Print( CBldTCA , 0);
Data( CBldTCA , -1);
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlasTCA , 0.25, 1, 3, 5, 10, 16, 24 );
Data( CPlasTCA , 104.576, 119.9356, 109.8048, 89.7066, 49.02, 7.6798, 5.2288 );
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Larson92b TCAmceB6aMorl_aq100
#### END Larson92b
##### END GROUP 8
}

##### BEGIN GROUP 9
Level {
#### BEGIN Merdink98
Experiment { # Begin Merdink98 TCEmceB6aM_iv_aq100
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.0225 ;

# Exposure/Dosing
IVDose = NDoses(2, 100 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0);
Data( CBldMix , -1);
Print( CBldTCA , 0.18, 0.359, 0.525, 0.65, 0.76, 1.02, 1.26, 1.52, 2.99, 6.01 );
Data( CBldTCA , 6.0458, 9.5589, 9.86936, 12.69618, 13.10468, 16.34, 18.791, 16.07856,
18.3008, 15.09816 );
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);

```

```

Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0);
Data( CTCOH , -1);
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0.18, 0.359, 0.525, 0.65, 0.76, 1.02, 1.26, 1.52, 2.99 );
Data( TotCTCOH , 7.13115, 5.8006, 3.6179, 2.40695, 2.6013, 2.3322, 0.79534, 0.617435,
    0.192855 );
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Merdink98 TCEmceB6aM_iv_aq100
#### END Merdink98
##### END GROUP 9
}

##### BEGIN GROUP 10
Level {
#### BEGIN Templin93
Experiment { # Begin Templin93 TCEmceB6aMorl_aq500
Species = 3 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.027 ;

# Exposure/Dosing
PDose = NDoses(2, 500 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0);
Data( AUrnTCOGTCOH , -1);
Print( CBldMix , 0.25, 0.5, 0.75, 1, 1.5, 2 );
Data( CBldMix , 28.3824, 24.7032, 21.9438, 11.826, 3.8106, 1.7082 );
Print( CBldTCA , 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 9, 12, 18, 24, 36 );
Data( CBldTCA , 10.7844, 18.791, 25.0002, 41.667, 46.569, 43.4644, 57.19, 64.8698,
    39.7062, 37.2552, 30.8826, 10.7844, 8.8236, 1.9608 );
Print( CFat , 0);
Data( CFat , -1);
Print( CInhPPM , 0);
Data( CInhPPM , -1);
Print( CKid , 0);
Data( CKid , -1);
Print( CLiv , 0);
Data( CLiv , -1);
Print( CLivTCA , 0);
Data( CLivTCA , -1);
Print( CLivTCOGTCOH , 0);
Data( CLivTCOGTCOH , -1);
Print( CLivTCOH , 0);
Data( CLivTCOH , -1);
Print( CPlastTCA , 0);
Data( CPlastTCA , -1);
Print( CTCOGTCOH , 0);
Data( CTCOGTCOH , -1);
Print( CTCOH , 0.25, 0.5, 0.75, 1, 1.5, 2, 3 );
Data( CTCOH , 17.9101, 27.7771, 35.5511, 40.2454, 30.199, 8.56635, 0.73255 );
Print( CVen , 0);
Data( CVen , -1);
Print( TotCTCOH , 0);
Data( TotCTCOH , -1);
Print( zAExhpost , 0);
Data( zAExhpost , -1);
Print( zAUrnTCA , 0);
Data( zAUrnTCA , -1);
} # End Templin93 TCEmceB6aMorl_aq500

```

```

#### END Templin93
##### END GROUP 10
}

};
};
End.

```

TCE.1.2.3.3.Mouse.pop.mean.x.5.out

```

iter   Ve_CInhPPM.1.  Ve_CVen.1.    Ve_CBldMix.1.  Ve_CFat.1.    Ve_CKid.1.    Ve_CLiv.1.
Ve_zAExhpost.1.  Ve_CTCOH.1.    Ve_CLivTCOH.1. Ve_CPlasTCA.1. Ve_CBldTCA.1. Ve_CLivTCA.1.
Ve_zAUrnTCA.1.   Ve_CTCOGTCOH.1. Ve_CLivTCOGTCOH.1. Ve_AUrnTCOGTCOH.1.
Ve_TotCTCOH.1.   M_lnQCC.1.     M_lnVPRC.1.    M_QFatC.1.    M_QGutC.1.    M_QLivC.1.
M_QSlwC.1. M_lnDRespC.1. M_QKidC.1.     M_FracPlasC.1. M_VFatC.1.    M_VGutC.1.
M_VLivC.1. M_VRapC.1.    M_VResplumC.1. M_VRespEffC.1. M_VKidC.1.    M_VBldC.1.
M_lnPBC.1. M_lnPFatC.1. M_lnPGutC.1.   M_lnPLivC.1.   M_lnPRapC.1.   M_lnPRespC.1.
M_lnPKidC.1. M_lnPSlwC.1. M_lnPRBCPlasTCAC.1. M_lnPBodTCAC.1.
M_lnPLivTCAC.1. M_lnKDissocC.1. M_lnBMaxkDC.1. M_lnPBodTCOHC.1.
M_lnPLivTCOHC.1. M_lnPBodTCOGC.1. M_lnPLivTCOGC.1. M_lnPeffDCVG.1.
M_lnKtSD.1. M_lnKAS.1. M_lnKTD.1.     M_lnKAD.1.    M_lnKASTCA.1. M_lnKASTCOH.1.
M_lnVMaxC.1. M_lnKMC.1.    M_lnFracOtherC.1. M_lnFracTCAC.1.
M_lnVMaxDCVGC.1. M_lnCLDCVGC.1. M_lnVMaxKidDCVGC.1. M_lnCLKidDCVGC.1.
M_lnVMaxLungLivC.1. M_lnKMClara.1. M_lnFracLungSysC.1. M_lnVMaxTCOHC.1.
M_lnKMTCOH.1. M_lnVMaxGlucC.1. M_lnKMGluc.1. M_lnKMetTCOHC.1.
M_lnKUrntCAC.1. M_lnKMetTCAC.1. M_lnkBileC.1. M_lnKEHRC.1. M_lnKUrntCOGC.1.
M_lnPGutC.1. M_lnKDCVGC.1. M_lnKATC.1. M_lnKKidBioactC.1. V_lnQCC.1.
V_lnVPRC.1. V_QFatC.1. V_QGutC.1. V_QLivC.1. V_QSlwC.1. V_lnDRespC.1.
V_QKidC.1. V_FracPlasC.1. V_VFatC.1. V_VGutC.1. V_VLivC.1. V_VRapC.1.
V_VResplumC.1. V_VRespEffC.1. V_VKidC.1. V_VBldC.1. V_lnPBC.1. V_lnPFatC.1.
V_lnPGutC.1. V_lnPLivC.1. V_lnPRapC.1. V_lnPRespC.1. V_lnPKidC.1. V_lnPSlwC.1.
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V_lnBMaxkDC.1. V_lnPBodTCOHC.1. V_lnPLivTCOHC.1. V_lnPBodTCOGC.1.
V_lnPLivTCOGC.1. V_lnPeffDCVG.1. V_lnKtSD.1. V_lnKAS.1. V_lnKTD.1.
V_lnKAD.1. V_lnKASTCA.1. V_lnKASTCOH.1. V_lnVMaxC.1. V_lnKMC.1. V_lnFracOtherC.1.
V_lnFracTCAC.1. V_lnVMaxDCVGC.1. V_lnCLDCVGC.1. V_lnVMaxKidDCVGC.1.
V_lnCLKidDCVGC.1. V_lnVMaxLungLivC.1. V_lnKMClara.1. V_lnFracLungSysC.1.
V_lnVMaxTCOHC.1. V_lnKMTCOH.1. V_lnVMaxGlucC.1. V_lnKMGluc.1. V_lnKMetTCOHC.1.
V_lnKUrntCAC.1. V_lnKMetTCAC.1. V_lnkBileC.1. V_lnKEHRC.1. V_lnKUrntCOGC.1.
V_lnFracKidDCVCC.1. V_lnKDCVGC.1. V_lnKATC.1. V_lnKKidBioactC.1. lnQCC.1.1.
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VResplumC.1.1. VRespEffC.1.1. VKidC.1.1. VBldC.1.1. lnPBC.1.1. lnPFatC.1.1.
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VResplumC.1.2. VRespEffC.1.2. VKidC.1.2. VBldC.1.2. lnPBC.1.2. lnPFatC.1.2.
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```

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 lnkAD.1.7. lnkASTCA.1.7. lnkASTCOH.1.7. lnVMaxC.1.7. lnKMC.1.7. lnFracOtherC.1.7.
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 lnUrntTCAC.1.7. lnkMetTCAC.1.7. lnkBileC.1.7. lnkEHRC.1.7. lnUrntTCOGC.1.7.
 lnFracKidDCVCC.1.7. lnkDCVGC.1.7. lnkNATC.1.7. lnkKidBioactC.1.7. lnQCC.1.8.
 lnVPRC.1.8. QFatC.1.8. QGutC.1.8. QLivC.1.8. QSlwC.1.8. lnDRespC.1.8.
 QKidC.1.8. FracPlasC.1.8. VFatC.1.8. VGutC.1.8. VLivC.1.8. VRapC.1.8.
 VRespLumC.1.8. VRespEffC.1.8. VKidC.1.8. VBldC.1.8. lnPBC.1.8. lnPFatC.1.8.
 lnPGutC.1.8. lnPLivC.1.8. lnPRapC.1.8. lnPRespC.1.8. lnPKidC.1.8. lnPSlwC.1.8.
 lnPRBCPlasTCAC.1.8. lnPBodTCAC.1.8. lnPLivTCAC.1.8. lnkDissocC.1.8.
 lnBMaxkDC.1.8. lnPBodTCOHC.1.8. lnPLivTCOHC.1.8. lnPBodTCOGC.1.8.
 lnPLivTCOGC.1.8. lnPeffDCVG.1.8. lnkTSD.1.8. lnkAS.1.8. lnkTD.1.8.
 lnkAD.1.8. lnkASTCA.1.8. lnkASTCOH.1.8. lnVMaxC.1.8. lnKMC.1.8. lnFracOtherC.1.8.
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 lnClKidDCVGC.1.8. lnVMaxLungLivC.1.8. lnKMClara.1.8. lnFracLungSysC.1.8.

0.1807	-0.1903	0.3283	-0.8682	-0.02329	-0.006428	3.002	0.3063	-2.3	-1.35		
1.219	-0.3202	-0.3867	-2.136	-3.714	-0.6557	0.9796	-0.992	0.9511	0.1999	1.195	-4.334
1.483	0.4326	0.0008282	4.304	3.219	1.239	-1.704	-0.1873	-0.03201			-4.435
2.222	0.4273	-1.676	-2.138	-2.427	-0.07327	-0.3272	0.8554	1.155	1.026	1.013	
0.2159	0.9947	0.8508	1.376	0.9815	0.7924	1	1	1	1.001	0.9845	0.2983
0.1863	-0.2909	0.1779	0.0005017	-0.001516	0.2056	-0.01837			0.6251	-0.1909	
-0.2996	0.09021	0.4198	-0.1957	0.2991	-0.8675	0.1113	-0.004539	2.8	0.736	-2.317	
-1.876	1.213	-0.305	-0.5503	-2.867	-3.742	-0.5882	0.9752	-0.9946	0.9509	0.2102	0.4614
-4.338	1.471	0.8723	-0.2125	4.24	3.462	1.178	-1.543	-0.1877	0.1019	-4.442	1.776
0.4356	-1.672	-2.16	-2.429	0.2555	-0.2257	1.019	1.112	1.02	0.9989	0.2308	0.9996
0.8688	1.292	0.9901	0.8842	0.9987	0.9994	0.9997	1	0.9945	0.02616	0.06875	-0.1962
0.2082	-0.03393		-0.007449		0.1973	0.001279		1.295	-0.09502		-0.2334
0.987	0.2931	-0.18	0.3658	-0.8665	-0.06241	-0.01731			0.8779	-0.508	-2.3
-1.991	1.228	-0.3371	-0.07415		-2.232	-3.649	-0.6589	0.9846	-0.9893	0.9492	0.2153
1.85	-4.438	1.452	0.8995	-0.1455	4.444	2.627	1.28	-3.008	-0.6281	-0.05987	
-4.413	3.969	0.4302	-1.666	-2.146	-2.428	0.08564	-0.3933	0.671	1.173	1.031	1.002
0.2547	0.9971	0.8928	1.369	0.9956	0.9045	0.9986	1	1.001	1	0.9968	-0.5723
-0.133	-0.1812	0.4028	-0.06227		-0.007895		-0.04468		-0.2902	0.9883	-
0.08722	-0.1897	0.5746	-0.01712	-0.04197	0.6228	-0.7739	0.5421	-0.007847			1.304
0.5695	-2.302	-1.261	1.212	-0.2819	-0.3721	-2.381	-3.687	-0.7124	0.9781	-1.009	0.9575
0.2181	1.115	-4.415	1.538	0.16	0.1028	4.278	3.68	1.329	-2.376	-0.6087	0.06862
-4.163	1.063	0.4263	-1.67	-2.149	-2.433	-0.1521	-0.395	1.17	1.136	1.026	1.028
0.225	0.9998	0.8887	1.222	0.9889	0.8499	0.9992	0.9994	1.001	1	0.993	0.4252
-0.03786	-0.2098	0.2066	-0.007257		-0.001485		0.2074	0.09782	0.7287	-0.1154	-0.242
0.2444	0.3493	-0.2946	0.2495	-0.8719	0.09919	-0.01514		0.6093	2.193	-2.306	-0.6433
2.144	-0.3354	-0.1777	-2.223	-3.768	-0.7506	0.9784	-0.9965	0.9496	0.2058	1.147	-4.356
1.519	0.1469	0.04324	3.943	4.062	1.08	-2.32	-0.5696	0.09306	-4.544	1.883	0.4335
-1.67	-2.152	-2.432	0.1923	-0.1453	1.018	1.108	1.021	0.9719	0.1897	0.9965	0.901
1.291	0.9902	0.8356	0.9968	1.001	1.001	0.9993	0.9945	-0.1656	0.02988	-0.2002	0.2097
-0.0505	-0.001705		0.1947	-0.05219		0.923	-0.04855		-0.2214	0.1	0.1681
-0.22	0.3568	-0.8837	0.03652	-0.01098		1.29	0.5643	-2.307	-1.289	1.209	-0.2949
-0.6747	-2.234	-3.691	-0.7415	0.9808	-1.002	0.953	0.2117	0.4987	-4.321	1.441	0.5847
-0.1488	4.372	3.175	1.3	-2.372	-0.6202	0.04133	-4.412	3.053	0.4352	-1.669	-2.155
-2.428	0.4212	-0.0929	1.042	1.12	1.024	0.9924	0.1837	0.9978	0.9046	1.18	0.9912
0.8936	0.9982	1	0.9999	0.9997	0.995	-0.2918	-0.03986		-0.1858	0.2228	-
0.03726	-0.004964	0.1981	-0.01771		0.9224	0.04575	-0.2314	-0.09587		0.08101	-0.2979
0.3171	-0.8674	-0.02216		-0.01727		0.837	0.566	-2.3	0.01877	1.196	-0.3051
0.03271	-2.578	-3.704	-0.9814	0.9806	-0.9958	0.9492	0.2084	0.8636	-4.362	1.462	0.5631
-0.1241	4.182	3.133	1.181	-2.442	-0.6577	-0.0174	-4.42	2.212	0.4283	-1.675	-2.154
-2.423	-585.4	-388.4	-241.8	-252.6	-56.07	-32.43	-25.96	-28.09	-39.99	-58.99	-96.03
-33.12	-205.2	-80.34	-236.2	-36.02	-45.36	-47.32	-56.15	-123.6	-58.11	-141.2	-172.1
-205.8	-93.23	-41.1	-54.56	-127.6	-40.6	-100.6	15.59	-7.499	-12.4	-1.252	-321.8
-93.72	-199.3	-32.63	-59.22	-43.74	-17.44	-28.74	-37.7	-84.31	-308.3	-4628	-4936

APPENDIX C

Rat MCSim Input and Output Files from Dr. Chiu

This is the MCSim input file for the rat provided by Dr. Weihsueh Chiu. It has been reformatted for better readability and some lines are now continued on additional lines due to the line length constriction in Word. While the output file is more easily read as an Excel file, it is included here for completeness.

TCE.1.2.3.3.Rat.seqpriors.test4.pop.1.1.in

```
# USEPA TCE MODEL VERSION 1.2.3.3
# Added exhaled breath mass balance data from Prout85
# Error variance at group level
# Priors for most uniformly distributed parameters based on mouse posteriors
# Removed DCVG compartment by:
# lnFracKidDCVCC -> 10; lnkDCVGC -> 10;
# Test 4 -- use 3.16-fold "extrapolation error"

Integrate(Lsodes, 1.0e-5, 1.0e-7, 1);
MCMC ("TCE.1.2.3.3.Rat.seqpriors.test4.pop.1.1.out", "", "", 250, 0, 5, 250, 482.6733);

Level { #Population level

# Population means
Distrib( M_lnQCC TruncNormal 0.0 0.14 -0.56 0.56 );
Distrib( M_lnVPRC TruncNormal 0.0 0.3 -1.2 1.2 );
Distrib( M_QFatC TruncNormal 1.0 0.46 0.08 1.92 );
Distrib( M_QGutC TruncNormal 1.0 0.17 0.66 1.34 );
Distrib( M_QLivC TruncNormal 1.0 0.17 0.66 1.34 );
Distrib( M_QSlwC TruncNormal 1.0 0.3 0.4 1.6 );
Distrib( M_lnDRespC TruncNormal 0.2 1.65 -11.513 2.303 );
Distrib( M_QKidC TruncNormal 1.0 0.13 0.74 1.26 );
Distrib( M_FracPlasC TruncNormal 1.0 0.2 0.4 1.6 );
Distrib( M_VFatC TruncNormal 1.0 0.45 0.1 1.9 );
Distrib( M_VGutC TruncNormal 1.0 0.13 0.74 1.26 );
Distrib( M_VLivC TruncNormal 1.0 0.18 0.64 1.36 );
Distrib( M_VRapC TruncNormal 1.0 0.12 0.76 1.24 );
Distrib( M_VRespLumC TruncNormal 1.0 0.18 0.64 1.36 );
Distrib( M_VRespEffC TruncNormal 1.0 0.18 0.64 1.36 );
Distrib( M_VKidC TruncNormal 1.0 0.15 0.7 1.3 );
Distrib( M_VBldC TruncNormal 1.0 0.12 0.76 1.24 );
Distrib( M_lnPBC TruncNormal 0.0 0.25 -0.75 0.75 );
Distrib( M_lnPFatC TruncNormal 0.0 0.3 -0.9 0.9 );
Distrib( M_lnPGutC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPLivC TruncNormal 0.0 0.15 -0.45 0.45 );
Distrib( M_lnPRapC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPRespC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPKidC TruncNormal 0.0 0.3 -0.9 0.9 );
Distrib( M_lnPSlwC TruncNormal 0.0 0.3 -0.9 0.9 );
Distrib( M_lnPRBCPlasTCAC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnPBodTCAC TruncNormal 0.0 0.693 -2.079 2.079 );
Distrib( M_lnPLivTCAC TruncNormal 0.0 0.693 -2.079 2.079 );
Distrib( M_lnKDissoC TruncNormal 0.0 0.61 -1.83 1.83 );
Distrib( M_lnBMaxkDC TruncNormal 0.0 0.47 -1.41 1.41 );
Distrib( M_lnPBodTCOHC TruncNormal 0.0 0.693 -2.079 2.079 );
Distrib( M_lnPLivTCOHC TruncNormal 0.0 0.693 -2.079 2.079 );
Distrib( M_lnPBodTCOGC TruncNormal -0.87 1.7 -4.605 4.605 );
Distrib( M_lnPLivTCOGC TruncNormal 0.01 1.67 -4.605 4.605 );
# Distrib( M_lnPeffDCVG Uniform -6.908 6.908 );
Distrib( M_lnKTSd Uniform -4.269 4.942 );
Distrib( M_lnKAS Uniform -6.571 7.244 );
Distrib( M_lnKTD Uniform -4.605 0 );
Distrib( M_lnKAD Uniform -7.195 6.62 );
Distrib( M_lnKASTCA Uniform -7.195 6.62 );
Distrib( M_lnKASTCOH Uniform -7.195 6.62 );
Distrib( M_lnVMaxC TruncNormal 0.0 0.693 -2.079 2.079 );
Distrib( M_lnKMC TruncNormal 0.0 1.386 -4.158 4.158 );
# Distrib( M_lnClC Normal 0 1 );
```

```

Distrib( M_lnFracOtherC TruncNormal -3.74 1.92 -6.908 6.908 );
Distrib( M_lnFracTCAC TruncNormal 0.0 1.163 -3.489 3.489 );
Distrib( M_lnVMaxDCVGC TruncNormal 0.96 3.75 -4.605 9.21 );
Distrib( M_lnClDCVGC TruncNormal -1.03 2.71 -4.605 9.21 );
# Distrib( M_lnKMDCVGC Normal 0 1 );
Distrib( M_lnVMaxKidDCVGC TruncNormal 0.94 3.12 -4.605 9.21 );
Distrib( M_lnClKidDCVGC TruncNormal 0.2 2.71 -4.605 9.21 );
# Distrib( M_lnKMKidDCVGC Normal 0 1 );
Distrib( M_lnVMaxLungLivC TruncNormal 1.02 1.82 -3.297 3.297 );
Distrib( M_lnKMClara TruncNormal -4.43 1.9 -6.908 6.908 );
Distrib( M_lnFracLungSysC TruncNormal 1.48 2.41 -6.908 6.908 );
Distrib( M_lnVMaxTCOHC TruncNormal 0.5 1.69 -9.21 9.21 );
# Distrib( M_lnClTCOHC Normal 0 1 );
Distrib( M_lnKMTCOH TruncNormal -0.07 1.73 -9.21 9.21 );
Distrib( M_lnVMaxGlucC TruncNormal 4.24 1.72 -9.21 9.21 );
# Distrib( M_lnClGlucC Normal 0 1 );
Distrib( M_lnKMGluc TruncNormal 3.42 1.81 -6.908 6.908 );
Distrib( M_lnKMetTCOHC TruncNormal 1.21 1.77 -11.513 6.908 );
Distrib( M_lnUrntTCAC TruncNormal -2.21 1.69 -4.605 4.605 );
Distrib( M_lnKMetTCAC TruncNormal -0.49 1.68 -9.21 4.605 );
Distrib( M_lnkBileC TruncNormal 0.01 1.74 -9.21 4.605 );
Distrib( M_lnKEHRC TruncNormal -4.42 1.89 -9.21 4.605 );
Distrib( M_lnUrntTCOGC TruncNormal 2.15 1.8 -6.908 6.908 );
# Distrib( M_lnFracKidDCVCC Uniform -6.908 6.908 );
# Distrib( M_lnKDCVGC Uniform -9.21 4.605 );
Distrib( M_lnKNATC Uniform -9.21 4.605 );
Distrib( M_lnKKidBioactC Uniform -9.21 4.605 );

## Population variances
Distrib( V_lnQCC InvGamma 2.25 0.0245 );
Distrib( V_lnVPRC InvGamma 2.25 0.1125 );
Distrib( V_QFatC InvGamma 6 1.058 );
Distrib( V_QGutC InvGamma 6 0.1445 );
Distrib( V_QLivC InvGamma 6 0.1445 );
Distrib( V_QSlwC InvGamma 6 0.45 );
Distrib( V_lnDRespC InvGamma 6 0.2 );
Distrib( V_QKidC InvGamma 6 0.0845 );
Distrib( V_FracPlasC InvGamma 6 0.2 );
Distrib( V_VFatC InvGamma 6 1.0125 );
Distrib( V_VGutC InvGamma 6 0.0845 );
Distrib( V_VLivC InvGamma 6 0.162 );
Distrib( V_VRapC InvGamma 6 0.072 );
Distrib( V_VRespLumC InvGamma 6 0.162 );
Distrib( V_VRespEffC InvGamma 6 0.162 );
Distrib( V_VKidC InvGamma 6 0.1125 );
Distrib( V_VBldC InvGamma 6 0.072 );
Distrib( V_lnPBC InvGamma 11.00018 0.62501125 );
Distrib( V_lnPFatC InvGamma 11.00018 0.9000162 );
Distrib( V_lnPGutC InvGamma 2.25 0.2 );
Distrib( V_lnPLivC InvGamma 11.00018 0.22500405 );
Distrib( V_lnPRapC InvGamma 2.25 0.2 );
Distrib( V_lnPRespC InvGamma 2.25 0.2 );
Distrib( V_lnPKidC InvGamma 5 0.36 );
Distrib( V_lnPSlwC InvGamma 11.00018 0.9000162 );
Distrib( V_lnPRBCPlasTCAC InvGamma 2.25 0.14112 );
Distrib( V_lnPBodTCAC InvGamma 2.25 0.60031125 );
Distrib( V_lnPLivTCAC InvGamma 2.25 0.60031125 );
Distrib( V_lnKDissoC InvGamma 2.25 0.465125 );
Distrib( V_lnBMaxkDC InvGamma 2.25 0.276125 );
Distrib( V_lnPBodTCOHC InvGamma 2.25 0.60031125 );
Distrib( V_lnPLivTCOHC InvGamma 2.25 0.60031125 );
Distrib( V_lnPBodTCOGC InvGamma 2.25 0.2 );
Distrib( V_lnPLivTCOGC InvGamma 2.25 0.2 );
# Distrib( V_lnPeffDCVG InvGamma 2.25 0.2 );
Distrib( V_lnKTSd InvGamma 2.25 5 );
Distrib( V_lnKAS InvGamma 2.25 5 );
Distrib( V_lnKTD InvGamma 2.25 5 );
Distrib( V_lnKAD InvGamma 2.25 5 );
Distrib( V_lnKASTCA InvGamma 2.25 5 );
Distrib( V_lnKASTCOH InvGamma 2.25 5 );
Distrib( V_lnVMaxC InvGamma 3 1.300806644 );

```

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Distrib( V_lnKMC InvGamma 3 2.879830961 );
# Distrib( V_lnClC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnFracOtherC InvGamma 2.25 0.3125 );
Distrib( V_lnFracTCAC InvGamma 2.25 0.3125 );
Distrib( V_lnVMaxDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnClDCVGC InvGamma 2.25 0.3125 );
# Distrib( V_lnKMDCVGC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnVMaxKidDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnClKidDCVGC InvGamma 2.25 0.3125 );
# Distrib( V_lnKMKidDCVGC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnVMaxLungLivC InvGamma 2.25 0.3125 );
Distrib( V_lnKMClara InvGamma 2.25 0.3125 );
Distrib( V_lnFracLungSysC InvGamma 2.25 0.3125 );
Distrib( V_lnVMaxTCOHC InvGamma 2.25 0.3125 );
# Distrib( V_lnClTCOHC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnKMTCOH InvGamma 2.25 0.3125 );
Distrib( V_lnVMaxGlucC InvGamma 2.25 0.3125 );
# Distrib( V_lnClGlucC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnKMGluc InvGamma 2.25 0.3125 );
Distrib( V_lnKMetTCOHC InvGamma 2.25 0.3125 );
Distrib( V_lnUrntCAC InvGamma 2.25 0.3125 );
Distrib( V_lnKMetTCAC InvGamma 2.25 0.3125 );
Distrib( V_lnkBileC InvGamma 2.25 0.3125 );
Distrib( V_lnKEHRC InvGamma 2.25 0.3125 );
Distrib( V_lnUrntCOGC InvGamma 2.25 0.3125 );
# Distrib( V_lnFracKidDCVCC InvGamma 2.25 0.3125 );
# Distrib( V_lnKDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnKNATC InvGamma 2.25 0.3125 );
Distrib( V_lnKKidBioactC InvGamma 2.25 0.3125 );

Level { #Subject level

#Error distributions
# Distrib( Ve_RetDose , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CAlv , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CAlvPPM , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CInhPPM , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CInh , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CMixExh , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CArt , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CVen , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CBldMix , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CFat , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CGut , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CRap , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CSlw , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CHrt , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CKid , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CLiv , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLung , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CMus , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CSpl , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CBrn , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAExh , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zAExhpost , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CKidTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLivTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLungTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CPlasTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CBldTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CBodTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CKidTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CLivTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLungTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zAUrnTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAUrnTCA_collect , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAUrnTCA_sat , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zABileTCOG , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CTCOG , LogUniform , 0.01 , 3.3 );

```

```

#       Distrib( Ve_CTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CKIdTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLivTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CLungTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_AUrntTCOGTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_AUrntTCOGTCOH_collect , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_AUrntTCOGTCOH_sat , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_CDCVGmol , LogUniform , 0.1 , 3.3 );
#       Distrib( Ve_zAurnNDCVC , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_AUrntCTotMole , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_TotCTCOH , LogUniform , 0.01 , 3.3 );
#       Distrib( Ve_QPsamp , LogUniform , 0.01 , 3.3 );

#Likelihoods
#       Likelihood( RetDose , LogNormal_v , Prediction( RetDose ) , Ve_RetDose );
#       Likelihood( CALv , LogNormal_v , Prediction( CALv ) , Ve_CALv );
#       Likelihood( CALvPPM , LogNormal_v , Prediction( CALvPPM ) , Ve_CALvPPM );
#       Likelihood( CInhPPM , LogNormal_v , Prediction( CInhPPM ) , Ve_CInhPPM );
#       Likelihood( CInh , LogNormal_v , Prediction( CInh ) , Ve_CInh );
#       Likelihood( CMixExh , LogNormal_v , Prediction( CMixExh ) , Ve_CMixExh );
#       Likelihood( CArt , LogNormal_v , Prediction( CArt ) , Ve_CArt );
#       Likelihood( CVen , LogNormal_v , Prediction( CVen ) , Ve_CVen );
#       Likelihood( CBldMix , LogNormal_v , Prediction( CBldMix ) , Ve_CBldMix );
#       Likelihood( CFat , LogNormal_v , Prediction( CFat ) , Ve_CFat );
#       Likelihood( CGut , LogNormal_v , Prediction( CGut ) , Ve_CGut );
#       Likelihood( CRap , LogNormal_v , Prediction( CRap ) , Ve_CRap );
#       Likelihood( CSLw , LogNormal_v , Prediction( CSLw ) , Ve_CSLw );
#       Likelihood( CHrt , LogNormal_v , Prediction( CHrt ) , Ve_CHrt );
#       Likelihood( CKid , LogNormal_v , Prediction( CKid ) , Ve_CKid );
#       Likelihood( CLiv , LogNormal_v , Prediction( CLiv ) , Ve_CLiv );
#       Likelihood( CLung , LogNormal_v , Prediction( CLung ) , Ve_CLung );
#       Likelihood( CMus , LogNormal_v , Prediction( CMus ) , Ve_CMus );
#       Likelihood( CSpl , LogNormal_v , Prediction( CSpl ) , Ve_CSpl );
#       Likelihood( CBrn , LogNormal_v , Prediction( CBrn ) , Ve_CBrn );
#       Likelihood( zAExh , LogNormal_v , Prediction( zAExh ) , Ve_zAExh );
#       Likelihood( zAExhpost , LogNormal_v , Prediction( zAExhpost ) , Ve_zAExhpost );
#       Likelihood( CTCOH , LogNormal_v , Prediction( CTCOH ) , Ve_CTCOH );
#       Likelihood( CKidTCOH , LogNormal_v , Prediction( CKidTCOH ) , Ve_CKidTCOH );
#       Likelihood( CLivTCOH , LogNormal_v , Prediction( CLivTCOH ) , Ve_CLivTCOH );
#       Likelihood( CLungTCOH , LogNormal_v , Prediction( CLungTCOH ) , Ve_CLungTCOH );
#       Likelihood( CPlastTCA , LogNormal_v , Prediction( CPlastTCA ) , Ve_CPlastTCA );
#       Likelihood( CBldTCA , LogNormal_v , Prediction( CBldTCA ) , Ve_CBldTCA );
#       Likelihood( CBodTCA , LogNormal_v , Prediction( CBodTCA ) , Ve_CBodTCA );
#       Likelihood( CKidTCA , LogNormal_v , Prediction( CKidTCA ) , Ve_CKidTCA );
#       Likelihood( CLivTCA , LogNormal_v , Prediction( CLivTCA ) , Ve_CLivTCA );
#       Likelihood( CLungTCA , LogNormal_v , Prediction( CLungTCA ) , Ve_CLungTCA );
#       Likelihood( zAurnTCA , LogNormal_v , Prediction( zAurnTCA ) , Ve_zAurnTCA );
#       Likelihood( zAurnTCA_collect , LogNormal_v , Prediction( zAurnTCA_collect ) ,
#       Ve_zAurnTCA_collect );
#       Likelihood( zAurnTCA_sat , LogNormal_v , Prediction( zAurnTCA_sat ) , Ve_zAurnTCA_sat );
#       Likelihood( zABileTCOG , LogNormal_v , Prediction( zABileTCOG ) , Ve_zABileTCOG );
#       Likelihood( CTCOG , LogNormal_v , Prediction( CTCOG ) , Ve_CTCOG );
#       Likelihood( CTCOGTCOH , LogNormal_v , Prediction( CTCOGTCOH ) , Ve_CTCOGTCOH );
#       Likelihood( CKidTCOGTCOH , LogNormal_v , Prediction( CKidTCOGTCOH ) , Ve_CKidTCOGTCOH );
#       Likelihood( CLivTCOGTCOH , LogNormal_v , Prediction( CLivTCOGTCOH ) , Ve_CLivTCOGTCOH );
#       Likelihood( CLungTCOGTCOH , LogNormal_v , Prediction( CLungTCOGTCOH ) , Ve_CLungTCOGTCOH );
#       Likelihood( AUrntTCOGTCOH , LogNormal_v , Prediction( AUrntTCOGTCOH ) , Ve_AUrntTCOGTCOH );
#       Likelihood( AUrntTCOGTCOH_collect , LogNormal_v , Prediction( AUrntTCOGTCOH_collect ) ,
#       Ve_AUrntTCOGTCOH_collect );
#       Likelihood( AUrntTCOGTCOH_sat , LogNormal_v , Prediction( AUrntTCOGTCOH_sat ) ,
#       Ve_AUrntTCOGTCOH_sat );
#       Likelihood( CDCVGmol , LogNormal_v , Prediction( CDCVGmol ) , Ve_CDCVGmol );
#       Likelihood( zAurnNDCVC , LogNormal_v , Prediction( zAurnNDCVC ) , Ve_zAurnNDCVC );
#       Likelihood( AurnTCTotMole , LogNormal_v , Prediction( AurnTCTotMole ) , Ve_AurnTCTotMole );
#       Likelihood( TotCTCOH , LogNormal_v , Prediction( TotCTCOH ) , Ve_TotCTCOH );
#       Likelihood( QPsamp , LogNormal_v , Prediction( QPsamp ) , Ve_QPsamp );

# Individual parameters
#       Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.56 0.56 );
#       Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -1.2 1.2 );
#       Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );

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Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.66 1.34 );
Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.66 1.34 );
Distrib( QSLwC TruncNormal_v M_QSLwC V_QSLwC 0.4 1.6 );
Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.74 1.26 );
Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.4 1.6 );
Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.74 1.26 );
Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.64 1.36 );
Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.76 1.24 );
Distrib( VRespLumC TruncNormal_v M_VRespLumC V_VRespLumC 0.64 1.36 );
Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.64 1.36 );
Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.7 1.3 );
Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.75 0.75 );
Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.9 0.9 );
Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -0.45 0.45 );
Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.9 0.9 );
Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -1.008 1.008 );
Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -2.079 2.079 );
Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -2.079 2.079 );
Distrib( lnkDissocC TruncNormal_v M_lnkDissocC V_lnkDissocC -1.83 1.83 );
Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -1.41 1.41 );
Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -2.079 2.079 );
Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -2.079 2.079 );
Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
# Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
Distrib( lnkTSD TruncNormal_v M_lnkTSD V_lnkTSD -4.269 4.942 );
Distrib( lnkAS TruncNormal_v M_lnkAS V_lnkAS -6.571 7.244 );
Distrib( lnkTD TruncNormal_v M_lnkTD V_lnkTD -4.605 0 );
Distrib( lnkAD TruncNormal_v M_lnkAD V_lnkAD -7.195 6.62 );
Distrib( lnkASTCA TruncNormal_v M_lnkASTCA V_lnkASTCA -7.195 6.62 );
Distrib( lnkASTCOH TruncNormal_v M_lnkASTCOH V_lnkASTCOH -7.195 6.62 );
Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
Distrib( lnkMC TruncNormal_v M_lnkMC V_lnkMC -4.158 4.158 );
# Distrib( lnClC TruncNormal_v M_lnClC V_lnClC 0 1 );
Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC -4.605 9.21 );
Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -4.605 9.21 );
# Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC 0 1 );
Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC -4.605 9.21 );
Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -4.605 9.21 );
# Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC 0 1 );
Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC -9.21 9.21 );
# Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC 0 1 );
Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC -9.21 9.21 );
# Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC 0 1 );
Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
Distrib( lnkUrnTCAC TruncNormal_v M_lnUrnTCAC V_lnUrnTCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
Distrib( lnkEHRC TruncNormal_v M_lnkEHRC V_lnkEHRC -9.21 4.605 );
Distrib( lnkUrnTCOGC TruncNormal_v M_lnUrnTCOGC V_lnUrnTCOGC -6.908 6.908 );
# Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );
# Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
Distrib( lnkNATC TruncNormal_v M_lnkNATC V_lnkNATC -9.21 4.605 );
Distrib( lnkKidBioactC TruncNormal_v M_lnkKidBioactC V_lnKKidBioactC -9.21 4.605 );

```

```

Species = 2;
lnFracKidDCVCC = 10; # Remove DCVG compartment
lnkDCVGC = 10; # Remove DCVG compartment

##### DATA USED IN CALIBRATION #####
#####

##### BEGIN GROUP 1
Level {
#### BEGIN Bernauer96
Experiment { # Begin Bernauer96 TCeratWSaMinh006040
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.325 ;

# Exposure/Dosing
Conc = NDoses( 2 , 40 0 , 0 6 );

# Data
Print( AUrnTCOGTCOH , 12, 24, 36, 48 );
Data( AUrnTCOGTCOH , 0.851813835, 0.973501526, 1.095189217, 1.156033062 );
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 12, 24, 36, 48 );
Data( zAUrnNDCVC , 0.000462562, 0.001002218, 0.001561147, 0.00213935 );
Print( zAUrnTCA , 12, 24, 36, 48 );
Data( zAUrnTCA , 0.055668023, 0.055668023, 0.055668023, 0.055668023 );
} # End Bernauer96 TCeratWSaMinh006040

Experiment { # Begin Bernauer96 TCeratWSaMinh006080
Species = 2 ;
Male = 1 ;

```

```

# Measured Covariates (if any)
  BWmeas = 0.325 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 80 0 , 0 6 );

# Data
  Print( AUrnTCOGTCOH , 12, 24, 36, 48 );
  Data( AUrnTCOGTCOH , 1.703627671, 2.068690743, 2.312066124, 2.433753815 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 12, 24, 36, 48 );
  Data( zAUrnNDCVC , 0.000510746, 0.000992581, 0.00149369, 0.002033346 );
  Print( zAUrnTCA , 12, 24, 36, 48 );
  Data( zAUrnTCA , 0.111336045, 0.167004068, 0.167004068, 0.167004068 );
} # End Bernauer96 TCeratWSaMinh006080

Experiment { # Begin Bernauer96 TCeratWSaMinh006160
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.325 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 160 0 , 0 6 );

# Data
  Print( AUrnTCOGTCOH , 12, 24, 36, 48 );
  Data( AUrnTCOGTCOH , 2.798816887, 3.16387996, 3.468099186, 3.711474568 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );

```



```

Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 12, 24, 36, 48 );
Data( zAUrnNDCVC , 0.000636023, 0.001618968, 0.002775373, 0.00360413 );
Print( zAUrnTCA , 12, 24, 36, 48 );
Data( zAUrnTCA , 0.334008135, 0.556680225, 0.668016271, 0.723684293 );
} # End Bernauer96 TCeratWSaMinh006160
#### END Bernauer96
##### END GROUP 1
}

##### BEGIN GROUP 2
Level {
#### BEGIN Dallas91
Experiment { # Begin Dallas91 TCeratSDaMinh002050
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.35 ;

# Exposure/Dosing
Conc = NDoses( 2 , 50 0 , 0 2 );

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CART , 0.027166667, 0.064666667, 0.100833333, 0.1335, 0.163833333,
0.253333333, 0.336666667, 0.42, 0.501666667, 0.756666667, 1.01, 1.258333333,
1.505, 1.75, 2, 2.033333333, 2.066666667, 2.1, 2.133333333, 2.166666667, 2.25,
2.333333333, 2.416666667, 2.5, 2.75, 3, 3.25, 3.516666667, 3.766666667,
4.016666667, 4.5 );
Data( CART , 0.203, 0.261, 0.335, 0.443, 0.402, 0.452, 0.491, 0.349, 0.49, 0.429,
0.55, 0.508, 0.639, 0.59, 0.601, 0.339, 0.268, 0.259, 0.158, 0.219, 0.148,
0.158, 0.0864, 0.119, 0.0797, 0.0685, 0.0492, 0.039, 0.0278, 0.0202, 0.0141 );
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );

```

```

Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0.023166667, 0.057333333, 0.089333333, 0.175, 0.26, 0.343333333,
      0.506666667, 0.671666667, 0.843333333, 1.008333333, 1.176666667, 1.335,
      1.501666667, 1.666666667, 1.816666667, 2, 2.016666667, 2.05, 2.083333333, 2.1,
      2.166666667, 2.25, 2.5, 2.75, 3, 3.25 ); #, 3.516666667, 3.75, 4, 4.5, 5 );
Data( CMixExh , 0.127, 0.146, 0.161, 0.155, 0.177, 0.176, 0.176, 0.18, 0.173, 0.179,
      0.187, 0.183, 0.192, 0.185, 0.182, 0.178, 0.0601, 0.0315, 0.0271, 0.00352,
      0.0129, 0.00946, 0.0063, 0.0025, 0.0045, 0.00128 ); #, -0.00277, -0.00326,
      -0.00105, 0.00334, 0.0021 );
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Dallas91 TCeratSDaMinh002050

Experiment { # Begin Dallas91 TCeratSDaMinh002500
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.35 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 500 0 , 0 2 );

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( Cart , 0.039833333, 0.0695, 0.107666667, 0.129333333, 0.173333333, 0.255,
      0.341666667, 0.421666667, 0.495, 0.748333333, 1.005, 1.253333333, 1.503333333,
      1.75, 2.016666667, 2.033333333, 2.066666667, 2.1, 2.133333333, 2.166666667,
      2.25, 2.333333333, 2.416666667, 2.516666667, 2.766666667, 3, 3.266666667, 3.5,
      3.75, 4, 4.516666667, 5.016666667 );
  Data( Cart , 2.88, 4.43, 4.7, 6.92, 7.23, 7.64, 10.2, 11.2, 12.2, 13.5, 15.2, 14.5,
      15.4, 15.3, 17.3, 12.9, 12.6, 11.5, 10.5, 10.3, 8.92, 7.55, 7.46, 6.69, 5.63,
      3.46, 2.58, 1.91, 1.6, 1.28, 1, 0.729 );
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );

```

```

Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0.012966667, 0.058166667, 0.092666667, 0.173333333, 0.258333333,
      0.341666667, 0.508333333, 0.675, 0.835, 1.003333333, 1.173333333, 1.338333333,
      1.506666667, 1.666666667, 1.85, 2.016666667, 2.033333333, 2.05, 2.083333333,
      2.116666667, 2.166666667, 2.25, 2.516666667, 2.766666667, 3.016666667,
      3.266666667, 3.516666667, 3.766666667, 4.016666667, 4.516666667, 5.016666667);
Data( CMixExh , 1.26, 1.44, 1.49, 1.56, 1.63, 1.61, 1.73, 1.73, 1.78, 1.82, 1.84,
      1.73, 1.83, 1.82, 1.91, 1.79, 0.702, 0.513, 0.465, 0.406, 0.382, 0.362, 0.222,
      0.153, 0.0991, 0.0806, 0.0621, 0.0258, 0.0324, 0.0312, 0.0121 );
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Dallas91 TCERatSDaMinh002500
#### END Dallas91
##### END GROUP 2
}

##### BEGIN GROUP 3
Level {
#### BEGIN Fisher89
Experiment { # Begin Fisher89 TCERatFR4Finhc9111e
Species = 2 ;
Male = 0 ;

# Measured Covariates (if any)
BWmeas = 0.159 ;

# Exposure/Dosing
CC = 1100 ;
NRodents = 4 ;
VChC = 9.1 ;
lnkLossC = -3.912 ;

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);

```

```

Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0.083, 0.167, 0.333, 0.5, 0.667, 0.833, 1, 1.167, 1.333, 1.5, 1.667,
      1.833, 2, 2.167, 2.333, 2.5, 2.667 );
Data( CInhPPM , 921, 760, 553, 423, 327, 267, 221, 185, 156, 133, 115, 100, 84, 70,
      58, 47, 37 );
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Fisher89 TCeratFR4Finhc9111e

Experiment { # Begin Fisher89 TCeratFR4Finhc9122e
  Species = 2 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.159 ;

# Exposure/Dosing
  CC = 2200 ;
  NRodents = 4 ;
  VChC = 9.1 ;
  lnLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0.083, 0.167, 0.333, 0.5, 0.667, 0.833, 1, 1.167, 1.333, 1.5, 1.667,
      1.833, 2, 2.167, 2.333, 2.5, 2.667, 2.833, 3, 3.167, 3.333, 3.5, 3.667, 3.833,
      4, 4.167, 4.333, 4.5, 4.667, 4.833, 5 );

```

```

Data( CInhPPM , 1918, 1629, 1331, 1092, 944, 802, 693, 607, 544, 492, 447, 418, 389,
      363, 339, 314, 292, 274, 257, 241, 227, 214, 201, 189, 176, 164, 151, 137, 124,
      113, 102 );
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Fisher89 TCERatFR4Finhc9122e

Experiment { # Begin Fisher89 TCERatFR4Finhc91300
  Species = 2 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.161 ;

# Exposure/Dosing
  CC = 300 ;
  NRodents = 4 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0.083, 0.5, 0.667, 0.833, 1, 1.167, 1.333, 1.5 );
  Data( CInhPPM , 214, 99, 70.3, 52.3, 38.1, 14, 11, 8 );
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);

```

```

Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Fisher89 TCeratFR4Finhc91300

Experiment { # Begin Fisher89 TCeratFR4Finhc9151e
  Species = 2 ;
  Male = 0 ;

# Measured Covariates (if any)
  BWmeas = 0.175 ;

# Exposure/Dosing
  CC = 5100 ;
  NRodents = 4 ;
  VChC = 9.1 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0.083, 0.167, 0.333, 0.5, 0.667, 0.833, 1, 1.167, 1.333, 1.5, 1.667,
    1.833, 2, 2.167, 2.333, 2.5, 2.667, 2.833, 3, 3.167, 3.333, 3.5, 3.667, 3.833,
    4, 4.167, 4.333, 4.5, 4.667, 4.833, 5, 5.167, 5.333, 5.5, 5.667, 5.833, 6 );
  Data( CInhPPM , 4507, 3951, 3079, 2553, 2152, 1797, 1544, 1373, 1214, 1093, 1004,
    934, 872, 826, 781, 743, 716, 695, 674, 651, 634, 619, 603, 589, 571, 561, 547,
    536, 528, 515, 507, 502, 492, 480, 468, 457, 448 );
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );

```

```

Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Fisher89 TCeratFR4Finhc9151e
#### END Fisher89
##### END GROUP 3
}

##### BEGIN GROUP 4
Level {
#### BEGIN Fisher91
Experiment { # Begin Fisher91 TCeratFRaFinh004600
Species = 2 ;
Male = 0 ;

# Measured Covariates (if any)
BWmeas = 0.186 ;

# Exposure/Dosing
Conc = NDoses( 2 , 600 0 , 0 4 );

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0.6, 3.75, 4.25, 5, 6, 8.75, 26, 32, 48 );
Data( CBldTCA , 1.672, 15.656, 14.972, 24.016, 25.232, 29.564, 8.284, 4.484, 0.988 );
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0.6, 3.75, 4.25, 5, 6, 8.75, 26, 32, 48 );
Data( CPlasTCA , 2.2, 20.6, 19.7, 31.6, 33.2, 38.9, 10.9, 5.9, 1.3 );
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0.6, 3.75, 4.25, 5, 6 );
Data( CVen , 9.3, 26.4, 19.7, 6.9, 3.5 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );

```

```

        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Fisher91 TCeratFRaFinh004600
#### END Fisher91
##### END GROUP 4
}

##### BEGIN GROUP 5
    Level {
#### BEGIN Fisher91
        Experiment { # Begin Fisher91 TCeratFRaMinh004505
            Species = 2 ;
            Male = 1 ;

# Measured Covariates (if any)
            BWmeas = 0.236 ;

# Exposure/Dosing
            Conc = NDoses( 2 , 505 0 , 0 4 );

# Data
            Print( AUrnTCOGTCOH , 0 );
            Data( AUrnTCOGTCOH , -1);
            Print( AUrnTCTotMole , 0 );
            Data( AUrnTCTotMole , -1);
            Print( CArt , 0 );
            Data( CArt , -1);
            Print( CBldMix , 0 );
            Data( CBldMix , -1);
            Print( CBldTCA , 2, 3.75, 6, 8, 10, 12, 26, 32 );
            Data( CBldTCA , 4.94, 8.284, 16.948, 16.34, 15.352, 13.3, 4.788, 3.42 );
            Print( CFat , 0 );
            Data( CFat , -1);
            Print( CGut , 0 );
            Data( CGut , -1);
            Print( CInhPPM , 0 );
            Data( CInhPPM , -1);
            Print( CKid , 0 );
            Data( CKid , -1);
            Print( CLiv , 0 );
            Data( CLiv , -1);
            Print( CLivTCA , 0 );
            Data( CLivTCA , -1);
            Print( CMixExh , 0 );
            Data( CMixExh , -1);
            Print( CMus , 0 );
            Data( CMus , -1);
            Print( CPlasTCA , 2, 3.75, 6, 8, 10, 12, 26, 32 );
            Data( CPlasTCA , 6.5, 10.9, 22.3, 21.5, 20.2, 17.5, 6.3, 4.5 );
            Print( CTCOG , 0 );
            Data( CTCOG , -1);
            Print( CTCOH , 0 );
            Data( CTCOH , -1);
            Print( CVen , 0 );
            Data( CVen , -1);
            Print( TotCTCOH , 0 );
            Data( TotCTCOH , -1);
            Print( zABileTCOG , 0 );
            Data( zABileTCOG , -1);
            Print( zAExhpost , 0 );
            Data( zAExhpost , -1);
            Print( zAUrnNDCVC , 0 );
            Data( zAUrnNDCVC , -1);
            Print( zAUrnTCA , 0 );
            Data( zAUrnTCA , -1);
        } # End Fisher91 TCeratFRaMinh004505
#### END Fisher91
##### END GROUP 5

```



```

}

##### BEGIN GROUP 6
  Level {
#### BEGIN Green85
    Experiment { # Begin Green85 TCAt0AaM_iv_aq010
      Species = 2 ;
      Male = 1 ;

# Measured Covariates (if any)
      BWmeas = 0.19 ;

# Exposure/Dosing
      IVDoseTCA = NDoses( 2 , 10 0 , 0 0.05 );
      TChng = 0.05 ;

# Data
      Print( AUrnTCOGTCOH , 0 );
      Data( AUrnTCOGTCOH , -1);
      Print( AUrnTCTotMole , 24 );
      Data( AUrnTCTotMole , 0.004011628 );
      Print( CART , 0 );
      Data( CART , -1);
      Print( CBldMix , 0 );
      Data( CBldMix , -1);
      Print( CBldTCA , 0 );
      Data( CBldTCA , -1);
      Print( CFat , 0 );
      Data( CFat , -1);
      Print( CGut , 0 );
      Data( CGut , -1);
      Print( CInhPPM , 0 );
      Data( CInhPPM , -1);
      Print( CKid , 0 );
      Data( CKid , -1);
      Print( CLiv , 0 );
      Data( CLiv , -1);
      Print( CLivTCA , 0 );
      Data( CLivTCA , -1);
      Print( CMixExh , 0 );
      Data( CMixExh , -1);
      Print( CMus , 0 );
      Data( CMus , -1);
      Print( CPlasTCA , 0 );
      Data( CPlasTCA , -1);
      Print( CTCOG , 0 );
      Data( CTCOG , -1);
      Print( CTCOH , 0 );
      Data( CTCOH , -1);
      Print( CVen , 0 );
      Data( CVen , -1);
      Print( TotCTCOH , 0 );
      Data( TotCTCOH , -1);
      Print( zABileTCOG , 0 );
      Data( zABileTCOG , -1);
      Print( zAExhpost , 0 );
      Data( zAExhpost , -1);
      Print( zAUrnNDCVC , 0 );
      Data( zAUrnNDCVC , -1);
      Print( zAUrnTCA , 0 );
      Data( zAUrnTCA , -1);
} # End Green85 TCAt0AaM_iv_aq010

    Experiment { # Begin Green85 TCAt0AaMorl_aq075
      Species = 2 ;
      Male = 1 ;

# Measured Covariates (if any)
      BWmeas = 0.19 ;

```

```
# Exposure/Dosing
  PODoseTCA = NDoses( 2 , 75 0 , 0 0.05 );
  TChng = 0.05 ;
```

```
# Data
```

```
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 24 );
  Data( AUrnTCTotMole , 0.05119186 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 0 );
  Data( zAUrnTCA , -1);
```

```
} # End Green85 TCAratOAaMorl_aq075
```

```
  Experiment { # Begin Green85 TCeratOAaMorloil500
    Species = 2 ;
    Male = 1 ;
```

```
# Measured Covariates (if any)
  BWmeas = 0.19 ;
```

```
# Exposure/Dosing
  PDose = NDoses( 2 , 500 0 , 0 0.05 );
  TChng = 0.05 ;
```

```
# Data
```

```
  Print( AUrnTCOGTCOH , 24 );
  Data( AUrnTCOGTCOH , 44.7973223 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
```

```

Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 24 );
Data( zAUrnTCA , 3.423565753 );
} # End Green85 TCerat0AaMorloil500

# Bile Cannulated
Experiment { # Begin Green85 TCerat0AaMorlocln500
  lnKEHRC = -100.;
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.19 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 500 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 24 );
  Data( AUrnTCTotMole , 0.187975647 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );

```

```

Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 24 );
Data( zABileTCOG , 18.35018265 );
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Green85 TCerat0AaMorlochn500
#### END Green85

#### BEGIN Prout85
# same group as Green85
  Experiment { # Begin Prout85 TCerat0AiMorloille3
    Species = 2 ;
    Male = 1 ;

# Measured Covariates (if any)
    BWmeas = 0.19 ;

# Exposure/Dosing
    PDose = NDoses( 2 , 1000 0 , 0 0.05 );
    TChng = 0.05 ;

# Data
    Print( AUrnTCOGTCOH , 0 );
    Data( AUrnTCOGTCOH , -1);
    Print( AUrnTCTotMole , 0 );
    Data( AUrnTCTotMole , -1);
    Print( CART , 0.25, 0.5, 0.75, 1, 1.5, 2, 2.5, 3, 4, 4.5, 5, 5.5, 6, 7, 8, 9, 10, 11);
    Data( CART , 5.77, 14.6, 20.1, 25.4, 20.2, 24, 42.4, 61.8, 43.7, 41.1, 29.6, 28.9,
      28.8, 21.2, 19.1, 13.4, 12, 8.25 );
    Print( CBldMix , 0 );
    Data( CBldMix , -1);
    Print( CBldTCA , 2.5, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 16, 17, 19, 20, 22, 23, 25,
      26, 28, 29, 30, 32, 34, 35, 36, 38, 40 );
    Data( CBldTCA , 3.4, 4.4, 10.7, 10.7, 15.2, 15.7, 27.7, 19.7, 47.1, 37.9, 48.8, 29.2,
      34.9, 44.5, 40.5, 23.8, 18.7, 14.6, 14.5, 22.5, 33.3, 39, 32.7, 18.9, 20.5,
      24.5, 21.6, 7.2 );
    Print( CFat , 0 );
    Data( CFat , -1);
    Print( CGut , 0 );
    Data( CGut , -1);
    Print( CInhPPM , 0 );
    Data( CInhPPM , -1);
    Print( CKid , 0 );
    Data( CKid , -1);
    Print( CLiv , 0 );
    Data( CLiv , -1);
    Print( CLivTCA , 0 );
    Data( CLivTCA , -1);
    Print( CMixExh , 0 );
    Data( CMixExh , -1);
    Print( CMus , 0 );

```

```

Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);

Print( CTCOH , 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 8, 9, 10, 11, 12,
      13, 14, 15, 16, 17, 18 );
Data( CTCOH , 0.81, 1.17, 1.08, 0.9, 0.81, 0.9, 1.17, 1.35, 0.9, 1.17, 0.99, 1.26,
      0.72, 1.17, 1.62, 7.39, 2.07, 2.34, 1.35, 0.81, 1.98, 0.81, 1.17, 0.81 );
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8,
      8.5, 10, 10.5, 11, 11.5 );
Data( zAExhpost , 3.4, 6, 9.1, 11.7, 15.7, 20.8, 27, 35.5, 41.1, 46.7, 50.8, 55.2,
      59.9, 63.5, 67.3, 71, 74.7, 83.3, 86, 88.6, 90.5 );
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Prout85 TCeratOAiMorloille3
#### END Prout85
##### END GROUP 6
}

##### BEGIN GROUP 7
Level {
#### BEGIN Hissink02
Experiment { # Begin Hissink02 TCeratWSaM_iv_aq010
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.275 ;

# Exposure/Dosing
IVDose = NDoses( 2 , 10 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 6, 12, 24, 48, 72, 96, 120, 144, 168 );
Data( AUrnTCTotMole , 0.010066591, 0.011866438, 0.012808219, 0.013164003,
      0.013247717, 0.013331431, 0.013331431, 0.013415145, 0.013436073 );
Print( CART , 0 );
Data( CART , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);

```

```

Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0.25, 0.5, 1, 1.5, 2, 3, 4, 6, 8 );
Data( CVen , 3.4821, 1.99728, 0.588672, 0.274626, 0.165564, 0.0614952, 0.0218124,
      0.00953964, 0.0026937 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Hissink02 TCeratWSaM_iv_aq010

Experiment { # Begin Hissink02 TCeratWSaM_iv_aq075
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.275 ;

# Exposure/Dosing
  IVDose = NDoses( 2 , 75 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 6, 12, 24, 48, 72, 96, 120, 144, 168 );
  Data( AUrnTCTotMole , 0.05744863, 0.075185502, 0.083818493, 0.086015982, 0.086486872,
      0.086957763, 0.086957763, 0.08774258, 0.08774258 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0.25, 0.5, 1, 1.5, 2, 3, 4, 6, 8 );
  Data( CVen , 48.618, 32.0616, 14.5854, 6.67512, 3.83688, 1.60308, 0.697734, 0.278568,
      0.1013094 );
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);

```

```

        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Hissink02 TCeratWSaM_iv_aq075

    Experiment { # Begin Hissink02 TCeratWSaMorloil100
        Species = 2 ;
        Male = 1 ;

    # Measured Covariates (if any)
        BWmeas = 0.275 ;

    # Exposure/Dosing
        PDose = NDoses( 2 , 100 0 , 0 0.05 );
        TChng = 0.05 ;

    # Data
        Print( AUrnTCOGTCOH , 0 );
        Data( AUrnTCOGTCOH , -1);
        Print( AUrnTCTotMole , 6, 12, 24, 48, 72, 96, 120, 144, 168 );
        Data( AUrnTCTotMole , 0.080993151, 0.144197108, 0.165334855, 0.169520548,
            0.171194825, 0.171822679, 0.172450533, 0.172869102, 0.172869102 );
        Print( CArt , 0 );
        Data( CArt , -1);
        Print( CBldMix , 0 );
        Data( CBldMix , -1);
        Print( CBldTCA , 0 );
        Data( CBldTCA , -1);
        Print( CFat , 0 );
        Data( CFat , -1);
        Print( CGut , 0 );
        Data( CGut , -1);
        Print( CInhPPM , 0 );
        Data( CInhPPM , -1);
        Print( CKid , 0 );
        Data( CKid , -1);
        Print( CLiv , 0 );
        Data( CLiv , -1);
        Print( CLivTCA , 0 );
        Data( CLivTCA , -1);
        Print( CMixExh , 0 );
        Data( CMixExh , -1);
        Print( CMus , 0 );
        Data( CMus , -1);
        Print( CPlasTCA , 0 );
        Data( CPlasTCA , -1);
        Print( CTCOG , 0 );
        Data( CTCOG , -1);
        Print( CTCOH , 0 );
        Data( CTCOH , -1);
        Print( CVen , 0.25, 0.5, 1, 1.5, 2, 3, 4, 6, 8 );
        Data( CVen , 5.70276, 6.75396, 5.54508, 4.69098, 3.6135, 1.73448, 0.67671, 0.140598,
            0.0865926 );
        Print( TotCTCOH , 0 );
        Data( TotCTCOH , -1);
        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Hissink02 TCeratWSaMorloil100

```

```

Experiment { # Begin Hissink02 TCeratWSaMorloille3
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.275 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 1000 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 6, 12, 24, 48, 72, 96, 120, 144, 168 );
  Data( AUrnTCTotMole , 0.073877473, 0.274162861, 0.655060883, 0.763888889,
    0.778538813, 0.782724505, 0.780631659, 0.784817352, 0.789003044 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0.25, 0.5, 1, 1.5, 2, 3, 4, 6, 8, 24 );
  Data( CVen , 69.7734, 54.6624, 44.8074, 42.8364, 38.6316, 44.9388, 54.9252, 66.0942,
    55.188, 0.178704 );
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 0 );
  Data( zAUrnTCA , -1);
} # End Hissink02 TCeratWSaMorloille3
#### END Hissink02
##### END GROUP 7
}

##### BEGIN GROUP 8
  Level {
#### BEGIN Kaneko94
    Experiment { # Begin Kaneko94 TCeratWSaMinh006050
      Species = 2 ;
      Male = 1 ;

```



```

# Measured Covariates (if any)

# Exposure/Dosing
  Conc = NDoses( 2 , 50 0 , 0 6 );

# Data
  Print( AUrnTCOGTCOH , 6, 12, 24, 48 );
  Data( AUrnTCOGTCOH , 0.37375, 0.743015, 0.84916, 0.89102 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 6, 8, 10 );
  Data( CVen , 0.385002, 0.0902718, 0.0254916 );
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 6, 12, 24, 48 );
  Data( zAUrnTCA , 0.00893798, 0.0339872, 0.0619286, 0.1379096 );
} # End Kaneko94 TCeratWSaMinh006050

Experiment { # Begin Kaneko94 TCeratWSaMinh006100
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)

# Exposure/Dosing
  Conc = NDoses( 2 , 100 0 , 0 6 );

# Data
  Print( AUrnTCOGTCOH , 6, 12, 24, 48 );
  Data( AUrnTCOGTCOH , 0.781885, 1.36643, 1.48902, 1.50995 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );

```

```

Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 6, 8, 10 );
Data( CVen , 0.772632, 0.248346, 0.054531 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 6, 12, 24, 48 );
Data( zAUrnTCA , 0.01550666, 0.0861118, 0.189544, 0.29412 );
} # End Kaneko94 TCeratWSaMinh006100

Experiment { # Begin Kaneko94 TCeratWSaMinh0061e3
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)

# Exposure/Dosing
  Conc = NDoses( 2 , 1000 0 , 0 6 );

# Data
  Print( AUrnTCOGTCOH , 6, 12, 24, 48 );
  Data( AUrnTCOGTCOH , 1.8239, 4.23085, 5.5913, 5.96505 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);

```

```

Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 6, 8, 10, 12 );
Data( CVen , 29.565, 11.60262, 4.6647, 1.78704 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 6, 12, 24, 48 );
Data( zAUrnTCA , 0.0856216, 0.4902, 1.197722, 1.62583 );
} # End Kaneko94 TCeratWSaMinh0061e3

Experiment { # Begin Kaneko94 TCeratWSaMinh006500
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)

# Exposure/Dosing
  Conc = NDoses( 2 , 500 0 , 0 6 );

# Data
  Print( AUrnTCOGTCOH , 6, 12, 24, 48 );
  Data( AUrnTCOGTCOH , 1.5249, 3.72255, 4.23085, 4.3654 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 6, 8, 10 );
  Data( CVen , 5.11146, 1.21545, 0.337698 );
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );

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```

        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 6, 12, 24, 48 );
        Data( zAUrnTCA , 0.062909, 0.328434, 0.617652, 0.861118 );
    } # End Kaneko94 TCeratWSaMinh006500
#### END Kaneko94
##### END GROUP 8
}

##### BEGIN GROUP 9
    Level {
#### BEGIN Keys03
        Experiment { # Begin Keys03 TCeratSDaM_ia_aq008
            Species = 2 ;
            Male = 1 ;

# Measured Covariates (if any)
            BWmeas = 0.355 ;

# Exposure/Dosing
            IADose = NDoses( 2 , 8 0 , 0 0.05 );
            TChng = 0.05 ;

# Data
            Print( AUrnTCOGTCOH , 0 );
            Data( AUrnTCOGTCOH , -1);
            Print( AUrnTCTotMole , 0 );
            Data( AUrnTCTotMole , -1);
            Print( CArt , 0 );
            Data( CArt , -1);
            Print( CBldMix , 0 );
            Data( CBldMix , -1);
            Print( CBldTCA , 0 );
            Data( CBldTCA , -1);
            Print( CFat , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 2.5, 4, 6, 8, 12, 16, 18, 24);
            Data( CFat , 12.92166667, 28.3185, 35.25533333, 28.5052, 18.1114, 19.24, 12.351,
                14.3292, 8.593666667, 4.881875, 3.50475, 2.228166667, 0.734, 0.1924, 0.009,
                0.007833333 );
            Print( CGut , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 2.5 );
            Data( CGut , 1.928333333, 1.332666667, 0.428833333, 0.3312, 0.0706, 0.0342, 0.0488,
                0.045166667, 0.024 );
            Print( CInhPPM , 0 );
            Data( CInhPPM , -1);
            Print( CKid , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 2.5 );
            Data( CKid , 3.177333333, 2.351666667, 0.639333333, 0.3044, 0.219, 0.077666667,
                0.071, 0.0436, 0.024166667 );
            Print( CLiv , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 2.5 );
            Data( CLiv , 5.34, 3.680166667, 1.1395, 0.4282, 0.284, 0.1285, 0.1206, 0.048833333,
                0.033666667 );
            Print( CLivTCA , 0 );
            Data( CLivTCA , -1);
            Print( CMixExh , 0 );
            Data( CMixExh , -1);
            Print( CMus , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 2.5 );
            Data( CMus , 2.430833333, 2.194833333, 1.216166667, 0.2778, 0.4538, 0.234833333,
                0.131, 0.131333333, 0.066333333 );
            Print( CPlasTCA , 0 );
            Data( CPlasTCA , -1);
            Print( CTCOG , 0 );
            Data( CTCOG , -1);
            Print( CTCOH , 0 );
            Data( CTCOH , -1);
            Print( CVen , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 2.5 );
            Data( CVen , 3.4475, 2.415666667, 0.908666667, 0.55475, 0.18, 0.084666667, 0.0744,
                0.040166667, 0.020833333 );
            Print( TotCTCOH , 0 );
            Data( TotCTCOH , -1);
            Print( zABileTCOG , 0 );
            Data( zABileTCOG , -1);
            Print( zAExhpost , 0 );

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```

        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Keys03 TCERatSDaM_ia_aq008

    Experiment { # Begin Keys03 TCERatSDaMinh002050
        Species = 2 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.291 ;

# Exposure/Dosing
        Conc = NDoses( 2 , 50 0 , 0 2 );

# Data
        Print( AUrnTCOGTCOH , 0 );
        Data( AUrnTCOGTCOH , -1);
        Print( AUrnTCTotMole , 0 );
        Data( AUrnTCTotMole , -1);
        Print( CArt , 0 );
        Data( CArt , -1);
        Print( CBldMix , 0 );
        Data( CBldMix , -1);
        Print( CBldTCA , 0 );
        Data( CBldTCA , -1);
        Print( CFat , 0.083, 0.333, 0.667, 1, 1.5, 2, 2.083, 2.167, 2.25, 2.5, 2.75, 3, 3.5,
            4, 5 );
        Data( CFat , 1.6636, 5.5892, 10.3988, 16.2034, 12.0516, 10.9364, 13.4514, 14.3444,
            11.9392, 12.2154, 10.5036, 8.4308, 10.26, 3.61, 5.92 );
        Print( CGut,0.083, 0.333, 0.667, 1, 1.5, 2, 2.083, 2.167, 2.25, 2.5, 2.75, 3, 3.5, 4);
        Data( CGut , 0.7058, 0.9556, 1.082, 1.4052, 0.9892, 0.9814, 0.6324, 0.60975, 0.364,
            0.3128, 0.3016, 0.1674, 0.11, 0.15 );
        Print( CInhPPM , 0 );
        Data( CInhPPM , -1);
        Print( CKid,0.083, 0.333, 0.667, 1, 1.5, 2, 2.083, 2.167, 2.25, 2.5, 2.75, 3, 3.5, 4);
        Data( CKid , 1.392, 1.2434, 1.548, 1.759, 1.272, 0.9038, 0.4354, 0.3874, 0.2428,
            0.1656, 0.1756, 0.1236, 0.056, 0.062 );
        Print( CLiv,0.083, 0.333, 0.667, 1, 1.5, 2, 2.083, 2.167, 2.25, 2.5, 2.75, 3, 3.5, 4);
        Data( CLiv , 0.5934, 0.4838, 0.5636, 0.7816, 0.4514, 0.3976, 0.1056, 0.1678, 0.1006,
            0.0782, 0.0414, 0.0692, 0.0435, 0.0436 );
        Print( CLivTCA , 0 );
        Data( CLivTCA , -1);
        Print( CMixExh , 0 );
        Data( CMixExh , -1);
        Print( CMus,0.083, 0.333, 0.667, 1, 1.5, 2, 2.083, 2.167, 2.25, 2.5, 2.75, 3, 3.5, 4);
        Data( CMus , 0.5354, 0.6714, 0.9312, 1.3028, 0.759, 0.5388, 0.5352, 0.3982, 0.3098,
            0.241, 0.2424, 0.1405, 0.127, 0.128 );
        Print( CPlasTCA , 0 );
        Data( CPlasTCA , -1);
        Print( CTCOG , 0 );
        Data( CTCOG , -1);
        Print( CTCOH , 0 );
        Data( CTCOH , -1);
        Print( CVen , 0.083, 0.333, 0.667, 1, 1.5, 2, 2.083, 2.167, 2.25, 2.5, 2.75, 3, 3.5,
            4, 5 );
        Data( CVen , 1.7216, 0.8474, 0.8866, 1.1678, 0.9346, 1.0914, 0.4452, 0.427, 0.333,
            0.2264, 0.108, 0.1068, 0.025, 0.048, 0.05 );
        Print( TotCTCOH , 0 );
        Data( TotCTCOH , -1);
        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Keys03 TCERatSDaMinh002050

```

```

Experiment { # Begin Keys03 TCERatSDaMinh002500
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.269 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 500 0 , 0 2 );

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0.083, 0.333, 1, 2, 2.083, 2.25, 2.75, 3.5, 5 );
  Data( CFat , 19.111, 66.285, 186.123, 323.977, 266.279, 493.956, 269.573, 298.914,
    150.91 );
  Print( CGut , 2.083, 2.25, 2.75, 3.5, 5 );
  Data( CGut , 14.987, 16.831, 7.856, 3.803, 0.876 );
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0.083, 0.333, 1, 2, 2.083, 2.25, 2.75, 3.5, 5 );
  Data( CKid , 14.408, 18.915, 20.26, 24.907, 11.504, 11.176, 5.177, 3.474, 0.846 );
  Print( CLiv , 0.083, 0.333, 1, 2, 2.083, 2.25, 2.75, 3.5, 5 );
  Data( CLiv , 18.211, 23.888, 27.611, 31.538, 13.564, 13.184, 4.335, 2.079, 0.251 );
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0.083, 0.333, 1, 2, 2.083, 2.25, 2.75, 3.5, 5 );
  Data( CMus , 5.956, 10.084, 15.028, 17.4, 9.141, 8.868, 4.547, 1.589, 1.113 );
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0.083, 0.333, 1, 2, 2.083, 2.25, 2.75, 3.5, 5 );
  Data( CVen , 6.25, 10.276, 11.503, 17.679, 11.806, 8.571, 3.118, 2.211, 0.608 );
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 0 );
  Data( zAUrnTCA , -1);
} # End Keys03 TCERatSDaMinh002500

Experiment { # Begin Keys03 TCERatSDaMorl_aq008
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.355 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 8 0 , 0 0.05 );
  TChng = 0.05 ;

```

```

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8, 12, 18, 24 );
Data( CFat , 14.97966667, 33.653, 36.5155, 28.9104, 18.803, 18.88566667, 24.3598,
      13.99866667, 8.718833333, 5.178875, 3.604625, 2.348333333, 0.784, 0.0306,
      0.0297 );
Print( CGut , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 3 );
Data( CGut , 2.360833333, 1.687833333, 0.796666667, 0.4382, 0.2488, 0.112833333,
      0.0958, 0.062166667, 0.029833333 );
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 3 );
Data( CKid , 3.730833333, 2.7075, 1.015333333, 0.3888, 0.3106, 0.1375, 0.0926,
      0.042833333, 0.026833333 );
Print( CLiv , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 3 );
Data( CLiv , 6.362666667, 3.914833333, 1.468333333, 0.5634, 0.4128, 0.197833333,
      0.144, 0.057166667, 0.037333333 );
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 3 );
Data( CMus , 2.8555, 2.4565, 1.3795, 0.3588, 0.5798, 0.318, 0.1614, 0.061,
      0.072833333 );
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0.083, 0.167, 0.333, 0.5, 0.75, 1, 1.5, 2, 3 );
Data( CVen , 3.934833333, 2.695666667, 1.061, 0.5296, 0.235, 0.128, 0.0934,
      0.030166667, 0.023 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Keys03 TCERatSDaMorl_aq008
#### END Keys03
##### END GROUP 9
}

##### BEGIN GROUP 10
Level {
#### BEGIN Kimmerle73
Experiment { # Begin Kimmerle73 TCERatWSaMinh004049
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.3 ;

# Exposure/Dosing
Conc = NDoses( 2 , 49 0 , 0 4 );

```

```

# Data
Print( AUrnTCOGTCOH , 28, 52 );
Data( AUrnTCOGTCOH , 0.848, 0.8591 );
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 5, 6, 7, 8 );
Data( zAExhpost , 0.0511, 0.0635, 0.0738, 0.0827 );
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 28, 52 );
Data( zAUrnTCA , 0.3425, 0.4252 );
} # End Kimmerle73 TCeratWSaMinh004049

Experiment { # Begin Kimmerle73 TCeratWSaMinh004054
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.3 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 54 0 , 0 4 );

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );

```



```

Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 4.083333333, 4.5, 5 );
Data( CTCOH , 0.8, 0.3, 0.2 );
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Kimmerle73 TCeratWSaMinh004054

Experiment { # Begin Kimmerle73 TCeratWSaMinh004175
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.3 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 175 0 , 0 4 );

# Data
  Print( AUrnTCOGTCOH , 28, 52, 76 );
  Data( AUrnTCOGTCOH , 2.2852, 2.306, 2.3092 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );

```

```

Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 5, 6, 7, 8, 9, 10, 11, 12 );
Data( zAExhpost , 0.3941, 0.5094, 0.5551, 0.5777, 0.5923, 0.5995, 0.6055, 0.6113 );
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 28, 52, 76 );
Data( zAUrnTCA , 0.8618, 1.0076, 1.0373 );
} # End Kimmerle73 TCeratWSaMinh004175

Experiment { # Begin Kimmerle73 TCeratWSaMinh004330
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.3 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 330 0 , 0 4 );

# Data
  Print( AUrnTCOGTCOH , 28, 52, 76 );
  Data( AUrnTCOGTCOH , 4.0664, 4.0828, 4.0851 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 5, 6, 7, 8, 9, 10, 11, 12 );
  Data( zAExhpost , 3.87, 4.445, 4.624, 4.711, 4.757, 4.783, 4.807, 4.824 );
  Print( zAUrnNDCVC , 0 );

```

```

        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 28, 52, 76 );
        Data( zAUrnTCA , 1.0291, 1.2373, 1.2713 );
    } # End Kimmerle73 TCeratWSaMinh004330

    Experiment { # Begin Kimmerle73 TCeratWSaMinh0043e3
        Species = 2 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.3 ;

# Exposure/Dosing
        Conc = NDoses( 2 , 3160 0 , 0 4 );

# Data
        Print( AUrnTCOGTCOH , 0 );
        Data( AUrnTCOGTCOH , -1);
        Print( AUrnTCTotMole , 0 );
        Data( AUrnTCTotMole , -1);
        Print( CArt , 0 );
        Data( CArt , -1);
        Print( CBldMix , 0 );
        Data( CBldMix , -1);
        Print( CBldTCA , 0 );
        Data( CBldTCA , -1);
        Print( CFat , 0 );
        Data( CFat , -1);
        Print( CGut , 0 );
        Data( CGut , -1);
        Print( CInhPPM , 0 );
        Data( CInhPPM , -1);
        Print( CKid , 0 );
        Data( CKid , -1);
        Print( CLiv , 0 );
        Data( CLiv , -1);
        Print( CLivTCA , 0 );
        Data( CLivTCA , -1);
        Print( CMixExh , 0 );
        Data( CMixExh , -1);
        Print( CMus , 0 );
        Data( CMus , -1);
        Print( CPlasTCA , 0 );
        Data( CPlasTCA , -1);
        Print( CTCOG , 0 );
        Data( CTCOG , -1);
        Print( CTCOH , 4.083333333, 4.5, 5 );
        Data( CTCOH , 1.74, 1.68, 1.75 );
        Print( CVen , 4.083333333, 4.5, 5 );
        Data( CVen , 89.2, 35.4, 19.4 );
        Print( TotCTCOH , 0 );
        Data( TotCTCOH , -1);
        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Kimmerle73 TCeratWSaMinh0043e3
#### END Kimmerle73
##### END GROUP 10
}

```

```

##### BEGIN GROUP 11
  Level {
#### BEGIN Larson92A
# oral metabolite
  Experiment { # Begin Larson92A TCAtFRAMorl_aq020
    Species = 2 ;
    Male = 1 ;

# Measured Covariates (if any)
    BWmeas = 0.331 ;

# Exposure/Dosing
    PODoseTCA = NDoses( 2 , 20 0 , 0 0.05 );
    TChng = 0.05 ;

# Data
    Print( AUrnTCOGTCOH , 0 );
    Data( AUrnTCOGTCOH , -1);
    Print( AUrnTCTotMole , 0 );
    Data( AUrnTCTotMole , -1);
    Print( CArt , 0 );
    Data( CArt , -1);
    Print( CBldMix , 0 );
    Data( CBldMix , -1);
    Print( CBldTCA , 0 );
    Data( CBldTCA , -1);
    Print( CFat , 0 );
    Data( CFat , -1);
    Print( CGut , 0 );
    Data( CGut , -1);
    Print( CInhPPM , 0 );
    Data( CInhPPM , -1);
    Print( CKid , 0 );
    Data( CKid , -1);
    Print( CLiv , 0 );
    Data( CLiv , -1);
    Print( CLivTCA , 0 );
    Data( CLivTCA , -1);
    Print( CMixExh , 0 );
    Data( CMixExh , -1);
    Print( CMus , 0 );
    Data( CMus , -1);
    Print( CPlasTCA , 0.25, 1, 3, 5, 10, 16, 24 );
    Data( CPlasTCA , 17.3204, 36.765, 36.1114, 30.229, 16.8302, 8.0066, 4.4118 );
    Print( CTCOG , 0 );
    Data( CTCOG , -1);
    Print( CTCOH , 0 );
    Data( CTCOH , -1);
    Print( CVen , 0 );
    Data( CVen , -1);
    Print( TotCTCOH , 0 );
    Data( TotCTCOH , -1);
    Print( zABileTCOG , 0 );
    Data( zABileTCOG , -1);
    Print( zAExhpost , 0 );
    Data( zAExhpost , -1);
    Print( zAUrnNDCVC , 0 );
    Data( zAUrnNDCVC , -1);
    Print( zAUrnTCA , 0 );
    Data( zAUrnTCA , -1);
  } # End Larson92A TCAtFRAMorl_aq020

# oral metabolite
  Experiment { # Begin Larson92A TCAtFRAMorl_aq100
    Species = 2 ;
    Male = 1 ;

# Measured Covariates (if any)
    BWmeas = 0.331 ;

```

```

# Exposure/Dosing
PODoseTCA = NDoses( 2 , 100 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0.25, 1, 3, 5, 10, 16, 24, 32 );
Data( CPlasTCA , 85.1314, 202.2892, 147.5502, 107.6806, 57.3534, 26.144, 10.621,
      4.4118 );
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Larson92A TCAtFrMorl_aq100
#### END Larson92A

#### BEGIN Larson92B
# same group as Larson92A
Experiment { # Begin Larson92B TCAtFrMorl_aq197
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.404 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 197.25 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);

```

```

Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 1, 2, 4, 8, 12, 24 );
Data( CBldTCA , 6.0458, 8.17, 12.7452, 13.2354, 10.621, 2.1242 );
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 1, 2, 4, 8, 12 );
Data( CTCOH , 1.196, 2.37705, 2.392, 0.61295, 0.1495 );
Print( CVen , 1, 2, 4, 8 );
Data( CVen , 11.18214, 6.42546, 2.50974, 1.14318 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Larson92B TCeratFRaMorl_aq197

# same group as Larson92A
Experiment { # Begin Larson92B TCeratFRaMorl_aq3e3
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.404 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 3024 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 1, 2, 4, 8, 12, 24, 48 );
  Data( CBldTCA , 4.2484, 9.804, 11.1112, 23.5296, 36.6016, 60.6214, 5.5556 );
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);

```

```

Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 1, 2, 4, 8, 12, 24 );
Data( CTCOH , 1.794, 2.99, 2.99, 3.289, 5.083, 3.4385 );
Print( CVen , 1, 2, 4, 8, 12, 24 );
Data( CVen , 61.6266, 164.5128, 101.178, 88.1694, 46.2528, 6.4386 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Larson92B TCeratFRaMorl_aq3e3

# same group as Larson92A
Experiment { # Begin Larson92B TCeratFRaMorl_aq592
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.404 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 591.75 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 1, 2, 4, 8, 12, 24, 48 );
  Data( CBldTCA , 2.7778, 6.76476, 9.08504, 20.16356, 24.49366, 17.18968, 1.53596 );
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);

```

```

Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 1, 2, 4, 8, 12, 24 );
Data( CTCOH , 1.30065, 1.59965, 2.43685, 4.44015, 1.92855, 0.43355 );
Print( CVen , 1, 2, 4, 8, 12 );
Data( CVen , 25.8201, 34.40052, 20.1699, 6.74082, 3.23244 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Larson92B TCERatFRaMorl_aq592
#### END Larson92B
##### END GROUP 11
}

##### BEGIN GROUP 12
Level {
#### BEGIN Lee00A
# blood and liver
Experiment { # Begin Lee00A TCERatSDaM_iv_aq016
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.275 ;

# Exposure/Dosing
IVDose = NDoses( 2 , 16 0 , 0 0.0028 );
TChng = 0.0028 ;

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0.01111111, 0.019444444, 0.036111111, 0.086111111 );
Data( CBldMix , 16, 25, 20, 11 );
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0.01111111, 0.019444444, 0.036111111, 0.086111111 );
Data( CLiv , 20, 22, 41, 17 );
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);

```



```

        Print( TotCTCOH , 0 );
        Data( TotCTCOH , -1);
        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Lee00A TCERatSDaM_iv_aq016

# blood and liver
    Experiment { # Begin Lee00A TCERatSDaM_pv_aq016
        Species = 2 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.275 ;

# Exposure/Dosing
        PVDose = NDoses( 2 , 16 0 , 0 0.0028 );
        TChng = 0.0028 ;

# Data
        Print( AUrnTCOGTCOH , 0 );
        Data( AUrnTCOGTCOH , -1);
        Print( AUrnTCTotMole , 0 );
        Data( AUrnTCTotMole , -1);
        Print( CArt , 0 );
        Data( CArt , -1);
        Print( CBldMix , 0.011111111, 0.019444444, 0.036111111, 0.086111111 );
        Data( CBldMix , 19, 25, 15, 8 );
        Print( CBldTCA , 0 );
        Data( CBldTCA , -1);
        Print( CFat , 0 );
        Data( CFat , -1);
        Print( CGut , 0 );
        Data( CGut , -1);
        Print( CInhPPM , 0 );
        Data( CInhPPM , -1);
        Print( CKid , 0 );
        Data( CKid , -1);
        Print( CLiv , 0.011111111, 0.019444444, 0.036111111, 0.086111111 );
        Data( CLiv , 82, 209, 44, 14 );
        Print( CLivTCA , 0 );
        Data( CLivTCA , -1);
        Print( CMixExh , 0 );
        Data( CMixExh , -1);
        Print( CMus , 0 );
        Data( CMus , -1);
        Print( CPlasTCA , 0 );
        Data( CPlasTCA , -1);
        Print( CTCOG , 0 );
        Data( CTCOG , -1);
        Print( CTCOH , 0 );
        Data( CTCOH , -1);
        Print( CVen , 0 );
        Data( CVen , -1);
        Print( TotCTCOH , 0 );
        Data( TotCTCOH , -1);
        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Lee00A TCERatSDaM_pv_aq016
##### END Lee00A

```

```

##### END GROUP 12
}

##### BEGIN GROUP 13
  Level {
#### BEGIN Merdink99
    Experiment { # Begin Merdink99 TCHratFRaMivf_aq100
      Species = 2 ;
      Male = 1 ;

# Measured Covariates (if any)
      BWmeas = 0.275 ;

# Exposure/Dosing
      IVDoseTCOH = NDoses( 2 , 100 0 , 0 3 );
      TChng = 3 ;

# Data
      Print( AUrnTCOGTCOH , 0 );
      Data( AUrnTCOGTCOH , -1);
      Print( AUrnTCTotMole , 0 );
      Data( AUrnTCTotMole , -1);
      Print( CArt , 0 );
      Data( CArt , -1);
      Print( CBldMix , 0 );
      Data( CBldMix , -1);
      Print( CBldTCA , 0 );
      Data( CBldTCA , -1);
      Print( CFat , 0 );
      Data( CFat , -1);
      Print( CGut , 0 );
      Data( CGut , -1);
      Print( CInhPPM , 0 );
      Data( CInhPPM , -1);
      Print( CKid , 0 );
      Data( CKid , -1);
      Print( CLiv , 0 );
      Data( CLiv , -1);
      Print( CLivTCA , 0 );
      Data( CLivTCA , -1);
      Print( CMixExh , 0 );
      Data( CMixExh , -1);
      Print( CMus , 0 );
      Data( CMus , -1);
      Print( CPlasTCA , 0 );
      Data( CPlasTCA , -1);
      Print( CTCOG , 0 );
      Data( CTCOG , -1);
      Print( CTCOH , 3.274, 3.509, 4.01, 4.99, 6, 8.01 );
      Data( CTCOH , 182.39, 130.5135, 72.059, 41.86, 28.2555, 14.4417 );
      Print( CVen , 0 );
      Data( CVen , -1);
      Print( TotCTCOH , 0 );
      Data( TotCTCOH , -1);
      Print( zABileTCOG , 0 );
      Data( zABileTCOG , -1);
      Print( zAExhpost , 0 );
      Data( zAExhpost , -1);
      Print( zAUrnNDCVC , 0 );
      Data( zAUrnNDCVC , -1);
      Print( zAUrnTCA , 0 );
      Data( zAUrnTCA , -1);
    } # End Merdink99 TCHratFRaMivf_aq100
#### END Merdink99
##### END GROUP 13
}

```

```

##### BEGIN GROUP 14
  Level {
#### BEGIN Prout85
# different strain
  Experiment { # Begin Prout85 TCeratAPaMorloil010
    Species = 2 ;
    Male = 1 ;

# Measured Covariates (if any)
    BWmeas = 0.19 ;

# Exposure/Dosing
    PDose = NDoses( 2 , 10 0 , 0 0.05 );
    TChng = 0.05 ;

# Data
    Print( AUrnTCOGTCOH , 0 );
    Data( AUrnTCOGTCOH , -1);
    Print( AUrnTCTotMole , 24, 48, 72 );
    Data( AUrnTCTotMole , 0.007894977, 0.008314307, 0.008429985 );
    Print( CART , 0 );
    Data( CART , -1);
    Print( CBldMix , 0 );
    Data( CBldMix , -1);
    Print( CBldTCA , 0 );
    Data( CBldTCA , -1);
    Print( CFat , 0 );
    Data( CFat , -1);
    Print( CGut , 0 );
    Data( CGut , -1);
    Print( CInhPPM , 0 );
    Data( CInhPPM , -1);
    Print( CKid , 0 );
    Data( CKid , -1);
    Print( CLiv , 0 );
    Data( CLiv , -1);
    Print( CLivTCA , 0 );
    Data( CLivTCA , -1);
    Print( CMixExh , 0 );
    Data( CMixExh , -1);
    Print( CMus , 0 );
    Data( CMus , -1);
    Print( CPlasTCA , 0 );
    Data( CPlasTCA , -1);
    Print( CTCOG , 0 );
    Data( CTCOG , -1);
    Print( CTCOH , 0 );
    Data( CTCOH , -1);
    Print( CVen , 0 );
    Data( CVen , -1);
    Print( TotCTCOH , 0 );
    Data( TotCTCOH , -1);
    Print( zABileTCOG , 0 );
    Data( zABileTCOG , -1);
    Print( zAExhpost , 24, 48 );
    Data( zAExhpost , 0.019, 0.019 );
    Print( zAUrnNDCVC , 0 );
    Data( zAUrnNDCVC , -1);
    Print( zAUrnTCA , 0 );
    Data( zAUrnTCA , -1);
} # End Prout85 TCeratAPaMorloil010

  Experiment { # Begin Prout85 TCeratAPaMorloil1e3
    Species = 2 ;
    Male = 1 ;

# Measured Covariates (if any)
    BWmeas = 0.19 ;

```

```

# Exposure/Dosing
  PDose = NDoses( 2 , 1000 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 24, 48, 72 );
  Data( AUrnTCTotMole , 0.247260274, 0.264611872, 0.270395738 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 24, 48 );
  Data( zAExhpost , 98.99, 98.99 );
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 0 );
  Data( zAUrnTCA , -1);
} # End Prout85 TCeratAPaMorloil1e3

Experiment { # Begin Prout85 TCeratAPaMorloil500
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.19 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 500 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 24, 48, 72 );
  Data( AUrnTCTotMole , 0.180022831, 0.18869863, 0.191590563 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);

```

```

Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 24, 48 );
Data( zAExhpost , 47.405, 47.405 );
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Prout85 TCeratAPaMorloil500
#### END Prout85
##### END GROUP 14
}

##### BEGIN GROUP 15
Level {
#### BEGIN Prout85
Experiment { # Begin Prout85 TCeratOMaMorloil010
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.19 ;

# Exposure/Dosing
PDose = NDoses( 2 , 10 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 24, 72 );
Data( AUrnTCTotMole , 0.009586758, 0.010035008 );
Print( CART , 0 );
Data( CART , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );

```

```

Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 24, 72 );
Data( zAExhpost , 0.0247, 0.0247 );
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Prout85 TCeratOMaMorloil010

Experiment { # Begin Prout85 TCeratOMaMorloil1e3
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.19 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 1000 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 24, 72 );
  Data( AUrnTCTotMole , 0.42222222, 0.449695586 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);

```

```

Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 24, 72 );
Data( zAExhpost , 106.78, 106.78 );
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Prout85 TCeratOMaMorloille3

Experiment { # Begin Prout85 TCeratOMaMorloille3
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.19 ;

# Exposure/Dosing
  PDose = NDoses( 2 , 2000 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 24, 72 );
  Data( AUrnTCTotMole , 0.38173516, 0.404870624 );
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 24, 72 );
  Data( zAExhpost , 295.64, 295.64 );
  Print( zAUrnNDCVC , 0 );

```

```

        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Prout85 TCeratOMaMorloil2e3

    Experiment { # Begin Prout85 TCeratOMaMorloil500
        Species = 2 ;
        Male = 1 ;

    # Measured Covariates (if any)
        BWmeas = 0.19 ;

    # Exposure/Dosing
        PDose = NDoses( 2 , 500 0 , 0 0.05 );
        TChng = 0.05 ;

    # Data
        Print( AUrnTCOGTCOH , 0 );
        Data( AUrnTCOGTCOH , -1);
        Print( AUrnTCTotMole , 24, 72 );
        Data( AUrnTCTotMole , 0.297869102, 0.3152207 );
        Print( CArt , 0 );
        Data( CArt , -1);
        Print( CBldMix , 0 );
        Data( CBldMix , -1);
        Print( CBldTCA , 0 );
        Data( CBldTCA , -1);
        Print( CFat , 0 );
        Data( CFat , -1);
        Print( CGut , 0 );
        Data( CGut , -1);
        Print( CInhPPM , 0 );
        Data( CInhPPM , -1);
        Print( CKid , 0 );
        Data( CKid , -1);
        Print( CLiv , 0 );
        Data( CLiv , -1);
        Print( CLivTCA , 0 );
        Data( CLivTCA , -1);
        Print( CMixExh , 0 );
        Data( CMixExh , -1);
        Print( CMus , 0 );
        Data( CMus , -1);
        Print( CPlasTCA , 0 );
        Data( CPlasTCA , -1);
        Print( CTCOG , 0 );
        Data( CTCOG , -1);
        Print( CTCOH , 0 );
        Data( CTCOH , -1);
        Print( CVen , 0 );
        Data( CVen , -1);
        Print( TotCTCOH , 0 );
        Data( TotCTCOH , -1);
        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 24, 72 );
        Data( zAExhpost , 40.565, 40.565 );
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Prout85 TCeratOMaMorloil500
    ##### END Prout85
    ##### END GROUP 15
}

```



```

##### BEGIN GROUP 16
Level {
#### BEGIN Simmons02
# for fixed inhalation, different simulations run since individual rat characteristics available
Experiment { # Begin Simmons02 TCERatLEaMinh0012e3
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.42014 ;
VFatCmeas = 0.0917 ;

# Exposure/Dosing
Conc = NDoses( 2 , 2000 0 , 0 1 );

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0.083, 0.333, 1, 2 );
Data( CFat , 13.5, 8.45, 256.6666667, 245 );
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0.083, 0.333, 1, 2 );
Data( CLiv , 24, 42, 79, 8.4 );
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0.083, 0.333, 1, 2 );
Data( CVen , 9.35, 12.15, 40.75, 4.75 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Simmons02 TCERatLEaMinh0012e3

Experiment { # Begin Simmons02 TCERatLEaMinh0014e3
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.40651 ;
VFatCmeas = 0.0875 ;

```

```

# Exposure/Dosing
  Conc = NDoses( 2 , 4000 0 , 0 1 );

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0.083, 0.333, 1, 2 );
  Data( CFat , 20.4, 200, 595.875, 670 );
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0.083, 0.333, 1, 2 );
  Data( CLiv , 69, 140, 189.025, 55 );
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0.083, 0.333, 1, 2 );
  Data( CVen , 31.5, 70.75, 57.05, 31.75 );
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 0 );
  Data( zAUrnTCA , -1);
} # End Simmons02 TCeratLEaMinh0014e3

Experiment { # Begin Simmons02 TCeratLEaMinh001200
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.3978625 ;
  VFatCmeas = 0.08125 ;

# Exposure/Dosing
  Conc = NDoses( 2 , 200 0 , 0 1 );

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );

```

```

Data( CBldTCA , -1);
Print( CFat , 0.083, 0.333, 1, 2 );
Data( CFat , 1.6, 4.875, 23, 11.1 );
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0.083, 0.333, 1, 2 );
Data( CLiv , 0.875, 1.275, 1.5, 0.015 );
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0.083, 0.333, 1, 2 );
Data( CVen , 0.79, 1.29, 1.2, 0.14 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Simmons02 TCeratLEaMinh001200

Experiment { # Begin Simmons02 TCeratLE3Minhc10100
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.408907143 ;

# Exposure/Dosing
  CC = 108 ;
  NRodents = 1 ;
  VChC = 10.4 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0.00598, 0.161, 0.316, 0.489, 0.661, 0.816, 0.989, 1.16, 1.32, 1.49,
    1.64, 1.82, 1.97, 2.14, 2.32, 2.47, 2.66, 2.82, 2.99, 3.14, 3.32, 3.49, 3.66,
    3.82, 3.99, 4.16, 4.31 );
  Data( CInhPPM , 108, 94.8, 85.1, 76.4, 70.1, 64.3, 59, 54.1, 50.7, 47.5, 44.5, 40.9,
    38.3, 35.9, 33.6, 31.5, 29.5, 27.1, 25.4, 23.3, 22.3, 20.9, 20, 18.4, 17.6,
    16.8, 16.1 );

```

```

Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Simmons02 TCeratLE3Minhc10100

Experiment { # Begin Simmons02 TCeratLE3Minhc101e3
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.408907143 ;

# Exposure/Dosing
  CC = 864 ;
  NRodents = 1 ;
  VChC = 10.4 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0.00598, 0.167, 0.323, 0.495, 0.667, 0.823, 0.995, 1.17, 1.32, 1.49,
    1.65, 1.8, 1.98, 2.15, 2.3, 2.49, 2.65, 2.8, 2.98, 3.15, 3.3, 3.48, 3.66,
    3.82, 3.97, 4.15, 4.32, 4.49, 4.66, 4.82, 4.99, 5.16, 5.34, 5.51, 5.66, 5.84);
  Data( CInhPPM , 864, 793, 697, 639, 599, 549, 504, 483, 462, 433, 415, 397, 372, 364,
    341, 320, 313, 293, 281, 275, 263, 252, 241, 231, 216, 207, 198, 190, 182, 170,
    163, 153, 143, 137, 129, 123 );
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );

```

```

Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Simmons02 TCERatLE3Minhc101e3

Experiment { # Begin Simmons02 TCERatLE3Minhc103e3
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.408907143 ;

# Exposure/Dosing
  CC = 2940 ;
  NRodents = 1 ;
  VChC = 10.4 ;
  lnLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0.00598, 0.161, 0.316, 0.489, 0.661, 0.816, 0.989, 1.16, 1.32, 1.49,
    1.66, 1.82, 1.97, 2.16, 2.33, 2.49, 2.66, 2.81, 2.99, 3.14, 3.31, 3.49, 3.64,
    3.81, 3.97, 4.16, 4.31, 4.48, 4.66, 4.81, 4.98, 5.15, 5.33, 5.5, 5.67, 5.83 );
  Data( CInhPPM , 2940, 2810, 2520, 2320, 2170, 1950, 1870, 1790, 1710, 1600, 1570,
    1470, 1440, 1350, 1350, 1290, 1260, 1230, 1180, 1160, 1130, 1110, 1080, 1060,
    1040, 1010, 1010, 991, 949, 948, 927, 907, 907, 887, 887, 867 );
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);

```

```

Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Simmons02 TCERatLE3Minhc103e3

Experiment { # Begin Simmons02 TCERatLE3Minhc10500
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.408907143 ;

# Exposure/Dosing
  CC = 506 ;
  NROdents = 1 ;
  VChC = 10.4 ;
  lnkLossC = -3.912 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0.00598, 0.17, 0.325, 0.481, 0.653, 0.825, 0.998, 1.15, 1.31, 1.48,
    1.65, 1.81, 1.98, 2.15, 2.33, 2.48, 2.65, 2.81, 3, 3.14, 3.31, 3.48, 3.65,
    3.82, 4, 4.17, 4.32, 4.5, 4.67, 4.82, 5, 5.17, 5.32, 5.5, 5.67, 5.82 );
  Data( CInhPPM , 506, 454, 408, 366, 343, 315, 282, 265, 243, 228, 209, 191, 176, 165,
    154, 142, 135, 127, 116, 109, 102, 95.9, 89.9, 84.2, 77.2, 74, 67.8, 63.6,
    58.3, 52.4, 48, 45, 43.1, 41.3, 37.9, 35.5 );
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );

```

```

        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);
        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
    } # End Simmons02 TCeratLE3Minhc10500
#### END Simmons02
##### END GROUP 16
}

##### BEGIN GROUP 17
    Level {
#### BEGIN Stenner97
# intraduodenal modeled as oral
    Experiment { # Begin Stenner97 TCeratFRaM_id_ns100
        Species = 2 ;
        Male = 1 ;

# Measured Covariates (if any)
        BWmeas = 0.3 ;

# Exposure/Dosing
        PDose = NDoses( 2 , 100 0 , 0 0.05 );
        TChng = 0.05 ;

# Data
        Print( AUrnTCOGTCOH , 0 );
        Data( AUrnTCOGTCOH , -1);
        Print( AUrnTCTotMole , 0 );
        Data( AUrnTCTotMole , -1);
        Print( CArt , 0 );
        Data( CArt , -1);
        Print( CBldMix , 0 );
        Data( CBldMix , -1);
        Print( CBldTCA , 0.251, 0.439, 0.966, 1.43, 2.42, 3.41, 4.47, 5.41, 8.4, 16.8 );
        Data( CBldTCA , 0.727, 1.64, 2.11, 2.46, 3.34, 3.97, 4.07, 4.07, 4.61, 3.77 );
        Print( CFat , 0 );
        Data( CFat , -1);
        Print( CGut , 0 );
        Data( CGut , -1);
        Print( CInhPPM , 0 );
        Data( CInhPPM , -1);
        Print( CKid , 0 );
        Data( CKid , -1);
        Print( CLiv , 0 );
        Data( CLiv , -1);
        Print( CLivTCA , 0 );
        Data( CLivTCA , -1);
        Print( CMixExh , 0 );
        Data( CMixExh , -1);
        Print( CMus , 0 );
        Data( CMus , -1);
        Print( CPlasTCA , 0 );
        Data( CPlasTCA , -1);
        Print( CTCOG , 0.251, 0.439, 0.966, 1.43, 2.42, 3.41, 4.47, 6.66 );
        Data( CTCOG , 0.412, 0.727, 0.791, 0.886, 0.668, 0.166, 0.105, 0.0462 );
        Print( CTCOH , 0.251, 0.439, 0.966, 1.43, 2.42, 3.41, 4.47, 5.41, 8.4 );
        Data( CTCOH , 2.02, 2.77, 2.93, 3.12, 2.4, 2.43, 2.28, 1.96, 0.364 );
        Print( CVen , 0 );
        Data( CVen , -1);
        Print( TotCTCOH , 0 );
        Data( TotCTCOH , -1);
        Print( zABileTCOG , 0 );
        Data( zABileTCOG , -1);
        Print( zAExhpost , 0 );
        Data( zAExhpost , -1);
        Print( zAUrnNDCVC , 0 );
        Data( zAUrnNDCVC , -1);

```

```

        Print( zAUrnTCA , 0 );
        Data( zAUrnTCA , -1);
} # End Stenner97 TCeratFRaM_id_ns100

Experiment { # Begin Stenner97 TCHratFRaM_iv_aq100
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.3 ;

# Exposure/Dosing
  IVDoseTCOH = NDoses( 2 , 100 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 48 );
  Data( AUrnTCOGTCOH , 7.9 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0.534, 0.979, 2.05, 3.03, 4.99, 8.01, 11, 16, 24 );
  Data( CBldTCA , 2.04, 3.7, 5.21, 5.5, 6.47, 7.1, 5.4, 4.57, 2.63 );
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0.979, 2.05, 3.03, 4.99, 8.01, 11 );
  Data( TotCTCOH , 72.8, 41.3, 27.5, 14.3, 6.89, 1.97 );
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 48 );
  Data( zAUrnTCA , 0.46 );
} # End Stenner97 TCHratFRaM_iv_aq100

# Bile Cannulated
Experiment { # Begin Stenner97 TCHratFRaM_ivacn005
  lnKEHRC = -100.;
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.3 ;

```



```

# Exposure/Dosing
  IVDoseTCOH = NDoses( 2 , 50 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 48 );
  Data( AUrnTCOGTCOH , 0.5 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0 );
  Data( CBldTCA , -1);
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0 );
  Data( CLivTCA , -1);
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0 );
  Data( CPlasTCA , -1);
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAUrnNDCVC , 0 );
  Data( zAUrnNDCVC , -1);
  Print( zAUrnTCA , 48 );
  Data( zAUrnTCA , 0.01 );
} # End Stenner97 TCHratFRaM_ivacn005

# Bile Cannulated
  Experiment { # Begin Stenner97 TCHratFRaM_ivacn020
    lnKEHRC = -100.;
    Species = 2 ;
    Male = 1 ;

# Measured Covariates (if any)
    BWmeas = 0.3 ;

# Exposure/Dosing
    IVDoseTCOH = NDoses( 2 , 200 , 0 0.05 );
    TChng = 0.05 ;

# Data
    Print( AUrnTCOGTCOH , 48 );
    Data( AUrnTCOGTCOH , 3.1 );
    Print( AUrnTCTotMole , 0 );
    Data( AUrnTCTotMole , -1);
    Print( CArt , 0 );
    Data( CArt , -1);

```

```

Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0 );
Data( CBldTCA , -1);
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 48 );
Data( zAUrnTCA , 0.03 );
} # End Stenner97 TCHratFRaM_ivacn020

# Bile Cannulated
Experiment { # Begin Stenner97 TCHratFRaM_ivacn100
  lnKEHRC = -100.;
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.3 ;

# Exposure/Dosing
  IVDoseTCOH = NDoses( 2 , 100 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 48 );
  Data( AUrnTCOGTCOH , 8.1 );
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( Cart , 0 );
  Data( Cart , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0.534, 1.07, 2.05, 3.03, 4.99, 8.01, 11, 16, 24 );
  Data( CBldTCA , 0.389, 0.973, 1.65, 2.38, 1.99, 1.8, 1.17, 0.827, 0.584 );
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );

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```

Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 1.07, 2.05, 3.03, 4.99 );
Data( TotCTCOH , 45.7, 9.84, 2.95, 0.984 );
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 48 );
Data( zAUrnTCA , 0.09 );
} # End Stenner97 TCHratFRaM_ivacn100
#### END Stenner97
##### END GROUP 17
}

##### BEGIN GROUP 18
Level {
#### BEGIN Templin95
Experiment { # Begin Templin95 TCERatFRaMorl_aq100
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.275 ;

# Exposure/Dosing
PDose = NDoses( 2 , 100 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0.25, 0.5, 0.75, 1, 1.5, 2, 2.5, 3, 4, 5, 6, 9, 12, 24, 48 );
Data( CBldTCA , 0.94772, 1.42158, 1.91178, 1.61766, 2.23858, 4.2484, 3.80722, 4.9837,
6.06214, 6.74842, 6.92816, 7.64712, 7.30398, 4.28108, 1.43792 );
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0 );
Data( CLivTCA , -1);
Print( CMixExh , 0 );

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```

Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0 );
Data( CPlasTCA , -1);
Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0.25, 0.5, 0.75, 1, 1.5, 2, 2.5, 3, 4, 5, 6, 9 );
Data( CTCOH , 0.91195, 1.56975, 1.9435, 2.0033, 2.04815, 2.70595, 3.39365, 2.67605,
      2.4817, 2.2126, 2.04815, 0.9867 );
Print( CVen , 0.25, 0.5, 0.75, 1, 1.5, 2, 2.5 );
Data( CVen , 5.67648, 9.21114, 10.52514, 6.79338, 2.32578, 1.55052, 0.94608 );
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 0 );
Data( zAUrnTCA , -1);
} # End Templin95 TCeratFRaMorl_aq100
#### END Templin95
##### END GROUP 18
}

##### BEGIN GROUP 19
Level {
#### BEGIN Yu00
Experiment { # Begin Yu00 TCAratFRaM_iv_aq001
Species = 2 ;
Male = 1 ;

# Measured Covariates (if any)
BWmeas = 0.215 ;

# Exposure/Dosing
IVDoseTCA = NDoses( 2 , 1 0 , 0 0.05 );
TChng = 0.05 ;

# Data
Print( AUrnTCOGTCOH , 0 );
Data( AUrnTCOGTCOH , -1);
Print( AUrnTCTotMole , 0 );
Data( AUrnTCTotMole , -1);
Print( CArt , 0 );
Data( CArt , -1);
Print( CBldMix , 0 );
Data( CBldMix , -1);
Print( CBldTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
Data( CBldTCA , 3.42323, 2.5835991, 2.2724038, 2.0143135, 1.6624316, 1.2100587,
      0.3230418 );
Print( CFat , 0 );
Data( CFat , -1);
Print( CGut , 0 );
Data( CGut , -1);
Print( CInhPPM , 0 );
Data( CInhPPM , -1);
Print( CKid , 0 );
Data( CKid , -1);
Print( CLiv , 0 );
Data( CLiv , -1);
Print( CLivTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
Data( CLivTCA , 1.86276, 1.034322, 0.9804, 1.245108, 1.367658, 1.099682, 0.545756 );
Print( CMixExh , 0 );
Data( CMixExh , -1);
Print( CMus , 0 );
Data( CMus , -1);
Print( CPlasTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
Data( CPlasTCA , 4.67324, 3.4314, 2.97388, 2.82682, 2.27126, 1.66668, 0.450984 );

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Print( CTCOG , 0 );
Data( CTCOG , -1);
Print( CTCOH , 0 );
Data( CTCOH , -1);
Print( CVen , 0 );
Data( CVen , -1);
Print( TotCTCOH , 0 );
Data( TotCTCOH , -1);
Print( zABileTCOG , 0 );
Data( zABileTCOG , -1);
Print( zAExhpost , 0 );
Data( zAExhpost , -1);
Print( zAUrnNDCVC , 0 );
Data( zAUrnNDCVC , -1);
Print( zAUrnTCA , 6, 9, 24 );
Data( zAUrnTCA , 0.066218422, 0.075218984, 0.101792073 );
} # End Yu00 TCARatFRaM_iv_aq001

Experiment { # Begin Yu00 TCARatFRaM_iv_aq010
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.215 ;

# Exposure/Dosing
  IVDoseTCA = NDoses( 2 , 10 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AUrnTCOGTCOH , 0 );
  Data( AUrnTCOGTCOH , -1);
  Print( AUrnTCTotMole , 0 );
  Data( AUrnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
  Data( CBldTCA , 35.35159, 29.26494, 25.210986, 21.347393, 13.804849, 10.840773,
    3.0365439 );
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
  Data( CLivTCA , 18.3008, 14.6243, 14.10142, 15.78444, 11.7648, 9.10138, 5.89874 );
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
  Data( CPlasTCA , 46.8958, 38.2356, 34.314, 29.5754, 17.974, 13.33344, 4.31376 );
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);

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        Print( zAurnNDCVC , 0 );
        Data( zAurnNDCVC , -1);
        Print( zAurnTCA , 6, 9, 24 );
        Data( zAurnTCA , 0.762904796, 0.919343139, 1.43580397 );
} # End Yu00 TCAtFRAm_iv_aq010

Experiment { # Begin Yu00 TCAtFRAm_iv_aq050
  Species = 2 ;
  Male = 1 ;

# Measured Covariates (if any)
  BWmeas = 0.215 ;

# Exposure/Dosing
  IVDoseTCA = NDoses( 2 , 50 0 , 0 0.05 );
  TChng = 0.05 ;

# Data
  Print( AurnTCOGTCOH , 0 );
  Data( AurnTCOGTCOH , -1);
  Print( AurnTCTotMole , 0 );
  Data( AurnTCTotMole , -1);
  Print( CArt , 0 );
  Data( CArt , -1);
  Print( CBldMix , 0 );
  Data( CBldMix , -1);
  Print( CBldTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
  Data( CBldTCA , 143.30997, 103.89789, 104.38809, 70.13945, 42.68825, 35.05747,
      8.812162 );
  Print( CFat , 0 );
  Data( CFat , -1);
  Print( CGut , 0 );
  Data( CGut , -1);
  Print( CInhPPM , 0 );
  Data( CInhPPM , -1);
  Print( CKid , 0 );
  Data( CKid , -1);
  Print( CLiv , 0 );
  Data( CLiv , -1);
  Print( CLivTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
  Data( CLivTCA , 78.9222, 69.2816, 68.1378, 57.6802, 44.4448, 45.4252, 20.2616 );
  Print( CMixExh , 0 );
  Data( CMixExh , -1);
  Print( CMus , 0 );
  Data( CMus , -1);
  Print( CPlasTCA , 0.083, 0.5, 1, 3, 6, 9, 24 );
  Data( CPlasTCA , 176.472, 130.8834, 128.4324, 90.3602, 57.0266, 48.3664, 12.8269 );
  Print( CTCOG , 0 );
  Data( CTCOG , -1);
  Print( CTCOH , 0 );
  Data( CTCOH , -1);
  Print( CVen , 0 );
  Data( CVen , -1);
  Print( TotCTCOH , 0 );
  Data( TotCTCOH , -1);
  Print( zABileTCOG , 0 );
  Data( zABileTCOG , -1);
  Print( zAExhpost , 0 );
  Data( zAExhpost , -1);
  Print( zAurnNDCVC , 0 );
  Data( zAurnNDCVC , -1);
  Print( zAurnTCA , 6, 9, 24 );
  Data( zAurnTCA , 6.407051256, 6.278050224, 9.08382267 );
} # End Yu00 TCAtFRAm_iv_aq050

#### END Yu00

##### END GROUP 19
}
}
}
End.

```

TCE.1.2.3.3.Rat.seqpriors.test4.pop.mean.x.10.out

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iter  M_lnQCC.1.    M_lnVPRC.1.    M_QFatC.1.    M_QGutC.1.    M_QLivC.1.    M_QSlwC.1.
      M_lnDRespC.1. M_QKidC.1.    M_FracPlasC.1. M_VFatC.1.    M_VGutC.1.    M_VLivC.1.
      M_VRapC.1.    M_VResplumC.1. M_VRespEffC.1. M_VKidC.1.    M_VBldC.1.    M_lnPBC.1.
      M_lnPFatC.1. M_lnPGutC.1.    M_lnPLivC.1.    M_lnPRapC.1.    M_lnPRespC.1. M_lnPKidC.1.
      M_lnPSlwC.1. M_lnPRBCPlasTCAC.1. M_lnPBodTCAC.1. M_lnPLivTCAC.1.
      M_lnDissocC.1. M_lnBMaxkDC.1. M_lnPBodTCOHC.1. M_lnPLivTCOHC.1.
      M_lnPBodTCOGC.1. M_lnPLivTCOGC.1. M_lnkTSD.1. M_lnkAS.1. M_lnkTD.1.
      M_lnkAD.1.    M_lnkASTCA.1. M_lnkASTCOH.1. M_lnVMaxC.1. M_lnkMCM.1.
      M_lnFracOtherC.1. M_lnFracTCAC.1. M_lnVMaxDCVGC.1. M_lnCldCVGC.1.
      M_lnVMaxKidDCVGC.1. M_lnCldKidDCVGC.1. M_lnVMaxLungLivC.1. M_lnkMCLara.1.
      M_lnFracLungSysC.1. M_lnVMaxTCOHC.1. M_lnkMTCOH.1. M_lnVMaxGlucC.1.
      M_lnkMGluc.1. M_lnkMetTCOHC.1. M_lnkUrnTCAC.1. M_lnkMetTCAC.1.
      M_lnkBileC.1. M_lnkEHRC.1. M_lnkUrnTCOGC.1. M_lnkNATC.1. M_lnkKidBioactC.1.
      V_lnQCC.1.    V_lnVPRC.1.    V_QFatC.1.    V_QGutC.1.    V_QLivC.1.    V_QSlwC.1.
      V_lnDRespC.1. V_QKidC.1.    V_FracPlasC.1. V_VFatC.1.    V_VGutC.1.    V_VLivC.1.
      V_VRapC.1.    V_VResplumC.1. V_VRespEffC.1. V_VKidC.1.    V_VBldC.1.    V_lnPBC.1.
      V_lnPFatC.1. V_lnPGutC.1.    V_lnPLivC.1.    V_lnPRapC.1.    V_lnPRespC.1. V_lnPKidC.1.
      V_lnPSlwC.1. V_lnPRBCPlasTCAC.1. V_lnPBodTCAC.1. V_lnPLivTCAC.1.
      V_lnDissocC.1. V_lnBMaxkDC.1. V_lnPBodTCOHC.1. V_lnPLivTCOHC.1.
      V_lnPBodTCOGC.1. V_lnPLivTCOGC.1. V_lnkTSD.1. V_lnkAS.1. V_lnkTD.1.
      V_lnkAD.1.    V_lnkASTCA.1. V_lnkASTCOH.1. V_lnVMaxC.1. V_lnkMCM.1.
      V_lnFracOtherC.1. V_lnFracTCAC.1. V_lnVMaxDCVGC.1. V_lnCldCVGC.1.
      V_lnVMaxKidDCVGC.1. V_lnCldKidDCVGC.1. V_lnVMaxLungLivC.1. V_lnkMCLara.1.
      V_lnFracLungSysC.1. V_lnVMaxTCOHC.1. V_lnkMTCOH.1. V_lnVMaxGlucC.1.
      V_lnkMGluc.1. V_lnkMetTCOHC.1. V_lnkUrnTCAC.1. V_lnkMetTCAC.1.
      V_lnkBileC.1. V_lnkEHRC.1. V_lnkUrnTCOGC.1. V_lnkNATC.1. V_lnkKidBioactC.1.
      Ve_CInhPPM.1.1. Ve_CMixExh.1.1. Ve_CART.1.1. Ve_CVen.1.1.
      Ve_CBldMix.1.1. Ve_CFat.1.1. Ve_CGut.1.1. Ve_CKid.1.1. Ve_CLiv.1.1.
      Ve_CMus.1.1. Ve_zAExhpost.1.1. Ve_CTCOH.1.1. Ve_CPlasTCA.1.1.
      Ve_CBldTCA.1.1. Ve_CLivTCA.1.1. Ve_zAurnTCA.1.1. Ve_zABileTCOG.1.1.
      Ve_CTCOG.1.1. Ve_AurnTCOGTCOH.1.1. Ve_zAurnNDCVC.1.1. Ve_AurnTCTotMole.1.1.
      Ve_TotCTCOH.1.1. lnQCC.1.1. lnVPRC.1.1. QFatC.1.1. QGutC.1.1.
      QLivC.1.1. QSlwC.1.1. lnDRespC.1.1. QKidC.1.1. FracPlasC.1.1. VFatC.1.1.
      VGutC.1.1. VLivC.1.1. VRapC.1.1. VResplumC.1.1. VRespEffC.1.1. VKidC.1.1.
      VBldC.1.1. lnPBC.1.1. lnPFatC.1.1. lnPGutC.1.1. lnPLivC.1.1. lnPRapC.1.1.
      lnPRespC.1.1. lnPKidC.1.1. lnPSlwC.1.1. lnPRBCPlasTCAC.1.1. lnPBodTCAC.1.1.
      lnPLivTCAC.1.1. lnkDissocC.1.1. lnBMaxkDC.1.1. lnPBodTCOHC.1.1.
      lnPLivTCOHC.1.1. lnPBodTCOGC.1.1. lnPLivTCOGC.1.1. lnkTSD.1.1.
      lnkAS.1.1. lnkTD.1.1. lnkAD.1.1. lnkASTCA.1.1. lnkASTCOH.1.1. lnVMaxC.1.1.
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 lnkEHRC.1.10. lnkUrnTCOGC.1.10. lnkNATC.1.10. lnkKidBioactC.1.10.
 Ve_CInhPPM.1.11. Ve_CMixExh.1.11. Ve_CArt.1.11. Ve_CVen.1.11.
 Ve_CBldMix.1.11. Ve_CFat.1.11. Ve_CGut.1.11. Ve_CKid.1.11. Ve_CLiv.1.11.
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Ve_TotCTCOH.1.11. lnQCC.1.11. lnVPRC.1.11. QFatC.1.11. QGutC.1.11.
 QLivC.1.11. QSlwC.1.11. lnDRespC.1.11. QKidC.1.11. FracPlasC.1.11.
 VFatC.1.11. VGutC.1.11. VlivC.1.11. VRapC.1.11. VRespLumC.1.11.
 VRespEffC.1.11. VKidC.1.11. VBldC.1.11. lnPBC.1.11. lnPFatC.1.11.
 lnPGutC.1.11. lnPlivC.1.11. lnPRapC.1.11. lnPRespC.1.11. lnPKidC.1.11. lnPSlwC.1.11.
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	-0.6728	1.197	1.089	1.02	0.9464	0.9434	1.001	1.045	0.9762	0.993	1	0.9961
	1.004	0.9942	0.9939	1.004	-0.128	0.09219	-0.1155	0.0393	0.1122	-0.04497		-
0.05696	0.2944	-0.08391		-0.04035		0.2897	0.1489	-0.05148		-0.1265	-0.1628	0.2039
	2.244	1.066	0.8737	-2.303	-1.65	0.3499	-0.3619	-0.1123	-2.992	-1.158	-1.716	2.483
	-0.9788	-1.537	5.197	0.8322	-3.775	0.6813	1.161	3.104	2.728	1.73	0.3424	-2.614
	-1.105	2.228	0.4481	2.92	-6.154	-4.971	0.7208	0.7065	0.7258	0.7216	0.7241	0.7026
	0.714	0.7192	0.7161	0.6993	0.7013	0.7125	0.02246	0.02231	0.719	0.7188	0.7129	0.7162
	0.7211	0.7138	0.7089	0.7181	0.1791	-0.4025	1.217	1.095	1.022	0.9341	0.9297	1.003
	1.044	0.8913	0.993	0.9749	0.9948	1.004	0.9946	0.9962	1.004	-0.07864		0.05264
	-0.1332	0.03756	0.07816	-0.03979		-0.05732		0.2297	-0.07442		0.1153	0.235
	0.07315	-0.05103		-0.09814		-0.04422		0.2085	2.167	1.056	0.8883	-2.297
	-1.65	0.3354	-0.3792	-0.2945	-2.779	-1.301	-1.484	2.485	-0.9819	-1.538	5.2	0.8736
	-3.771	0.6785	0.8404	3.092	3.128	1.737	0.6063	-2.677	-1.158	2.041	0.4211	3.016
	-6.156	-4.964	0.7125	0.7047	0.1979	0.7249	0.7299	0.702	0.7142	0.7027	0.7032	0.718
	0.02025	0.2592	0.714	0.2278	0.7154	0.7408	0.8221	0.7123	0.4842	0.7173	0.3833	0.7141
	0.338	-0.2794	1.423	1.109	1.022	0.9122	0.9228	1.002	1.048	1.093	0.9909	0.9396
	0.994	1.003	0.9944	0.9939	1.001	-0.2202	0.1652	-0.1529	0.03181	0.08067	-0.04767	
	-0.05623		0.2768	-0.03451		0.2741	0.1295	0.05878	-0.0987	0.02328	-0.02936	
	0.227	1.95	2.391	-1.228	-2.3	-2.197	0.6178	-0.3664	-0.1988	-3.103	-1.684	-1.254
	2.476	-0.9818	-1.54	5.196	0.7363	-3.738	0.6795	0.8718	2.966	4.023	1.311	0.6471
	-2.631	-1.231	1.567	0.1926	3.137	-6.153	-4.973	0.7118	0.7203	0.7116	0.2778	0.7023
	0.7329	0.7137	0.708	0.7052	0.7172	0.7233	0.7126	0.7154	0.7185	0.7127	0.7138	0.7054
	0.7108	0.7232	0.7065	0.01301	0.7205	0.1156	-0.5876	1.341	1.073	1.018	0.9401	0.9365
	1.002	1.029	0.9574	0.9916	0.9648	0.9975	1.004	0.994	0.9967	1.002	-0.05765	
	0.07328	-0.1284	0.04057	0.1484	-0.04043		-0.05507		0.416	-0.04814		0.02076
	0.1044	-0.02347		-0.04477		0.09384	-0.3144	0.3198	2.184	-0.7061	-0.7796	-2.308
	-2.387	0.3474	-0.3646	-0.1247	-3.664	-2.889	-1.397	2.481	-0.9893	-1.525	5.223	0.7185
	-3.705	0.6274	0.6672	3.106	4.164	1.584	0.03244	-2.446	-1.224	1.946	0.3118	2.85
	-6.152	-4.972	0.7003	0.7049	0.7138	0.1863	0.7087	0.6962	0.716	0.7196	0.7114	0.7116
	0.7019	0.7023	0.7306	0.705	0.716	0.04434	0.7161	0.7121	0.01307	0.7176	0.7125	0.7172
	-0.06705		-0.9964	1.376	1.137	1.029	0.9334	0.9714	1.001	1.082	1.051	0.994
	1.032	0.9968	1.002	0.9921	0.9952	1.003	-0.05771		0.1342	-0.1173	0.03934	0.1058
	-0.04229		-0.05231		0.3019	0.00948	0.6295	0.2974	-0.02417		-0.01847	
	-0.2396	0.2273	0.1833	2.342	1.079	0.8924	-2.292	-1.649	0.3751	-0.361	-0.1098	-3.335
	-0.3912	-1.835	2.48	-0.9877	-1.538	5.199	1.073	-3.712	0.7261	0.427	3.403	2.005
	1.578	1.051	-3.208	-1.139	2.561	0.5122	2.863	-6.157	-4.969	0.7105	0.7237	0.6962
	0.2119	0.7055	0.3903	0.3944	0.1531	0.3505	0.2627	0.721	0.7124	0.7028	0.7098	0.7161
	0.7068	0.702	0.717	0.7181	0.7288	0.7247	0.7079	0.4882	-0.324	0.7644	1.252	1.052
	0.6715	0.931	1.012	1.037	1.233	0.9588	0.9116	0.9782	1.003	0.9941	0.9874	0.9786
	-0.4479	0.3992	-0.4268	0.1047	0.03982	-0.05015		-0.2352	0.5769	-0.03645		0.1023
	0.2306	-0.02253		-0.04779		-0.04638		-0.02991		0.2155	2.146	2.666
	5.366	-2.292	-0.9199	0.3564	-0.3786	-0.2442	-2.726	-1.154	-1.367	2.485	-0.9823	-1.53
	5.226	1.577	-3.926	0.6827	0.6999	3.115	3.308	1.717	0.6396	-2.597	-1.126	1.981
	0.3704	3.005	-6.149	-4.971	0.7124	0.7185	0.7148	2.204	0.7046	0.7171	0.6976	0.7195
	0.7109	0.7138	0.0136	0.09655	0.7108	0.7125	0.7122	0.04006	0.7079	0.7183	0.02406	0.7184
	0.7156	0.7072	0.4251	-0.235	1.322	1.169	1.034	0.9322	1.019	1.002	1.034	0.8143
	0.9953	1.012	0.9949	1.004	0.9942	0.9952	1.002	0.4386	-0.006005		-0.1134	0.04337
	0.08983	-0.04763		-0.0575	0.2799	-0.03975		0.04778	0.1945	-0.02322		-
0.04798	-0.26	0.3415	0.2154	2.092	1.06	0.8886	-2.294	-1.666	0.3602	-0.3539	0.007359	
	-3.916	0.5416	-1.272	2.482	-1.006	-1.541	5.194	2.01	-4.522	0.8252	0.8976	2.731
	3.289	2.479	1.701	-2.559	-1.133	1.913	0.3712	3.061	-6.155	-4.965	0.7251	0.7182
	0.7024	0.2524	0.7085	0.718	0.7066	0.7119	0.7065	0.7259	0.7136	0.1863	0.04239	0.141
	0.7064	0.7303	0.7099	0.7141	0.7171	0.7087	0.7145	0.7212	0.2739	-0.3249	1.298	1.097
	1.021	0.9372	0.9248	1.003	1.083	1.313	0.9912	0.9828	0.9953	1.004	0.9936	0.9952
	1.008	-0.1992	0.3549	-0.1484	0.03338	0.04729	-0.04476		-0.05654		0.1663	-2.18E-
03	-0.1359	0.437	-0.2816	-0.1544	0.02555	-0.005487		0.2038	2.031	1.607	1.696	-2.293
	-2.337	0.6068	-0.3551	-0.1322	-2.822	-1.364	-1.205	2.488	-0.981	-1.544	5.198	0.933
	-3.771	0.6946	0.9393	2.994	3.539	1.053	0.6927	-2.367	-0.9786	1.745	0.4854	3.124
	-6.155	-4.97	0.7215	0.7081	0.7172	0.7082	0.2029	0.7173	0.6934	0.7239	0.3786	0.7096
	0.7129	0.7125	0.7039	0.714	0.7059	0.7157	0.7028	0.705	0.7175	0.7049	0.7055	0.7183
	0.3081	-0.3831	1.154	1.071	1.017	0.9802	0.9299	0.9908	1.038	0.9805	1.004	1.061
	0.9995	1.004	0.9929	0.9978	1.002	-0.141	0.1064	-0.01684		0.05758	0.1261	-
0.04333	-0.03185		0.2144	-0.03559		0.1035	0.2333	-0.02017		-0.04459		-0.0507
	-0.02614		0.2084	2.136	1.079	0.8793	-2.314	-1.643	0.3482	-0.3677	-0.1407	-2.484
	-1.147	-1.364	2.483	-0.9845	-1.538	5.195	0.8942	-3.75	0.6806	0.7012	3.107	3.278
	1.73	0.6525	-2.601	-1.125	1.957	0.3643	3.013	-6.156	-4.971	0.7062	0.716	0.7139
	0.7169	0.7043	0.7237	0.7204	0.7082	0.7144	0.7172	0.7139	0.3712	0.7281	0.7166	0.7095
	0.695	0.7133	0.7073	0.7227	0.7206	0.7026	0.709	0.1049	-0.4071	1.128	1.088	1.021
	0.9353	0.9327	1.003	1.037	0.9805	0.9925	0.9931	0.9945	1.003	0.995	0.9939	1.002
	-0.1302	0.1068	-0.133	0.03533	0.06505	-0.04163		-0.05713		0.2134	-0.03365	
	0.1043	0.232	-0.0248	-0.04962		-0.5542	-0.2169	0.212	2.228	1.058	0.8927	-2.309

	-1.647	0.3663	-0.3795	-0.05106		-2.586	-1.146	-1.368	2.483	-0.9755	-1.539	5.194
	0.8874	-3.761	0.6831	0.6155	3.156	2.545	2.1	0.292	-2.603	-1.123	2.212	0.4225
	2.907	-6.151	-4.97	0.7026	0.7054	0.713	0.7242	0.7219	0.7184	0.7142	0.7185	0.6954
	0.702	0.03778	0.7108	0.698	0.7103	0.7008	0.6981	0.7381	0.7154	0.7143	0.7101	0.01547
	0.7184	0.05703	-0.5475	1.078	1.091	1.022	0.9331	0.9521	1.001	1.036	1.036	0.9929
	1.024	0.9956	1.004	0.9944	0.9938	1.001	-0.06654		0.1344	-0.1279	0.03749	0.068
	-0.04304		-0.05608		0.2133	-0.03776		0.09624	0.2331	-0.02791		-
0.04691	-0.04089		0.01058	0.2124	2.093	0.5874	0.1235	-2.304	-1.045	0.3663	-0.3727	0.5062
	-3.563	-1.184	-1.332	2.481	-0.9719	-1.541	5.205	1.133	-3.879	0.6738	0.7369	3.097
	3.614	1.752	0.8241	-2.6	-1.113	1.874	0.4073	3.064	-6.157	-4.97	0.7146	0.7193
	0.7227	0.7105	0.7256	0.7094	0.7083	0.7059	0.7118	0.7216	0.01757	0.7123	0.7297	0.7085
	0.7117	0.7147	0.7211	0.7083	0.7055	0.7063	0.03064	0.718	0.1005	-0.5392	1.156	1.096
	1.021	0.9354	0.9475	1.001	1.037	0.9683	0.993	1.003	0.995	1.002	0.9943	0.9951
	1.002	-0.07325		0.09493	-0.1324	0.03665	0.07068	-0.04199		-0.06017		0.2185
	-0.03767		0.07781	0.2309	-0.02285		-0.05284		-0.02832		-0.1035	0.2069
	2.055	1.334	-0.6951	-2.304	-1.213	0.3824	-0.371	0.2499	-3.526	-1.776	-1.35	2.485
	-0.9826	-1.543	5.195	1.073	-3.872	0.6946	0.709	3.102	3.982	1.584	0.5045	-2.582
	-1.128	1.778	0.4085	3.09	-6.15	-4.967	0.01033	0.7125	0.7193	0.4696	0.7072	0.9955
	0.7188	0.7195	0.3577	0.7119	0.7064	0.7192	0.7033	0.7032	0.7132	0.7116	0.7106	0.7144
	0.722	0.7119	0.7049	0.715	0.08684	-0.6036	0.9433	1.13	1.034	0.9363	0.8161	1.008
	1.041	0.4669	1.002	0.9862	0.9972	1.016	0.974	0.9794	1.002	-0.2708	0.1042	-
0.04803	0.0644	0.2395	-0.08795		-0.01744		0.5481	-0.04601		0.08357	0.2624	-0.0306
	-0.03706		-0.01595		-0.01489		0.2089	2.148	1.079	0.9033	-2.302	-1.658
	0.3694	-0.3671	-0.1245	-3.026	-1.08	-1.285	2.503	-0.9819	-1.565	5.176	-0.7041	-3.531
	0.6761	0.7014	3.11	3.077	1.782	0.6445	-2.593	-1.125	1.934	0.394	2.992	-6.169
	-4.964	0.7205	0.7068	0.7131	0.6985	0.7177	0.7078	0.7118	0.7057	0.7186	0.7118	0.7109
	0.176	0.6959	0.1408	0.7181	0.5295	0.7084	1.202	0.8559	0.7099	0.7151	0.2105	0.03431
	-0.1529	1.1	1.021	1.011	0.9348	0.9189	1.001	1.067	0.9352	0.9922	1.029	0.996
	1.005	0.9933	0.9944	1.003	-0.2342	0.08137	-0.1409	0.03514	0.05351	-0.04151		-0.0551
	0.1826	-0.005202		0.1704	0.3774	9.34E-03		0.0214	0.3578	-0.194	0.2459	2.258
	0.7595	2.681	-2.306	-2.364	0.3693	-0.3849	0.3097	-2.375	-0.6711	-1.327	2.48	-0.9805
	-1.533	5.194	0.873	-3.739	0.6688	0.1585	3.545	4.058	2.933	0.4544	-2.978	-1.066
	2.44	1.131	3.5	-6.155	-4.975	0.7121	0.6975	0.7072	0.464	0.7165	0.7118	0.6989
	0.7152	0.7299	0.7093	0.7036	0.02122	0.7148	0.03529	0.7155	0.712	0.7058	0.7214	0.7205
	0.7174	0.7019	0.7158	0.04632	-0.3357	1.106	1.111	1.023	0.939	0.9279	1.002	0.9912
	1.008	0.9907	0.9874	0.9956	1.004	0.9942	0.9956	0.9998	-0.1611	0.1286	-0.1494	0.03692
	0.07587	-0.03929		-0.05458		0.2287	0.004913		0.6365	0.1175	-0.04196	
	-0.0619	0.2105	-0.007234		0.2088	2.152	1.831	0.8283	-2.302	-1.533	0.3398	-0.3642
	0.05665	-2.637	-1.26	-1.275	2.48	-0.9766	-1.532	5.195	0.8809	-3.757	0.6819	0.6422
	3.171	3.538	2.04	0.7598	-2.601	-1.105	1.945	0.3044	3.003	-6.152	-4.968	0.7025
	0.714	0.7081	0.7195	0.6998	0.7179	0.7126	0.725	0.7011	0.7209	0.7115	0.7126	0.03653
	0.04074	0.2812	0.1012	0.7165	0.7024	0.7191	0.7132	0.7098	0.7155	0.06022	-0.4038	1.124
	1.111	1.023	0.9365	0.9285	1.003	1.037	0.9835	0.9923	0.9542	0.9949	1.002	0.9947
	0.9955	1.025	-0.1306	0.1078	-0.1315	0.03599	0.06883	-0.04334		-0.05766		0.2154
	-0.1202	-0.206	0.1942	-0.14	-0.003423		-0.03991		-0.03149		0.2161	2.136
	1.067	0.8914	-2.305	-1.634	0.3626	-0.3567	-0.05501		-2.609	-1.15	-1.368	2.485
	-0.9838	-1.542	5.194	0.9019	-3.754	0.6838	0.7074	3.11	3.275	1.739	0.651	-2.535
	-1.402	1.967	0.3704	3.006	-6.154	-4.966	42.35	36.01	27.64	117.3	-30.6	-79.65
	-158.4	-28.44	-211.7	-37.87	-25.69	4.658	2.544	-6.244	-2.701	-251.5	59.99	18.23
	14.45	-33.46	26.36	16.54	-7.192	1.274	-12.21	-17.76	-154.4	-21.42	18.29	2.23
	14.12	-5.831	-18.88	-18.57	-28.26	-26.57	-59.57	-36.83	-28.56	-33.05	-28.11	26.7
	-1.444	1.809	19.86	-5.14	-6.893	-1.629	-54.12	-63.83	-15.35	-71.6	-161.7	-211.2
	-136.7	-23.59	-39.75	3.711	0.5522	-18.3	-28.04	-1.265	-57.75	-98.53	-441.3	-1906
	-2347											

APPENDIX D

Human MCSim Input and Output Files from Dr. Chiu

This is the MCSim input file for the human provided by Dr. Weihsueh Chiu. It has been reformatted for better readability and some lines are now continued on additional lines due to the line length constriction in Word. While the output file is more easily read as an Excel file, it is included here for completeness.

TCE.1.2.3.3.Human.seqpriors.v1.pop.1.1.in

```
# USEPA TCE MODEL VERSION 1.2.3.3
# Include non-detects for DCVG in blood
# Error variances at study level
# Priors for most uniformly distributed parameters
# based on combined mouse and rat posteriors
# Ver 1: based on previous rat "seqpriors.test4" chains
#   set lnFracKidDCVCC -> 10 (all kidney GSH conjugation is
#   "locally" processed)
# Lsodes tolerances reduced to 0.3e-5 and 0.3e-5 based on problems in
# "Human.newpriors" chains
# Removed unused individual-level parameters to increase computational speed
# FISHER -- removed DCVC parameters
# PAYCOK -- kept only physiological and TCA parameter
# KIMMERLE, MONSTER, CHIU -- removed DCVG and DCVC parameters
# MULLER -- kept only physiological, TCA, TCOH, and TCOG parameters
# Muller -- both studies use same parameters (grouped data anyway)

Integrate(Lsodes, 0.3e-5, 0.3e-5, 1);
MCMC ("TCE.1.2.3.3.Human.seqpriors.v1.pop.1.1.out", "TCE.1.2.3.3.Human.seqpriors.v1.pop.1.0.out"
, "", 250 , 0 , 5 , 250 , 482.6733);

Level { #Population level

# Population means
Distrib( M_lnQCC TruncNormal 0.0 0.2 -0.8 0.8 );
Distrib( M_lnVPRC TruncNormal 0.0 0.2 -0.8 0.8 );
Distrib( M_QFatC TruncNormal 1.0 0.46 0.08 1.92 );
Distrib( M_QGutC TruncNormal 1.0 0.18 0.64 1.36 );
Distrib( M_QLivC TruncNormal 1.0 0.45 0.1 1.9 );
Distrib( M_QSlwC TruncNormal 1.0 0.32 0.36 1.64 );
Distrib( M_lnDRspC TruncNormal 0.61 1.43 -11.513 2.303 );
Distrib( M_QKidC TruncNormal 1.0 0.12 0.76 1.24 );
Distrib( M_FracPlasC TruncNormal 1.0 0.05 0.85 1.15 );
Distrib( M_VFatC TruncNormal 1.0 0.45 0.1 1.9 );
Distrib( M_VGutC TruncNormal 1.0 0.08 0.84 1.16 );
Distrib( M_VLivC TruncNormal 1.0 0.23 0.54 1.46 );
Distrib( M_VRapC TruncNormal 1.0 0.08 0.84 1.16 );
Distrib( M_VResplumC TruncNormal 1.0 0.2 0.6 1.4 );
Distrib( M_VRespEffC TruncNormal 1.0 0.2 0.6 1.4 );
Distrib( M_VKidC TruncNormal 1.0 0.17 0.66 1.34 );
Distrib( M_VBldC TruncNormal 1.0 0.12 0.76 1.24 );
Distrib( M_lnPBC TruncNormal 0.0 0.2 -0.6 0.6 );
Distrib( M_lnPFatC TruncNormal 0.0 0.2 -0.6 0.6 );
Distrib( M_lnPGutC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPLivC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPRapC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPRespC TruncNormal 0.0 0.4 -1.2 1.2 );
Distrib( M_lnPKidC TruncNormal 0.0 0.2 -0.6 0.6 );
Distrib( M_lnPSlwC TruncNormal 0.0 0.3 -0.9 0.9 );
Distrib( M_lnPRBCPlasTCAC Uniform -4.605 4.605 );
Distrib( M_lnPBodTCAC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnPLivTCAC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnKDissocC TruncNormal 0.0 0.06 -0.18 0.18 );
Distrib( M_lnBMaxkDC TruncNormal 0.0 0.182 -0.546 0.546 );
Distrib( M_lnPBodTCOHC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnPLivTCOHC TruncNormal 0.0 0.336 -1.008 1.008 );
Distrib( M_lnPBodTCOGC TruncNormal -0.21 1.63 -4.605 4.605 );
Distrib( M_lnPLivTCOGC TruncNormal 1.07 1.46 -4.605 4.605 );
```

```

Distrib( M_lnPeffDCVG Uniform -6.908 6.908 );
#### Distrib( M_lnkTSD Uniform -4.269 4.942 );
#### Distrib( M_lnkAS Uniform -6.571 7.244 );
#### Distrib( M_lnkTD Uniform -4.605 0 );
#### Distrib( M_lnkAD Uniform -7.195 6.62 );
Distrib( M_lnkASTCA Uniform -7.195 6.62 );
Distrib( M_lnkASTCOH Uniform -7.195 6.62 );
Distrib( M_lnVMaxC TruncNormal 0.0 0.693 -2.079 2.079 );
# Distrib( M_lnkMC Normal 0 1 );
Distrib( M_lnCIC TruncNormal 0.0 1.386 -4.158 4.158 );
Distrib( M_lnFracOtherC TruncNormal -1.98 1.56 -6.908 6.908 );
Distrib( M_lnFracTCAC TruncNormal 0.0 1.163 -3.489 3.489 );
# Distrib( M_lnVMaxDCVGC Normal 0 1 );
Distrib( M_lnCICDCVGC TruncNormal 0.0 4.605 -13.815 13.815 );
Distrib( M_lnkMDCVGC TruncNormal 0.0 1.386 -4.158 4.158 );
# Distrib( M_lnVMaxKidDCVGC Normal 0 1 );
Distrib( M_lnCICKidDCVGC TruncNormal 0.0 4.605 -13.815 13.815 );
Distrib( M_lnkMKidDCVGC TruncNormal 0.0 1.386 -4.158 4.158 );
Distrib( M_lnVMaxLungLivC TruncNormal 1.03 1.55 -3.297 3.297 );
Distrib( M_lnkMClara TruncNormal -3.93 1.58 -6.908 6.908 );
Distrib( M_lnFracLungSysC TruncNormal 1.13 2.09 -6.908 6.908 );
# Distrib( M_lnVMaxTCOHC Normal 0 1 );
Distrib( M_lnCITCOHC TruncNormal -1 1.49 -11.513 6.908 );
Distrib( M_lnkMTCOH TruncNormal 1.57 1.51 -9.21 9.21 );
# Distrib( M_lnVMaxGlucC Normal 0 1 );
Distrib( M_lnCIGlucC TruncNormal 1.22 1.47 -9.21 4.605 );
Distrib( M_lnkMGluc TruncNormal 2.41 1.52 -6.908 6.908 );
Distrib( M_lnkMetTCOHC TruncNormal 0.87 1.53 -11.513 6.908 );
Distrib( M_lnkUrnTCAC TruncNormal -2.42 1.44 -4.605 4.605 );
Distrib( M_lnkMetTCAC TruncNormal -0.8 1.45 -9.21 4.605 );
Distrib( M_lnkBileC TruncNormal 1.22 1.49 -9.21 4.605 );
Distrib( M_lnkEHRC TruncNormal -1.51 1.55 -9.21 4.605 );
Distrib( M_lnkUrnTCOGC TruncNormal 2.78 1.57 -6.908 6.908 );
## Distrib( M_lnFracKidDCVCC Uniform -6.908 6.908 );
Distrib( M_lnkDCVGC Uniform -9.21 4.605 );
Distrib( M_lnkNATC TruncNormal -6.12 1.81 -9.21 4.605 );
Distrib( M_lnkKidBioactC TruncNormal -5.12 1.87 -9.21 4.605 );

#### Population variance parameters
Distrib( V_lnQCC InvGamma 2.25 0.05 );
Distrib( V_lnVPRC InvGamma 2.25 0.05 );
Distrib( V_QFatC InvGamma 6 1.058 );
Distrib( V_QGutC InvGamma 6 0.162 );
Distrib( V_QLivC InvGamma 6 1.0125 );
Distrib( V_QSlwC InvGamma 6 0.512 );
Distrib( V_lnDRespC InvGamma 6 0.2 );
Distrib( V_QKidC InvGamma 6 0.072 );
Distrib( V_FracPlasC InvGamma 6 0.0125 );
Distrib( V_VFatC InvGamma 6 1.0125 );
Distrib( V_VGutC InvGamma 6 0.032 );
Distrib( V_VLivC InvGamma 6 0.2645 );
Distrib( V_VRapC InvGamma 6 0.032 );
Distrib( V_VRespLumC InvGamma 6 0.2 );
Distrib( V_VRespEffC InvGamma 6 0.2 );
Distrib( V_VKidC InvGamma 6 0.1445 );
Distrib( V_VBldC InvGamma 6 0.072 );
Distrib( V_lnPBC InvGamma 11.00018 0.342256161 );
Distrib( V_lnPFatC InvGamma 3 0.08 );
Distrib( V_lnPGutC InvGamma 2.25 0.2 );
Distrib( V_lnPLivC InvGamma 2.5 0.24 );
Distrib( V_lnPRapC InvGamma 2.25 0.2 );
Distrib( V_lnPRespC InvGamma 2.25 0.2 );
Distrib( V_lnPKidC InvGamma 2.5 0.06 );
Distrib( V_lnPSlwC InvGamma 2.5 0.135 );
Distrib( V_lnPRBCPlasTCAC InvGamma 2.25 0.14112 );
Distrib( V_lnPBodTCAC InvGamma 2.25 0.14112 );
Distrib( V_lnPLivTCAC InvGamma 2.25 0.14112 );
Distrib( V_lnkDissoC InvGamma 2.25 0.0045 );
Distrib( V_lnBMaxkDC InvGamma 2.25 0.041405 );
Distrib( V_lnPBodTCOHC InvGamma 2.25 0.14112 );
Distrib( V_lnPLivTCOHC InvGamma 2.25 0.14112 );

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Distrib( V_lnPBodTCOGC InvGamma 2.25 0.2 );
Distrib( V_lnPLivTCOGC InvGamma 2.25 0.2 );
Distrib( V_lnPeffDCVG InvGamma 2.25 0.2 );
#### Distrib( V_lnkTSD InvGamma 2.25 5 );
#### Distrib( V_lnkAS InvGamma 2.25 5 );
#### Distrib( V_lnkTD InvGamma 2.25 5 );
#### Distrib( V_lnkAD InvGamma 2.25 5 );
Distrib( V_lnkASTCA InvGamma 2.25 5 );
Distrib( V_lnkASTCOH InvGamma 2.25 5 );
Distrib( V_lnVMaxC InvGamma 16.79289941 7.91721238 );
# Distrib( V_lnkMC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnClC InvGamma 2.502992807 1.339103986 );
Distrib( V_lnFracOtherC InvGamma 2.25 0.3125 );
Distrib( V_lnFracTCAC InvGamma 2.25 4.05 );
# Distrib( V_lnVMaxDCVGC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnClDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnkMDCVGC InvGamma 2.25 0.3125 );
# Distrib( V_lnVMaxKidDCVGC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnClKidDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnkMKidDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnVMaxLungLivC InvGamma 2.25 0.3125 );
Distrib( V_lnkMClara InvGamma 2.25 0.3125 );
Distrib( V_lnFracLungSysC InvGamma 2.25 0.3125 );
# Distrib( V_lnVMaxTCOHC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnClTCOHC InvGamma 2.25 0.3125 );
Distrib( V_lnkMTCOH InvGamma 2.25 0.3125 );
# Distrib( V_lnVMaxGlucC InvGamma #DIV/0! #DIV/0! );
Distrib( V_lnClGlucC InvGamma 2.25 0.3125 );
Distrib( V_lnkMGluc InvGamma 2.25 0.3125 );
Distrib( V_lnkMetTCOHC InvGamma 2.25 0.3125 );
Distrib( V_lnkUrnTCAC InvGamma 2.25 0.3125 );
Distrib( V_lnkMetTCAC InvGamma 2.25 0.3125 );
Distrib( V_lnkBileC InvGamma 2.25 0.3125 );
Distrib( V_lnkEHRC InvGamma 2.25 0.3125 );
Distrib( V_lnkUrnTCOGC InvGamma 2.25 0.3125 );
## Distrib( V_lnFracKidDCVCC InvGamma 2.25 0.3125 );
Distrib( V_lnkDCVGC InvGamma 2.25 0.3125 );
Distrib( V_lnkNATC InvGamma 2.25 0.3125 );
Distrib( V_lnkKidBioactC InvGamma 2.25 0.3125 );

Level { # Study Level
#Error distributions
Distrib( Ve_RetDose , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CALv , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CALvPPM , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CInhPPM , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CInh , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CMixExh , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CArt , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CVen , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CBldMix , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CFat , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CGut , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CRap , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CSlw , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CHrt , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CKid , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLiv , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLung , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CMus , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CSpl , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CBrn , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAEExh , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_zAEExhpost , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CKidTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLivTCOH , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CLungTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CPlasTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CBldTCA , LogUniform , 0.01 , 3.3 );
# Distrib( Ve_CBodTCA , LogUniform , 0.01 , 3.3 );

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#      Distrib( Ve_CKidTCA , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_CLivTCA , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_CLungTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zAurnTCA , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zAurnTCA_collect , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_zAurnTCA_sat , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_zABileTCOG , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_CTCOG , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_CTCOGTCOH , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_CKidTCOGTCOH , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_CLivTCOGTCOH , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_CLungTCOGTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_AurnTCOGTCOH , LogUniform , 0.01 , 3.3 );
Distrib( Ve_AurnTCOGTCOH_collect , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_AurnTCOGTCOH_sat , LogUniform , 0.01 , 3.3 );
Distrib( Ve_CDCVGmol , LogUniform , 0.01 , 3.3 );
Distrib( Ve_zAurnNDCVC , LogUniform , 0.01 , 3.3 );
Distrib( Ve_AurnTCTotMole , LogUniform , 0.01 , 3.3 );
Distrib( Ve_TotCTCOH , LogUniform , 0.01 , 3.3 );
#      Distrib( Ve_QPsamp , LogUniform , 0.01 , 3.3 );

#Likelihoods
Likelihood( RetDose , LogNormal_v , Prediction( RetDose ) , Ve_RetDose );
#      Likelihood( CALv , LogNormal_v , Prediction( CALv ) , Ve_CALv );
Likelihood( CALvPPM , LogNormal_v , Prediction( CALvPPM ) , Ve_CALvPPM );
#      Likelihood( CInhPPM , LogNormal_v , Prediction( CInhPPM ) , Ve_CInhPPM );
#      Likelihood( CInh , LogNormal_v , Prediction( CInh ) , Ve_CInh );
#      Likelihood( CMixExh , LogNormal_v , Prediction( CMixExh ) , Ve_CMixExh );
#      Likelihood( CART , LogNormal_v , Prediction( CART ) , Ve_CART );
Likelihood( CVen , LogNormal_v , Prediction( CVen ) , Ve_CVen );
#      Likelihood( CBldMix , LogNormal_v , Prediction( CBldMix ) , Ve_CBldMix );
#      Likelihood( CFat , LogNormal_v , Prediction( CFat ) , Ve_CFat );
#      Likelihood( CGut , LogNormal_v , Prediction( CGut ) , Ve_CGut );
#      Likelihood( CRap , LogNormal_v , Prediction( CRap ) , Ve_CRap );
#      Likelihood( CSLw , LogNormal_v , Prediction( CSLw ) , Ve_CSLw );
#      Likelihood( CHrt , LogNormal_v , Prediction( CHrt ) , Ve_CHrt );
#      Likelihood( CKid , LogNormal_v , Prediction( CKid ) , Ve_CKid );
#      Likelihood( CLiv , LogNormal_v , Prediction( CLiv ) , Ve_CLiv );
#      Likelihood( CLung , LogNormal_v , Prediction( CLung ) , Ve_CLung );
#      Likelihood( CMus , LogNormal_v , Prediction( CMus ) , Ve_CMus );
#      Likelihood( CSpl , LogNormal_v , Prediction( CSpl ) , Ve_CSpl );
#      Likelihood( CBrn , LogNormal_v , Prediction( CBrn ) , Ve_CBrn );
#      Likelihood( zAExh , LogNormal_v , Prediction( zAExh ) , Ve_zAExh );
#      Likelihood( zAExhpost , LogNormal_v , Prediction( zAExhpost ) , Ve_zAExhpost );
Likelihood( CTCOH , LogNormal_v , Prediction( CTCOH ) , Ve_CTCOH );
#      Likelihood( CKidTCOH , LogNormal_v , Prediction( CKidTCOH ) , Ve_CKidTCOH );
#      Likelihood( CLivTCOH , LogNormal_v , Prediction( CLivTCOH ) , Ve_CLivTCOH );
#      Likelihood( CLungTCOH , LogNormal_v , Prediction( CLungTCOH ) , Ve_CLungTCOH );
Likelihood( CPlasTCA , LogNormal_v , Prediction( CPlasTCA ) , Ve_CPlasTCA );
Likelihood( CBldTCA , LogNormal_v , Prediction( CBldTCA ) , Ve_CBldTCA );
#      Likelihood( CBodTCA , LogNormal_v , Prediction( CBodTCA ) , Ve_CBodTCA );
#      Likelihood( CKidTCA , LogNormal_v , Prediction( CKidTCA ) , Ve_CKidTCA );
#      Likelihood( CLivTCA , LogNormal_v , Prediction( CLivTCA ) , Ve_CLivTCA );
#      Likelihood( CLungTCA , LogNormal_v , Prediction( CLungTCA ) , Ve_CLungTCA );
Likelihood( zAurnTCA , LogNormal_v , Prediction( zAurnTCA ) , Ve_zAurnTCA );
Likelihood( zAurnTCA_collect , LogNormal_v , Prediction( zAurnTCA_collect ) ,
Ve_zAurnTCA_collect );
#      Likelihood( zAurnTCA_sat , LogNormal_v , Prediction( zAurnTCA_sat ) , Ve_zAurnTCA_sat );
#      Likelihood( zABileTCOG , LogNormal_v , Prediction( zABileTCOG ) , Ve_zABileTCOG );
#      Likelihood( CTCOG , LogNormal_v , Prediction( CTCOG ) , Ve_CTCOG );
#      Likelihood( CTCOGTCOH , LogNormal_v , Prediction( CTCOGTCOH ) , Ve_CTCOGTCOH );
#      Likelihood( CKidTCOGTCOH , LogNormal_v , Prediction( CKidTCOGTCOH ) , Ve_CKidTCOGTCOH );
#      Likelihood( CLivTCOGTCOH , LogNormal_v , Prediction( CLivTCOGTCOH ) , Ve_CLivTCOGTCOH );
#      Likelihood( CLungTCOGTCOH , LogNormal_v , Prediction( CLungTCOGTCOH ) , Ve_CLungTCOGTCOH );
Likelihood( AurnTCOGTCOH , LogNormal_v , Prediction( AurnTCOGTCOH ) , Ve_AurnTCOGTCOH );
Likelihood( AurnTCOGTCOH_collect , LogNormal_v , Prediction( AurnTCOGTCOH_collect ) ,
Ve_AurnTCOGTCOH_collect );
#      Likelihood( AurnTCOGTCOH_sat , LogNormal_v , Prediction( AurnTCOGTCOH_sat ) ,
Ve_AurnTCOGTCOH_sat );
#      Likelihood( CDCVGmol , LogNormal_v , Prediction( CDCVGmol ) , Ve_CDCVGmol );
Likelihood( zAurnNDCVC , LogNormal_v , Prediction( zAurnNDCVC ) , Ve_zAurnNDCVC );

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Likelihood( AURNtCTotMole , LogNormal_v , Prediction( AURNtCTotMole ) , Ve_AURNtCTotMole );
Likelihood( TotCTCOH , LogNormal_v , Prediction( TotCTCOH ) , Ve_TotCTCOH );
# Likelihood( QPsamp , LogNormal_v , Prediction( QPsamp ) , Ve_QPsamp );
Likelihood( CDCVG_ND , Poisson , Prediction( CDCVG_ND ) );

#### For non-detects, LD = 5e-5 mM, where LD is the detection limit.
#### Code calculates -lnlikelihood, so poisson(0,lambda) gives
#### likelihood

Species = 1;
lnFracKidDCVCC = 10; # All kidney GSH conjugation is locally processed

##### BEGIN Individual Data #####

##### BEGIN FISHER et al. 1998 individual data #####
Level { #Subject level
### FOR FISHER, NO DCVC
Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );
Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.64 1.36 );
Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.1 1.9 );
Distrib( QSLwC TruncNormal_v M_QSLwC V_QSLwC 0.36 1.64 );
Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.76 1.24 );
Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.85 1.15 );
Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.84 1.16 );
Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.54 1.46 );
Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.84 1.16 );
Distrib( VResplumC TruncNormal_v M_VResplumC V_VResplumC 0.6 1.4 );
Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.6 1.4 );
Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.66 1.34 );
Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.6 0.6 );
Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.6 0.6 );
Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.6 0.6 );
Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
Distrib( lnkDissocC TruncNormal_v M_lnkDissocC V_lnkDissocC -0.18 0.18 );
Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -0.546 0.546 );
Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );
Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
#### Distrib( lnkTSD TruncNormal_v M_lnkTSD V_lnkTSD -4.269 4.942 );
#### Distrib( lnkAS TruncNormal_v M_lnkAS V_lnkAS -6.571 7.244 );
#### Distrib( lnkTD TruncNormal_v M_lnkTD V_lnkTD -4.605 0 );
#### Distrib( lnkAD TruncNormal_v M_lnkAD V_lnkAD -7.195 6.62 );
#### Distrib( lnkASTCA TruncNormal_v M_lnkASTCA V_lnkASTCA -7.195 6.62 );
#### Distrib( lnkASTCOH TruncNormal_v M_lnkASTCOH V_lnkASTCOH -7.195 6.62 );
Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
# Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC 0 1 );
Distrib( lnClC TruncNormal_v M_lnClC V_lnClC -4.158 4.158 );
Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
# Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC 0 1 );
Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -13.815 13.815 );
Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC -4.158 4.158 );
# Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC 0 1 );
Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -13.815 13.815 );
Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC -4.158 4.158 );
Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );

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Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
# Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC 0 1 );
Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC -11.513 6.908 );
Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
# Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC 0 1 );
Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC -9.21 4.605 );
Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
Distrib( lnkUrnTCAC TruncNormal_v M_lnkUrnTCAC V_lnkUrnTCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
Distrib( lnkEHRC TruncNormal_v M_lnkEHRC V_lnkEHRC -9.21 4.605 );
Distrib( lnkUrnTCOGC TruncNormal_v M_lnkUrnTCOGC V_lnkUrnTCOGC -6.908 6.908 );
## Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );
Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
#### Distrib( lnkNATC TruncNormal_v M_lnkNATC V_lnkNATC -9.21 4.605 );
#### Distrib( lnkKidBioactC TruncNormal_v M_lnkKidBioactC V_lnkKidBioactC -9.21 4.605 );

Level { # Fisher et al. 1998 Male subject 1
#Subject=13;
Experiment { # 1
# PROCED M100_1
# Data from Fisher et al. (1998)
# Data from procedure M100_1 (in Bld_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 1
# lnBW=4.27; VFatC=0.79; lnPB=2.44;
# BWmeas = 71.4;
# VFatCmeas = 0.17;
# PBmeas = 11.49;

# CC= 0;
# Conc=NDoses(2, 105.5 0, 0.0 4.0);

# M100_1a (T, CVen)
Print (CVen, 0.52, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18);
Data (CVen, 1.98, 2.69, 3.38, 3.76, 3.95, 3.26, 2.54, 1.12, 0.72, 0.52, 0.31,
0.28, 0.23, 0.17, 0.15);

# M100_1b (T, CTCOH)
Print (CTCOH, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
Data (CTCOH, 0.39, 1.3, 2.18, 2.83, 2.94, 3.21, 2.78, 2.84, 2.52, 2.03, 1.56,
1.56, 1.31, 1.21, 1.15);

# M100_1c (T, CBldTCA)
Print (CBldTCA, 0.52, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03,
22.02, 45.83, 69.74, 93.75);
Data (CBldTCA, 0.15, 0.5, 1.07, 2.11, 3.12, 2.87, 3.39, 4, 4.09, 4.76, 5.52, 6.16,
6.48, 8.12, 7.18, 8.56, 8.14, 9.3, 7.37, 6.97);

# M100_1d (T, AUrnTCA),
Print (zAUrnTCA, 4.5, 6.1, 8, 10.1, 11.4, 12.1, 14.1, 16, 18, 20.23, 21.97, 26,
31.5, 34.25, 35.5, 36.75, 44.75, 52, 54.5, 56.5, 59.5, 60.5, 68.5, 70.25,
73, 79.5, 81.5, 84.67);
Data (zAUrnTCA, 1.47, 2.82, 5.02, 7.1, 8.87, 10.22, 12.67, 15.33, 16.85, 22.83,
25.23, 30.03, 33.1, 39.59, 42.21, 48.47, 52.39, 55.28, 58.64, 59.8, 62.4,
65, 79.17, 83.51, 88.15, 99.19, 100.11, 100.62);

# M100_1e (T, AUrnTCOGTCOH),
Print (AUrnTCOGTCOH, 4.5, 6.1, 8, 10.1, 11.4, 12.1, 14.1, 16, 18, 20.23, 21.97,
26, 31.5, 34.25, 35.5, 36.75, 44.75, 52, 54.5, 56.5, 59.5, 60.5, 68.5,
70.25, 73, 79.5, 81.5, 84.67);
Data (AUrnTCOGTCOH, 13.94, 23.22, 30.95, 37.58, 43.49, 46.17, 50.32, 56.69, 61.37,
65.35, 68.94, 74.63, 79.76, 82.89, 84.29, 86.91, 90.23, 91.8,
93.75, 94.88, 96.1, 96.99, 99.59, 100.64, 102.16, 104.07,
104.74, 104.94);

# Total = Free in Fisher data
Print (TotCTCOH, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
Data (TotCTCOH, 0.39, 1.3, 2.18, 2.83, 2.94, 3.21, 2.78, 2.84, 2.52, 2.03, 1.56,
1.56, 1.31, 1.21, 1.15);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Data (CALvPPM, -1);

```

```

Print(CPlasTCA, 1);
Print(AUrntCTotMole, 1);
Print(zAurnNDCVC, 1);
Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
      0.000671);
Print(CDCVGmol0, 12); # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12); # No detect at 12 hr in males
Data(CDCVG_ND, 0);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAurnTCA_collect, 1);
Data(zAurnTCA_collect, -1);
Print(AUrntCOGTCOH_collect, 1);
Data(AUrntCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Male subject 2
#Subject=14;
Experiment { # 2
# PROCED M50_2
# Data from Fisher et al. (1998)
# Data from procedure M50_2 (in Bld50_M and Urin50_M) in HumanB.cmd
# Male 50 ppm exposure
# Male vol #2
# lnBW=4.24; VFatC=1.3; lnPB=2.31;
# CC= 0;
      BWmeas = 69.3;
      VFatCmeas = 0.27;
      PBmeas = 10.1;
      Conc=NDoses(2, 49.3 0, 0.0 4.0);
# M50_2a (T, CVen),
      Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5);
      Data (CVen, 0.61, 0.74, 1.11, 1.01, 1.05, 0.81, 0.46);
# M50_2b (T, CTCOH),
      Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 14, 16, 18, 20);
      Data (CTCOH, 0.44, 0.55, 0.83, 1.08, 1.35, 1.26, 1.34, 1.11, 1.01, 0.9, 0.76,
            0.66, 0.63, 0.56, 0.51);
# M50_2c (T, CBldTCA),
      Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20, 22,
            49.08, 71.72, 97.47);
      Data (CBldTCA, 0.29, 0.65, 1.47, 2.27, 2.91, 2.99, 3.12, 3.49, 3.66, 4.29, 4.69,
            5.11, 5.17, 5.26, 5.66, 5.18, 5.69, 6.67, 6.49, 6.01);
# M50_2d (T, AurnTCA),
      Print (zAurnTCA, 4.55, 5.08, 6.06, 8.08, 10.06, 12.08, 14.08, 16.08, 18.08, 20.08,
            22.17, 31.33, 49, 64.33, 77, 86.25);
      Data (zAurnTCA, 0.041, 0.062, 0.15, 0.26, 0.41, 0.53, 0.65, 0.8, 0.92, 1.05, 1.18,
            1.46, 2.2, 3.61, 4.36, 5.03);
# M50_2e (T, AurnTCOGTCOH),
      Print (AurnTCOGTCOH, 4.55, 5.08, 6.06, 8.08, 10.06, 12.08, 14.08, 16.08, 18.08,
            20.08, 22.17, 31.33, 49, 64.33, 77, 86.25);
      Data (AurnTCOGTCOH, 8.45, 15.2, 21.6, 28.09, 35.67, 39.98, 43.78, 47.68, 50.54,
            53.03, 55.3, 60.62, 69.8, 73.15, 74.82, 76.02);

```

```

# Total = Free in Fisher data
Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 14, 16, 18, 20);
Data (TotCTCOH, 0.44, 0.55, 0.83, 1.08, 1.35, 1.26, 1.34, 1.11, 1.01, 0.9, 0.76,
      0.66, 0.63, 0.56, 0.51);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Data (CALvPPM, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);
Print(CALvPPM, 1);

Print(CDCVGmol, 0);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 0);
Data(CDCVG_ND, -1);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect, -1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Male subject 3
#Subject=15;
Experiment { # 3 ## Low exposure
# PROCED M60
# Data from Fisher et al. (1998)
# Data from procedure M60 (in Bld50_M and Urin50_M) in HumanB.cmd
# Male 50 ppm exposure
# Male vol 3
# lnBW=4.26; VFatC=0.654; lnPB=2.41;
# CC= 0;
      BWmeas = 71.1;
      VFatCmeas = 0.14;
      PBmeas = 11.1;
      Conc=NDoses(2, 55.2 0, 0.0 4.0);
# M60a (T, CVen),
      Print (CVen, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8);
      Data (CVen, 1.89, 1.36, 2.68, 2.67, 2.79, 2.42, 1.52, 0.82, 0.37, 0.29);
# M60b (T, CTCOH),
      Print (CTCOH, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8, 10, 12,
            14.17, 16.02, 18.02, 20);
      Data (CTCOH, 0.63, 1.07, 1.57, 1.9, 1.94, 2.02, 2.26, 1.02, 0.96, 1.65, 1.38,
            1.26, 1.13, 1.03, 1.05, 0.9);
# M60c (T, CBldTCA),
      Print (CBldTCA, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8, 10, 12,
            14.17, 16.02, 18.02, 20, 22, 44.83, 68.72, 93.12);
      Data (CBldTCA, 0.43, 0.55, 1.07, 1.57, 1.96, 2.01, 2.19, 2.28, 2.52, 2.92, 3.2,
            3.56, 4.19, 3.9, 4.95, 5.04, 5.08, 5.51, 9.45, 4.27);
# M60d (T, AUrnTCA),
      Print (zAUrnTCA, 0.5, 3.12, 4.63, 5.45, 6.45, 8.13, 10.17, 12.15, 14.27, 16.13,
            18.15, 20.2, 22.22, 24.22, 32.85, 34.22, 39.85, 44.25, 47.25,
            52.13, 58.59, 67.75, 72.37, 77.15, 82.92, 91.83);

```

```

        Data (zAurnTCA, 0.002, 0.082, 0.184, 0.249, 0.307, 0.539, 0.852, 1.35, 1.78, 2.12,
              2.48, 2.89, 3.48, 4.28, 5.35, 5.66, 6.72, 7.42, 8.14, 8.93, 10.17,
              11.19, 12.56, 13.78, 14.44, 15.63);
# M60e (T, AurnTCOGTCOH),
    Print (AurnTCOGTCOH, 3.12, 4.63, 5.45, 6.45, 8.13, 10.17, 12.15, 14.27, 16.13,
          18.15, 20.2, 22.22, 24.22, 32.85, 34.22, 39.85, 44.25, 47.25,
          52.13, 58.59, 67.75, 72.37, 77.15, 82.92, 91.83);
    Data (AurnTCOGTCOH, 8.24, 11.6, 13.64, 15.64, 19.73, 23.26, 28.95, 28.95, 29.79,
          32.07, 34.21, 38.49, 43.06, 47.48, 48.6, 52.15, 53.88, 55.21,
          57.21, 59.15, 60.89, 61.46, 61.84, 62.2, 62.56);
# Total = Free in Fisher data
    Print (TotCTCOH, 0.58, 0.98, 2.02, 3.02, 4.02, 4.25, 4.44, 5.02, 5.83, 8, 10, 12,
          14.17, 16.02, 18.02, 20);
    Data (TotCTCOH, 0.63, 1.07, 1.57, 1.9, 1.94, 2.02, 2.26, 1.02, 0.96, 1.65, 1.38,
          1.26, 1.13, 1.03, 1.05, 0.9);
    Data (CPlastTCA, -1);
    Data (AurnTCTotMole, -1);
    Data (zAurnNDCVC, -1);
    Data (CALvPPM, -1);
    Print(CPlastTCA, 1);
    Print(AurnTCTotMole, 1);
    Print(zAurnNDCVC, 1);
    Print(CALvPPM, 1);

    Print(CDCVGmol, 0);
    Data(CDCVGmol, -1);
    Print(CDCVG_ND, 0);
    Data(CDCVG_ND, -1);

#
    Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
    Print(RetDose, 1);
    Data(RetDose, -1);
    Print(zAurnTCA_collect, 1);
    Data(zAurnTCA_collect, -1);
    Print(AurnTCOGTCOH_collect, 1);
    Data(AurnTCOGTCOH_collect, -1);
};

#Subject=15; # 16
    Experiment { # 4 ## High exposure
# PROCED M100_4
# Data from Fisher et al. (1998)
# Data from procedure M100_4 (in Bld_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 3
# lnBW=4.26; VFatC=0.654; lnPB=2.41;
# CC= 0;
        BWmeas = 71.1;
        VFatCmeas = 0.14;
        PBmeas = 11.1;
        Conc=NDoses(2, 101.5 0, 0.0 4.0);

# M100_4a (T, CVen)
        Print (CVen, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5);
        Data (CVen, 3.1, 3.76, 3.46, 3.83, 3.78, 2.9, 2.11, 1.09);
# M100_4b (T, CTCOH)
        Print (CTCOH, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10, 12.05, 14, 16, 18, 20,
              22.05);
        Data (CTCOH, 0.56, 1.12, 1.75, 2.55, 3.48, 3.73, 3.52, 3.78, 3.79, 3.3, 2.96,
              2.71, 2.38, 2.04, 1.89, 1.57, 1.4);

```

```

# M100_4c (T, CBldTCA)
  Print (CBldTCA, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10, 12.05, 14, 16, 18, 20,
        22.05, 50.52, 74.03, 98.58);
  Data (CBldTCA, 0.3, 0.75, 1.42, 2.34, 3.01, 2.58, 3.1, 3.26, 4.21, 4.99, 5.46,
        5.74, 6.69, 6.85, 7.14, 9.85, 9.32, 8.87, 8.08, 3.82);
# M100_4d (T, zAurnTCA),
  Print (zAurnTCA, 4.35, 5.03, 6.07, 8.07, 10.04, 12.07, 14.06, 16.03, 18.02, 20.04,
        22.13, 25.5, 36.5, 44.1, 47, 54, 61.45, 69.3, 85, 93.55);
  Data (zAurnTCA, 0.98, 1.21, 1.42, 2.05, 3.12, 3.6, 4.09, 4.57, 4.86, 5.28, 5.98,
        8.14, 8.94, 10.97, 11.58, 13.48, 15.33, 17.47, 21.65, 21.65);
# M100_4e (T, AurnTCOGTCOH),
  Print (AurnTCOGTCOH, 4.35, 5.03, 6.07, 8.07, 10.04, 12.07, 14.06, 16.03, 18.02,
        20.04, 22.13, 25.5, 36.5, 44.1, 47, 54, 61.45, 69.3, 85,
        93.55);
  Data (AurnTCOGTCOH, 28.92, 31.85, 40.01, 56.31, 68.48, 78.8, 89.82, 98.66, 105.25,
        112.29, 122.73, 141.62, 150.29, 162.32, 165.74, 173.84, 178.3,
        182.24, 185.01, 186.89);
# Total = Free in Fisher data
  Print (TotCTCOH, 0.5, 1, 2, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10, 12.05, 14, 16, 18,
        20, 22.05);
  Data (TotCTCOH, 0.56, 1.12, 1.75, 2.55, 3.48, 3.73, 3.52, 3.78, 3.79, 3.3, 2.96,
        2.71, 2.38, 2.04, 1.89, 1.57, 1.4);
  Data (CPlasTCA, -1);
  Data (AurnTCTotMole, -1);
  Data (zAurnNDCVC, -1);
  Data (CALvPPM, -1);
  Print(CPlasTCA, 1);
  Print(AurnTCTotMole, 1);
  Print(zAurnNDCVC, 1);
  Print(CALvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
  Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
  Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
        0.000671);
  Print(CDCVGmol0, 12); # No detect at 12 hr in males
  Data(CDCVGmol0, 0.000025); # Half the detection limit
  Print(CDCVG_ND, 12); # No detect at 12 hr in males
  Data(CDCVG_ND, 0);

#
  Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
  Print(RetDose, 1);
  Data(RetDose, -1);
  Print(zAurnTCA_collect, 1);
  Data(zAurnTCA_collect, -1);
  Print(AurnTCOGTCOH_collect, 1);
  Data(AurnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Male subject 4
#Subject=16; # 17
  Experiment { # 5 ## Low exposure
# PROCED M50_1
# Data from Fisher et al. (1998)
# Data from procedure M50_1 (in Bld50_M and Urin50_M) in HumanB.cmd
# Male 50 ppm exposure
# Male vol 4
# lnBW=3.96; VFatC=0.467; lnPB=2.49;
# CC= 0;

```



```

        BWmeas = 52.3;
        VFatCmeas = 0.1;
        PBmeas = 12.1;
        Conc=NDoses(2, 53.1 0, 0.0 4.0);
# M50_1a (T, CVen)
    Print (CVen, 0.5, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10);
    Data (CVen, 0.67, 1.37, 1.96, 1.92, 2.08, 1.13, 0.76, 0.42, 0.3, 0.21, 0.15);
# M50_1b (T, CTCOH)
    Print (CTCOH, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10, 12, 14, 16, 18,
           20, 22);
    Data (CTCOH, 0.43, 1.2, 1.26, 1.69, 1.66, 1.6, 1.58, 1.51, 1.44, 1.52, 1.14, 1.05,
           1.04, 1.06, 0.45, 0.75);
# M50_1c (T, CBldTCA)
    Print (CBldTCA, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10, 12, 14, 16, 18,
           20, 22, 44.78, 68.72, 100.4);
    Data (CBldTCA, 0.29, 0.77, 1.33, 1.84, 1.93, 2.07, 2.27, 2.94, 3.58, 3.72, 3.98,
           4.4, 4.58, 4.86, 5.73, 4.22, 5, 4.72, 4.47);
# M50_1d (T, AUrnTCA)
    Print (zAUrnTCA, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17, 22.17,
           25, 29.83, 37.83, 44.83, 45.67, 49.67, 53.33, 61.23, 62.83,
           79.1);
    Data (zAUrnTCA, 1, 1.53, 3.34, 6.01, 7.6, 13.02, 14.83, 16.67, 18.69, 21.3, 21.95,
           26.24, 31.79, 40.44, 40.86, 42.64, 42.94, 43.8, 44.54, 48.73);
# M50_1e (T, AUrnTCOGTCOH),
    Print (AUrnTCOGTCOH, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17,
           22.17, 25, 29.83, 37.83, 44.83, 45.67, 49.67, 53.33, 61.23,
           62.83, 79.1);
    Data (AUrnTCOGTCOH, 5.26, 8.23, 13.05, 16.3, 19.05, 24.62, 26.97, 29.06, 30.62,
           32.53, 33.35, 35.43, 37.99, 38.21, 39.06, 39.63, 39.7, 39.9,
           40.23, 40.67);
# Total = Free in Fisher data
    Print (TotCTCOH, 1, 2.03, 3, 4.02, 4.25, 4.5, 5.02, 6.02, 8.08, 10, 12, 14, 16,
           18, 20, 22);
    Data (TotCTCOH, 0.43, 1.2, 1.26, 1.69, 1.66, 1.6, 1.58, 1.51, 1.44, 1.52, 1.14,
           1.05, 1.04, 1.06, 0.45, 0.75);
    Data (CPlasTCA, -1);
    Data (AUrnTCTotMole, -1);
    Data (zAUrnNDCVC, -1);
    Data (CALvPPM, -1);
    Print(CPlasTCA, 1);
    Print(AUrnTCTotMole, 1);
    Print(zAUrnNDCVC, 1);
    Print(CALvPPM, 1);

    Print(CDCVGmol, 0);
    Data(CDCVGmol, -1);
    Print(CDCVG_ND, 0);
    Data(CDCVG_ND, -1);

#
    Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
    Print(RetDose, 1);
    Data(RetDose, -1);
    Print(zAUrnTCA_collect, 1);
    Data(zAUrnTCA_collect, -1);
    Print(AUrnTCOGTCOH_collect, 1);
    Data(AUrnTCOGTCOH_collect, -1);
};

```

```

#Subject=16; # 18
Experiment { # 6 ## High exposure
# PROCED M100_6
# Data from Fisher et al. (1998)
# Data from procedure M100_6 (in Bld_M, Exh_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 4
# lnBW=3.96; VFatC=0.467; lnPB=2.49;
# CC= 0;

        BWmeas = 52.3;
        VFatCmeas = 0.1;
        PBmeas = 12.1;
        Conc=NDoses(2, 97.8 0, 0.0 4.0);

# M100_6a (T, CVen),
        Print (CVen, 0.5, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03);
        Data (CVen, 0.64, 0.94, 1.35, 1.62, 1.56, 1.16, 0.77, 0.37, 0.23, 0.19, 0.17);
# M100_6b (T, CTCOH),
        Print (CTCOH, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03, 16, 18,
                19.97, 22.07);
        Data (CTCOH, 0.47, 1.1, 1.58, 2.1, 2.21, 2.2, 2.15, 1.94, 1.88, 1.61, 1.39, 1.26,
                1.06, 0.95, 0.88, 0.77);
# M100_6c (T, CBldTCA),
        Print (CBldTCA, 0.5, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03,
                16, 18, 19.97, 22.07, 48, 71.83, 101.08);
        Data (CBldTCA, 0.21, 0.49, 1.1, 1.67, 2.52, 2.44, 2.71, 3.18, 3.46, 4.26, 4.93,
                5.43, 5.85, 6.02, 6.18, 6.35, 6.52, 12.88, 6.25, 5.07);
# M100_6d (T, CALVPPM),
        Print (CALVPPM, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03, 16);
        Data (CALVPPM, 24.679, 6.422, 4.394, 2.691, 1.388, 1.198, 0.592, 0.47, 0.369,
                0.351);
# M100_6e (T, zAurnTCA),
        Print (zAurnTCA, 4.55, 5.12, 6.08, 8.13, 10.13, 12.1, 14.1, 16.1, 18.12, 20.08,
                22.3, 30.42, 35.67, 51.83, 56.67, 61.5, 70.17, 72.67, 76.92,
                82.67, 85.75, 93.67);
        Data (zAurnTCA, 0.32, 0.41, 1.04, 1.32, 2.51, 4.77, 7.29, 10.23, 11.5, 13.03,
                14.26, 17.65, 18.58, 18.58, 18.58, 18.95, 20.95, 22.77, 25.76,
                30.01, 30.7, 34.88);
# M100_6f (T, AurnTCOGTCOH),
        Print (AurnTCOGTCOH, 4.55, 5.12, 6.08, 8.13, 10.13, 12.1, 14.1, 16.1, 18.12,
                20.08, 22.3, 30.42, 35.67, 51.83, 56.67, 61.5, 70.17, 72.67,
                76.92, 82.67, 85.75, 93.67);
        Data (AurnTCOGTCOH, 11.6, 13.64, 18.54, 25, 33.99, 42.1, 50.19, 60.58, 64.73,
                70.85, 77.69, 79.75, 80.14, 80.23, 80.32, 80.66, 81.44, 82.38,
                82.74, 83.28, 83.35, 83.79);

# Total = Free in Fisher data
        Print (TotCTCOH, 1, 2.02, 3, 4.02, 4.25, 4.5, 5, 6, 8, 10.03, 12.02, 14.03, 16,
                18, 19.97, 22.07);
        Data (TotCTCOH, 0.47, 1.1, 1.58, 2.1, 2.21, 2.2, 2.15, 1.94, 1.88, 1.61, 1.39,
                1.26, 1.06, 0.95, 0.88, 0.77);
        Data (CPlasTCA, -1);
        Data (AurnTCTotMole, -1);
        Data (zAurnNDCVC, -1);
        Print(CPlasTCA, 1);
        Print(AurnTCTotMole, 1);
        Print(zAurnNDCVC, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
        Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
        Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
                0.000671);
        Print(CDCVGmol0, 12); # No detect at 12 hr in males
        Data(CDCVGmol0, 0.000025); # Half the detection limit
        Print(CDCVG_ND, 12); # No detect at 12 hr in males
        Data(CDCVG_ND, 0);

#
        Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
        Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);

```

```

#           Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose, -1);
#           Print(zAurnTCA_collect, 1);
#           Data(zAurnTCA_collect, -1);
#           Print(AurnTCOGTCOH_collect, 1);
#           Data(AurnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Male subject 5
#Subject=17; # 19
  Experiment { # 7
# PROCED M100_2
# Data from Fisher et al. (1998)
# Data from procedure M100_2 (in Bld_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 5
# lnBW=4.41; VFatC=0.65; lnPB=2.48;
# CC= 0;
    BWmeas = 82.3;
    VFatCmeas = 0.14;
    PBmeas = 11.91;
    Conc=NDoses(2, 105.5 0, 0.0 4.0);

# M100_2a (T, CVen),
    Print (CVen, 0.52, 1, 2.02, 3.02, 4.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 12);
    Data (CVen, 1.69, 2.5, 3.5, 4.24, 4.75, 3.76, 2.2, 0.96, 0.53, 0.26, 0.17, 0.17);
# M100_2b (T, CTCOH)
    Print (CTCOH, 1, 2.02, 3.02, 4.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 12, 14, 16, 18,
    20, 22.03);
    Data (CTCOH, 0.37, 1.41, 2.4, 3.59, 4.16, 3.73, 3.65, 3.63, 2.6, 2.82, 1.84, 1.55,
    1.59, 1.06, 1.23, 0.75);
# M100_2c (T, CBldTCA)
    Print (CBldTCA, 0.52, 1, 2.02, 3.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 14, 16, 18,
    20, 22.03, 69.72, 93.61);
    Data (CBldTCA, 0.24, 0.6, 1.24, 2.71, 4.23, 3.86, 3.92, 4.54, 5.71, 6.21, 7.96,
    9.08, 8.3, 8.43, 8.95, 5.51, 3.55);
# M100_2d (T, CDCA)
#           Print (CDCA, 0.52, 1, 2.02, 3.02, 4.27, 8);
#           Data (CDCA, 0.004, 0.004, 0.004, 0.004, 0.005, 0.007);
# M100_2e (T, AurnTCA),
    Print (zAurnTCA, 4.38, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24.42, 31, 35.42, 44.9,
    49.75, 53.75, 54.76, 59.42, 68.9, 70.83, 72, 74.58, 77, 83.92,
    86, 92.67);
    Data (zAurnTCA, 1.74, 2.77, 3.94, 5.52, 7.66, 9.62, 11.69, 13.57, 20.39, 26.25,
    30.32, 40.91, 50.7, 65.02, 65.02, 78.15, 79.79, 83.82, 93.09,
    98.82, 100.66, 112.13, 117.83, 118.82, 119.3, 120.02);
# M100_2f (T, AurnTCOGTCOH),
    Print (AurnTCOGTCOH, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24.42, 31, 35.42, 44.9,
    49.75, 53.75, 54.76, 59.42, 68.9, 70.83, 72, 74.58, 77,
    83.92, 86, 92.67);
    Data (AurnTCOGTCOH, 8.69, 18.39, 27.48, 37.49, 44.58, 51.78, 56.11, 60.47, 64.77,
    66.98, 75.49, 79.43, 82.13, 85.29, 88.15, 88.66, 89.44, 90.6,
    91.71, 91.84, 92.37, 93.07, 93.79, 94.17, 94.55);

# Total = Free
    Print (TotCTCOH, 1, 2.02, 3.02, 4.02, 4.27, 4.52, 5.02, 6.42, 8, 10, 12, 14, 16,
    18, 20, 22.03);
    Data (TotCTCOH, 0.37, 1.41, 2.4, 3.59, 4.16, 3.73, 3.65, 3.63, 2.6, 2.82, 1.84,
    1.55, 1.59, 1.06, 1.23, 0.75);
    Data (CPlasTCA, -1);
    Data (AurnTCTotMole, -1);
    Data (zAurnNDCVC, -1);
    Data (CAIvPPM, -1);

```

```

Print(CPlasTCA, 1);
Print(AUrntCTotMole, 1);
Print(zAurnNDCVC, 1);
Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
0.000671);
Print(CDCVGmol0, 12); # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12); # No detect at 12 hr in males
Data(CDCVG_ND, 0);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAurnTCA_collect, 1);
Data(zAurnTCA_collect, -1);
Print(AUrntCOGTCOH_collect, 1);
Data(AUrntCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Male subject 6
#Subject=18;# 20
Experiment { # 8
# PROCED M100_3
# Data from Fisher et al. (1998)
# Data from procedure M100_3 (in Bld_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 6
# lnBW=4.42; VFatC=0.65; lnPB=2.39;
# CC= 0;
BWmeas = 82.7;
VFatCmeas = 0.14;
PBmeas = 10.85;
Conc=NDoses(2, 102.6 0, 0.0 4.0);

# M100_3a (T, CVen),
Print (CVen, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6);
Data (CVen, 1.93, 2.34, 2.84, 3.4, 3.41, 2.2, 1.66, 0.89, 0.38);
# M100_3b (T, CTCOH)
Print (CTCOH, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6, 8, 10.02, 12, 14, 16.02,
18.07, 20, 22);
Data (CTCOH, 0.45, 0.77, 1.51, 2.41, 3.3, 3.64, 3.67, 3.48, 3.05, 2.52, 2.38,
2.16, 1.73, 1.48, 1.12, 1.01, 0.85);
# M100_3c (T, CBldTCA)
Print (CBldTCA, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6, 8, 10.02, 12, 14, 16.02,
18.07, 20, 22, 46.85, 71.47, 95.5);
Data (CBldTCA, 0.23, 0.49, 1.07, 1.89, 2.87, 3.69, 3.87, 3.59, 4.18, 4.71, 5.46,
5.67, 5.97, 6.05, 6.22, 7.54, 7.26, 8.43, 3.86, 3.55);
# M100_3d (T, zAurnTCA)
Print (zAurnTCA, 3.03, 4.75, 6.7, 8.25, 10.17, 12.08, 14.19, 15.58, 17.6, 18.23,
19.58, 20.05, 21.33, 22.17, 23.2, 35.42, 40.67, 46.67, 47.17,
52.33, 55.25, 68.17, 69.75);
Data (zAurnTCA, 0.488, 0.961, 2.09, 2.96, 5.56, 7.17, 8.37, 9.09, 9.7, 10.13,
10.99, 11.24, 11.88, 12.36, 13.03, 14.18, 16.14, 18.07, 19.06,
20.35, 23.68, 24.71, 27.02);

```

```

# M100_3e (T, AUrnTCOGTCOH)
  Print (AUrnTCOGTCOH, 3.03, 4.75, 6.7, 8.25, 10.17, 12.08, 14.19, 15.58, 17.6,
        18.23, 19.58, 20.05, 21.33, 22.17, 23.2, 35.42, 40.67, 46.67,
        47.17, 52.33, 55.25, 68.17, 69.75);
  Data (AUrnTCOGTCOH, 32.7, 60.26, 97.98, 130.67, 182.9, 204.64, 224.53, 233.79,
        240.99, 245.36, 253.46, 255.9, 261.17, 265.4, 269.76, 271.64,
        276.15, 277.54, 277.83, 278.12, 278.81, 278.88, 279.07);

# Total = Free in Fisher data
  Print (TotCTCOH, 0.5, 1.07, 2, 3, 3.98, 4.25, 4.5, 5, 6, 8, 10.02, 12, 14, 16.02,
        18.07, 20, 22);
  Data (TotCTCOH, 0.45, 0.77, 1.51, 2.41, 3.3, 3.64, 3.67, 3.48, 3.05, 2.52, 2.38,
        2.16, 1.73, 1.48, 1.12, 1.01, 0.85);
  Data (CPlasTCA, -1);
  Data (AUrnTCTotMole, -1);
  Data (zAUrnNDCVC, -1);
  Data (CAlvPPM, -1);
  Print(CPlasTCA, 1);
  Print(AUrnTCTotMole, 1);
  Print(zAUrnNDCVC, 1);
  Print(CAlvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
  Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
  Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
        0.000671);
  Print(CDCVGmol0, 12);      # No detect at 12 hr in males
  Data(CDCVGmol0, 0.000025); # Half the detection limit
  Print(CDCVG_ND, 12);      # No detect at 12 hr in males
  Data(CDCVG_ND, 0);

#
  Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
  Print(RetDose, 1);
  Data(RetDose, -1);
  Print(zAUrnTCA_collect, 1);
  Data(zAUrnTCA_collect, -1);
  Print(AUrnTCOGTCOH_collect, 1);
  Data(AUrnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Male subject 7
  #Subject=19;# 21
  Experiment { # 9
# PROCED M100_5
# Data from Fisher et al. (1998)
# Data from procedure M100_5 (in Bld_M, Exh_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 7
# lnBW=4.29; VFatC=0.84; lnPB=2.35;
# CC= 0;

    BWmeas = 73.2;
    VFatCmeas = 0.18;
    PBmeas = 10.47;
    Conc=NDoses(2, 102.0 0, 0.0 4.0);

# M100_5a (T, CVen),
    Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8);
    Data (CVen, 0.76, 0.86, 1.15, 1.15, 1.23, 0.77, 0.46, 0.34, 0.21, 0.15);

```

```

# M100_5b (T, CTCOH),
    Print (CTCOH, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8, 10, 12, 14, 16.03, 18, 20, 22);
    Data (CTCOH, 0.52, 1.35, 1.87, 2.5, 2.59, 2.58, 2.25, 2.15, 1.98, 1.56, 1.02,
          1.26, 0.89, 0.79, 0.73, 0.7);
# M100_5c (T, CBldTCA),
    Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8, 10, 12, 14, 16.03, 18, 20,
          22, 51, 78.08, 100.83);
    Data (CBldTCA, 0.11, 0.36, 1.07, 1.55, 2.31, 2.03, 2.16, 2.35, 2.53, 3.61, 3.93,
          4.57, 4.5, 5.02, 5.1, 5.07, 5.91, 6.38, 5.33, 4.01);
# M100_5d (T, CALvPPM),
    Print (CALvPPM, 4, 4.25, 4.53, 5, 6, 8, 10);
    Data (CALvPPM, 12.386, 3.305, 2.478, 1.567, 0.577, 0.317, 0.286);
# M100_5e (T, zAurnTCA),
    Print (zAurnTCA, 4.67, 5.05, 6.3, 8.05, 10.07, 12.07, 14.07, 16.15, 18.08, 20.05,
          22.15, 25.33, 31.92, 35.33, 43.58, 51.08, 53.25, 56.92, 58.33,
          59.67, 63.75, 67.42, 73.08, 78, 80.58, 82.75, 84.25, 84.92,
          87.58, 91.83);
    Data (zAurnTCA, 1.36, 1.66, 2.7, 4.22, 6.04, 8.04, 10.37, 13.33, 16.55, 20.04,
          23.89, 30.02, 35.07, 38.42, 43.06, 46.65, 48.88, 54.83, 57.31,
          59.49, 62.36, 66.44, 70.15, 73.57, 75.42, 77.73, 78.87, 80.37,
          83.6, 86.81);
# M100_5f (T, AurnTCOGTCOH),
    Print (AurnTCOGTCOH, 4.67, 5.05, 6.3, 8.05, 10.07, 12.07, 14.07, 16.15, 18.08,
          20.05, 22.15, 25.33, 31.92, 35.33, 43.58, 51.08, 53.25,
          56.92, 58.33, 59.67, 63.75, 67.42, 73.08, 78, 80.58, 82.75,
          84.25, 84.92, 87.58, 91.83);
    Data (AurnTCOGTCOH, 16.05, 18.22, 25.28, 34.46, 43.49, 49.91, 55.78, 59.33, 65.07,
          68.36, 71.48, 76.1, 81.25, 83.82, 86.11, 87.66, 88.38, 89.39,
          89.71, 89.92, 89.92, 90.38, 91.07, 91.55, 91.79, 91.94, 92.03,
          92.22, 92.37, 92.55);
# Total = Free in Fisher data
    Print (TotCTCOH, 1, 2, 3, 4, 4.25, 4.53, 5, 6, 8, 10, 12, 14, 16.03, 18, 20, 22);
    Data (TotCTCOH, 0.52, 1.35, 1.87, 2.5, 2.59, 2.58, 2.25, 2.15, 1.98, 1.56, 1.02,
          1.26, 0.89, 0.79, 0.73, 0.7);
    Data (CPlasTCA, -1);
    Data (AurnTCTotMole, -1);
    Data (zAurnNDCVC, -1);
    Print(CPlasTCA, 1);
    Print(AurnTCTotMole, 1);
    Print(zAurnNDCVC, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
    Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
    Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
          0.000671);
    Print(CDCVGmol0, 12);          # No detect at 12 hr in males
    Data(CDCVGmol0, 0.000025);    # Half the detection limit
    Print(CDCVG_ND, 12);          # No detect at 12 hr in males
    Data(CDCVG_ND, 0);

#
    Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
    Print(RetDose, 1);
    Data(RetDose, -1);
    Print(zAurnTCA_collect, 1);
    Data(zAurnTCA_collect, -1);
    Print(AurnTCOGTCOH_collect, 1);
    Data(AurnTCOGTCOH_collect, -1);
};
}

```

```

Level { # Fisher et al. 1998 Male subject 8
#Subject=20;#22
  Experiment { # 10
# PROCED M100_7
# Data from Fisher et al. (1998)
# Data from procedure M100_7 (in Bld_M, Exh_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 8
# lnBW=4.11; VFatC=0.47;
# CC= 0;
      BWmeas = 60.9;
      VFatCmeas = 0.1;
      Conc=NDoses(2, 101.1 0, 0.0 4.0);

# M100_7a (T, CVen),
      Print (CVen, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5);
      Data (CVen, 0.59, 0.85, 1.1, 1.04, 1.18, 0.64, 0.42, 0.19);
# M100_7b (T, CTCOH),
      Print (CTCOH, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
      Data (CTCOH, 0.28, 0.76, 1.92, 1.69, 2.34, 2.34, 2.16, 2.13, 1.95, 1.61, 1.33,
            1.58, 0.84, 0.77, 0.57, 0.76);
# M100_7c (T, CBldTCA),
      Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03,
            49.75, 73.8, 95.24, 264);
      Data (CBldTCA, 0.36, 0.84, 1.73, 2.6, 3.42, 3.9, 3.67, 4.47, 5, 5.95, 6.74, 7.12,
            7.75, 8.22, 8.17, 9.01, 10.66, 8.6, 7.46, 3.13);
# M100_7d (T, CALvPPM),
      Print (CALvPPM, 4, 4.03, 4.05, 4.08, 4.167, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16,
            18);
      Data (CALvPPM, 21.575, 14.272, 10.77, 7.056, 5.876, 5.773, 5.01, 2.498, 1.713,
            1.263, 1.029, 0.936, 0.809, 0.738, 0.683);
# M100_7e (T, CDCA),
#      Print (CDCA, 1, 2, 4);
#      Data (CDCA, 0.006, 0.008, 0.012);
# M100_7f (T, zAurnTCA),
      Print (zAurnTCA, 4.75, 7.95, 14.08, 16.08, 18.1, 20.25, 24.67, 29.17, 32.67,
            35.33, 38.83, 44.25, 49.67, 55.92, 58.75, 68.25, 73.83, 75.92,
            77.92, 81.17, 82.58, 92.17);
      Data (zAurnTCA, 0.93, 3.02, 5.95, 7.07, 8.28, 9.63, 13.46, 15.73, 20.11, 22.71,
            24.07, 25.6, 27.51, 29.6, 33.36, 39.61, 43.7, 45.78, 48.52, 51.21,
            53.54, 60.72);
# M100_7g (T, AurnTCOGTCOH),
      Print (AurnTCOGTCOH, 4.75, 7.95, 14.08, 16.08, 18.1, 20.25, 24.67, 29.17, 32.67,
            35.33, 38.83, 44.25, 49.67, 55.92, 58.75, 68.25, 73.83,
            75.92, 77.92, 81.17, 82.58, 92.17);
      Data (AurnTCOGTCOH, 40.71, 69.81, 89.76, 96.8, 102.69, 107.93, 121.3, 128.51,
            135.51, 138.05, 140.2, 142.48, 144.47, 144.96, 145.55, 146.67,
            147.09, 147.25, 147.38, 147.5, 147.62, 147.98);
# Total = Free in Fisher data
      Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.3, 4.5, 5, 6, 8, 10, 12, 14, 16, 18, 20.03);
      Data (TotCTCOH, 0.28, 0.76, 1.92, 1.69, 2.34, 2.34, 2.16, 2.13, 1.95, 1.61, 1.33,
            1.58, 0.84, 0.77, 0.57, 0.76);
      Data (CPlasTCA, -1);
      Data (AurnTCTotMole, -1);
      Data (zAurnNDCVC, -1);
      Print(CPlasTCA, 1);
      Print(AurnTCTotMole, 1);
      Print(zAurnNDCVC, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
      Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
      Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
            0.000671);
      Print(CDCVGmol0, 12); # No detect at 12 hr in males
      Data(CDCVGmol0, 0.000025); # Half the detection limit
      Print(CDCVG_ND, 12); # No detect at 12 hr in males
      Data(CDCVG_ND, 0);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);

```

```

#           Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose, -1);
#           Print(zAurnTCA_collect, 1);
#           Data(zAurnTCA_collect, -1);
#           Print(AurnTCOGTCOH_collect, 1);
#           Data(AurnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Male subject 9
#Subject=21;#23
Experiment { # 11
# PROCED M100_8
# Data from Fisher et al. (1998)
# Data from procedure M100_8 (in Bld_M and Urine_M) in HumanB.cmd
# Male 100 ppm exposure
# Male vol 9
# lnBW=4.26; VFatC=0.84;
# CC= 0;
      BWmeas = 70.9;
      VFatCmeas = 0.18;
      Conc=NDoses(2, 103.4 0, 0.0 4.0);

# M100_8a (T, CVen),
      Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20, 22);
      Data (CVen, 2.69, 2.98, 3.51, 3.58, 2.88, 1.96, 1.53, 0.81, 0.52, 0.32, 0.27,
            0.24, 0.22, 0.22, 0.2, 0.16, 0.16);

# M100_8b (T, CTCOH)
      Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20, 22);
      Data (CTCOH, 0.47, 0.68, 1.51, 3.58, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59, 1.28,
            1.23, 1.06, 0.98, 0.72, 0.71);

# M100_8c (T, CBldTCA)
      Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20,
            22, 44.98, 68.9, 93.08, 264);
      Data (CBldTCA, 0.43, 1, 2.15, 3.4, 4.94, 5.42, 5.67, 5.83, 5.99, 7.23, 7.96, 8.14,
            8.39, 8.36, 8.83, 8.96, 9.51, 10.75, 9.21, 7.94, 1.94);

# M100_8d (T, CDCA)
#           Print (CDCA, 2, 3, 4, 4.25, 4.5, 5.75, 8, 16);
#           Data (CDCA, 0.004, 0.01, 0.008, 0.005, 0.005, 0.004, 0.005, 0.005);
# M100_8e (T, zAurnTCA)
      Print (zAurnTCA, 4.58, 5.03, 6.03, 8.05, 10.03, 12.03, 14.07, 16.05, 18.03, 20.02,
            22.08, 45.42, 47.42, 48.92, 50.42, 53.92, 57.33, 59.17, 60.92,
            63.92, 67.92, 74.58, 80.25, 82.42, 84.33, 85.58, 86.92);
      Data (zAurnTCA, 40.02, 40.67, 57.48, 76.6, 99.19, 115.98, 126, 136.55, 143.51,
            150.54, 163.57, 196.37, 197.62, 198.48, 199.33, 201.12, 201.12,
            201.73, 202.15, 202.88, 203.6, 204.11, 204.47, 204.92, 205.07,
            205.15, 205.3);

# M100_8f (T, AurnTCOGTCOH)
      Print (AurnTCOGTCOH, 4.58, 5.03, 6.03, 8.05, 10.03, 12.03, 14.07, 16.05, 18.03,
            20.02, 22.08, 45.42, 47.42, 48.92, 50.42, 53.92, 57.33,
            59.17, 60.92, 63.92, 67.92, 74.58, 80.25, 82.42, 84.33,
            85.58, 86.92);
      Data (AurnTCOGTCOH, 0.935, 1.34, 4.1, 6.1, 9.74, 13.29, 16.29, 20.29, 22.87,
            24.83, 29.98, 56.81, 61.82, 64.84, 67.02, 74.27, 76.87, 78.68,
            61.05, 88.53, 90.31, 92.43, 95.17, 97.12, 100.02, 100.76,
            103.23);

# Total = Free in Fisher data
      Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5.75, 6, 8, 10, 12, 14, 16, 18, 20,
            22);
      Data (TotCTCOH, 0.47, 0.68, 1.51, 3.58, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59,
            1.28, 1.23, 1.06, 0.98, 0.72, 0.71);
      Data (CPlasTCA, -1);

```



```

Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Data (CALvPPM, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);
Print(CALvPPM, 1);

# This is average male data points -- high CV (~0.3, based on peaks)
Print(CDCVGmol, 0.579 1.01 2 3 4.02 4.24 4.5 5.01 6.02 8.01);
Data(CDCVGmol, 0.00886 0.0349 0.0461 0.0337 0.0313 0.0241 0.0132 0.00552 0.00417
      0.000671);
Print(CDCVGmol0, 12); # No detect at 12 hr in males
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 12); # No detect at 12 hr in males
Data(CDCVG_ND, 0);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect, -1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Female subject 1
#Subject=22;#24
Experiment { # 12 ## Low exposure
# PROCED F60_1
# Data from Fisher et al. (1998)
# Data from procedure F60_1 (in Bld50_F and Urin50_F) in HumanB.cmd
# Female 50 ppm exposure
# Female vol 1
# lnBW=4.20; VFatC=1.50; lnPB=2.29;
# CC= 0;

BWmeas = 66.5;
VFatCmeas = 0.32;
PBmeas = 9.88;
Male = 0.0;
Conc=NDoses(2, 55.1 0, 0.0 4.0);

# F60_1a (T, CVen)
Print (CVen, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 6, 8.03);
Data (CVen, 1, 1.29, 1.38, 1.7, 1.72, 1.08, 1.17, 0.55, 0.39, 0.22);
# F60_1b (T, CTCOH)
Print (CTCOH, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 9.98, 12, 14.02, 16, 18.03, 20,
      22);
Data (CTCOH, 0.32, 0.49, 0.85, 0.97, 1.2, 1.14, 1.18, 1.13, 0.7, 0.6, 0.52, 0.55,
      0.54, 0.45, 0.35);
# F60_1c (T, CBldTCA)
Print (CBldTCA, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 6, 8.03, 9.98, 12, 14.02, 16,
      18.03, 20, 22, 44.33, 68.32, 93.38);
Data (CBldTCA, 0.16, 0.46, 1.15, 1.53, 1.9, 2.1, 2.18, 2.13, 2.56, 3.32, 2.83,
      2.98, 3.42, 3.44, 3.31, 4.15, 4.07, 3.7, 3.31, 1.02);

```

```

# F60_1d (T, AUrnTCA)
  Print (zAUrnTCA, 4.58, 5.26, 6.12, 8.12, 10.18, 12.18, 14.32, 16.18, 18.16, 20.25,
          22.53, 23.25, 25.25, 27.58, 29.5, 30.92, 32.92, 35, 39.83, 42,
          43.08, 44.72, 46.5, 49.83, 52, 53.59, 54.53, 56.83, 58.5, 59.25,
          63.83, 68.28, 70.67, 72.78, 74.75, 76.92, 80.33, 81.5, 82.42,
          83.5, 90.25, 91.42, 92.33);
  Data (zAUrnTCA, 0.64, 0.76, 0.85, 1.83, 2.57, 3.36, 3.94, 5.12, 6.03, 6.67, 7.3,
        7.6, 7.96, 8.6, 8.89, 9.21, 9.86, 9.66, 11.19, 11.85, 12.35,
        12.73, 13.49, 14.31, 15.73, 16.12, 16.34, 16.93, 17.24, 17.85,
        18.13, 18.53, 19.18, 19.42, 20, 20.58, 20.79, 20.93, 21.82, 21.37,
        21.56, 21.69, 21.87);

# F60_1e (T, AUrnTCOGTCOH)
  Print (AUrnTCOGTCOH, 4.58, 5.26, 6.12, 8.12, 10.18, 12.18, 14.32, 16.18, 18.16,
        20.25, 22.53, 23.25, 25.25, 27.58, 29.5, 30.92, 32.92, 35,
        39.83, 42, 43.08, 44.72, 46.5, 49.83, 52, 53.59, 54.53,
        56.83, 58.5, 59.25, 63.83, 68.28, 70.67, 72.78, 74.75, 76.92,
        80.33, 81.5, 82.42, 83.5, 90.25, 91.42, 92.33);
  Data (AUrnTCOGTCOH, 20.08, 22.91, 24.87, 28.94, 36.46, 39.14, 42.64, 45.16, 53.64,
        56.34, 57.08, 57.64, 58.45, 60.33, 61.44, 62.83, 67.36, 68.3,
        69.92, 70.88, 71.09, 71.59, 71.99, 72.6, 73.6, 73.93, 74.27,
        74.26, 74.56, 74.71, 74.77, 75.16, 75.34, 75.52, 75.75, 75.81,
        76.05, 76.06, 76.12, 76.15, 76.3, 76.34, 76.39);

# Total = Free in Fisher data
  Print (TotCTCOH, 0.58, 1.02, 2, 3, 4, 4.25, 4.47, 5, 9.98, 12, 14.02, 16, 18.03,
        20, 22);
  Data (TotCTCOH, 0.32, 0.49, 0.85, 0.97, 1.2, 1.14, 1.18, 1.13, 0.7, 0.6, 0.52,
        0.55, 0.54, 0.45, 0.35);
  Data (CPlasTCA, -1);
  Data (AUrnTCTotMole, -1);
  Data (zAUrnNDCVC, -1);
  Data (CALvPPM, -1);
  Print(CPlasTCA, 1);
  Print(AUrnTCTotMole, 1);
  Print(zAUrnNDCVC, 1);
  Print(CALvPPM, 1);

  Print(CDCVGmol, 0);
  Data(CDCVGmol, -1);
  Print(CDCVG_ND, 0);
  Data(CDCVG_ND, -1);

#
  Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
  Print(RetDose, 1);
  Data(RetDose, -1);
  Print(zAUrnTCA_collect, 1);
  Data(zAUrnTCA_collect, -1);
  Print(AUrnTCOGTCOH_collect, 1);
  Data(AUrnTCOGTCOH_collect, -1);
};

#Subject=22;#25
  Experiment { # 13 ## high exposure
# PROCED F100_2
# Data from Fisher et al. (1998)
# Data from procedure F100_2 (in Bld_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 1
# lnBW=4.20; VFatC=1.50; lnPB=2.29;
# CC= 0;

```

```

        BWmeas = 66.5;
        VFatCmeas = 0.32;
        PBmeas = 9.88;
        Male = 0.0;
        Conc=NDoses(2, 101.4 0, 0.0 4.0);

#F100_2a (T, Cven),
    Print (Cven, 0.5, 1, 2, 3, 4, 4.23, 4.5, 5, 6);
    Data (Cven, 1.18, 2.17, 2.3, 2.41, 2.65, 1.84, 1.17, 0.62, 0.38);
# F100_2b (T, CTCOH),
    Print (CTCOH, 1, 2, 3, 4, 4.23, 4.5, 5, 6, 8.05, 10, 12, 14.02, 16, 18, 20,
        22.02);
    Data (CTCOH, 0.74, 1.38, 1.93, 2.41, 2.4, 2.33, 2.17, 1.94, 1.81, 1.38, 1.17,
        1.25, 1.01, 0.88, 0.74, 0.7);
# F100_2c (T, CBldTCA),
    Print (CBldTCA, 2, 3, 4, 4.23, 4.5, 5, 6, 8.05, 10, 12, 14.02, 16, 18, 20, 22.02,
        46.7, 70.25, 93.72);
    Data (CBldTCA, 0.91, 1.75, 2.65, 2.54, 2.65, 2.73, 3.26, 3.58, 4.5, 4.02, 4.17,
        4.45, 4.9, 5.26, 5.94, 6.68, 5.2, 3.6);
# F100_2d (T, zAurnTCA)
    Print (zAurnTCA, 4.37, 5.03, 6.1, 8.1, 10.07, 12.03, 14.1, 16.05, 18.05, 20.06,
        22.15, 24.32, 27.05, 28.3, 30.1, 32.45, 34.2, 36.1, 43.2, 45.4,
        48, 51.4, 54.05, 56.4, 58.2, 59.55, 67.55, 70.2, 72.2, 75, 77.55,
        81.55, 84.1, 89.1, 91.35);
    Data (zAurnTCA, 0.31, 0.39, 0.64, 1.21, 1.66, 2.16, 2.96, 3.66, 4.37, 5.44, 6.66,
        7.63, 8.16, 8.71, 10.3, 10.92, 11.77, 12.45, 13.71, 14.04, 15.07,
        15.98, 16.51, 17, 17.6, 19.57, 19.76, 20.25, 21.31, 22.08, 22.65,
        24.79, 30.86, 31.05, 31.06);
# F100_2e (T, AurnTCOGTCOH)
    Print (AurnTCOGTCOH, 4.37, 5.03, 6.1, 8.1, 10.07, 12.03, 14.1, 16.05, 18.05,
        20.06, 22.15, 24.32, 27.05, 28.3, 30.1, 32.45, 34.2, 36.1,
        43.2, 45.4, 48, 51.4, 54.05, 56.4, 58.2, 59.55, 67.55, 70.2,
        72.2, 75, 77.55, 81.55, 84.1, 89.1, 91.35);
    Data (AurnTCOGTCOH, 35.78, 44.4, 54.4, 72.58, 90.61, 104.44, 116.9, 127.49,
        127.49, 136.49, 144.45, 147.89, 150.61, 154.52, 157.72,
        160.74, 163.47, 165.86, 167.54, 168.21, 169.24, 170.26,
        171.66, 172.85, 173.7, 175.02, 175.31, 175.67, 176.21, 176.6,
        177.07, 178.04, 178.43, 178.65, 178.94);
# Total = Free in Fisher data
    Print (TotCTCOH, 1, 2, 3, 4, 4.23, 4.5, 5, 6, 8.05, 10, 12, 14.02, 16, 18, 20,
        22.02);
    Data (TotCTCOH, 0.74, 1.38, 1.93, 2.41, 2.4, 2.33, 2.17, 1.94, 1.81, 1.38, 1.17,
        1.25, 1.01, 0.88, 0.74, 0.7);
    Data (CPlasTCA, -1);
    Data (AurnTCTotMole, -1);
    Data (zAurnNDCVC, -1);
    Data (CALvPPM, -1);
    Print(CPlasTCA, 1);
    Print(AurnTCTotMole, 1);
    Print(zAurnNDCVC, 1);
    Print(CALvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
    Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
    Data(CDCVGmol,0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074);
    Print(CDCVGmol0, 10);          # No detect at 10 hr in females
    Data(CDCVGmol0, 0.000025); # Half the detection limit
    Print(CDCVG_ND, 10);          # No detect at 10 hr in females
    Data(CDCVG_ND, 0);

#
    Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);

```

```

#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose, -1);
#           Print(zAurnTCA_collect, 1);
#           Data(zAurnTCA_collect, -1);
#           Print(AurnTCOGTCOH_collect, 1);
#           Data(AurnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Female subject 2
#Subject=23;#26
Experiment { # 14 ## Low exposure
# PROCED F50_1
# Data from Fisher et al. (1998)
# Data from procedure F50_1 (in Bld50_F and Urin50_F) in HumanB.cmd
# Female 50 ppm exposure, n=2
# Female vol 2
# lnBW=4.13; VFatC=1.12; lnPB=2.25;
# CC= 0;

      BWmeas = 62.3;
      VFatCmeas = 0.24;
      PBmeas = 9.45;
      Male = 0.0;
      Conc=NDoses(2, 53.0 0, 0.0 4.0);

# F50_1a (T, CVen)
      Print (CVen, 0.5, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6);
      Data (CVen, 0.93, 1.33, 1.65, 1.85, 1.45, 0.94, 0.63, 0.32, 0.18);
# F50_1b (T, CTCOH)
      Print (CTCOH, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6, 8, 10, 12, 14, 16.05, 18, 22);
      Data (CTCOH, 0.33, 0.63, 0.79, 0.98, 0.83, 0.83, 0.9, 0.89, 0.76, 0.66, 0.67,
            0.54, 0.48, 0.47, 0.35);
# F50_1c (T, CBldTCA)
      Print (CBldTCA, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6, 8, 10, 12, 14, 16.05, 18, 20.02,
            22, 44.92, 68.86, 100.44);
      Data (CBldTCA, 0.38, 1.23, 1.96, 2.8, 2.81, 3.23, 3.34, 3.72, 4.88, 4.93, 5.28,
            5.18, 5.37, 6.03, 4.87, 6.66, 6.66, 5.27, 2.27);
# F50_1d (T, AurnTCA)
      Print (zAurnTCA, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17, 22.17,
            25, 29.83, 37.83, 44.83, 49.67, 53.33, 61.23, 62.83, 67.92,
            75.75, 79.63, 96.67, 96.92);
      Data (zAurnTCA, 1.35, 4.49, 7.17, 9.38, 10.36, 11.91, 13.46, 14.7, 15.64, 16.49,
            22.11, 23.27, 26.03, 27.35, 33.94, 35.83, 42.58, 43.36, 50.68,
            52.36, 53.79, 54.16, 55.93);
# F50_1e (T, AurnTCOGTCOH)
      Print (AurnTCOGTCOH, 5.25, 5.97, 8, 10.17, 12.17, 14.17, 16.17, 18.17, 20.17,
            22.17, 25, 29.83, 37.83, 44.83, 49.67, 53.33, 61.23, 62.83,
            67.92, 75.75, 79.63, 96.67, 96.92);
      Data (AurnTCOGTCOH, 4.42, 6.71, 12, 15.4, 16.73, 20.35, 23.49, 25.44, 25.44,
            26.96, 30.55, 32.71, 34.38, 34.88, 37.25, 38.53, 41.16, 41.38,
            43.01, 43.29, 43.53, 43.66, 43.85);

# Total = Free in Fisher data
      Print (TotCTCOH, 1, 2, 3, 4, 4.27, 4.55, 5.1, 6, 8, 10, 12, 14, 16.05, 18, 22);
      Data (TotCTCOH, 0.33, 0.63, 0.79, 0.98, 0.83, 0.83, 0.9, 0.89, 0.76, 0.66, 0.67,
            0.54, 0.48, 0.47, 0.35);
      Data (CPlasTCA, -1);
      Data (AurnTCTotMole, -1);
      Data (zAurnNDCVC, -1);
      Data (CAlvPPM, -1);
      Print(CPlasTCA, 1);
      Print(AurnTCTotMole, 1);
      Print(zAurnNDCVC, 1);
      Print(CAlvPPM, 1);

      Print(CDCVGmol, 0);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 0);
      Data(CDCVG_ND, -1);

```

```

#           Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose, -1);
#           Print(zAurnTCA_collect, 1);
#           Data(zAurnTCA_collect, -1);
#           Print(AurnTCOGTCOH_collect, 1);
#           Data(AurnTCOGTCOH_collect, -1);
};

#Subject=23;#27
Experiment { # 15 ## High exposure
# PROCED F100_6
# Data from Fisher et al. (1998)
# Data from procedure F100_6 (in Bld_F, Exh_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 2
# lnBW=4.13; VFatC=1.12; lnPB=2.25;
# CC= 0;

#           BWmeas = 62.3;
#           VFatCmeas = 0.24;
#           PBmeas = 9.45;
#           Male = 0.0;
#           Conc=NDoses(2, 97.7 0, 0.0 4.0);

# F100_6a (T, CVen)
#           Print (CVen, 0.5, 1, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10);
#           Data (CVen, 0.83, 0.99, 1.2, 1.59, 2.03, 1.33, 0.87, 0.42, 0.21, 0.22, 0.15);
# F100_6b (T, CTCOH),
#           Print (CTCOH, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03, 16.03, 18.07, 20);
#           Data (CTCOH, 0.53, 0.83, 1.27, 0.92, 0.85, 1.17, 1.03, 0.86, 0.8, 0.71, 0.62,
#           0.55, 0.48, 0.41);
# F100_6c (T, CBldTCA),
#           Print (CBldTCA, 0.5, 1, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03, 16.03,
#           18.07, 20, 22, 47.95, 71.98, 101.22);
#           Data (CBldTCA, 0.44, 0.97, 2.16, 3.79, 5.12, 5.35, 5.6, 5.88, 6.55, 7.3, 7.66,
#           8.61, 8.73, 9.65, 8.29, 8.6, 10.2, 6.15, 7.11, 6.73);
# F100_6d (T, CALvPPM),
#           Print (CALvPPM, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03);
#           Data (CALvPPM, 22.398, 7.317, 5.917, 2.903, 1.382, 0.982, 0.691, 0.524, 0.428);
# F100_6e (T, CDCA),
#           Print (CDCA, 1, 2.03, 3);
#           Data (CDCA, 0.005, 0.014, 0.005);
# F100_6f (T, zAurnTCA),
#           Print (zAurnTCA, 4.55, 5.12, 6.08, 8.19, 10.19, 12.17, 14.33, 16.23, 18.19, 20.13,
#           22.38, 31.92, 34.25, 36.92, 48.67, 55.83, 59, 63.5, 70.8, 76,
#           85.5, 87.25, 88.08, 94.75);
#           Data (zAurnTCA, 0.3, 0.56, 1.75, 1.97, 3.75, 6.58, 6.81, 8.64, 10.3, 12.13, 13.64,
#           15.77, 18.03, 18.16, 22.69, 28.52, 30.85, 31.36, 33.88, 37.2,
#           41.32, 42.86, 49.42, 54.14);
# F100_6g (T, AurnTCOGTCOH),
#           Print (AurnTCOGTCOH, 4.55, 5.12, 6.08, 8.19, 10.19, 12.17, 14.33, 16.23, 18.19,
#           20.13, 22.38, 31.92, 34.25, 36.92, 48.67, 55.83, 59, 63.5,
#           70.8, 76, 85.5, 87.25, 88.08, 94.75);
#           Data (AurnTCOGTCOH, 11.67, 14.56, 20.78, 25.55, 34.83, 45.33, 45.98, 54.21, 60.91,
#           68.01, 73.35, 75.14, 79.52, 79.97, 85.95, 90.84, 91.82, 92.13,
#           92.13, 95.09, 96.05, 96.34, 96.45, 97.45);
# Total = Free in Fisher data
#           Print (TotCTCOH, 2.03, 3, 4.03, 4.25, 4.5, 5, 6, 8, 10, 12, 14.03, 16.03, 18.07,
#           20);

```

```

        Data (TotCTCOH, 0.53, 0.83, 1.27, 0.92, 0.85, 1.17, 1.03, 0.86, 0.8, 0.71, 0.62,
              0.55, 0.48, 0.41);
        Data (CPlasTCA, -1);
        Data (AUrnTCTotMole, -1);
        Data (zAUrnNDCVC, -1);
        Print(CPlasTCA, 1);
        Print(AUrnTCTotMole, 1);
        Print(zAUrnNDCVC, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
        Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
        Data(CDCVGmol,0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074);
        Print(CDCVGmol0, 10);          # No detect at 10 hr in females
        Data(CDCVGmol0, 0.000025); # Half the detection limit
        Print(CDCVG_ND, 10);          # No detect at 10 hr in females
        Data(CDCVG_ND, 0);

#
        Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
        Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
        Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
        Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
        Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
        Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
        Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
        Print(RetDose, 1);
        Data(RetDose,-1);
        Print(zAUrnTCA_collect, 1);
        Data(zAUrnTCA_collect,-1);
        Print(AUrnTCOGTCOH_collect, 1);
        Data(AUrnTCOGTCOH_collect,-1);
    };
}

Level { # Fisher et al. 1998 Female subject 3
    #Subject=24;#28
    Experiment { # 16
# PROCED F100_1
# Data from Fisher et al. (1998)
# Data from procedure F100_1 (in Bld_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 3
# lnBW=4.05; VFatC=0.98; lnPB=1.87;
# CC= 0;
        BWmeas = 57.5;
        VFatCmeas = 0.21;
        PBmeas = 6.47;
        Male = 0.0;
        Conc=NDoses(2, 102.5 0, 0.0 4.0);

# F100_1a (T, CVen)
        Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6);
        Data (CVen, 1.11, 1.36, 2.11, 1.92, 2.3, 1.56, 1.26, 0.73, 0.42);
# F100_1b (T, CTCOH)
        Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16.05, 18, 20.02,
              22.02, 46.17);
        Data (CTCOH, 0.22, 0.46, 1.18, 2.18, 3.03, 3.29, 3.67, 3.13, 2.57, 2.46, 1.93,
              1.57, 1.3, 1.08, 0.89, 0.56, 0.65, 0.3);
# F100_1c (T, CBldTCA),
        Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16.05, 18, 20.02,
              22.02, 46.17, 69.83, 94.67);
        Data (CBldTCA, 0.21, 0.39, 1.05, 1.86, 3.46, 3.78, 3.91, 4.22, 4.67, 5.71, 6.29,
              7.76, 7.78, 8.11, 8.79, 9.05, 9.34, 9.58, 7.93, 6.69);
# F100_1d (T, zAUrnTCA),
        Print (zAUrnTCA, 4.62, 5.08, 6.86, 8.33, 10.25, 12.13, 14.08, 16.15, 18, 20.05,
              22.17, 30.67, 33.67, 35.42, 40.67, 46.67, 47.17, 52.33, 55.25, 68.17,
              69.75, 73.92, 76, 78.17, 80.33, 81.5, 82.25, 92.58, 93.67, 94.17);
    }
}

```

```

        Data (zAurnTCA, 0.51, 0.65, 1.26, 1.85, 2.92, 3.91, 4.92, 5.91, 5.91, 7.12, 9.55,
              15.22, 17.85, 19.66, 24.08, 26.68, 27.91, 30.49, 35.74, 35.75,
              36.78, 37.71, 41.25, 45.21, 46.43, 47.22, 47.91, 49.66, 50.98,
              51.67);
# F100_1e (T, AurnTCOGTCOH),
    Print (AurnTCOGTCOH, 4.62, 5.08, 6.86, 8.33, 10.25, 12.13, 14.08, 16.15, 18,
           20.05, 22.17, 30.67, 33.67, 35.42, 40.67, 46.67, 47.17,
           52.33, 55.25, 68.17, 69.75, 73.92, 76, 78.17, 80.33, 81.5,
           82.25, 92.58, 93.67, 94.17);
    Data (AurnTCOGTCOH, 44.83, 52.08, 77.84, 89.76, 108.58, 122.65, 133.38, 140.85,
          147.19, 151.76, 155.86, 169.38, 174.67, 175.78, 179.31,
          179.77, 179.97, 180.44, 181.52, 184.09, 184.16, 184.26, 184.7,
          185.2, 185.35, 185.42, 185.51, 185.81, 185.91, 185.95);
# Total = Free in Fisher data
    Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8, 10, 12, 14, 16.05, 18,
           20.02, 22.02, 46.17);
    Data (TotCTCOH, 0.22, 0.46, 1.18, 2.18, 3.03, 3.29, 3.67, 3.13, 2.57, 2.46, 1.93,
           1.57, 1.3, 1.08, 0.89, 0.56, 0.65, 0.3);
    Data (CPlasTCA, -1);
    Data (AurnTCTotMole, -1);
    Data (zAurnNDCVC, -1);
    Data (CALvPPM, -1);
    Print(CPlasTCA, 1);
    Print(AurnTCTotMole, 1);
    Print(zAurnNDCVC, 1);
    Print(CALvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
    Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
    Data(CDCVGmol, 0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074
);
    Print(CDCVGmol0, 10);          # No detect at 10 hr in females
    Data(CDCVGmol0, 0.000025); # Half the detection limit
    Print(CDCVG_ND, 10);          # No detect at 10 hr in females
    Data(CDCVG_ND, 0);

#
    Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
    Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
    Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
    Print(RetDose, 1);
    Data(RetDose, -1);
    Print(zAurnTCA_collect, 1);
    Data(zAurnTCA_collect, -1);
    Print(AurnTCOGTCOH_collect, 1);
    Data(AurnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Female subject 4
#Subject=25;#29
    Experiment { # 17
# PROCED F100_3
# Data from Fisher et al. (1998)
# Data from procedure F100_3 (in Bld_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 4
# lnBW=4.02; VFatC=1.07; lnPB=2.03;
# CC= 0;

        BWmeas = 55.5;
        VFatCmeas = 0.23;
        PBmeas = 7.63;

```

```

Male = 0.0;
Conc=NDoses(2, 102.0 0, 0.0 4.0);

# F100_3a (T, CVen)
Print (CVen, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02);
Data (CVen, 0.81, 0.88, 1.09, 1.03, 1.13, 0.59, 0.47, 0.3, 0.18, 0.15);

# F100_3b (T, CTCOH)
Print (CTCOH, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02, 10.02, 12.02, 14.03, 16,
18, 20, 22);
Data (CTCOH, 0.33, 0.57, 1.01, 1.25, 1.79, 1.64, 1.54, 1.43, 1.27, 0.95, 1.01,
0.9, 0.88, 0.74, 0.69, 0.63, 0.61);

# F100_3c (T, CBldTCA)
Print (CBldTCA, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02, 10.02, 12.02, 14.03, 16,
18, 20, 22, 46.08, 75.67, 94.25);
Data (CBldTCA, 0.4, 0.97, 1.72, 2.64, 3.41, 3.62, 3.86, 4.39, 4.8, 5.73, 6.79,
7.55, 7.68, 7.98, 9.27, 8.91, 9.12, 11.31, 10.49, 8.47);

# F100_3d (T, zAurnTCA)
Print (zAurnTCA, 4.58, 6.03, 8.12, 10.08, 12.1, 14.1, 16.05, 18.1, 20.05, 21.92,
26.17, 33.25, 37.92, 44.92, 49, 54.92, 58.42, 61.42, 66.42,
70.67, 74.75, 80.42, 82.42, 84.92, 93.42);
Data (zAurnTCA, 0.44, 0.71, 1.31, 2.28, 3.48, 4.64, 5.64, 6.76, 7.66, 8.89, 10.64,
13.81, 14.11, 15.44, 16, 23.2, 22.4, 24.1, 29.1, 32.6, 36.2, 36.8,
37.5, 37.79, 45.72);

# F100_3e (T, AurnTCOGTCOH)
Print (AurnTCOGTCOH, 4.58, 6.03, 8.12, 10.08, 12.1, 14.1, 16.05, 18.1, 20.05,
21.92, 26.17, 33.25, 37.92, 44.92, 49, 54.92, 58.42, 61.42,
66.42, 70.67, 74.75, 80.42, 82.42, 84.92, 93.42);
Data (AurnTCOGTCOH, 12.63, 17.83, 26.05, 30.4, 36.72, 41.26, 44.27, 47.94, 50.31,
53.17, 57.9, 65.27, 65.8, 69.74, 69.74, 72.07, 73.58, 75.39,
76.98, 79.89, 80.98, 82.2, 82.57, 82.74, 83.41);

# Total = Free in Fisher data
Print (TotCTCOH, 0.58, 1, 2, 3, 4, 4.17, 4.5, 5, 6, 8.02, 10.02, 12.02, 14.03, 16,
18, 20, 22);
Data (TotCTCOH, 0.33, 0.57, 1.01, 1.25, 1.79, 1.64, 1.54, 1.43, 1.27, 0.95, 1.01,
0.9, 0.88, 0.74, 0.69, 0.63, 0.61);
Data (CPlasTCA, -1);
Data (AurnTCTotMole, -1);
Data (zAurnNDCVC, -1);
Data (CALvPPM, -1);
Print(CPlasTCA, 1);
Print(AurnTCTotMole, 1);
Print(zAurnNDCVC, 1);
Print(CALvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
Data(CDCVGmol, 0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074);
Print(CDCVGmol0, 10); # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10); # No detect at 10 hr in females
Data(CDCVG_ND, 0);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAurnTCA_collect, 1);
Data(zAurnTCA_collect, -1);
Print(AurnTCOGTCOH_collect, 1);
Data(AurnTCOGTCOH_collect, -1);
};

```



```

}

Level { # Fisher et al. 1998 Female subject 5
#Subject=26;#30
Experiment { # 18
# PROCED F100_5
# Data from Fisher et al. (1998)
# Data from procedure F100_5 (in Bld_F, Exh_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 5
# lnBW=4.21; VFatC=1.64; lnPB=2.40;
# CC= 0;

      BWmeas = 67.3;
      VFatCmeas = 0.35;
      PBmeas = 11.0;
      Male = 0.0;
      Conc=NDoses(2, 102.0 0, 0.0 4.0);

# F100_5a (T, CVen),
      Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.55, 5, 6.02, 8.02);
      Data (CVen, 0.74, 1, 1.27, 1.45, 1.19, 0.81, 0.66, 0.46, 0.25, 0.19);
# F100_5b (T, CTCOH),
      Print (CTCOH, 1, 2, 3, 4, 4.25, 4.55, 5, 8.02, 10, 12, 14, 18.02, 20);
      Data (CTCOH, 0.41, 0.78, 1.04, 1.18, 1.17, 1.18, 1.18, 0.84, 0.72, 0.82, 0.56,
            0.49, 0.41);
# F100_5c (T, CBldTCA),
      Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.55, 5, 6.02, 8.02, 10, 12, 14, 18.02, 20,
            22, 46.58, 70.5);
      Data (CBldTCA, 0.25, 0.76, 1.48, 2.21, 2.79, 2.78, 3.12, 3.23, 3.52, 4.76, 4.95,
            5.29, 5.33, 6.46, 6.91, 7.1, 6.63, 5.28);
# F100_5d (T, CALVPPM),
      Print (CALVPPM, 4.25, 4.55, 5, 6.02, 8.02, 10, 12, 14);
      Data (CALVPPM, 4.243, 2.798, 1.849, 1.467, 0.681, 0.452, 0.409, 0.356);
# F100_5e (T, zAurnTCA)
      Print (zAurnTCA, 4.67, 5, 6.3, 8.08, 10.08, 12.07, 14.08, 16.12, 18.11, 20.1,
            22.12, 22.67, 26.5, 29.67, 34.17, 35.67, 40.67, 43.67, 47.17,
            49.67, 53.42, 56.17, 58, 59.67, 60.17, 61.67, 67.67, 72.67,
            76.67, 82.67, 84.17, 85.67, 91.67);
      Data (zAurnTCA, 0.69, 0.8, 1.64, 3.16, 4.95, 7.19, 9.89, 13.14, 17.46, 21.67,
            26.4, 29.05, 35.18, 41.73, 49.36, 50.76, 56.47, 60.68, 69, 73.32,
            76.81, 79.16, 81.7, 83.84, 84.56, 86.11, 91.59, 95.63, 100.35,
            110.14, 111.45, 112.62, 115.92);
# F100_5f (T, AurnTCOGTCOH)
      Print (AurnTCOGTCOH, 4.67, 5, 6.3, 8.08, 10.08, 12.07, 14.08, 16.12, 18.11, 20.1,
            22.12, 22.67, 26.5, 29.67, 34.17, 35.67, 40.67, 43.67, 47.17,
            49.67, 53.42, 56.17, 58, 59.67, 60.17, 61.67, 67.67, 72.67,
            76.67, 82.67, 84.17, 85.67, 91.67);
      Data (AurnTCOGTCOH, 9.98, 9.98, 12.41, 16.09, 18.99, 20.96, 23.08, 24.46, 26.22,
            27.92, 29.05, 29.64, 32.31, 34.4, 36.58, 37.14, 38.8, 39.86,
            40.61, 41.58, 42.31, 42.94, 43.3, 43.53, 43.6, 43.78, 44.79,
            45.19, 45.69, 46.42, 46.54, 46.6, 47.13);

# Total = Free in Fisher data
      Print (TotCTCOH, 1, 2, 3, 4, 4.25, 4.55, 5, 8.02, 10, 12, 14, 18.02, 20);
      Data (TotCTCOH, 0.41, 0.78, 1.04, 1.18, 1.17, 1.18, 1.18, 0.84, 0.72, 0.82, 0.56,
            0.49, 0.41);
      Data (CPlasTCA, -1);
      Data (AurnTCTotMole, -1);
      Data (zAurnNDCVC, -1);
      Print(CPlasTCA, 1);
      Print(AurnTCTotMole, 1);
      Print(zAurnNDCVC, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
      Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
      Data(CDCVGmol,0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074);
      Print(CDCVGmol0, 10);          # No detect at 10 hr in females
      Data(CDCVGmol0, 0.000025);    # Half the detection limit
      Print(CDCVG_ND, 10);          # No detect at 10 hr in females
      Data(CDCVG_ND, 0);

```

```

#           Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose, -1);
#           Print(zAurnTCA_collect, 1);
#           Data(zAurnTCA_collect, -1);
#           Print(AurnTCOGTCOH_collect, 1);
#           Data(AurnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Female subject 6
#Subject=27;#31
  Experiment { # 19
# PROCED F100_7
# Data from Fisher et al. (1998)
# Data from procedure F100_7 (in Bld_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 6
# lnBW=4.15; VFatC=1.21;
# CC= 0;

    BWmeas = 63.2;
    VFatCmeas = 0.26;
    Male = 0.0;
    Conc=NDoses(2, 101.0 0, 0.0 4.0);

# F100_7a (T, CVen),
    Print (CVen, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5);
    Data (CVen, 0.53, 1, 0.97, 1.31, 1.48, 0.84, 0.58, 0.39);
# F100_7b (T, CTCOH)
    Print (CTCOH, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5, 6.05, 8, 10, 12);
    Data (CTCOH, 0.35, 0.58, 0.86, 1.6, 2.03, 2.04, 1.93, 1.95, 1.79, 1.29, 1.14,
          1.03);
# F100_7c (T, CBldTCA)
    Print (CBldTCA, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5, 6.05, 8, 10, 12, 46.75, 73.97,
          95.42);
    Data (CBldTCA, 0.39, 1.08, 1.9, 3.83, 4.48, 4.65, 4.8, 4.73, 6.02, 6.02, 7.12,
          7.13, 9.1, 6.92, 6.14);
# F100_7d (T, zAurnTCA)
    Print (zAurnTCA, 4.67, 5.17, 6.25, 8.08, 10.13, 12.08, 14.12, 16.02, 18.02, 20.17,
          25.27, 25.75, 30, 34.5, 37.92, 45.08, 49.33, 56.92, 60.42, 68.33,
          72.58, 80.5, 84.33, 86.17, 93.5);
    Data (zAurnTCA, 2.51, 3.07, 6.21, 9.97, 13.01, 16.35, 20.65, 23.23, 26.31, 26.31,
          34.28, 34.84, 42.19, 51.62, 61.19, 75.52, 81.43, 92.21, 104.12,
          116.32, 121.17, 131.94, 134.71, 136.09, 142.3);
# F100_7e (T, AurnTCOGTCOH)
    Print (AurnTCOGTCOH, 4.67, 5.17, 6.25, 8.08, 10.13, 12.08, 14.12, 16.02, 18.02,
          20.17, 25.27, 25.75, 30, 34.5, 37.92, 45.08, 49.33, 56.92,
          60.42, 68.33, 72.58, 80.5, 84.33, 86.17, 93.5);
    Data (AurnTCOGTCOH, 37.76, 42.18, 48.68, 60.91, 72.32, 81.05, 86.76, 94.78,
          100.92, 105.91, 115.12, 116.22, 125.29, 131.36, 135.91,
          143.62, 146.34, 149.7, 151.17, 153.38, 154.28, 155.7, 155.93,
          156.09, 156.7);
# Total = Free in Fisher data
    Print (TotCTCOH, 0.52, 1, 2, 3, 4, 4.28, 4.5, 5, 6.05, 8, 10, 12);
    Data (TotCTCOH, 0.35, 0.58, 0.86, 1.6, 2.03, 2.04, 1.93, 1.95, 1.79, 1.29, 1.14,
          1.03);
    Data (CPlasTCA, -1);
    Data (AurnTCOTotMole, -1);
    Data (zAurnNDCVC, -1);
  }
}

```

```

Data (CALvPPM, -1);
Print(CPlasTCA, 1);
Print(AUrntCTotMole, 1);
Print(zAUrnNDCVC, 1);
Print(CALvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
Data(CDCVGmol,0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074);
Print(CDCVGmol0, 10); # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10); # No detect at 10 hr in females
Data(CDCVG_ND, 0);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose,-1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect,-1);
Print(AUrntCOGTCOH_collect, 1);
Data(AUrntCOGTCOH_collect,-1);
};
}

Level { # Fisher et al. 1998 Female subject 7
#Subject=28;#32
Experiment { # 20
# PROCED F100_8
# Data from Fisher et al. (1998)
# Data from procedure F100_8 (in Bld_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 7
# lnBW=3.88; VFatC=1.07;
# CC= 0;

BWmeas = 48.6;
VFatCmeas = 0.23;
Male = 0.0;
Conc=NDoses(2, 103.3 0, 0.0 4.0);

# F100_8a (T, CVen)
Print (CVen, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03);
Data (CVen, 1.32, 1.68, 1.86, 2.37, 2.66, 2.1, 1.23, 0.83, 0.42, 0.33, 0.3);
# F100_8b (T, CTCOH)
Print (CTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03, 12.05, 14.02, 16, 18,
20, 22);
Data (CTCOH, 0.47, 0.68, 1.51, 2.15, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59, 1.28,
1.23, 1.1, 0.98, 0.72, 0.71);
# F100_8c (T, CBldTCA)
Print (CBldTCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03, 12.05, 14.02, 16,
18, 20, 22, 45.03, 69.03, 93.13, 264);
Data (CBldTCA, 0.27, 0.7, 1.48, 2.8, 3.92, 3.86, 3.98, 4.55, 4.8, 5.96, 6.09,
6.41, 7.01, 7.23, 7.57, 7.68, 8.46, 8.75, 7.73, 5.72, 0.53);
# F100_8d (T, CDCA)
Print (CDCA, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 12.05, 16, 18, 22, 45.03,
69.03);
Data (CDCA, 0.008, 0.008, 0.007, 0.007, 0.006, 0.009, 0.013, 0.012, 0.011, 0.005,
0.005, 0.004, 0.004, 0.005, 0.006, 0.004);

```

```

# F100_8e (T, zAurnTCA)
  Print (zAurnTCA, 4.58, 5.05, 6.05, 8.08, 10.07, 12.08, 14.31, 16.05, 18.05, 20.03,
    22.08, 43.33, 45.58, 47.58, 49.17, 53.58, 61.33, 67.33, 70.58,
    74.58, 77.25, 83.25, 84.25, 85.17, 90.5);
  Data (zAurnTCA, 2.34, 2.92, 5.27, 8.33, 12.15, 17.02, 21.46, 26.02, 28.88, 32.6,
    37.96, 80.45, 85.25, 87.93, 91.55, 99.63, 110.21, 114.43, 118.52,
    123.23, 128.78, 133.51, 134.95, 136.29, 143.83);

# F100_8f (T, AurnTCOGTCOH)
  Print (AurnTCOGTCOH, 4.58, 5.05, 6.05, 8.08, 10.07, 12.08, 14.31, 16.05, 18.05,
    20.03, 22.08, 43.33, 45.58, 47.58, 49.17, 53.58, 61.33,
    67.33, 70.58, 74.58, 77.25, 83.25, 84.25, 85.17, 90.5);
  Data (AurnTCOGTCOH, 15.54, 18.22, 24.58, 33.76, 41.25, 47.8, 54.36, 59.99, 63.23,
    68.23, 73.9, 110.18, 112.61, 113.7, 115.14, 118.2, 122.07,
    124.3, 125.29, 126.29, 127.48, 128.07, 128.31, 128.49,
    129.56);

# Total = Free in Fisher data
  Print (TotCTCOH, 0.5, 1, 2, 3, 4, 4.25, 4.5, 5, 6, 8.05, 10.03, 12.05, 14.02, 16,
    18, 20, 22);
  Data (TotCTCOH, 0.47, 0.68, 1.51, 2.15, 2.72, 2.87, 2.77, 2.63, 2.3, 1.9, 1.59,
    1.28, 1.23, 1.1, 0.98, 0.72, 0.71);
  Data (CPlasTCA, -1);
  Data (AurnTCTotMole, -1);
  Data (zAurnNDCVC, -1);
  Data (CALvPPM, -1);
  Print(CPlasTCA, 1);
  Print(AurnTCTotMole, 1);
  Print(zAurnNDCVC, 1);
  Print(CALvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
  Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
  Data(CDCVGmol,0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074);
  Print(CDCVGmol0, 10);      # No detect at 10 hr in females
  Data(CDCVGmol0, 0.000025); # Half the detection limit
  Print(CDCVG_ND, 10);      # No detect at 10 hr in females
  Data(CDCVG_ND, 0);

#
  Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
  Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
  Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
  Print(RetDose, 1);
  Data(RetDose, -1);
  Print(zAurnTCA_collect, 1);
  Data(zAurnTCA_collect, -1);
  Print(AurnTCOGTCOH_collect, 1);
  Data(AurnTCOGTCOH_collect, -1);
};
}

Level { # Fisher et al. 1998 Female subject 8
  #Subject=29;#33
  Experiment { # 21
# PROCED F100_4
# Data from Fisher et al. (1998)
# Data from procedure F100_4 (in Bld_F and Urine_F) in HumanB.cmd
# Female 100 ppm exposure
# Female vol 8
# lnBW=4.12; VFatC=1.54; lnPB=2.34;
# CC= 0;

    BWmeas = 61.8;
    VFatCmeas = 0.33;

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```

PBmeas = 10.37;
Male = 0.0;
Conc=NDoses(2, 102.0 0, 0.0 4.0);

# F100_4a (T, CVen)
Print (CVen, 0.55, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6);
Data (CVen, 0.55, 0.81, 1.3, 1.37, 1.43, 0.81, 0.54, 0.35, 0.18);

# F100_4b (T, CTCOH)
Print (CTCOH, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6, 8.05, 10.08, 14.03, 18.02,
22.02);
Data (CTCOH, 0.39, 1.2, 1.59, 1.93, 1.97, 1.75, 1.63, 1.32, 1.1, 0.91, 0.83, 0.69,
0.54);

# F100_4c (T, CBldTCA)
Print (CBldTCA, 0.55, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6, 8.05, 10.08, 14.03,
18.02, 22.02, 46.08, 75.67, 94.25);
Data (CBldTCA, 0.47, 1.05, 2.73, 3.85, 4.82, 5.02, 5.29, 5.37, 6.01, 7.6, 6.77,
8.65, 9.49, 10.64, 9.58, 8.55, 7.82);

# F100_4d (T, zAurnTCA),
Print (zAurnTCA, 2.33, 4.57, 5.12, 6.12, 8.12, 10.33, 12.08, 14.12, 16, 18.08, 20,
21.92, 25.08, 29.25, 32.58, 35.83, 38.33, 41, 45, 48.83, 50.33,
53.67, 56.33, 59.33, 66.83, 73.25, 80.58, 83.5, 86, 93);
Data (zAurnTCA, 0.29, 1.62, 2.09, 4.01, 5.81, 8.27, 10.21, 13.06, 16.29, 19.09,
21.96, 24.17, 27.09, 29.05, 35.13, 45.84, 56.12, 65.21, 75.98,
81.05, 83.74, 87.89, 91.72, 97.13, 100.34, 102.88, 106.5, 110.02,
113.61, 117.51);

# F100_4e (T, AurnTCOGTCOH),
Print (AurnTCOGTCOH, 2.33, 4.57, 5.12, 6.12, 8.12, 10.33, 12.08, 14.12, 16, 18.08,
20, 21.92, 25.08, 29.25, 32.58, 35.83, 38.33, 41, 45, 48.83,
50.33, 53.67, 56.33, 59.33, 66.83, 73.25, 80.58, 83.5, 86,
93);
Data (AurnTCOGTCOH, 4.52, 8.37, 12.49, 19.46, 29.26, 35.93, 40.21, 44.9, 48.15,
51.04, 55.72, 58.76, 60.75, 62.24, 72.07, 76.15, 79.24, 81.48,
83.84, 86.37, 87.44, 88.84, 90.9, 92.91, 94.07, 94.96, 96.17,
96.82, 97.41, 98.54);

# Total = Free in Fisher data
Print (TotCTCOH, 1, 2.12, 3.05, 4, 4.25, 4.5, 5, 6, 8.05, 10.08, 14.03, 18.02,
22.02);
Data (TotCTCOH, 0.39, 1.2, 1.59, 1.93, 1.97, 1.75, 1.63, 1.32, 1.1, 0.91, 0.83,
0.69, 0.54);
Data (CPlasTCA, -1);
Data (AurnTCTotMole, -1);
Data (zAurnNDCVC, -1);
Data (CALvPPM, -1);
Print(CPlasTCA, 1);
Print(AurnTCTotMole, 1);
Print(zAurnNDCVC, 1);
Print(CALvPPM, 1);

# This is average female data points -- high CV (~0.5, based on peaks)
Print(CDCVGmol, 0.51 0.985 1.99 2.96 4.02 4.23 4.52 5.01 6.03 );
Data(CDCVGmol,0.0032 0.00868 0.0106 0.0127 0.0133 0.0087 0.00508 0.00229 0.00074);
Print(CDCVGmol0, 10); # No detect at 10 hr in females
Data(CDCVGmol0, 0.000025); # Half the detection limit
Print(CDCVG_ND, 10); # No detect at 10 hr in females
Data(CDCVG_ND, 0);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAurnTCA_collect, 1);

```

```

        Data(zAurnTCA_collect,-1);
        Print(AurnTCOGTCOH_collect, 1);
        Data(AurnTCOGTCOH_collect,-1);
    };
}
}
##### END FISHER et al. 1998 individual data #####

##### BEGIN Paykoc and Powell 1945 individual data #####
Level { #Subject level
### FOR PAYKOC, ONLY PHYSIOLOGICAL AND TCA PARAMETERS
    Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
    Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );
    Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
    Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.64 1.36 );
    Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.1 1.9 );
    Distrib( QSlwC TruncNormal_v M_QSlwC V_QSlwC 0.36 1.64 );
####
    Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
    Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.76 1.24 );
    Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.85 1.15 );
    Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
    Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.84 1.16 );
    Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.54 1.46 );
    Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.84 1.16 );
    Distrib( VRespLumC TruncNormal_v M_VRespLumC V_VRespLumC 0.6 1.4 );
    Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.6 1.4 );
    Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.66 1.34 );
    Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
####
    Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.6 0.6 );
####
    Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.6 0.6 );
####
    Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
####
    Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
####
    Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
####
    Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
####
    Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.6 0.6 );
####
    Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
    Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
    Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
    Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
    Distrib( lnkDissocC TruncNormal_v M_lnkDissocC V_lnkDissocC -0.18 0.18 );
    Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -0.546 0.546 );
####
    Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
####
    Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );
####
    Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
####
    Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
####
    Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
####
    Distrib( lnkTSD TruncNormal_v M_lnkTSD V_lnkTSD -4.269 4.942 );
####
    Distrib( lnkAS TruncNormal_v M_lnkAS V_lnkAS -6.571 7.244 );
####
    Distrib( lnkTD TruncNormal_v M_lnkTD V_lnkTD -4.605 0 );
####
    Distrib( lnkAD TruncNormal_v M_lnkAD V_lnkAD -7.195 6.62 );
####
    Distrib( lnkASTCA TruncNormal_v M_lnkASTCA V_lnkASTCA -7.195 6.62 );
####
    Distrib( lnkASTCOH TruncNormal_v M_lnkASTCOH V_lnkASTCOH -7.195 6.62 );
####
    Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
####
    Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC 0 1 );
####
    Distrib( lnClC TruncNormal_v M_lnClC V_lnClC -4.158 4.158 );
    Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
####
    Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
####
    Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC 0 1 );
####
    Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -13.815 13.815 );
####
    Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC -4.158 4.158 );
####
    Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC 0 1 );
####
    Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -13.815 13.815 );
####
    Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC -4.158 4.158 );
####
    Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
);
####
    Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
####
    Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
);
#####
    Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC 0 1 );
####
    Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC -11.513 6.908 );
####
    Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );

```

```

#####      Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC 0 1 );
#####      Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC -9.21 4.605 );
#####      Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
#####      Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
Distrib( lnkUrnTCAC TruncNormal_v M_lnkUrnTCAC V_lnkUrnTCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
#####      Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
#####      Distrib( lnkEHRC TruncNormal_v M_lnkEHRC V_lnkEHRC -9.21 4.605 );
#####      Distrib( lnkUrnTCOGC TruncNormal_v M_lnkUrnTCOGC V_lnkUrnTCOGC -6.908 6.908 );
#####      Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908
);
#####      Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
#####      Distrib( lnkNATC TruncNormal_v M_lnkNATC V_lnkNATC -9.21 4.605 );
#####      Distrib( lnkKidBioactC TruncNormal_v M_lnkKidBioactC V_lnkKidBioactC -9.21 4.605 );

Experiment { # 22 ## Paykoc and Powell 1945
# #Subject 1, TCA iv, 1.7 g sodium TCA, 45.6 kg
# 0.03728 g sodium TCA/kg = 37.2 mg NaTCA/kg = 32.9 mg TCA/kg
# NaTCA MW = 185.4
# TCA MW = 163.5
# 1 mg NaTCA equiv to 0.8819 mg TCA
# lnBW=3.82; ## ln(45.6)

      BWmeas = 45.6;
      Hematocritmeas = 0.39;

# CC= 0;
#Conc= 0;

      TChng = 1; # 1 hr infusion
      IVDoseTCA=NDoses(2, 32.9 0, 0 1); # Converted to dose-rate in model

      Print( CBldTCA, 10 34 58 82 106 130 154);
      Data( CBldTCA, 80 57 44 35 28 24 21);
      Print(CPlasTCA, 10 34 58 82 106 130 154);
      Data (CPlasTCA, 140 100 77 61 50 42 37);

      Print( zAUrnTCA, 10 34 58 82 106 130 154 178 202 );
      Data( zAUrnTCA, 189 453 703 928 1075 1148 1224 1284 1332);

      Print( AUrnTCOGTCOH, 0 );
      Data( AUrnTCOGTCOH, -1 );
      Print( CVen, 0);
      Data( CVen, -1);
      Print( CTCOH, 0);
      Data( CTCOH, -1);
      Print( CALvPPM, 0);
      Data( CALvPPM, -1);
      Print(TotCTCOH, 1);
      Data (TotCTCOH, -1);
      Data (AUrnTCTotMole, -1);
      Data (zAUrnNDCVC, -1);
      Print(AUrnTCTotMole, 1);
      Print(zAUrnNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 0);
      Data(CDCVG_ND, -1);

#      Print(MassBaltTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBaltTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBaltTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBaltTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);

```

```

#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose,-1);
#           Print(zAUrnTCA_collect, 1);
#           Data(zAUrnTCA_collect,-1);
#           Print(AUrnTCOGTCOH_collect, 1);
#           Data(AUrnTCOGTCOH_collect,-1);
};

      Experiment { # 23 ## Paykoc and Powell 1945
# Subject 2, TCA iv, 2.9 g sodium TCA, 48.2 kg
# 0.06016 g sodium TCA/kg = 60.16 mg NaTCA/kg = 53.06 mg TCA/kg
# NaTCA MW = 185.4
# TCA MW = 163.5
# 1 mg NaTCA equiv to 0.8819 mg TCA
# lnBW=3.875; ## ln(48.2)

      BWmeas = 48.2;
      Hematocritmeas = 0.40;

# CC= 0;
#Conc= 0;

      TChng = 1; # 1 hr infusion
      IVDoseTCA=NDoses(2, 53.06 0, 0 1); # Converted to dose-rate in model

      Print( CBldTCA, 34 58 82 106 130);
      Data( CBldTCA, 102 78 62 48 40);
      Print(CPlasTCA, 34 58 82 106 130);
      Data (CPlasTCA, 179 136 108 84 70);

      Print( zAUrnTCA, 34 58 82 106 130 154 178 202);
      Data( zAUrnTCA, 900 1260 1500 1690 1816 1856 1878 1932);

      Print( AUrnTCOGTCOH, 0 );
      Data( AUrnTCOGTCOH, -1 );
      Print( CVen, 0);
      Data( CVen, -1);
      Print( CTCOH, 0);
      Data( CTCOH, -1);
      Print( CALvPPM, 0);
      Data( CALvPPM, -1);
      Print(TotCTCOH, 1);
      Data (TotCTCOH, -1);
      Data (AUrnTCTotMole, -1);
      Data (zAUrnNDCVC, -1);
      Print(AUrnTCTotMole, 1);
      Print(zAUrnNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 1);
      Data(CDCVG_ND, -1);

#           Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose,-1);
#           Print(zAUrnTCA_collect, 1);
#           Data(zAUrnTCA_collect,-1);
#           Print(AUrnTCOGTCOH_collect, 1);
#           Data(AUrnTCOGTCOH_collect,-1);

```



```

};

      Experiment { # 24 ## Paykoc and Powell 1945
# Subject 3, TCA iv, 1.8 g sodium TCA, 64 kg
# 0.028125 g sodium TCA/kg = 28.125 mg NaTCA/kg = 24.80 mg TCA/kg
# NaTCA MW = 185.4
# TCA MW = 163.5
# 1 mg NaTCA equiv to 0.8819 mg TCA
# CC= 0;
#Conc= 0;

      BWmeas = 64;
      Hematocritmeas = 0.45;
      TChng = 1; # 1 hr infusion
      IVDoseTCA=NDoses(2, 24.8 0, 0 1); # Converted to dose-rate in model

      Print( CBldTCA, 34 58 82 106);
      Data( CBldTCA, 65 50 44 32);
      Print(CPlasTCA, 34 58 82 106);
      Data (CPlasTCA, 119 95 83 61);

      Print( zAUrnTCA, 0);
      Data( zAUrnTCA, -1);

      Print( AUrnTCOGTCOH, 0 );
      Data( AUrnTCOGTCOH, -1 );
      Print( CVen, 0);
      Data( CVen, -1);
      Print( CTCOH, 0);
      Data( CTCOH, -1);
      Print( CALvPPM, 0);
      Data( CALvPPM, -1);
      Print(TotCTCOH, 1);
      Data (TotCTCOH, -1);
      Data (AUrnTCTotMole, -1);
      Data (zAUrnNDCVC, -1);
      Print(AUrnTCTotMole, 1);
      Print(zAUrnNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 1);
      Data(CDCVG_ND, -1);

#      Print(MassBaltCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBaltCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBaltTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBaltCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBaltCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
      Print(RetDose, 1);
      Data(RetDose, -1);
      Print(zAUrnTCA_collect, 1);
      Data(zAUrnTCA_collect, -1);
      Print(AUrnTCOGTCOH_collect, 1);
      Data(AUrnTCOGTCOH_collect, -1);
};
}

##### END Paykoc and Powell 1945 individual data #####

##### BEGIN Kimmerle et al. 1973 individual data #####
      Level { #Subject level
### FOR KIMMERLE, NO DCVG, DCVC PARAMETERS
      Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
      Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );

```

```

Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.64 1.36 );
Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.1 1.9 );
Distrib( QSlwC TruncNormal_v M_QSlwC V_QSlwC 0.36 1.64 );
Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.76 1.24 );
Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.85 1.15 );
Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.84 1.16 );
Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.54 1.46 );
Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.84 1.16 );
Distrib( VResplumC TruncNormal_v M_VResplumC V_VResplumC 0.6 1.4 );
Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.6 1.4 );
Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.66 1.34 );
Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.6 0.6 );
Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.6 0.6 );
Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.6 0.6 );
Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
Distrib( lnkDissocC TruncNormal_v M_lnkdissocC V_lnkdissocC -0.18 0.18 );
Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -0.546 0.546 );
Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );
Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
#### Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
#### Distrib( lnkTSD TruncNormal_v M_lnktSD V_lnktSD -4.269 4.942 );
#### Distrib( lnkAS TruncNormal_v M_lnktAS V_lnktAS -6.571 7.244 );
#### Distrib( lnkTD TruncNormal_v M_lnktD V_lnktD -4.605 0 );
#### Distrib( lnkAD TruncNormal_v M_lnktAD V_lnktAD -7.195 6.62 );
#### Distrib( lnkASTCA TruncNormal_v M_lnktASTCA V_lnktASTCA -7.195 6.62 );
#### Distrib( lnkASTCOH TruncNormal_v M_lnktASTCOH V_lnktASTCOH -7.195 6.62 );
Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
# Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC 0 1 );
Distrib( lnClC TruncNormal_v M_lnClC V_lnClC -4.158 4.158 );
Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
# Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC 0 1 );
Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -13.815 13.815 );
Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC -4.158 4.158 );
# Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC 0 1 );
Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -13.815 13.815 );
Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC -4.158 4.158 );
Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
# Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC 0 1 );
Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC -11.513 6.908 );
Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
# Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC 0 1 );
Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC -9.21 4.605 );
Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
Distrib( lnkUrntTCAC TruncNormal_v M_lnkUrntTCAC V_lnkUrntTCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
Distrib( lnkEHRC TruncNormal_v M_lnkEHRC V_lnkEHRC -9.21 4.605 );
Distrib( lnkUrntCOGC TruncNormal_v M_lnkUrntCOGC V_lnkUrntCOGC -6.908 6.908 );
#### Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );
#### );
#### Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
#### Distrib( lnkNATC TruncNormal_v M_lnkNATC V_lnkNATC -9.21 4.605 );
#### Distrib( lnkKidBioactC TruncNormal_v M_lnkKidBioactC V_lnkKidBioactC -9.21 4.605 );

```

```

Experiment { # 33 ## Kimmerle & Eben 1973; Single exposure;
# Subject A - Female, 40 +/- 4 ppm
#
# CC= 0;

Male = 0.0;
Conc= NDoses(2, 40 0, 0 4 );

Print( CALvPPM, 0); ## only group mean available
Data( CALvPPM, -1);

Print( CVen, 4 5 6);
Data( CVen, 0.196 0.104 0.078);
Print( CTCOH, 4 5 6 7 8 24 48 72); ## Assume is free -- need to check
Data( CTCOH, 0.706 0.693 0.614 0.574 0.602 0.473 0.244 0.2);
Print( AUrnTCOGTCOH, 4 8 24 48 72 96 120);
Data( AUrnTCOGTCOH, 12.046 15.644 41.741 61.959 75.097 81.615 85.263);
Print( zAUrnTCA, 4 8 24 48 72 96 120);
Data( zAUrnTCA, 1.32 1.645 5.803 18.403 32.335 40.805 48.605);

# Separate the 8th day collection
UrnMissing= NDoses( 3, 1 0 1 0 168 192);
Print( AUrnTCOGTCOH_collect, 192);
Data( AUrnTCOGTCOH_collect, 1.297);
Print( zAUrnTCA_collect, 192);
Data( zAUrnTCA_collect, 2.322);

Print(TotCTCOH, 1);
Data( TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#
# Print(MassBaltCE, 1, 2, 4, 8, 16, 32);
# Data(MassBaltCE, 0, 0, 0, 0, 0, 0);
# Print(MassBaltTCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBaltTCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBaltTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBaltTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBaltTCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBaltTCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
# Print(RetDose, 1);
# Data(RetDose, -1);
};

Experiment { # 34 ## Kimmerle & Eben 1973; Single exposure;
# Subject B - Female, 44 +/- 4 ppm
#
# CC= 0;

Male = 0.0;
Conc= NDoses(2, 44 0, 0 4 );

Print( CALvPPM, 0); ## only group mean available
Data( CALvPPM, -1);

```

```

Print( CVen, 4 5 6 7);
Data( CVen, 0.479 0.151 0.109 0.077);
Print( CTCOH, 4 5 6 7 8 24 32 48 72); ## Assume is free -- need to check
Data( CTCOH, 1.636 1.621 1.335 1.195 1.302 0.525 0.659 0.134 0.096);
Print( AUrnTCOGTCOH, 4 8 24 48 72 96);
Data( AUrnTCOGTCOH, 8.816 24.94 44.218 60.919 68.921 70.903);
Print( zAUrnTCA, 4 8 24 48 72 96);
Data( zAUrnTCA, 0.294 1.842 7.027 19.845 31.698 38.408);

# Separate the 8th day collection
UrnMissing= NDoses( 3, 1 0 1 0 168 192);
Print( AUrnTCOGTCOH_collect, 192);
Data( AUrnTCOGTCOH_collect, 0.239);
Print( zAUrnTCA_collect, 192);
Data( zAUrnTCA_collect, 3.682);

Print(TotCTCOH, 1);
Data( TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
};

Experiment { # 35 ## Kimmerle & Eben 1973; Single exposure;
# Subject C - Female, 44 +/- 4 ppm
#
# CC= 0;

Male = 0.0;
Conc= NDoses(2, 44 0, 0 4 );

Print( CalvPPM, 0); ## only group mean available
Data( CalvPPM, -1);

Print( CVen, 4 5 6 7);
Data( CVen, 0.277 0.216 0.113 0.077);
Print( CTCOH, 4 5 6 7 8 24 32 48 72); ## Assume is free -- need to check
Data( CTCOH, 1.776 1.712 1.465 1.32 1.545 0.521 0.543 0.108 0.05);
Print( AUrnTCOGTCOH, 4 8 24 48 72 96);
Data( AUrnTCOGTCOH, 23.797 28.703 58.809 85.586 93.276 95.967);
Print( zAUrnTCA, 4 8 24 48 72 96);
Data( zAUrnTCA, 0.467 1.333 14.093 30.235 42.643 51.288);

# Separate the 8th day collection
UrnMissing= NDoses( 3, 1 0 1 0 168 192);
Print( AUrnTCOGTCOH_collect, 192);

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Data( AUrnTCOGTCOH_collect, 0.268);
Print( zAUrnTCA_collect, 192);
Data( zAUrnTCA_collect, 1.518);

Print(TotCTCOH, 1);
Data (TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
};

Experiment { # 36 ## Kimmerle & Eben 1973; Single exposure;
# Subject D - Female, 44 +/- 4 ppm
#
# CC= 0;

Male = 0.0;
Conc= NDoses(2, 44 0, 0 4 );

Print( CalvPPM, 0); ## only group mean available
Data( CalvPPM, -1);

Print( CVen, 4 5 6 7);
Data( CVen, 0.256 0.194 0.097 0.077);
Print( CTCOH, 4 5 6 7 8 24 32 48 72); ## Assume is free -- need to check
Data( CTCOH, 1.49 1.335 1.239 1.172 1.356 0.696 0.668 0.232 0.129);
Print( AUrnTCOGTCOH, 4 8 24 48 72 96);
Data( AUrnTCOGTCOH, 14.848 44.609 82.283 113.34 126.783 131.251);
Print( zAUrnTCA, 4 8 24 48 72 96);
Data( zAUrnTCA, 1.273 3.715 18.435 40.529 57.932 69.431);

# Separate the 8th day collection
UrnMissing= NDoses( 3, 1 0 1 0 168 192);
Print( AUrnTCOGTCOH_collect, 192);
Data( AUrnTCOGTCOH_collect, -1);
Print( zAUrnTCA_collect, 192);
Data( zAUrnTCA_collect, -1);

Print(TotCTCOH, 1);
Data (TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(CPlasTCA, 1);

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Print(AUrntCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#       Print(MassBaltCE, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCE, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltCOH, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCOH, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltTCA, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltTCA, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltCOG, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCOG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
};

Experiment { # 37 ## Kimmerle & Eben 1973; Single exposure;
# Subject E - Male, 40 +/- 4 ppm
#
# CC= 0;

Conc= NDoses(2, 40 0, 0 4 );

Print( CALvPPM, 0); ## only group mean available
Data( CALvPPM, -1);

Print( CVen, 4 5 6);
Data( CVen, 0.322 0.117 0.117);
Print( CTCOH, 4 5 6 7 8 24 48 72); ## Assume is free -- need to check
Data( CTCOH, 0.775 0.66 0.638 0.585 0.574 0.438 0.2 0.141);
Print( AUrnTCOGTCOH, 4 8 24 48 72 96 120);
Data( AUrnTCOGTCOH, 6.262 15.15 29.19 36.782 42.539 44.553 46.221);
Print( zAUrnTCA, 4 8 24 48 72 96 120);
Data( zAUrnTCA, 0.426 1.195 6.565 11.965 23.235 32.775 37.96);

# Separate the 8th day collection
UrnMissing= NDoses( 3, 1 0 1 0 168 192);
Print( AUrnTCOGTCOH_collect, 192);
Data( AUrnTCOGTCOH_collect, 1.126);
Print( zAUrnTCA_collect, 192);
Data( zAUrnTCA_collect, 1.280);

Print(TotCTCOH, 1);
Data( TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrntCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#       Print(MassBaltCE, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCE, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltCOH, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCOH, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltTCA, 1, 2, 4, 8, 16, 32);

```

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#           Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose, -1);
};

      Experiment { # 38 ## Kimmerle & Eben 1973; Single exposure;
# Subject F - Male, 40 +/- 4 ppm
#
# CC= 0;

      Conc= NDoses(2, 40 0, 0 4 );

      Print( CalvPPM, 0); ## only group mean available
      Data( CalvPPM, -1);

      Print( CVen, 4 5 6);
      Data( CVen, 0.252 0.132 0.08);
      Print( CTCOH, 4 5 6 7 8 24 48); ## Assume is free -- need to check
      Data( CTCOH, 0.806 0.681 0.614 0.551 0.504 0.243 0.08);
      Print( AUrnTCOGTCOH, 4 8 24 48 72 96 120);
      Data( AUrnTCOGTCOH, 12.878 24.712 58.083 72.72 76.4 77.744 78.599);
      Print( zAUrnTCA, 4 8 24 48 72 96 120);
      Data( zAUrnTCA, 0.205 0.489 4.818 17.241 28.511 38.051 43.199);

# Separate the 8th day collection
      UrnMissing= NDoses( 3, 1 0 1 0 168 192);
      Print( AUrnTCOGTCOH_collect, 192);
      Data( AUrnTCOGTCOH_collect, 0.297);
      Print( zAUrnTCA_collect, 192);
      Data( zAUrnTCA_collect, 2.695);

      Print(TotCTCOH, 1);
      Data( TotCTCOH, -1);
      Print( CBldTCA, 0);
      Data( CBldTCA, -1);
      Data( CPlasTCA, -1);
      Data( AUrnTCTotMole, -1);
      Data( zAUrnNDCVC, -1);
      Print(CPlasTCA, 1);
      Print(AUrnTCTotMole, 1);
      Print(zAUrnNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 1);
      Data(CDCVG_ND, -1);

#           Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print(RetDose, 1);
#           Data(RetDose, -1);
};

```

```

Experiment { # 39 ## Kimmerle & Eben 1973; Single exposure;
# Subject G - Male, 40 +/- 4 ppm
#
# CC= 0;

Conc= NDoses(2, 40 0, 0 4 );

Print( CalvPPM, 0); ## only group mean available
Data( CalvPPM, -1);

Print( CVen, 4 5 6);
Data( CVen, 0.266 0.127 0.078);
Print( CTCOH, 4 5 6 7 8 24 48 72); ## Assume is free -- need to check
Data( CTCOH, 0.939 0.69 0.812 0.696 0.658 0.339 0.128 0.09);
Print( AUrnTCOGTCOH, 4 8 24 48 72 96 120);
Data( AUrnTCOGTCOH, 15.053 21.897 62.789 85.28 93.302 95.789 97.177);
Print( zAUrnTCA, 4 8 24 48 72 96 120);
Data( zAUrnTCA, 0.462 0.822 8.42 19.045 27.681 33.457 39.762);

# Separate the 8th day collection
UrnMissing= NDoses( 3, 1 0 1 0 168 192);
Print( AUrnTCOGTCOH_collect, 192);
Data( AUrnTCOGTCOH_collect, 0.324);
Print( zAUrnTCA_collect, 192);
Data( zAUrnTCA_collect, 3.610);

Print(TotCTCOH, 1);
Data( TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#
# Print(MassBaltCE, 1, 2, 4, 8, 16, 32);
# Data(MassBaltCE, 0, 0, 0, 0, 0, 0);
# Print(MassBaltCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBaltCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBaltTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBaltTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBaltCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBaltCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
};

Experiment { # 40 ## Kimmerle & Eben 1973; Single exposure;
# Subject H - Male, 44 +/- 4 ppm
#
# CC= 0;

Conc= NDoses(2, 44 0, 0 4 );

Print( CalvPPM, 0); ## only group mean available
Data( CalvPPM, -1);

Print( CVen, 4 5 6 7);
Data( CVen, 0.246 0.131 0.077 0.077);
Print( CTCOH, 4 5 6 7 8 24 32 48 72 96); ## Assume is free -- need to check

```



```

Data( CTCOH, 1.323 1.283 1.191 1.035 1.093 0.551 0.403 0.155 0.098 0.044);
Print( AUrnTCOGTCOH, 4 8 24 48 72 96);
Data( AUrnTCOGTCOH, 11.722 37.419 92.855 114.296 121.185 123.768);
Print( zAUrnTCA, 8 24 48 72 96);
Data( zAUrnTCA, 0.585 4.673 11.492 18.063 23.734);

# Separate the 8th day collection
UrnMissing= NDoses( 3, 1 0 1 0 168 192);
Print( AUrnTCOGTCOH_collect, 192);
Data( AUrnTCOGTCOH_collect, 0.234);
Print( zAUrnTCA_collect, 192);
Data( zAUrnTCA_collect, 2.108);

Print(TotCTCOH, 1);
Data( TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#
Print(MassBaltTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBaltTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBaltTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBaltTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBaltTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBaltTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBaltTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBaltTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
};

Experiment { # 41 ## Kimmerle & Eben 1973; Repeated exposure;
# Subject J - 48 +/- 3 ppm, 4 hr/day for 5 days
# Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

Conc= NDoses(10, 48 0 48 0 48 0 48 0 48 0, 0 4 24 28 48 52 72 76 96 100);

Print( CVen, 4 5 8 28 33 52 76 100);
Data( CVen, 0.42 0.13 0.085 0.51 0.17 0.408 0.51 0.85);
Print( CTCOH, 4 5 8 9 10 24 28 33 48 52 57 72 76 81 96 100 104 105 120 144 168 192
216 240 264); ## Assume is free -- need to check
Data( CTCOH, 2.047 1.672 1.596 1.406 1.26 1.174 2.002 1.801 0.917 2.38 1.72 0.946
2.58 2.064 1.267 2.509 2.142 2.113 2.11 0.507 0.272 0.138 0.08 0.054
0.03);
Print( AUrnTCOGTCOH, 24 48 72 96 120 144 168);
Data( AUrnTCOGTCOH, 46.14 121.6 175.55 238.17 358.26 378.55 396.33);
Print( zAUrnTCA, 24 48 72 96 120 144 168);
Data( zAUrnTCA, 4.175 19.16 46.72 72.82 124.285 153.321 168.271);

# Separate the 11-12th day post-exposure collection
UrnMissing= NDoses( 3, 1 0 1 0 384 408);
Print( AUrnTCOGTCOH_collect, 408);
Data( AUrnTCOGTCOH_collect, 0.20);
Print( zAUrnTCA_collect, 408);
Data( zAUrnTCA_collect, 1.365);

```

```

Print( CALvPPM, 0);
Data( CALvPPM, -1);
Print(TotCTCOH, 1);
Data (TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
};

Experiment { # 42 ## Kimmerle & Eben 1973; Repeated exposure;
# Subject K - 48 +/- 3 ppm, 4 hr/day for 5 days
# Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

Conc= NDoses(10, 48 0 48 0 48 0 48 0 48 0, 0 4 24 28 48 52 72 76 96 100);

Print( Cven, 4 5 8 28 52 76 100);
Data( Cven, 0.34 0.23 0.13 0.34 0.476 0.272 0.782);
Print( CTCOH, 4 5 8 9 10 24 28 33 48 52 57 72 76 81 96 100 104 105 120 144 168 192);
## Assume is free -- need to check
Data( CTCOH, 1.958 1.596 1.368 1.204 1.152 1.036 1.82 1.674 0.812 2.01 1.87 0.591
2.322 1.909 0.845 2.509 2.016 2.016 1.01 0.386 0.102 0.04);
Print( AUrnTCOGTCOH, 24 48 72 96 120 144 168 192 216 240 264);
Data( AUrnTCOGTCOH, 88.46 214.54 335.72 453.37 557.89 600.5 638.16 643.27 647.1
649.13 650.17);
Print( zAUrnTCA, 24 48 72 96 120 144 168 192 216 240 264);
Data( zAUrnTCA, 6.613 25.399 75.391 139.375 229.037 271.661 304.179 328.651 346.571
360.221 371.781);

# Separate the 11-12th day post-exposure collection
UrnMissing= NDoses( 3, 1 0 1 0 384 408);
Print( AUrnTCOGTCOH_collect, 408);
Data( AUrnTCOGTCOH_collect, 0.08);
Print( zAUrnTCA_collect, 408);
Data( zAUrnTCA_collect, 2.1);

Print( CALvPPM, 0);
Data( CALvPPM, -1);
Print(TotCTCOH, 1);
Data (TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(CPlasTCA, 1);

```

```

Print(AUrntCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#       Print(MassBaltCE, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCE, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltCOH, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCOH, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltCA, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCA, 0, 0, 0, 0, 0, 0);
#       Print(MassBaltCOG, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCOG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
};

Experiment { # 43 ## Kimmerle & Eben 1973; Repeated exposure;
# Subject L - 48 +/- 3 ppm, 4 hr/day for 5 days
# Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

Conc= NDoses(10, 48 0 48 0 48 0 48 0 48 0, 0 4 24 28 48 52 72 76 96 100);

Print( CVen, 4 5 8 28 52 76 100);
Data( CVen, 0.28 1.18 0.09 0.34 0.34 0.34 0.51);
Print( CTCOH, 4 5 8 9 10 24 28 33 48 52 57 72 76 81 96 100 104 105 120 144 192 216);
## Assume is free -- need to check
Data( CTCOH, 1.275 1.014 0.9 0.803 0.72 0.567 1.44 1.85 0.55 2.09 1.4 0.676 1.565
1.248 0.507 1.974 1.638 1.323 0.51 0.179 0.045 0.028);
Print( AUrnTCOGTCOH, 24 48 72 96 120 144 168 192 216 240 264);
Data( AUrnTCOGTCOH, 63.33 149.89 234.33 320.33 409.94 434.46 440.59 444.02 446.58
447.9 448.61);
Print( zAUrnTCA, 24 48 72 96 120 144 168 192 216 240 264);
Data( zAUrnTCA, 5.341 17.631 49.311 110.463 187.167 234.983 283.309 319.077 337.788
356.118 372.468);

# Separate the 11-12th day post-exposure collection
UrnMissing= NDoses( 3, 1 0 1 0 384 408);
Print( AUrnTCOGTCOH_collect, 408);
Data( AUrnTCOGTCOH_collect, 0.07);
Print( zAUrnTCA_collect, 408);
Data( zAUrnTCA_collect, 2.184);

Print( CALvPPM, 0);
Data( CALvPPM, -1);
Print(TotCTCOH, 1);
Data( TotCTCOH, -1);
Print( CBldTCA, 0);
Data( CBldTCA, -1);
Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrntCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#       Print(MassBaltCE, 1, 2, 4, 8, 16, 32);
#       Data(MassBaltCE, 0, 0, 0, 0, 0, 0);

```

```

#         Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#         Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#         Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#         Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#         Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#         Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#         Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#         Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#         Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#         Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
#         Print(RetDose, 1);
#         Data(RetDose, -1);
};

      Experiment { # 44 ## Kimmerle & Eben 1973; Repeated exposure;
# Subject M - 48 +/- 3 ppm, 4 hr/day for 5 days
# Not clear if M or F (3 males, 1 female in these experiments)
# CC= 0;

      Conc= NDoses(10, 48 0 48 0 48 0 48 0 48 0, 0 4 24 28 48 52 72 76 96 100);

      Print( CVen, 4 5 8 28 52);
      Data( CVen, 0.17 0.17 0.09 0.34 0.272);
      Print( CTCOH, 4 5 8 9 10 24 28 33 48 52 57 72 76 81 96 100 104 105 120 144 168);
## Assume is free -- need to check
      Data( CTCOH, 2.849 2.394 2.28 2.052 1.976 1.296 2.912 2.429 0.825 2.53 2.26 0.473
            2.322 2.418 0.76 2.87 2.52 2.293 1.01 0.198 0.034);
      Print( AUrnTCOGTCOH, 24 48 72 96 120 144 168 192 216 240 264);
      Data( AUrnTCOGTCOH, 116.1 246.68 363.79 458.92 556.48 597.53 638.45 641.52 642.45
            642.84 642.97);
      Print( zAUrnTCA, 24 48 72 96 120 144 168 192 216 240 264);
      Data( zAUrnTCA, 2.928 12.19 29.482 48.094 111.934 169.81 186.895 206.764 218.839
            230.578 239.119);

# Separate the 11-12th day post-exposure collection
      UrnMissing= NDoses( 3, 1 0 1 0 384 408);
      Print( AUrnTCOGTCOH_collect, 408);
      Data( AUrnTCOGTCOH_collect, -1);
      Print( zAUrnTCA_collect, 408);
      Data( zAUrnTCA_collect, 3.564);

      Print( CALvPPM, 0);
      Data( CALvPPM, -1);
      Print(TotCTCOH, 1);
      Data( TotCTCOH, -1);
      Print( CBldTCA, 0);
      Data( CBldTCA, -1);
      Data( CPlasTCA, -1);
      Data( AUrnTCTotMole, -1);
      Data( zAUrnNDCVC, -1);
      Print(CPlasTCA, 1);
      Print(AUrnTCTotMole, 1);
      Print(zAUrnNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 1);
      Data(CDCVG_ND, -1);

#         Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#         Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#         Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#         Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#         Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#         Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#         Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#         Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#         Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#         Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#         Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#         Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);

```

```

        Print(RetDose, 1);
        Data(RetDose, -1);
    };
}
##### END Kimmerle et al. 1973 individual data #####

##### BEGIN Monster et al. 1976 individual data #####
Level { #Subject level
### FOR MONSTER, NO DCVG OR DCVC PARAMETERS
    Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
    Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );
    Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
    Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.64 1.36 );
    Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.1 1.9 );
    Distrib( QSlwC TruncNormal_v M_QSlwC V_QSlwC 0.36 1.64 );
    Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
    Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.76 1.24 );
    Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.85 1.15 );
    Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
    Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.84 1.16 );
    Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.54 1.46 );
    Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.84 1.16 );
    Distrib( VRespLumC TruncNormal_v M_VRespLumC V_VRespLumC 0.6 1.4 );
    Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.6 1.4 );
    Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.66 1.34 );
    Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
    Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.6 0.6 );
    Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.6 0.6 );
    Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
    Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
    Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
    Distrib( lnPResC TruncNormal_v M_lnPResC V_lnPResC -1.2 1.2 );
    Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.6 0.6 );
    Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
    Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
    Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
    Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
    Distrib( lnkDissocC TruncNormal_v M_lnkDissocC V_lnkDissocC -0.18 0.18 );
    Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -0.546 0.546 );
    Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
    Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );
    Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
    Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
#####
    Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
#####
    Distrib( lnkTSD TruncNormal_v M_lnkTSD V_lnkTSD -4.269 4.942 );
#####
    Distrib( lnkAS TruncNormal_v M_lnkAS V_lnkAS -6.571 7.244 );
#####
    Distrib( lnkTD TruncNormal_v M_lnkTD V_lnkTD -4.605 0 );
#####
    Distrib( lnkAD TruncNormal_v M_lnkAD V_lnkAD -7.195 6.62 );
#####
    Distrib( lnkASTCA TruncNormal_v M_lnkASTCA V_lnkASTCA -7.195 6.62 );
#####
    Distrib( lnkASTCOH TruncNormal_v M_lnkASTCOH V_lnkASTCOH -7.195 6.62 );
    Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
#
    Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC 0 1 );
    Distrib( lnClC TruncNormal_v M_lnClC V_lnClC -4.158 4.158 );
    Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
    Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
#
    Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC 0 1 );
    Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -13.815 13.815 );
    Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC -4.158 4.158 );
#
    Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC 0 1 );
    Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -13.815 13.815 );
    Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC -4.158 4.158 );
    Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
    Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
    Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
#
    Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC 0 1 );
    Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC -11.513 6.908 );
    Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
#
    Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC 0 1 );
    Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC -9.21 4.605 );
    Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
    Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );

```

```

Distrib( lnkUrnTCAC TruncNormal_v M_lnUrnTCAC V_lnUrnTCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnMetTCAC V_lnMetTCAC -9.21 4.605 );
Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
Distrib( lnkEHRC TruncNormal_v M_lnEHRC V_lnEHRC -9.21 4.605 );
Distrib( lnkUrnTCOGC TruncNormal_v M_lnUrnTCOGC V_lnUrnTCOGC -6.908 6.908 );
#### Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );
#### Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
#### Distrib( lnkNATC TruncNormal_v M_lnNATC V_lnNATC -9.21 4.605 );
#### Distrib( lnkKidBioactC TruncNormal_v M_lnKidBioactC V_lnKidBioactC -9.21 4.605 );

Level { # Subject A
Experiment { # 45 ## Monster Subject A, lower dose
# Data from Monster et al. (1976)
# Male
# CC= 0;

# BW= 70 PctFat= 0.12
# lnBW= 4.248495242 ; VFatC= 0.560747664 ;
      BWmeas = 70.0;
      VFatCmeas = 0.12;

# MV= 7.7
      Conc= NDoses(2, 65 0, 0 4 );
      QPmeas= 210; # NDoses(2, 210 0, 0.0 4.0);

      Print( RetDose, 4);
      Data( RetDose, 320);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 210 );
      Print( CALvPPM, 4.5 6 23.75 48 72 );
      Data( CALvPPM, 3.766118721 1.842123288 0.122808219 0.034795662 0.020877397 );
      Print( CVen, 3.5 6 23.75 );
      Data( CVen, 1.2 0.13 0.01 );
      Print( TotCTCOH, 3.5 6 23.75 );
      Data( TotCTCOH, 4.3 4.4 1.1 );
      Print( CBldTCA, 3.5 6 23.75 48 72 );
      Data( CBldTCA, 3.6 5.7 10.1 11.4 11.8 );
      Print( AUrnTCOGTCOH, 16 24 32 40 48 56 64 72 80 88 );
      Data( AUrnTCOGTCOH, 31.5445 84.4675 119.4505 146.3605 157.573 163.553 169.0845
          176.709 179.699 182.5395 );
      Print( zAUrnTCA, 16 24 32 40 48 56 64 72 80 88 );
      Data( zAUrnTCA, 1.1445 3.27 5.232 8.502 9.9735 10.791 12.099 14.388 15.5325
          16.8405 );

      Print(CTCOH, 1);
      Data(CTCOH, -1);
      Data(CPlasTCA, -1);
      Data(AUrnTCTotMole, -1);
      Data(zAUrnNDCVC, -1);
      Print(CPlasTCA, 1);
      Print(AUrnTCTotMole, 1);
      Print(zAUrnNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 1);
      Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
      Print(zAUrnTCA_collect, 1);

```

```

        Data(zAurnTCA_collect, -1);
        Print(AurnTCOGTCOH_collect, 1);
        Data(AurnTCOGTCOH_collect, -1);
};

Experiment { # 46 ## Monster Subject A, higher dose
# Data from Monster et al. (1976)
# Male
# CC= 0;

# BW= 70 PctFat= 0.12
# lnBW= 4.248495242 ; VFatC= 0.560747664 ;
        BWmeas = 70.0;
        VFatCmeas = 0.12;

# MV= 8.9

        Conc= NDoses(2, 140 0, 0 4 );
        QPmeas= 282; # NDoses(2, 282 0, 0.0 4.0);
        Print( RetDose, 4);
        Data( RetDose, 740);
#       Print( QPsamp, 1 );
#       Data( QPsamp, 282 );
        Print( CALvPPM, 4.5 6.5 23.5 48 );
        Data( CALvPPM, 5.989968911 2.572163121 0.28188089 0.070470222 );
        Print( CVen, 6.5 23.5 48 72 );
        Data( CVen, 0.28 0.014 0.005 0.0025 );
        Print( TotCTCOH, 3.99 6.5 23.5 48 72 );
        Data( TotCTCOH, 6.1 7.2 2.9 0.72 0.15 );
        Print( CBldTCA, 3.99 6.5 23.5 48 72 142 214 479 );
        Data( CBldTCA, 5.2 9 15 20 17.5 12.5 7.4 1.5 );
        Print( AurnTCOGTCOH, 16 24 32 40 48 56 64 72 80 );
        Data( AurnTCOGTCOH, 58.305 164.5995 246.675 295.113 326.209 340.561 353.418
                360.594 364.481 );
        Print( zAurnTCA, 16 24 32 40 48 56 64 72 80 );
        Data( zAurnTCA, 0.8175 3.597 5.559 9.81 13.8975 17.1675 22.563 26.9775 28.9395 );

        Print(CTCOH, 1);
        Data (CTCOH, -1);
        Data (CPlasTCA, -1);
        Data (AurnTCTotMole, -1);
        Data (zAurnNDCVC, -1);
        Print(CPlasTCA, 1);
        Print(AurnTCTotMole, 1);
        Print(zAurnNDCVC, 1);

        Print(CDCVGmol, 1);
        Data(CDCVGmol, -1);
        Print(CDCVG_ND, 1);
        Data(CDCVG_ND, -1);

#       Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
        Print(zAurnTCA_collect, 1);
        Data(zAurnTCA_collect, -1);
        Print(AurnTCOGTCOH_collect, 1);
        Data(AurnTCOGTCOH_collect, -1);
};
}

```

```

Level { # Subject B
  Experiment { # 47 ## Monster Subject B, lower dose
# Data from Monster et al. (1976)
# Male
# CC= 0;

# BW= 80 PctFat= 0.26
# lnBW= 4.382026635 ; VFatC= 1.214953271 ;
      BWmeas = 80.0;
      VFatCmeas = 0.26;

# MV= 10.7
      Conc= NDoses(2, 68 0, 0 4 );
      QPmeas= 390; # NDoses(2, 390 0, 0.0 4.0);
      Print( RetDose, 4);
      Data( RetDose, 430);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 390 );
      Print( CALvPPM, 4.083 4.5 22 48 80 );
      Data( CALvPPM, 3.675658588 1.531524412 0.245043906 0.110269758 0.076882525 );
      Print( CVen, 3.5 6 22.83333333 47 72 );
      Data( CVen, 1.5 0.16 0.0156 0.0065 0.0034 );
      Print( TotCTCOH, 3.5 6 22.83333333 47 );
      Data( TotCTCOH, 2.9 2.5 0.45 0.15 );
      Print( CBldTCA, 3.5 6 22.83333333 47 72 142 214 );
      Data( CBldTCA, 4 6.6 9.1 8.9 8.8 4.5 2.4 );
      Print( AUrnTCOGTCOH, 16 24 32 40 48 56 64 72 80 88 );
      Data( AUrnTCOGTCOH, 41.86 92.391 117.507 136.4935 148.1545 155.6295 162.5065
          167.2905 170.729 176.8585 );
      Print( zAUrnTCA, 8 16 24 32 40 48 56 64 72 80 88 );
      Data( zAUrnTCA, 0.4905 2.1255 7.0305 11.9355 19.7835 25.3425 29.103 34.989 41.856
          46.2705 51.5025 );

      Print(CTCOH, 1);
      Data (CTCOH, -1);
      Data (CPlasTCA, -1);
      Data (AUrnTCTotMole, -1);
      Data (zAUrnNDCVC, -1);
      Print(CPlasTCA, 1);
      Print(AUrnTCTotMole, 1);
      Print(zAUrnNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 1);
      Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
      Print(zAUrnTCA_collect, 1);
      Data(zAUrnTCA_collect, -1);
      Print(AUrnTCOGTCOH_collect, 1);
      Data(AUrnTCOGTCOH_collect, -1);
};

Experiment { # 48 ## Monster Subject B, higher dose
# Data from Monster et al. (1976)
# Male
# CC= 0;

```



```

# BW= 80 PctFat= 0.26
# lnBW= 4.382026635 ; VFatC= 1.214953271 ;
      BWmeas = 80.0;
      VFatCmeas = 0.26;
# MV= 10.4
      Conc= NDoses(2, 138 0, 0 4 );
      QPmeas= 372; # NDoses(2, 372 0, 0.0 4.0);
      Print( RetDose, 4);
      Data( RetDose, 790);
#       Print( QPsamp, 1 );
#       Data( QPsamp, 372 );
      Print( CALvPPM, 4.083 6 24 56 95 );
      Data( CALvPPM, 4.993960819 3.433348063 0.343334806 0.103000442 0.043697157 );
      Print( CVen, 6.5 23 47.33333333 72.33333333 94.5 );
      Data( CVen, 0.22 0.028 0.0085 0.0048 0.0011 );
      Print( TotCTCOH, 3.99 6.5 23 47.33333333 72.33333333 94.5 );
      Data( TotCTCOH, 4.5 3.9 1.2 0.35 0.11 0.03 );
      Print( CBldTCA, 3.99 6.5 23 47.33333333 72.33333333 94.5 164 260 404 );
      Data( CBldTCA, 4 6.6 12 13 11 10 5.4 1.6 0.04 );
      Print( AURNtCOGTCOH, 16 24 32 40 48 56 64 72 80 );
      Data( AURNtCOGTCOH, 74.75 181.493 232.7715 272.09 301.99 315.445 324.415 331.292
          336.076 );
      Print( zAURNtTCA, 16 24 32 40 48 56 64 72 80 );
      Data( zAURNtTCA, 1.7985 8.829 14.715 26.487 39.24 47.415 55.59 64.419 71.1225 );

      Print(CTCOH, 1);
      Data(CTCOH, -1);
      Data(CPlasTCA, -1);
      Data(AURNtCTotMole, -1);
      Data(zAURNtNDCVC, -1);
      Print(CPlasTCA, 1);
      Print(AURNtCTotMole, 1);
      Print(zAURNtNDCVC, 1);

      Print(CDCVGmol, 1);
      Data(CDCVGmol, -1);
      Print(CDCVG_ND, 1);
      Data(CDCVG_ND, -1);

#       Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
      Print(zAURNtTCA_collect, 1);
      Data(zAURNtTCA_collect, -1);
      Print(AURNtCOGTCOH_collect, 1);
      Data(AURNtCOGTCOH_collect, -1);
};
}

Level { # Subject C
      Experiment { # 49 ## Monster Subject C, lower dose
# Data from Monster et al. (1976)
# Male
# CC= 0;

# BW= 62 PctFat= 0.14
# lnBW= 4.127134385 ; VFatC= 0.654205607 ;
      BWmeas = 62.0;
      VFatCmeas = 0.14;

```

```

# MV= 8.5
Conc= NDoses(2, 70 0, 0 4 );
QPmeas= 258; # NDoses(2, 258 0, 0.0 4.0);
Print( RetDose, 4);
Data( RetDose, 330);
#   Print( QPsamp, 1 );
#   Data( QPsamp, 258 );
Print( CALvPPM, 4.5 6 22.5 47.75 70.5 );
Data( CALvPPM, 5.517282574 3.678188383 0.239082245 0.062529203 0.018390942 );
Print( CVen, 3.583333333 6 22.5 47.75 );
Data( CVen, 1.6 0.18 0.011 0.0023 );
Print( TotCTCOH, 3.583333333 6 22.5 );
Data( TotCTCOH, 2.8 2.7 0.51 );
Print( CBldTCA, 3.583333333 6 22.5 47.75 70.5 134 214 454 );
Data( CBldTCA, 3.1 5.2 7.8 8.1 6.2 4.1 2.1 0.04 );
Print( AURNtCOGTcoH, 16 24 32 40 48 56 64 72 80 88 );
Data( AURNtCOGTcoH, 35.88 91.6435 116.909 134.849 145.1645 149.6495 153.088 155.48
      156.676 157.1245 );
Print( zAURNtCA, 16 24 32 40 48 56 64 72 80 88 );
Data( zAURNtCA, 1.4715 4.7415 7.521 14.715 20.4375 22.563 26.814 31.2285 33.354
      36.1335 );

Print(CTCOH, 1);
Data (CTCOH, -1);
Data (CPlasTCA, -1);
Data (AURNtCTotMole, -1);
Data (zAURNtDCVC, -1);
Print(CPlasTCA, 1);
Print(AURNtCTotMole, 1);
Print(zAURNtDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#   Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#   Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#   Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#   Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#   Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#   Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#   Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#   Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#   Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#   Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#   Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#   Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAURNtCA_collect, 1);
Data(zAURNtCA_collect, -1);
Print(AURNtCOGTcoH_collect, 1);
Data(AURNtCOGTcoH_collect, -1);
};

Experiment { # 50 ## Monster Subject C, higher dose
# Data from Monster et al. (1976)
# Male
# CC= 0;

# BW= 62 PctFat= 0.14
# lnBW= 4.127134385 ; VFatC= 0.654205607 ;
      BWmeas = 62.0;
      VFatCmeas = 0.14;

# MV= 9.8
Conc= NDoses(2, 142 0, 0 4 );
QPmeas= 336; # NDoses(2, 336 0, 0.0 4.0);
Print( RetDose, 4);
Data( RetDose, 710);
#   Print( QPsamp, 1 );
#   Data( QPsamp, 336 );
Print( CALvPPM, 4.5 6 23.33333333 48.16666667 71.5 );

```

```

Data( CALvPPM, 4.884417808 2.767836758 0.325627854 0.11071347 0.035819064 );
Print( CVen, 6 23.33333333 48.16666667 71.5 );
Data( CVen, 0.25 0.022 0.0054 0.0025 );
Print( TotCTCOH, 3.99 6 23.33333333 48.16666667 71.5 );
Data( TotCTCOH, 5.2 5.1 1.6 0.34 0.06 );
Print( CBldTCA, 3.99 6 23.33333333 48.16666667 71.5 191 263 407 );
Data( CBldTCA, 3.6 6.5 12 11 10 5.8 3.8 1.5 );
Print( AUrnTCOGTCOH, 16 24 32 40 48 56 64 72 80 88 96 104 );
Data( AUrnTCOGTCOH, 49.933 132.457 178.204 210.3465 226.7915 239.499 242.19
      247.871 250.861 251.758 251.9075 252.5055 );
Print( zAUrnTCA, 16 24 32 40 48 56 64 72 80 88 96 104 );
Data( zAUrnTCA, 0.654 2.4525 4.251 11.118 15.696 22.7265 25.3425 31.2285 36.297
      41.202 45.6165 48.069 );

Print(CTCOH, 1);
Data (CTCOH, -1);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect, -1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect, -1);
};
}

Level { # Subject D
  Experiment { # 51 ## Monster Subject D, lower dose
# Data from Monster et al. (1976)
# Male
#CC= 0;

# BW= 67 PctFat= 0.09
# lnBW= 4.204692619 ; VFatC= 0.420560748 ;
      BWmeas = 67.;
      VFatCmeas = 0.09;
# MV= 11.6
      Conc= NDoses(2, 76 0, 0 4 );
      QPmeas= 444; # NDoses(2, 444 0, 0.0 4.0);
      Print( RetDose, 4);
      Data( RetDose, 470);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 444 );
      Print( CALvPPM, 4.5 6 24.08333333 48.16666667 72 );
      Data( CALvPPM, 4.666913489 2.10011107 0.204177465 0.06125324 0.020417747 );
      Print( CVen, 6 24.08333333 48.16666667 );
      Data( CVen, 0.175 0.0088 0.0025 );
      Print( TotCTCOH, 3.416666667 6 24.08333333 48.16666667 );
      Data( TotCTCOH, 3.2 3.2 0.6 0.11 );
      Print( CBldTCA, 3.416666667 6 24.08333333 48.16666667 72 142 214 504 );

```

```

Data( CBldTCA, 2.4 4.5 9 11.6 9.8 5.4 2.6 0.25 );
Print( AurnTCOGTCOH, 16 24 32 40 48 56 64 72 80 88 96 );
Data( AurnTCOGTCOH, 49.7835 121.5435 153.088 179.5495 192.257 198.237 202.124
      207.3565 209.4495 211.2435 212.29 );
Print( zAurnTCA, 16 24 32 40 48 56 64 72 80 88 96 );
Data( zAurnTCA, 1.308 3.27 5.886 12.9165 21.582 25.6695 30.2475 35.316 39.4035
      44.799 51.339 );

Print(CTCOH, 1);
Data (CTCOH, -1);
Data (CPlasTCA, -1);
Data (AurnTCTotMole, -1);
Data (zAurnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AurnTCTotMole, 1);
Print(zAurnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAurnTCA_collect, 1);
Data(zAurnTCA_collect, -1);
Print(AurnTCOGTCOH_collect, 1);
Data(AurnTCOGTCOH_collect, -1);
};

Experiment { # 52 ## Monster Subject D, higher dose
# Data from Monster et al. (1976)
# Male
#CC= 0;

# BW= 67 PctFat= 0.09
# lnBW= 4.204692619 ; VFatC= 0.420560748 ;
      BWmeas = 67.0;
      VFatCmeas = 0.09;

# MV= 12.3
      Conc= NDoses(2, 140 0, 0 4 );
      QPmeas= 486; # NDoses(2, 486 0, 0.0 4.0);
      Print( RetDose, 4);
      Data( RetDose, 790);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 486 );
      Print( CALvPPM, 4.5 6.416666667 23.25 48.91666667 72.66666667 );
      Data( CALvPPM, 4.520886183 2.542998478 0.268427617 0.062162185 0.025429985 );
      Print( CVen, 3.99 6.416666667 23.25 48.91666667 72.66666667 );
      Data( CVen, 3.1 0.26 0.019 0.004 0.002 );
      Print( TotCTCOH, 3.99 6.416666667 23.25 48.91666667 72.66666667 );
      Data( TotCTCOH, 5 5.5 1.7 0.35 0.06 );
      Print( CBldTCA, 3.99 6.416666667 23.25 48.91666667 72.66666667 144 216 );
      Data( CBldTCA, 3.3 6.4 11 14 12.5 5.3 3.4 );
      Print( AurnTCOGTCOH, 16 24 32 40 48 56 64 72 80 88 96 104 );
      Data( AurnTCOGTCOH, 74.75 222.755 290.7775 332.6375 355.0625 366.1255 374.4975
            380.029 382.421 383.7665 384.215 384.6635 );
      Print( zAurnTCA, 16 24 32 40 48 56 64 72 80 88 96 104 );
      Data( zAurnTCA, 1.635 8.829 17.004 25.6695 40.548 49.8675 60.168 74.229 80.9325
            89.271 100.5525 106.1115 );

```

```

Print(CTCOH, 1);
Data (CTCOH, -1);
Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#
# Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect, -1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect, -1);
};
}
}
##### END Monster et al. 1976 individual data #####

##### BEGIN CHIU et al. 2006 individual data #####
Level { #Subject level
### FOR CHIU, NO DCVG OR DCVC PARAMETERS
Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );
Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.64 1.36 );
Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.1 1.9 );
Distrib( QSlwC TruncNormal_v M_QSlwC V_QSlwC 0.36 1.64 );
Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.76 1.24 );
Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.85 1.15 );
Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.84 1.16 );
Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.54 1.46 );
Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.84 1.16 );
Distrib( VRespLumC TruncNormal_v M_VRespLumC V_VRespLumC 0.6 1.4 );
Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.6 1.4 );
Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.66 1.34 );
Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.6 0.6 );
Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.6 0.6 );
Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.6 0.6 );
Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
Distrib( lnkDissocC TruncNormal_v M_lnkDissocC V_lnkDissocC -0.18 0.18 );
Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -0.546 0.546 );
Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );

```

```

Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
#### Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
#### Distrib( lnkTSD TruncNormal_v M_lnTSD V_lnTSD -4.269 4.942 );
#### Distrib( lnkAS TruncNormal_v M_lnAS V_lnAS -6.571 7.244 );
#### Distrib( lnkTD TruncNormal_v M_lnTD V_lnTD -4.605 0 );
#### Distrib( lnkAD TruncNormal_v M_lnAD V_lnAD -7.195 6.62 );
#### Distrib( lnkASTCA TruncNormal_v M_lnASTCA V_lnASTCA -7.195 6.62 );
#### Distrib( lnkASTCOH TruncNormal_v M_lnASTCOH V_lnASTCOH -7.195 6.62 );
Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
# Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC 0 1 );
Distrib( lnClC TruncNormal_v M_lnClC V_lnClC -4.158 4.158 );
Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
# Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC 0 1 );
Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -13.815 13.815 );
Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC -4.158 4.158 );
# Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC 0 1 );
Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -13.815 13.815 );
Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC -4.158 4.158 );
Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
# Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC 0 1 );
Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC -11.513 6.908 );
Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
# Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC 0 1 );
Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC -9.21 4.605 );
Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
Distrib( lnkUrnTCAC TruncNormal_v M_lnkUrnTCAC V_lnkUrnTCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
Distrib( lnkEHRC TruncNormal_v M_lnkEHRC V_lnkEHRC -9.21 4.605 );
Distrib( lnkUrnTCOGC TruncNormal_v M_lnUrnTCOGC V_lnUrnTCOGC -6.908 6.908 );
#### Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );
);
#### Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
#### Distrib( lnkNATC TruncNormal_v M_lnNATC V_lnNATC -9.21 4.605 );
#### Distrib( lnkKidBioactC TruncNormal_v M_lnkKidBioactC V_lnkKidBioactC -9.21 4.605 );

#### Chiu et al. 2006 data
Level { # Subject A
  Experiment { # 61 # Experiment A-TRI-1
#CC=0;

    BWmeas= 70.5; VFatCmeas= 0.11;
#lnBW= 4.25561271 ; VFatC= 0.514018692 ;

    QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#    Print( QPsamp, 1 );
#    Data( QPsamp, 310.8 );

    Conc = NDoses( 17 1.155 1.185 1.322 1.262 1.357 1.282 1.339 1.330 1.284 1.248
1.077 1.257 1.182 1.175 1.149 1.053 0.000 0.000 0.283 0.617
1.117 1.367 1.867 2.117 2.367 2.783 2.950 3.700 4.117 4.533 4.950
5.533 6.000 6.001 );

    Print( CALvPPM, 0.3333 0.3343 0.6667 0.6677 1 1.001 1.3333 1.3343 1.6667
1.6677 1.6687 1.6697 2 2.001 2.6667 2.6677 3 3.6667 3.6677 4
4.001 4.3333 4.3343 4.6667 4.6677 5 5.001 5.3333 5.3343 5.6667
5.6677 5.8333 5.8343 6.0333 6.0667 6.1 6.1333 6.1667 6.2833
6.3333 6.4167 6.5 6.6667 6.8333 7 7.5 8 9 10 11 14.3833 15.4167
22.8667 27.1167 46.45 46.6167 51.1167 58.3667 71.9833 75.4 94.8333
103.9167 );
    Data( CALvPPM, 0.259221 0.26847 0.34737 0.389423 0.351313 0.417967 0.495419
0.424781 0.437765 0.452817 0.49446 0.446217 0.493601 0.409691
0.474658 0.451876 0.416239 0.389068 0.390245 0.444807 0.398569
0.326154 0.300993 0.412284 0.420992 0.267463 0.302049 0.353893
0.244604 0.261695 0.294977 0.366387 0.290711 0.142397 0.118484
0.104238 0.099659 0.097115 0.123063 0.080043 0.053037 0.054674

```

```

0.062257 0.056389 0.043814 0.04124 0.02635 0.018905 0.017538
0.014803 0.01106 0.006724 0.007639 0.003938 0.001551 0.002001
0.000819 0.000466 0.000741 0.000246 0.000318 0.000148 );

Print( CVen, 1 2 4 5.7833 6.1167 7.0333 8.0333 );
Data( CVen, 0.0045 0.0045 0.005 0.004 0.002 0.002 0.001 );
Print( CBldTCA, 1 2 4 5.7833 6.1167 7.0333 8.0333 40.7833 98.2833 122.55 );
Data( CBldTCA, 0.002 0.004 0.01 0.019 0.0265 0.0275 0.0375 0.047 0.024 0.0175 );
Print( TotCTCOH, 1 2 4 5.7833 6.1167 7.0333 8.0333 40.7833 77.6167 98.2833 );
Data( TotCTCOH, 0.007 0.048 0.066 0.0995 0.088 0.104 0.037 0.0035 0.0015 0.003 );
Print( CTCOH, 1 2 4 5.7833 6.1167 7.0333 8.0333 40.7833 );
Data( CTCOH, 0.005 0.007 0.011 0.027 0.0165 0.0195 0.02 0.002 );

#      TCAUrnSat= NDoses( 18 1 1 1 1 0 1 0 0 1 1 1 1 0 0 0 0 0 6.2833 7.6167
#      14.45 22.9167 29.7 31.2333 36.3667 38.6167 39.4 46.4167
#      65.7167 75.5667 86.7333 94.7333 114.0667 121.4 134.7333);
UrnMissing= NDoses( 18 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 6.2833 7.6167
14.45 22.9167 29.7 31.2333 36.3667 38.6167 39.4 46.4167
65.7167 75.5667 86.7333 94.7333 114.0667 121.4 134.7333 );
#      Print( zAUrnTCA_sat, 6.2833 7.6167 14.45 22.9167 29.7 36.3667 46.4167 75.5667
#      94.7333 );
#      Data( zAUrnTCA_sat, 0.0167 0.0234 0.0259 0.0449 0.0617 0.0878 0.1053 0.1321
#      0.1478 );
Print( zAUrnTCA_collect, 31.2333 38.6167 39.4 121.4 );
Data( zAUrnTCA_collect, 0.0101 0.0165 0.0277 0.0465 );
#      TCOGUrnSat= NDoses( 18 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6.2833 7.6167
#      14.45 22.9167 29.7 31.2333 36.3667 38.6167 39.4 46.4167
#      65.7167 75.5667 86.7333 94.7333 114.0667 121.4 134.7333 );

#      Print( AUrnTCOGTCOH_sat, 6.2833 7.6167 14.45);
#      Data( AUrnTCOGTCOH_sat, 0.6353 0.8059 0.8711 );

Print( AUrnTCOGTCOH_collect, 22.9167 29.7 31.2333 36.3667 38.6167 39.4 46.4167
75.5667 94.7333 121.4 );
Data( AUrnTCOGTCOH_collect, 0.5003 0.6866 0.7662 1.0048 1.0342 1.0736 1.1472
1.1793 1.1995 1.2039 );

Print( AUrnTCOGTCOH, 1);
Data( AUrnTCOGTCOH, -1);
Print( zAUrnTCA, 1);
Data( zAUrnTCA, -1);

Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print( CPlasTCA, 1);
Print( AUrnTCTotMole, 1);
Print( zAUrnNDCVC, 1);

Print( CDCVGmol, 1);
Data( CDCVGmol, -1);
Print( CDCVG_ND, 1);
Data( CDCVG_ND, -1);

#      Print( MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data( MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print( MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data( MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print( MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data( MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print( MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data( MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print( MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data( MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print( MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data( MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print( RetDose, 1);
Data( RetDose, -1);
}

```

```

Experiment { # 62 # Experiment A-TRI-2

#CC=0;

      BWmeas= 70.5; VFatCmeas= 0.11 ;
#lnBW= 4.25561271 ; VFatC= 0.514018692 ;

      QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 310.8 );

      Conc = NDoses( 21 1.019 0.932 1.085 1.031 1.035 1.165 1.238 1.194 1.200 1.171
1.249 1.194 1.147 1.136 1.234 1.173 1.181 1.300 1.143 1.162 0.000
0.000 0.300 0.717 1.050 1.383 1.717 2.050 2.383 2.633 3.050 3.383
3.800 4.300 4.467 4.800 5.383 5.550 5.800 5.967 6.000 6.001 );

      Print( CALvPPM, 0.3333 0.3343 0.6667 0.6677 1 1.001 1.3333 1.3343 1.6667
1.6677 2 2.001 2.3333 2.3343 2.6667 2.6677 3 3.3333 3.3343
3.6667 3.6677 4 4.3333 4.3343 4.6667 4.6677 5 5.001 5.3333
5.3343 5.6667 5.6677 5.8333 6.0333 6.0667 6.1 6.1333 6.1667 6.25
6.3333 6.5 6.501 6.6667 6.6677 6.8333 6.8343 7 7.001 7.5
7.501 8 8.001 30.4667 34.4667 34.4677 39.1167 46.7167 46.7177
51.7167 51.7177 56.4667 56.4677 56.4687 70.9167 79.2167
79.2177 86.8 86.801 86.9667 96.8167 96.8177 96.8187 );
      Data( CALvPPM, 0.249519 0.262734 0.378056 0.382217 0.350707 0.385927 0.354557
0.314386 0.307842 0.387507 0.33907 0.34747 0.357612 0.427078
0.414282 0.231707 0.437608 0.472409 0.499564 0.470648 0.427958
0.391077 0.395443 0.412294 0.378057 0.474724 0.479064 0.406866
0.476614 0.492051 0.580758 0.463621 0.47456 0.173685 0.157038
0.132661 0.124388 0.095374 0.146307 0.108293 0.033362 0.036
0.063939 0.063 0.054916 0.061 0.050446 0.047 0.035078 0.039
0.024738 0.032 0.004378 0.001287 0.002111 0.003002 0.001518
0.001805 0.000979 0.001069 0.000348 0.000465 0.000458 0.000189
0.000313 0.000196 0.000667 0.000864 0.000388 0.000097 0.000164
0.000246 );

      Print( CVen, 0.8 2.05 5.8833 6.2167 8.05 122.9667 );
      Data( CVen, 0.003 0.003 0.006 0.0015 0.0005 0.001 );
      Print( CBldTCA, 0.8 2.05 5.8833 6.2167 8.05 25.6333 73.8 98.7167 122.9667 122.9677 );
      Data( CBldTCA, 0.001 0.002 0.0105 0.0115 0.0125 0.0205 0.0325 0.024 0.0285 0.024 );
      Print( TotCTCOH, 0.8 2.05 4.05 5.8833 6.2167 8.05 25.6333 );
      Data( TotCTCOH, 0.007 0.011 0.041 0.057 0.0595 0.044 0.01 );
      Print( CTCOH, 5.8833 6.2167 8.05 122.9667 );
      Data( CTCOH, 0.0025 0.003 0.0025 0.0055 );

#      TCAUrnSat= NDoses( 19 0 1 0 1 0 0 1 1 0 1 0 0 0 0 0 0 0 0 0 6.2167 10.3
#      14.3667 23.7167 27.4667 31.4667 37.2167 39.0667 42.0167
#      47.6333 63.9333 69.5167 92.45 96.85 109.4667 120.85 133.9667
#      142.5 );
      UrnMissing= NDoses( 19 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 6.2167 10.3
14.3667 23.7167 27.4667 31.4667 37.2167 39.0667 42.0167
47.6333 63.9333 69.5167 92.45 96.85 109.4667 120.85 133.9667
142.5 );
#      Print( zAUrnTCA_sat, 10.3 23.7167 37.2167 39.0667 47.6333 );
#      Data( zAUrnTCA_sat, 0.0043 0.0225 0.0288 0.0391 0.0478 );
      Print( zAUrnTCA_collect, 6.2167 14.3667 31.4667 42.0167 69.5167 96.85 120.85
142.5 );
      Data( zAUrnTCA_collect, 0.017 0.0336 0.039 0.0491 0.062 0.0709 0.0847 0.0962 );

#      TCOGUrnSat= NDoses( 19 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 6.2167 10.3
#      14.3667 23.7167 27.4667 31.4667 37.2167 39.0667 42.0167
#      47.6333 63.9333 69.5167 92.45 96.85 109.4667 120.85 133.9667
#      142.5 );
#      Print( AUrnTCOGTCOH_sat, 6.2167 10.3 );
#      Data( AUrnTCOGTCOH_sat, 0.778 0.9838 );
      Print( AUrnTCOGTCOH_collect, 14.3667 23.7167 31.4667 37.2167 39.0667 42.0167
47.6333 69.5167 96.85 120.85 142.5 );
      Data( AUrnTCOGTCOH_collect, 0.5175 0.9178 0.9796 1.0985 1.1677 1.2565 1.3254
1.3535 1.3605 1.365 1.3664 );

      Print( AUrnTCOGTCOH, 1);
      Data( AUrnTCOGTCOH, -1);

```



```

Print( zAurnTCA, 1);
Data( zAurnTCA, -1);

Data (CPlasTCA, -1);
Data (AurnTCTotMole, -1);
Data (zAurnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AurnTCTotMole, 1);
Print(zAurnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
}
}

Level { # Subject B
      Experiment { # 63 # Experiment B-TRI-1
#CC=0;

      BWmeas= 75.6; VFatCmeas= 0.204 ;
#lnBW= 4.325456283 ; VFatC= 0.953271028 ;

      QPmeas= 319.2; # NDoses(2, 319.2 0, 0.0 6.0);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 319.2 );

      Conc = NDoses( 23 1.117 1.080 1.107 1.060 1.011 1.067 1.114 1.142 1.153 1.116
1.133 1.122 1.196 1.142 1.213 1.159 1.175 1.211 1.111 1.176 1.142
1.142 0.000 0.000 0.150 0.317 0.983 1.150 1.483 1.733 2.233 2.483
2.900 3.150 3.400 3.567 3.900 4.150 4.317 4.650 4.900 5.567 5.733
5.983 6.000 6.001 );

      Print( CALvPPM, 0.3333 0.3343 0.3353 0.6667 0.6677 0.6687 1 1.001 1.3667
1.3677 1.6667 2.3333 2.3343 2.3353 2.6667 2.6677 3 3.3333
3.3343 3.6667 4 4.001 4.3333 4.3343 4.6667 4.6677 5 5.001
5.3333 5.3343 5.6667 5.6677 5.8333 5.8343 6.0333 6.0667 6.1
6.1333 6.1667 6.25 6.3333 6.4167 6.5 6.7167 6.8333 7 7.5 7.501 8
9 10.5 11 14.2333 24.2333 26.4833 38.4833 47.2333 47.2343 62.9167
71.9833 77.9833 84.4833 93.2333 93.2343 105.4833 );
      Data( CALvPPM, 0.297425 0.284702 0.27631 0.280924 0.269558 0.28923 0.254859
0.28093 0.29746 0.343662 0.361015 0.381184 0.384937 0.340788
0.324214 0.337734 0.298919 0.32549 0.36164 0.342242 0.310441
0.329029 0.334923 0.296386 0.329482 0.350791 0.313065 0.353667
0.355003 0.336777 0.344067 0.348624 0.343156 0.332677 0.225231
0.157472 0.149624 0.150308 0.129402 0.134187 0.125676 0.075
0.086772 0.078 0.065 0.05 0.035353 0.044 0.044 0.024978 0.019178
0.016161 0.011541 0.006049 0.005569 0.003943 0.002919 0.003068
0.002467 0.002008 0.001714 0.001331 0.000976 0.001209 0.000651 );

      Print( CVen, 1 2 4 5.8333 7 8 );
      Data( CVen, 0.002 0.0045 0.003 0.004 0.001 0.001 );
      Print( CBldTCA, 1 2 4 5.8333 7 8 26.5 47.75 72.8333 );
      Data( CBldTCA, 0.002 0.005 0.12 0.031 0.035 0.0425 0.0725 0.0685 0.0485 );
      Print( TotCTCOH, 1 2 4 6.1667 7 8 26.5 47.75 72.8333 98.5 );

```

```

Data( TotCTCOH, 0.0055 0.011 0.034 0.053 0.04 0.04 0.007 0.0025 0.001 0.0015 );
Print( CTCOH, 1 2 4 5.8333 7 8 26.5 47.75 );
Data( CTCOH, 0.003 0.006 0.008 0.011 0.026 0.0135 0.0055 0.0025 );

#           TCAUrnSat= NDoses( 18 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 6.4833 11.4833
#                               14.2333 20.4833 22.9833 26.2333 29.4833 34.4833 39.4833
#                               47.2333 62.9833 71.4833 84.4833 91.4833 109.4833 116.4833
#                               131.9833 );
UrnMissing= NDoses( 18 0 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 6.4833 11.4833
                    14.2333 20.4833 22.9833 26.2333 29.4833 34.4833 39.4833
                    47.2333 62.9833 71.4833 84.4833 91.4833 109.4833 116.4833
                    131.9833 );
#           Print( zAUrnTCA_sat, 6.4833 11.4833 14.2333 20.4833 22.9833 26.2333 29.4833
#                               34.4833 39.4833 47.2333 71.4833 );
#           Data( zAUrnTCA_sat, 0.0204 0.0361 0.0444 0.072 0.0888 0.0994 0.1234 0.1334 0.1481
#                               0.1703 0.1778 );
#           Print( zAUrnTCA_collect, 0 );
#           Data( zAUrnTCA_collect, -1 );

#           TCOGUrnSat= NDoses( 18 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6.4833 11.4833
#                               14.2333 20.4833 22.9833 26.2333 29.4833 34.4833 39.4833
#                               47.2333 62.9833 71.4833 84.4833 91.4833 109.4833 116.4833
#                               131.9833 );

#           Print( AUrnTCOGTCOH_sat, 11.4833 14.2333 );
#           Data( AUrnTCOGTCOH_sat, 0.4522 0.6758 );
Print( AUrnTCOGTCOH_collect, 6.4833 20.4833 22.9833 26.2333 29.4833 34.4833
      39.4833 47.2333 71.4833 91.4833 116.4833 );
Data( AUrnTCOGTCOH_collect, 0.6936 1.1404 1.3606 1.4823 1.6973 1.8812 2.0137
      2.1577 2.1792 2.2126 2.2329 );

Print( AUrnTCOGTCOH, 1);
Data( AUrnTCOGTCOH, -1);
Print( zAUrnTCA, 1);
Data( zAUrnTCA, -1);

Data( CPlastTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print( CPlastTCA, 1);
Print( AUrnTCTotMole, 1);
Print( zAUrnNDCVC, 1);

Print( CDCVGmol, 1);
Data( CDCVGmol, -1);
Print( CDCVG_ND, 1);
Data( CDCVG_ND, -1);

#           Print( MassBalTCE, 1, 2, 4, 8, 16, 32);
#           Data( MassBalTCE, 0, 0, 0, 0, 0, 0);
#           Print( MassBalTCOH, 1, 2, 4, 8, 16, 32);
#           Data( MassBalTCOH, 0, 0, 0, 0, 0, 0);
#           Print( MassBalTCA, 1, 2, 4, 8, 16, 32);
#           Data( MassBalTCA, 0, 0, 0, 0, 0, 0);
#           Print( MassBalTCOG, 1, 2, 4, 8, 16, 32);
#           Data( MassBalTCOG, 0, 0, 0, 0, 0, 0);
#           Print( MassBalDCVG, 1, 2, 4, 8, 16, 32);
#           Data( MassBalDCVG, 0, 0, 0, 0, 0, 0);
#           Print( MassBalDCVC, 1, 2, 4, 8, 16, 32);
#           Data( MassBalDCVC, 0, 0, 0, 0, 0, 0);
#           Print( RetDose, 1);
#           Data( RetDose, -1);
}

Experiment { # 64 # Experiment B-TRI-2
#CC=0;

      BWmeas= 75.6; VFatCmeas= 0.204 ;
#lnBW= 4.325456283 ; VFatC= 0.953271028 ;

```

```

QPmeas= 319.2; # NDoses(2, 319.2 0, 0.0 6.0);
#   Print( QPsamp, 1 );
#   Data( QPsamp, 319.2 );

Conc = NDoses( 31 1.424 1.305 1.367 1.341 1.353 0.492 0.248 0.302 1.594 1.876
1.642 1.583 1.465 0.825 1.259 1.284 1.450 1.386 1.240 1.303 1.315
1.401 1.435 1.381 1.261 1.339 1.436 1.128 1.205 1.166 0.000 0.000
0.133 0.300 0.467 0.717 1.050 1.300 1.383 1.550 1.633 1.717 1.800
1.883 1.967 2.100 2.133 2.267 2.333 2.383 2.717 2.967 3.467 3.967
4.050 4.467 4.800 5.133 5.383 5.883 6.000 6.001 );

Print( CALvPPM, 0.3333 0.3343 0.6667 0.6677 1 1.001 1.3333 1.6667 1.6677
2.3333 2.3343 2.6667 2.6677 3 3.001 3.3333 3.3343 3.6667
3.6677 4 4.001 4.3333 4.3343 4.6667 4.6677 5 5.001 5.3333
5.3343 5.6667 5.8333 6.0333 6.0667 6.1 6.1333 6.1667 6.25 6.3333
6.45 6.8333 7 7.5 8 11.1333 14.1333 24.1333 25.6333 25.6343
35.1333 40.6333 49.6333 53.6333 62.3833 72.6333 76.3833 86.3833
94.6333 99.6333 );
Data( CALvPPM, 0.292512 0.230086 0.25225 0.233197 0.195014 0.249061 0.073272
0.0486764 0.0822443 0.238585 0.250825 0.29416 0.341965 0.335391
0.36076 0.273437 0.271976 0.393574 0.343947 0.358395 0.412402
0.358135 0.334281 0.407889 0.404538 0.458073 0.377995 0.376453
0.324713 0.348042 0.372123 0.166853 0.111252 0.129059 0.101955
0.100765 0.098608 0.090289 0.058627 0.061 0.05 0.037 0.034 0.030738
0.019318 0.008817 0.009376 0.009201 0.006491 0.007261 0.004046
0.005629 0.003618 0.003276 0.002677 0.002406 0.000952 0.000978 );

Print( CVen, 0.95 5.7833 6.1167 6.95 7.95 );
Data( CVen, 0.0025 0.006 0.003 0.001 0.001 );
Print( CBldTCA, 0.95 5.7833 6.1167 6.95 7.95 26.4667 50.2167 74.1333 144.6667 );
Data( CBldTCA, 0.002 0.041 0.034 0.0325 0.042 0.057 0.06 0.068 0.0405 );
Print( TotCTCOH, 5.7833 6.1167 6.95 7.95 26.4667 50.2167 74.1333 99.6333 );
Data( TotCTCOH, 0.0425 0.037 0.036 0.0325 0.011 0.004 0.0025 0.001 );
Print( CTCOH, 5.7833 6.1167 6.95 7.95 );
Data( CTCOH, 0.011 0.0075 0.0065 0.008 );
#   TCAUrnSat= NDoses( 17 1 1 1 1 1 1 1 1 0 1 1 1 1 0 0 0 6.3 9.1333 11.6333
#   15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 65.1333
#   73.1333 87.3833 94.6333 111.3833 117.9667 135.6333 );
UrnMissing= NDoses( 17 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 6.3 9.1333 11.6333
15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 65.1333
73.1333 87.3833 94.6333 111.3833 117.9667 135.6333 );
#   Print( zAUrnTCA_sat, 6.3 9.1333 11.6333 15.1333 26.1333 32.1333 36.1333 41.6333
#   50.1333 73.1333 94.6333 117.9667 );
#   Data( zAUrnTCA_sat, 0.0143 0.0228 0.0304 0.0425 0.0659 0.073 0.0846 0.0917 0.1043
#   0.1149 0.1227 0.1365 );
Print( zAUrnTCA_collect, 0 );
Data( zAUrnTCA_collect, -1 );
#   TCOGUrnSat= NDoses( 17 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 6.3 9.1333 11.6333
#   15.1333 26.1333 32.1333 36.1333 41.6333 50.1333 65.1333
#   73.1333 87.3833 94.6333 111.3833 117.9667 135.6333 );
#   Print( AUrnTCOGTCOH_sat, 6.3 9.1333 11.6333 );
#   Data( AUrnTCOGTCOH_sat, 0.7941 1.3632 1.6546 );
Print( AUrnTCOGTCOH_collect, 15.1333 26.1333 32.1333 36.1333 41.6333 50.1333
73.1333 94.6333 117.9667);
Data( AUrnTCOGTCOH_collect, 0.2776 0.8985 1.1068 1.3213 1.4584 1.6555 1.7119
1.7378 1.7532 );

Print( AUrnTCOGTCOH, 1);
Data( AUrnTCOGTCOH, -1);
Print( zAUrnTCA, 1);
Data( zAUrnTCA, -1);

Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);

```

```

Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#       Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#       Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#       Print(MassBalDVC, 1, 2, 4, 8, 16, 32);
#       Data(MassBalDVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
}
}

Level { # Subject C
      Experiment { # 65 # Experiment C-TRI-1
#CC=0;

      BWmeas= 75.2; VFatCmeas= 0.204 ;
#lnBW= 4.320151231 ; VFatC= 0.953271028 ;

      QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#       Print( QPsamp, 1 );
#       Data( QPsamp, 310.8 );

      Conc = NDoses( 18 1.218 1.155 1.185 1.322 1.262 1.357 1.282 1.339 1.330 1.284
1.248 1.077 1.257 1.182 1.175 1.149 1.053 0.000 0.000 0.050 0.550
0.883 1.383 1.633 2.133 2.383 2.633 3.050 3.217 3.967 4.383 4.800
5.217 5.800 6.000 6.001 );

      Print( CALvPPM, 0.3333 0.3343 0.6667 0.6677 1 1.001 1.3333 1.3343 1.6667
1.6677 2 2.001 2.3333 2.3343 2.6667 2.6677 3 3.001 3.3333
3.3343 3.6667 3.6677 4 4.3333 4.3343 4.6667 5 5.001 5.3333
5.6667 5.6677 5.8333 5.8343 6.0333 6.0667 6.1 6.1333 6.1667
6.2833 6.3333 6.4167 6.5333 6.6667 6.8333 7 7.5 8 8.1333 9.25
9.251 10.25 11 14.05 14.051 22.8833 27.05 33.2167 38.3833 45.8
51.8833 62.3833 69.8 75 80.7167 86.2167 93.6333 94.3833 94.3843
103.6333 103.6343 );
      Data( CALvPPM, 0.401675 0.330756 0.377474 0.356618 0.403155 0.375551 0.331179
0.328483 0.309511 0.319748 0.385379 0.388993 0.460043 0.44499
0.480806 0.422521 0.406884 0.394325 0.322196 0.355099 0.330437
0.320814 0.379121 0.233554 0.3079 0.307107 0.224368 0.255573
0.27075 0.259446 0.291828 0.268891 0.225715 0.105026 0.078629
0.073664 0.083212 0.075192 0.063266 0.066949 0.054265 0.049763
0.050582 0.049355 0.045262 0.024803 0.032 0.032289 0.021 0.023554
0.015935 0.012913 0.020003 0.01928 0.007244 0.007512 0.003531
0.003104 0.003364 0.001355 0.003528 0.001538 0.000655 0.000321
0.001165 0.00036 0.000689 0.000681 0.000388 0.000452 );

      Print( CVen, 1 2 4 5.8333 7.05 51.8833 );
      Data( CVen, 0.001 0.004 0.004 0.0025 0.001 0.0005 );
      Print( CBldTCA, 1 2 4 5.8333 7.05 28.55 51.8833 74.9667 98.6 120.8833 );
      Data( CBldTCA, 0.001 0.004 0.014 0.015 0.035 0.055 0.053 0.045 0.033 0.027 );
      Print( TotCTCOH, 1 2 4 5.8333 6.1667 7.05 8.3833 28.55 51.8833 74.9667 120.8833 );
      Data(TotCTCOH,0.005 0.0165 0.213 0.094 0.095 0.088 0.075 0.012 0.014 0.012 0.001);
      Print( CTCOH, 1 2 4 5.8333 7.05 28.55 51.8833 74.9667 );
      Data( CTCOH, 0.003 0.006 0.02 0.016 0.024 0.006 0.0015 0.001 );

#       TCAUrnSat= NDoses( 16 0 1 1 0 0 1 0 1 0 1 0 0 0 0 0 7.2167 14.1333 22.3833
#       28.3833 32.8833 38.3833 45.6333 62.3833 69.8833 86.2167
#       94.4667 110.3833 118.3833 133.4667 141.3833 );
      UrnMissing= NDoses( 16 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 7.2167 14.1333 22.3833
28.3833 32.8833 38.3833 45.6333 62.3833 69.8833 86.2167
94.4667 110.3833 118.3833 133.4667 141.3833 );
#       Print( zAUrnTCA_sat, 14.1333 22.3833 38.3833 );

```

```

#      Data( zAurnTCA_sat, 0.0114 0.0237 0.0317 );
Print(zAurnTCA_collect, 7.2167 28.3833 45.6333 69.8833 94.4667 118.3833 141.3833);
Data( zAurnTCA_collect, 0.0106 0.0213 0.0333 0.0527 0.067 0.0823 0.0951 );
#      TCOGurnSat= NDoses( 16 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7.2167 14.1333
#                          22.3833 28.3833 32.8833 38.3833 45.6333 62.3833 69.8833
#                          86.2167 94.4667 110.3833 118.3833 133.4667 141.3833 );
#      Print( AurnTCOGTCOH_sat, 14.1333 22.3833 );
#      Data( AurnTCOGTCOH_sat, 0.6721 1.2857 );
Print( AurnTCOGTCOH_collect, 7.2167 28.3833 38.3833 45.6333 69.8833 94.4667
      118.3833 141.3833 );
Data( AurnTCOGTCOH_collect, 0.5381 0.9118 1.1632 1.3584 1.4847 1.5212 1.5427
      1.5485 );

Print( AurnTCOGTCOH, 1);
Data( AurnTCOGTCOH, -1);
Print( zAurnTCA, 1);
Data( zAurnTCA, -1);

Data (CPlasTCA, -1);
Data (AurnTCTotMole, -1);
Data (zAurnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AurnTCTotMole, 1);
Print(zAurnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
}

Experiment { # 66 # Experiment C-TRI-2
#CC=0;
      BWmeas= 75.2; VFatCmeas= 0.204 ;
#lnBW= 4.320151231 ; VFatC= 0.953271028 ;

      QPmeas= 310.8; # NDoses(2, 310.8 0, 0.0 6.0);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 310.8 );

      Conc = NDoses( 21 0.965 1.019 0.932 1.085 1.031 1.035 1.165 1.238 1.194 1.200
      1.171 1.249 1.194 1.147 1.136 1.234 1.173 1.181 1.300 1.143 0.000
      0.000 0.133 0.467 0.883 1.217 1.550 1.883 2.217 2.550 2.800 3.217
      3.550 3.967 4.467 4.633 4.967 5.550 5.717 5.967 6.000 6.001 );

      Print( CALvPPM, 0.3833 0.3843 0.6667 0.6677 0.95 0.951 1.3667 1.3677 1.65
      1.651 2 2.001 2.3333 2.3343 2.75 2.751 3.3833 3.3843 3.6667
      3.6677 4 4.001 4.3333 4.3343 4.6667 4.6677 5.3333 5.3343
      5.6667 5.6677 5.8333 5.8343 6.0333 6.0667 6.1 6.1333 6.1667 6.25
      6.3333 6.4167 6.5 6.6667 6.8333 7.0667 7.5167 8.0667 9.1333
      10.3333 22.3 22.301 22.302 27.8833 27.9667 33.4667 33.4677
      33.4687 33.8833 33.8843 37.7167 46.1333 46.1343 53.1333 53.1343
      70.6333 70.6343 74.8 74.801 74.802 80.9167 80.9177 86.5833
      86.5843 94.1333 109.8833 );

```

```

Data( CALvPPM, 0.253178 0.257009 0.254465 0.29185 0.301115 0.312384 0.340338
0.287822 0.370802 0.30183 0.251879 0.247645 0.288842 0.256194
0.347955 0.343899 0.381599 0.354656 0.302258 0.282438 0.333418
0.279138 0.248589 0.280191 0.262212 0.238468 0.314908 0.320199
0.23351 0.273286 0.293398 0.31403 0.104011 0.08682 0.07929
0.077221 0.050574 0.050266 0.044009 0.041885 0.04326 0.03298
0.027589 0.035016 0.011413 0.000367 0.018218 0.011661 0.004863
0.004727 0.005205 0.001923 0.002692 0.002092 0.002603 0.002335
0.001203 0.000656 0.002035 0.002554 0.002702 0.001537 0.001002
0.000237 0.000666 0.000391 0.001138 0.00068 0.000141 0.000181
0.000631 0.000813 0.000729 0.000656 );

Print( CVen, 1 1.9 3.9833 5.8833 6.2167 7.0667 8.0667 );
Data( CVen, 0.002 0.002 0.003 0.003 0.001 0.0005 0.001 );
Print( CBldTCA, 1 1.9 3.9833 5.8833 6.2167 7.0667 8.0667 25.6333 52.6333 74.8 97.8
124.1333 );
Data( CBldTCA, 0.001 0.004 0.0065 0.012 0.0135 0.018 0.0155 0.048 0.058 0.051
0.038 0.036 );
Print( TotCTCOH, 1 1.9 3.9833 5.8833 6.2167 7.0667 8.0667 25.6333 52.6333 74.8 );
Data( TotCTCOH, 0.006 0.013 0.055 0.097 0.066 0.069 0.079 0.013 0.0095 0.004 );
Print( CTCOH, 3.9833 5.8833 6.2167 7.0667 8.0667 25.6333 );
Data( CTCOH, 0.002 0.003 0.004 0.003 0.003 0.002 );
# TCAUrnSat= NDoses( 17 0 1 1 0 1 0 1 0 0 1 1 0 0 0 0 0 7.9667 13.6333
# 22.1333 29.1333 33.4667 37.6333 46.1333 50.8 63.8 70.1333
# 86.55 94.1333 110.1333 122.4667 134.8 141.6333 );
UrnMissing= NDoses( 17 0 0 0 0 0 0 0 1 0 1 0 1 1 0 0 0 7.9667 13.6333
22.1333 29.1333 33.4667 37.6333 46.1333 50.8 63.8 70.1333
86.55 94.1333 110.1333 122.4667 134.8 141.6333 );
# Print( zAUrnTCA_sat, 13.6333 22.1333 33.4667 46.1333 70.1333 );
# Data( zAUrnTCA_sat, 0.0103 0.0233 0.032 0.0465 0.0542 );
Print( zAUrnTCA_collect, 7.9667 29.1333 37.6333 50.8 94.1333 141.6333 );
Data( zAUrnTCA_collect, 0.0133 0.0232 0.0315 0.0454 0.0542 0.0575 );
# TCOGUrnSat= NDoses( 17 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7.9667 13.6333
# 22.1333 29.1333 33.4667 37.6333 46.1333 50.8 63.8 70.1333
# 86.55 94.1333 110.1333 122.4667 134.8 141.6333 );
# Print( AUrnTCOGTCOH_sat, 7.9667 13.6333 );
# Data( AUrnTCOGTCOH_sat, 0.8675 1.6259 );
Print( AUrnTCOGTCOH_collect, 22.1333 29.1333 33.4667 37.6333 46.1333 50.8 70.1333
94.1333 141.6333 );
Data( AUrnTCOGTCOH_collect, 0.5968 0.9005 1.0882 1.2845 1.556 1.6346 1.6844 1.706
1.7109 );

Print( AUrnTCOGTCOH, 1);
Data( AUrnTCOGTCOH, -1);
Print( zAUrnTCA, 1);
Data( zAUrnTCA, -1);

Data( CPlasTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

# Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);

```

```

        Print(RetDose, 1);
        Data(RetDose, -1);
    }
}

Level { # Subject D
    Experiment { # 67 # Experiment D-TRI-1
#CC=0;

        BWmeas= 70.5; VFatCmeas= 0.129 ;
#lnBW= 4.25561271 ; VFatC= 0.602803738 ;

        QPmeas= 298.2; # NDoses(2, 298.2 0, 0.0 6.0);
#        Print( QPsamp, 1 );
#        Data( QPsamp, 298.2 );

        Conc = NDoses( 22 1.080 1.117 1.080 1.107 1.060 1.011 1.067 1.114 1.142 1.153
                        1.116 1.133 1.122 1.196 1.142 1.213 1.159 1.175 1.211 1.111 1.176
                        0.000 0.000 0.050 0.550 0.717 1.383 1.550 1.883 2.133 2.633 2.883
                        3.300 3.550 3.800 3.967 4.300 4.550 4.717 5.050 5.300 5.967 6.000
                        6.001 );
        Print( CALvPPM, 0.3333 0.3343 0.6667 0.6677 1 1.001 1.3333 1.3343 1.6667
                        1.6677 2 2.001 2.3333 2.3343 2.6667 2.6677 3 3.001 3.3333
                        3.3343 3.6667 3.6677 4 4.001 4.3333 4.3343 4.6667 4.6677 5
                        5.001 5.3333 5.3343 5.6667 5.6677 5.8333 5.8343 6.0333 6.0667
                        6.1 6.1333 6.1667 6.25 6.3333 6.4167 6.5 6.6667 6.8333 7 7.5
                        7.501 8 8.001 9 9.001 11 22.7167 26.8833 26.8843 71.8833
                        71.8843 74.3833 80.8833 99.8833 );
        Data( CALvPPM, 0.339106 0.340422 0.424221 0.398335 0.393694 0.396775 0.309778
                        0.348686 0.301157 0.313293 0.481734 0.436713 0.386535 0.373559
                        0.399467 0.377011 0.428886 0.441738 0.285831 0.31491 0.336511
                        0.33477 0.355122 0.337867 0.35645 0.356892 0.377994 0.345809
                        0.460963 0.434667 0.335875 0.378302 0.421981 0.404211 0.658911
                        0.525865 0.243293 0.164947 0.150146 0.079 0.128442 0.108595
                        0.101212 0.062 0.076 0.075 0.066 0.081382 0.045 0.032546 0.031561
                        0.052 0.009309 0.014 0.011843 0.007562 0.006445 0.014 0.000948
                        0.000915 0.001914 0.000675 0.000462 );

        Print( CVen, 1 4 5.8333 6.1667 8 );
        Data( CVen, 0.004 0.0035 0.007 0.0025 0.001 );
        Print( CBldTCA, 1 4 5.8333 6.1667 8 25.2167 49.8833 73.7333 );
        Data( CBldTCA, 0.003 0.032 0.056 0.047 0.072 0.0595 0.0875 0.052 );
        Print( TotCTCOH, 1 2 4 5.8333 6.1667 7 8 25.2167 73.7333 99.6333 );
        Data( TotCTCOH, 0.006 0.011 0.035 0.073 0.104 0.366 0.133 0.01 0.0025 0.001 );
        Print( CTCOH, 1 4 5.8333 6.1667 8 25.2167 49.8833 );
        Data( CTCOH, 0.0025 0.016 0.022 0.014 0.0095 0.005 0.003 );

#        TCAUrnSat= NDoses( 19 0 1 1 1 1 1 1 0 1 1 1 0 0 0 0 0 0 0 0 6.3 8.7167
#                        12.6333 22.7167 25.9667 31.8833 33.3833 35.55 40.4167 48.55
#                        61.3 72.3833 84.5 93.55 108.3833 118.1333 130.6333 132.8833 );
        UrnMissing= NDoses( 19 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 0 6.3 8.7167
                        12.6333 22.7167 25.9667 31.8833 33.3833 35.55 40.4167 48.55
                        61.3 72.3833 84.5 93.55 108.3833 118.1333 130.6333 132.8833 );
#        Print( zAUrnTCA_sat, 8.7167 12.6333 22.7167 25.9667 31.8833 33.3833 35.55 48.55
#                        72.3833 );
#        Data( zAUrnTCA_sat, 0.0117 0.0168 0.0313 0.041 0.05 0.0511 0.0568 0.0782 0.0972);
        Print( zAUrnTCA_collect, 6.3 40.4167 );
        Data( zAUrnTCA_collect, 0.0141 0.0171 );
#        TCOGUrnSat= NDoses( 19 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6.3 8.7167
#                        12.6333 22.7167 25.9667 31.8833 33.3833 35.55 40.4167 48.55
#                        61.3 72.3833 84.5 93.55 108.3833 118.1333 130.6333 132.8833);

#        Print( AUrnTCOGTCOH_sat, 6.3 8.7167 12.6333 22.7167 );
#        Data( AUrnTCOGTCOH_sat, 0.7557 1.1772 1.4037 2.0733 );
        Print( AUrnTCOGTCOH_collect, 25.9667 31.8833 33.3833 35.55 40.4167 48.55 72.3833
                        93.55 118.1333 132.8833 );
        Data( AUrnTCOGTCOH_collect, 0.2368 0.3721 0.3835 0.4405 0.4633 0.6079 0.6947
                        0.7139 0.728 0.7312 );

        Print( AUrnTCOGTCOH, 1);
        Data( AUrnTCOGTCOH, -1);

```



```

Print( CTCOH, 1 4 5.8333 6.1667 7 8 25.6667 49.8333 73.8333 );
Data( CTCOH, 0.002 0.008 0.0095 0.0175 0.01 0.01 0.003 0.001 0.001 );

#       TCAUrnSat= NDoses( 21 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 0 0 0 0 0 0 6.3 8.1667
#                               9.1667 12.6667 14.6667 24.6667 29.6667 31.6667 36.6667 39.1667
#                               41.6667 48.4167 62.6667 72.1667 88.6667 97.6667 112.6667
#                               122.1667 134.6667 143.4167 );
UrnMissing= NDoses( 21 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 0 6.3 8.1667
                    9.1667 12.6667 14.6667 24.6667 29.6667 31.6667 36.6667 39.1667
                    41.6667 48.4167 62.6667 72.1667 88.6667 97.6667 112.6667
                    122.1667 134.6667 143.4167 );
#       Print( zAUrnTCA_sat, 6.3 8.1667 9.1667 12.6667 14.6667 24.6667 29.6667 36.6667
#                               39.1667 41.6667 48.4167 72.1667 97.6667 );
#       Data( zAUrnTCA_sat, 0.0002 0.0094 0.01 0.0201 0.0249 0.0378 0.0515 0.0691 0.0936
#                               0.1106 0.1211 0.1386 0.1475 );
Print( zAUrnTCA_collect, 31.6667 );
Data( zAUrnTCA_collect, 0.0088 );
#       TCOGUrnSat= NDoses( 21 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6.3 8.1667
#                               9.1667 12.6667 14.6667 24.6667 29.6667 31.6667 36.6667
#                               39.1667 41.6667 48.4167 62.6667 72.1667 88.6667 97.6667
#                               112.6667 122.1667 134.6667 143.4167 );

#       Print( AUrnTCOGTCOH_sat, 9.1667 );
#       Data( AUrnTCOGTCOH_sat, 0.0788 );
Print( AUrnTCOGTCOH_collect, 6.3 8.1667 12.6667 14.6667 24.6667 29.6667 31.6667
        36.6667 39.1667 41.6667 48.4167 72.1667 97.6667
        122.1667 143.4167 );
Data( AUrnTCOGTCOH_collect, 0.0063 0.2254 0.4775 0.6152 0.9452 1.0952 1.143 1.2548
        1.3098 1.3584 1.3788 1.4181 1.4272 1.4363 1.4402 );

Print( AUrnTCOGTCOH, 1);
Data( AUrnTCOGTCOH, -1);
Print( zAUrnTCA, 1);
Data( zAUrnTCA, -1);

Data( CPlastTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print( CPlastTCA, 1);
Print( AUrnTCTotMole, 1);
Print( zAUrnNDCVC, 1);

Print( CDCVGmol, 1);
Data( CDCVGmol, -1);
Print( CDCVG_ND, 1);
Data( CDCVG_ND, -1);

#       Print( MassBalTCE, 1, 2, 4, 8, 16, 32);
#       Data( MassBalTCE, 0, 0, 0, 0, 0, 0);
#       Print( MassBalTCOH, 1, 2, 4, 8, 16, 32);
#       Data( MassBalTCOH, 0, 0, 0, 0, 0, 0);
#       Print( MassBalTCA, 1, 2, 4, 8, 16, 32);
#       Data( MassBalTCA, 0, 0, 0, 0, 0, 0);
#       Print( MassBalTCOG, 1, 2, 4, 8, 16, 32);
#       Data( MassBalTCOG, 0, 0, 0, 0, 0, 0);
#       Print( MassBalDCVG, 1, 2, 4, 8, 16, 32);
#       Data( MassBalDCVG, 0, 0, 0, 0, 0, 0);
#       Print( MassBalDCVC, 1, 2, 4, 8, 16, 32);
#       Data( MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print( RetDose, 1);
Data( RetDose, -1);
}

Experiment { # 69 # Experiment F-TRI-2

#CC=0;

        BWmeas= 69.5; VFatCmeas= 0.18 ;
#lnBW= 4.241326753 ; VFatC= 0.841121495 ;

```

```

QPmeas= 327.6; # NDoses(2, 327.6 0, 0.0 6.0);
#   Print( QPsamp, 1 );
#   Data( QPsamp, 327.6 );

Conc = NDoses( 32 1.344 1.252 1.424 1.305 1.367 1.341 1.353 0.492 0.248 0.302
1.594 1.876 1.642 1.583 1.465 0.825 1.259 1.284 1.450 1.386 1.240
1.303 1.315 1.401 1.435 1.381 1.261 1.339 1.436 1.128 1.205 0.000
0.000 0.300 0.383 0.633 0.800 0.967 1.217 1.550 1.800 1.883 2.050
2.133 2.217 2.300 2.383 2.467 2.600 2.633 2.767 2.833 2.883 3.217
3.467 3.967 4.467 4.550 4.967 5.300 5.633 5.883 6.000 6.001 );
Print( CALvPPM, 0.3333 0.3343 0.6667 0.6677 1 1.001 1.3333 1.3343 1.6667
1.6677 2 2.001 2.3333 2.3343 2.6667 2.6677 3 3.001 3.3333
3.3343 3.6667 3.6677 4 4.001 4.4667 4.4677 4.6667 4.6677 5
5.001 5.3333 5.3343 5.6667 5.6677 5.8333 6.0333 6.0667 6.1
6.1333 6.1667 6.25 6.3333 6.4167 6.5 6.6667 6.8333 7 7.5 8 16.15
22.8833 27.6333 34.1333 35.6333 39.3833 48.6333 51.6333 58.6333
58.6343 58.6353 72.3833 75.6333 75.6343 82.6333 92.8833 99.6333
99.6343 99.6353 );
Data( CALvPPM, 0.42561 0.351669 0.416291 0.294322 0.39137 0.543459 0.347941
0.392029 0.072125 0.074234 0.059767 0.054379 0.159857 0.492105
0.386478 0.344507 0.530141 0.497122 0.545553 0.544988 0.445338
0.413655 0.331208 0.544767 0.505634 0.529838 0.417287 0.327814
0.440222 0.511302 0.317899 0.312976 0.308524 0.478391 0.412262
0.179332 0.134678 0.092383 0.059 0.09907 0.050897 0.059 0.051
0.045315 0.045715 0.043 0.038 0.03 0.015 0.010247 0.007517 0.00535
0.00279 0.006341 0.003194 0.001592 0.001841 0.001643 0.002178
0.002056 0.001587 0.001208 0.000874 0.00112 0.000748 0.00031
0.000223 0.000584 );

Print( CVen, 1 2 4 5.8333 6.2333 8 );
Data( CVen, 0.0035 0.001 0.005 0.006 0.002 0.001 );
Print( CBldTCA, 1 2 4 5.8333 6.2333 8 26.6333 73.3833 94.3833 128.6333 );
Data( CBldTCA, 0.002 0.0035 0.02 0.039 0.0425 0.048 0.074 0.067 0.0545 0.036 );
Print( TotCTCOH, 1 2 4 5.8333 6.2333 7 8 26.6333 50.55 73.3833 );
Data( TotCTCOH, 0.0065 0.018 0.038 0.065 0.043 0.041 0.036 0.012 0.0025 0.001 );
Print( CTCOH, 4 5.8333 6.2333 8 26.6333 );
Data( CTCOH, 0.008 0.009 0.009 0.007 0.002 );

#   TCAUrnSat= NDoses( 20 0 1 0 1 1 1 1 1 0 1 0 1 1 0 0 0 1 0 0 6.1333 8.1333
#   9.6333 15.6333 22.8 26.6333 30.3833 34.1333 39.3833 40.6333
#   48.6333 63.6333 72.1333 86.6333 93.6333 110.6333 118.6333
#   135.1333 143.1333 );
UrnMissing= NDoses( 20 0 0 0 0 0 0 0 0 0 0 1 0 1 0 1 0 1 0 0 6.1333 8.1333
9.6333 15.6333 22.8 26.6333 30.3833 34.1333 39.3833 40.6333
48.6333 63.6333 72.1333 86.6333 93.6333 110.6333 118.6333
135.1333 143.1333 );

#   Print( zAUrnTCA_sat, 8.1333 15.6333 22.8 26.6333 30.3833 34.1333 39.3833 48.6333
#   72.1333 93.6333 143.1333 );
#   Data( zAUrnTCA_sat, 0.0115 0.028 0.049 0.0561 0.0688 0.0897 0.0959 0.1072 0.1216
#   0.1282 0.133 );
Print( zAUrnTCA_collect, 40.6333 118.6333 );
Data( zAUrnTCA_collect, 0.0198 0.024 );

#   TCOGUrnSat= NDoses( 20 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6.1333 8.1333
#   9.6333 15.6333 22.8 26.6333 30.3833 34.1333 39.3833 40.6333
#   48.6333 63.6333 72.1333 86.6333 93.6333 110.6333 118.6333
#   135.1333 143.1333 );

#   Print( AUrnTCOGTCOH_sat, 8.1333 );
#   Data( AUrnTCOGTCOH_sat, 0.635 );
Print( AUrnTCOGTCOH_collect, 6.1333 9.6333 15.6333 22.8 26.6333 30.3833 34.1333
39.3833 40.6333 48.6333 72.1333 93.6333 118.6333
143.1333 );
Data( AUrnTCOGTCOH_collect, 0.5917 1.0628 1.4811 1.9016 2.0542 2.1926 2.3728
2.4387 2.4618 2.5126 2.5518 2.566 2.5684 2.5711 );

Print( AUrnTCOGTCOH, 1);
Data( AUrnTCOGTCOH, -1);
Print( zAUrnTCA, 1);
Data( zAUrnTCA, -1);

```

```

Data (CPlasTCA, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(CPlasTCA, 1);
Print(AUrnTCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#      Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#      Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#      Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#      Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
}
}

Level { # Subject G
      Experiment { # 70 # Experiment G-TRI-2
#CC=0;

      BWmeas= 71; VFatCmeas= 0.096 ;
#lnBW= 4.262679877 ; VFatC= 0.448598131 ;

      QPmeas= 302.4; # NDoses(2, 302.4 0, 0.0 6.0);
#      Print( QPsamp, 1 );
#      Data( QPsamp, 302.4 );

      Conc = NDoses( 32 1.344 1.252 1.424 1.305 1.367 1.341 1.353 0.492 0.248 0.302
1.594 1.876 1.642 1.583 1.465 0.825 1.259 1.284 1.450 1.386 1.240
1.303 1.315 1.401 1.435 1.381 1.261 1.339 1.436 1.128 1.205 0.000
0.000 0.050 0.133 0.383 0.550 0.717 0.967 1.300 1.550 1.633 1.800
1.883 1.967 2.050 2.133 2.217 2.350 2.383 2.517 2.583 2.633 2.967
3.217 3.717 4.217 4.300 4.717 5.050 5.383 5.633 6.000 6.001 );
      Print( CALvPPM, 0.3333 0.3343 0.6667 0.6677 1 1.001 1.3333 1.3343 1.6667
1.6677 2 2.001 2.3333 2.3343 2.6667 2.6677 3 3.001 3.3833
3.3843 3.6667 3.6677 4 4.001 4.3333 4.3343 4.6667 4.6677 5
5.001 5.3333 5.3343 5.6667 5.6677 5.8333 6.0667 6.1 6.1333
6.1667 6.3333 6.4167 6.5 6.6667 6.8333 7 7.5 9.4 10.7167 12.8833
24.3833 24.3843 27.1333 27.1343 32.3833 32.3843 37.3833 48.3833
48.3843 51.3833 51.3843 57.3833 57.3843 71.1333 71.1343 81.3833
81.3843 85.3833 85.3843 96.3833 101.3833 );
      Data( CALvPPM, 0.313836 0.289407 0.358654 0.330007 0.286794 0.351549 0.098419
0.111763 0.055313 0.056352 0.477732 0.560644 0.280315 0.307747
0.420583 0.32215 0.494522 0.568965 0.38854 0.352325 0.383471
0.353154 0.401385 0.384194 0.449241 0.413776 0.421671 0.405174
0.510643 0.454817 0.47175 0.523048 0.392709 0.37841 0.416564
0.09573 0.104838 0.082287 0.075879 0.076577 0.046446 0.039067
0.027451 0.023355 0.051239 0.0165 0.042249 0.027713 0.025106
0.011491 0.010796 0.006405 0.007495 0.003457 0.003741 0.005975
0.002303 0.001115 0.001783 0.001744 0.003287 0.002935 0.001309
0.003156 0.000455 0.000346 0.000209 0.001095 0.000518 0.000259 );

      Print( CVen, 1 2 4 5.8333 6.2 );
      Data( CVen, 0.002 0.004 0.004 0.005 0.001 );
      Print( CBldTCA, 1 2 4 5.8333 6.2 51.1333 71.8833 98.55 143.75 );
      Data( CBldTCA, 0.001 0.002 0.0135 0.0255 0.027 0.0665 0.0635 0.0445 0.0385 );
      Print( TotCTCOH, 1 4 5.8333 6.2 7 8.05 27.3833 51.1333 );
      Data( TotCTCOH, 0.008 0.024 0.0455 0.049 0.049 0.041 0.009 0.006 );

```

```

Print( CTCOH, 4 5.8333 6.2 );
Data( CTCOH, 0.008 0.011 0.013 );

#          TCAUrnSat= NDoses( 16 1 1 0 1 1 1 1 1 1 1 1 0 0 1 0 0 6.2167 10.8833 13.3833
#                               24.3833 29.8833 33.3833 36.8833 48.3833 62.8833 71.1333
#                               88.8833 96.3833 108.3833 120.3833 134.3833 );
UrnMissing= NDoses( 16 0 0 0 0 0 1 1 1 1 0 1 0 1 1 1 0 0 6.2167 10.8833 13.3833
                    24.3833 29.8833 33.3833 36.8833 48.3833 62.8833 71.1333
                    88.8833 96.3833 108.3833 120.3833 134.3833 );
#          Print( zAUrnTCA_sat, 6.2167 10.8833 24.3833 29.8833 71.1333 96.3833 );
#          Data( zAUrnTCA_sat, 0.0085 0.0176 0.0381 0.0463 0.0563 0.0641 );
Print( zAUrnTCA_collect, 13.3833 );
Data( zAUrnTCA_collect, 0.0037 );

#          TCOGUrnSat= NDoses( 16 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 6.2167 10.8833
#                               13.3833 24.3833 29.8833 33.3833 36.8833 48.3833 62.8833
#                               71.1333 88.8833 96.3833 108.3833 120.3833 134.3833 );

#          Print( AUrnTCOGTCOH_sat, 6.2167 10.8833 13.3833 );
#          Data( AUrnTCOGTCOH_sat, 0.7646 1.2333 1.4698 );
Print( AUrnTCOGTCOH_collect, 24.3833 29.8833 71.1333 96.3833 );
Data( AUrnTCOGTCOH_collect, 0.778 0.9906 1.0389 1.0529 );

Print( AUrnTCOGTCOH, 1);
Data( AUrnTCOGTCOH, -1);
Print( zAUrnTCA, 1);
Data( zAUrnTCA, -1);

Data( CPlastTCA, -1);
Data( AUrnTCTotMole, -1);
Data( zAUrnNDCVC, -1);
Print( CPlastTCA, 1);
Print( AUrnTCTotMole, 1);
Print( zAUrnNDCVC, 1);

Print( CDCVGmol, 1);
Data( CDCVGmol, -1);
Print( CDCVG_ND, 1);
Data( CDCVG_ND, -1);

#          Print( MassBalTCE, 1, 2, 4, 8, 16, 32);
#          Data( MassBalTCE, 0, 0, 0, 0, 0, 0);
#          Print( MassBalTCOH, 1, 2, 4, 8, 16, 32);
#          Data( MassBalTCOH, 0, 0, 0, 0, 0, 0);
#          Print( MassBalTCA, 1, 2, 4, 8, 16, 32);
#          Data( MassBalTCA, 0, 0, 0, 0, 0, 0);
#          Print( MassBalTCOG, 1, 2, 4, 8, 16, 32);
#          Data( MassBalTCOG, 0, 0, 0, 0, 0, 0);
#          Print( MassBalDCVG, 1, 2, 4, 8, 16, 32);
#          Data( MassBalDCVG, 0, 0, 0, 0, 0, 0);
#          Print( MassBalDCVC, 1, 2, 4, 8, 16, 32);
#          Data( MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print( RetDose, 1);
Data( RetDose, -1);
}
}
}
##### END CHIU et al. 2006 individual data #####
##### END Individual Data #####

##### BEGIN GROUPED DATA THAT ARE UNIQUE #####
##### BEGIN BERNAUER ET AL DATA #####
Level { #Subject level
### FOR BERNAUER, ALL PARAMETERS
Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );
Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.64 1.36 );
Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.1 1.9 );
Distrib( QSlwC TruncNormal_v M_QSlwC V_QSlwC 0.36 1.64 );

```

```

Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.76 1.24 );
Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.85 1.15 );
Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.84 1.16 );
Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.54 1.46 );
Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.84 1.16 );
Distrib( VRespLumC TruncNormal_v M_VRespLumC V_VRespLumC 0.6 1.4 );
Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.6 1.4 );
Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.66 1.34 );
Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.6 0.6 );
Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.6 0.6 );
Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.6 0.6 );
Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
Distrib( lnkDissocC TruncNormal_v M_lnDissocC V_lnDissocC -0.18 0.18 );
Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -0.546 0.546 );
Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );
Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
#### Distrib( lnkTSD TruncNormal_v M_lnTSD V_lnTSD -4.269 4.942 );
#### Distrib( lnkAS TruncNormal_v M_lnAS V_lnAS -6.571 7.244 );
#### Distrib( lnkTD TruncNormal_v M_lnTD V_lnTD -4.605 0 );
#### Distrib( lnkAD TruncNormal_v M_lnAD V_lnAD -7.195 6.62 );
#### Distrib( lnkASTCA TruncNormal_v M_lnASTCA V_lnASTCA -7.195 6.62 );
#### Distrib( lnkASTCOH TruncNormal_v M_lnASTCOH V_lnASTCOH -7.195 6.62 );
Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
# Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC 0 1 );
Distrib( lnClC TruncNormal_v M_lnClC V_lnClC -4.158 4.158 );
Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
# Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC 0 1 );
Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -13.815 13.815 );
Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC -4.158 4.158 );
# Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC 0 1 );
Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -13.815 13.815 );
Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC -4.158 4.158 );
Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
# Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC 0 1 );
Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC -11.513 6.908 );
Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
# Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC 0 1 );
Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC -9.21 4.605 );
Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
Distrib( lnkUrntCAC TruncNormal_v M_lnkUrntCAC V_lnkUrntCAC -4.605 4.605 );
Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
Distrib( lnkEHRC TruncNormal_v M_lnkEHRC V_lnkEHRC -9.21 4.605 );
Distrib( lnkUrntCOGC TruncNormal_v M_lnkUrntCOGC V_lnkUrntCOGC -6.908 6.908 );
## Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );
Distrib( lnkDCVGC TruncNormal_v M_lnkDCVGC V_lnkDCVGC -9.21 4.605 );
Distrib( lnkNATC TruncNormal_v M_lnkNATC V_lnkNATC -9.21 4.605 );
Distrib( lnkKidBioactC TruncNormal_v M_lnKKidBioactC V_lnKKidBioactC -9.21 4.605 );

Level {# Bernauer et al. (1996) - Urinary mercapturates from GSH conjugation
# Subject=1;
# Experiment { # 85
#PROCED BernH
#! Data from Bernauer et al. (1996) -- Human

```

```

#! From procedure BernH in TCENew.cmd
#! Human -- 40, 80, 160 ppm TCE for 6 hours
# CC=0;
Conc=NDoses(2, 40.0 0, 0.0 6.0);
##
BernH1 (T, AUrnTCTotMole)
####
Print (AUrnTCTotMole, 54);
####
Data (AUrnTCTotMole, 0.823);
##
BernH2 (T, AUrnNDCVCMole)
#
Print(AUrnNDCVCMole, 54);
#
Data (AUrnNDCVCMole, 0.00025);
##
BernH3 (T, AUrnTCA)
####
Print (zAUrnTCA, 6, 11, 16, 23, 30, 35, 40, 47, 54);
####
Data (zAUrnTCA, 0.84, 1.56, 3.37, 6.19, 9.73, 11.49, 13.2, 15.14, 16.46);
##
BernH4 (T, AUrnTCOGTCOH)
####
Print (AUrnTCOGTCOH, 6, 11, 16, 23, 30, 35, 40, 47, 54);
####
Data (AUrnTCOGTCOH, 12.65, 28.58, 43.41, 53.72, 65.12, 73.7, 81.61, 88.4,
#
93.21);
##
BernH5 (T, AUrnNDCVC)
####
Print (zAUrnNDCVC, 6, 11, 16, 23, 30, 35, 40, 47, 54);
####
Data (zAUrnNDCVC, 0.0015, 0.0028, 0.0049, 0.0068, 0.0124, 0.0144, 0.0163,
#
0.018, 0.0193);
# Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
Print (AUrnTCTotMole, 0);
Data (AUrnTCTotMole, -1);
Print (zAUrnTCA, 6 11 16 23 30 35 40 47 54 );
Data (zAUrnTCA, 1.557452405 3.14839841 5.681351918 8.719500561 11.70391989
14.45667515 16.84309415 19.6760945 21.54196714 );
Print (AUrnTCOGTCOH, 6 11 16 23 30 35 40 47 54 );
Data (AUrnTCOGTCOH, 13.63675325 33.61944879 51.78263372 61.25685742 71.08859899
81.97374145 91.93316798 98.27911027 103.3290503 );
Print (zAUrnNDCVC, 6 11 16 23 30 35 40 47 54 );
Data (zAUrnNDCVC, 0.005309749 0.012434097 0.019694974 0.025776734 0.035646562
0.042820557 0.05376152 0.060468832 0.0647 );

Data (CBldTCA, -1);
Data (CPlasTCA, -1);
Data (CVen, -1);
Data (CTCOH, -1);
Data (TotCTCOH, -1);
Data (CALvPPM, -1);
Print(CBldTCA, 1);
Print(CPlasTCA, 1);
Print(CVen, 1);
Print(CTCOH, 1);
Print(TotCTCOH, 1);
Print(CALvPPM, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

#
Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
#
Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
#
Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
#
Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect, -1);
Print(AUrnTCOGTCOH_collect, 1);
Data(AUrnTCOGTCOH_collect, -1);
};

```

```

#Subject=2;
Experiment { # 86
# CC=0;
Conc=NDoses(2, 80.0 0, 0.0 6.0);
# Conc=80.0;
## Print(AUrntCTotMole, 54);
## Data(AUrntCTotMole, 1.775);
# Print (AUrnNDCVCMole, 54);
# Data (AUrnNDCVCMole, 0.00037);
#### Print (zAUrnTCA, 6, 11, 16, 23, 30, 35, 40, 47, 54);
#### Data(zAUrnTCA, 2.06, 4.27, 6.52, 10.49, 17.08, 21.57, 26.87, 31.84, 37.96);
#### Print (AUrnTCOGTCOH, 6, 11, 16, 23, 30, 35, 40, 47, 54);
#### Data (AUrnTCOGTCOH, 37.44, 79.43, 112.69, 145.3, 173.21, 188.35, 201.73,
# 217.09, 230.08);
#### Print (zAUrnNDCVC, 6, 11, 16, 23, 30, 35, 40, 47, 54);
#### Data (zAUrnNDCVC, 0.0035, 0.0055, 0.0113, 0.0152, 0.0262, 0.0306, 0.0347,
# 0.0384, 0.0416);

# Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
Print (AUrnCTotMole, 0);
Data (AUrnCTotMole, -1);
Print (zAUrnTCA, 6 11 16 23 30 35 40 47 54 );
Data (zAUrnTCA, 1.941365664 4.874486405 7.841594641 11.14857782 16.28748693
21.28364856 27.26544753 31.66206976 36.99130884 );
Print (AUrnTCOGTCOH, 6 11 16 23 30 35 40 47 54 );
Data (AUrnTCOGTCOH, 36.6438435 86.08691135 124.9572477 151.426392 174.630428
192.4174939 208.1833023 220.8519223 231.5179426 );
Print (zAUrnNDCVC, 6 11 16 23 30 35 40 47 54 );
Data (zAUrnNDCVC, 0.007553303 0.013224905 0.027986974 0.036437397 0.057308365
0.068022128 0.078623254 0.088400143 0.095756 );

Data (CBldTCA, -1);
Data (CPlasTCA, -1);
Data (CVen, -1);
Data (CTCOH, -1);
Data (TotCTCOH, -1);
Data (CALvPPM, -1);
Print(CBldTCA, 1);
Print(CPlasTCA, 1);
Print(CVen, 1);
Print(CTCOH, 1);
Print(TotCTCOH, 1);
Print(CALvPPM, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

# Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect, -1);
Print(AUrntCOGTCOH_collect, 1);
Data(AUrntCOGTCOH_collect, -1);
};

```

```

#Subject=3;
Experiment{ # 87
# CC=0;
Conc=NDoses(2, 160.0 0, 0.0 6.0);
#### Print(AUrntCTotMole, 54);
#### Data(AUrntCTotMole, 3.08);
#### #Print(AUrntNDCVCMole, 54);
#### #Data (AUrntNDCVCMole, 0.00043);
#### Print (zAUrntTCA, 6, 11, 16, 23, 30, 35, 40, 47, 54);
#### Data (zAUrntTCA, 2.29, 5.71, 10.74, 18.57, 28.08, 34.58, 41.75, 49.31, 57.51);
#### Print(AUrntTCOGTCOH, 6, 11, 16, 23, 30, 35, 40, 47, 54);
#### Data (AUrntTCOGTCOH, 52.5, 113.78, 168.73, 222.17, 243.14, 263.43, 280.17,
# 294.98, 311.45);
#### Print (zAUrntNDCVC, 6, 11, 16, 23, 30, 35, 40, 47, 54);
#### Data (zAUrntNDCVC, 0.0051, 0.0118, 0.0225, 0.0301, 0.0368, 0.0382, 0.0447,
# 0.0531, 0.0577);
# Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
Print (AUrntCTotMole, 0);
Data (AUrntCTotMole, -1);
Print (zAUrntTCA, 6 11 16 23 30 35 40 47 54 );
Data (zAUrntTCA, 2.838297949 8.369594126 16.2537551 24.5176767 35.0353951
44.90091589 55.13794165 63.40186326 73.34168504 );
Print (AUrntTCOGTCOH, 6 11 16 23 30 35 40 47 54 );
Data (AUrntTCOGTCOH, 62.99517723 150.9920375 229.5471746 284.5357705 305.7381042
334.9696792 359.5181595 375.6974964 393.3572955 );
Print (zAUrntNDCVC, 6 11 16 23 30 35 40 47 54 );
Data (zAUrntNDCVC, 0.01122279 0.026161736 0.053723225 0.064310553 0.073536529
0.078057851 0.091739498 0.102725693 0.111284 );
Data (CBldTCA, -1);
Data (CPlastTCA, -1);
Data (CVen, -1);
Data (CTCOH, -1);
Data (TotCTCOH, -1);
Data (CALvPPM, -1);
Print(CBldTCA, 1);
Print(CPlastTCA, 1);
Print(CVen, 1);
Print(CTCOH, 1);
Print(TotCTCOH, 1);
Print(CALvPPM, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

# Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAUrntTCA_collect, 1);
Data(zAUrntTCA_collect, -1);
Print(AUrntTCOGTCOH_collect, 1);
Data(AUrntTCOGTCOH_collect, -1);
};
} # Bernauer
}
##### END BERNAUER ET AL DATA #####

```



```

##### BEGIN Muller et al. 1974 (TCA, TCOH dosing)
Level { #Subject level
### FOR MULLER, ONLY PHYSIOLOGICAL, TCA, TCOH, and TCOG PARAMETERS
  Distrib( lnQCC TruncNormal_v M_lnQCC V_lnQCC -0.8 0.8 );
  Distrib( lnVPRC TruncNormal_v M_lnVPRC V_lnVPRC -0.8 0.8 );
  Distrib( QFatC TruncNormal_v M_QFatC V_QFatC 0.08 1.92 );
  Distrib( QGutC TruncNormal_v M_QGutC V_QGutC 0.64 1.36 );
  Distrib( QLivC TruncNormal_v M_QLivC V_QLivC 0.1 1.9 );
  Distrib( QSlwC TruncNormal_v M_QSlwC V_QSlwC 0.36 1.64 );
####
  Distrib( lnDRespC TruncNormal_v M_lnDRespC V_lnDRespC -11.513 2.303 );
  Distrib( QKidC TruncNormal_v M_QKidC V_QKidC 0.76 1.24 );
  Distrib( FracPlasC TruncNormal_v M_FracPlasC V_FracPlasC 0.85 1.15 );
  Distrib( VFatC TruncNormal_v M_VFatC V_VFatC 0.1 1.9 );
  Distrib( VGutC TruncNormal_v M_VGutC V_VGutC 0.84 1.16 );
  Distrib( VLivC TruncNormal_v M_VLivC V_VLivC 0.54 1.46 );
  Distrib( VRapC TruncNormal_v M_VRapC V_VRapC 0.84 1.16 );
  Distrib( VRespLumC TruncNormal_v M_VRespLumC V_VRespLumC 0.6 1.4 );
  Distrib( VRespEffC TruncNormal_v M_VRespEffC V_VRespEffC 0.6 1.4 );
  Distrib( VKidC TruncNormal_v M_VKidC V_VKidC 0.66 1.34 );
  Distrib( VBldC TruncNormal_v M_VBldC V_VBldC 0.76 1.24 );
####
  Distrib( lnPBC TruncNormal_v M_lnPBC V_lnPBC -0.6 0.6 );
####
  Distrib( lnPFatC TruncNormal_v M_lnPFatC V_lnPFatC -0.6 0.6 );
####
  Distrib( lnPGutC TruncNormal_v M_lnPGutC V_lnPGutC -1.2 1.2 );
####
  Distrib( lnPLivC TruncNormal_v M_lnPLivC V_lnPLivC -1.2 1.2 );
####
  Distrib( lnPRapC TruncNormal_v M_lnPRapC V_lnPRapC -1.2 1.2 );
####
  Distrib( lnPRespC TruncNormal_v M_lnPRespC V_lnPRespC -1.2 1.2 );
####
  Distrib( lnPKidC TruncNormal_v M_lnPKidC V_lnPKidC -0.6 0.6 );
####
  Distrib( lnPSlwC TruncNormal_v M_lnPSlwC V_lnPSlwC -0.9 0.9 );
  Distrib( lnPRBCPlasTCAC TruncNormal_v M_lnPRBCPlasTCAC V_lnPRBCPlasTCAC -4.605 4.605 );
  Distrib( lnPBodTCAC TruncNormal_v M_lnPBodTCAC V_lnPBodTCAC -1.008 1.008 );
  Distrib( lnPLivTCAC TruncNormal_v M_lnPLivTCAC V_lnPLivTCAC -1.008 1.008 );
  Distrib( lnkDissocC TruncNormal_v M_lnkDissocC V_lnkDissocC -0.18 0.18 );
  Distrib( lnBMaxkDC TruncNormal_v M_lnBMaxkDC V_lnBMaxkDC -0.546 0.546 );
  Distrib( lnPBodTCOHC TruncNormal_v M_lnPBodTCOHC V_lnPBodTCOHC -1.008 1.008 );
  Distrib( lnPLivTCOHC TruncNormal_v M_lnPLivTCOHC V_lnPLivTCOHC -1.008 1.008 );
  Distrib( lnPBodTCOGC TruncNormal_v M_lnPBodTCOGC V_lnPBodTCOGC -4.605 4.605 );
  Distrib( lnPLivTCOGC TruncNormal_v M_lnPLivTCOGC V_lnPLivTCOGC -4.605 4.605 );
####
  Distrib( lnPeffDCVG TruncNormal_v M_lnPeffDCVG V_lnPeffDCVG -6.908 6.908 );
####
  Distrib( lnkTSD TruncNormal_v M_lnkTSD V_lnkTSD -4.269 4.942 );
####
  Distrib( lnkAS TruncNormal_v M_lnkAS V_lnkAS -6.571 7.244 );
####
  Distrib( lnkTD TruncNormal_v M_lnkTD V_lnkTD -4.605 0 );
####
  Distrib( lnkAD TruncNormal_v M_lnkAD V_lnkAD -7.195 6.62 );
  Distrib( lnkASTCA TruncNormal_v M_lnkASTCA V_lnkASTCA -7.195 6.62 );
  Distrib( lnkASTCOH TruncNormal_v M_lnkASTCOH V_lnkASTCOH -7.195 6.62 );
####
  Distrib( lnVMaxC TruncNormal_v M_lnVMaxC V_lnVMaxC -2.079 2.079 );
#####
  Distrib( lnKMC TruncNormal_v M_lnKMC V_lnKMC 0 1 );
####
  Distrib( lnClC TruncNormal_v M_lnClC V_lnClC -4.158 4.158 );
####
  Distrib( lnFracOtherC TruncNormal_v M_lnFracOtherC V_lnFracOtherC -6.908 6.908 );
####
  Distrib( lnFracTCAC TruncNormal_v M_lnFracTCAC V_lnFracTCAC -3.489 3.489 );
#####
  Distrib( lnVMaxDCVGC TruncNormal_v M_lnVMaxDCVGC V_lnVMaxDCVGC 0 1 );
####
  Distrib( lnClDCVGC TruncNormal_v M_lnClDCVGC V_lnClDCVGC -13.815 13.815 );
####
  Distrib( lnKMDCVGC TruncNormal_v M_lnKMDCVGC V_lnKMDCVGC -4.158 4.158 );
#####
  Distrib( lnVMaxKidDCVGC TruncNormal_v M_lnVMaxKidDCVGC V_lnVMaxKidDCVGC 0 1 );
####
  Distrib( lnClKidDCVGC TruncNormal_v M_lnClKidDCVGC V_lnClKidDCVGC -13.815 13.815 );
####
  Distrib( lnKMKidDCVGC TruncNormal_v M_lnKMKidDCVGC V_lnKMKidDCVGC -4.158 4.158 );
#####
  Distrib( lnVMaxLungLivC TruncNormal_v M_lnVMaxLungLivC V_lnVMaxLungLivC -3.297 3.297 );
####
  Distrib( lnKMClara TruncNormal_v M_lnKMClara V_lnKMClara -6.908 6.908 );
####
  Distrib( lnFracLungSysC TruncNormal_v M_lnFracLungSysC V_lnFracLungSysC -6.908 6.908 );
#
  Distrib( lnVMaxTCOHC TruncNormal_v M_lnVMaxTCOHC V_lnVMaxTCOHC 0 1 );
  Distrib( lnClTCOHC TruncNormal_v M_lnClTCOHC V_lnClTCOHC -11.513 6.908 );
  Distrib( lnKMTCOH TruncNormal_v M_lnKMTCOH V_lnKMTCOH -9.21 9.21 );
#
  Distrib( lnVMaxGlucC TruncNormal_v M_lnVMaxGlucC V_lnVMaxGlucC 0 1 );
  Distrib( lnClGlucC TruncNormal_v M_lnClGlucC V_lnClGlucC -9.21 4.605 );
  Distrib( lnKMGluc TruncNormal_v M_lnKMGluc V_lnKMGluc -6.908 6.908 );
  Distrib( lnkMetTCOHC TruncNormal_v M_lnkMetTCOHC V_lnkMetTCOHC -11.513 6.908 );
  Distrib( lnkUrnTCAC TruncNormal_v M_lnkUrnTCAC V_lnkUrnTCAC -4.605 4.605 );
  Distrib( lnkMetTCAC TruncNormal_v M_lnkMetTCAC V_lnkMetTCAC -9.21 4.605 );
  Distrib( lnkBileC TruncNormal_v M_lnkBileC V_lnkBileC -9.21 4.605 );
  Distrib( lnkEHRC TruncNormal_v M_lnkEHRC V_lnkEHRC -9.21 4.605 );
  Distrib( lnkUrnTCOGC TruncNormal_v M_lnkUrnTCOGC V_lnkUrnTCOGC -6.908 6.908 );
####
  Distrib( lnFracKidDCVCC TruncNormal_v M_lnFracKidDCVCC V_lnFracKidDCVCC -6.908 6.908 );

```

```

##### Distrib( lnkDCVGC TruncNormal_v M_lnkdCVGC V_lnkdCVGC -9.21 4.605 );
##### Distrib( lnkNATC TruncNormal_v M_lnknATC V_lnknATC -9.21 4.605 );
##### Distrib( lnkKidBioactC TruncNormal_v M_lnkkidBioactC V_lnkkidBioactC -9.21 4.605 );

Level {
  Experiment { # 88 # Muller et al. 1974
# TCA Dosing (3 mg/kg NaTCA = 2.646 mg/kg TCA)
# NaTCA MW = 185.4
# TCA MW = 163.5
# 1 mg NaTCA equiv to 0.8819 mg TCA
# CC= 0;
# Conc=0;

PODoseTCA = NDoses(2, 2.646 0,0 0.01); # Drink over 0.01 hr = 36 seconds

Print(CPlasTCA, 0.496 0.993 2.98 5.46 9.93 23.8 34.2 48.9 58.8 72 81.6 95.8 106
120 148 168 );
Data (CPlasTCA, 22.7 29.4 23 24.4 21.8 17.2 15.6 14 11.4 8.95 8.48 5.4 5.82 5 3.38
2.42 );

Print(zAUrnTCA, 24 48 72 96 120 144 168 );
Data (zAUrnTCA, 43.4 59.7 75 88.7 98.58 107.98 113.03 );

Print (CALvPPM, 0);
Data (CALvPPM, -1);

Print(AUrntCOGTCOH, 0);
Data (AUrnTCOGTCOH, -1);

Print (CVen, 0);
Data (CVen, -1);

Print (CTCOH, 0);
Data (CTCOH, -1);

Print (CBldTCA, 0);
Data (CBldTCA, -1);

Data (TotCTCOH, -1);
Data (AUrnTCTotMole, -1);
Data (zAUrnNDCVC, -1);
Print(TotCTCOH, 1);
Print(AUrntCTotMole, 1);
Print(zAUrnNDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

# Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAUrnTCA_collect, 1);
Data(zAUrnTCA_collect, -1);
Print(AUrntCOGTCOH_collect, 1);
Data(AUrntCOGTCOH_collect, -1);
};

```

```

Experiment { # 89 # Muller et al. 1974
# TCOH Dosing (10 mg/kg)
# CC= 0;
# Conc=0;

PODoseTCOH = NDoses(2,10 0 ,0 0.01); # Drink over 0.01 hr = 36 seconds

Print (CTCOH, 0.402 0.415 0.807 1.57 3.11 5.97 10.9 24 35.2 47.9 72.2 96.2 );
Data (CTCOH, 5.79 4.93 4.1 3.76 2.58 1.91 1.22 0.498 0.276 0.163 0.0487 0.0196 );

Print(AUrntCOGTCOH, 24 48 72 96 120 );
Data (AUrntCOGTCOH, 84.2 100.9 109.26 113.16 115.39 );

Print(CPlasTCA, 0.496 0.993 1.49 3.47 5.96 10.9 23.8 34.7 47.6 71.7 95.5 122 146
170 );
Data (CPlasTCA, 4.8 3.88 6.57 6.86 11.5 18.7 24.2 20.8 17.1 12.1 9.28 8.72 5.73
5.3 );

Print(zAUrntTCA, 24 48 72 96 120 144 168 );
Data (zAUrntTCA, 27.8 70.2 101 125.8 147.9 156.74 161.23 );

Print (CALvPPM, 0);
Data (CALvPPM, -1);

Print (CVen, 0);
Data (CVen, -1);

Print (CBldTCA, 0);
Data (CBldTCA, -1);

Data (TotCTCOH, -1);
Data (AUrntCTotMole, -1);
Data (zAUrntDCVC, -1);
Print(TotCTCOH, 1);
Print(AUrntCTotMole, 1);
Print(zAUrntDCVC, 1);

Print(CDCVGmol, 1);
Data(CDCVGmol, -1);
Print(CDCVG_ND, 1);
Data(CDCVG_ND, -1);

# Print(MassBalTCE, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCE, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOH, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOH, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCA, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCA, 0, 0, 0, 0, 0, 0);
# Print(MassBalTCOG, 1, 2, 4, 8, 16, 32);
# Data(MassBalTCOG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVG, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVG, 0, 0, 0, 0, 0, 0);
# Print(MassBalDCVC, 1, 2, 4, 8, 16, 32);
# Data(MassBalDCVC, 0, 0, 0, 0, 0, 0);
Print(RetDose, 1);
Data(RetDose, -1);
Print(zAUrntTCA_collect, 1);
Data(zAUrntTCA_collect, -1);
Print(AUrntCOGTCOH_collect, 1);
Data(AUrntCOGTCOH_collect, -1);
};
}
}
##### END Muller et al. 1974 (TCA, TCOH dosing)
}
#### END STUDIES
}
#### END POPULATION
End.

```

TCE.1.2.3.3.Human.seqpriors.v1.pop.mean.x.23.out

```

iter  M_lnQCC.1.      M_lnVPRC.1.      M_QFatC.1.      M_QGutC.1.      M_QLivC.1.      M_QSlwC.1.
      M_lnDRespC.1. M_QKidC.1.      M_FracPlasC.1. M_VFatC.1.      M_VGutC.1.      M_VLivC.1.
      M_VRapC.1.      M_VRespLumC.1. M_VRespEffC.1. M_VKidC.1.      M_VBldC.1.      M_lnPBC.1.
      M_lnPFatC.1.    M_lnPGutC.1.    M_lnPLivC.1.    M_lnPRapC.1.    M_lnPRespC.1.  M_lnPKidC.1.
      M_lnPSlwC.1.    M_lnPRBCPlasTCAC.1. M_lnPBodTCAC.1. M_lnPLivTCAC.1.
      M_lnDissocC.1. M_lnBMaxkDC.1. M_lnPBodTCOHC.1. M_lnPLivTCOHC.1.
      M_lnPBodTCOGC.1. M_lnPLivTCOGC.1. M_lnPeffDCVG.1. M_lnASTCA.1.
      M_lnASTCOH.1. M_lnVMaxC.1. M_lnClC.1.      M_lnFracOtherC.1. M_lnFracTCAC.1.
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      M_lnVMaxLungLivC.1. M_lnKMClara.1. M_lnFracLungSysC.1. M_lnClTCOHC.1. M_lnKMTCOH.1.
      M_lnClGlucC.1. M_lnKMGluc.1. M_lnMetTCOHC.1. M_lnUrnTCAC.1.
      M_lnMetTCAC.1. M_lnkBileC.1. M_lnKEHRC.1. M_lnUrnTCOGC.1. M_lnKDCVGC.1.
      M_lnNATC.1. M_lnKidBioactC.1. V_lnQCC.1.      V_lnVPRC.1.      V_QFatC.1.
      V_QGutC.1.      V_QLivC.1.      V_QSlwC.1.      V_lnDRespC.1. V_QKidC.1.      V_FracPlasC.1.
      V_VFatC.1.      V_VGutC.1.      V_VLivC.1.      V_VRapC.1.      V_VRespLumC.1. V_VRespEffC.1.
      V_VKidC.1.      V_VBldC.1.      V_lnPBC.1.      V_lnPFatC.1. V_lnPGutC.1. V_lnPLivC.1.
      V_lnPRapC.1.    V_lnPRespC.1. V_lnPKidC.1. V_lnPSlwC.1. V_lnPRBCPlasTCAC.1.
      V_lnPBodTCAC.1. V_lnPLivTCAC.1. V_lnDissocC.1. V_lnBMaxkDC.1.
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      V_lnPeffDCVG.1. V_lnASTCA.1. V_lnASTCOH.1. V_lnVMaxC.1. V_lnClC.1.
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      V_lnKEHRC.1. V_lnUrnTCOGC.1. V_lnKDCVGC.1. V_lnNATC.1. V_lnKidBioactC.1.
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      Ve_zAUrnTCA_collect.1.1. Ve_AUrnTCOGTCOH.1.1. Ve_AUrnTCOGTCOH_collect.1.1.
      Ve_CDCVmol.1.1. Ve_zAUrnNDCVC.1.1. Ve_AUrnTCTotMole.1.1. Ve_TotCTCOH.1.1.
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```

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LnLike.1.6.1.3.	LnLike.1.7.1.1.	LnLike.1.7.1.2.	LnPrior LnData
LnPosterior			
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	-1.172	1.243	-1.413
	-1.857	2.829	1.97
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	0.01954	0.009687	0.037
	0.07023	0.05544	0.001576
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	0.7911	0.4142	0.1688
	0.7092	0.3903	0.4016
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	1.003	1.038	0.9977
0.03649	-0.0202	0.0108	0.002403
	0.1466	-1.181	2.804
	0.9143	-0.2875	3.152
	3.634	1.526	-0.5473
	0.9982	1.108	0.9954
	-0.0165	-0.1969	0.009981
	-0.03426	0.7631	0.09317
	0.1225	-3.841	-1.18
	-1.64	1.731	-1.956
	1.004	1.001	0.8353
	-0.1256	-0.09889	-0.05422
0.07777	0.3829	0.291	-0.00655
	-3.348	-1.958	3.315
	5.328	-0.6691	-3.636
	0.4624	0.7285	-0.4967
	0.9991	-0.02819	-0.125
	0.0607	-1.9	0.3001
	-1.226	3.248	-0.4119
	-1.265	-0.05082	-2.063
	0.2135	0.6421	0.2538
	1.002	1.003	1.001
	0.7914	0.5071	0.7196
	0.9969	1.012	-0.03055
	-1.242	0.173	0.1764
	1.988	-0.9906	2.569
	-1.734	0.8201	-1.269
	-2.768	0.1294	0.1515
	0.1294	0.004368	0.03691
	0.02661	0.1005	0.07683
	0.01799	0.1101	0.05681
	0.9174	1.924	0.3502
	0.3812	0.7613	0.1743
	0.03481	0.6943	0.01671
	0.7034	0.2731	0.7927
	1.002	0.9937	1.02
	-1.92	0.1731	0.2072
	-0.793	-2.012	0.2746
	0.3735	-2.715	-1.577
	0.6431	0.7689	-0.5575
	1.027	-0.02547	-0.1364
	-0.1326	1.897	0.01505
	-4.569	-0.436	1.881
	-2.241	1.404	-1.481
	-0.2856	0.7586	0.142
	0.9951	1.001	0.9995
	-0.2783	0.008021	-0.002051
	-0.1596	0.4757	-0.0756
	-1.212	2.467	-1.169
	-1.623	3.21	2.43
	0.09131	-0.01829	-0.09973
	-0.1735	0.4905	0.09361
	-3.691	-1.17	0.8331
	-2.763	-1.917	1.769
	-0.5824	1.004	0.9996
	-0.02676	-0.1375	0.1926
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
	0.9955	0.9936	-0.02676
	0.06881	-3.691	-1.17
	0.166	0.06374	-2.763
	0.388	0.9642	-0.5824
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	0.166	0.06374	-2.763
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	0.06881	-3.691	-1.17
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	0.388	0.9642	-0.5824
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	0.388	0.9642	-0.5824
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	0.06		

	-0.00212	-0.01794	-1.238	0.06862	0.1971	-0.005918	-0.1256	-0.01895	
	0.126	1.968	2.045	-4.606	-1.054	0.7196	-1.379	-1.404	0.792
	0.7311	0.4316	3.156	-1.537	0.6825	-2.159	4.764	0.1139	-2.665
	2.349	2.33	0.2176	0.5528	0.1667	0.8214	0.5839	0.9516	-0.5404
	1.001	1.015	0.9982	1.002	0.9987	0.9968	1.006	-0.02555	-0.1156
0.009342	0.001754	0.01455	0.001069	-0.1933	-1.205	0.06315	0.2156	-0.005581	
	-0.09734	0.2656	0.06288	-0.9757	-0.02716	-4.581	-1.126	0.7623	-2.322
	1.136	0.6727	-3.616	-1.186	0.869	-0.5259	3.157	-2.189	1.199
	-3.195	-0.702	1.765	-1.818	4.335	2.227	0.1533	0.01945	0.2427
	-0.3711	1.005	1.001	0.8337	1.005	1.089	0.9961	1.001	1
0.02605	-0.1081	0.2106	0.01904	-0.1506	0.007256	-0.0004935	-0.1686	-2.133	0.3902
	-0.006328	-0.209	0.2865	0.08275	-0.8924	3.004	-4.592	-1.027	1.473
	2.15	0.5358	-2.758	-1.143	0.8322	-0.5452	3.149	-1.558	0.825
	-2.614	-2.017	2.135	-1.898	3.585	2.035	0.09095	0.3758	1.104
	-0.4949	1.008	1.004	0.8383	0.9983	1.023	0.9917	1.002	1.001
0.09951	-0.09029	0.0191	-0.05305	-0.3456	0.01022	-0.002676	-0.215	-1.602	0.4921
	0.09447	-0.007442	-0.172	0.4208	0.0863	-1.268	1.561	-4.578	-1.751
	-1.297	1.159	0.7963	-2.174	-1.125	1.072	-0.9449	3.156	-1.416
	-0.1107	-3.397	-2.236	2.074	-1.945	4.376	1.349	0.6146	0.688
	0.7095	-0.6003	1.006	0.9957	0.8436	1.001	1.125	0.9952	1.001
	0.4009	-0.05255	0.1346	-0.043	-0.08555	0.0104	0.002348	0.3666	-2.081
	0.2183	0.1366	-0.006609	-0.1993	0.5316	0.06023	3.199	4.093	-4.57
	-2.935	-1.658	-0.3832	0.9315	-3.994	-1.192	1.032	-0.8883	3.158
	4.896	-1.531	-1.5	-1.985	1.944	-2.367	0.6239	1.491	-0.4473
	0.5502	0.912	-0.7694	1.005	1.004	0.8455	0.9952	1.148	0.9954
	1.033	-0.02712	-0.1362	-0.1537	-0.05687	-0.2124	0.01205	-0.002706	-0.362
	-1.519	0.02386	0.4049	-0.006333	-0.1595	0.6259	-0.003897	-0.8931	2.866
	0.2816	0.7692	-2.965	-2.156	1.384	-1.387	-3.598	-1.201	1.144
	-1.416	-0.8554	5.098	-1.096	-3.311	0.8055	2.009	-1.663	4.134
	0.6691	0.7531	0.4301	0.8764	-0.5633	1.006	1.003	0.8318	0.996
	0.9992	0.9963	0.9882	-0.02744	-0.1574	-0.0735	-0.03112	-0.1347	0.009825
	-6.73E-04	-0.2955	-1.19	-0.05746	0.2318	-0.004569	-0.09852	0.8274	
	0.04269	2.384	1.666	-4.613	-1.159	2.751	-1.269	-1.149	1.426
	0.7996	0.7621	3.149	-1.247	0.4108	-1.492	5.139	-0.2322	-2.86
	3.342	1.949	0.1334	0.369	0.2131	0.6928	0.2731	1.164	-0.4997
	1.018	1.069	1.014	1.004	0.9987	0.9927	0.9922	-0.02833	-0.1354
	0.5885	0.00771	0.003418	-0.1691	-0.8683	0.07778	0.1218	-0.006192	-0.08044
	0.3904	0.1102	-1.32	2.358	-4.609	-0.6464	1.319	-2.946	-2.446
	-1.199	0.5932	0.785	3.145	-1.936	1.638	-1.035	4.982	-1.316
	-2.019	4.724	2.206	-0.3415	0.4848	0.719	0.8915	0.72	0.7992
	0.8321	0.9978	0.9869	0.9949	1.004	1	0.9947	1.008	-0.02965
0.01946	-0.04244	-0.1918	0.01051	-0.00215	-0.1221	-0.7691	0.167	0.1553	-0.006106
	-0.09579	0.6796	0.06078	0.01188	2.795	-4.56	-1.665	3.021	-1.786
	0.4604	-3.241	-1.157	1.027	-0.7253	3.153	-1.51	1.223	-1.257
	-1.292	2.003	-1.77	3.437	1.853	-0.4112	0.5076	1.037	0.8728
	1.006	0.9977	0.8319	0.997	0.96	0.9923	1.002	1	0.9988
	-0.1378	-0.04094	-0.0378	-0.2997	0.008272	-0.0005029	-0.03105	-1.696	
	0.2254	0.1563	-0.008516	-0.1668	0.6712	0.07201	-1.114	3.404	-4.562
	-1.121	-2.073	1.017	0.4379	-3.125	-1.153	1.143	-1.151	3.136
	4.816	0.0486	-2.402	-1.358	2.249	-1.89	3.684	1.879	-0.08211
	0.8156	0.5814	0.9672	-0.5006	1.005	0.9991	0.8394	1	1.022
	0.9974	1.022	-0.04408	-0.1116	0.1009	-0.006	-0.005949	0.01226	-0.001502
	-0.2806	-1.793	0.3742	0.1293	-0.007246	-0.1848	0.7667	0.05295	-1.042
	-1.191	2.648	-2.519	-1.367	1.221	0.398	-3.449	-1.165	0.9733
	0.8955	-0.8262	4.83	-0.8113	-2.378	-1.921	2.17	-1.913	4.378
	0.7996	0.7657	0.4607	0.8889	-0.5578	1.005	0.9975	0.8391	1.002
	0.9976	0.9947	1.028	0.1715	-0.1309	0.1319	-0.004193	0.05846	0.01232
	0.1848	-2.022	0.3119	0.1623	-0.006615	-0.2115	0.4237	0.05835	0.6687
	-1.517	2.91	-2.477	-2.009	-0.02194	0.5301	-3.815	-1.185	1.012
	-1.513	1.407	-0.5618	4.813	-0.9745	-1.972	-1.803	2.359	-2.112
0.04296	0.2525	0.7046	0.8735	0.6836	0.9031	-0.4961	1.004	0.9999	0.8372
	1.001	1.003	0.998	1.017	-0.02657	-0.1209	0.0636	-0.02186	-0.02441
	0.00671	-0.001782	-0.06088	-1.565	0.1334	0.1305	-0.007274	-0.1306	0.6208
	0.04735	0.4686	3.441	-4.545	-1.421	2.563	-1.829	-0.9969	0.8936
	0.9712	-0.7131	3.156	-1.343	1.085	-0.7567	4.723	-0.7947	-2.592
	2.725	2.048	0.7023	0.7206	0.7191	0.7329	0.01354	0.01415	0.0123
	0.6943	0.727	0.6916	0.7113	-0.138	0.2614	0.9029	0.8678	0.683
	0.8444	1.002	0.9911	0.9979	1.004	0.997	0.9961	1.024	-2.722
0.01463	-0.2248	-2.789	-2.329	-0.1228	0.2516	0.9	0.8656	0.6758	0.8244
	1	1.021	0.9977	1.005	1.001	0.998	1.013	-2.548	0.1717
	-0.1007	-3.062	-1.594	-0.1245	0.2583	0.898	0.8678	0.6809	0.829

1	1.026	0.9968	1.004	1.002	0.9976	1.01	-2.488	0.1442	0.1443	-0.006148
-0.09001	-3.416	-1.544	0.7189	0.7042	0.2402	0.03783	0.7157	0.718	0.04786	0.5922
0.01114	0.1439	0.7117	0.7046	0.7113	0.7147	-0.5552	0.381	1.193	0.8117	0.5694
-0.463	1.005	0.9984	0.7506	0.9987	1.032	0.9955	1.005	1.002	0.9982	1.001
0.01061	-0.1502	0.03254	-0.01123	-0.08826	0.009566	0.0007956	0.2006	-1.134		
0.17	0.138	-0.006118	-0.1277	0.8913	0.02974	-1.637	2.352	-0.3799	2.316	-2.718
-0.7729	0.8885	0.1369	-3.557	-1.152	1.758	-3.047	3.176	-2.584	0.4131	-1.062
-1.283	-2.448	-1.49	2.321	-1.621	3.674	-0.2357	0.4634	0.829	0.8383	0.6254
-0.5313	1.005	1.001	0.7378	1	1.038	0.9973	1.004	0.9997	0.9967	1.008
-0.1537	0.07643	-0.008422	-0.02607	0.0139	-0.001116	0.191	-1.013	0.1524		
0.1687	-0.006934	-0.1182	0.452	0.05794	-1.168	2.008	-0.6782	2.241	-2.513	-1.617
0.8449	0.1166	-3.625	-1.163	1.221	-1.429	3.158	-1.946	1.069	-1.774	4.824
-3.048	-1.254	2.071	-1.786	3.421	-0.5331	0.5044	0.8095	0.7981	0.535	0.9182
1.005	1.001	0.8141	0.9989	1.059	0.9987	1.002	0.9983	0.994	1.007	0.01811
0.04539	-0.004629	0.0263	0.01471	-9.94E-04	0.202	-1.194	0.0987	0.1836	-	
0.006039	-0.1169	0.5993	0.0474	-1.696	0.4139	-0.1913	2.151	-2.748	-2.377	0.8435
-3.655	-1.173	1.931	-3.181	3.196	-1.7	0.9047	-1.862	4.832	-0.4911	-2.838
1.96	-1.808	4.026	-0.1268	0.4601	1.04	0.854	0.6524	0.8741	-0.5152	1.003
0.6871	1	1.037	0.9974	1.002	0.9976	0.9965	1.002	0.03984	-0.1552	0.07172
0.008973	-0.001591	0.002955	-0.0009718	0.2583	-1.373	0.07811	0.1576	-		
0.006033	-0.1249	0.7288	0.03783	-1.021	1.511	-0.5427	2.48	-2.804	-1.102	0.7208
-3.693	-1.171	1.384	-2.004	3.162	-2.22	0.8346	-1.468	4.86	-0.9599	-2.266
1.972	-1.792	3.465	-0.5427	0.3292	0.9091	0.8114	0.5642	0.8096	-0.4983	1.005
0.8656	0.9996	1.058	0.9955	1.001	1.003	0.9976	1.004	-0.03557	-0.1362	0.04664
-0.01309	-0.1006	0.01088	-1.97E-03	0.0899	-1.144	0.1128	0.1866	-0.00646		
-0.126	0.7269	0.04749	-1.381	2.728	-0.5761	2.199	-2.52	-1.517	0.9163	0.1038
-1.159	1.443	-2.256	3.161	-2.263	0.9229	-1.32	4.848	-0.4392	-2.744	-0.8753
-2.138	3.446	-0.2594	0.2054	1.045	0.8811	0.6971	0.8099	-0.4899	1.006	1.001
0.9995	0.9959	0.9971	1.004	0.9978	1	1.012	-0.009202	-0.1199	0.07877	-
0.01466	-0.0403	0.00735	0.0002116	0.2747	-1.265	0.1578	0.1261	-0.00664	-0.106	0.7897
0.04191	-1.221	1.416	-0.8461	2.36	-2.472	-2.551	0.8102	0.1269	-3.53	-1.167
-0.6811	3.159	-1.562	0.5454	-1.16	4.806	-1.074	-3.127	-1.832	1.987	-1.764
-0.3325	0.2937	1.08	0.8681	0.6905	0.7835	-0.5017	1.006	1.001	0.7599	0.9992
0.9953	1.004	0.9988	0.9952	1.006	-0.03103	-0.1621	0.04852	-0.006927	-	
0.09673	0.005195	8.60E-04	0.1873	-1.159	0.1509	0.1394	-0.007749	-0.1134	0.7964	
0.04064	-1.4	1.704	-0.6222	2.344	-2.544	-1.698	0.8668	0.1404	-3.426	-1.165
-1.949	3.163	-2.089	0.8804	-1.175	4.813	-1.05	-2.826	-1.554	2.144	-1.65
-0.02508	0.1823	1.133	0.8869	0.7198	0.8119	-0.4899	1.005	1.002	0.6913	1.001
1.03	0.9971	1.004	0.9998	0.9963	1.009	-0.02189	-0.1664	0.08537	-0.007206	
-0.02253	0.009954	-0.0007209	0.272	-0.9877	0.1728	0.1708	-0.007156			
-0.1102	0.5723	0.04561	-0.3154	1.881	-0.7783	2.372	-2.539	-2.22	0.8781	0.1553
-1.161	1.081	-1.053	3.152	-2.307	0.7671	-1.314	4.844	-0.917	-3.233	-1.289
-1.694	2.795	-0.3844	0.4084	0.8899	0.843	0.6289	0.7734	-0.521	1.006	1.002
1.001	1.035	0.9942	1.003	0.9985	0.9938	1.007	0.03933	-0.1217	0.06954	-0.0174
0.07337	0.01698	-0.00111	0.4954	-0.9745	0.1379	0.1856	-0.006488	-0.1096	0.3278	0.06052
-0.6795	1.455	-0.7779	2.173	-2.448	-2.185	0.8144	0.156	-3.82	-1.169	1.099
3.154	-2.352	1.488	-2.185	4.794	-0.4832	-3.229	-0.9928	1.945	-1.916	3.089
0.3524	0.7457	0.8778	0.6882	0.903	-0.5034	1.007	1.001	0.6497	1.001	0.1017
1.002	0.9999	0.9955	1.008	-0.002505	-0.1587	0.07864	-0.0121	0.02558	0.01328	
0.0004914	0.4553	-1.223	0.1346	0.1426	-0.00667	-0.1055	0.5935	0.04473	-0.725	
0.5259	-0.5404	2.339	-2.692	-2.156	0.8334	0.1227	-3.625	-1.161	1.366	-2.024
-1.936	1.408	-1.734	4.8	-0.8644	-3.125	-1.517	1.863	-1.683	3.475	-0.369
1.034	0.8607	0.6717	1.052	-0.5066	1.006	1.002	0.7765	1	1	1.002
1.002	0.9933	1.014	0.03459	-0.1449	0.06024	-0.009742	0.2056	0.002782		
0.001611	0.3519	-1.232	0.1478	0.1335	-0.006969	-0.0992	0.5819	0.04954	-0.709	
0.7692	-0.7165	2.321	-2.655	-2.187	0.7976	0.1172	-3.717	-1.172	1.2	-1.307
-1.703	1.561	-1.708	4.8	-0.7096	-3.347	-1.714	1.878	-1.777	3.31	-0.01923
0.09533	1.061	0.9053	0.7701	0.8819	-0.4849	1.005	1.004	0.4744	1.002	1.017
1.004	1	0.9955	1.016	-0.03337	-0.1848	0.0895	-0.01221	0.01761		
0.008449	-0.0004444	0.4069	-0.7073	0.2419	0.1181	-0.007391	-0.08745			
0.1917	0.05958	-0.8056	0.1318	-0.6013	2.546	-2.641	-2.332	0.8645	0.1757	-3.286
1.255	-1.767	3.161	-2.12	1.605	-1.975	4.796	-0.402	-3.799	-1.795	1.83
3.575	0.01892	0.1812	0.3053	0.7119	0.7224	0.1612	0.1891	0.685	0.01399	0.7115
0.7084	0.6925	0.05217	-0.1199	0.1007	0.8002	0.8663	0.6635	0.8466	-0.2538	1.005
0.8286	1.001	0.9969	1	1.004	1.003	0.9917	1.003	-0.07682	-0.2317	0.09209
-0.009756	0.08031	0.01321	0.0001807	0.2968	1.909	-0.08126	0.1311	-		
0.006295	-0.02636	-0.03075	0.0212	3.039	-0.6359	-0.5486	2.169	-3.378	-2.175	
0.8055	0.2643	-4.174	-1.177	2.069	-5.056	3.317	-2.099	0.2524	-1.998	4.527
-3.426	-1.498	1.651	-1.72	1.983	-0.1228	-0.267	1.54	0.8803	0.715	0.6772
1.01	1.001	0.8298	1.001	1.073	0.9909	0.9995	1.003	0.9962	0.9878	0.01003
0.07334	-0.0104	-0.2298	0.009339	-0.003613	0.4747	0.4623	-0.08336	0.2428		

-0.006587	-0.06531	0.2956	0.05229	3.268	0.8726	-0.7491	2.582	-2.709	-2.444
0.8823	0.1916	-3.685	-1.171	1.039	-1.305	3.166	-1.072	-0.1106	-1.499
-3.417	-0.186	1.836	-1.486	2.401	-0.1205	-0.2215	0.9979	0.8843	0.7647
1.008	0.9947	0.8351	0.9948	0.89	1.006	1.002	1.006	0.989	0.9895
-0.3274	0.06148	0.01499	0.0003522		0.01377	-0.002287		0.05308	0.4398
0.1605	-0.009244	-0.03098			0.03393	0.09547	3.084	-0.3212	-1.736
-2.315	1.641	0.8001	-4.034	-1.158	1.779	-3.046	3.201	-1.617	-0.04427
4.473	-0.9879	-3.412	-0.8377	1.773	-1.794	2.31	-0.1194	0.09635	0.8129
0.6717	-0.3342	1.003	1.003	0.8367	1.001	1.019	0.996	1.002	0.9978
-0.09536	-0.2062	0.07469	-0.01149		-0.1626	0.007477		0.00122	0.1441
0.1208	0.1632	-0.006579	-0.08601		0.3355	0.05835	3.258	0.03575	-1.007
-2.466	-2.431	1.028	0.2177	-3.455	-1.174	0.9594	-1.277	3.158	-1.505
4.645	-0.7518	-3.528	-1.304	1.736	-1.737	2.485	0.7373	0.1335	1.2
0.1344	0.7259	1.123	0.7312	0.2401	0.7148	0.7034	0.7044	0.2823	-0.1284
0.9566	0.8574	0.4968	-0.338	1.024	1.005	0.8323	1.001	1.022	0.9983
1.009	1.01	-0.01373	-0.1353	0.1376	-0.008821			0.2684	0.007976
0.002149	0.7907	-1.386	0.247	0.1869	-0.005983	-0.1213	0.3486	0.06573	-2.114
-0.8867	1.88	-1.294	-2.636	1.405	0.1352	-1.569	-1.153	0.8653	0.3951
0.8097	-0.44	4.79	-0.4175	-3.604	-1.287	1.848	-2.621	-1.288	-0.1273
0.8111	0.5454	0.5614	-0.6401	0.9948	1.001	0.8366	1.001	1.01	0.9982
0.9971	1.021	-0.09733	-0.1161	0.1216	0.004203			0.03324	0.008357
0.001943	0.2662	-1.408	0.1923	0.1737	-0.005723	-0.124	0.4672	0.07053	-2.012
0.6806	-0.8916	1.057	-1.737	-2.089	1.259	0.1478	-3.624	-1.16	0.8465
-1.924	0.8319	-0.7954	4.803	-0.1899	-3.108	-1.348	1.85	-1.955	-0.07733
0.1663	1.205	1.012	0.9866	0.4249	-0.1482	1.035	1.006	0.8358	1.002
1.001	0.9999	1.012	1.008	-0.169	-0.3831	0.1986	0.003193	0.2376	0.008923
0.001055	0.7559	-1.186	0.1781	0.1652	-0.006132	-0.08687		0.5207	0.06285
-2.376	-0.4508	-0.9466	2.049	-1.002	-2.75	1.605	0.1514	-0.8563	-1.164
3.151	-2.259	0.806	-0.4472	4.791	-0.7718	-3.869	-1.53	1.705	-1.565
-0.02098	1.445	0.8494	0.6398	0.8168	-0.3895	1.004	1.003	0.8329	1.003
0.9918	1.001	1.001	0.9959	1.014	-0.2826	-0.1512	0.1181	-0.008879	-0.3414
0.009401	-0.003796	-0.5513	-0.9182	0.1957	0.2046	-0.006007		-0.115	0.2267
0.1133	-2.327	-0.2367	-0.9227	1.749	-1.858	-1.933	1.273	0.162	-3.363
0.9068	3.144	-1.89	0.8214	-1.3	4.8	1.475	-3.378	-0.8987	1.727
-0.1235	-0.1372	1.454	0.9169	0.7844	0.4888	-0.2905	1.006	1.006	0.8385
0.986	1.004	0.9994	1.004	1.009	-0.2841	-0.1609	0.1121	-0.009983	-0.5118
0.002232	0.1425	-0.02351			0.1437	0.2012	-0.005837	-0.07543	0.374
0.06333	-0.7807	-0.494	-0.9263	1.895	-1.079	-2.609	1.742	0.138	-2.183
0.871	3.157	-2.107	0.8402	-0.7444	4.794	-0.5277	-3.97	-1.078	1.679
-0.1199	0.196	1.484	0.9124	0.786	0.529	-0.3227	1.009	1.004	0.8377
0.9845	1.001	0.9974	1.002	1.012	-0.1067	-0.1217	0.1313	-0.003567	-0.5044
0.009022	-0.006406	0.6543	-1.407	0.2631	0.1727	-0.007101		-0.1239	0.3197
0.07013	-1.14	1.019	-0.9264	1.87	-1.296	-2.795	1.471	0.1612	-2.101
0.7435	3.163	-2.665	0.8383	-1.345	4.783	-0.6224	-3.586	-1.414	1.895
0.719	0.7126	0.719	0.6875	0.707	0.7046	0.02301	0.709	0.01316	0.7315
0.7155	0.725	-0.284	0.3376	0.7828	0.8727	0.7032	0.7753	-0.5413	1.007
0.9985	1.065	0.995	1.002	0.9992	1.001	1.006	-0.1069	-0.1242	0.03852
-0.204	0.01069	-0.0007935	-0.2332	-0.3612	0.2268	0.1539	-0.00544	-0.1199	0.4626
0.06856	0.2308	2.194	-4.562	-0.05249	2.987	-2.453	-0.9738	-0.7986	-0.8467
-1.381	1.083	-0.1584	3.143	-2.098	-0.1025	-1.119	4.923	-0.3403	-2.755
-1.984	2.172	2.067	-8.177	-2.6	0.7048	0.7001	0.6908	0.1355	0.02561
0.7054	0.02495	0.7222	0.7219	0.7206	0.728	0.7017	-0.4473	0.2588	0.8996
0.8238	1.005	1.004	0.8339	0.9995	1.129	0.9966	1.002	1.001	1.001
0.1968	0.232	-0.007878	-0.1828	0.8733	0.1816	-0.7252	3.408	1.886	2.167
1.854	0.6634	5.269	3.95	-3.127	-0.1446	2.318	-1.305	0.3659	-188.8
-151.7	-166.7	-158.9	-174.6	-139	-165.3	-148.8	-285.5	-229.2	-181.4
-173.6	-73.96	-138.4	-133.7	-140.8	-156.8	-92.94	-82.79	-25.14	-29.38
-23.96	-18.14	-18.94	-23.3	-8.86	-40.54	-96.95	-90.42	-108.3	-74.65
-75.86	-88.56	-107.6	-84.64	-116.6	286.5	308.6	270.8	214.4	320.3
280.8	276	272.9	-8.177	-23.01	-34.11	-51.39	-64.8	-936.6	-2186

APPENDIX E

Utility M Files for Simulations

The following M files are called within various M files utilized for this work. As noted in Tables 1 through 4 of the main report, QRapC is calculated as 1.0 minus sum of other blood flows; VSlwC is calculated as VPerfC minus sum of fractional volumes for blood, fat, gut, kidney, liver, rapid and respiratory tissue; and kTD set to zero because it is set in the MCSim model definition file as $kTD=0.0*\exp(\ln kTD)$.

Init.m

```
prepare @All

xerror (["AInhResp", "AExhResp", "AResp"], [1.0e-11, 1.0e-11, 1.0e-11])
xerror (["AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw"], [1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8])
xerror (["ASTom", "ADuod"], [1.0e-8, 1.0e-8])

xerror (["APlasTCA", "ABodTCA", "ALivTCA"], [1.0e-8, 1.0e-8, 1.0e-8])
xerror (["ABodTCOH", "ALivTCOH"], [1.0e-8, 1.0e-8])
xerror (["ABodTCOG", "ALivTCOG", "ABileTCOG"], [1.0e-8, 1.0e-8, 1.0e-8])

HVDPRN=0;
WESITG=0;
```

ResetDoses.m

```
% Setting concentration parameters with loop because lines were longer than 510 characters and
% were too long
```

```
CC=0; NRODENTS=1.0; KLOSSC=0.0; VCHC=1.0;
for iter = [1 : 150]
    CONCLIST(iter) = 0.0;
    STRTNEXTLIST(iter)=0.0;
end
STRTNXTLIST(1)=50000.0;
IVDOSE=0.0; TCHNG=1.0; DAYS=1.0; TMAX=24.0;
PDOSE=0.0; DRINK=0.0; IADOSE=0.0; PVDLOSE=0.0;
IVDOSETCA=0.0; PODOSETCA=0.0;
IVDOSETCOH=0.0; PODOSETCOH=0.0;
URNMISSLIST=[100000.0 100000.0 100000.0 100000.0 100000.0 100000.0 100000.0 100000.0 100000.0 100000.0
100000.0];
CINT=0.01; DOSEINT=100000.0;
```

MousePrior.m

```
xerror (["AInhResp", "AExhResp", "AResp"], [1.0e-11, 1.0e-11, 1.0e-11])
xerror (["AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw"], [1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8])
xerror (["ASTom", "ADuod"], [1.0e-8, 1.0e-8])
xerror (["APlasTCA", "ABodTCA", "ALivTCA"], [1.0e-8, 1.0e-8, 1.0e-8])
xerror (["ABodTCOH", "ALivTCOH"], [1.0e-8, 1.0e-8])
xerror (["ABodTCOG", "ALivTCOG", "ABileTCOG"], [1.0e-8, 1.0e-8, 1.0e-8])

% Prior parameters for mouse
% DRespC, PEffDCVG, kAS, kTSD, kAD, kASTCA, kASTCOH, FracOtherC, KMClara, FracLungSysC,
% VMaxTCOHC, KMTCOH, VMaxGlucC, KMGluc, kMetTCOHC, kMetTCAC, kBileC, KEHRC, KDCVGC,
% FracKidDCVCC, kNATC, kKidBioactC from Table 3-37 in report
SPECIES=3;
BW=0.03; QCC=11.6; VPR=2.5; DRESPC=0.00813;
QFATC=0.07; QGUTC=0.141; QKIDC=0.091; QLIVC=0.02; QRAP=0.461; QSLWC=0.217;
VBLDC=0.049; VFATC=0.07; VGUTC=0.049; VKIDC=0.017; VLIVC=0.055; VPERFC=0.8897; VRAPC=0.1;
VRESPC=0.0007; VRESPLUMC=0.0046667; VSLWC=0.549; FRACPLAS=0.52;
PB=15.0; PFAT=36.0; PGUT=1.9; PKID=2.1; PLIV=1.7; PRAP=1.9; PRESP=2.6; PSLW=2.4;
PRBCPLASTCA=0.5; PBODTCAC=0.88; PLIVTCAC=1.18;
PBODTCOH=1.11; PLIVTCOH=1.3;
PBODTCOG=1.11; PLIVTCOG=1.3; PEFFDCVG=1.25;
BMAXKDC=0.88; KDISSOC=107.0;
```



```

KAS=1.7; KTS=1.4; KAD=1.2; KTD=0.0; KASTCA=0.63; KASTCOH=0.75
VMAXC=2700.0; KMC=36.0; CL=1.0; FRACCTAC=0.32; FRACOTHERC=0.75;
VMAXDCVGC=300.0; KMDCVGC=1.0; CLDCVG=1.53;
VMAXKIDDCVGC=60.0; KMKIDDCVGC=1.0; CLKIDDCVG=0.34;
VMAXLUNGLIV=0.070102; KMCLARA=1.5; FRACLUNGSSYS=0.52;
VMAXTCOHC=0.89; KMTCOH=1.4; CLTCOH=1.0;
VMAXGLUCC=1.53; KMGLUC=1.8; CLGLUC=1.0; KMETTCOHC=0.079;
KURNTCAC=0.6; KMETTCAC=0.05;
KBILEC=0.13; KEHRC=0.087; KURNTCOGC=0.6;
KDCVGC=0.1; FRACKIDDCVCC=1.9;
KNATC=0.12; KKIDBIOACTC=0.075;

```

MousePost.m

```

xerror(["AInhResp", "AExhResp", "AResp"], [1.0e-11, 1.0e-11, 1.0e-11])
xerror(["AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw"], [1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8, 1.0e-8])
xerror(["ASTom", "ADuod"], [1.0e-8, 1.0e-8])
xerror(["APlasTCA", "ABodTCA", "ALivTCA"], [1.0e-8, 1.0e-8, 1.0e-8])
xerror(["ABodTCOH", "ALivTCOH"], [1.0e-8, 1.0e-8])
xerror(["ABodTCOG", "ALivTCOG", "ABileTCOG"], [1.0e-8, 1.0e-8, 1.0e-8])

```

% Mean posterior parameters for mouse

```

SPECIES=3;
BW=0.03; QCC=14.24071; VPR=2.01857; DRESPC=1.22067;
QFATC=0.072310; QGUTC=0.16610; QKIDC=0.090390; QLIVC=0.020660; QRAPC=0.43697; QSLWC=0.21357;
VLDC=0.048613; VFATC=0.092960; VGUTC=0.048358; VKIDC=0.0170; VLIVC=0.044440; VPERFC=0.88970;
VRAPC=0.099680; VRESPC=0.0007; VRESPLUMC=0.0046667; VSLWC=0.53795; FRACPLAS=0.45334;
PB=13.94569; PFAT=35.56845; PGUT=1.53427; PKID=2.65843; PLIV=2.18153; PRAP=1.81543;
PRESP=2.58620; PSLW=2.22194;
PRBCPLASTCA=1.23485; PBODTCAC=0.78096; PLIVTCAC=0.94801;
PBODTCOH=0.89240; PLIVTCOH=1.94637;
PBODTCOG=0.46620; PLIVTCOG=1.31905; PEFFDCVG=0.98705;
BMAXKDC=1.09173; KDISSOC=126.01851;
KAS=1.79751; KTS=5.25931; KAD=0.26767; KTD=0.0; KASTCA=3.97490; KASTCOH=0.73001;
VMAXC=1810.95037; KMC=2.62353; CL=1.0; FRACCTAC=0.15585; FRACOTHERC=0.023707;
VMAXDCVGC=786.41329; KMDCVGC=1.0; CLDCVG=0.54896;
VMAXKIDDCVGC=154.35337; KMKIDDCVGC=1.0; CLKIDDCVG=0.41337;
VMAXLUNGLIV=0.19499; KMCLARA=0.011950; FRACLUNGSSYS=4.38417;
VMAXTCOHC=1.64280; KMTCOH=0.93257; CLTCOH=1.0;
VMAXGLUCC=69.54681; KMGLUC=30.44738; CLGLUC=1.0; KMETTCOHC=3.36693;
KURNTCAC=0.065755; KMETTCAC=0.61275;
KBILEC=1.01433; KEHRC=0.012082; KURNTCOGC=5.15607;
KDCVGC=0.1890; FRACKIDDCVCC=1.53664;
KNATC=0.11648; KKIDBIOACTC=0.087861;

```

RatPrior.m

```

xerror(["AInhResp", "AExhResp", "AResp"], [1.0e-13, 1.0e-13, 1.0e-13])
xerror(["ACh", "AExh", "AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw", "ABld"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ASTom", "ADuod", "AExc"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["AMetLng", "AMetKid", "AMetLiv1", "AMetLiv2"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["APlasTCA", "ABodTCA", "ASTomTCA", "ALivTCA", "AMetTCA", "AurnTCA"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOH", "ASTomTCOH", "ALivTCOH", "AMetTCOHTCA", "AMetTCOHgluc", "AMetTCOHOther"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOG", "ALivTCOG", "ABileTCOG", "ARecircTCOG", "AurnTCOG"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVC", "ABioactDCVC", "AurnDCVC"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVG_mMole", "AMetDCVG_mMole"], [1.0e-9, 1.0e-9])

```

% Prior parameters for rat

```

% DRespC, KAS, KTS, KAD, KASTCA, FracOtherC, KMclara, FracLungSysC, VMaxTCOHC, KMTCOH,
% VMaxGlucC, KMgluc, kMetTCOHC, kMetTCAC, kBileC, KEHRC, KNATC, kKidBioactC from Table 3-38
% in report
% KASTCOH from Table A-12
SPECIES=2;
BW=0.3; QCC=13.3; VPR=1.9; DRESPC=0.99;
QFATC=0.07; QGUTC=0.153; QKIDC=0.141; QLIVC=0.021; QRAP=0.279; QSLWC=0.336;
VLDC=0.074; VFATC=0.07; VGUTC=0.032; VKIDC=0.007; VLIVC=0.034; VPERFC=0.8995; VRAPC=0.088;
VRESPC=0.0005; VRESPLUMC=0.0046667; VSLWC=0.594; FRACPLAS=0.53;

```

PB=22.0; PFAT=27.0; PGUT=1.4; PKID=1.3; PLIV=1.5; PRAP=1.3; PRES=1.0; PSLW=0.58;
 PRBCPLASTCA=0.5; PBODTCAC=0.88; PLIVTCAC=1.18;
 PBODTCOH=1.11; PLIVTCOH=1.3;
 PBODTCOG=1.11; PLIVTCOG=1.3; PEFFDCVG=1.0;
 BMAXKDC=1.22; KDISSOC=275.0;
 KAS=0.73; KTS=1.4; KAD=0.96; KTD=0.0; KASTCA=0.83; KASTCOH=0.69;
 VMAXC=600.0; KMC=21.0; CL=1.0; FRACTCAC=0.32; FRACOTHERC=0.028;
 VMAXDCVGC=66.0; KMDCVGC=1.0; CLDCVG=0.25;
 VMAXKIDDCVGC=6.0; KMKIDDCVGC=1.0; CLKIDDCVG=0.026;
 VMAXLUNGLIV=0.014347; KMCLARA=0.016; FRACLUNGSYS=4.6;
 VMAXTCOHC=1.9; KMTCOH=1.0; CLTCOH=1.0;
 VMAXGLUCC=67.0; KMGLUC=31.0; CLGLUC=1.0; KMETTCOHC=3.1;
 KURNTCAC=0.522; KMETTCAC=0.56;
 KBILEC=1.0; KEHRC=0.0096; KURNTCOGC=0.522;
 KDCVGC=22206.46579; FRACKIDDCVCC=22206.46579;
 KNATC=0.11; KKIDBIOACTC=0.09;

RatPost.m

```

xerror (["AInhResp", "AExhResp", "AResp"], [1.0e-13, 1.0e-13, 1.0e-13])
xerror (["ACH", "AExh", "AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw", "ABld"],
        [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror (["Astom", "ADuod", "AExc"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror (["AMetLng", "AMetKid", "AMetLiv1", "AMetLiv2"],
        [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror (["APlasTCA", "ABodTCA", "ASTomTCA", "ALivTCA", "AMetTCA", "AUrnTCA"],
        [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror (["ABodTCOH", "ASTomTCOH", "ALivTCOH", "AMetTCOHTCA", "AMetTCOHGluc", "AMetTCOHOther"],
        [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror (["ABodTCOG", "ALivTCOG", "ABileTCOG", "ARecircTCOG", "AUrnTCOG"],
        [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror (["ADCVC", "ABioactDCVC", "AUrnDCVC"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror (["ADCVG_mMole", "AMetDCVG_mMole"], [1.0e-9, 1.0e-9])
  
```

% Mean posterior parameters for rat

SPECIES=2;
 BW=0.3; QCC=15.84833; VPR=1.18359; DRESPC=2.55308;
 QFATC=0.083090; QGUTC=0.17549; QKIDC=0.14128; QLIVC=0.021672; QRAPC=0.27512; QSLWC=0.30334;
 VBLDC=0.074148; VFATC=0.068040; VGUTC=0.031654; VKIDC=0.0069489; VLIVC=0.033470;
 VPERFC=0.89950; VRAPC=0.087393; VRESPC=0.00049585; VRESPLUMC=0.0046900; VSLWC=0.59735;
 FRACPLAS=0.55226;
 PB=18.79597; PFAT=30.50031; PGUT=1.21152; PKID=1.22174; PLIV=1.56356; PRAP=1.40279;
 PRES=0.95547; PSLW=0.74929;
 PRBCPLASTCA=0.48121; PBODTCAC=0.98262; PLIVTCAC=1.51333;
 PBODTCOH=1.05556; PLIVTCOH=1.24815;
 PBODTCOG=1.37638; PLIVTCOG=11.16032; PEFFDCVG=1.0;
 BMAXKDC=1.16098; KDISSOC=268.46783;
 KAS=2.72100; KTS=4.16618; KAD=0.18105; KTD=0.0; KASTCA=1.48750; KASTCOH=0.68805;
 VMAXC=571.68015; KMC=0.73825; CL=1.0; FRACTCAC=0.079624; FRACOTHERC=0.30975;
 VMAXDCVGC=790.49137; KMDCVGC=1.0; CLDCVG=0.093015;
 VMAXKIDDCVGC=1.26460; KMKIDDCVGC=1.0; CLKIDDCVG=4.72724;
 VMAXLUNGLIV=0.047682; KMCLARA=0.020775; FRACLUNGSYS=1.98080;
 VMAXTCOHC=2.01819; KMTCOH=22.42104; CLTCOH=1.0;
 VMAXGLUCC=27.16692; KMGLUC=5.87673; CLGLUC=1.0; KMETTCOHC=1.97605;
 KURNTCAC=0.037512; KMETTCAC=0.32530;
 KBILEC=7.55342; KEHRC=1.46756; KURNTCOGC=10.70716;
 KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
 KNATC=0.0020891; KKIDBIOACTC=0.0069016;

FemalePrior.m

```
xerror(["AIInhResp", "AExhResp", "AResp"], [1.0e-13, 1.0e-13, 1.0e-13])
xerror(["ACh", "AExh", "AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw", "ABld"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ASTom", "ADuod", "AExc"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["AMetLng", "AMetKid", "AMetLiv1", "AMetLiv2"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["APlasTCA", "ABodTCA", "ASTomTCA", "ALivTCA", "AMetTCA", "AurnTCA"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOH", "ASTomTCOH", "ALivTCOH", "AMetTCOHTCA", "AMetTCOHGluc", "AMetTCOHOther"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOG", "ALivTCOG", "ABileTCOG", "AREcircTCOG", "AurnTCOG"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVC", "ABioactDCVC", "AurnDCVC"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVG_mMole", "AMetDCVG_mMole"], [1.0e-9, 1.0e-9])

% Mean prior parameters for female human
% DRespc, PEffDCVG, KAS, KTSd, KAD, KASTCA, KASTCOH, FracOtherC, KMClara, FracLungSysC, KMTCOH,
% CLTCOH, KMGLuc, CLGLuc, kMetTCOHC, kMetTCAC, kBileC, kEHRC, kDCVGC, kNATC, kKidBioactC from
% Table 3-39 in report
% FrackidDCVC from model code (comment from model - "In ".in" files, set to 1, so that all
% kidney GSH conjugation is assumed to directly produce DCVC (model lacks identifiability
% otherwise)"
SPECIES=1;
BW=60.0; QCC=16.0; VPR=0.96; DRESPC=1.47;
QFATC=0.085; QGUTC=0.21; QKIDC=0.17; QLIVC=0.065; QRAPC=0.3; QSLWC=0.17;
VLDC=0.068; VFATC=0.317; VGUTC=0.022; VKIDC=0.0046; VLIVC=0.023; VPERFC=0.85778; VRAPC=0.093;
VRESPC=0.00018; VRESPLUMC=0.0023857; VSLWC=0.33; FRACPLAS=0.615;
PB=9.5; PFAT=67; PGUT=2.6; PKID=1.6; PLIV=4.1; PRAP=2.6; PRESP=1.3; PSLW=2.1;
PRBCPLASTCA=0.5; PBODTCAC=0.52; PLIVTCAC=0.66;
PBODTCOH=0.91; PLIVTCOH=0.59;
PBODTCOG=0.91; PLIVTCOG=0.59; PEFDCVG=1.24;
BMAXKDC=4.62; KDISSOC=182.0;
KAS=1.4; KTSd=1.4; KAD=0.75; KTD=0.0; KASTCA=0.58; KASTCOH=0.49;
VMAXC=255.0; KMC=1.0; CL=66.0; FRACTCAC=0.32; FRACOTHERC=0.14;
VMAXDCVGC=1.0; KMDCVGC=2.9; CLDCVG=19.0;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=2.7; CLKIDDCVGC=230.0;
VMAXLUNGLIV=0.027273; KMCLARA=0.019; FRACLUNGSYSC=3.0;
VMAXTCOHC=1.0; KMTCOH=5.0; CLTCOH=0.35;
VMAXGLUC=1.0; KMGLUC=10.0; CLGLUC=3.0; KMETTCOHC=2.47;
KURNTCAC=0.108; KMETTCAC=0.55;
KBILEC=3.47; KEHRC=0.21; KURNTCOGC=0.108;
KDCVGC=0.127; FRACKIDDCVCC=22026.46579;
KNATC=0.0025; KKIDBIOACTC=0.0064;
```

FemalePost.m

```
xerror(["AIInhResp", "AExhResp", "AResp"], [1.0e-13, 1.0e-13, 1.0e-13])
xerror(["ACh", "AExh", "AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw", "ABld"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ASTom", "ADuod", "AExc"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["AMetLng", "AMetKid", "AMetLiv1", "AMetLiv2"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["APlasTCA", "ABodTCA", "ASTomTCA", "ALivTCA", "AMetTCA", "AurnTCA"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOH", "ASTomTCOH", "ALivTCOH", "AMetTCOHTCA", "AMetTCOHGluc", "AMetTCOHOther"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOG", "ALivTCOG", "ABileTCOG", "AREcircTCOG", "AurnTCOG"],
       [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVC", "ABioactDCVC", "AurnDCVC"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVG_mMole", "AMetDCVG_mMole"], [1.0e-9, 1.0e-9])

% Mean posterior parameters for female human
SPECIES=1;
BW=60.0; QCC=13.36432; VPR=1.46518; DRESPC=0.60799;
QFATC=0.066156; QGUTC=0.16619; QKIDC=0.17136; QLIVC=0.032962; QRAPC=0.44100; QSLWC=0.12233;
VLDC=0.068816; VFATC=0.24799; VGUTC=0.022022; VKIDC=0.0045857; VLIVC=0.024012; VPERFC=0.85778;
VRAPC=0.092619; VRESPC=0.00017998; VRESPLUMC=0.0023929; VSLWC=0.39756; FRACPLAS=0.61562;
PB=9.21416; PFAT=57.04798; PGUT=2.83403; PKID=1.59940; PLIV=4.05470; PRAP=2.40664;
PRESP=1.31422; PSLW=2.43522;
PRBCPLASTCA=0.14440; PBODTCAC=0.61821; PLIVTCAC=0.78732;
PBODTCOH=1.56375; PLIVTCOH=0.62940;
```

```

PBODTCOG=0.62057; PLIVTCOG=3.84344; PEFDCVG=0.010275;
BMAXKDC=4.07143; KDISSOC=180.77365;
KAS=0.0; KTSO=0.0; KAD=0.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=94.69522; KMC=1.0; CL=861.48250; FRACTCAC=0.040908; FRACOTHERC=0.10721;
VMAXDCVGC=1.0; KMDCVGC=3.61760; CLDCVG=52.79619;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83632; CLKIDDCVG=7.94132;
VMAXLUNGLIV=0.094527; KMCLARA=0.24341; FRACLUNGSYS=23.57060;
VMAXTCOHC=1.0; KMTCOH=2.27073; CLTCOH=0.17658;
VMAXGLUC=1.0; KMGLUC=129.28251; CLGLUC=0.28111; KMETTCOHC=0.69907;
KURNTCAC=0.0048995; KMETTCAC=0.27555;
KBILEC=7.24274; KEHRC=0.15614; KURNTCOGC=1.82828;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

```

MalePrior.m

```

xerror(["AInhResp", "AExhResp", "AResp"], [1.0e-13, 1.0e-13, 1.0e-13])
xerror(["ACh", "AExh", "AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw", "ABld"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ASTom", "ADuod", "AExc"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["AMetLng", "AMetKid", "AMetLiv1", "AMetLiv2"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["APlasTCA", "ABodTCA", "ASTomTCA", "ALivTCA", "AMetTCA", "AurnTCA"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOH", "ASTomTCOH", "ALivTCOH", "AMetTCOHTCA", "AMetTCOHGluc", "AMetTCOHOther"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOG", "ALivTCOG", "ABileTCOG", "ARecircTCOG", "AurnTCOG"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVC", "ABioactDCVC", "AurnDCVC"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ADCVG_mMole", "AMetDCVG_mMole"], [1.0e-9, 1.0e-9])

% Mean prior parameters for male human
% DRespc, Pefdcvg, KAS, KTSO, KAD, KASTCA, KASTCOH, FracOtherC, KMclara, FracLungSysC, KMTCOH,
% CLTCOH, KMGLUC, CLGLUC, kMetTCOHC, kMetTCAC, kBileC, KEHRC, KDCVGC, KNATC, kKidBioactC from
% Table 3-39 in report
% FrackIDDCVC from model code (comment from model - "In ".in" files, set to 1, so that all
% kidney GSH conjugation is assumed to directly produce DCVC (model lacks identifiability
% otherwise))
SPECIES=1;
BW=70.0; QCC=16; VPR=0.96; DRESPC=1.47;
QFATC=0.05; QGUTC=0.19; QKIDC=0.19; QLIVC=0.065; QRAPC=0.285; QSLWC=0.22;
VBLDC=0.077; VFATC=0.199; VGUTC=0.02; VKIDC=0.0043; VLIVC=0.025; VPERFC=0.856; VRAPC=0.088;
VRESPC=0.00018; VRESPLUMC=0.0023857; VSLWC=0.44252; FRACPLAS=0.567;
PB=9.5; PFAT=67.0; PGUT=2.6; PKID=1.6; PLIV=4.1; PRAP=2.6; PRESP=1.3; PSLW=2.1;
PRBCPLASTCA=0.5; PBODTCAC=0.52; PLIVTCAC=0.66;
PBODTCOH=0.91; PLIVTCOH=0.59;
PBODTCOG=0.91; PLIVTCOG=0.59; PEFDCVG=1.24;
BMAXKDC=4.62; KDISSOC=182.0;
KAS=1.4; KTSO=1.4; KAD=0.75; KTD=0.0; KASTCA=0.58; KASTCOH=0.49;
VMAXC=255.0; KMC=1.0; CL=66.0; FRACTCAC=0.32; FRACOTHERC=0.14;
VMAXDCVGC=1.0; KMDCVGC=2.9; CLDCVG=19.0;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=2.7; CLKIDDCVG=230.0;
VMAXLUNGLIV=0.025253; KMCLARA=0.019; FRACLUNGSYS=3.0;
VMAXTCOHC=1.0; KMTCOH=5.0; CLTCOH=0.35;
VMAXGLUC=1.0; KMGLUC=10.0; CLGLUC=3.0; KMETTCOHC=2.47;
KURNTCAC=0.108; KMETTCAC=0.55;
KBILEC=3.47; KEHRC=0.21; KURNTCOGC=0.108;
KDCVGC=0.127; FRACKIDDCVCC=22026.46579;
KNATC=0.0025; KKIDBIOACTC=0.0064;

```

MalePost.m

```

xerror(["AInhResp", "AExhResp", "AResp"], [1.0e-13, 1.0e-13, 1.0e-13])
xerror(["ACh", "AExh", "AFat", "AGut", "AKid", "ALiv", "ARap", "ASlw", "ABld"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ASTom", "ADuod", "AExc"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror(["AMetLng", "AMetKid", "AMetLiv1", "AMetLiv2"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["APlasTCA", "ABodTCA", "ASTomTCA", "ALivTCA", "AMetTCA", "AurnTCA"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ABodTCOH", "ASTomTCOH", "ALivTCOH", "AMetTCOHTCA", "AMetTCOHGluc", "AMetTCOHOther"],
[1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])

```

```

xerror (["ABodTCOG", "ALivTCOG", "ABileTCOG", "ARecircTCOG", "AurnTCOG"],
        [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror (["ADCVC", "ABioactDCVC", "AurnDCVC"], [1.0e-9, 1.0e-9, 1.0e-9])
xerror (["ADCVG_mMole", "AMetDCVG_mMole"], [1.0e-9, 1.0e-9])

% Mean posterior parameters for male human
SPECIES=1;
BW=70.0; QCC=13.36432; VPR=1.46518; DRESPC=0.60799;
QFATC=0.038915; QGUTC=0.15037; QKIDC=0.19152; QLIVC=0.032962; QRAPC=0.42793; QSLWC=0.15831;
VBLDC=0.077924; VFATC=0.15568; VGUTC=0.020020; VKIDC=0.0042867; VLIVC=0.026100; VPERFC=0.85600;
VRAPC=0.087639; VRESPC=0.00017998; VRESPLUMC=0.0023929; VSLWC=0.48417; FRACPLAS=0.56757;
PB=9.21416; PFAT=57.04798; PGUT=2.83403; PKID=1.59940; PLIV=4.05470; PRAP=2.40664;
PRESP=1.31422; PSLW=2.43522;
PRBCPLASTCA=0.14440; PBODTCAC=0.61821; PLIVTCAC=0.78732;
PBODTCOH=1.56375; PLIVTCOH=0.62940;
PBODTCOG=0.62057; PLIVTCOG=3.84344; PEFDCVG=0.010275;
BMAXKDC=4.07143; KDISSOC=180.77365;
KAS=0.0; KTSO=0.0; KAD=0.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=94.69522; KMC=1.0; CL=861.48250; FRACTCAC=0.040908; FRACOTHERC=0.10721;
VMAXDCVGC=1.0; KMDCVGC=3.61760; CLDCVG=52.79619;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83632; CLKIDDCVG=7.94132;
VMAXLUNGLIV=0.087525; KMCLARA=0.24341; FRACLUNGSYSYSC=23.57060;
VMAXTCOHC=1.0; KMTCOH=2.27073; CLTCOH=0.17658;
VMAXGLUCC=1.0; KMGLUC=129.28251; CLGLUC=0.28111; KMETTCOHC=0.69907;
KURNTCAC=0.0048995; KMETTCAC=0.27555;
KBILEC=7.24274; KEHRC=0.15614; KURNTCOGC=1.82828;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

```

Output Check.m

```
% Output parameters to check that all parameters are within range
```

```

Params(i,1) = QC;
Params(i,2) = QP;
Params(i,3) = QM;
Params(i,4) = DRESP;
Params(i,5) = QFAT;
Params(i,6) = QGUT;
Params(i,7) = QKID;
Params(i,8) = QLIV;
Params(i,9) = QRAP;
Params(i,10) = QSLW;
Params(i,11) = QGUTLIV;
Params(i,12) = QBOD;
Params(i,13) = QCPLAS;
Params(i,14) = QBODPLAS;
Params(i,15) = QGUTLIVPLAS;
Params(i,16) = VBLD;
Params(i,17) = VFAT;
Params(i,18) = VGUT;
Params(i,19) = VKID;
Params(i,20) = VLIV;
Params(i,21) = VPERFC;
Params(i,22) = VRAP;
Params(i,23) = VRESPLUM;
Params(i,24) = VRESP;
Params(i,25) = VRESPEFF;
Params(i,26) = VSLW;
Params(i,27) = VPLAS;
Params(i,28) = VBOD;
Params(i,29) = VDCVG;
Params(i,30) = TCAPLAS;
Params(i,31) = PBODTCA;
Params(i,32) = PLIVTCA;
Params(i,33) = BMAX;
Params(i,34) = VMAX;
Params(i,35) = KM;
Params(i,36) = FRACOTHER;
Params(i,37) = FRACTCA;
Params(i,38) = VMAXDCVG;

```

```

Params(i,39) = KMDCVG;
Params(i,40) = VMAXKIDDCVG;
Params(i,41) = KMKIDDCVG;
Params(i,42) = VMAXCLARA;
Params(i,43) = FRACLUNGSYS;
Params(i,44) = KMETTCOH;
Params(i,45) = VMAXTCOH;
Params(i,46) = VMAXGLUC;
Params(i,47) = KURNTCA;
Params(i,48) = KMETTCA;
Params(i,49) = KBILE;
Params(i,50) = KEHR;
Params(i,51) = KURNTCOG;
Params(i,52) = KDCVG;
Params(i,53) = FRACKIDDCVC;
Params(i,54) = KNAT;
Params(i,55) = KKIDBIOACT;
Params(i,56) = CC;
Params(i,57) = RODENTS;
Params(i,58) = KLOSS;
Params(i,59) = VCH;
Params(i,60) = ACH0;
Params(i,61) = KDRINK;

```

```

TmpCheckOutput = [];
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottissue, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _totmetab, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltce, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _rinhdose, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _totdose, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _retdose, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ach, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ainhresp, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aexhresp, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aresp, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametlng, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cart, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _calv, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _exhfactor, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _exhfac_den, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aexh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aexhpost, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _afat, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _astom, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aduod, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aexc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _rao, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _agut, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _akid, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametkid, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aliv, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametliv1, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametliv2, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _arap, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aslw, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cven, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottissuetca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aplastca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cplastcafree, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aplastcafree, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cplastcabnd, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _abodtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _astomtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _alivtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _amettca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aurntca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aotca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcain, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottissuetcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _totmetabtc, @Justification = 'begin');

```

```

TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ctcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _abodtcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _astomtcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _alivtcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _amettcohtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _amettcohgluc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _amettcohothet, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aotcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcohin, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcohdose, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottissuetcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ctcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _abodtcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _alivtcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _abiletcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _arecirtcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aurntcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcogin, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaldcvc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _advcin, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _adcvc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _abioactdcvc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aurndcvc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaldcvg, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _adcvgin, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _adcvg_mmole, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametdcvg_mmole, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cinh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kia, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kiv, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kpv, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kivtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kivtcoh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kstom, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kstomtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kstomtcoh, @Justification = 'begin');

CheckOutput = atrrowsj(CheckOutput, max(TmpCheckOutput), @Justification = 'begin');
CheckOutput = atrrowsj(CheckOutput, min(TmpCheckOutput), @Justification = 'begin');

```

Output_Check_Reset.m

```

% Output parameters to check that all parameters are reset with each run
ParamsReset=[];

```

```

ParamsReset(1,1) = BW;
ParamsReset(2,1) = QCC;
ParamsReset(3,1) = VPR;
ParamsReset(4,1) = DRESPC;
ParamsReset(5,1) = QFATC;
ParamsReset(6,1) = QGUTC;
ParamsReset(7,1) = QKIDC;
ParamsReset(8,1) = QLIVC;
ParamsReset(9,1) = QRAPC;
ParamsReset(10,1) = QSLWC;
ParamsReset(11,1) = VBLDC;
ParamsReset(12,1) = VFATC;
ParamsReset(13,1) = VGUTC;
ParamsReset(14,1) = VKIDC;
ParamsReset(15,1) = VLIVC;
ParamsReset(16,1) = VPERFC;
ParamsReset(17,1) = VRAPC;
ParamsReset(18,1) = VRESPC;
ParamsReset(19,1) = VRESPLUMC;
ParamsReset(20,1) = VSLWC;
ParamsReset(21,1) = FRACPLAS;
ParamsReset(22,1) = MWTCE;
ParamsReset(23,1) = MWDCVC;
ParamsReset(24,1) = MWTCA;

```

```

ParamsReset(25,1) = MWTCOH;
ParamsReset(26,1) = MWTCOHGLUC;
ParamsReset(27,1) = MWNADCVC;
ParamsReset(28,1) = PB;
ParamsReset(29,1) = PFAT;
ParamsReset(30,1) = PGUT;
ParamsReset(31,1) = PKID;
ParamsReset(32,1) = PLIV;
ParamsReset(33,1) = PRAP;
ParamsReset(34,1) = PRES;
ParamsReset(35,1) = PSLW;
ParamsReset(36,1) = PRBCPLASTCA;
ParamsReset(37,1) = PBODTCAC;
ParamsReset(38,1) = PLIVTCAC;
ParamsReset(39,1) = PBODTCOH;
ParamsReset(40,1) = PLIVTCOH;
ParamsReset(41,1) = PBODTCOG;
ParamsReset(42,1) = PLIVTCOG;
ParamsReset(43,1) = PEFDCVGC;
ParamsReset(44,1) = BMAXKDC;
ParamsReset(45,1) = KDISSOC;
ParamsReset(46,1) = KAS;
ParamsReset(47,1) = KTS;
ParamsReset(48,1) = KAD;
ParamsReset(49,1) = KTD;
ParamsReset(50,1) = KASTCA;
ParamsReset(51,1) = KASTCOH;
ParamsReset(52,1) = VMAXC;
ParamsReset(53,1) = KMC;
ParamsReset(54,1) = CL;
ParamsReset(55,1) = FRACCTAC;
ParamsReset(56,1) = FRACOTHERC;
ParamsReset(57,1) = VMAXDCVGC;
ParamsReset(58,1) = KMDCVGC;
ParamsReset(59,1) = CLDCVGC;
ParamsReset(60,1) = VMAXKIDDCVGC;
ParamsReset(61,1) = KMKIDDCVGC;
ParamsReset(62,1) = CLKIDDCVGC;
ParamsReset(63,1) = VMAXLUNGLIV;
ParamsReset(64,1) = KMCLARA;
ParamsReset(65,1) = FRACLUNGSYSC;
ParamsReset(66,1) = VMAXTCOHC;
ParamsReset(67,1) = KMTCOH;
ParamsReset(68,1) = CLTCOH;
ParamsReset(69,1) = VMAXGLUCC;
ParamsReset(70,1) = KMGLUC;
ParamsReset(71,1) = CLGLUC;
ParamsReset(72,1) = KMETTCOHC;
ParamsReset(73,1) = KURNTCAC;
ParamsReset(74,1) = KMETTCAC;
ParamsReset(75,1) = KBILEC;
ParamsReset(76,1) = KEHRC;
ParamsReset(77,1) = KURNTCOGC;
ParamsReset(78,1) = KDCVGC;
ParamsReset(79,1) = FRACKIDDCVCC;
ParamsReset(80,1) = KNATC;
ParamsReset(81,1) = KKIDBIOACTC;
ParamsReset(82,1) = CC;
ParamsReset(83,1) = NRODENTS;
ParamsReset(84,1) = KLOSSC;
ParamsReset(85,1) = VCHC;
ParamsReset(86,1) = CONCLIST(1);
ParamsReset(87,1) = STRTNEXTLIST(1);
ParamsReset(88,1) = TSTR;
ParamsReset(89,1) = IVDOS;
ParamsReset(90,1) = TCHNG;
ParamsReset(91,1) = DAYS;
ParamsReset(92,1) = TMAX;
ParamsReset(93,1) = PDOS;
ParamsReset(94,1) = DRINK;
ParamsReset(95,1) = IADOS;

```


ParamsReset(96,1) = PVD0SE;
 ParamsReset(97,1) = IVD0SETCA;
 ParamsReset(98,1) = POD0SETCA;
 ParamsReset(99,1) = IVD0SETCOH;
 ParamsReset(100,1) = POD0SETCOH;
 ParamsReset(101,1) = SPECIES;
 ParamsReset(102,1) = TURN;
 ParamsReset(103,1) = URNMISSLIST(1);
 ParamsReset(104,1) = URNMISSING;
 ParamsReset(105,1) = TSTP;
 ParamsReset(106,1) = CINT;
 ParamsReset(107,1) = QC;
 ParamsReset(108,1) = QP;
 ParamsReset(109,1) = QM;
 ParamsReset(110,1) = DRESP;
 ParamsReset(111,1) = QADJUS;
 ParamsReset(112,1) = QFAT;
 ParamsReset(113,1) = QGUT;
 ParamsReset(114,1) = QKID;
 ParamsReset(115,1) = QLIV;
 ParamsReset(116,1) = QRAP;
 ParamsReset(117,1) = QSLW;
 ParamsReset(118,1) = QGUTLIV;
 ParamsReset(119,1) = QBOD;
 ParamsReset(120,1) = QCPLAS;
 ParamsReset(121,1) = QBODPLAS;
 ParamsReset(122,1) = QGUTLIVPLAS;
 ParamsReset(123,1) = VTOTC;
 ParamsReset(124,1) = VADJUS;
 ParamsReset(125,1) = VBLD;
 ParamsReset(126,1) = VFAT;
 ParamsReset(127,1) = VGUT;
 ParamsReset(128,1) = VKID;
 ParamsReset(129,1) = VLIV;
 ParamsReset(130,1) = VRAP;
 ParamsReset(131,1) = VRESP;
 ParamsReset(132,1) = VSLW;
 ParamsReset(133,1) = VPLAS;
 ParamsReset(134,1) = VBOD;
 ParamsReset(135,1) = VBODTCOH;
 ParamsReset(136,1) = VDCVG;
 ParamsReset(137,1) = VRESPLUM;
 ParamsReset(138,1) = VRESPEFF;
 ParamsReset(139,1) = STOCHTCATCE;
 ParamsReset(140,1) = STOCHTCATCOH;
 ParamsReset(141,1) = STOCHTCOHTCE;
 ParamsReset(142,1) = STOCHGLUCTCOH;
 ParamsReset(143,1) = STOCHTCOHLUC;
 ParamsReset(144,1) = STOCHDCVCTCE;
 ParamsReset(145,1) = STOCHN;
 ParamsReset(146,1) = TCAPLAS;
 ParamsReset(147,1) = PBODTCA;
 ParamsReset(148,1) = PLIVTCA;
 ParamsReset(149,1) = BMAX;
 ParamsReset(150,1) = VMAX;
 ParamsReset(151,1) = FRACOTHER;
 ParamsReset(152,1) = FRACTCA;
 ParamsReset(153,1) = KM;
 ParamsReset(154,1) = VMAXDCVG;
 ParamsReset(155,1) = KMDCVG;
 ParamsReset(156,1) = VMAXKIDDCVG;
 ParamsReset(157,1) = KMKIDDCVG;
 ParamsReset(158,1) = VMAXCLARA;
 ParamsReset(159,1) = FRACLUNGSYS;
 ParamsReset(160,1) = KMETTCOH;
 ParamsReset(161,1) = VMAXTCOH;
 ParamsReset(162,1) = VMAXGLUC;
 ParamsReset(163,1) = KURNTCA;
 ParamsReset(164,1) = KMETTCA;
 ParamsReset(165,1) = KBILE;
 ParamsReset(166,1) = KEHR;

```

ParamsReset(167,1) = KURNTCOG;
ParamsReset(168,1) = KDCVG;
ParamsReset(169,1) = FRACKIDDCVC;
ParamsReset(170,1) = KNAT;
ParamsReset(171,1) = KKIDBIOACT;
ParamsReset(172,1) = RODENTS;
ParamsReset(173,1) = KLOSS;
ParamsReset(174,1) = VCH;
ParamsReset(175,1) = ACH0;
ParamsReset(176,1) = _day(1,1);
ParamsReset(177,1) = _cinh(1,1);
ParamsReset(178,1) = _kdrink(1,1);
ParamsReset(179,1) = _kia(1,1);
ParamsReset(180,1) = _kiv(1,1);
ParamsReset(181,1) = _kivtca(1,1);
ParamsReset(182,1) = _kivtcoh(1,1);
ParamsReset(183,1) = _kpv(1,1);
ParamsReset(184,1) = _kstom(1,1);
ParamsReset(185,1) = _kstomtca(1,1);
ParamsReset(186,1) = _kstomtcoh(1,1);
ParamsReset(187,1) = _aurntca_coll(1,1);
ParamsReset(188,1) = _aurntcog_coll(1,1);
ParamsReset(189,1) = _paucbld(1,1);
ParamsReset(190,1) = _aucblddm(1,1);
ParamsReset(191,1) = _paucplastca(1,1);
ParamsReset(192,1) = _aucplastcadm(1,1);
ParamsReset(193,1) = _paucplastcafree(1,1);
ParamsReset(194,1) = _aucplastcafreedm(1,1);
ParamsReset(195,1) = _paucctcoh(1,1);
ParamsReset(196,1) = _aucctcohdm(1,1);
ParamsReset(197,1) = _paucctcog(1,1);
ParamsReset(198,1) = _aucctcogdm(1,1);
ParamsReset(199,1) = _pauctotctcoh(1,1);
ParamsReset(200,1) = _auctotctcohdm(1,1);
ParamsReset(201,1) = _pauccliv(1,1);
ParamsReset(202,1) = _aucclivdm(1,1);
ParamsReset(203,1) = _paucclivtca(1,1);
ParamsReset(204,1) = _aucclivtcadm(1,1);
ParamsReset(205,1) = _paucclivtcoh(1,1);
ParamsReset(206,1) = _aucclivtcohdm(1,1);
ParamsReset(207,1) = _paucclivtcog(1,1);
ParamsReset(208,1) = _aucclivtcogdm(1,1);
ParamsReset(209,1) = _pametliv1tcavliv(1,1);
ParamsReset(210,1) = _ametliv1tcavlivdm(1,1);
ParamsReset(211,1) = _pametliv1tcabw34(1,1);
ParamsReset(212,1) = _ametliv1tcabw34dm(1,1);
ParamsReset(213,1) = _pametliv1tcohvliv(1,1);
ParamsReset(214,1) = _ametliv1tcohvlivdm(1,1);
ParamsReset(215,1) = _pametliv1tcohbw34(1,1);
ParamsReset(216,1) = _ametliv1tcohbw34dm(1,1);
ParamsReset(217,1) = _pametliv2vliv(1,1);
ParamsReset(218,1) = _ametliv2vlivdm(1,1);
ParamsReset(219,1) = _pametliv2bw34(1,1);
ParamsReset(220,1) = _ametliv2bw34dm(1,1);
ParamsReset(221,1) = _pametlivothervliv(1,1);
ParamsReset(222,1) = _ametlivothervlivdm(1,1);
ParamsReset(223,1) = _pametlivotherbw34(1,1);
ParamsReset(224,1) = _ametlivotherbw34dm(1,1);
ParamsReset(225,1) = _pamettcavliv(1,1);
ParamsReset(226,1) = _amettcavlivdm(1,1);
ParamsReset(227,1) = _pamettcabw34(1,1);
ParamsReset(228,1) = _amettcabw34dm(1,1);
ParamsReset(229,1) = _pamettcohtcavliv(1,1);
ParamsReset(230,1) = _amettcohtcavlivdm(1,1);
ParamsReset(231,1) = _pamettcohtcabw34(1,1);
ParamsReset(232,1) = _amettcohtcabw34dm(1,1);
ParamsReset(233,1) = _pamettcohglucvliv(1,1);
ParamsReset(234,1) = _amettcohglucvlivdm(1,1);
ParamsReset(235,1) = _pamettcohglucbw34(1,1);
ParamsReset(236,1) = _amettcohglucbw34dm(1,1);
ParamsReset(237,1) = _pamettcothervliv(1,1);

```

```

ParamsReset(238,1) = _amettcoothervlivdm(1,1);
ParamsReset(239,1) = _pamettcootherbw34(1,1);
ParamsReset(240,1) = _amettcootherbw34dm(1,1);
ParamsReset(241,1) = _hours(1,1);
ParamsReset(242,1) = _rach(1,1);
ParamsReset(243,1) = _ach(1,1);
ParamsReset(244,1) = _cinhppm(1,1);
ParamsReset(245,1) = _cinh(1,1);
ParamsReset(246,1) = _rainhresp(1,1);
ParamsReset(247,1) = _ainhresp(1,1);
ParamsReset(248,1) = _cinhresp(1,1);
ParamsReset(249,1) = _raexhresp(1,1);
ParamsReset(250,1) = _aexhresp(1,1);
ParamsReset(251,1) = _cexhresp(1,1);
ParamsReset(252,1) = _raresp(1,1);
ParamsReset(253,1) = _aresp(1,1);
ParamsReset(254,1) = _cresp(1,1);
ParamsReset(255,1) = _rametlng(1,1);
ParamsReset(256,1) = _ametlng(1,1);
ParamsReset(257,1) = _ametlngbw34(1,1);
ParamsReset(258,1) = _ametlngvresp(1,1);
ParamsReset(259,1) = _cart(1,1);
ParamsReset(260,1) = _auccbld(1,1);
ParamsReset(261,1) = _calv(1,1);
ParamsReset(262,1) = _calvppm(1,1);
ParamsReset(263,1) = _exhfac_den(1,1);
ParamsReset(264,1) = _exhfactor(1,1);
ParamsReset(265,1) = _raexh(1,1);
ParamsReset(266,1) = _aexh(1,1);
ParamsReset(267,1) = _aexhpost(1,1);
ParamsReset(268,1) = _aexhexp(1,1);
ParamsReset(269,1) = _rafat(1,1);
ParamsReset(270,1) = _afat(1,1);
ParamsReset(271,1) = _cfat(1,1);
ParamsReset(272,1) = _cvfat(1,1);
ParamsReset(273,1) = _rastom(1,1);
ParamsReset(274,1) = _astom(1,1);
ParamsReset(275,1) = _raduod(1,1);
ParamsReset(276,1) = _aduod(1,1);
ParamsReset(277,1) = _raexc(1,1);
ParamsReset(278,1) = _aexc(1,1);
ParamsReset(279,1) = _rao(1,1);
ParamsReset(280,1) = _ragut(1,1);
ParamsReset(281,1) = _agut(1,1);
ParamsReset(282,1) = _cgut(1,1);
ParamsReset(283,1) = _cvgut(1,1);
ParamsReset(284,1) = _rakid(1,1);
ParamsReset(285,1) = _akid(1,1);
ParamsReset(286,1) = _ckid(1,1);
ParamsReset(287,1) = _cvkid(1,1);
ParamsReset(288,1) = _aucckid(1,1);
ParamsReset(289,1) = _rametkid(1,1);
ParamsReset(290,1) = _ametkid(1,1);
ParamsReset(291,1) = _raliv(1,1);
ParamsReset(292,1) = _aliv(1,1);
ParamsReset(293,1) = _cliv(1,1);
ParamsReset(294,1) = _cvliv(1,1);
ParamsReset(295,1) = _auccliv(1,1);
ParamsReset(296,1) = _rametliv1(1,1);
ParamsReset(297,1) = _ametliv1(1,1);
ParamsReset(298,1) = _ametliv1vliv(1,1);
ParamsReset(299,1) = _ametliv1bw34(1,1);
ParamsReset(300,1) = _ametliv1tca(1,1);
ParamsReset(301,1) = _ametliv1tcavliv(1,1);
ParamsReset(302,1) = _ametliv1tcabw34(1,1);
ParamsReset(303,1) = _ametliv1tcoh(1,1);
ParamsReset(304,1) = _ametliv1tcohvliv(1,1);
ParamsReset(305,1) = _ametliv1tcohbw34(1,1);
ParamsReset(306,1) = _ametlivother(1,1);
ParamsReset(307,1) = _ametlivothervliv(1,1);
ParamsReset(308,1) = _ametlivotherbw34(1,1);

```

```

ParamsReset(309,1) = _rametliv2(1,1);
ParamsReset(310,1) = _ametliv2(1,1);
ParamsReset(311,1) = _ametliv2vliv(1,1);
ParamsReset(312,1) = _ametliv2bw34(1,1);
ParamsReset(313,1) = _ametgsh(1,1);
ParamsReset(314,1) = _ametgshbw34(1,1);
ParamsReset(315,1) = _rarap(1,1);
ParamsReset(316,1) = _arap(1,1);
ParamsReset(317,1) = _crap(1,1);
ParamsReset(318,1) = _cvrap(1,1);
ParamsReset(319,1) = _auccrap(1,1);
ParamsReset(320,1) = _chrt(1,1);
ParamsReset(321,1) = _clung(1,1);
ParamsReset(322,1) = _cspl(1,1);
ParamsReset(323,1) = _cbrn(1,1);
ParamsReset(324,1) = _raslw(1,1);
ParamsReset(325,1) = _aslw(1,1);
ParamsReset(326,1) = _cslw(1,1);
ParamsReset(327,1) = _cvslw(1,1);
ParamsReset(328,1) = _cmus(1,1);
ParamsReset(329,1) = _rabld(1,1);
ParamsReset(330,1) = _abld(1,1);
ParamsReset(331,1) = _cven(1,1);
ParamsReset(332,1) = _cven_mmole(1,1);
ParamsReset(333,1) = _cbldmix(1,1);
ParamsReset(334,1) = _rinhdose(1,1);
ParamsReset(335,1) = _retdose(1,1);
ParamsReset(336,1) = _totdose(1,1);
ParamsReset(337,1) = _tottissue(1,1);
ParamsReset(338,1) = _totmetab(1,1);
ParamsReset(339,1) = _massbaltce(1,1);
ParamsReset(340,1) = _totdosebw34(1,1);
ParamsReset(341,1) = _totmetabbw34(1,1);
ParamsReset(342,1) = _totoxmetbw34(1,1);
ParamsReset(343,1) = _raplastca(1,1);
ParamsReset(344,1) = _aplastca(1,1);
ParamsReset(345,1) = _cplastca(1,1);
ParamsReset(346,1) = _cbldtca(1,1);
ParamsReset(347,1) = _auccplastca(1,1);
ParamsReset(348,1) = _aplastcafree(1,1);
ParamsReset(349,1) = _auccplastcafree(1,1);
ParamsReset(350,1) = _a(1,1);
ParamsReset(351,1) = _b(1,1);
ParamsReset(352,1) = _cplastcafree(1,1);
ParamsReset(353,1) = _cplastcabnd(1,1);
ParamsReset(354,1) = _rabodtca(1,1);
ParamsReset(355,1) = _abodtca(1,1);
ParamsReset(356,1) = _cbodtca(1,1);
ParamsReset(357,1) = _cvbodtca(1,1);
ParamsReset(358,1) = _cvbodtcafree(1,1);
ParamsReset(359,1) = _ckidtca(1,1);
ParamsReset(360,1) = _clungtca(1,1);
ParamsReset(361,1) = _rastomtca(1,1);
ParamsReset(362,1) = _astomtca(1,1);
ParamsReset(363,1) = _ralivtca(1,1);
ParamsReset(364,1) = _alivtca(1,1);
ParamsReset(365,1) = _clivtca(1,1);
ParamsReset(366,1) = _cvlivtca(1,1);
ParamsReset(367,1) = _cvlivtcafree(1,1);
ParamsReset(368,1) = _aucclivtca(1,1);
ParamsReset(369,1) = _ramettca(1,1);
ParamsReset(370,1) = _amettca(1,1);
ParamsReset(371,1) = _amettcavliv(1,1);
ParamsReset(372,1) = _amettcabw34(1,1);
ParamsReset(373,1) = _raurntca(1,1);
ParamsReset(374,1) = _aurntca(1,1);
ParamsReset(375,1) = _aurntca_coll(1,1);
ParamsReset(376,1) = _aotca(1,1);
ParamsReset(377,1) = _tottcain(1,1);
ParamsReset(378,1) = _tottissuetca(1,1);
ParamsReset(379,1) = _massbaltca(1,1);

```

```

ParamsReset(380,1) = _tottcainbw(1,1);
ParamsReset(381,1) = _ctcoh(1,1);
ParamsReset(382,1) = _aucctcoh(1,1);
ParamsReset(383,1) = _rabodtcoh(1,1);
ParamsReset(384,1) = _abodtcoh(1,1);
ParamsReset(385,1) = _cbodtcoh(1,1);
ParamsReset(386,1) = _cvbodtcoh(1,1);
ParamsReset(387,1) = _auccbodtcoh(1,1);
ParamsReset(388,1) = _ckidtcoh(1,1);
ParamsReset(389,1) = _clungtcoh(1,1);
ParamsReset(390,1) = _cbodtcogtcoh(1,1);
ParamsReset(391,1) = _ckidtcogtcoh(1,1);
ParamsReset(392,1) = _clungtcogtcoh(1,1);
ParamsReset(393,1) = _rastomtcoh(1,1);
ParamsReset(394,1) = _astomtcoh(1,1);
ParamsReset(395,1) = _ralivtcoh(1,1);
ParamsReset(396,1) = _alivtcoh(1,1);
ParamsReset(397,1) = _clivtcoh(1,1);
ParamsReset(398,1) = _cvlivtcoh(1,1);
ParamsReset(399,1) = _aucclivtcoh(1,1);
ParamsReset(400,1) = _clivtcogtcoh(1,1);
ParamsReset(401,1) = _ramettcohtca(1,1);
ParamsReset(402,1) = _amettcohtca(1,1);
ParamsReset(403,1) = _amettcohtcavliv(1,1);
ParamsReset(404,1) = _amettcohtcabw34(1,1);
ParamsReset(405,1) = _ramettcohgluc(1,1);
ParamsReset(406,1) = _amettcohgluc(1,1);
ParamsReset(407,1) = _amettcohglucvliv(1,1);
ParamsReset(408,1) = _amettcohglucbw34(1,1);
ParamsReset(409,1) = _ramettcohoth(1,1);
ParamsReset(410,1) = _amettcohoth(1,1);
ParamsReset(411,1) = _amettcohothervliv(1,1);
ParamsReset(412,1) = _amettcohotherbw34(1,1);
ParamsReset(413,1) = _aotcoh(1,1);
ParamsReset(414,1) = _tottcohin(1,1);
ParamsReset(415,1) = _tottissuetcoh(1,1);
ParamsReset(416,1) = _totmetabtcogh(1,1);
ParamsReset(417,1) = _massbaltcogh(1,1);
ParamsReset(418,1) = _tottcohdose(1,1);
ParamsReset(419,1) = _ctcog(1,1);
ParamsReset(420,1) = _aucctcog(1,1);
ParamsReset(421,1) = _ctcogtcoh(1,1);
ParamsReset(422,1) = _rabodtcog(1,1);
ParamsReset(423,1) = _abodtcog(1,1);
ParamsReset(424,1) = _cvbodtcog(1,1);
ParamsReset(425,1) = _ralivtcog(1,1);
ParamsReset(426,1) = _alivtcog(1,1);
ParamsReset(427,1) = _cvlivtcog(1,1);
ParamsReset(428,1) = _aucclivtcog(1,1);
ParamsReset(429,1) = _rabiletcog(1,1);
ParamsReset(430,1) = _abiletcog(1,1);
ParamsReset(431,1) = _rarecircctcog(1,1);
ParamsReset(432,1) = _arecircctcog(1,1);
ParamsReset(433,1) = _aurntcog(1,1);
ParamsReset(434,1) = _aurntcog(1,1);
ParamsReset(435,1) = _aurntcogtcoh(1,1);
ParamsReset(436,1) = _aurntcog_coll(1,1);
ParamsReset(437,1) = _aurntcogtcoh_coll(1,1);
ParamsReset(438,1) = _aurntctot_mmole(1,1);
ParamsReset(439,1) = _atcog(1,1);
ParamsReset(440,1) = _totctcoh(1,1);
ParamsReset(441,1) = _auctotctcoh(1,1);
ParamsReset(442,1) = _tottcogin(1,1);
ParamsReset(443,1) = _tottissuetcog(1,1);
ParamsReset(444,1) = _massbaltcog(1,1);
ParamsReset(445,1) = _radcvc(1,1);
ParamsReset(446,1) = _adcvc(1,1);
ParamsReset(447,1) = _radioactdcvc(1,1);
ParamsReset(448,1) = _abioactdcvc(1,1);
ParamsReset(449,1) = _abioactdcvcvkid(1,1);
ParamsReset(450,1) = _abioactdcvcbw34(1,1);

```

```

ParamsReset(451,1) = _raurndcvc(1,1);
ParamsReset(452,1) = _aurndcvc(1,1);
ParamsReset(453,1) = _aurndcvc_eq(1,1);
ParamsReset(454,1) = _aurndcvc(1,1);
ParamsReset(455,1) = _adcvcin(1,1);
ParamsReset(456,1) = _massbaldcvc(1,1);
ParamsReset(457,1) = _radcvg_mmole(1,1);
ParamsReset(458,1) = _adcvg_mmole(1,1);
ParamsReset(459,1) = _cdcvg_mmole(1,1);
ParamsReset(460,1) = _auccdcvg_mmole(1,1);
ParamsReset(461,1) = _rametdcvg_mmole(1,1);
ParamsReset(462,1) = _ametdcvg_mmole(1,1);
ParamsReset(463,1) = _adcvgin(1,1);
ParamsReset(464,1) = _massbaldcvg(1,1);

```

```

OutputReset = addcolsj(OutputReset, ParamsReset, @Justification = 'begin');

```

RunFigures.m

```

% Mouse
CheckOutput = []; OutputReset=[]; Params=[]; i=0;
Abbas97a_Mouse
Abbas97b_Mouse
Fisher91_Mouse
Fisher93_Mouse
Green85_Mouse
Greenberg99_Mouse
Larson92a_Mouse
Larson92b_Mouse
Merdink98_Mouse
Prout85_Mouse
Templin93_Mouse
save CheckOutput @file='CheckOutput_MouseFigures.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_MouseFigures.txt' @format=ascii
save Params @file='Params_MouseFigures.txt' @format=ascii

% Rat
CheckOutput = []; OutputReset=[]; Params=[]; i=0;
Bernauer96_Rat
Dallas91_Rat
Fisher89_Rat
Fisher91_Rat
Green85_Rat
Hissink02_Rat
Kaneko94_Rat
Keys03_Rat
Kimmerle73_Rat
Larson92a_Rat
Larson92b_Rat
Lee00_Rat
Merdink99_Rat
Prout85_Rat
Simmons02_Rat
Stenner97_Rat
Templin95_Rat
Yu00_Rat
save CheckOutput @file='CheckOutput_RatFigures.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_RatFigures.txt' @format=ascii
save Params @file='Params_RatFigures.txt' @format=ascii

% Human
CheckOutput = []; OutputReset=[]; Params=[]; i=0;
Bernauer96_Human
Chiu07_Human
Fisher98_Human
Kimmerle73_Human
Monster76_Human
Muller74_Human
Paykoc45_Human

```

```

save CheckOutput @file='CheckOutput_HumanFigures.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_HumanFigures.txt' @format=ascii
save Params @file='Params_HumanFigures.txt' @format=ascii

```

RunSA.m

```

load @format=model @file=New_EPA
Init
Mouse_SARun
Rat_SARun
Male_SARun
Female_SARun

```

RunDMS.m

```

load @format=model @file=New_EPA
init

% Mouse
CheckOutput=[]; DMOutput=[]; Params=[]; i=0;
Cosby92_MouseDM
George85_MouseDM
Griffin00_MouseDM
Kaneko00_MouseDM
Kjellstrand83_MouseDM
Land81_MouseDM
Ramdhan10_MouseDM
Sanders82_MouseDM
Schwetz75_MouseDM
save CheckOutput @file='CheckOutput_MouseDMS.txt' @format=ascii
save DMOutput @file='MouseDMS.txt' @format=ascii
save Params @file='Params_MouseDMS.txt' @format=ascii

% Rat
CheckOutput=[]; DMOutput=[]; Params=[]; i=0;
Adams51_RatDM
Albee06_RatDM
Arito94_RatDM
Bushnell97_RatDM
Carney06_RatDM
Crofton97_RatDM
Fisher01_RatDM
Healy82_RatDM
Jaspers93_RatDM
Kumar00a_01a_RatDM
Maltoni88_RatDM
Manson84_RatDM
Narotsky95_RatDM
Schwetz75_RatDM
Woolhiser06_RatDM
Wu07_RatDM
save CheckOutput @file='CheckOutput_RatDMS.txt' @format=ascii
save DMOutput @file='RatDMS.txt' @format=ascii
save Params @file='Params_RatDMS.txt' @format=ascii

```

RunHECs.m

```

load @format=model @file=New_EPA
init

% Human
CheckOutput=[]; DMOutput=[]; Params=[]; i=0;
Male_Fit_DMS_ContInh
save CheckOutput @file='CheckOutput_MaleContDMS.txt' @format=ascii
CheckOutput=[]; i=0;
Male_Fit_DMS_OccInh
save CheckOutput @file='CheckOutput_MaleOccDMS.txt' @format=ascii
CheckOutput=[]; i=0;
Female_Fit_DMS_ContInh
save CheckOutput @file='CheckOutput_FemaleContDMS.txt' @format=ascii
CheckOutput=[]; i=0;

```

```
Female_Fit_DMs_OccInh
save CheckOutput @file='CheckOutput_FemaleOccDMs.txt' @format=ascii
save Params @file='Params_HumanDMs.txt' @format=ascii
```

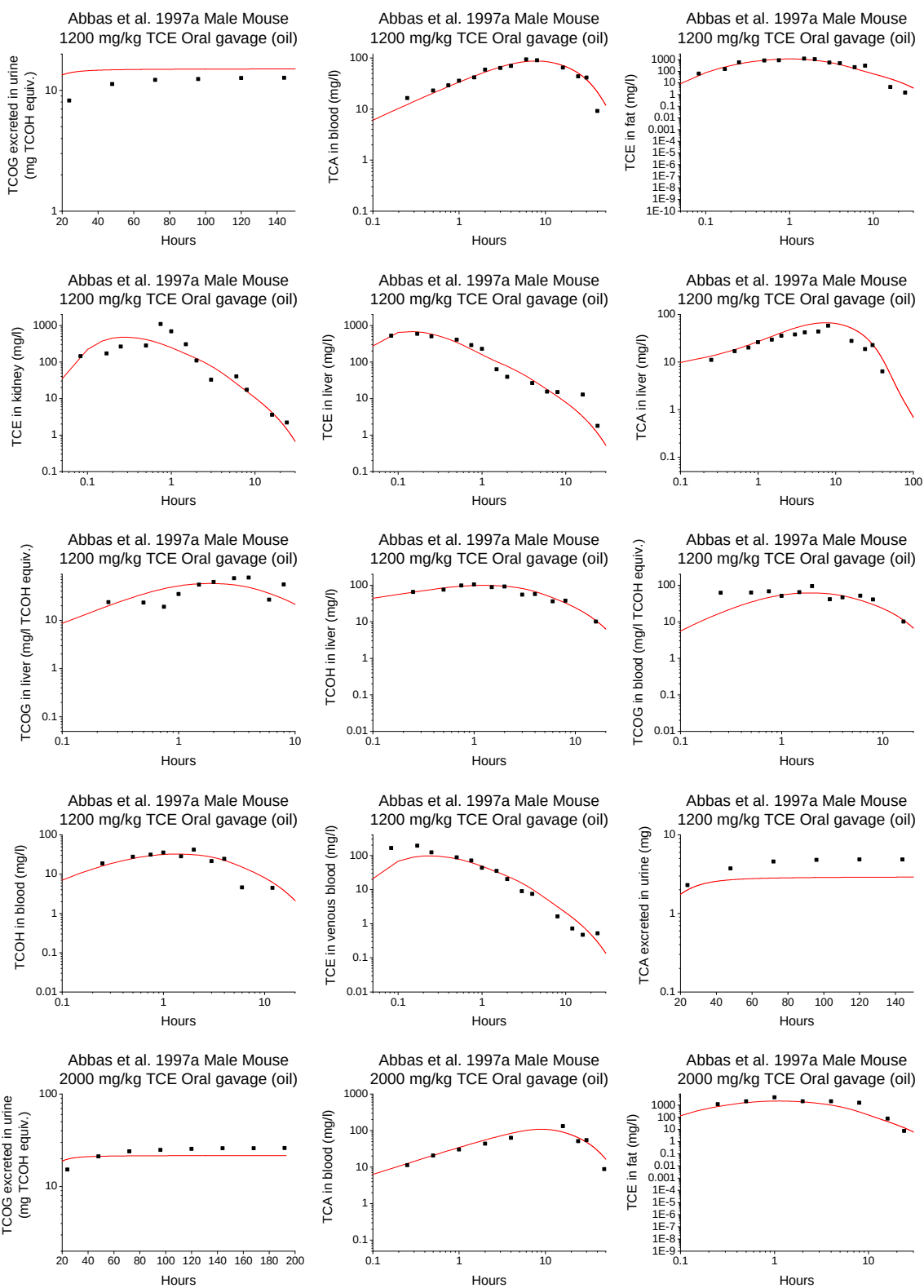
SavedDMs.m

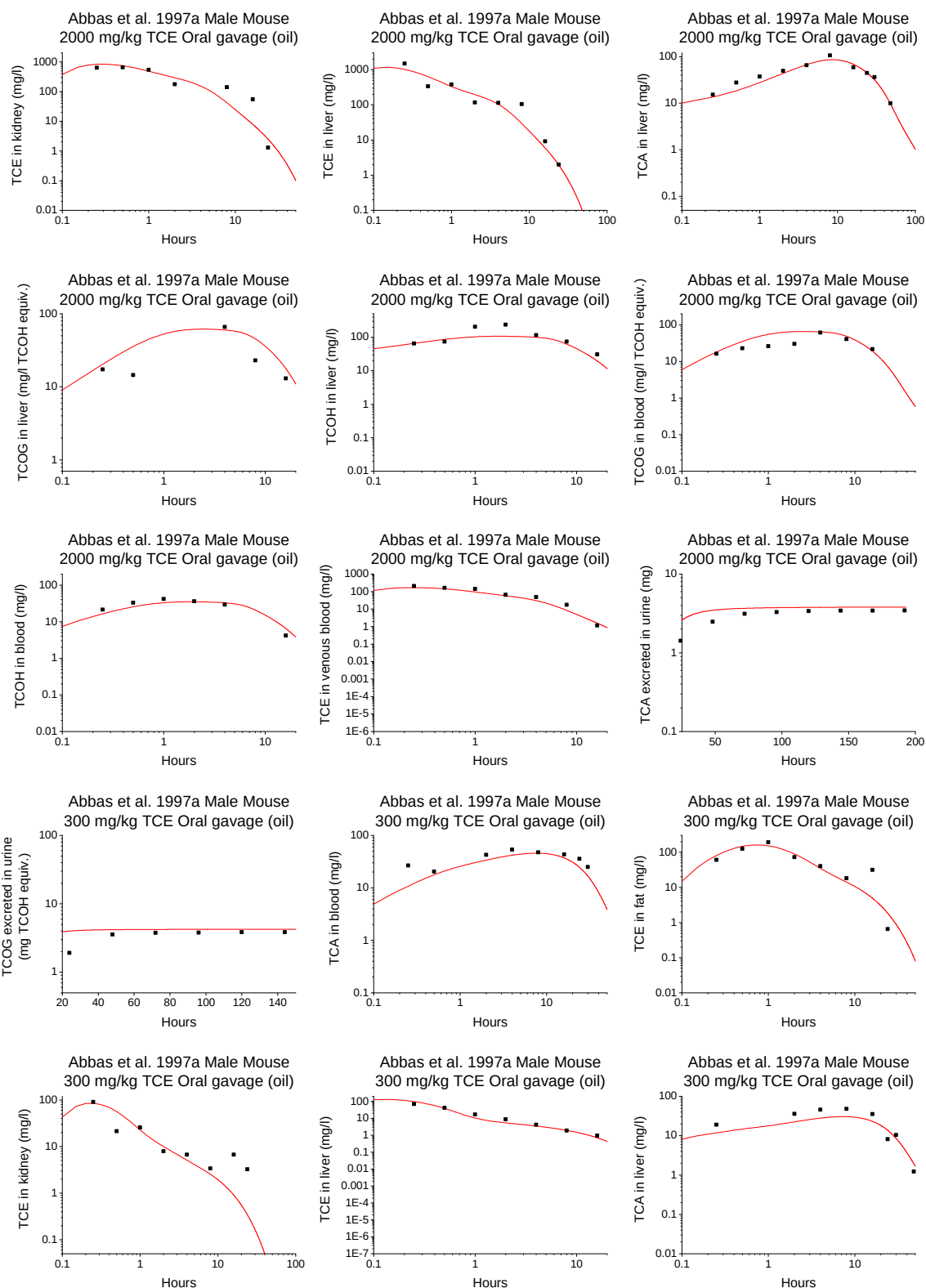
```
DMOutput(i,1) = max(_cart);
DMOutput(i,2) = max(_cplastca);
DMOutput(i,3) = max(_cplastcafree);
DMOutput(i,4) = max(_ctcoh);
DMOutput(i,5) = max(_ctcog);
DMOutput(i,6) = max(_totctcoh);
DMOutput(i,7) = AUCCBLDDM;
DMOutput(i,8) = AUCCPLASTCADM;
DMOutput(i,9) = AUCCPLASTCAFREEDM;
DMOutput(i,10) = AUCCTCOHDM;
DMOutput(i,11) = AUCCTCOGDM;
DMOutput(i,12) = AUCTOTCTCOHDM;
DMOutput(i,13) = TOTMETABBW34DM;
DMOutput(i,14) = TOTOXMETBW34DM;
DMOutput(i,15) = max(_cliv);
DMOutput(i,16) = max(_clivtca);
DMOutput(i,17) = max(_clivtcoh);
DMOutput(i,18) = max(_clivtcog);
DMOutput(i,19) = AUCCLIVDM;
DMOutput(i,20) = AUCCLIVTCADM;
DMOutput(i,21) = AUCCLIVTCOHDM;
DMOutput(i,22) = AUCCLIVTCOGDM;
DMOutput(i,23) = AMETLIV1VLIVDM;
DMOutput(i,24) = AMETLIV1TCAVLIVDM;
DMOutput(i,25) = AMETLIV1TCOHVLIVDM;
DMOutput(i,26) = AMETLIV2VLIVDM;
DMOutput(i,27) = AMETLIVOTHERVLIVDM;
DMOutput(i,28) = AMETTCAVLIVDM;
DMOutput(i,29) = AMETTCOHTCAVLIVDM;
DMOutput(i,30) = AMETTCOHLUCVLIVDM;
DMOutput(i,31) = AMETTCOHOTHERVLIVDM;
DMOutput(i,32) = AMETLIV1BW34DM;
DMOutput(i,33) = AMETLIV1TCABW34DM;
DMOutput(i,34) = AMETLIV1TCOHBW34DM;
DMOutput(i,35) = AMETLIV2BW34DM;
DMOutput(i,36) = AMETLIVOTHERBW34DM;
DMOutput(i,37) = AMETTCABW34DM;
DMOutput(i,38) = AMETTCOHTCABW34DM;
DMOutput(i,39) = AMETTCOHLUCBW34DM;
DMOutput(i,40) = AMETTCOHOTHERBW34DM;
DMOutput(i,41) = max(_ckid);
DMOutput(i,42) = max(_cdcvg_mmole);
DMOutput(i,43) = AUCCKIDDM;
DMOutput(i,44) = AUCCDCVG_MMOLEDm;
DMOutput(i,45) = AMETKIDVKIDDM;
DMOutput(i,46) = AMETDCVG_MMOLVVKIDDM;
DMOutput(i,47) = AMETKIDBW34DM;
DMOutput(i,48) = AMETDCVG_MMOLVKBW34DM;
```

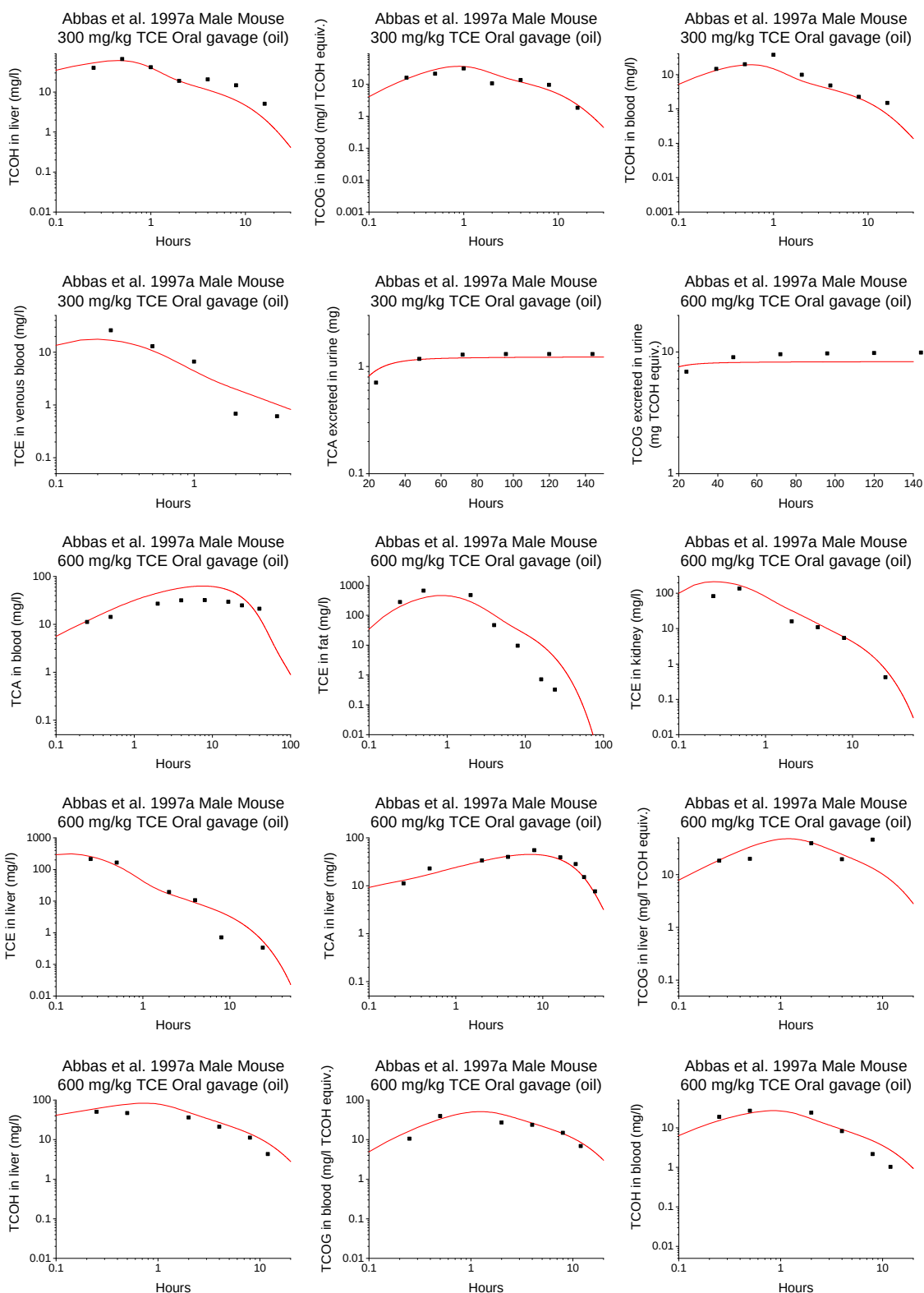

APPENDIX F

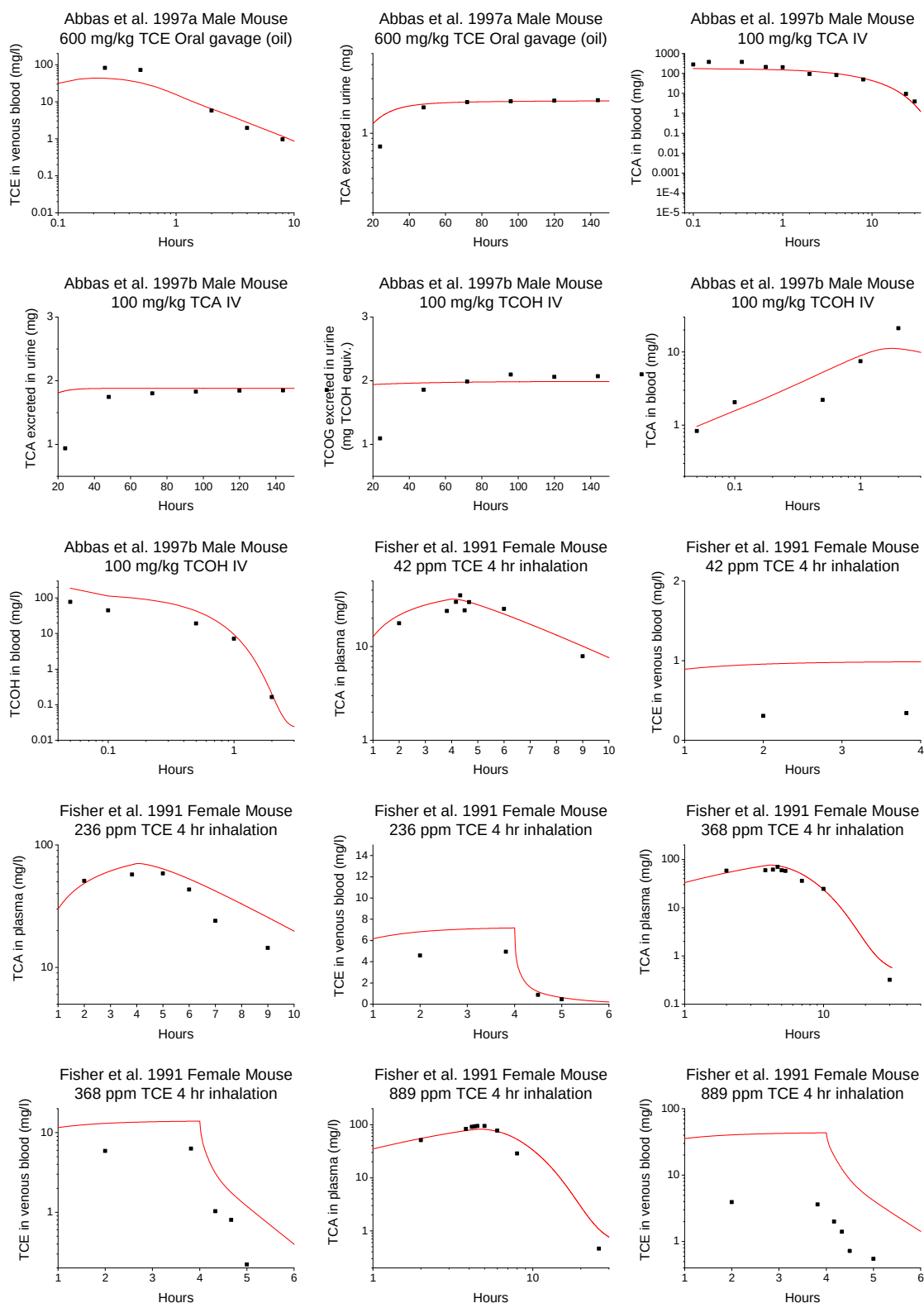
Mouse Validation Figures

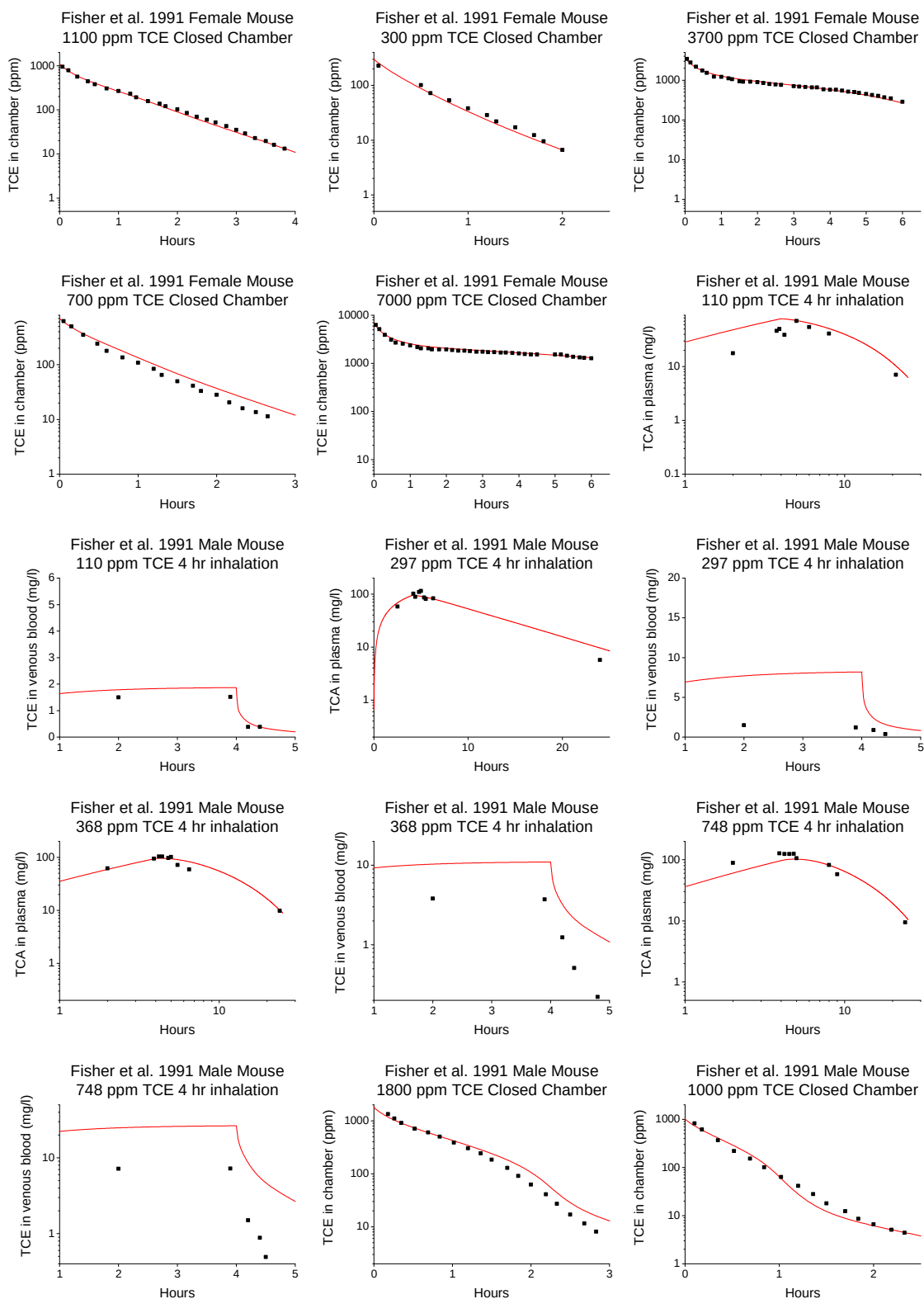
Mouse figures correspond to Figure A-31 in Appendix A of USEPA [1]. Red lines represent model simulations using the study-specific posterior parameter values. Citations for the original studies for these data are in Section 9.0 of the main report.

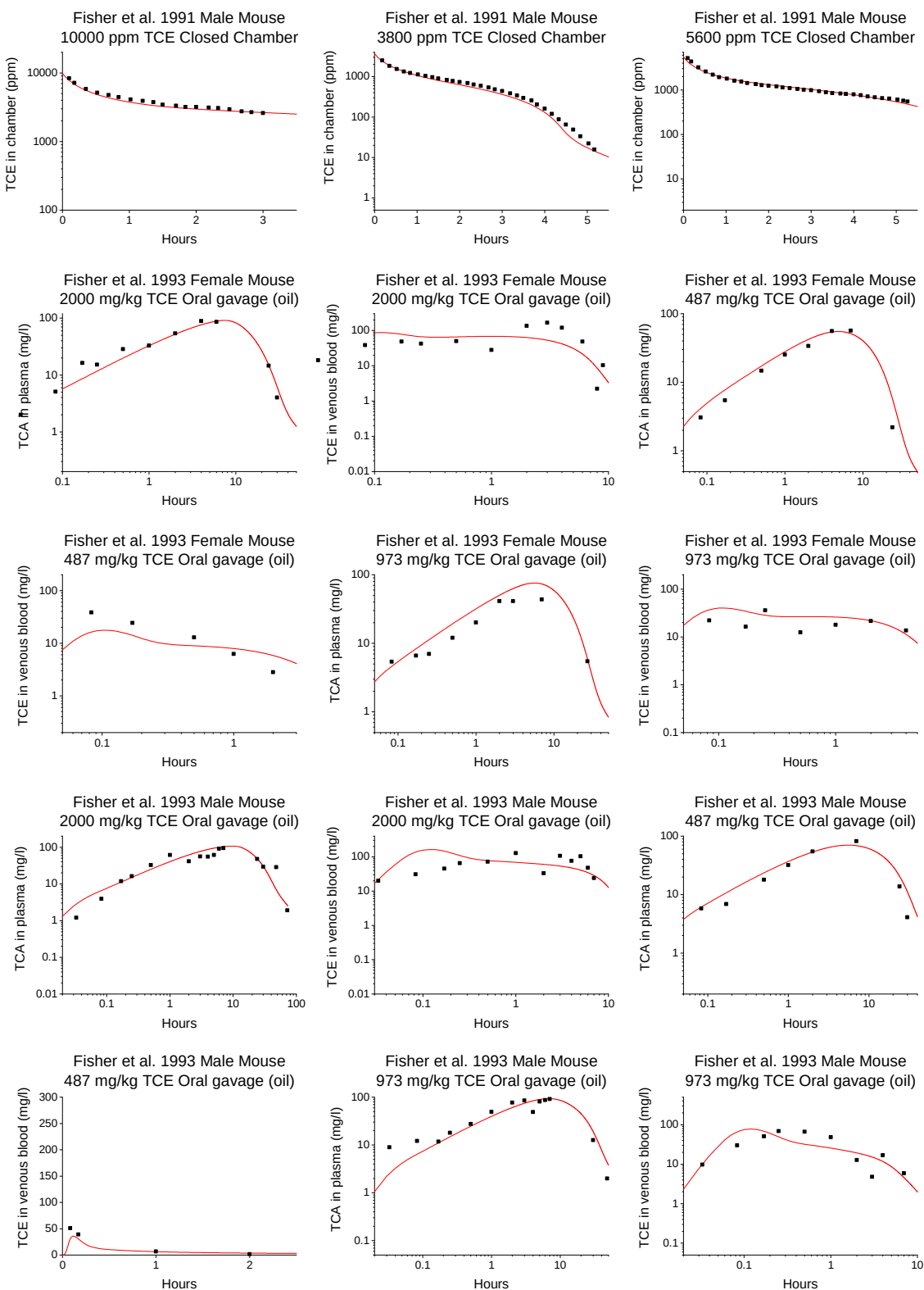


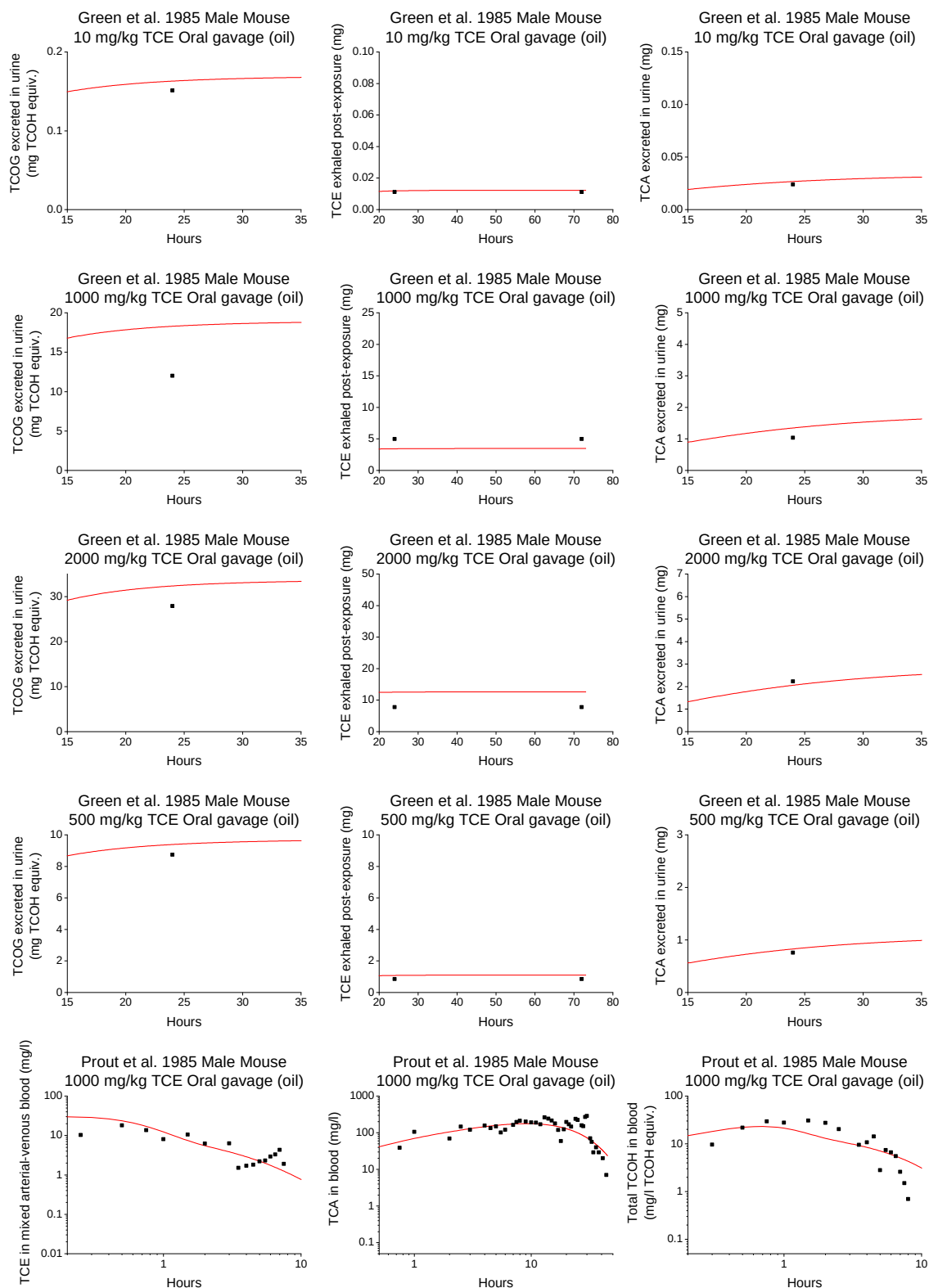


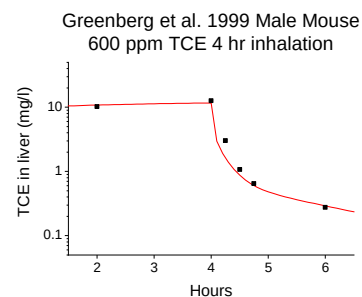
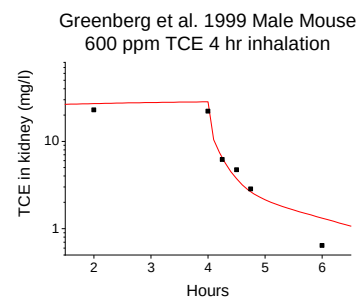
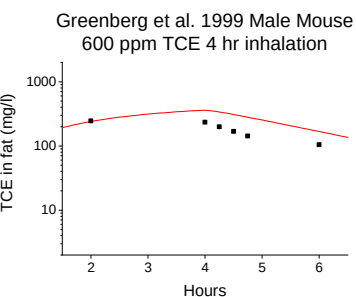
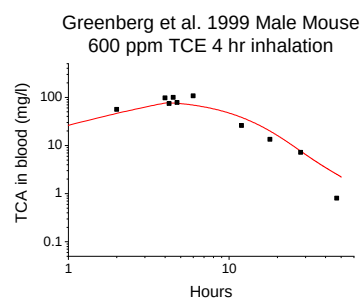
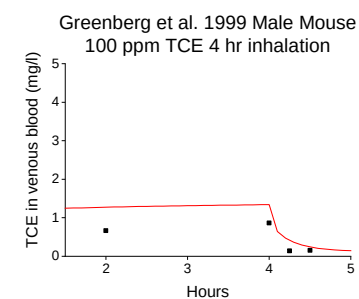
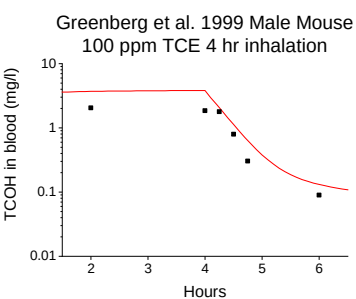
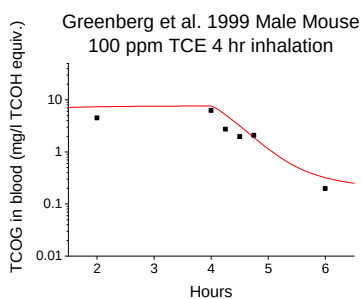
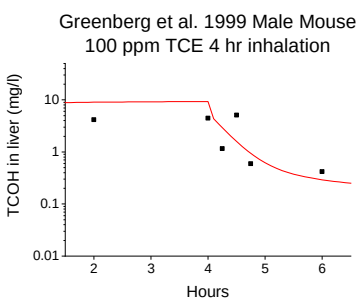
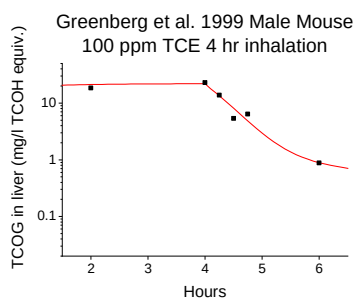
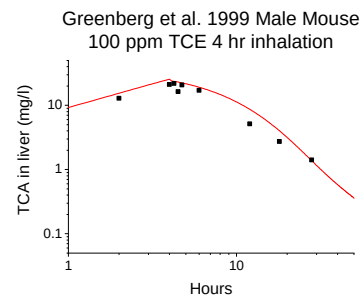
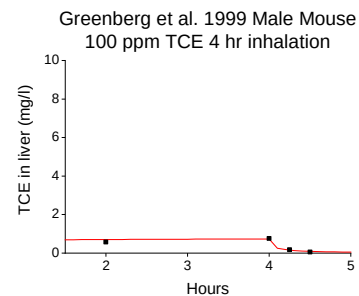
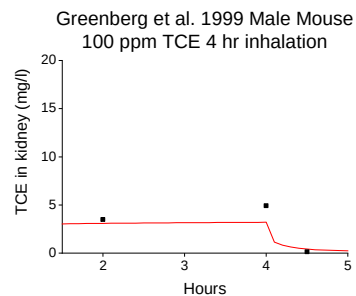
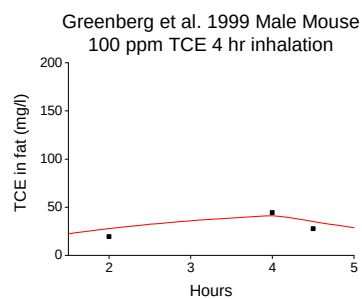
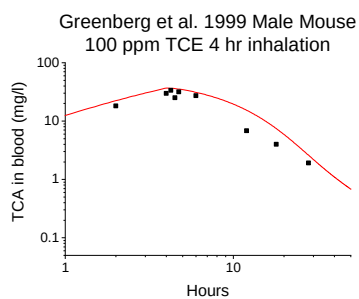
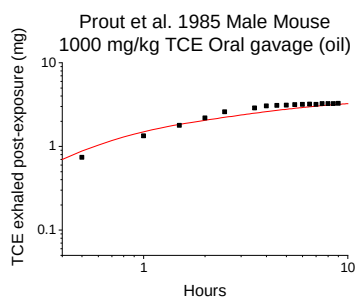


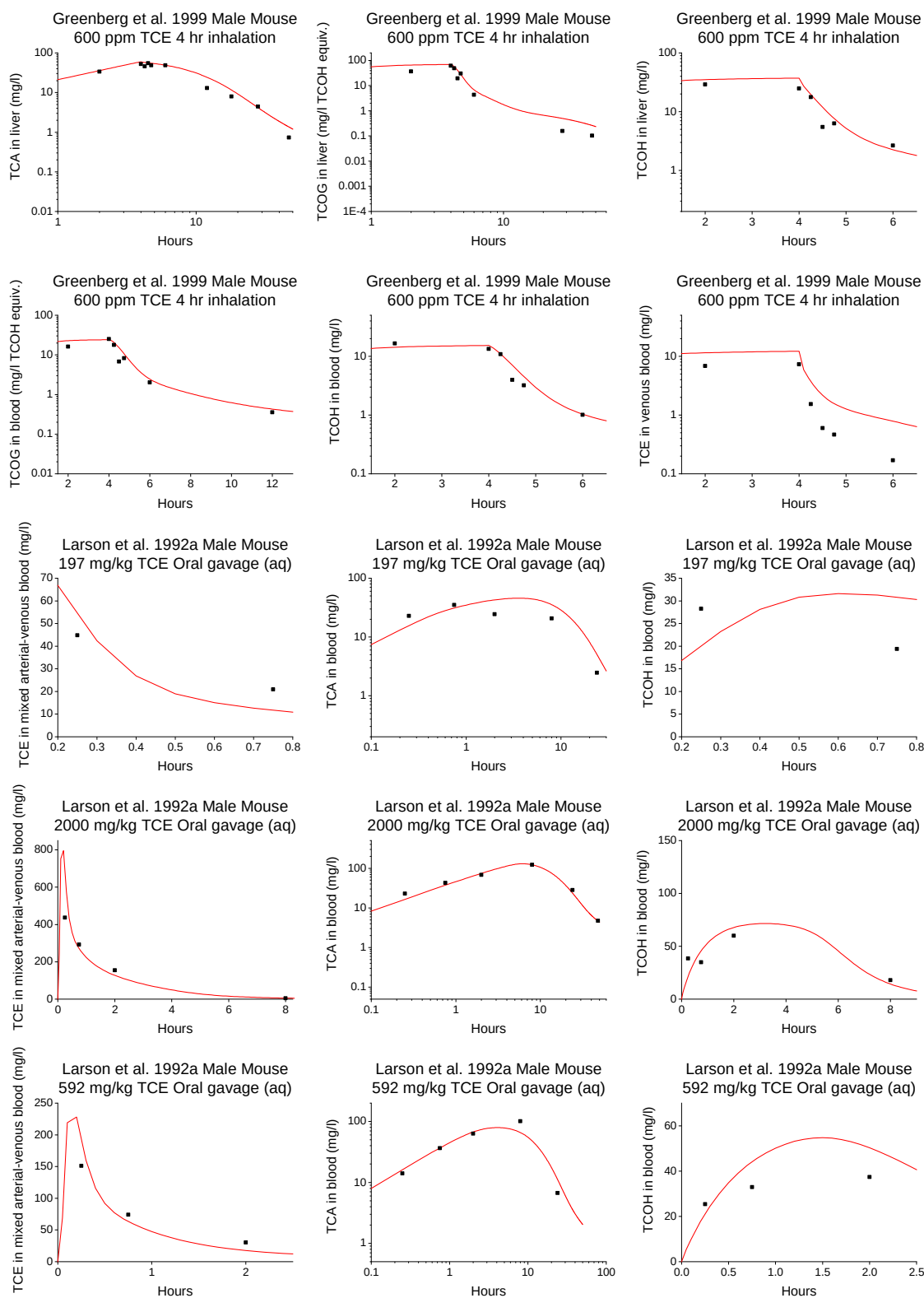


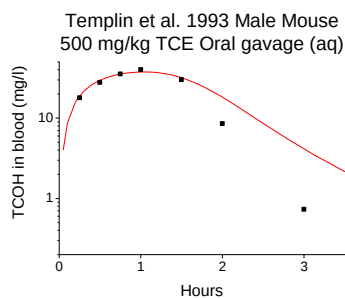
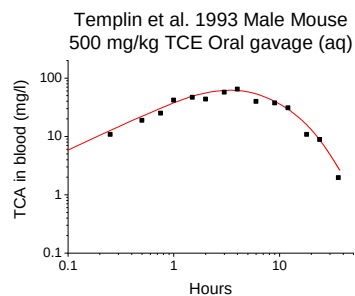
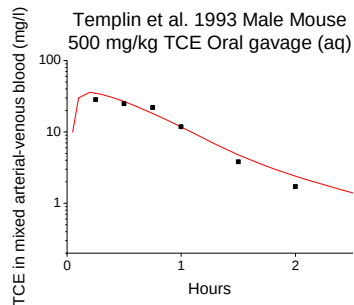
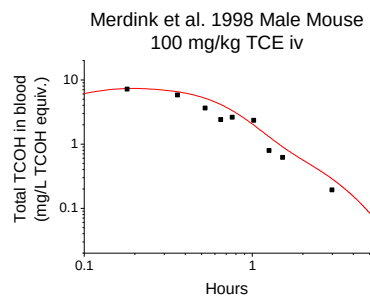
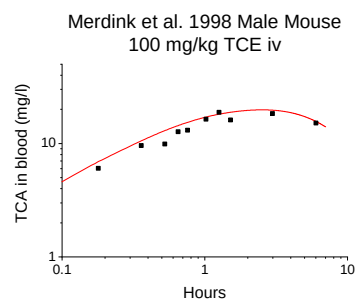
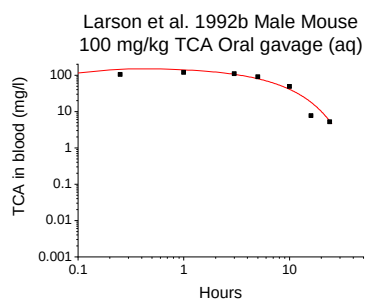
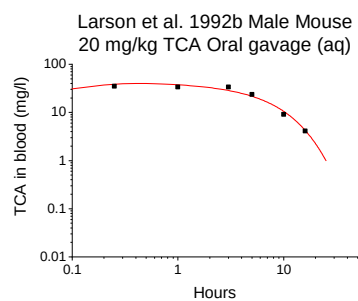












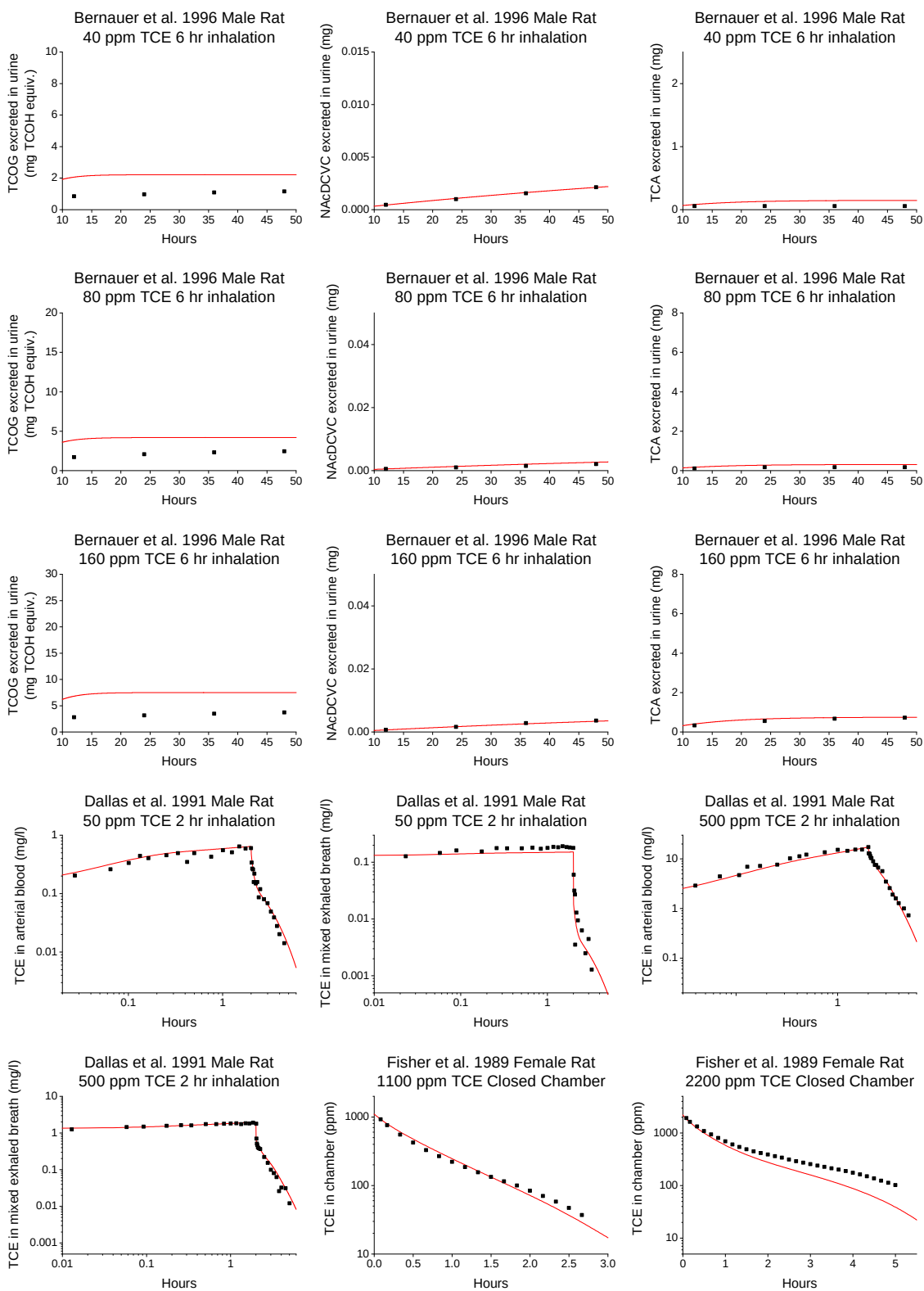
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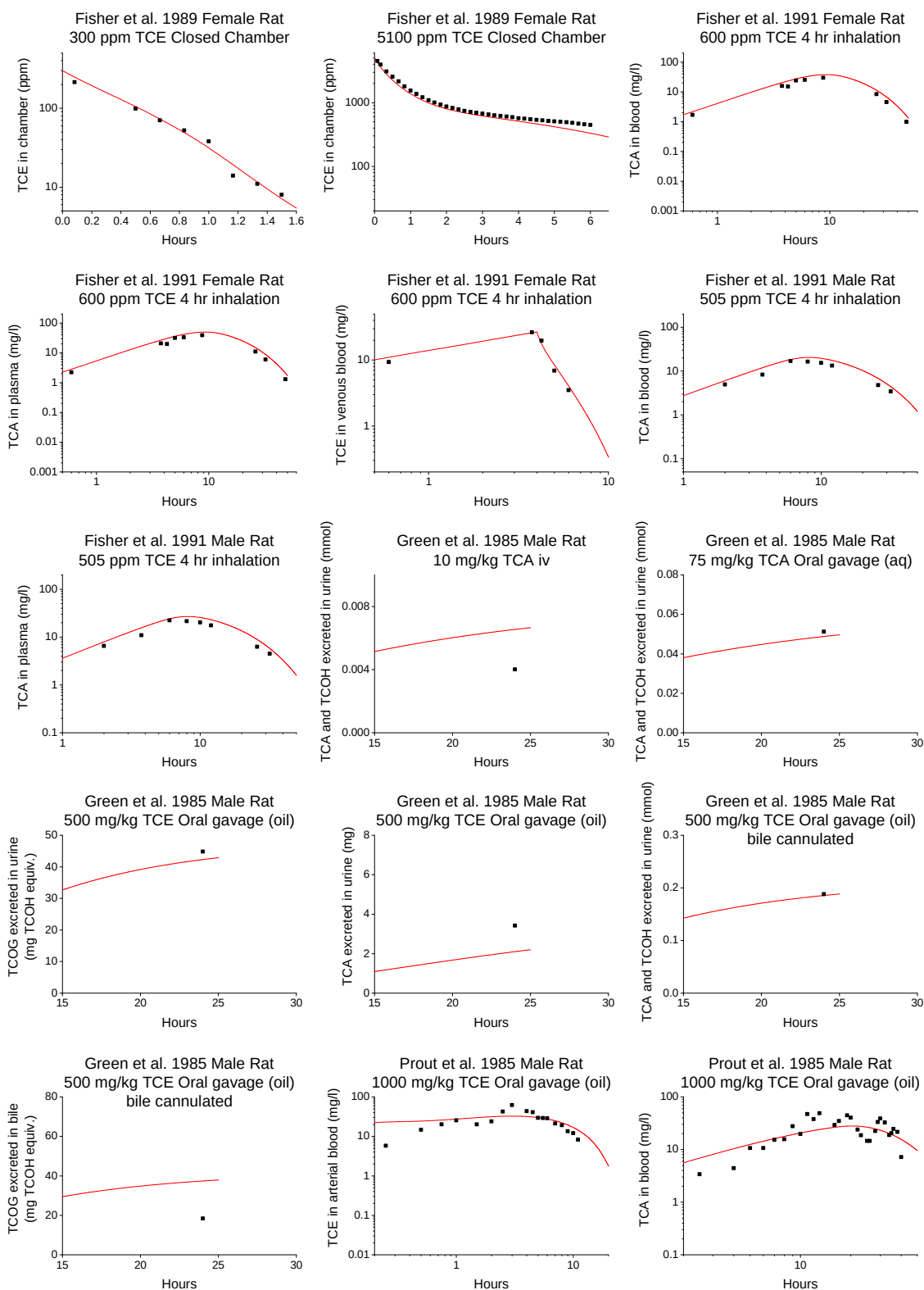
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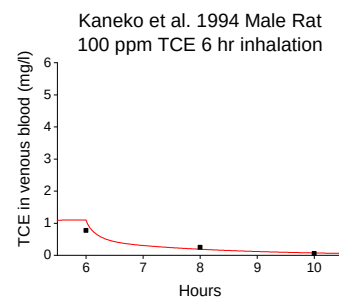
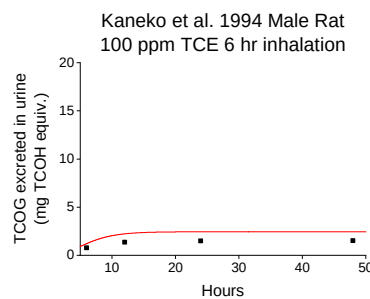
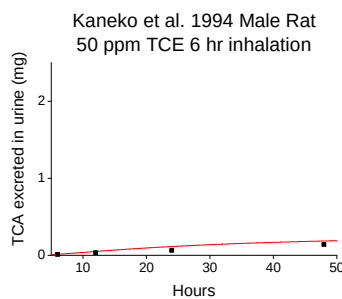
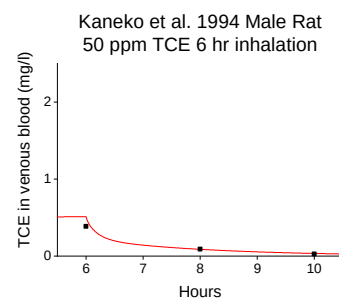
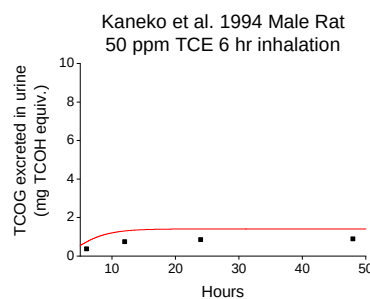
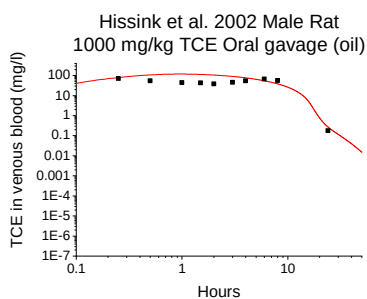
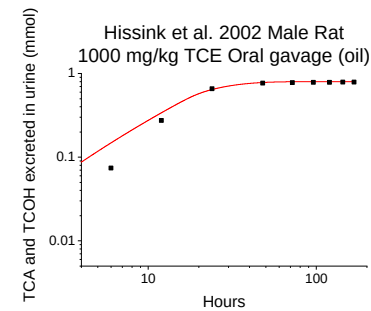
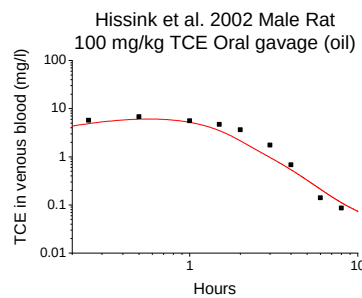
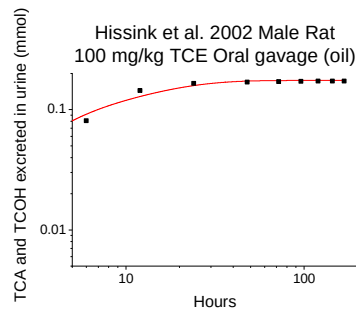
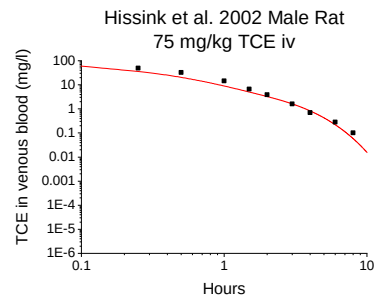
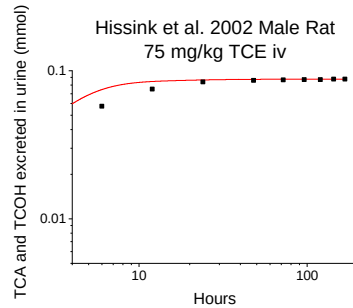
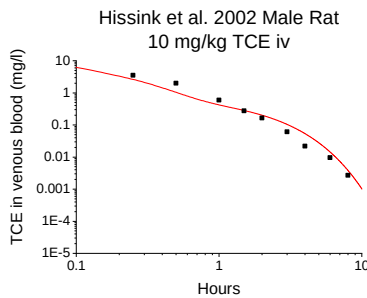
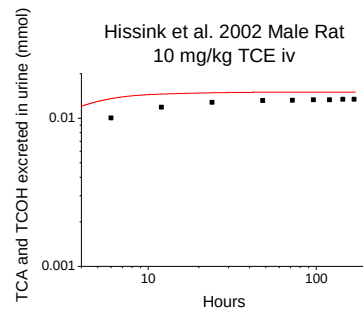
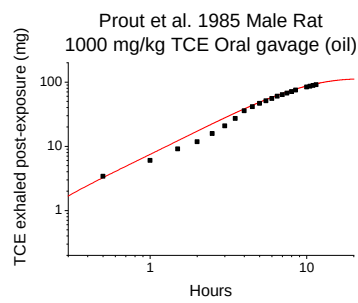
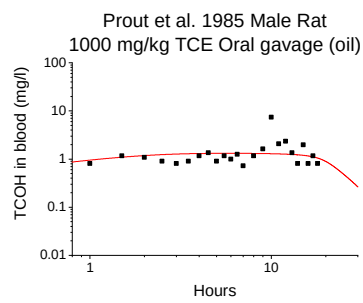
APPENDIX G

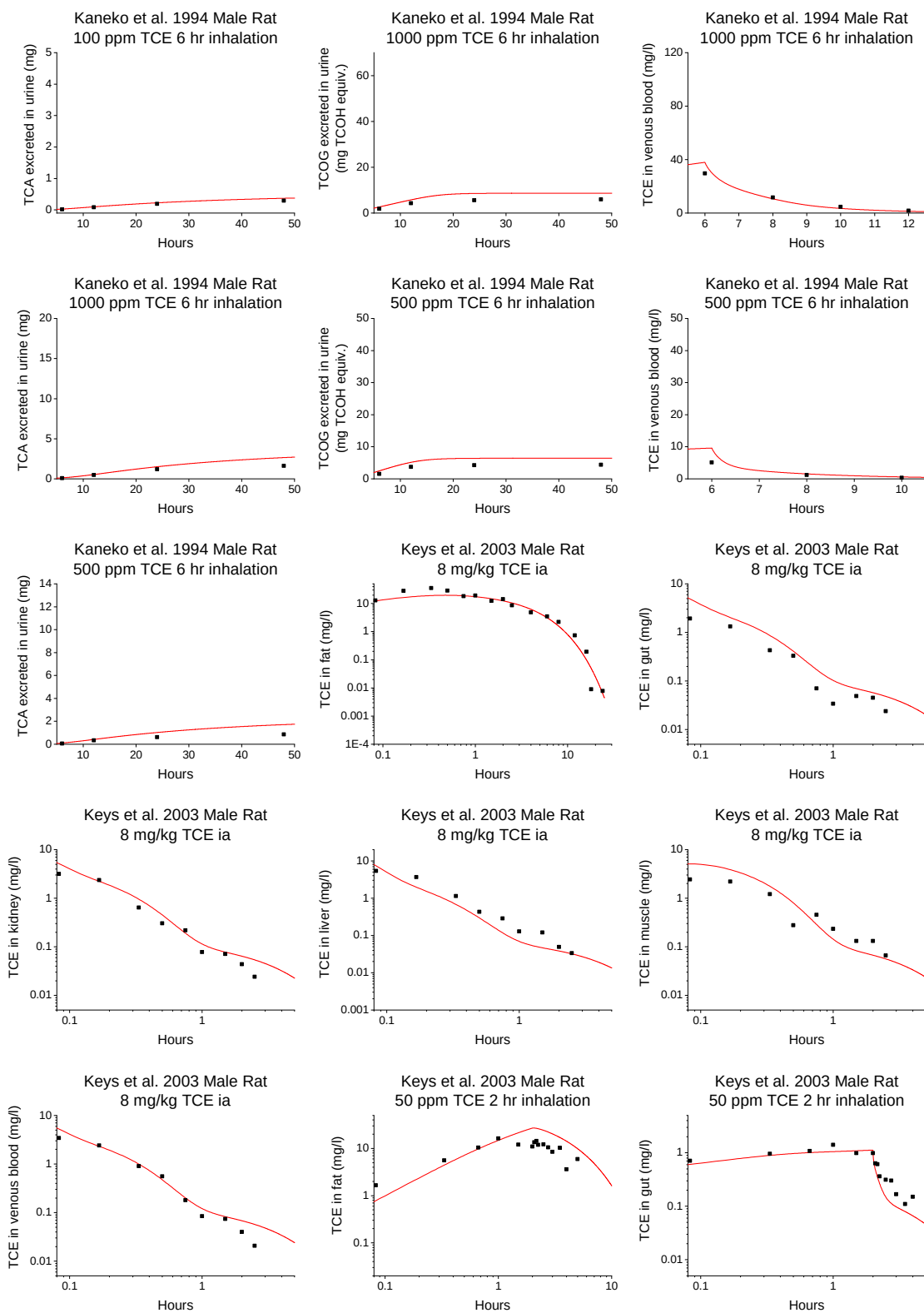
Rat Validation Figures

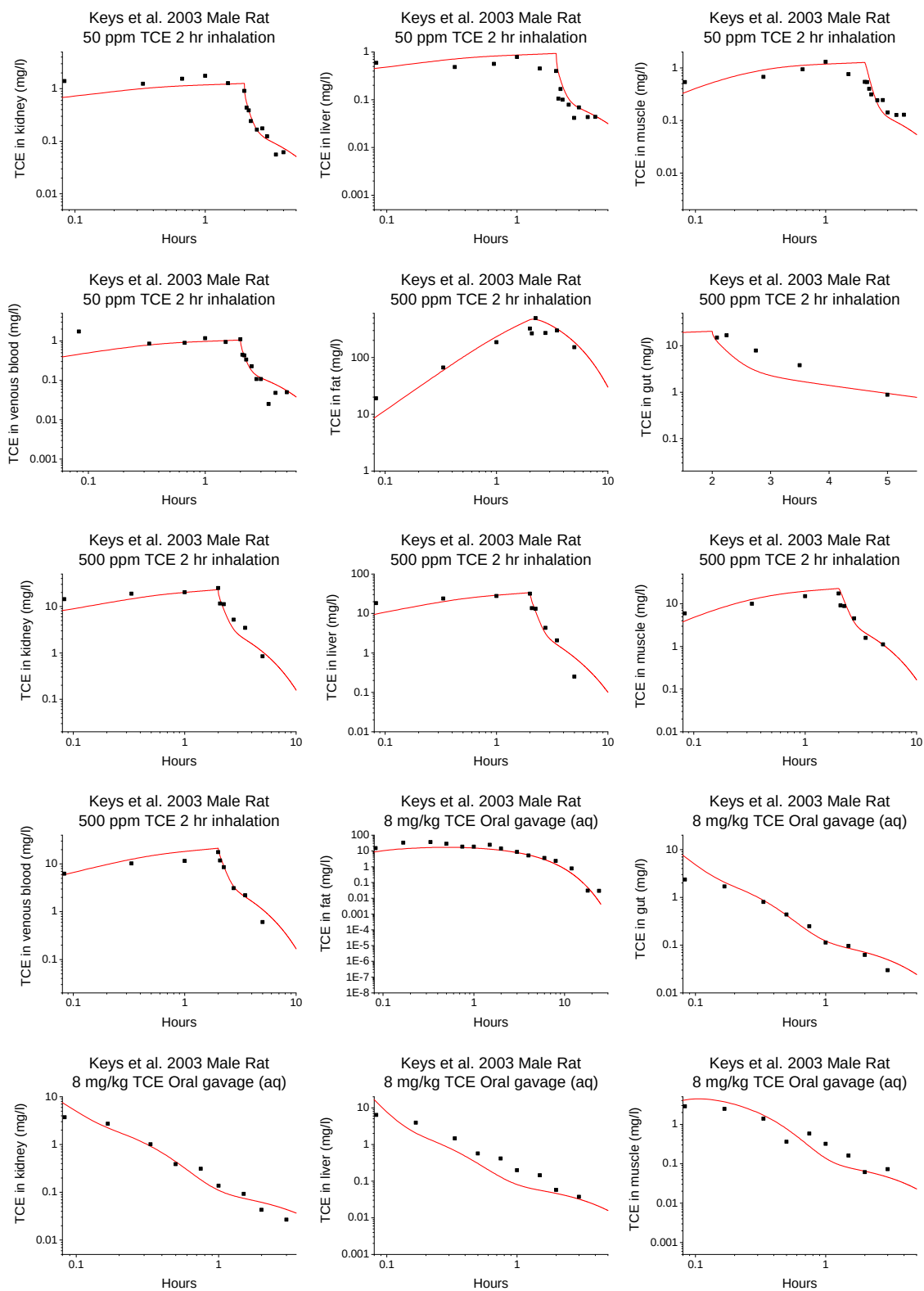
Rat figures correspond to Figure A-32 in Appendix A of USEPA [1]. Red lines represent model simulations using the study-specific posterior parameter values. Citations for the original studies are in Section 9.0 of the main report.

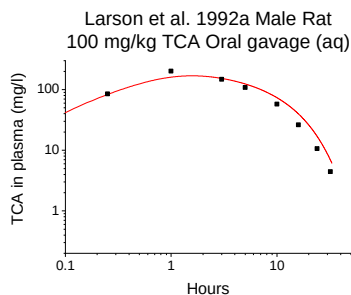
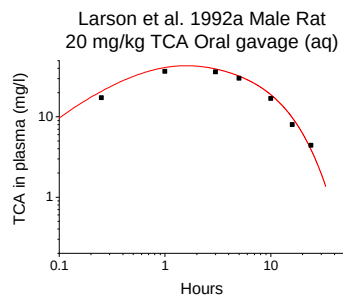
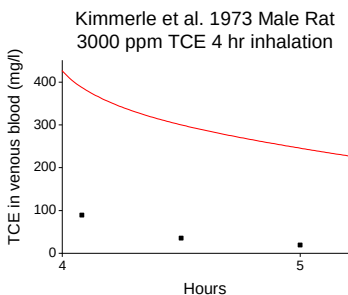
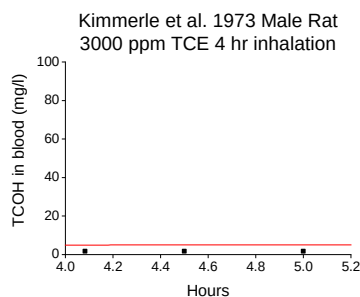
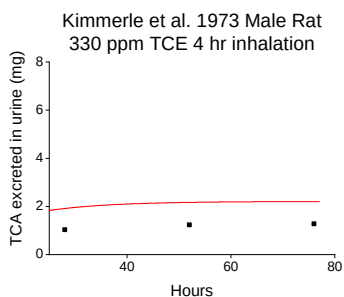
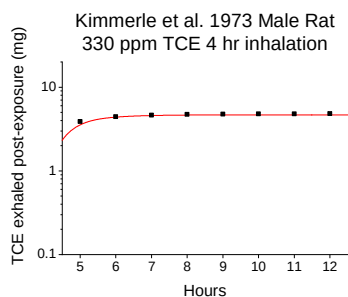
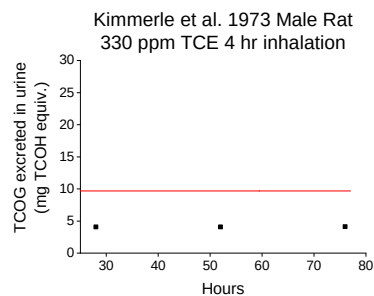
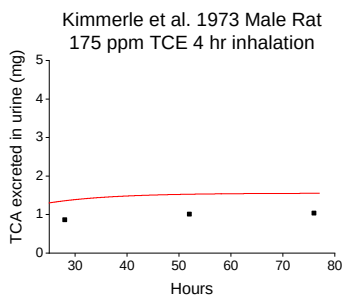
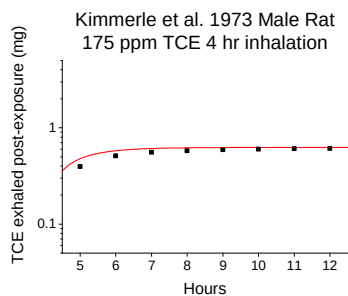
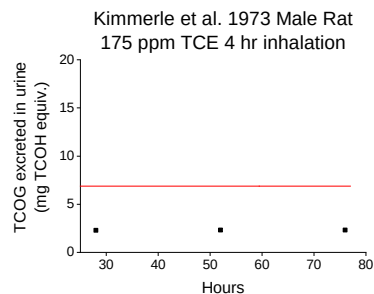
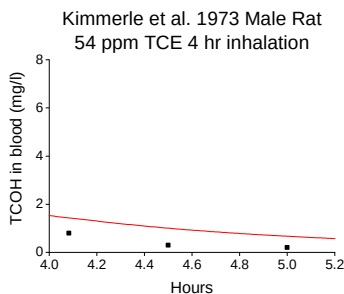
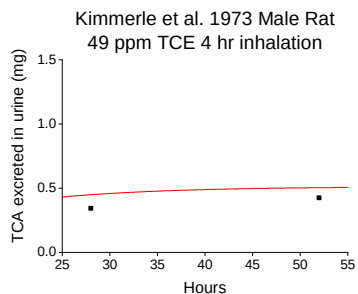
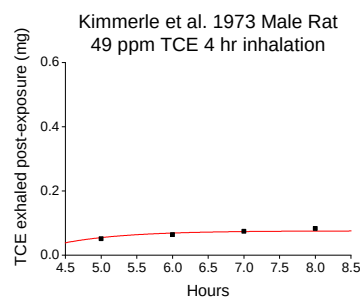
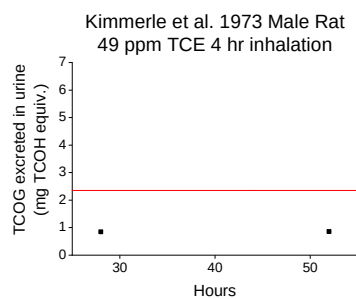
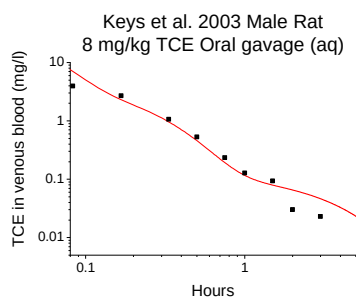


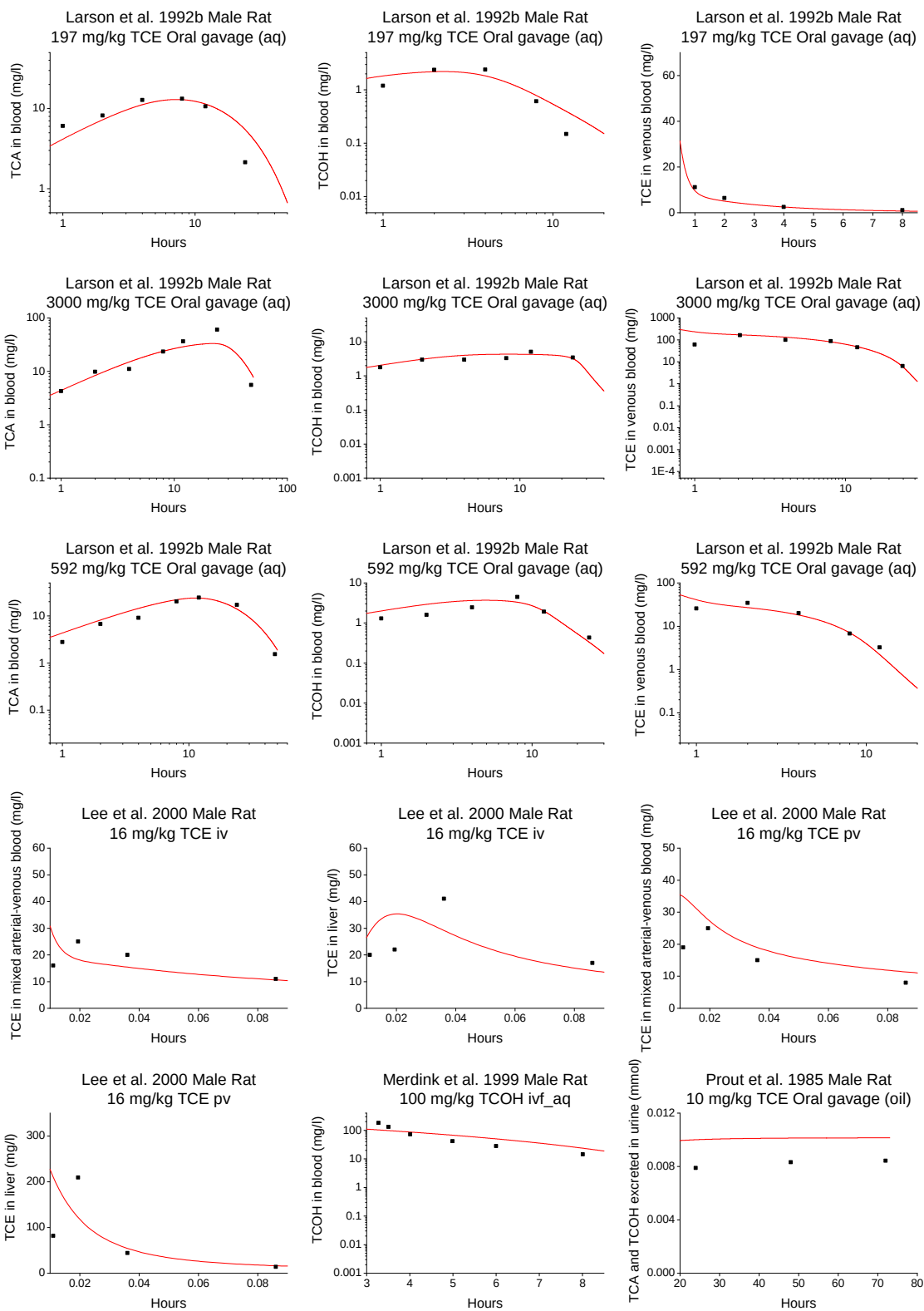


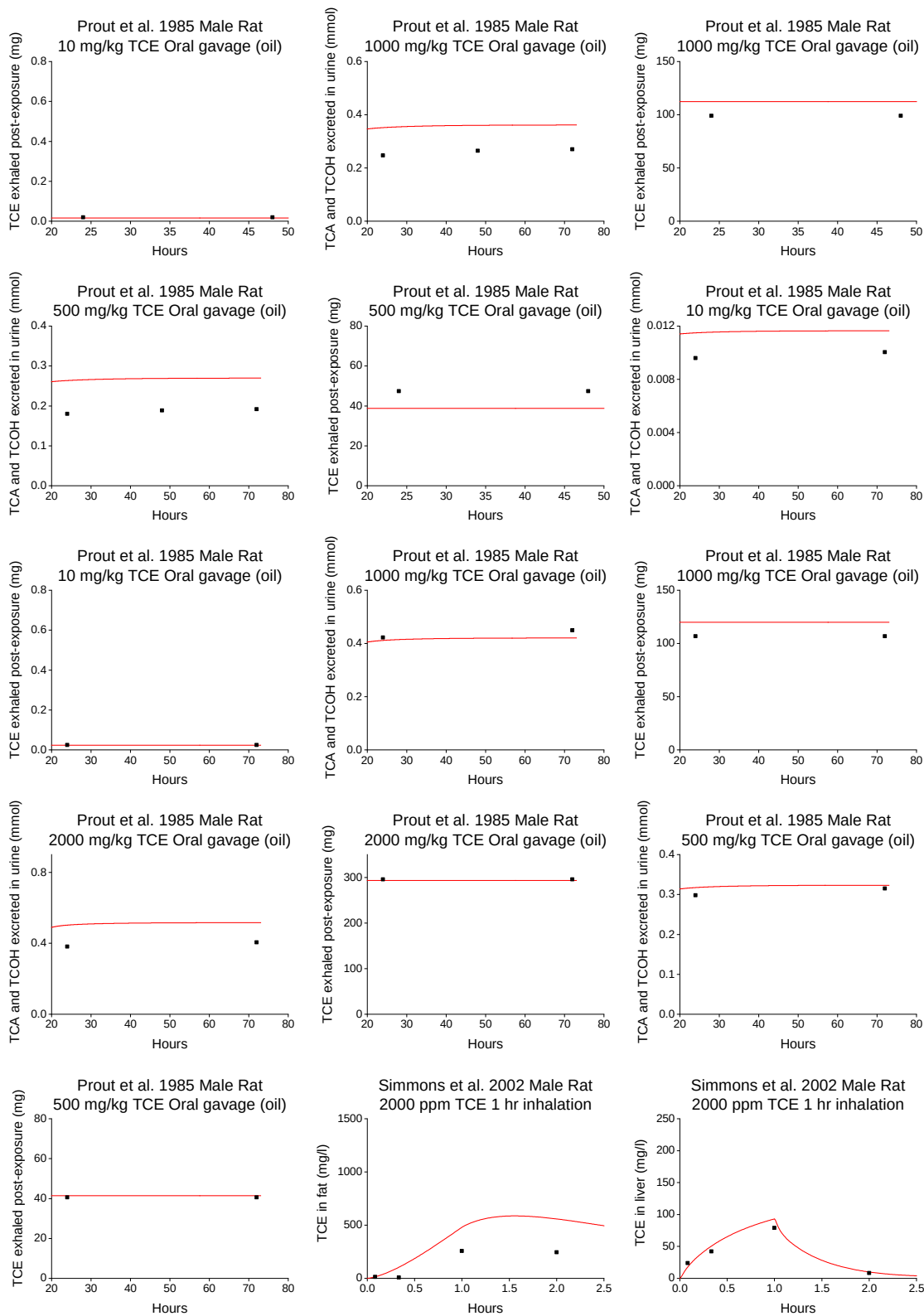


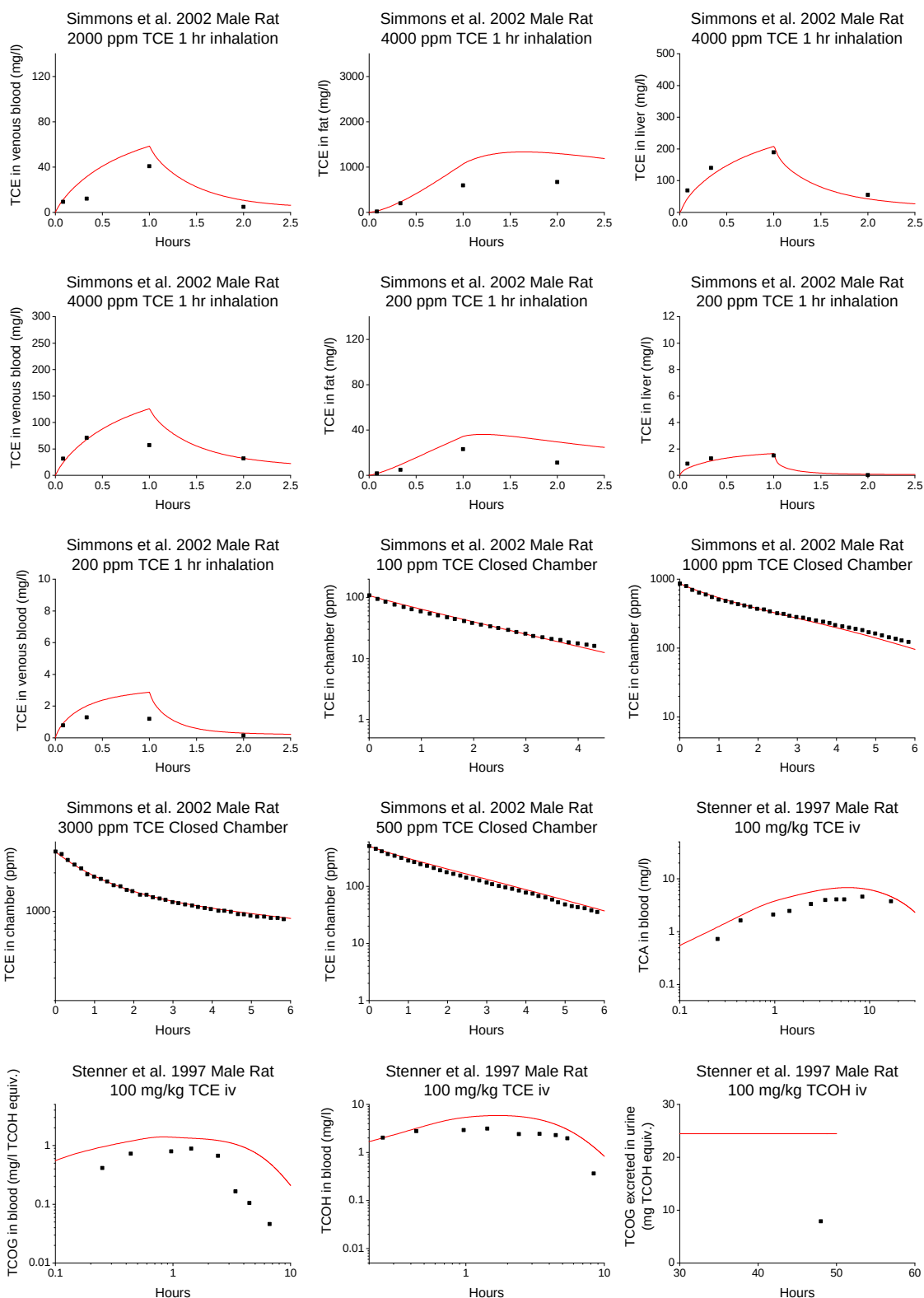


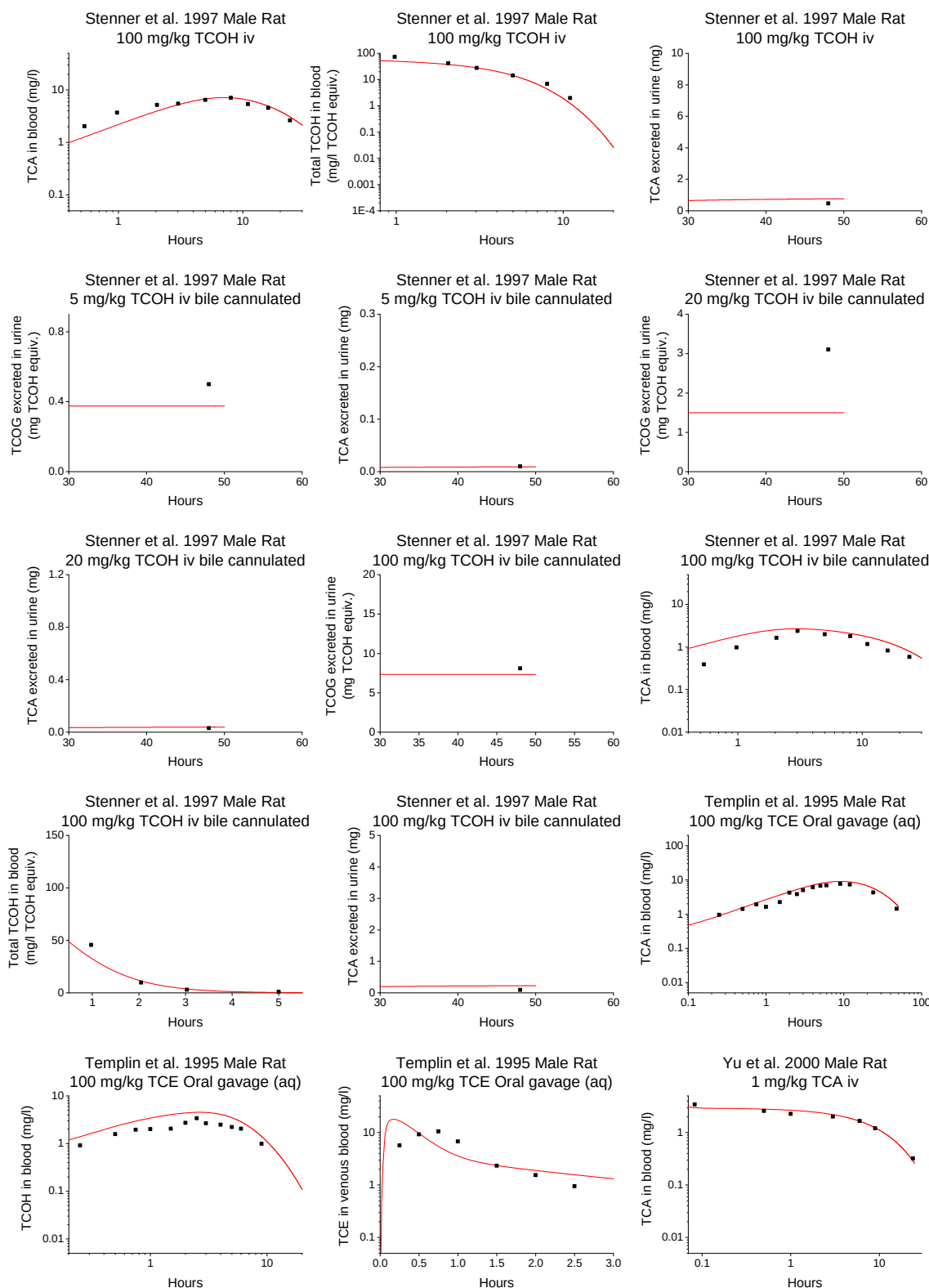


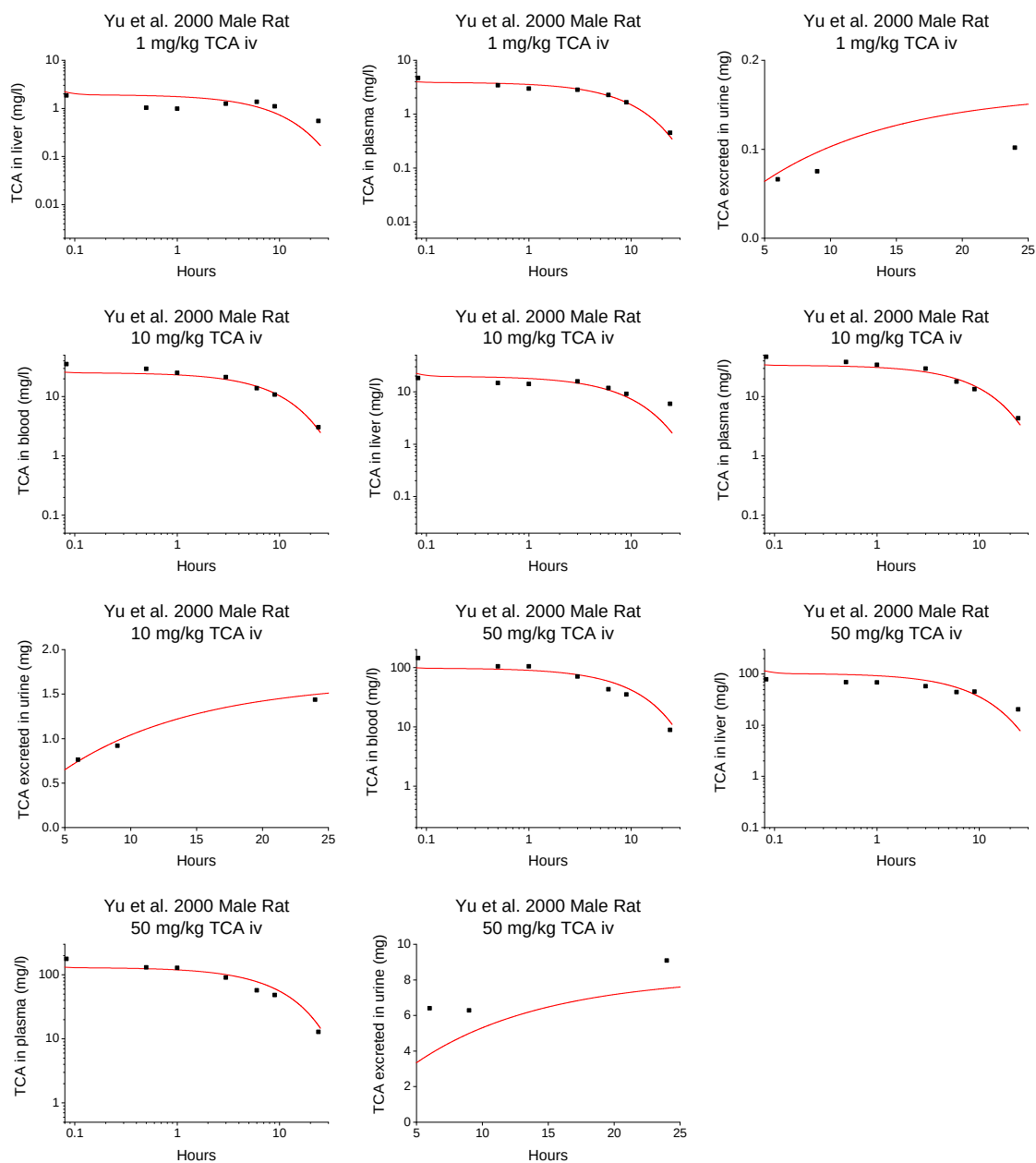












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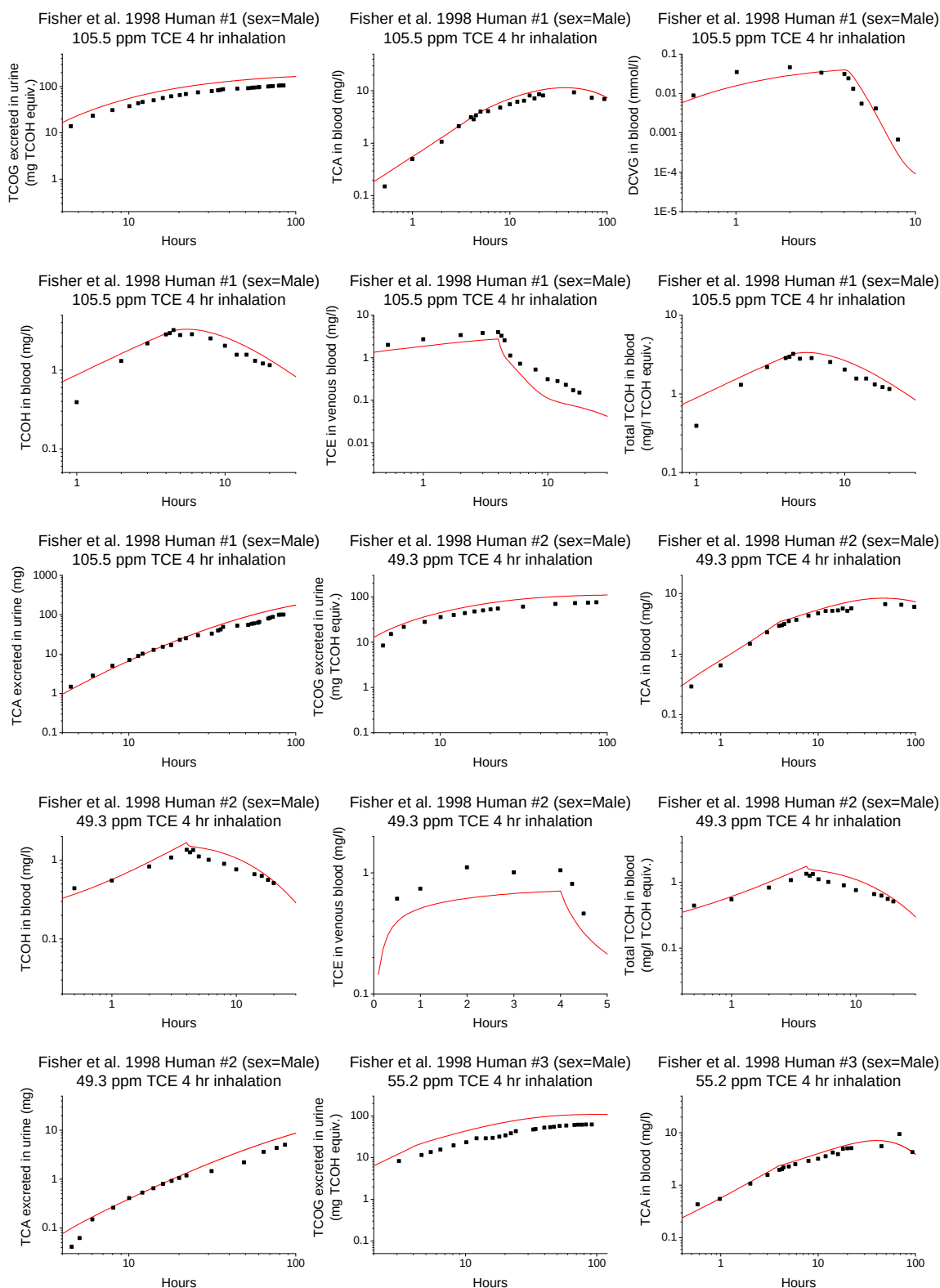
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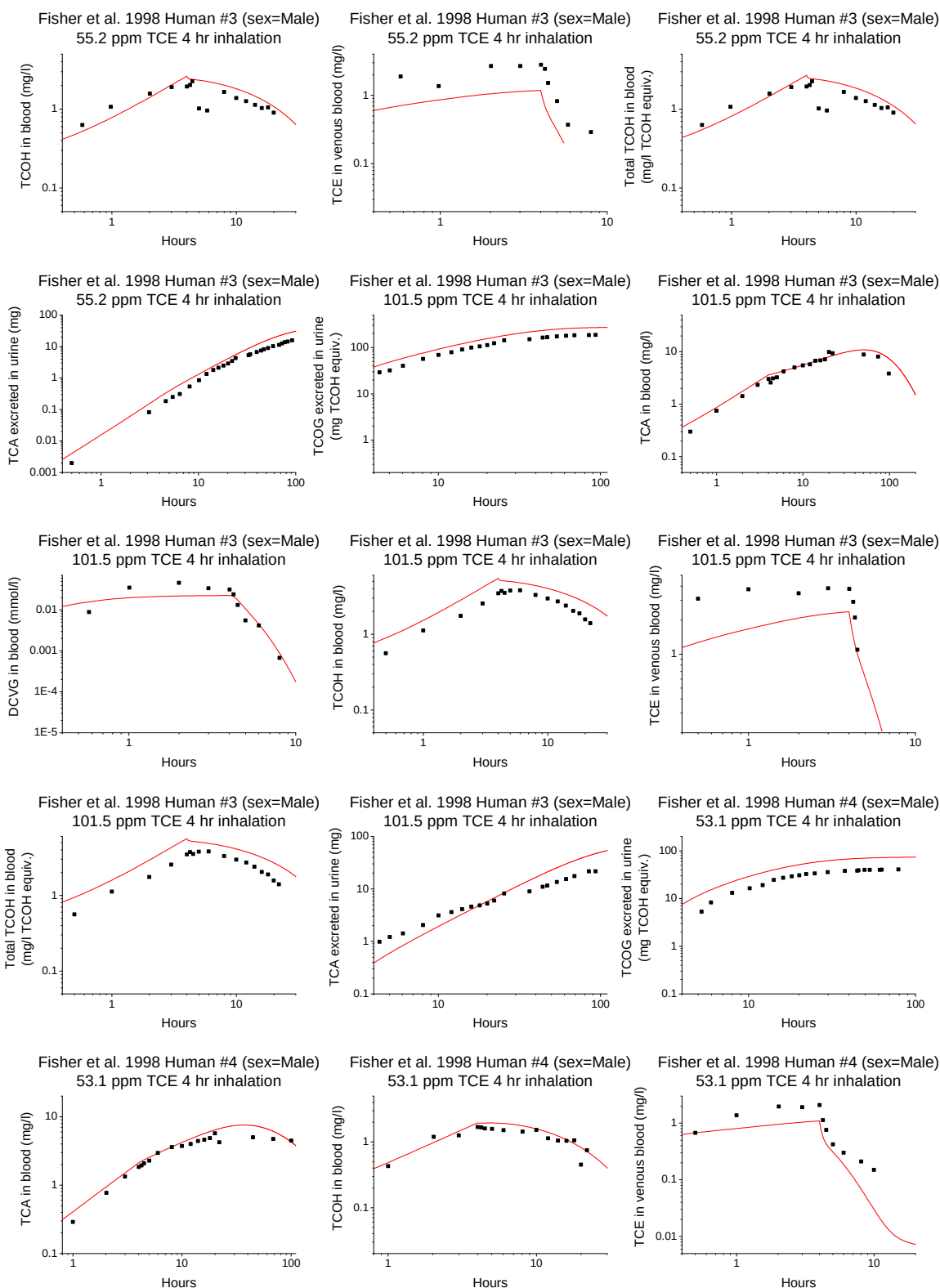
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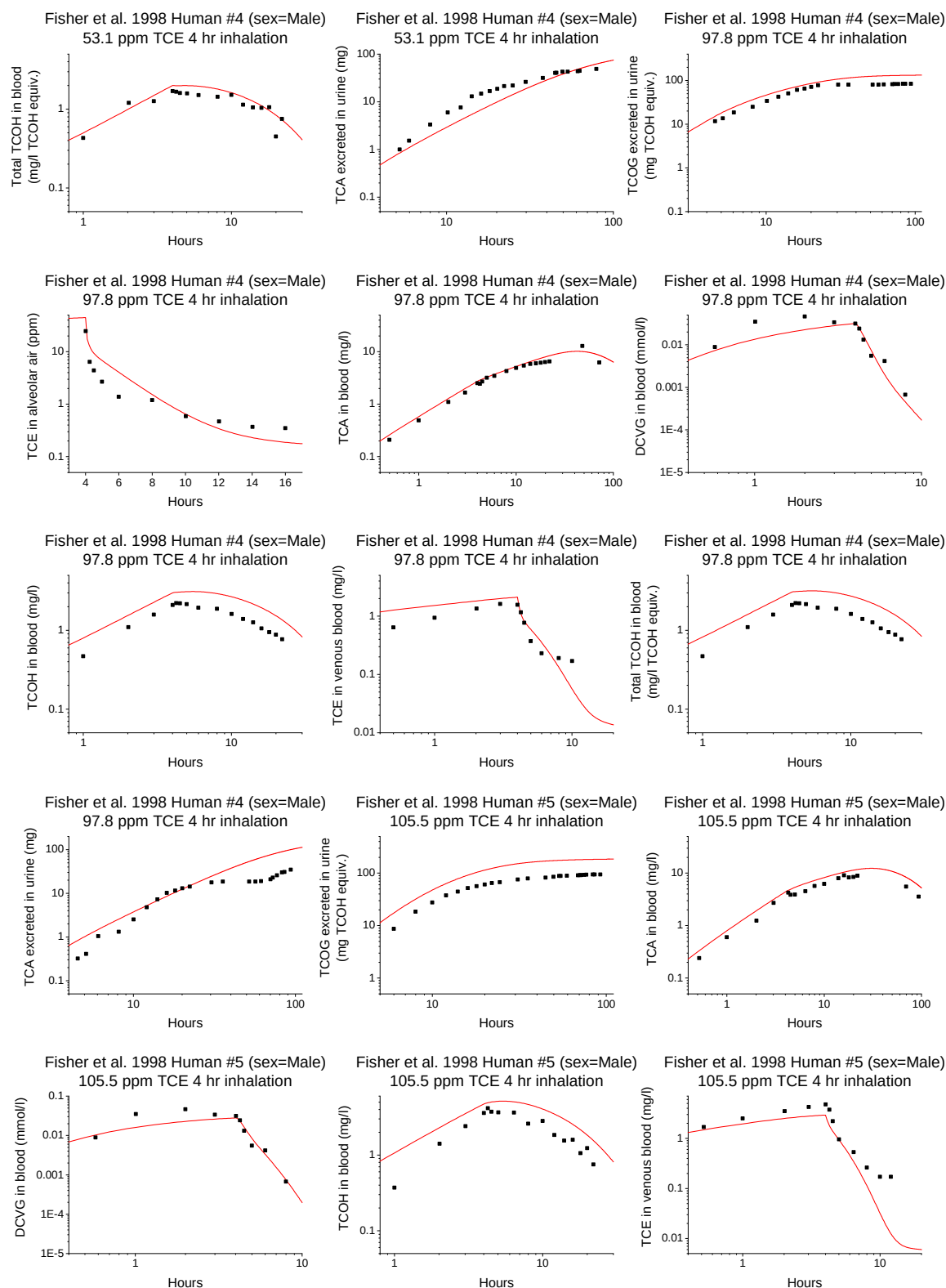
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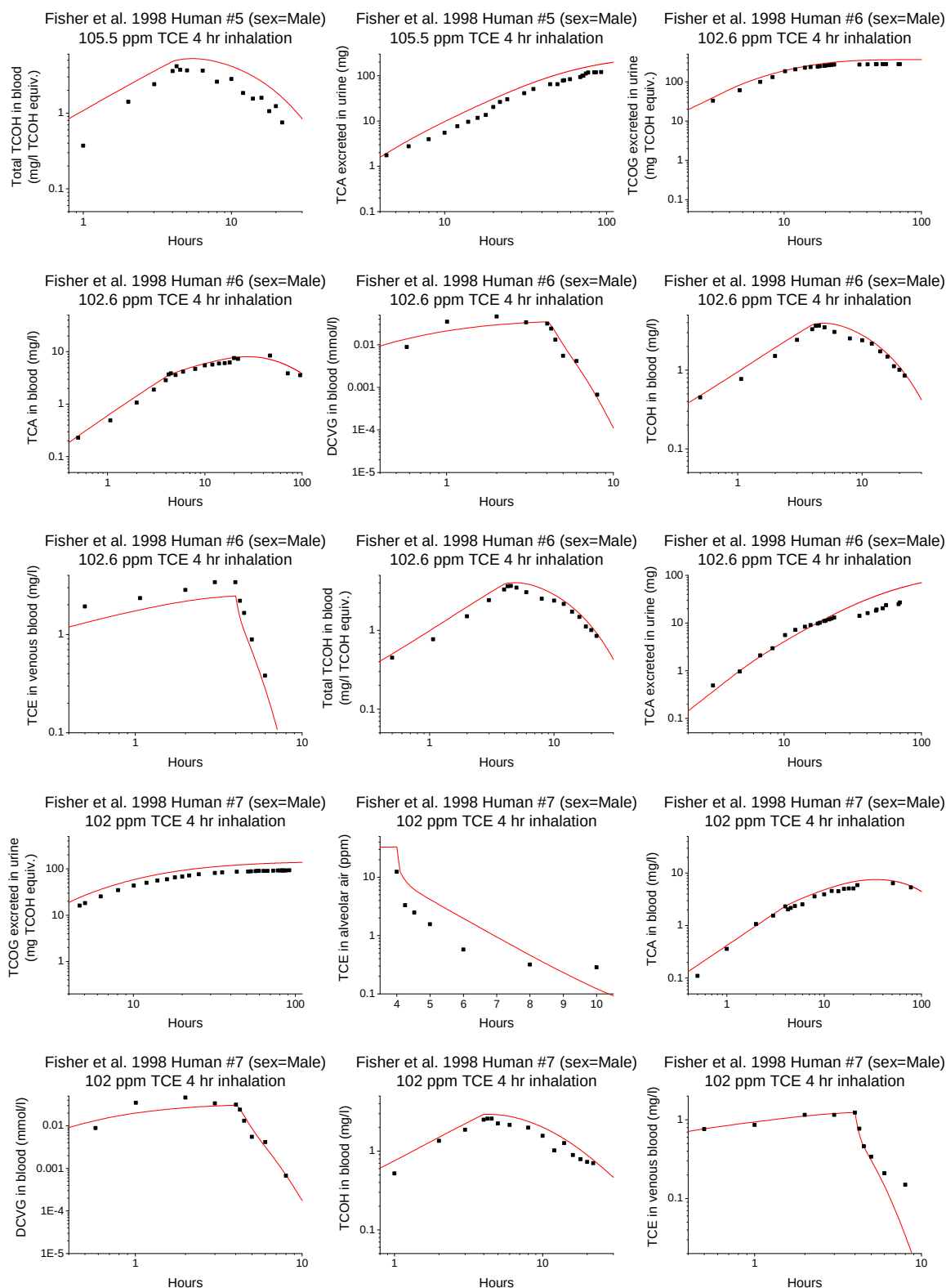
Human Validation Figures

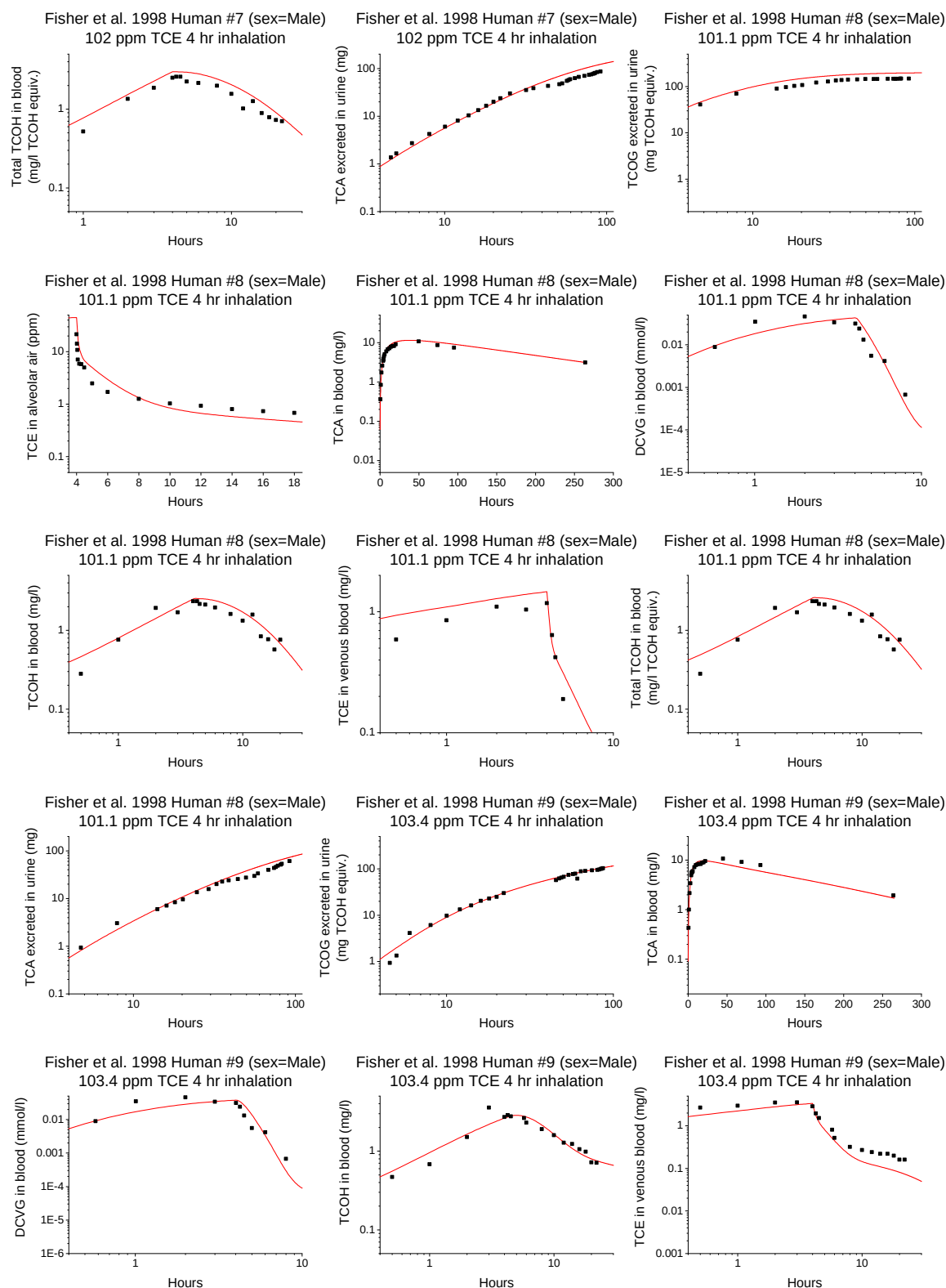
Human figures correspond to Figure A-33 in Appendix A of USEPA [1]. Red lines represent model simulations using the study- and subject-specific posterior parameter values. Citations for the original studies are in Section 9.0 of the main report.

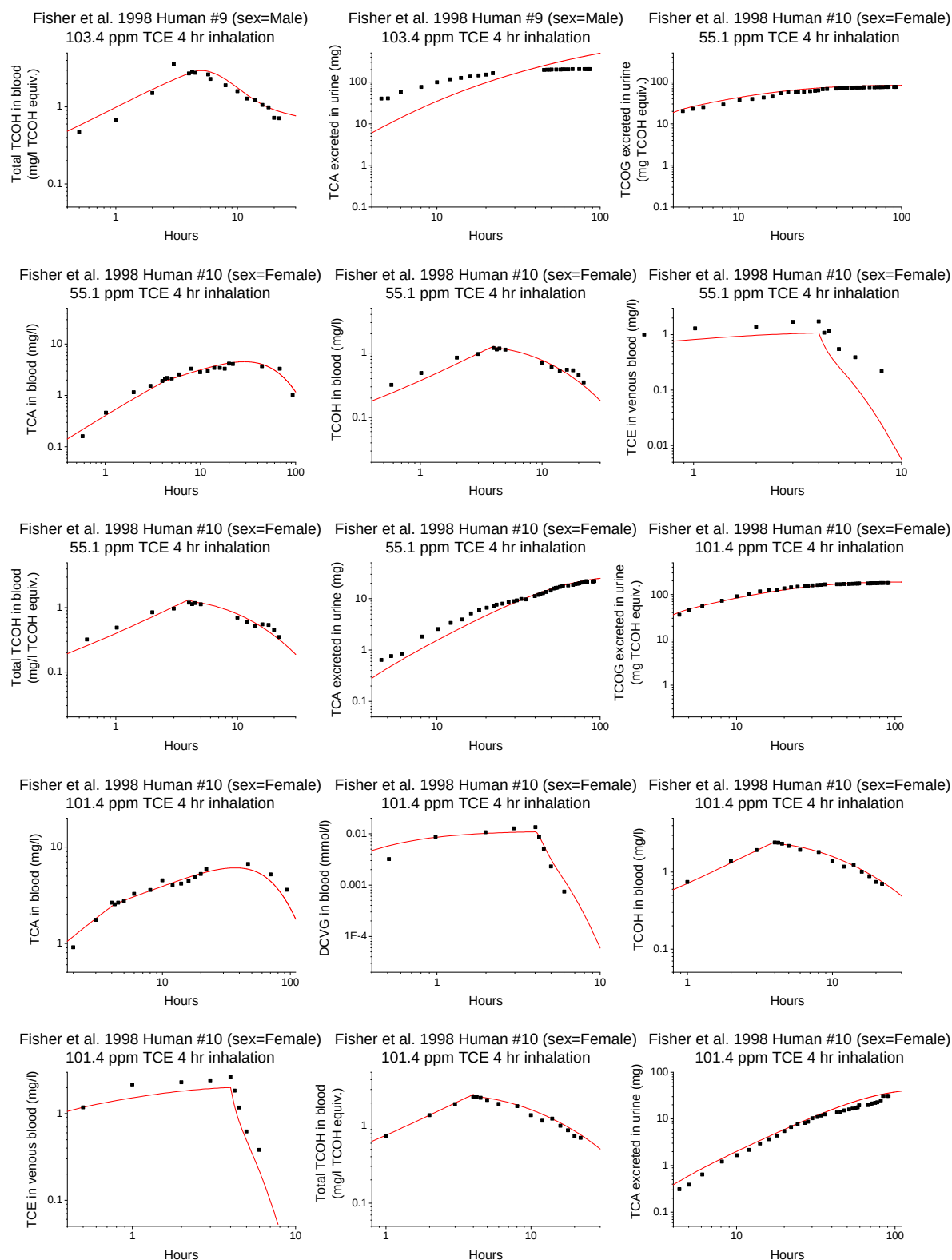


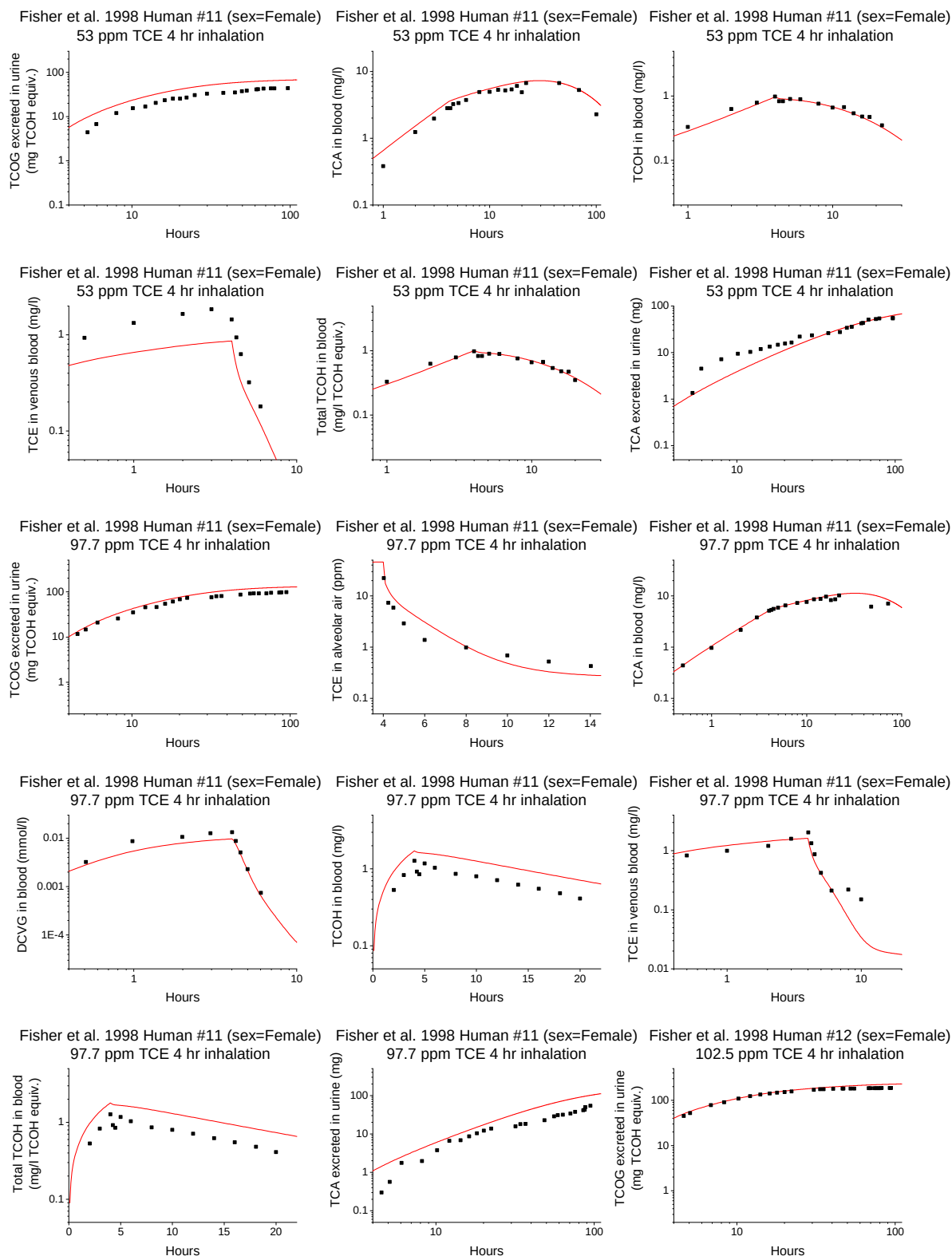




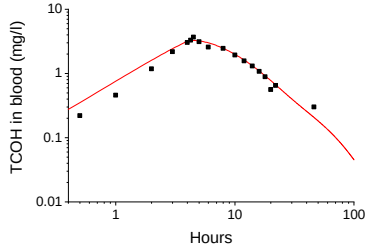
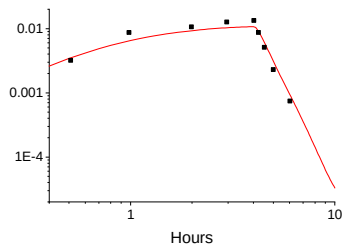
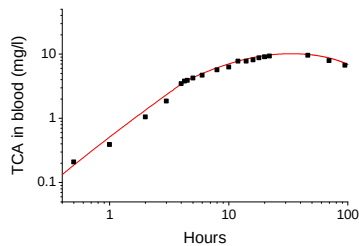




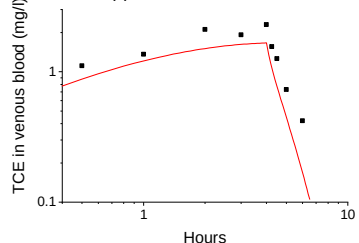




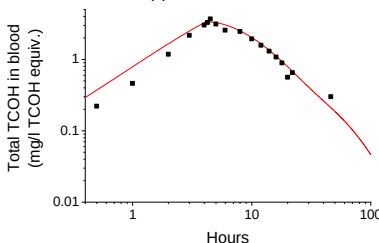
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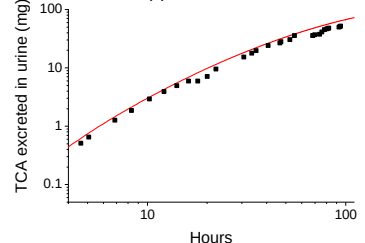
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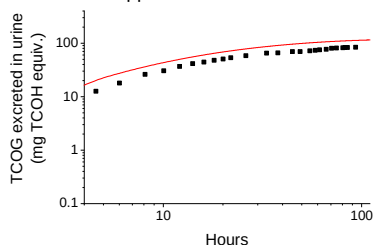
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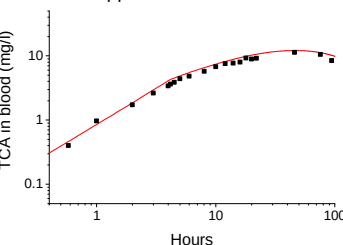
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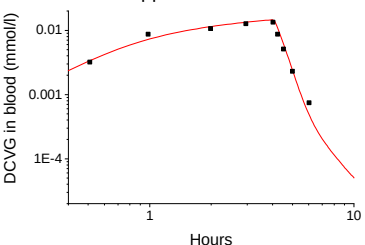
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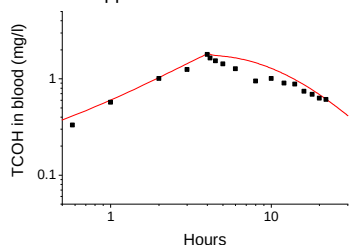
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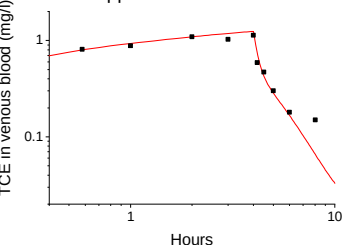
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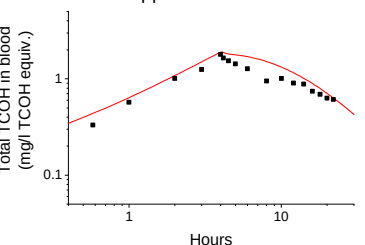
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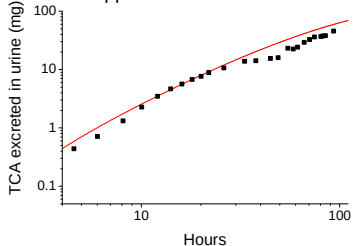
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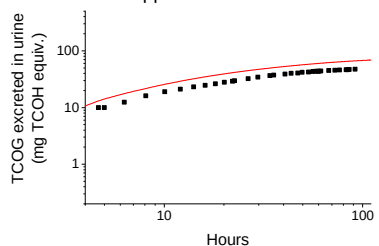
Fisher et al. 1998 Human #13 (sex=Female) 102 ppm TCE 4 hr inhalation



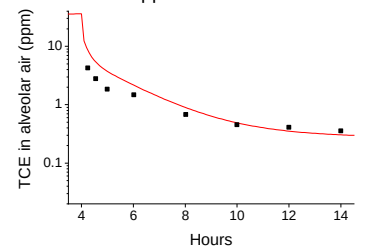
Fisher et al. 1998 Human #13 (sex=Female) 102 ppm TCE 4 hr inhalation



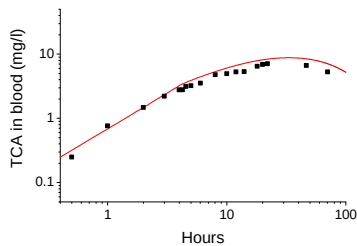
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



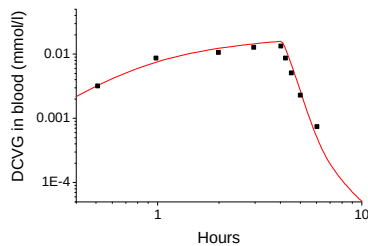
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



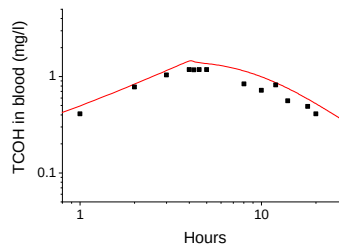
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



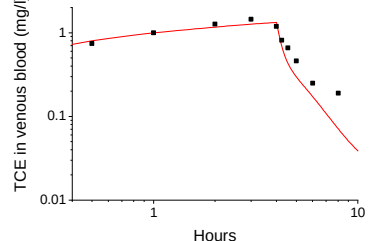
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



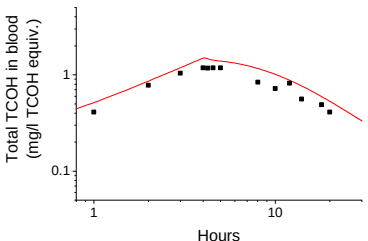
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



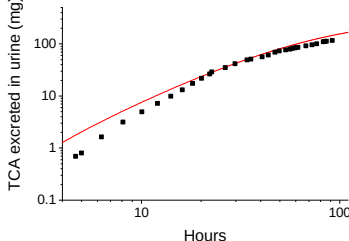
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



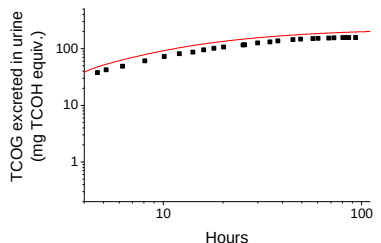
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



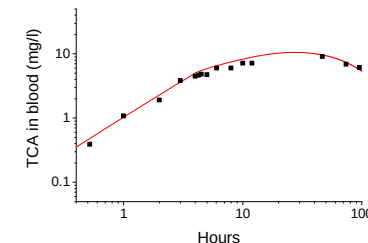
Fisher et al. 1998 Human #14 (sex=Female) 102 ppm TCE 4 hr inhalation



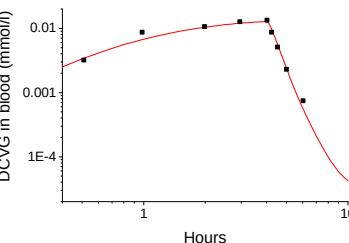
Fisher et al. 1998 Human #15 (sex=Female) 101 ppm TCE 4 hr inhalation



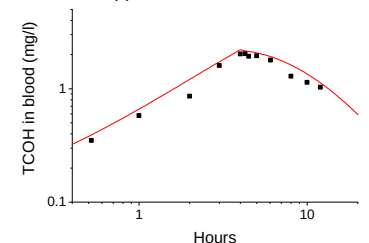
Fisher et al. 1998 Human #15 (sex=Female) 101 ppm TCE 4 hr inhalation



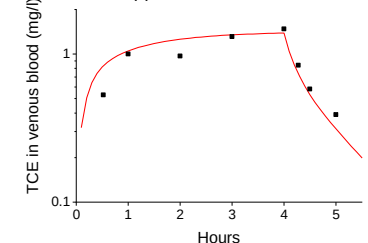
Fisher et al. 1998 Human #15 (sex=Female) 101 ppm TCE 4 hr inhalation



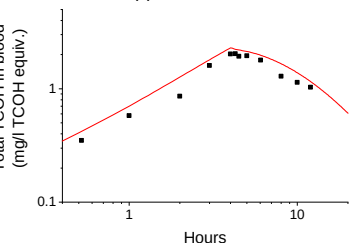
Fisher et al. 1998 Human #15 (sex=Female) 101 ppm TCE 4 hr inhalation



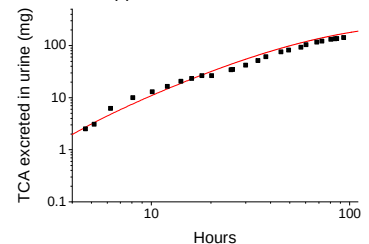
Fisher et al. 1998 Human #15 (sex=Female) 101 ppm TCE 4 hr inhalation



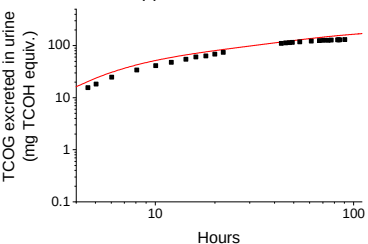
Fisher et al. 1998 Human #15 (sex=Female) 101 ppm TCE 4 hr inhalation



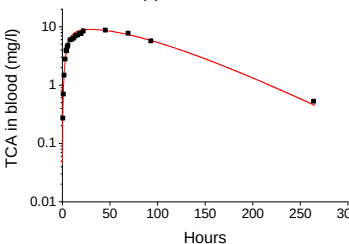
Fisher et al. 1998 Human #15 (sex=Female) 101 ppm TCE 4 hr inhalation

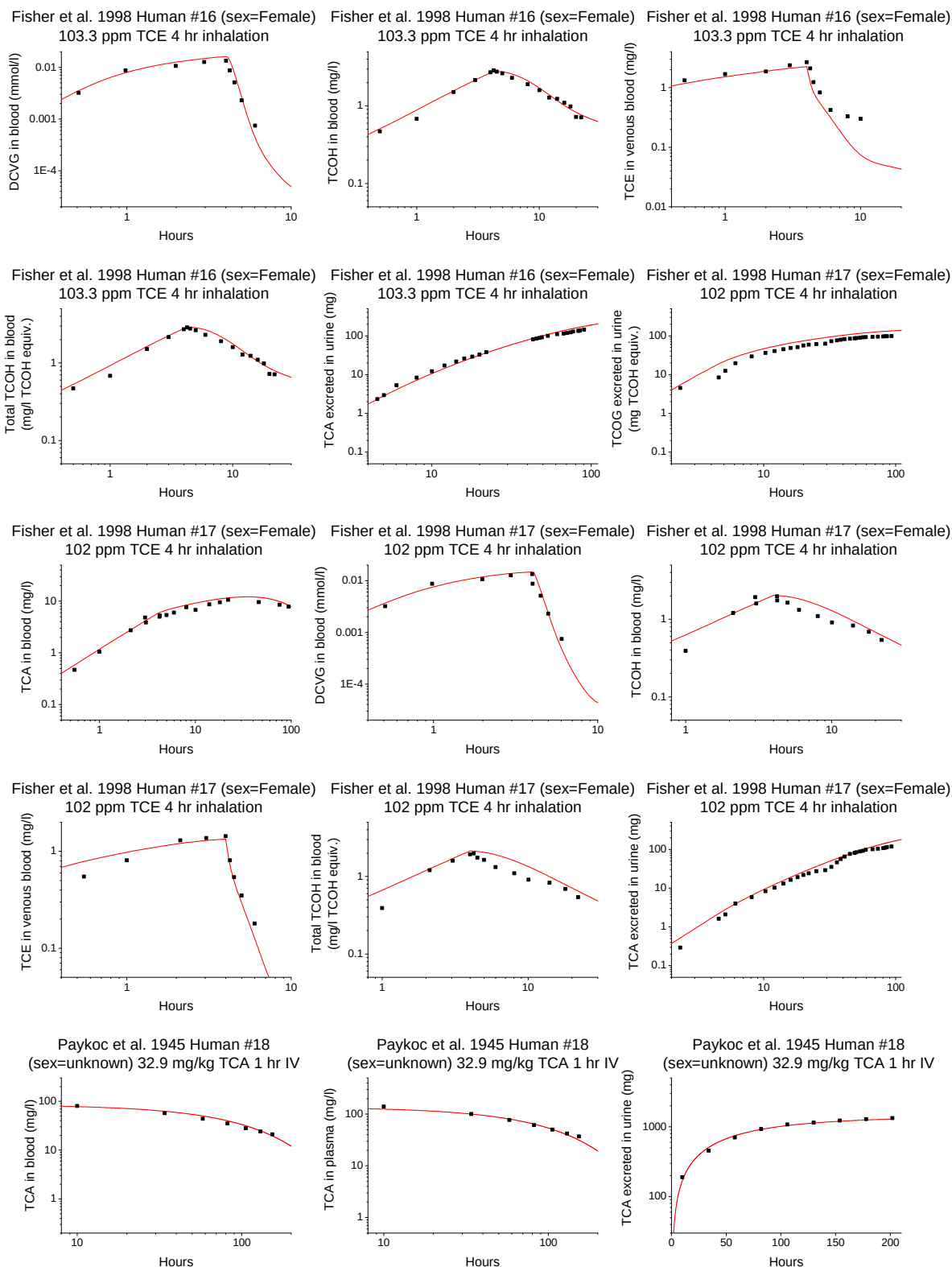


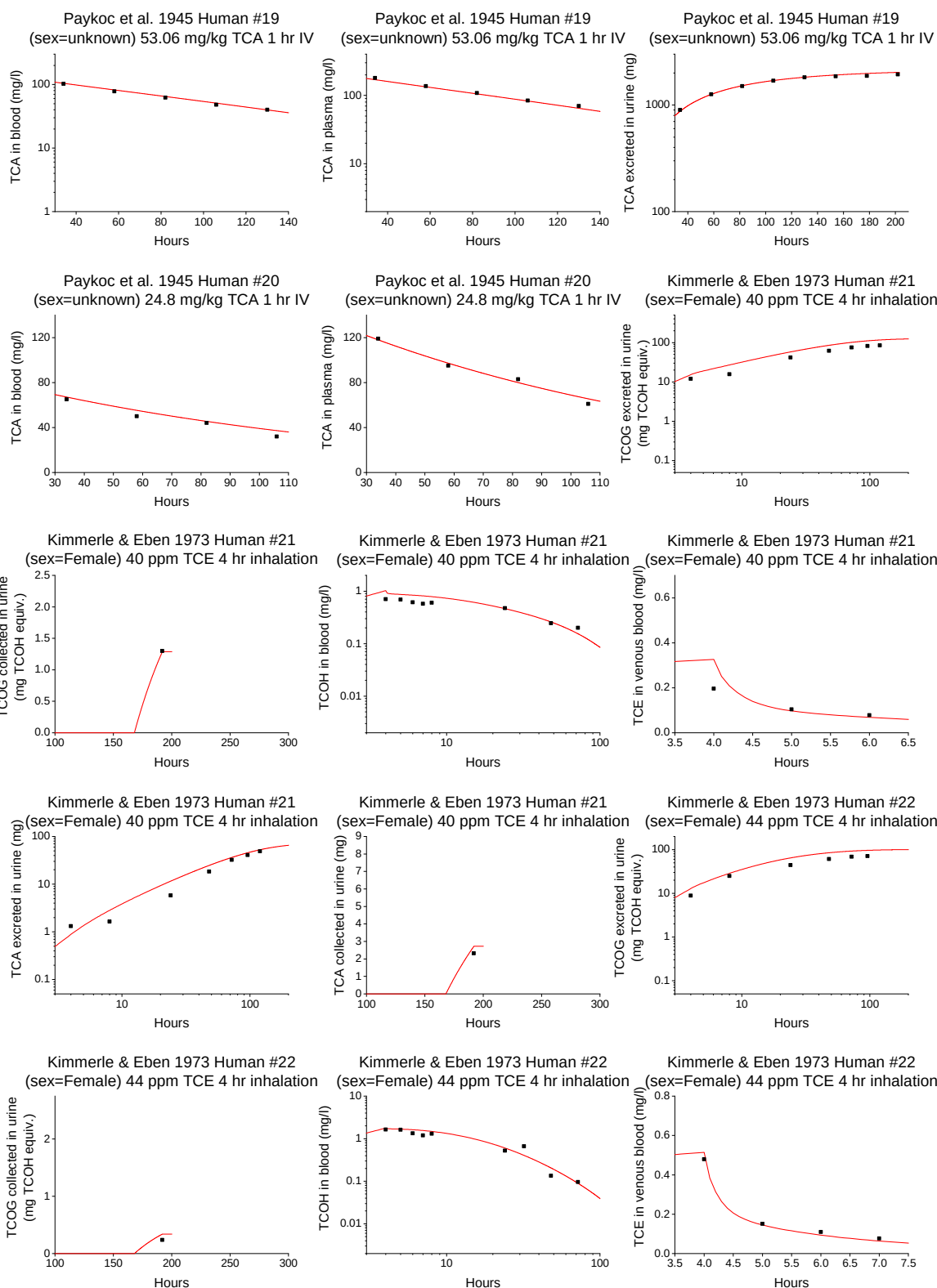
Fisher et al. 1998 Human #16 (sex=Female) 103.3 ppm TCE 4 hr inhalation

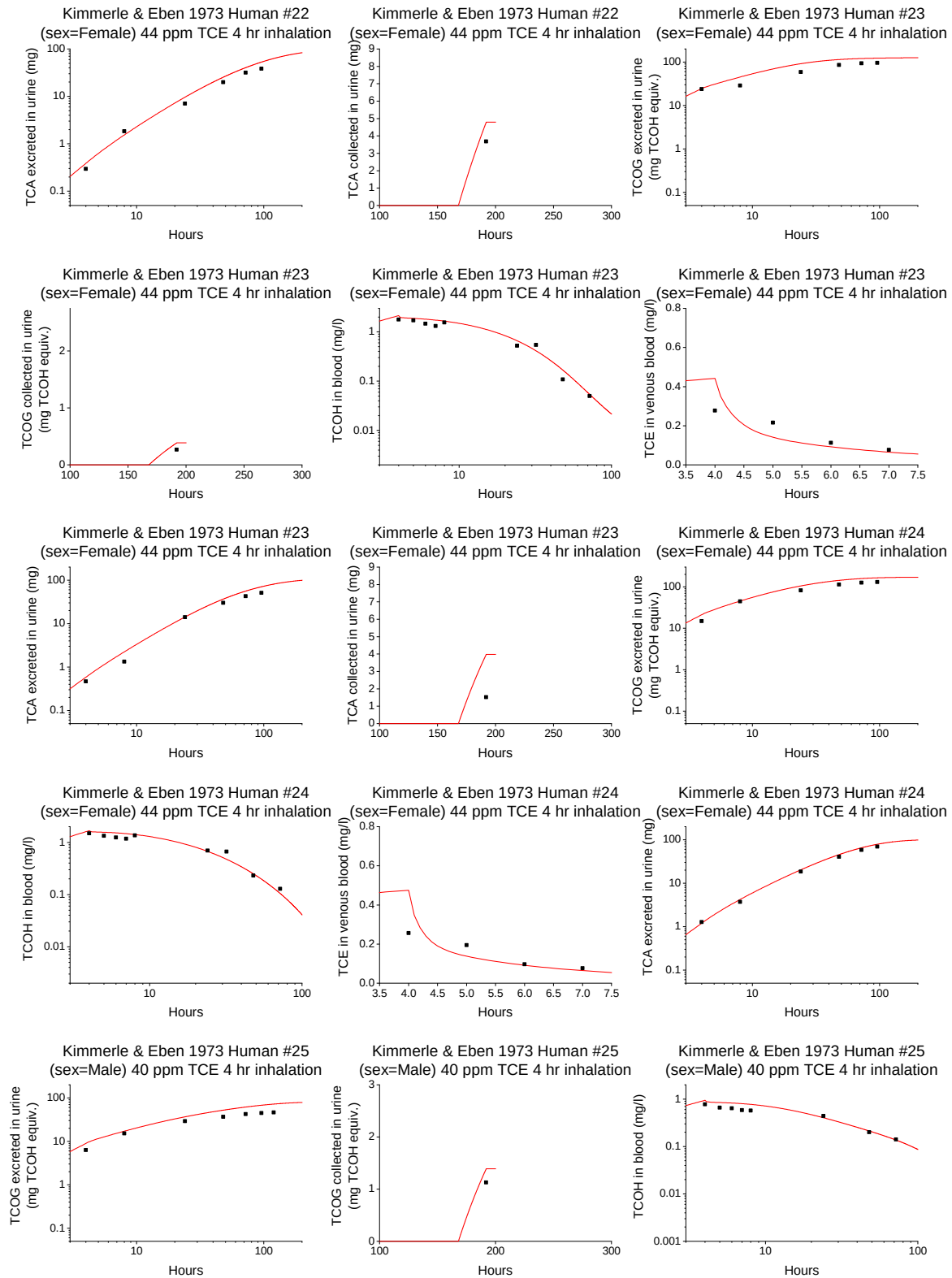


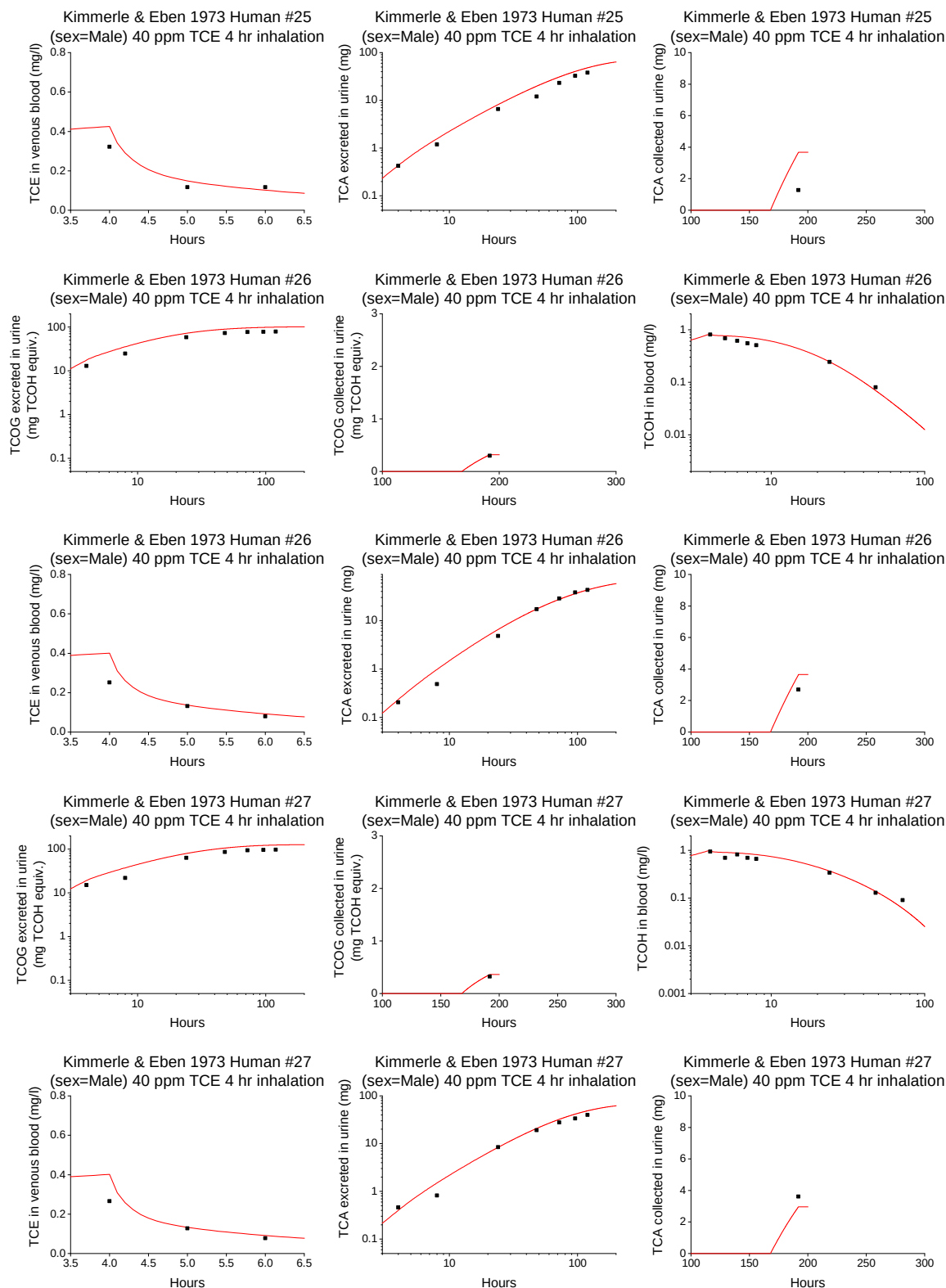
Fisher et al. 1998 Human #16 (sex=Female) 103.3 ppm TCE 4 hr inhalation

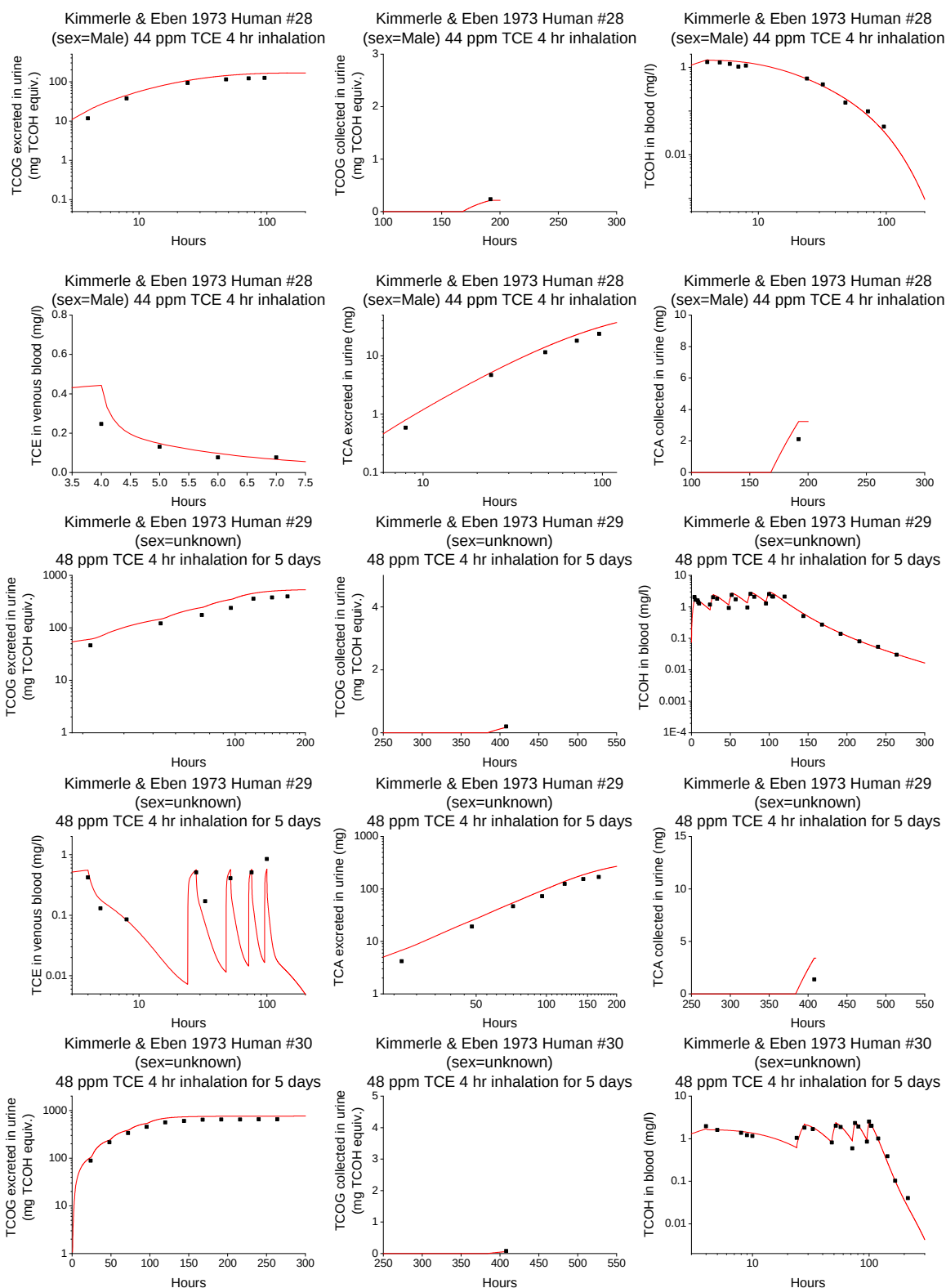


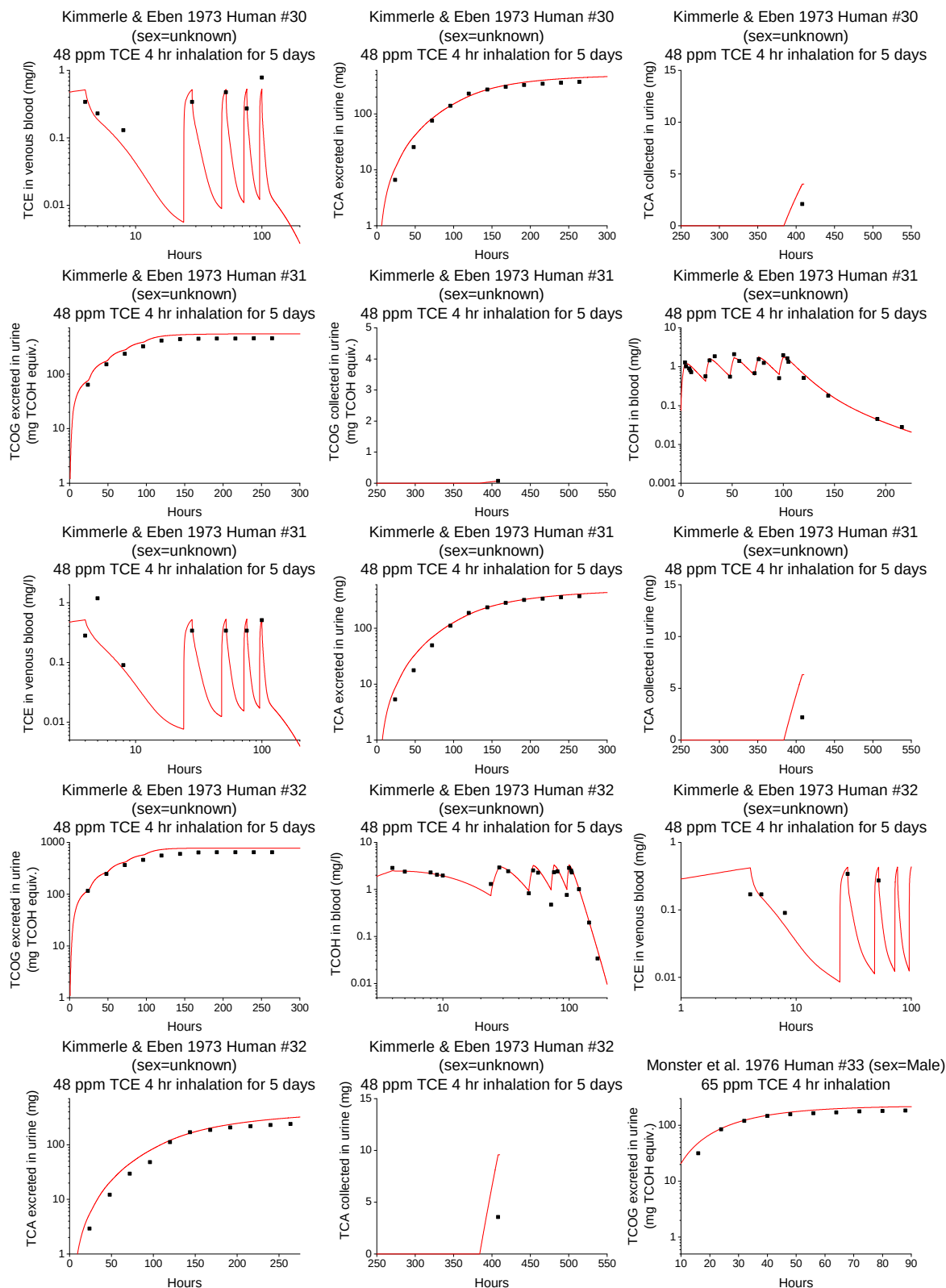


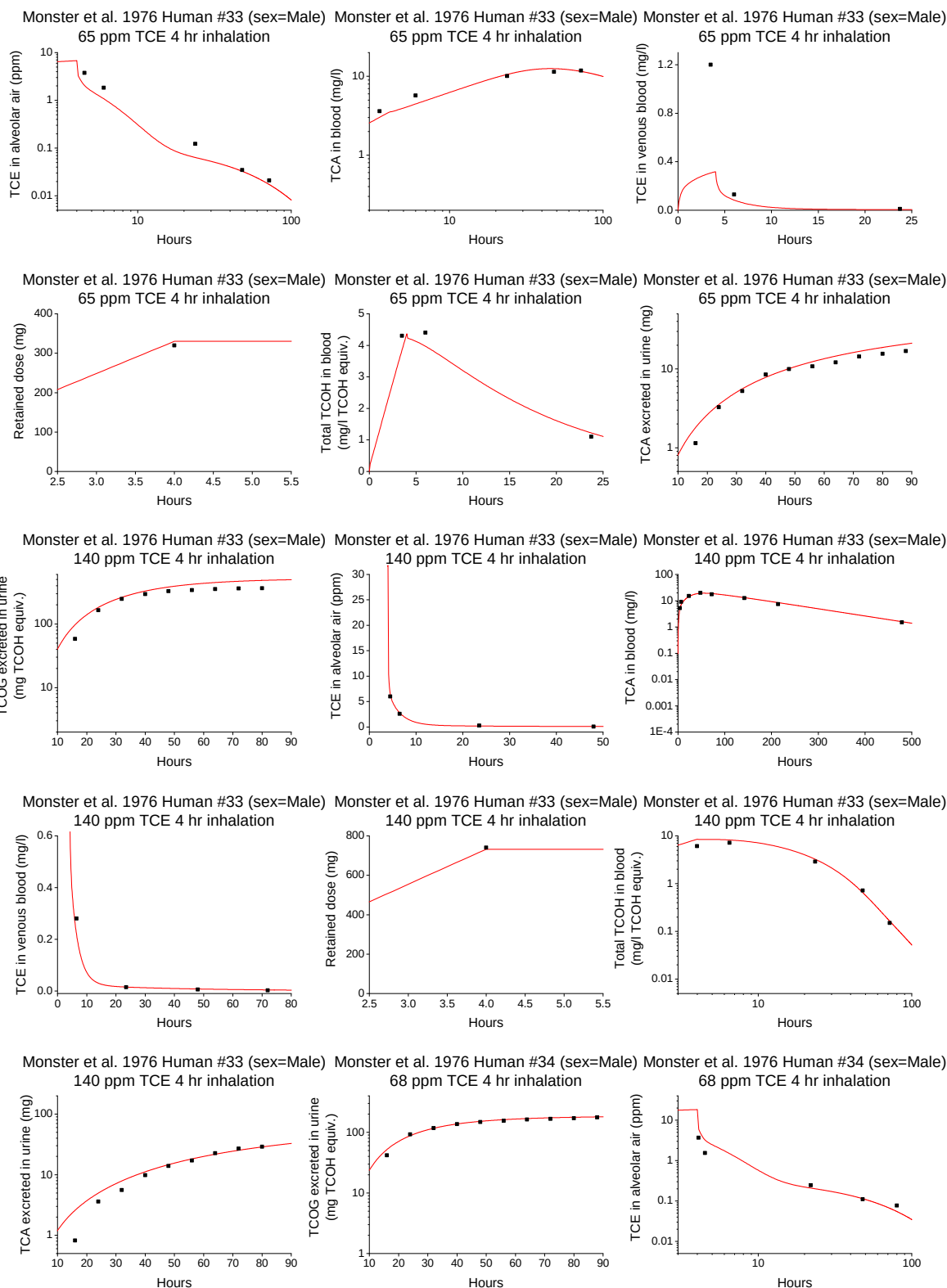


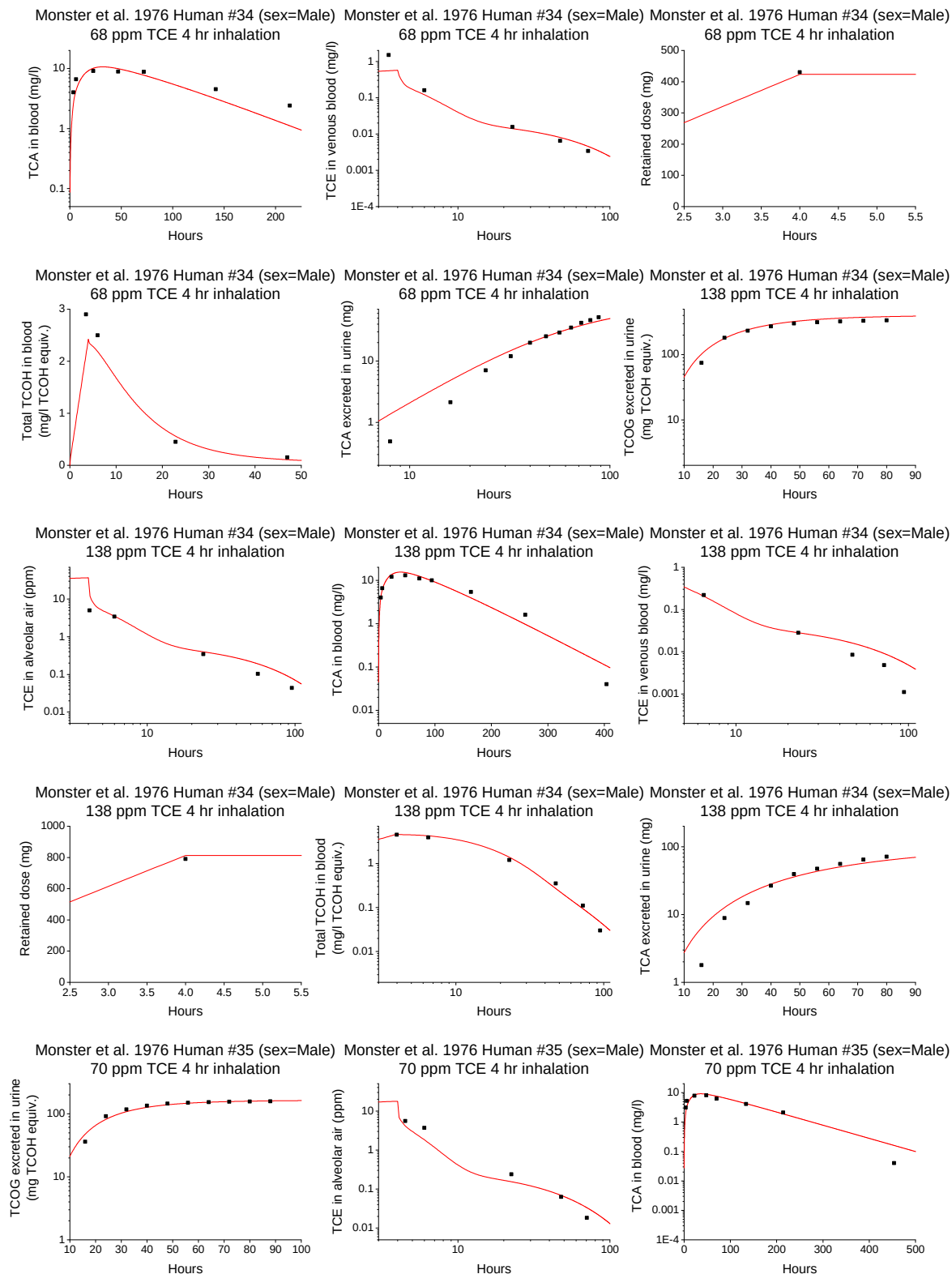




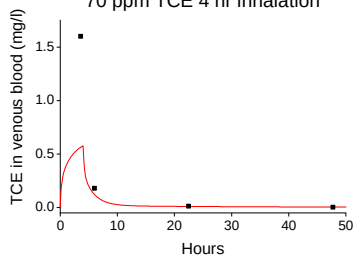




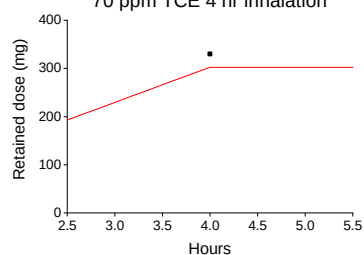




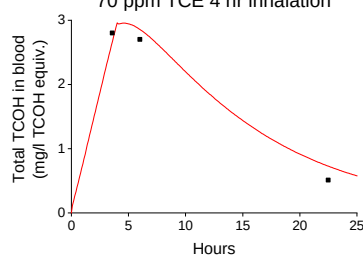
Monster et al. 1976 Human #35 (sex=Male) 70 ppm TCE 4 hr inhalation



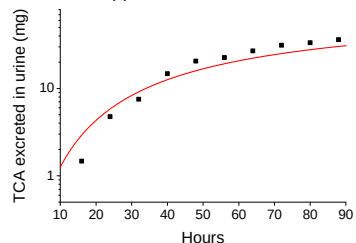
Monster et al. 1976 Human #35 (sex=Male) 70 ppm TCE 4 hr inhalation



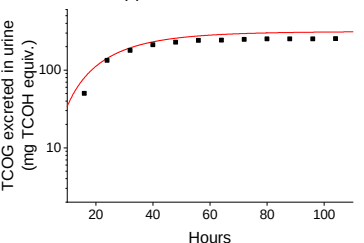
Monster et al. 1976 Human #35 (sex=Male) 70 ppm TCE 4 hr inhalation



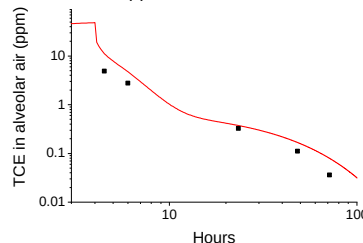
Monster et al. 1976 Human #35 (sex=Male) 70 ppm TCE 4 hr inhalation



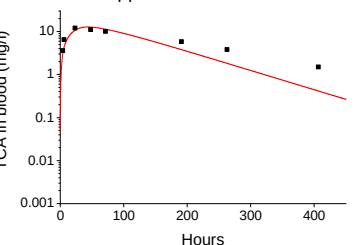
Monster et al. 1976 Human #35 (sex=Male) 142 ppm TCE 4 hr inhalation



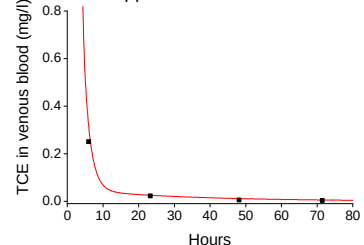
Monster et al. 1976 Human #35 (sex=Male) 142 ppm TCE 4 hr inhalation



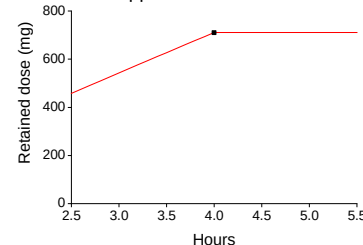
Monster et al. 1976 Human #35 (sex=Male) 142 ppm TCE 4 hr inhalation



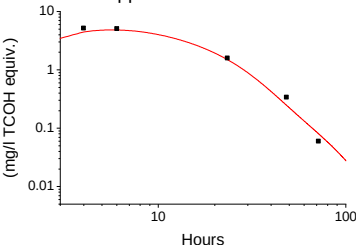
Monster et al. 1976 Human #35 (sex=Male) 142 ppm TCE 4 hr inhalation



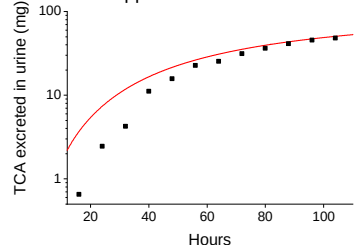
Monster et al. 1976 Human #35 (sex=Male) 142 ppm TCE 4 hr inhalation



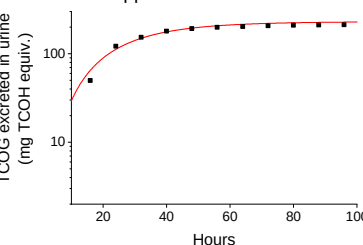
Monster et al. 1976 Human #35 (sex=Male) 142 ppm TCE 4 hr inhalation



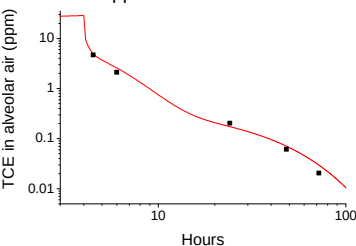
Monster et al. 1976 Human #35 (sex=Male) 142 ppm TCE 4 hr inhalation



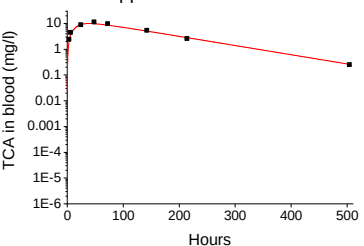
Monster et al. 1976 Human #36 (sex=Male) 76 ppm TCE 4 hr inhalation



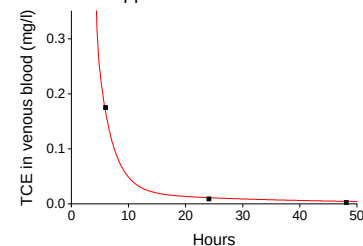
Monster et al. 1976 Human #36 (sex=Male) 76 ppm TCE 4 hr inhalation

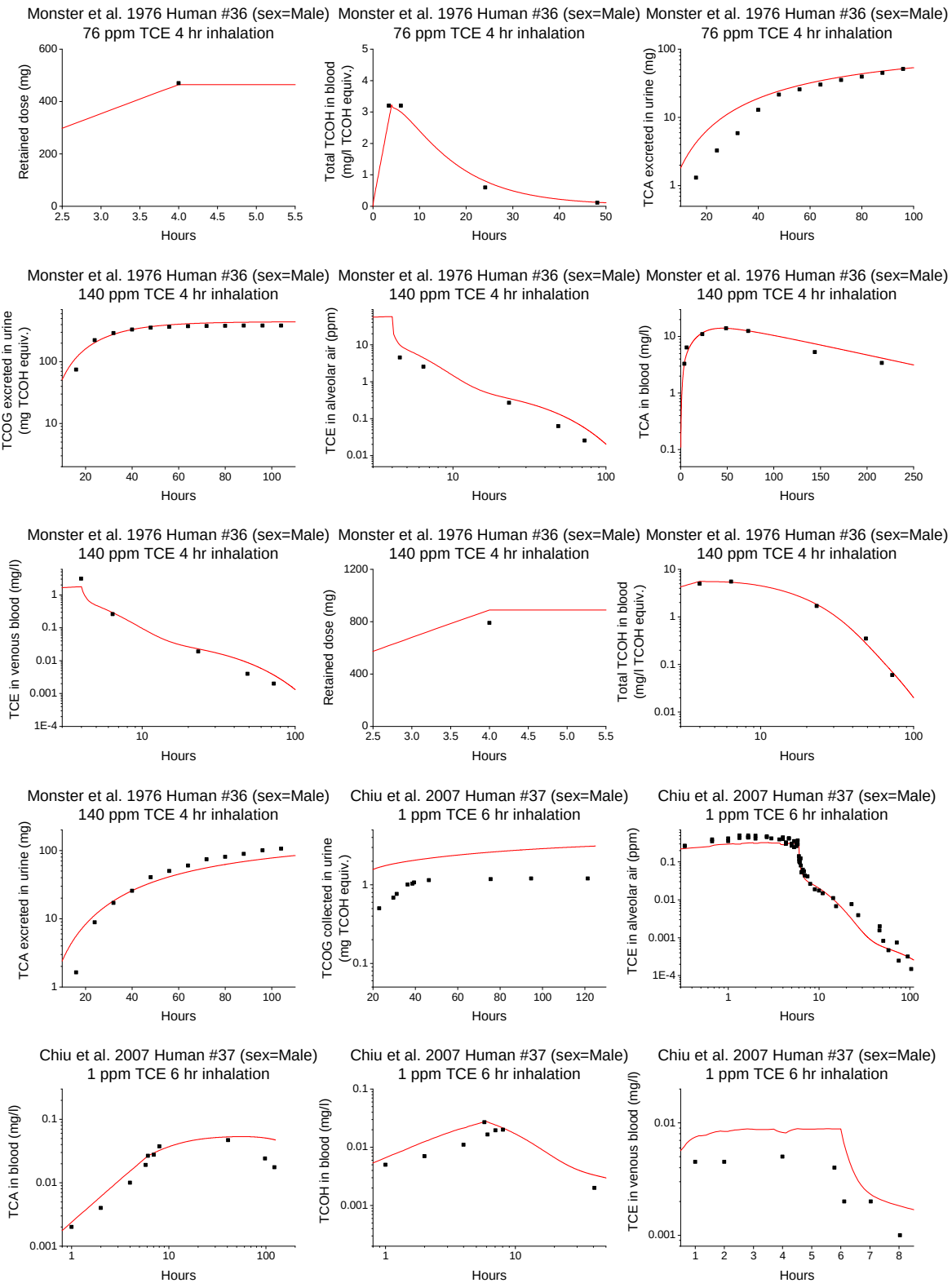


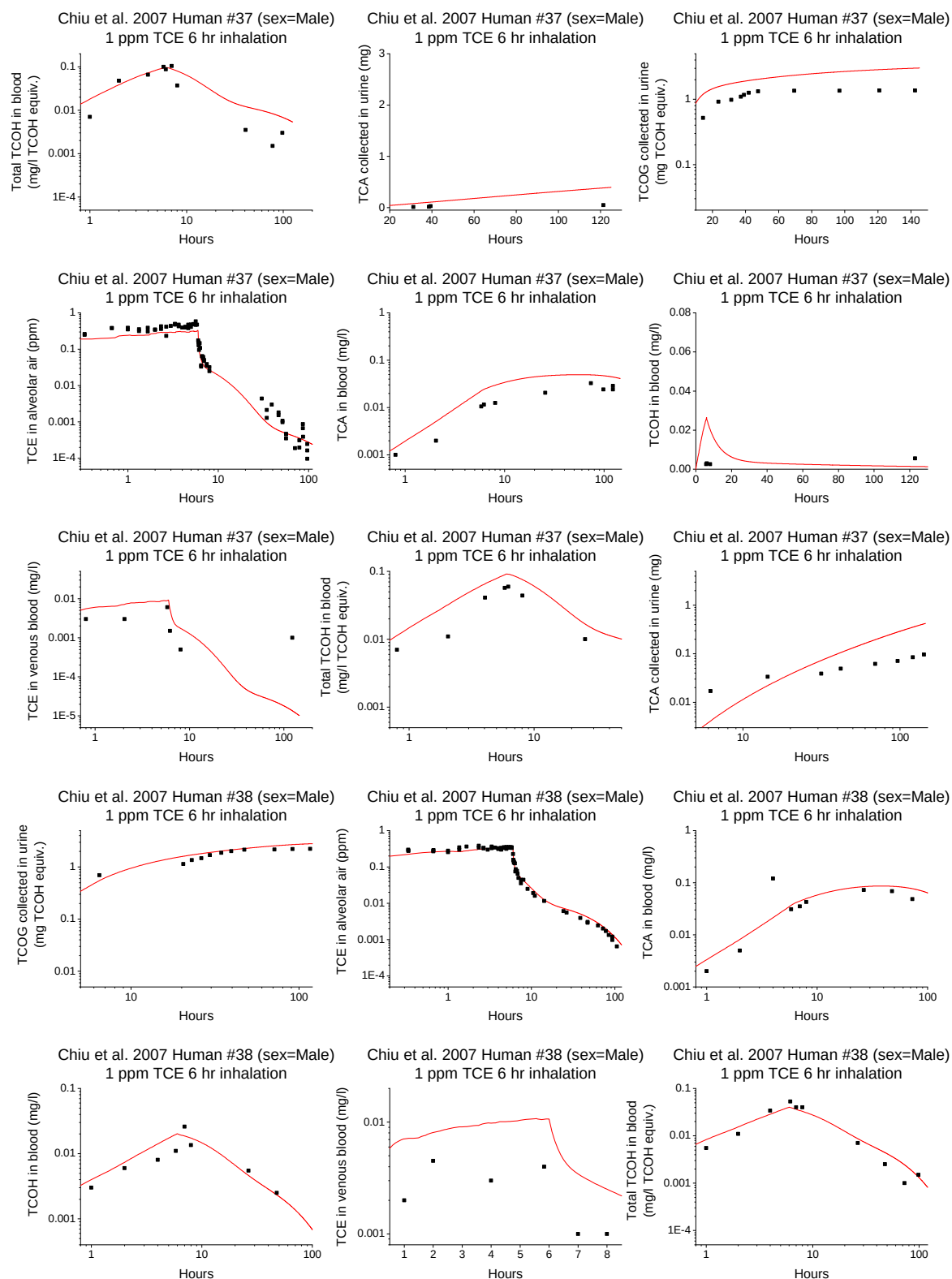
Monster et al. 1976 Human #36 (sex=Male) 76 ppm TCE 4 hr inhalation

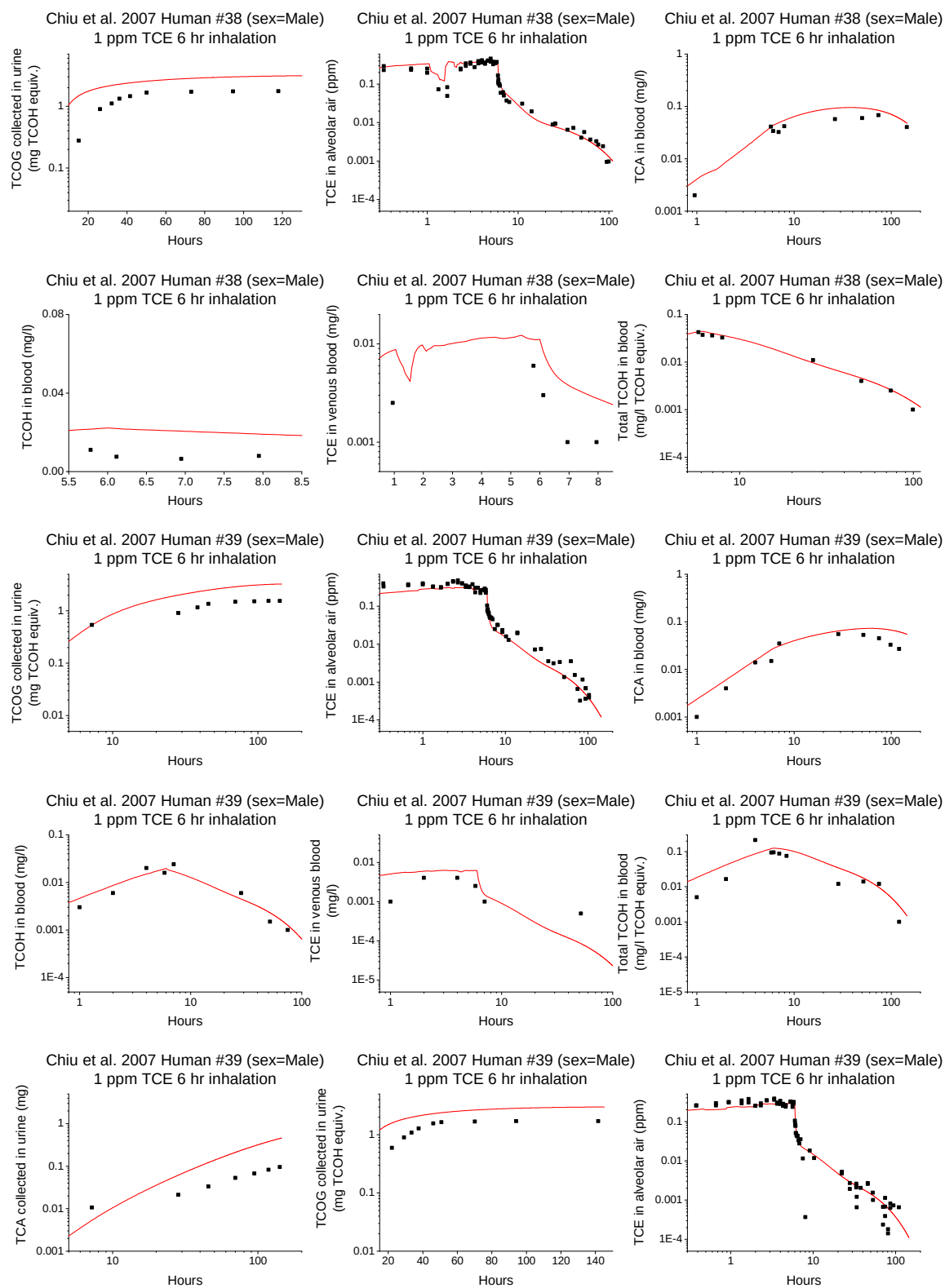


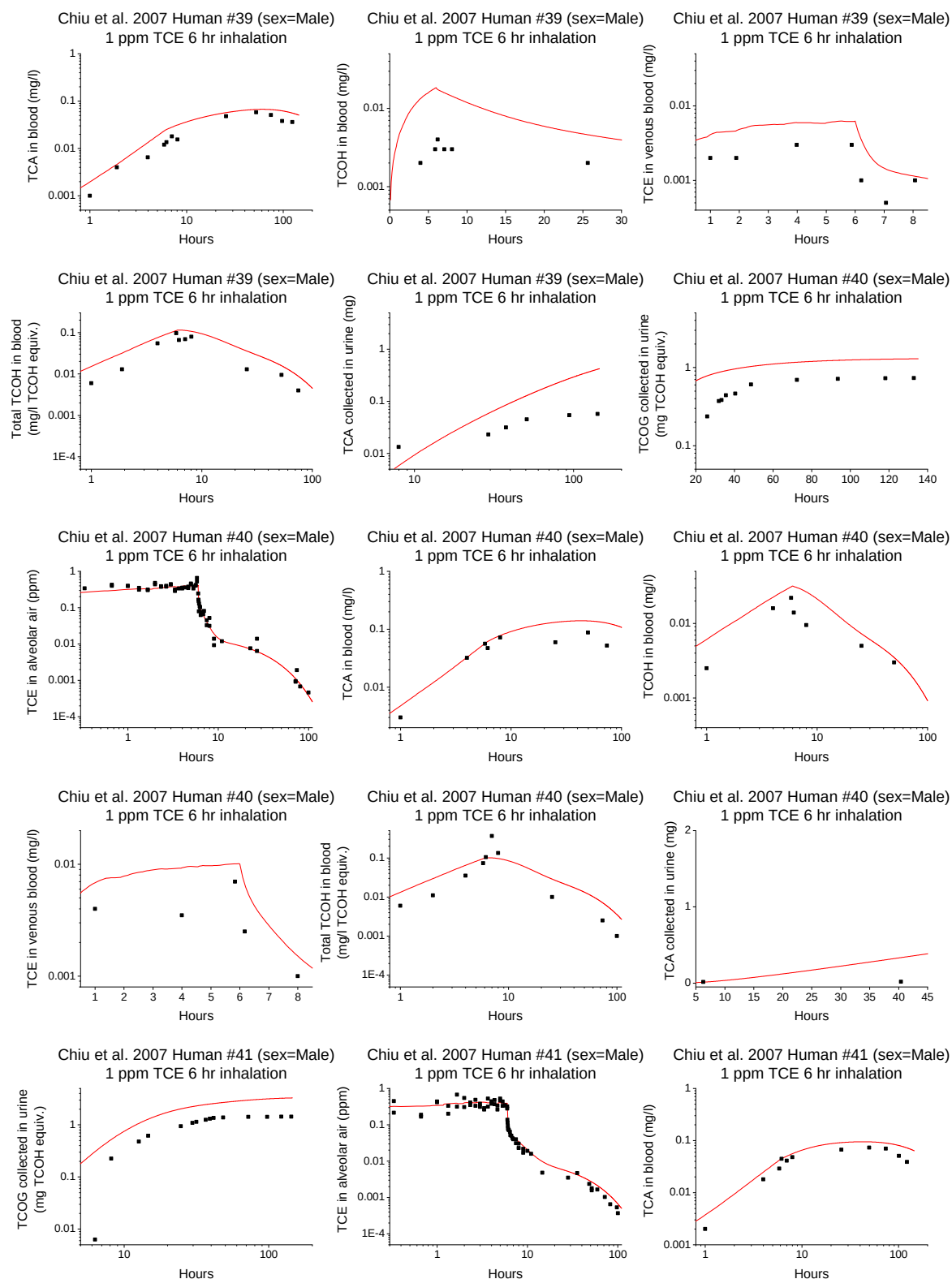
Monster et al. 1976 Human #36 (sex=Male) 76 ppm TCE 4 hr inhalation

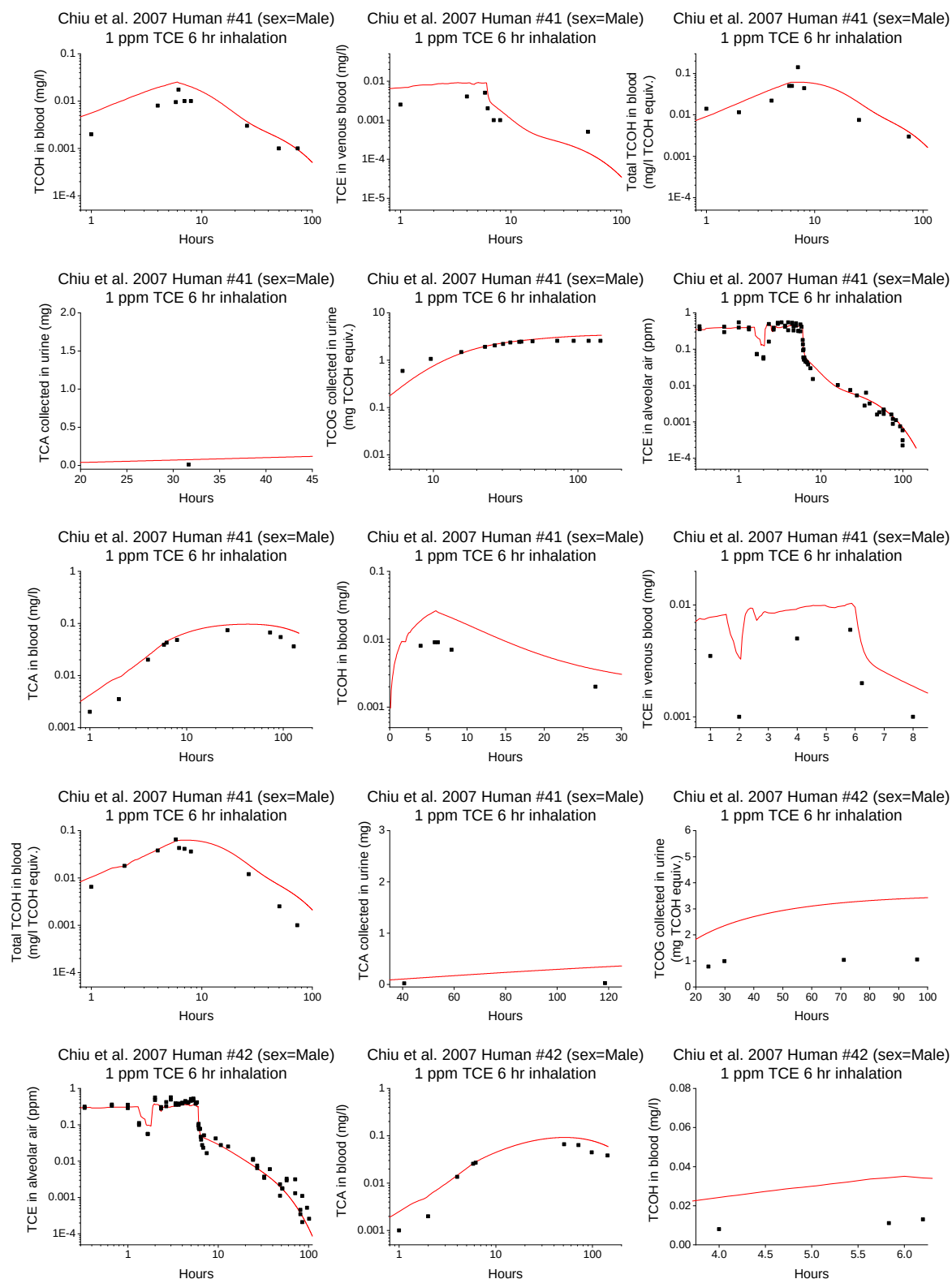


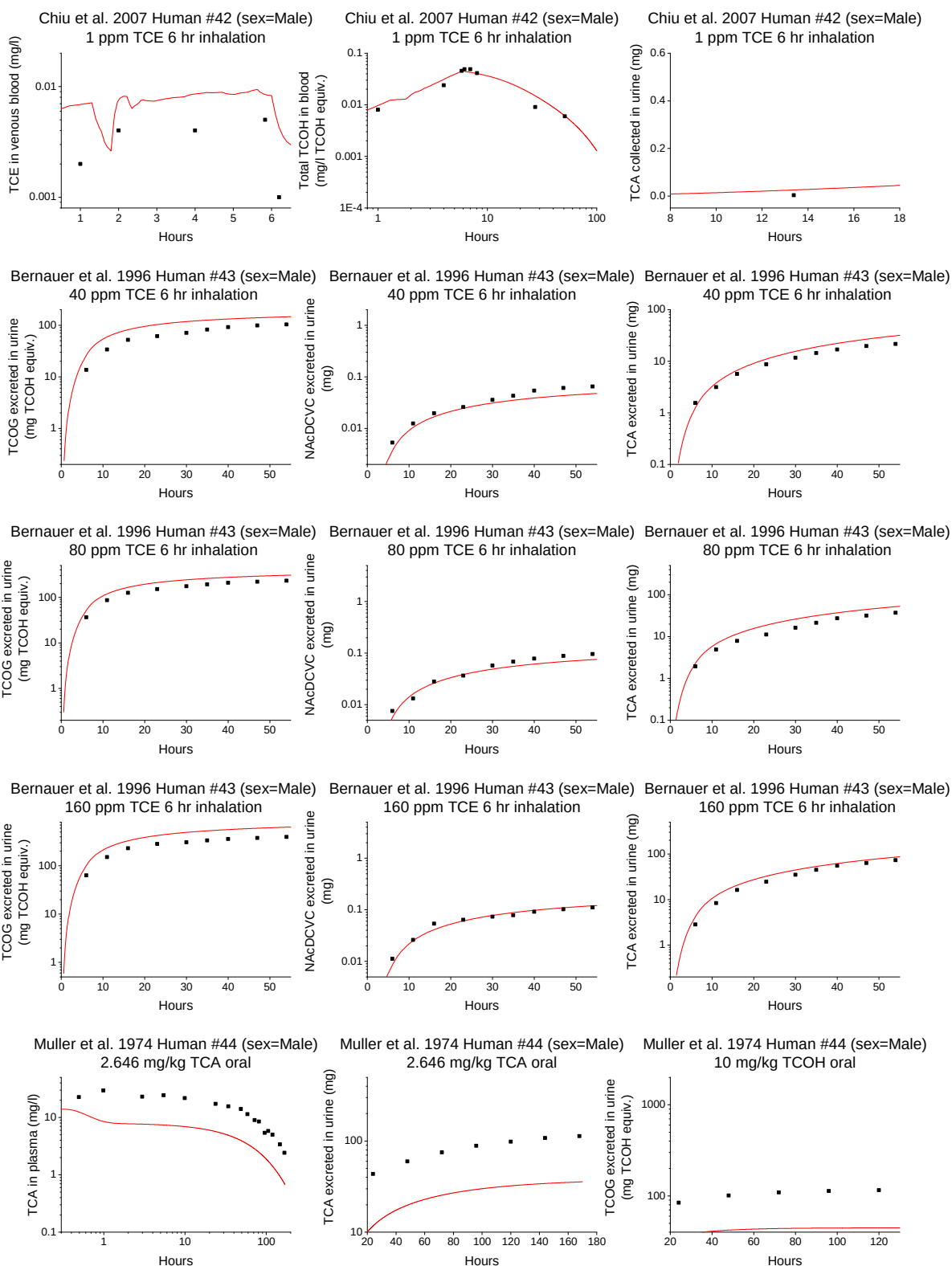


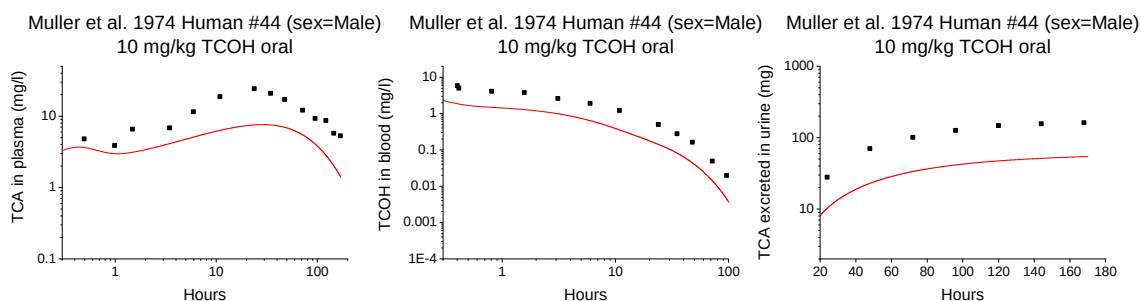












REFERENCES

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- Paykoc ZV, Powell JF. The excretion of sodium trichloracetate. *J Pharmacol Exp Ther.* 1945, 85:289-293.

APPENDIX I

M Files for Mouse Validation Figures

The following M files are for generating mouse output for validation figures in Appendix F.

Abbas97a_Mouse.m

```
% Abbas R and Fisher J. 1997. A physiologically based pharmacokinetic model for trichloroethylene
%   and its metabolites, chloral hydrate, trichloroacetate, dichloroacetate, trichloroethanol,
%   and trichloroethanol glucuronide in B6C3F1 mice. Toxicol Appl Pharmacol 147: 15-30.
% Male B6C3F1 mice, 25-30 grams
% Oral dosing of 300, 600, 1200 or 2000 mg/kg TCE in corn oil (dose volume of 0.5 mL, 20 mL corn
%   oil/kg BW)
```

```
PlotOutput=[];
ResetDoses
MousePost
```

```
% Individual posterior parameters for Abbas97a_Mouse and Abbas97b_Mouse
QCC=13.64680; VPR=1.74681; DRESC=1.27367;
QFATC=0.075810; QGUTC=0.16709; QKIDC=0.088634; QLIVC=0.020660; QRAPC=0.42821; QSLWC=0.21960;
VBLDC=0.048716; VFATC=0.079870; VGUTC=0.048236; VKIDC=0.017017; VLIVC=0.043302; VPERFC=0.88970;
VRAPC=0.09980; VRESC=0.0007; VRESPLUMC=0.0046713; VSLWC=0.55206; FRACPLAS=0.37560;
PB=21.90358; PFAT=25.89420; PGUT=1.45028; PKID=5.33739; PLIV=3.08616; PRAP=1.79924;
PRES=2.59676; PSLW=1.95359;
PRBCPLASTCA=1.61584; PBODTCAC=0.72156; PLIVTCAC=0.90648;
PBODTCOH=0.72207; PLIVTCOH=3.04641;
PBODTCOG=0.42663; PLIVTCOG=0.82264; PEFFDCVG=0.98693;
BMAXKDC=1.26550; KDISSOC=68.74671;
KAS=1.26529; KTS=3.12677; KAD=0.11943; KTD=0.0; KASTCA=3.33676; KASTCOH=0.72928;
VMAXC=2118.38027; KMC=5.74034; CL=1.0; FRACTCAC=0.10673; FRACOTHERC=0.019644;
VMAXDCVGC=769.22420; KMDCVGC=1.0; CLDCVG=0.53863;
VMAXKIDDCVGC=153.86023; KMKIDDCVGC=1.0; CLKIDDCVGC=0.40446;
VMAXLUNGLIV=0.22905; KMCLARA=0.012253; FRACLUNGSYS=4.82591;
VMAXTCOH=1.28685; KMTCOH=0.92839; CLTCOH=1.0;
VMAXGLUC=65.56225; KMGLUC=50.95791; CLGLUC=1.0; KMETTCOH=2.98023;
KURNTCAC=0.076933; KMETTCAC=0.54313;
KBILEC=1.01747; KEHRC=0.012070; KURNTCOG=0.92060;
KDCVGC=0.18900; FRACKIDDCVCC=1.53634;
KNATC=0.11579; KKIDBIOACTC=0.087861;
```

```
BW=0.0275; PDOSE=300.0; TCHNG=0.05; TSTP=193.0; CINT=0.05;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurtca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
PDSE=600.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
```

```

PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=1200.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=2000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Abbas97a_Mouse_Output.txt' @format=ascii

```

Abbas97b_Mouse.m

```

% Abbas R, Seckel C, MacMahon K and Fisher J. 1997. Determination of kinetic rate constants for
% chloral hydrate, trichloroethanol, trichloroacetic acid and dichloroacetic acid: A
% physiologically based modeling approach. Toxicologist 36: 32-33.
% B6C3FI mice
% IV dose of 100 mg/kg TCA or TCOH

```

```

PlotOutput=[];
ResetDoses
MousePost

```

```

% Individual posterior parameters for Abbas97a_Mouse and Abbas97b_Mouse
QCC=13.64680; VPR=1.74681; DRESC=1.27367;
QFATC=0.075810; QGUTC=0.16709; QKIDC=0.088634; QLIVC=0.020660; QRAPC=0.42821; QSLWC=0.21960;
VBLDC=0.048716; VFATC=0.079870; VGUTC=0.048236; VKIDC=0.017017; VLIVC=0.043302; VPERFC=0.88970;
VRAPC=0.09980; VRESC=0.0007; VRESPLUMC=0.0046713; VSLWC=0.55206; FRACPLAS=0.37560;
PB=21.90358; PFAT=25.89420; PGUT=1.45028; PKID=5.33739; PLIV=3.08616; PRAP=1.79924;
PRES=2.59676; PSLW=1.95359;
PRBCPLASTCA=1.61584; PBODTCAC=0.72156; PLIVTCAC=0.90648;

```

```

PBODTCOH=0.72207; PLIVTCOH=3.04641;
PBODTCOG=0.42663; PLIVTCOG=0.82264; PEFDCVGC=0.98693;
BMAXKDC=1.26550; KDISSOC=68.74671;
KAS=1.26529; KTS=3.12677; KAD=0.11943; KTD=0.0; KASTCA=3.33676; KASTCOH=0.72928;
VMAXC=2118.38027; KMC=5.74034; CL=1.0; FRACTCAC=0.10673; FRACOTHERC=0.019644;
VMAXDCVGC=769.22420; KMDCVGC=1.0; CLDCVGC=0.53863;
VMAXKIDDCVGC=153.86023; KMKIDDCVGC=1.0; CLKIDDCVGC=0.40446;
VMAXLUNGLIV=0.22905; KMCLARA=0.012253; FRACLUNGSYS=4.82591;
VMAXTCOH=1.28685; KMTCOH=0.92839; CLTCOH=1.0;
VMAXGLUCC=65.56225; KMGLUC=50.95791; CLGLUC=1.0; KMETTCOH=2.98023;
KURNTCAC=0.076933; KMETTCAC=0.54313;
KBILEC=1.01747; KEHRC=0.012070; KURNTCOG=0.92060;
KDCVGC=0.18900; FRACKIDDCVCC=1.53634;
KNATC=0.11579; KKIDBI0ACTC=0.087861;

```

```

BW=0.035; IVDOSSETCA=100.0; TCHNG=0.05; TSTP=170.0; CINT=0.05;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

IVDOSSETCA=0.0; IVDOSSETCOH=100.0;
start @NoCallback
plot(_t, _ctcoh)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

save PlotOutput @file='Abbas97b_Mouse_Output.txt' @format=ascii

```

Fisher91_Mouse.m

```

% Fisher J, Gargas M, Allen B and Andersen M. 1991. Physiologically based pharmacokinetic
% modeling with trichloroethylene and its metabolite, trichloroacetic acid, in the rat and
% mouse. Toxicol Appl Pharmacol 109: 183-195.
% B6C3F1 female and male mice
% Open or closed chamber inhalation of various concentrations of TCE for 4 hours

% Female mice -- inhalation of 42, 236, 368 or 889 ppm TCE for 4 hours
PlotOutput=[];
ResetDoses
MousePost

% Individual posterior parameters for Fisher91_Mouse female
QCC=23.59666; VPR=2.19875; DRESPC=1.19602;
QFATC=0.070280; QGUTC=0.17357; QKIDC=0.090936; QLIVC=0.020940; QRAPC=0.42910; QSLWC=0.21518;
VBLDC=0.048716; VFATC=0.09030; VGUTC=0.048672; VKIDC=0.0170; VLIVC=0.047306; VPERFC=0.88970;
VRAPC=0.099790; VRESPC=0.0007; VRESPLUMC=0.0046657; VSLWC=0.53722; FRACPLAS=0.46717;
PB=11.03035; PFAT=35.36522; PGUT=1.58590; PKID=2.56264; PLIV=2.12003; PRAP=1.83836;
PRESP=2.58842; PSLW=2.27830;
PRBCPLASTCA=1.01405; PBODTCAC=0.66210; PLIVTCAC=1.03047;
PBODTCOH=0.90218; PLIVTCOH=1.82862;
PBODTCOG=0.46587; PLIVTCOG=1.19497; PEFDCVGC=0.99014;
BMAXKDC=1.12701; KDISSOC=123.79523;
KAS=1.78425; KTS=3.69138; KAD=0.28280; KTD=0.0; KASTCA=3.30026; KASTCOH=0.73499;
VMAXC=1459.00073; KMC=0.68627; CL=1.0; FRACTCAC=0.16756; FRACOTHERC=0.023873;
VMAXDCVGC=779.91308; KMDCVGC=1.0; CLDCVGC=0.54622;
VMAXKIDDCVGC=153.43002; KMKIDDCVGC=1.0; CLKIDDCVGC=0.41532;
VMAXLUNGLIV=0.025228; KMCLARA=0.017810; FRACLUNGSYS=4.44598;
VMAXTCOH=1.89250; KMTCOH=0.86918; CLTCOH=1.0;
VMAXGLUCC=65.82502; KMGLUC=34.63969; CLGLUC=1.0; KMETTCOH=3.40076;
KURNTCAC=0.099976; KMETTCAC=0.78286;
KBILEC=0.92533; KEHRC=0.011154; KURNTCOG=7.39774;
KDCVGC=0.18787; FRACKIDDCVCC=1.54574;

```

```

KNATC=0.11695; KKIDBIOACTC=0.088037;
BW=0.025; CONCLIST=[42.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=31.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.023; CONCLIST=[236.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.024; CONCLIST=[368.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.03; CONCLIST=[889.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female mice -- closed chamber inhalation of 300, 700, 1100, 3700 or 7000 ppm TCE
ResetDoses
BW=0.024; CC=1; CONCLIST(1)=300.0; STRTNEXTLIST(1)=10.0; TSTRT=0.0; NRODENTS=14.0; VCHC=9.1;
KLOSSC=exp(-3.912); TSTP=2.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
BW=0.021; CONCLIST(1)=700.0; STRTNEXTLIST(1)=10.0; TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022; CONCLIST(1)=1100.0; STRTNEXTLIST(1)=10.0; TSTP=4.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022; CONCLIST(1)=3700.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check

```



```

Output_Check_Reset
BW=0.022; CONCLIST(1)=7000.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male mice -- inhalation of 110, 297, 368 or 748 ppm TCE for 4 hours
ResetDoses
MousePost

% Individual posterior parameters for Fisher91_Mouse male
QCC=22.02119; VPR=2.41566; DRESPC=1.09032;
QFATC=0.09240; QGUTC=0.16328; QKIDC=0.090527; QLIVC=0.020540; QRAPC=0.44653; QSLWC=0.18673;
VLDC=0.048775; VFATC=0.101640; VGUTC=0.048490; VKIDC=0.016952; VLIVC=0.038104; VPERFC=0.88970;
VRAPC=0.099390; VRESPC=0.0007; VRESPLUMC=0.0046634; VSLWC=0.53565; FRACPLAS=0.46883;
PB=7.77373; PFAT=41.78423; PGUT=1.49414; PKID=2.45969; PLIV=1.96507; PRAP=1.63895;
PRES=2.58200; PSLW=1.84185;
PRBCPLASTCA=1.11377; PBODTCAC=0.75259; PLIVTCAC=0.93764;
PBODTCOH=0.91097; PLIVTCOH=1.81333;
PBODTCOG=0.46452; PLIVTCOG=1.33564; PEFFDCVG=0.98370;
BMAXKDC=1.01650; KDISSOC=136.66448;
KAS=1.76562; KTS=3.75092; KAD=0.27665; KTD=0.0; KASTCA=3.30686; KASTCOH=0.73301;
VMAXC=866.97232; KMC=0.73090; CL=1.0; FRACTCAC=0.20986; FRACOTHERC=0.023849;
VMAXDCVGC=758.22674; KMDCVGC=1.0; CLDCVG=0.50171;
VMAXKIDDCVGC=150.33176; KMKIDDCVGC=1.0; CLKIDDCVG=0.39820;
VMAXLUNGLIV=1.52989; KMCLARA=0.0068741; FRACLUNGSYS=3.77349;
VMAXTCOHC=1.51255; KMTCOH=1.01194; CLTCOH=1.0;
VMAXGLUCC=74.29176; KMGLUC=24.23990; CLGLUC=1.0; KMETTCOHC=3.39397;
KURNTCAC=0.055198; KMETTCAC=0.56762;
KBILEC=1.01444; KEHRC=0.012095; KURNTCOG=4.63750;
KDCVGC=0.18938; FRACKIDDCVCC=1.53449;
KNATC=0.11614; KKIDBIOACTC=0.088037;

BW=0.031; CONCLIST=[110.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=25.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[297.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[368.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[748.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check

```

```

Output_Check_Reset
% Male mice -- closed chamber inhalation of 1020, 1800, 3800, 5600 or 10000 ppm TCE
ResetDoses
BW=0.03; CC=1; CONCLIST(1)=1020.0; STRTNEXTLIST(1)=10.0; TSTRT=0.0; NRODENTS=14.0; VCHC=9.1;
KLOSSC=exp(-3.912); TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.026; CONCLIST(1)=1800.0; STRTNEXTLIST(1)=10.0; TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.03; CONCLIST(1)=3800.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.028; CONCLIST(1)=5600.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.026; CONCLIST(1)=10000.0; STRTNEXTLIST(1)=10.0; TSTP=4.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher91_Mouse_Output.txt' @format=ascii

```

Fisher93_Mouse.m

```

% Fisher J and Allen B. 1993. Evaluating the risk of liver cancer in humans exposed to
% trichloroethylene using physiological models. Risk Anal 13: 87-95.
% Female and male mice
% Oral gavage of various doses of TCE

% Female mice -- oral gavage of 487, 973 or 1947 mg/kg TCE
PlotOutput=[];
ResetDoses
MousePost

% Individual posterior parameters for Fisher93_Mouse female
QCC=13.54890; VPR=1.94700; DRESPC=1.20925;
QFATC=0.077070; QGUTC=0.16201; QKIDC=0.091273; QLIVC=0.020520; QRAPC=0.43315; QSLWC=0.21598;
VBLDC=0.048441; VFATC=0.086730; VGUTC=0.048285; VKIDC=0.0170; VLIVC=0.046486; VPERFC=0.88970;
VRAPC=0.099760; VRESPC=0.0007; VRESPLUMC=0.0046667; VSLWC=0.54230; FRACPLAS=0.44642;
PB=16.73078; PFAT=36.28491; PGUT=1.47146; PKID=2.55368; PLIV=2.00176; PRAP=1.84136;
PRES=2.60091; PSLW=2.46105;
PRBCPLASTCA=1.19155; PBODTCAC=0.78739; PLIVTCAC=0.95305;
PBODTCOH=0.91765; PLIVTCOH=1.80519;
PBODTCOG=0.46587; PLIVTCOG=1.27007; PEFDCVG=0.99359;
BMAXKDC=1.05429; KDISSOC=92.90048;
KAS=1.35839; KTS=20.12575; KAD=0.25924; KTD=0.0; KASTCA=3.38380; KASTCOH=0.72600;
VMAXC=1834.09610; KMC=4.25255; CL=1.0; FRACTCAC=0.16611; FRACOTHERC=0.024380;

```

```

VMAXDCVGC=799.01720; KMDCVGC=1.0; CLDCVG=0.56738;
VMAXKIDDCVGC=155.31333; KMKIDDCVGC=1.0; CLKIDDCVG=0.41524;
VMAXLUNGLIV=0.23159; KMCLARA=0.013115; FRACLUNGSYS=4.40614;
VMAXTCOHC=1.54126; KMTCOH=1.00083; CLTCOH=1.0;
VMAXGLUCC=73.99518; KMGLUC=25.00310; CLGLUC=1.0; KMETTCOHC=3.45216;
KURNTCAC=0.109173; KMETTCAC=0.82919;
KBILEC=0.96850; KEHRC=0.011855; KURNTCOGC=5.53546;
KDCVGC=0.18712; FRACKIDDCVCC=1.53311;
KNATC=0.11789; KKIDBIOACTC=0.088301;

BW=0.0273; PDOSE=487.0; TCHNG=0.05; TSTP=73.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.0238; PDOSE=973.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.0257; PDOSE=1947.0; TCHNG=0.05; TSTP=73.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male mice -- oral gavage of 487, 973 or 1947 mg/kg TCE
ResetDoses
MousePost

% Individual posterior parameters for Fisher93_Mouse male
QCC=10.78046; VPR=1.80235; DRESPC=1.24098;
QFATC=0.059878; QGUTC=0.16286; QKIDC=0.090518; QLIVC=0.020520; QRAPC=0.44641; QSLWC=0.21982;
VBLDC=0.048241; VFATC=0.096320; VGUTC=0.048094; VKIDC=0.017017; VLIVC=0.043582; VPERFC=0.88970;
VRAPC=0.10; VRESPC=0.0007; VRESPLUMC=0.0046667; VSLWC=0.53575; FRACPLAS=0.44242;
PB=20.21349; PFAT=43.37221; PGUT=1.42042; PKID=2.57935; PLIV=2.03100; PRAP=1.90095;
PRESP=2.59606; PSLW=2.35631;
PRBCPLASTCA=0.93422; PBODTCAC=0.72707; PLIVTCAC=0.87452;
PBODTCOH=0.91271; PLIVTCOH=1.75324;
PBODTCOG=0.46620; PLIVTCOG=1.45305; PEFDCVG=0.99547;
BMAXKDC=1.33906; KDISSOC=117.10124;
KAS=2.08757; KTS=16.44465; KAD=0.15320; KTD=0.0; KASTCA=3.36356; KASTCOH=0.73712;
VMAXC=1557.29723; KMC=2.04729; CL=1.0; FRACTCAC=0.17770; FRACOTHERC=0.023707;
VMAXDCVGC=795.50925; KMDCVGC=1.0; CLDCVG=0.56590;
VMAXKIDDCVGC=155.28227; KMKIDDCVGC=1.0; CLKIDDCVG=0.41953;
VMAXLUNGLIV=0.11120; KMCLARA=0.013063; FRACLUNGSYS=4.35359;
VMAXTCOHC=2.39241; KMTCOH=0.80856; CLTCOH=1.0;
VMAXGLUCC=69.40785; KMGLUC=31.88067; CLGLUC=1.0; KMETTCOHC=3.24787;
KURNTCAC=0.128243; KMETTCAC=0.82886;
KBILEC=1.10727; KEHRC=0.011772; KURNTCOGC=3.54371;
KDCVGC=0.18787; FRACKIDDCVCC=1.54589;
KNATC=0.11533; KKIDBIOACTC=0.088125;

BW=0.0338; PDOSE=487.0; TCHNG=0.05; TSTP=73.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');

```

```

i = i + 1;
Output_Check
Output_Check_Reset

BW=0.0306; PD0SE=973.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.0306; PD0SE=1947.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher93_Mouse_Output.txt' @format=ascii

```

Green85_Mouse.m

```

% Green T and Prout M. 1985. Species differences in response to trichloroethylene: II.
% Biotransformation in rats and mice. Toxicol Appl Pharmacol 79: 401-411.
% Male mice (25 to 32 g) of the B6C3FI and Swiss-Webster strains (N=4 each/group)
% Oral dosing of 10, 500, 1000 or 2000 mg/kg containing 10 uCi trichloro[1,2-14C]ethylene in corn
% oil (0.5 mL to mice)

```

```

PlotOutput=[];
ResetDoses
MousePost

```

```

% Individual posterior parameters for Green85_Mouse and Prout85_Mouse
QCC=14.97684; VPR=1.99489; DRESPC=1.25961;
QFATC=0.071330; QGUTC=0.15679; QKIDC=0.090964; QLIVC=0.02040; QRAPC=0.44375; QSLWC=0.21676;
VBLDC=0.048731; VFATC=0.090440; VGUTC=0.048515; VKIDC=0.0170; VLIVC=0.048631; VPERFC=0.88970;
VRAPC=0.099870; VRESPC=0.0007; VRESPLUMC=0.0046639; VSLWC=0.53581; FRACPLAS=0.45178;
PB=15.39758; PFAT=38.56206; PGUT=1.56151; PKID=2.55803; PLIV=2.09348; PRAP=1.83661;
PRESP=2.58070; PSLW=2.40307;
PRBCPLASTCA=1.82550; PBODTCAC=0.80023; PLIVTCAC=0.93437;
PBODTCOH=0.92715; PLIVTCOH=1.87417;
PBODTCOG=0.46667; PLIVTCOG=1.22135; PEFDCVGC=0.98284;
BMAXKDC=1.17971; KDISSOC=287.09950;
KAS=0.60170; KTSO=2.40584; KAD=0.13656; KTD=0.0; KASTCA=3.41439; KASTCOH=0.71384;
VMAXC=2507.03749; KMC=3.86329; CL=1.0; FRACTCAC=0.16557; FRACOTHERC=0.026017;
VMAXDCVGC=803.02229; KMDCVGC=1.0; CLDCVGC=0.56891;
VMAXKIDDCVGC=155.01852; KMKIDDCVGC=1.0; CLKIDDCVGC=0.42168;
VMAXLUNGLIV=0.44584; KMCLARA=0.011820; FRACLUNGSYS=4.27165;
VMAXTCOHC=2.45837; KMTCOH=0.86459; CLTCOH=1.0;
VMAXGLUCC=85.11472; KMGLUC=13.83221; CLGLUC=1.0; KMETTCOHC=3.59664;
KURNTCAC=0.029634; KMETTCAC=0.53360;
KBILEC=0.94189; KEHRC=0.012119; KURNTCOGC=31.75894;
KDCVGC=0.1890; FRACKIDDCVCC=1.53757;
KNATC=0.11695; KKIDBIOACTC=0.088213;

```

```

BW=0.0285; PD0SE=10.0; TCHNG=0.05; TSTP=73.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

PDOSE=500.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

PDOSE=1000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

PDOSE=2000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

save PlotOutput @file='Green85_Mouse_Output.txt' @format=ascii

```

Greenberg99_Mouse.m

```

% Greenberg M, Burton G and Fisher J. 1999. Physiologically based pharmacokinetic modeling of
%   inhaled trichloroethylene and its oxidative metabolites in B6C3F1 mice. Toxicol Appl
%   Pharmacol 154: 264-278.
% Male B6C3F1 mice, 28-32 grams (N=6/time point)
% Inhalation of 100 or 600 ppm TCE for 4 hours

```

```

PlotOutput=[];
ResetDoses
MousePost

```

```

% Individual posterior parameters for Greenberg99_Mouse
QCC=12.63720; VPR=1.68707; DRESPEC=1.29007;
QFATC=0.046970; QGUTC=0.16539; QKIDC=0.090736; QLIVC=0.020620; QRAPC=0.45885; QSLWC=0.21743;
VBLDC=0.048843; VFATC=0.095830; VGUTC=0.048784; VKIDC=0.0170; VLIVC=0.049748; VPERFC=0.88970;
VRAPC=0.099860; VRESPEC=0.0007; VRESPLUMC=0.0046667; VSLWC=0.52893; FRACPLAS=0.46426;
PB=8.46339; PFAT=31.51674; PGUT=1.58511; PKID=2.00824; PLIV=2.54321; PRAP=1.78530;
PRESPEC=2.57955; PSLW=1.79547;
PRBCPLASTCA=1.34333; PBODTCAC=0.80650; PLIVTCAC=0.97610;
PBODTCOH=1.06438; PLIVTCOH=2.42338;
PBODTCOG=0.51194; PLIVTCOG=2.23550; PEFDCVGC=0.99218;
BMAXKDC=0.86506; KDISSOC=190.07692;
KAS=1.76738; KTSR=3.6840; KAD=0.28337; KTD=0.0; KASTCA=3.36020; KASTCOH=0.75435;
VMAXC=1861.07034; KMC=3.32849; CL=1.0; FRACTCAC=0.15695; FRACOTHERC=0.025047;
VMAXDCVGC=797.81957; KMDCVGC=1.0; CLDCVGC=0.55781;
VMAXKIDDCVGC=156.31052; KMKIDDCVGC=1.0; CLKIDDCVGC=0.42286;
VMAXLUNGLIV=0.21378; KMCLARA=0.012095; FRACLUNGSSYS=4.65527;
VMAXTCOH=1.17351; KMTCOH=1.10827; CLTCOH=1.0;
VMAXGLUCC=72.09610; KMGLUC=39.64639; CLGLUC=1.0; KMETTCOH=3.77726;
KURNTCAC=0.055753; KMETTCAC=0.54406;
KBILEC=1.07103; KEHRC=0.015561; KURNTCOGC=1.73703;
KDCVGC=0.18825; FRACKIDDCVCC=1.53158;
KNATC=0.11660; KKIDBIOACTC=0.087773;

```

```

BW=0.03; CONCLIST=[100.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=50.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)

```

```

PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[600.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Greenberg99_Mouse_Output.txt' @format=ascii

```

Larson92a_Mouse.m

```

% Larson J and Bull R. 1992. Species differences in the metabolism of trichloroethylene to the
% carcinogenic metabolites trichloroacetate and dichloroacetate. Toxicol Appl Pharmacol 115:
% 278-285.
% Male B6C3F1 mice (26.4 +/- 3.2 grams) (N=5-6/time point)
% Fasted 4 hr
% Oral dosing of 1.5, 4.5 or 15 mmol TCE/kg in Tween 80 (constant volume of 10 mL/kg to mice)
% (197.25, 591.75 and 1972.5 mg/kg)

PlotOutput=[];
ResetDoses
MousePost

% Individual posterior parameters for Larson92a_Mouse and Larson92b_Mouse
QCC=9.96327; VPR=1.68420; DRESPC=1.25232;
QFATC=0.08190; QGUTC=0.16018; QKIDC=0.090982; QLIVC=0.020520; QRAPC=0.42335; QSLWC=0.22308;
VBLDC=0.048657; VFATC=0.085540; VGUTC=0.048456; VKIDC=0.0170; VLIVC=0.046745; VPERFC=0.88970;
VRAPC=0.099920; VRESPC=0.0007; VRESPLUMC=0.0046639; VSLWC=0.54268; FRACPLAS=0.46212;
PB=22.94845; PFAT=34.66252; PGUT=1.54042; PKID=2.5840; PLIV=2.09013; PRAP=1.88626;
PRES=2.59614; PSLW=2.64663;
PRBCPLASTCA=1.03619; PBODTCAC=0.78409; PLIVTCAC=0.92637;
PBODTCOH=0.82676; PLIVTCOH=1.66840;
PBODTCOG=0.46415; PLIVTCOG=1.43556; PEFDCVGC=0.98497;
BMAXKDC=1.24791; KDISSOC=136.62348;
KAS=8.96206; KTS=1.83914; KAD=0.52556; KTD=0.0; KASTCA=8.53350; KASTCOH=0.71505;
VMAXC=2260.42257; KMC=3.89822; CL=1.0; FRACTCAC=0.15107; FRACOTHERC=0.023098;
VMAXDCVGC=798.05896; KMDCVGC=1.0; CLDCVGC=0.56483;
VMAXKIDDCVGC=155.08053; KMKIDDCVGC=1.0; CLKIDDCVGC=0.41769;
VMAXLUNGLIV=0.22073; KMCLARA=0.012830; FRACLUNGSYS=4.56766;
VMAXTCOHC=1.15824; KMTCOH=1.04419; CLTCOH=1.0;
VMAXGLUCC=51.57309; KMGLUC=58.09038; CLGLUC=1.0; KMETTCOHC=2.94468;
KURNTCAC=0.058964; KMETTCAC=0.56575;
KBILEC=1.09753; KEHRC=0.010631; KURNTCOGC=3.94392;
KDCVGC=0.18825; FRACKIDDCVCC=1.54265;
KNATC=0.11625; KKIDBIOACTC=0.087861;

```

```

BW=0.0264; PDOSE=197.25; TCHNG=0.05; TSTP=50.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=591.75;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=1972.5;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Larson92a_Mouse_Output.txt' @format=ascii

```

Larson92b_Mouse.m

```

% Larson J and Bull R. 1992. Metabolism and lipoperoxidative activity of trichloroacetate and
% dichloroacetate in rats and mice. Toxicol Appl Pharmacol 115: 268-277.
% Male B6C3FI mice (27 +/- 2 grams)
% Oral gavage of 5, 20 or 100 mg/kg TCA (5-20 uCi of [14C]TCA)

PlotOutput=[];
ResetDoses
MousePost

% Individual posterior parameters for Larson92a_Mouse and Larson92b_Mouse
QCC=9.96327; VPR=1.68420; DRESPC=1.25232;
QFATC=0.08190; QGUTC=0.16018; QKIDC=0.090982; QLIVC=0.020520; QRAPC=0.42335; QSLWC=0.22308;
VBLDC=0.048657; VFATC=0.085540; VGUTC=0.048456; VKIDC=0.0170; VLIVC=0.046745; VPERFC=0.88970;
VRAPC=0.099920; VRESPC=0.0007; VRESPLUMC=0.0046639; VSLWC=0.54268; FRACPLAS=0.46212;
PB=22.94845; PFAT=34.66252; PGUT=1.54042; PKID=2.5840; PLIV=2.09013; PRAP=1.88626;
PRES=2.59614; PSLW=2.64663;
PRBCPLASTCA=1.03619; PBODTCAC=0.78409; PLIVTCAC=0.92637;
PBODTCOH=0.82676; PLIVTCOH=1.66840;
PBODTCOG=0.46415; PLIVTCOG=1.43556; PEFDCVGC=0.98497;
BMAXKDC=1.24791; KDISSOC=136.62348;
KAS=8.96206; KTS=1.83914; KAD=0.52556; KTD=0.0; KASTCA=8.53350; KASTCOH=0.71505;
VMAXC=2260.42257; KMC=3.89822; CL=1.0; FRACTCAC=0.15107; FRACOTHERC=0.023098;
VMAXDCVGC=798.05896; KMDCVGC=1.0; CLDCVGC=0.56483;
VMAXKIDDCVGC=155.08053; KMKIDDCVGC=1.0; CLKIDDCVGC=0.41769;
VMAXLUNGLIV=0.22073; KMCLARA=0.012830; FRACLUNGSYS=4.56766;
VMAXTCOH=1.15824; KMTCOH=1.04419; CLTCOH=1.0;
VMAXGLUCC=51.57309; KMGLUC=58.09038; CLGLUC=1.0; KMETTCOH=2.94468;
KURNTCAC=0.058964; KMETTCAC=0.56575;
KBILEC=1.09753; KEHRC=0.010631; KURNTCOG=3.94392;
KDCVGC=0.18825; FRACKIDDCVCC=1.54265;
KNATC=0.11625; KKIDBIOACTC=0.087861;

BW=0.0264; PDOSETCA=20.0; TCHNG=0.05; TSTP=25.0; CINT=0.1;
start @NoCallback
plot(_t, _cplastca)

```

```

PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PODOSETCA=100.0;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Larson92b_Mouse_Output.txt' @format=ascii

```

Merdink98_Mouse.m

```

% Merdink J, Gonzalez-Leon A, Bull R and Schultz I. 1998. The extent of dichloroacetate formation
% from trichloroethylene, chloral hydrate, trichloroacetate, and trichloroethanol in B6C3F1
% mice. Toxicol Sci 45: 33-41.
% Male B6C3F1 mice (20-25 grams)
% Fasted 4-8 h prior to dosing
% IV dosing of 100 mg/kg TCE, as a suspension in 5% Alkamuls, into either an indwelling jugular
% vein cannula or a lateral tail vein

```

```

PlotOutput=[];
ResetDoses
MousePost

```

```

% Individual posterior parameters for Merdink98_Mouse
QCC=14.05960; VPR=2.16191; DRESPC=1.20889;
QFATC=0.071260; QGUTC=0.15623; QKIDC=0.090682; QLIVC=0.020420; QRAPC=0.45051; QSLWC=0.21090;
VBLDC=0.048731; VFATC=0.090370; VGUTC=0.048520; VKIDC=0.016988; VLIVC=0.045958; VPERFC=0.88970;
VRAPC=0.099680; VRESPC=0.0007; VRESPLUMC=0.0046713; VSLWC=0.53875; FRACPLAS=0.46852;
PB=12.71078; PFAT=37.09191; PGUT=1.55528; PKID=2.55139; PLIV=2.09662; PRAP=1.80643;
PRESP=2.59557; PSLW=2.27796;
PRBCPLASTCA=1.25841; PBODTCAC=0.83830; PLIVTCAC=0.94565;
PBODTCOH=0.89080; PLIVTCOH=1.85738;
PBODTCOG=0.45871; PLIVTCOG=1.34835; PEFDCVG=0.98908;
BMAXKDC=1.04109; KDISSOC=118.25329;
KAS=1.75822; KTSO=3.63279; KAD=0.27555; KTD=0.0; KASTCA=3.35013; KASTCOH=0.74461;
VMAXC=1375.13481; KMC=3.85557; CL=1.0; FRACTCAC=0.15245; FRACOTHERC=0.024947;
VMAXDCVGC=799.97660; KMDCVGC=1.0; CLDCVG=0.56173;
VMAXKIDDCVGC=155.60871; KMKIDDCVGC=1.0; CLKIDDCVG=0.42016;
VMAXLUNGLIV=0.11543; KMCLARA=0.013287; FRACLUNGYSYC=4.22492;
VMAXTCOHC=1.79445; KMTCOH=0.86174; CLTCOH=1.0;
VMAXGLUCC=79.20188; KMGLUC=23.92682; CLGLUC=1.0; KMETTCOHC=3.66930;
KURNTCAC=0.055976; KMETTCAC=0.53784;
KBILEC=1.04220; KEHRC=0.012131; KURNTCOGC=12.70727;
KDCVGC=0.18844; FRACKIDDCVCC=1.54527;
KNATC=0.11590; KKIDBIOACTC=0.088213;

BW=0.0225; IVDOSE=100.0; TCHNG=0.05; TSTP=7.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Merdink98_Mouse_Output.txt' @format=ascii

```


Prout85_Mouse.m

```
% Prout M, Provan W and Green T. 1985. Species differences in response to trichloroethylene: I
% pharmacokinetics in rats and mice. Toxicol Appl Pharmacol 79: 389-400.
% Male B6C3F1 and Swiss-Webster mice, 25-32 grams (N=4 or 2 mice/group)
% Oral dosing of 10, 500, 1000 or 2000 mg/kg trichloro[14C]ethylene in corn oil (0.5 mL)
% (containing 10 uCi)
```

```
PlotOutput=[];
ResetDoses
MousePost
```

```
% Individual posterior parameters for Green85_Mouse and Prout85_Mouse
QCC=14.97684; VPR=1.99489; DRESPC=1.25961;
QFATC=0.071330; QGUTC=0.15679; QKIDC=0.090964; QLIVC=0.02040; QRAPC=0.44375; QSLWC=0.21676;
VBLDC=0.048731; VFATC=0.090440; VGUTC=0.048515; VKIDC=0.0170; VLIVC=0.048631; VPERFC=0.88970;
VRAPC=0.099870; VRESPC=0.0007; VRESPLUMC=0.0046639; VSLWC=0.53581; FRACPLAS=0.45178;
PB=15.39758; PFAT=38.56206; PGUT=1.56151; PKID=2.55803; PLIV=2.09348; PRAP=1.83661;
PRES=2.58070; PSLW=2.40307;
PRBCPLASTCA=1.82550; PBODTCAC=0.80023; PLIVTCAC=0.93437;
PBODTCOH=0.92715; PLIVTCOH=1.87417;
PBODTCOG=0.46667; PLIVTCOG=1.22135; PEFDCVG=0.98284;
BMAXKDC=1.17971; KDISSOC=287.09950;
KAS=0.60170; KTS=2.40584; KAD=0.13656; KTD=0.0; KASTCA=3.41439; KASTCOH=0.71384;
VMAXC=2507.03749; KMC=3.86329; CL=1.0; FRACTCAC=0.16557; FRACOTHERC=0.026017;
VMAXDCVGC=803.02229; KMDCVGC=1.0; CLDCVG=0.56891;
VMAXKIDDCVGC=155.01852; KMKIDDCVGC=1.0; CLKIDDCVG=0.42168;
VMAXLUNGLIV=0.44584; KMCLARA=0.011820; FRACLUNGSYS=4.27165;
VMAXTCOH=2.45837; KMTCOH=0.86459; CLTCOH=1.0;
VMAXGLUC=85.11472; KMGLUC=13.83221; CLGLUC=1.0; KMETTCOH=3.59664;
KURNTCAC=0.029634; KMETTCAC=0.53360;
KBILEC=0.94189; KEHRC=0.012119; KURNTCOG=31.75894;
KDCVGC=0.1890; FRACKIDDCVCC=1.53757;
KNATC=0.11695; KKIDBIOACTC=0.088213;

BW=0.0295; PDOSE=1000.0; TCHNG=0.05; TSTP=45.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Prout85_Mouse_Output.txt' @format=ascii
```

Templin93_Mouse.m

```
% Templin M, Parker J and Bull R. 1993. Relative formation of dichloroacetate and
% trichloroacetate from trichloroethylene in male B6C3F1 mice. Toxicol Appl Pharmacol 123: 1-8.
% Male B6C3F1 mice, 7 weeks of age (N=4/time point)
% Oral dosing of 3.8 mmol/kg (499.282 mg/kg) trichloroethylene in 2% polyoxyethylcnc-sorbitan
% monooleate (Tween 80)
```

```
PlotOutput=[];
ResetDoses
MousePost
```

```
% Individual posterior parameters for Templin93_Mouse
QCC=17.67595; VPR=2.27821; DRESPC=1.20166;
QFATC=0.072940; QGUTC=0.15792; QKIDC=0.09080; QLIVC=0.020480; QRAPC=0.44251; QSLWC=0.21535;
VBLDC=0.048755; VFATC=0.08260; VGUTC=0.048569; VKIDC=0.016995; VLIVC=0.049148; VPERFC=0.88970;
VRAPC=0.099820; VRESPC=0.0007; VRESPLUMC=0.0046667; VSLWC=0.54311; FRACPLAS=0.47039;
PB=11.20377; PFAT=34.59326; PGUT=1.57784; PKID=2.56008; PLIV=2.12427; PRAP=1.83051;
PRES=2.58713; PSLW=2.35787;
PRBCPLASTCA=1.25766; PBODTCAC=0.92120; PLIVTCAC=0.93624;
```

```

PBODTCOH=0.82404; PLIVTCOH=1.78508;
PBODTCOG=0.46625; PLIVTCOG=1.27151; PEFDCVG=0.98288;
BMAXKDC=0.95426; KDISSOC=97.21829;
KAS=1.76121; KTS=2.30943; KAD=1.01895; KTD=0.0; KASTCA=3.30686; KASTCOH=0.73705;
VMAXC=2789.77730; KMC=2.73333; CL=1.0; FRACTCAC=0.11993; FRACOTHERC=0.024625;
VMAXDCVGC=799.81662; KMDCVGC=1.0; CLDCVG=0.56522;
VMAXKIDDCVGC=155.01852; KMKIDDCVGC=1.0; CLKIDDCVG=0.41878;
VMAXLUNGLIV=0.16626; KMCLARA=0.012753; FRACLUNGSYS=4.31458;
VMAXTCOH=1.75611; KMTCOH=0.88329; CLTCOH=1.0;
VMAXGLUC=65.49672; KMGLUC=22.94270; CLGLUC=1.0; KMETTCOH=3.25763;
KURNTCAC=0.052192; KMETTCAC=0.51804;
KBILEC=0.98275; KEHRC=0.012034; KURNTCOG=5.48038;
KDCVGC=0.18731; FRACKIDDCVCC=1.53465;
KNATC=0.11602; KKIDBIOACTC=0.088655;

BW=0.027; PDSE=500.0; TCHNG=0.05; TSTP=37.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Templin93_Mouse_Output.txt' @format=ascii

```

APPENDIX J

M Files for Rat Validation Figures

The following M files are for generating rat output for validation figures in Appendix G.

Bernauer96_Rat.m

```
% Bernauer U, Birner G, Dekant W and Henschler D. 1996. Biotransformation of trichloroethene:
% Dose-dependent excretion of 2,2,2-trichloro-metabolites and mercapturic acids in rats and
% humans after inhalation. Arch Toxicol 70: 338-346.
% http://dx.doi.org/10.1007/s002040050283.
% 2 male Wistar (300-350 g) and 2 female Wistar (200-250 g) exposed simultaneously with humans
% Inhalation of 40, 80 or 160 ppm TCE stabilized with diisopropylamine (40 ppm) for 6 hours
```

```
PlotOutput=[];
ResetDoses
RatPost
```

```
% Individual posterior parameters for Bernauer96_Rat
QCC=13.19330; VPR=1.04305; DRESPC=2.54187;
QFATC=0.077980; QGUTC=0.16493; QKIDC=0.14128; QLIVC=0.021420; QRAPC=0.28056; QSLWC=0.31382;
VBLDC=0.074148; VFATC=0.061670; VGUTC=0.031757; VKIDC=0.0069321; VLIVC=0.034816;
VPERFC=0.89950; VRAPC=0.087507; VRESPC=0.00049655; VRESPLUMC=0.0046807; VSLWC=0.60217;
FRACPLAS=0.54696;
PB=18.67232; PFAT=28.66041; PGUT=1.22039; PKID=1.22695; PLIV=1.55674; PRAP=1.37828;
PRESP=0.96017; PSLW=0.71418;
PRBCPLASTCA=0.48207; PBODTCAC=0.76076; PLIVTCAC=1.94160;
PBODTCOH=1.03652; PLIVTCOH=1.22823;
PBODTCOG=1.40405; PLIVTCOG=13.08366; PEFFDCVG=1.0;
BMAXKDC=1.14697; KDISSOC=268.22632;
KAS=2.37121; KTS=2.86051; KAD=0.19340; KTD=0.0; KASTCA=1.40621; KASTCOH=0.69496;
VMAXC=647.86974; KMC=1.06027; CL=1.0; FRACTCAC=0.058400; FRACOTHERC=1.09635;
VMAXDCVGC=792.07394; KMDCVGC=1.0; CLDCVG=0.084307;
VMAXKIDDCVGC=0.91554; KMKIDDCVGC=1.0; CLKIDDCVG=5.96161;
VMAXLUNGLIV=0.023221; KMCLARA=0.026944; FRACLUNGSYS=1.73343;
VMAXTCOHC=1.71275; KMTCOH=28.24736; CLTCOH=1.0;
VMAXGLUCC=10.30882; KMGLUC=1.41213; CLGLUC=1.0; KMETTCOHC=2.40608;
KURNTCAC=0.039121; KMETTCAC=0.42431;
KBILEC=10.88080; KEHRC=1.22581; KURNTCOGC=9.28047;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0016189; KKIDBIOACTC=0.0062324;
```

```
BW=0.325; CONCLIST=[40.0 0.0 0.0]; STRTNEXTLIST=[6.0 50.0]; TSTRT=0.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
CONCLIST=[80.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
CONCLIST=[160.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
```

```

Output_Check
Output_Check_Reset

save PlotOutput @file='Bernauer96_Rat_Output.txt' @format=ascii

Dallas91_Rat.m
% Dallas C, Gallo J, Ramanathan R, Muralidhara S and Bruckner J. 1991. Physiological
% pharmacokinetic modeling of inhaled trichloroethylene in rats. Toxicol Appl Pharmacol 110:
% 303-314.
% Male SD rats (325-375 g)
% Nose-only inhalation of 50 or 500 ppm TCE for 2 hours

PlotOutput=[];
ResetDoses
RatPost

% Individual posterior parameters for Dallas91_Rat
QCC=20.79399; VPR=0.65958; DRESPC=2.71801;
QFATC=0.065422; QGUTC=0.19324; QKIDC=0.14128; QLIVC=0.022260; QRAPC=0.27456; QSLWC=0.30324;
VBLDC=0.073882; VFATC=0.060424; VGUTC=0.031526; VKIDC=0.0069923; VLIVC=0.030760;
VPERFC=0.89950; VRAPC=0.086918; VRESPC=0.00049750; VRESPLUMC=0.0046947; VSLWC=0.60850;
FRACPLAS=0.55067;
PB=12.75652; PFAT=26.63076; PGUT=1.09809; PKID=1.22312; PLIV=1.52054; PRAP=1.19236;
PRES=0.95535; PSLW=0.50579;
PRBCPLASTCA=0.48411; PBODTCAC=0.96831; PLIVTCAC=1.48708;
PBODTCOH=1.06038; PLIVTCOH=1.25775;
PBODTCOG=1.37377; PLIVTCOG=10.98317; PEFFDCVG=1.0;
BMAXKDC=1.16170; KDISSOC=267.97162;
KAS=2.40176; KTS=2.90955; KAD=0.19301; KTD=0.0; KASTCA=1.40804; KASTCOH=0.69267;
VMAXC=256.67987; KMC=0.38080; CL=1.0; FRACTCAC=0.082049; FRACOTHERC=0.31664;
VMAXDCVGC=787.33572; KMDCVGC=1.0; CLDCVG=0.093015;
VMAXKIDDCVGC=1.29792; KMKIDDCVGC=1.0; CLKIDDCVG=4.89073;
VMAXLUNGLIV=0.019579; KMCLARA=0.035084; FRACLUNGSYS=1.98695;
VMAXTCOHC=2.01114; KMTCOH=22.30922; CLTCOH=1.0;
VMAXGLUCC=26.52267; KMGLUC=5.65760; CLGLUC=1.0; KMETTCOHC=1.92745;
KURNTCAC=0.038926; KMETTCAC=0.32693;
KBILEC=7.12066; KEHRC=1.43735; KURNTCOGC=10.61122;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021356; KKIDBIOACTC=0.0068741;

BW=0.35; CONCLIST=[50.0 0.0 0.0]; STRTNEXTLIST=[2.0 10.0]; TSTRT=0.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cart, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cexhresp, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[500.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cart, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cexhresp, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Dallas91_Rat_Output.txt' @format=ascii

```

Fisher89_Rat.m

% Fisher J, Whittaker T, Taylor D, Clewell H III and Andersen M. 1989. Physiologically based
% pharmacokinetic modeling of the pregnant rat: A multiroute exposure model for
% trichloroethylene and its metabolite, trichloroacetic acid. Toxicol Appl Pharmacol 99: 395-
% 414. [http://dx.doi.org/10.1016/0041-008X\(89\)90149-X](http://dx.doi.org/10.1016/0041-008X(89)90149-X).
% Female F344 rats
% Closed-chamber inhalation of 300, 1100, 2200 or 5100 ppm TCE

```
PlotOutput=[];  
ResetDoses  
RatPost
```

% Individual posterior parameters for Fisher89_Rat

```
QCC=17.65226; VPR=1.46925; DRESPC=2.57796;  
QFATC=0.079870; QGUTC=0.17151; QKIDC=0.14100; QLIVC=0.021546; QRAPC=0.27319; QSLWC=0.31288;  
VBLDC=0.073993; VFATC=0.077000; VGUTC=0.031766; VKIDC=0.0069671; VLIVC=0.033225;  
VPERFC=0.89950; VRAPC=0.087322; VRESPC=0.00049555; VRESPLUMC=0.0046900; VSLWC=0.58873;  
FRACPLAS=0.55067;  
PB=17.18510; PFAT=30.86543; PGUT=1.18836; PKID=1.22781; PLIV=1.54695; PRAP=1.28901;  
PRES=0.94884; PSLW=0.61901;  
PRBCPLASTCA=0.48195; PBODTCAC=0.97459; PLIVTCAC=1.46905;  
PBODTCOH=1.06368; PLIVTCOH=1.25477;  
PBODTCOG=1.37501; PLIVTCOG=11.02719; PEFFDCVG=1.0;  
BMAXKDC=1.15955; KDISSOC=268.27192;  
KAS=2.46231; KTS=2.93880; KAD=0.19090; KTD=0.0; KASTCA=1.42775; KASTCOH=0.69205;  
VMAXC=799.37459; KMC=5.03555; CL=1.0; FRACCTCAC=0.081314; FRACOTHERC=0.33387;  
VMAXDCVGC=796.84067; KMDCVGC=1.0; CLDCVG=0.094025;  
VMAXKIDDCVGC=1.28629; KMKIDDCVGC=1.0; CLKIDDCVG=4.69426;  
VMAXLUNGLIV=0.268689; KMCLARA=0.014066; FRACLUNGSYS=1.93964;  
VMAXTCOH=2.00712; KMTTCOH=22.42104; CLTCOH=1.0;  
VMAXGLUC=26.60236; KMGLUC=5.66326; CLGLUC=1.0; KMETTCOH=1.91210;  
KURNTCAC=0.038577; KMETTCAC=0.32368;  
KBILEC=7.14920; KEHRC=1.45995; KURNTCOG=10.53720;  
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;  
KNATC=0.0021250; KKIDBIOACTC=0.0069570;
```

```
BW=0.161; CC=1; CONCLIST(1)=300.0; STRTNEXTLIST(1)=10.0; TSTRT=0.0; NRODENTS=4.0; VCHC=9.1;  
KLOSSC=exp(-3.912); TSTP=2.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
BW=0.159; CONCLIST(1)=1100.0; STRTNEXTLIST(1)=10.0; TSTP=3.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
BW=0.159; CONCLIST(1)=2200.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
BW=0.175; CONCLIST(1)=5100.0; STRTNEXTLIST(1)=10.0; TSTP=7.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');  
i = i + 1;  
Output_Check
```

```

Output_Check_Reset
save PlotOutput @file='Fisher89_Rat_Output.txt' @format=ascii

Fisher91_Rat.m
% Fisher J, Gargas M, Allen B and Andersen M. 1991. Physiologically based pharmacokinetic
% modeling with trichloroethylene and its metabolite, trichloroacetic acid, in the rat and
% mouse. Toxicol Appl Pharmacol 109: 183-195.
% Female and male Fischer 344 rats
% Inhalation of 600 or 505 ppm TCE for 4 hours

PlotOutput=[];
ResetDoses
RatPost

% Individual posterior parameters for Fisher91_Rat female
QCC=14.01228; VPR=0.96953; DRESPC=2.56870;
QFATC=0.083790; QGUTC=0.16662; QKIDC=0.14114; QLIVC=0.021420; QRAPC=0.26904; QSLWC=0.31799;
VBLDC=0.074296; VFATC=0.068334; VGUTC=0.031776; VKIDC=0.0069573; VLIVC=0.034000;
VPERFC=0.89950; VRAPC=0.087657; VRESPC=0.00049710; VRESPLUMC=0.0046853; VSLWC=0.59598;
FRACPLAS=0.55385;
PB=19.35677; PFAT=29.60748; PGUT=1.24729; PKID=1.22802; PLIV=1.56012; PRAP=1.45436;
PRES=0.95603; PSLW=0.77855;
PRBCPLASTCA=0.45976; PBODTCAC=0.84520; PLIVTCAC=1.57651;
PBODTCOH=0.97810; PLIVTCOH=1.10469;
PBODTCOG=1.36105; PLIVTCOG=12.26027; PEFFDCVG=1.0;
BMAXKDC=1.15878; KDISSOC=319.15316;
KAS=2.39576; KTS=2.90374; KAD=0.19205; KTD=0.0; KASTCA=1.41893; KASTCOH=0.69635;
VMAXC=536.26565; KMC=1.05393; CL=1.0; FRACTCAC=0.057531; FRACOTHERC=0.31411;
VMAXDCVGC=790.49137; KMDCVGC=1.0; CLDCVG=0.093940;
VMAXKIDDCVGC=1.29015; KMKIDDCVGC=1.0; CLKIDDCVG=4.69896;
VMAXLUNGLIV=0.032975; KMCLARA=0.022937; FRACLUNGSYS=1.97645;
VMAXTCOH=3.19312; KMTCOH=22.28692; CLTCOH=1.0;
VMAXGLUC=15.30225; KMGLUC=5.64065; CLGLUC=1.0; KMETTCOH=1.40832;
KURNTCAC=0.038232; KMETTCAC=0.33121;
KBILEC=9.28128; KEHRC=1.56534; KURNTCOG=9.67855;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021250; KKIDBIOACTC=0.0069362;

BW=0.186; CONCLIST=[600.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

ResetDoses
RatPost

% Individual posterior parameters for Fisher91_Rat male
QCC=15.90867; VPR=1.27043; DRESPC=2.53375;
QFATC=0.085190; QGUTC=0.16754; QKIDC=0.14142; QLIVC=0.021462; QRAPC=0.27053; QSLWC=0.31386;
VBLDC=0.074296; VFATC=0.062391; VGUTC=0.031776; VKIDC=0.0069734; VLIVC=0.033147;
VPERFC=0.89950; VRAPC=0.087542; VRESPC=0.00049730; VRESPLUMC=0.0046853; VSLWC=0.60288;
FRACPLAS=0.55332;
PB=20.33620; PFAT=28.45935; PGUT=1.22541; PKID=1.22758; PLIV=1.55741; PRAP=1.40568;
PRES=0.96099; PSLW=0.72977;
PRBCPLASTCA=0.46414; PBODTCAC=0.98754; PLIVTCAC=1.49259;
PBODTCOH=1.00624; PLIVTCOH=1.24377;
PBODTCOG=1.36733; PLIVTCOG=11.35166; PEFFDCVG=1.0;
BMAXKDC=1.15931; KDISSOC=295.87027;
KAS=2.43099; KTS=2.87485; KAD=0.19205; KTD=0.0; KASTCA=1.39850; KASTCOH=0.68441;
VMAXC=446.94237; KMC=1.30411; CL=1.0; FRACTCAC=0.072553; FRACOTHERC=0.27226;
VMAXDCVGC=792.07394; KMDCVGC=1.0; CLDCVG=0.093650;
VMAXKIDDCVGC=1.28886; KMKIDDCVGC=1.0; CLKIDDCVG=4.71308;

```

```

VMAXLUNGLIV=0.034369; KMCLARA=0.023029; FRACLUNGSYSC=1.97092;
VMAXTCOHC=2.31729; KMTCOH=22.02108; CLTCOH=1.0;
VMAXGLUCC=22.82828; KMGLUC=5.68028; CLGLUC=1.0; KMETTCOHC=1.83363;
KURNTCAC=0.035897; KMETTCAC=0.31411;
KBILEC=7.69830; KEHRC=1.52364; KURNTCOGC=10.65375;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021207; KKIDBIOACTC=0.0069849;

BW=0.236; CONCLIST=[505.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher91_Rat_Output.txt' @format=ascii

```

Green85_Rat.m

```

% Green T and Prout M. 1985. Species differences in response to trichloroethylene: II.
% Biotransformation in rats and mice. Toxicol Appl Pharmacol 79: 401-411.
% http://dx.doi.org/10.1016/0041-008X\(85\)90138-3.
% Male rats (180 to 200 g) of the Osborne-Mendel and Alderley Park (Wistar derived) strains
% IV dose of 10 mg/kg Trichloro[2-14C]acetic acid (12.5 uCi) in water (0.25 mL) injected in tail
% vein
% OR oral dose of 75 mg/kg Trichloro[2-14C]acetic acid (9 uCi) in water
% OR oral dose of 500 mg/kg TCE (10 uCi) in corn oil (5 mL/kg) with or without bile cannulated

```

```

PlotOutput=[];
ResetDoses
RatPost

```

```

% Individual posterior parameters for Green85_Rat and Prout85_Rat (non-specified rats)
QCC=18.64847; VPR=1.43685; DRESPC=2.51633;
QFATC=0.099610; QGUTC=0.16968; QKIDC=0.14128; QLIVC=0.021462; QRAPC=0.26147; QSLWC=0.30650;
VBLDC=0.074074; VFATC=0.076510; VGUTC=0.031709; VKIDC=0.0069573; VLIVC=0.031946;
VPERFC=0.89950; VRAPC=0.087472; VRESPC=0.00049720; VRESPLUMC=0.0046807; VSLWC=0.59033;
FRACPLAS=0.55544;
PB=17.65188; PFAT=31.84998; PGUT=1.20150; PKID=1.22892; PLIV=1.54848; PRAP=1.40922;
PRESP=0.95345; PSLW=0.76496;
PRBCPLASTCA=0.48304; PBODTCAC=1.15750; PLIVTCAC=1.34315;
PBODTCOH=1.13614; PLIVTCOH=1.26239;
PBODTCOG=1.39286; PLIVTCOG=9.13729; PEFDCVGC=1.0;
BMAXKDC=1.10534; KDISSOC=291.64902;
KAS=0.29288; KTS=10.92441; KAD=0.11114; KTD=0.0; KASTCA=1.85484; KASTCOH=0.69323;
VMAXC=491.82829; KMC=0.94320; CL=1.0; FRACCTC=0.091316; FRACOTHERC=0.18563;
VMAXDCVGC=784.97725; KMDCVGC=1.0; CLDCVGC=0.093659;
VMAXKIDDCVGC=1.28629; KMKIDDCVGC=1.0; CLKIDDCVGC=4.69426;
VMAXLUNGLIV=0.029960; KMCLARA=0.023802; FRACLUNGSYSC=1.97289;
VMAXTCOHC=2.39121; KMTCOH=19.41411; CLTCOH=1.0;
VMAXGLUCC=55.86846; KMGLUC=3.70988; CLGLUC=1.0; KMETTCOHC=1.90999;
KURNTCAC=0.037587; KMETTCAC=0.29200;
KBILEC=4.79225; KEHRC=1.21240; KURNTCOGC=12.02409;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021271; KKIDBIOACTC=0.0069223;

```

```

BW=0.19; IVDOSSETCA=10.0; TCHNG=0.05; TSTP=25.0;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

IVDOSSETCA=0.0; PODOSSETCA=75.0;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');

```

```

i = i + 1;
Output_Check
Output_Check_Reset

PODOSETCA=0.0; PDOSE=500.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Bile Cannulated
KEHRC=exp(-100.0);
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _abiletcog, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Green85_Rat_Output.txt' @format=ascii

```

Hissink02_Rat.m

```

% Hissink E, Bogaards J, Freidig A, Commandeur J, Vermeulen N and van Bladeren P. 2002. The use
% of in vitro metabolic parameters and physiologically based pharmacokinetic (PBPK) modeling to
% explore the risk assessment of trichloroethylene. Environ Toxicol Pharmacol 11: 259-271.
% http://dx.doi.org/10.1016/S1382-6689(02)00019-4.
% Adult male Wistar rats (250-300 g, 9-10 weeks old)
% IV dosing of 10 or 75 mg/kg [1,2-14C]-trichloroethylene in Intralipid† 30% (specific activity:
% 61.3 or 5.70 KBq/mg)
% OR oral dose of 100 or 1000 mg/kg [1,2-14C]-trichloroethylene in corn oil (specific activity:
% 9.22 or 0.83 KBq/mg)

```

```

PlotOutput=[];
ResetDoses
RatPost

```

```

% Individual posterior parameters for Hissink02_Rat
QCC=14.92987; VPR=1.05575; DRESPC=2.55104;
QFATC=0.093870; QGUTC=0.16417; QKIDC=0.14128; QLIVC=0.021378; QRAPC=0.26343; QSLWC=0.31587;
VBLDC=0.074148; VFATC=0.067018; VGUTC=0.031731; VKIDC=0.0069769; VLIVC=0.032803;
VPERFC=0.89950; VRAPC=0.087780; VRESPC=0.00049700; VRESPLUMC=0.0046853; VSLWC=0.59855;
FRACPLAS=0.54537;
PB=20.76757; PFAT=29.05286; PGUT=1.23130; PKID=1.23034; PLIV=1.56211; PRAP=1.50797;
PRESP=0.96038; PSLW=0.87921;
PRBCPLASTCA=0.47650; PBODTCAC=0.89846; PLIVTCAC=1.30985;
PBODTCOH=1.21921; PLIVTCOH=0.94929;
PBODTCOG=1.52831; PLIVTCOG=11.54629; PEFFDCVG=1.0;
BMAXKDC=1.16659; KDISSOC=268.62090;
KAS=0.45859; KTSO=0.49357; KAD=0.09190; KTD=0.0; KASTCA=1.41538; KASTCOH=0.69447;
VMAXC=529.65701; KMC=0.53823; CL=1.0; FRACTCAC=0.079148; FRACOTHERC=0.05563;
VMAXDCVGC=788.91197; KMDCVGC=1.0; CLDCVG=0.092959;
VMAXKIDDCVGC=1.30573; KMKIDDCVGC=1.0; CLKIDDCVG=4.82274;
VMAXLUNGLIV=0.029431; KMCLARA=0.024600; FRACLUNGSSYS=1.87274;
VMAXTCOHC=1.94877; KMTCOH=22.33154; CLTCOH=1.0;
VMAXGLUCC=64.32832; KMGLUC=4.87441; CLGLUC=1.0; KMETTCOHC=1.03297;
KURNTCAC=0.045226; KMETTCAC=0.29405;
KBILEC=7.00063; KEHRC=1.36588; KURNTCOGC=9.02422;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021292; KKIDBIOACTC=0.0069293;

BW=0.275; IVDSE=10.0; TCHNG=0.05; TSTP=170.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');

```



```

i = i + 1;
Output_Check
Output_Check_Reset

IVDOSE=75.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

IVDOSE=0.0; PDOSE=100.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=1000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Hissink02_Rat_Output.txt' @format=ascii

```

Kaneko94_Rat.m

```

% Kaneko T, Wang P-Y and Sato A. 1994. Enzymes induced by ethanol differently affect the
% pharmacokinetics of trichloroethylene and 1,1,1-trichloroethane. Occup Environ Med 51: 113-
% 119.
% Male Wistar rats, 8 weeks old, put on study at 10 weeks
% Inhalation of 50, 100, 500 or 1000 ppm TCE for 6 hours

PlotOutput=[];
ResetDoses
RatPost

% Individual posterior parameters for Kaneko94_Rat
QCC=12.43747; VPR=0.70149; DRESPC=2.64164;
QFATC=0.096320; QGUTC=0.17396; QKIDC=0.14114; QLIVC=0.021609; QRAPC=0.25335; QSLWC=0.31362;
VBLDC=0.074222; VFATC=0.073570; VGUTC=0.031808; VKIDC=0.0069664; VLIVC=0.035088;
VPERFC=0.89950; VRAPC=0.087718; VRESPC=0.00049605; VRESPLUMC=0.0046760; VSLWC=0.58963;
FRACPLAS=0.57346;
PB=20.76632; PFAT=30.87778; PGUT=1.24505; PKID=1.23375; PLIV=1.56019; PRAP=1.44508;
PRESP=0.95859; PSLW=0.78441;
PRBCPLASTCA=0.50476; PBODTCAC=1.65147; PLIVTCAC=1.58870;
PBODTCOH=0.87351; PLIVTCOH=1.63177;
PBODTCOG=1.33330; PLIVTCOG=13.52263; PEFFDCVG=1.0;
BMAXKDC=1.19767; KDISSOC=268.43293;
KAS=2.44098; KTS=2.94174; KAD=0.19224; KTD=0.0; KASTCA=1.45514; KASTCOH=0.69698;
VMAXC=537.60799; KMC=0.74791; CL=1.0; FRACTCAC=0.051076; FRACOTHERC=0.67624;
VMAXDCVGC=788.12345; KMDCVGC=1.0; CLDCVG=0.093108;
VMAXKIDDCVGC=1.28886; KMKIDDCVGC=1.0; CLKIDDCVG=4.70837;
VMAXLUNGLIV=0.041953; KMCLARA=0.024429; FRACLUNGSYS=2.06700;
VMAXTCOH=1.53265; KMTTCOH=30.05413; CLTCOH=1.0;
VMAXGLUC=7.42609; KMGLUC=4.84526; CLGLUC=1.0; KMETTCOH=2.86051;
KURNTCAC=0.021108; KMETTCAC=0.32014;
KBILEC=12.94876; KEHRC=1.66896; KURNTCOG=9.14230;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021186; KKIDBIOACTC=0.0069501;

```

```

CONCLIST=[50.0 0.0 0.0]; STRTNEXTLIST=[6.0 50.0]; TSTRT=0.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[100.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[500.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[1000.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Kaneko94_Rat_Output.txt' @format=ascii

```

Keys03_Rat.m

```

% Keys D, Bruckner J, Muralidhara S and Fisher J. 2003. Tissue dosimetry expansion and cross-
% validation of rat and mouse physiologically based pharmacokinetic models for
% trichloroethylene. Toxicol Sci 76: 35-50.
% http://dx.doi.org/10.1093/toxsci/kfg212.
% Male SD rats (0.291-0.355 g)
% Intra-arterial dosing of 8 mg/kg TCE in 5% Alkamuls® aqueous emulsion (injected volume of
% 0.3 ml/animal) injected over 30-second period
% OR inhalation of 50 or 500 ppm TCE for 2 hr
% OR oral dosing of 8 mg TCE/kg TCE in 5% Alkamuls® (total volume 0.7 to 1.0 ml per rat)

```

```

PlotOutput=[];
ResetDoses
RatPost

```

```

% Individual posterior parameters for Keys03_Rat
QCC=21.67076; VPR=1.37418; DRESPC=2.53704;
QFATC=0.053508; QGUTC=0.19156; QKIDC=0.14269; QLIVC=0.022092; QRAPC=0.36453; QSLWC=0.22562;
VBLDC=0.072416; VFATC=0.086310; VGUTC=0.030682; VKIDC=0.0069118; VLIVC=0.030994;
VPERFC=0.89950; VRAPC=0.086082; VRESPC=0.00049705; VRESPLUMC=0.0046807; VSLWC=0.58561;
FRACPLAS=0.54961;
PB=14.05731; PFAT=40.24706; PGUT=0.91363; PKID=1.02754; PLIV=1.66557; PRAP=1.35281;
PRES=0.95109; PSLW=1.03270;
PRBCPLASTCA=0.48210; PBODTCAC=0.97479; PLIVTCAC=1.48604;
PBODTCOH=1.05969; PLIVTCOH=1.26169;
PBODTCOG=1.37694; PLIVTCOG=11.11576; PEFDCVG=1.0;
BMAXKDC=1.16307; KDISSOC=268.87352;

```

```

KAS=214.00513; KTS=14.38232; KAD=0.39856; KTD=0.0; KASTCA=1.42818; KASTCOH=0.68482;
VMAXC=469.99857; KMC=1.37509; CL=1.0; FRACTCAC=0.081559; FRACOTHERC=0.31537;
VMAXDCVGC=792.07394; KMDCVGC=1.0; CLDCVG=0.093612;
VMAXKIDDCVGC=1.29921; KMKIDDCVGC=1.0; CLKIDDCVG=4.83723;
VMAXLUNGLIV=0.069446; KMCLARA=0.019722; FRACLUNGSYS=1.97921;
VMAXTCOHC=2.01355; KMTCOH=22.53343; CLTCOH=1.0;
VMAXGLUC=27.33041; KMGLUC=5.56780; CLGLUC=1.0; KMETTCOHC=1.89572;
KURNTCAC=0.038887; KMETTCAC=0.32433;
KBILEC=7.24999; KEHRC=1.44831; KURNTCOGC=10.53720;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021356; KKIDBIOACTC=0.0069362;

```

```

BW=0.355; IADOSE=8.0; TCHNG=0.05; TSTP=25.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cgut, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cmus, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

IADOSE=0.0;
BW=0.291; CONCLIST=[50.0 0.0 0.0]; STRTNEXTLIST=[2.0 50.0]; TSTRT=0.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cgut, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cmus, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

BW=0.269; CONCLIST=[500.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cgut, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cmus, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

CONCLIST=[0.0 0.0 0.0]; STRTNEXTLIST=[50000.0 0.0];
BW=0.355; PDOSE=8.0; TCHNG=0.05;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cgut, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cmus, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

save PlotOutput @file='Keys03_Rat_Output.txt' @format=ascii

```

Kimmerle73_Rat.m

```
% Kimmerle G and Eben A. 1973. Metabolism, excretion and toxicology of trichloroethylene after
% inhalation: 1. Experimental exposure on rats. Arch Toxicol 30: 115-126.
% http://dx.doi.org/10.1007/BF02425929.
% Male Wistar rats
% Inhalation of 0, 49, 54, 175, 330 or 3160 ppm TCE for 4 hr
```

```
PlotOutput=[];
ResetDoses
RatPost
```

```
% Individual posterior parameters for Kimmerle73_Rat
```

```
QCC=20.34559; VPR=1.50208; DRESPC=2.77042;
QFATC=0.092540; QGUTC=0.17886; QKIDC=0.14128; QLIVC=0.021714; QRAPC=0.25239; QSLWC=0.31322;
VBLDC=0.074148; VFATC=0.057001; VGUTC=0.031850; VKIDC=0.0069664; VLIVC=0.034408;
VPERFC=0.89950; VRAPC=0.087551; VRESPC=0.00049710; VRESPLUMC=0.0046853; VSLWC=0.60708;
FRACPLAS=0.54802;
PB=34.11177; PFAT=26.83835; PGUT=1.24991; PKID=1.22736; PLIV=1.56649; PRAP=1.42218;
PRES=0.95349; PSLW=0.76734;
PRBCPLASTCA=0.48051; PBODTCAC=0.92307; PLIVTCAC=1.43335;
PBODTCOH=0.85587; PLIVTCOH=1.82917;
PBODTCOG=1.37680; PLIVTCOG=10.53143; PEFFDCVG=1.0;
BMAXKDC=1.16285; KDISSOC=268.68807;
KAS=2.43172; KTD=2.88637; KAD=0.18900; KTD=0.0; KASTCA=1.43362; KASTCOH=0.70195;
VMAXC=604.43169; KMC=0.41833; CL=1.0; FRACTCAC=0.089687; FRACOTHERC=1.71875;
VMAXDCVGC=789.70128; KMDCVGC=1.0; CLDCVG=0.091420;
VMAXKIDDCVGC=1.28500; KMKIDDCVGC=1.0; CLKIDDCVG=4.68488;
VMAXLUNGLIV=0.107078; KMCLARA=0.010867; FRACLUNGYSYC=2.28234;
VMAXTCOHC=2.45371; KMTCOH=15.34823; CLTCOH=1.0;
VMAXGLUCC=26.81603; KMGLUC=11.92933; CLGLUC=1.0; KMETTCOHC=5.47942;
KURNTCAC=0.040393; KMETTCAC=0.32207;
KBILEC=6.77338; KEHRC=1.44947; KURNTCOGC=11.14412;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021228; KKIDBIOACTC=0.0069780;
```

```
BW=0.3; CONCLIST=[49.0 0.0 0.0]; STRTNEXTLIST=[4.0 100.0]; TSTRT=0.0; TSTP=77.0;
```

```
start @NoCallback
```

```
plot(_t, _cart)
```

```
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
```

```
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
```

```
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
```

```
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
```

```
i = i + 1;
```

```
Output_Check
```

```
Output_Check_Reset
```

```
CONCLIST=[54.0 0.0 0.0];
```

```
start @NoCallback
```

```
plot(_t, _cart)
```

```
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
```

```
i = i + 1;
```

```
Output_Check
```

```
Output_Check_Reset
```

```
CONCLIST=[175.0 0.0 0.0];
```

```
start @NoCallback
```

```
plot(_t, _cart)
```

```
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
```

```
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
```

```
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
```

```
i = i + 1;
```

```
Output_Check
```

```
Output_Check_Reset
```

```
CONCLIST=[330.0 0.0 0.0];
```

```
start @NoCallback
```

```
plot(_t, _cart)
```

```
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
```

```
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
```

```
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
```

```
i = i + 1;
```

```

Output_Check
Output_Check_Reset

CONCLIST=[3160.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Kimmerle73_Rat_Output.txt' @format=ascii

```

Larson92a_Rat.m

```

% Larson J and Bull R. 1992. Metabolism and lipoperoxidative activity of trichloroacetate and
% dichloroacetate in rats and mice. Toxicol Appl Pharmacol 115: 268-277.
% http://dx.doi.org/10.1016/0041-008X\(92\)90332-M.
% Male F344 rats (331 +/- 24 g)
% Oral dosing of 20 or 100 mg/kg TCA following fasting for 24 hrs

```

```

PlotOutput=[];
ResetDoses
RatPost

```

```

% Individual posterior parameters for Larson92a_Rat and Larson92b_Rat
QCC=17.49061; VPR=1.37294; DRESPC=2.52136;
QFATC=0.090860; QGUTC=0.16784; QKIDC=0.14142; QLIVC=0.021441; QRAPC=0.26354; QSLWC=0.31490;
VBLDC=0.074592; VFATC=0.091910; VGUTC=0.031718; VKIDC=0.0069664; VLIVC=0.033415;
VPERFC=0.89950; VRAPC=0.087586; VRESPC=0.00049680; VRESPLUMC=0.0046853; VSLWC=0.57281;
FRACPLAS=0.57399;
PB=18.02649; PFAT=38.50303; PGUT=1.20692; PKID=1.22854; PLIV=1.55092; PRAP=1.36295;
PRES=0.95623; PSLW=0.68494;
PRBCPLASTCA=0.49891; PBODTCAC=0.76818; PLIVTCAC=1.82671;
PBODTCOH=1.13873; PLIVTCOH=1.29289;
PBODTCOG=1.36092; PLIVTCOG=9.90822; PEFDCVG=1.0;
BMAXKDC=1.04545; KDISSOC=207.50825;
KAS=5.45210; KTS=4.98783; KAD=0.09662; KTD=0.0; KASTCA=1.83455; KASTCOH=0.70110;
VMAXC=525.69945; KMC=1.24922; CL=1.0; FRACCTC=0.095901; FRACOTHERC=0.25564;
VMAXDCVGC=794.45373; KMDCVGC=1.0; CLDCVG=0.093734;
VMAXKIDDCVGC=1.28115; KMKIDDCVGC=1.0; CLKIDDCVG=4.70366;
VMAXLUNGLIV=0.036472; KMCLARA=0.023029; FRACLUNGSYS=2.00291;
VMAXTCOH=2.55819; KMTCOH=19.96538; CLTCOH=1.0;
VMAXGLUC=34.43247; KMGLUC=2.86624; CLGLUC=1.0; KMETTCOH=1.99911;
KURNTCAC=0.048944; KMETTCAC=0.37584;
KBILEC=5.72590; KEHRC=1.62482; KURNTCOG=11.86879;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021228; KKIDBIOACTC=0.0069431;

```

```

BW=0.331; PODOSETCA=20.0; TCHNG=0.05; TSTP=33.0;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

PODOSETCA=100.0;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');

```

```

i = i + 1;
Output_Check
Output_Check_Reset

```

```

save PlotOutput @file='Larson92a_Rat_Output.txt' @format=ascii

```

Larson92b_Rat.m

```
% Larson J and Bull R. 1992. Species differences in the metabolism of trichloroethylene to the
% carcinogenic metabolites trichloroacetate and dichloroacetate. Toxicol Appl Pharmacol 115:
% 278-285. http://dx.doi.org/10.1016/0041-008X(92)90333-N.
% Male Sprague-Dawley rats (404 +/- 91 g)
% Oral dosing of 1.5, 4.5 or 23 mmol TCE/kg in Tween 80 (constant volume of 3 ml/kg) after
% fasting for 24 hours
```

```
PlotOutput=[];
ResetDoses
RatPost
```

```
% Individual posterior parameters for Larson92a_Rat and Larson92b_Rat
```

```
QCC=17.49061; VPR=1.37294; DRESPC=2.52136;
QFATC=0.090860; QGUTC=0.16784; QKIDC=0.14142; QLIVC=0.021441; QRAPC=0.26354; QSLWC=0.31490;
VBLDC=0.074592; VFATC=0.091910; VGUTC=0.031718; VKIDC=0.0069664; VLIVC=0.033415;
VPERFC=0.89950; VRAPC=0.087586; VRESPC=0.00049680; VRESPLUMC=0.0046853; VSLWC=0.57281;
FRACPLAS=0.57399;
PB=18.02649; PFAT=38.50303; PGUT=1.20692; PKID=1.22854; PLIV=1.55092; PRAP=1.36295;
PRES=0.95623; PSLW=0.68494;
PRBCPLASTCA=0.49891; PBODTCAC=0.76818; PLIVTCAC=1.82671;
PBODTCOH=1.13873; PLIVTCOH=1.29289;
PBODTCOG=1.36092; PLIVTCOG=9.90822; PEFDCVG=1.0;
BMAXKDC=1.04545; KDISSOC=207.50825;
KAS=5.45210; KTS=4.98783; KAD=0.09662; KTD=0.0; KASTCA=1.83455; KASTCOH=0.70110;
VMAXC=525.69945; KMC=1.24922; CL=1.0; FRACCTCAC=0.095901; FRACOTHERC=0.25564;
VMAXDCVGC=794.45373; KMDCVGC=1.0; CLDCVG=0.093734;
VMAXKIDDCVGC=1.28115; KMKIDDCVGC=1.0; CLKIDDCVG=4.70366;
VMAXLUNGLIV=0.036472; KMCLARA=0.023029; FRACLUNGSYS=2.00291;
VMAXTCOH=2.55819; KMTTCOH=19.96538; CLTCOH=1.0;
VMAXGLUC=34.43247; KMGLUC=2.86624; CLGLUC=1.0; KMETTCOH=1.99911;
KURNTCAC=0.048944; KMETTCAC=0.37584;
KBILEC=5.72590; KEHRC=1.62482; KURNTCOG=11.86879;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021228; KKIDBIOACTC=0.0069431;
```

```
BW=0.404; PDOSE=197.25; TCHNG=0.05; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
PDOSE=591.75;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
PDOSE=3024.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
```

```
i = i + 1;
Output_Check
Output_Check_Reset
```

```
save PlotOutput @file='Larson92b_Rat_Output.txt' @format=ascii
```

Lee00_Rat.m

% Lee K, Muralidhara S, Schnellmann R and Bruckner J. 2000. Contribution of direct solvent injury
% to the dose-dependent kinetics of trichloroethylene: Portal vein administration to rats.
% Toxicol Appl Pharmacol 164: 46-54.
% <http://dx.doi.org/10.1006/taap.2000.8891>.
% Adult male Sprague-Dawley rats (320-380 g at experimentation)
% Injected dosing of 16 mg TCE/kg BW in 10-sec IV or PV injection

```
PlotOutput=[];  
ResetDoses  
RatPost
```

% Individual posterior parameters for Lee00_Rat

```
QCC=18.09913; VPR=1.29531; DRESPC=2.53426;  
QFATC=0.080780; QGUTC=0.16386; QKIDC=0.13970; QLIVC=0.021357; QRAPC=0.26495; QSLWC=0.32935;  
VBLDC=0.074148; VFATC=0.068635; VGUTC=0.032128; VKIDC=0.0069846; VLIVC=0.036074;  
VPERFC=0.89950; VRAPC=0.087956; VRESPC=0.00049645; VRESPLUMC=0.0046853; VSLWC=0.59308;  
FRACPLAS=0.55014;  
PB=19.10676; PFAT=30.03120; PGUT=1.37662; PKID=1.25925; PLIV=1.58891; PRAP=1.47471;  
PRES=0.95760; PSLW=0.71869;  
PRBCPLASTCA=0.48252; PBODTCAC=0.97596; PLIVTCAC=1.49006;  
PBODTCOH=1.05513; PLIVTCOH=1.26646;  
PBODTCOG=1.36719; PLIVTCOG=11.00516; PEFFDCVG=1.0;  
BMAXKDC=1.16680; KDISSOC=269.50881;  
KAS=2.40921; KTS=2.94174; KAD=0.19340; KTD=0.0; KASTCA=1.41652; KASTCOH=0.69232;  
VMAXC=521.24994; KMC=1.75159; CL=1.0; FRACCTCAC=0.081804; FRACOTHERC=0.31759;  
VMAXDCVGC=790.49137; KMDCVGC=1.0; CLDCVG=0.093406;  
VMAXKIDDCVGC=1.28886; KMKIDDCVGC=1.0; CLKIDDCVG=4.68957;  
VMAXLUNGLIV=0.035084; KMCLARA=0.023518; FRACLUNGSYS=1.97506;  
VMAXTCOH=2.01617; KMTTCOH=22.35388; CLTCOH=1.0;  
VMAXGLUC=26.52267; KMGLUC=5.64065; CLGLUC=1.0; KMETTCOH=1.92034;  
KURNTCAC=0.038732; KMETTCAC=0.32465;  
KBILEC=7.07806; KEHRC=1.43951; KURNTCOGC=10.62184;  
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;  
KNATC=0.0021207; KKIDBIOACTC=0.0069362;
```

```
BW=0.275; IVDSE=16.0; TCHNG=0.0028; TSTP=0.1; CINT=0.001;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
IVDOSE=0.0; PVDSE=16.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
save PlotOutput @file='Lee00_Rat_Output.txt' @format=ascii
```

Merdink99_Rat.m

% Merdink J, Stenner R, Stevens D, Parker J and Bull R. 1999. Effect of enterohepatic circulation
% on the pharmacokinetics of chloral hydrate and its metabolites in F344 rats. J Toxicol
% Environ Health A 57: 357-368.
% <http://dx.doi.org/10.1080/009841099157665>.
% Male Fischer 344 rats (250-300 g)
% IV dosing of 100 mg/kg TCOH

```
PlotOutput=[];  
ResetDoses  
RatPost
```

```
% Individual posterior parameters for Merdink99_Rat.m
QCC=14.77097; VPR=1.26460; DRESPEC=2.54136;
QFATC=0.078960; QGUTC=0.16646; QKIDC=0.14142; QLIVC=0.021441; QRAPC=0.27745; QSLWC=0.31426;
VBLDC=0.074148; VFATC=0.068635; VGUTC=0.031760; VKIDC=0.0069573; VLIVC=0.033765;
VPERFC=0.89950; VRAPC=0.087516; VRESPEC=0.00049750; VRESPLUMC=0.0046807; VSLWC=0.59622;
FRACPLAS=0.54961;
PB=19.31424; PFAT=30.04322; PGUT=1.22565; PKID=1.22781; PLIV=1.55394; PRAP=1.38738;
PRESPEC=0.95922; PSLW=0.71797;
PRBCPLASTCA=0.48345; PBODTCAC=0.97674; PLIVTCAC=1.48812;
PBODTCOH=0.63773; PLIVTCOH=1.04651;
PBODTCOG=1.37212; PLIVTCOG=12.06567; PEFFDCVG=1.0;
BMAXKDC=1.16094; KDISSOC=268.26387;
KAS=2.44171; KTS=2.88060; KAD=0.19263; KTD=0.0; KASTCA=1.44239; KASTCOH=0.68420;
VMAXC=570.13299; KMC=1.58174; CL=1.0; FRACTCAC=0.081477; FRACOTHERC=0.31791;
VMAXDCVGC=790.49137; KMDCVGC=1.0; CLDCVG=0.094251;
VMAXKIDDCVGC=1.28757; KMKIDDCVGC=1.0; CLKIDDCVG=4.68488;
VMAXLUNGLIV=0.034847; KMCLARA=0.023260; FRACLUNGSYS=1.98001;
VMAXTCOHC=1.85058; KMTCOH=23.47650; CLTCOH=1.0;
VMAXGLUC=12.74323; KMGLUC=8.16617; CLGLUC=1.0; KMETTCOHC=1.33910;
KURNTCAC=0.038655; KMETTCAC=0.32530;
KBILEC=9.13397; KEHRC=1.52577; KURNTCOGC=9.55355;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021313; KKIDBIOACTC=0.0069431;

BW=0.275; IVDOSCTCOH=100.0; TCHNG=3.0; TSTP=9.0;
start @NoCallback
plot(_t, _ctcoh)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Merdink99_Rat_Output.txt' @format=ascii
```

Prout85_Rat.m

```
% Prout M, Provan W and Green T. 1985. Species differences in response to trichloroethylene: I
% pharmacokinetics in rats and mice. Toxicol Appl Pharmacol 79: 389-400.
% Male Alderley Park Wistar OR Osborne-Mendel derived rats, 180-200g
% Oral dosing of 10, 500, 1000 or 2000 mg/kg trichloro[14C]ethylene (10 uCi) in corn oil
```

```
PlotOutput=[];
```

```
% Non-specified rats
ResetDoses
RatPost
```

```
% Individual posterior parameters for Green85_Rat and Prout85_Rat (non-specified rats)
QCC=18.64847; VPR=1.43685; DRESPEC=2.51633;
QFATC=0.099610; QGUTC=0.16968; QKIDC=0.14128; QLIVC=0.021462; QRAPC=0.26147; QSLWC=0.30650;
VBLDC=0.074074; VFATC=0.076510; VGUTC=0.031709; VKIDC=0.0069573; VLIVC=0.031946;
VPERFC=0.89950; VRAPC=0.087472; VRESPEC=0.00049720; VRESPLUMC=0.0046807; VSLWC=0.59033;
FRACPLAS=0.55544;
PB=17.65188; PFAT=31.84998; PGUT=1.20150; PKID=1.22892; PLIV=1.54848; PRAP=1.40922;
PRESPEC=0.95345; PSLW=0.76496;
PRBCPLASTCA=0.48304; PBODTCAC=1.15750; PLIVTCAC=1.34315;
PBODTCOH=1.13614; PLIVTCOH=1.26239;
PBODTCOG=1.39286; PLIVTCOG=9.13729; PEFFDCVG=1.0;
BMAXKDC=1.10534; KDISSOC=291.64902;
KAS=0.29288; KTS=10.92441; KAD=0.11114; KTD=0.0; KASTCA=1.85484; KASTCOH=0.69323;
VMAXC=491.82829; KMC=0.94320; CL=1.0; FRACTCAC=0.091316; FRACOTHERC=0.18563;
VMAXDCVGC=784.97725; KMDCVGC=1.0; CLDCVG=0.093659;
VMAXKIDDCVGC=1.28629; KMKIDDCVGC=1.0; CLKIDDCVG=4.69426;
VMAXLUNGLIV=0.029960; KMCLARA=0.023802; FRACLUNGSYS=1.97289;
VMAXTCOHC=2.39121; KMTCOH=19.41411; CLTCOH=1.0;
VMAXGLUC=55.86846; KMGLUC=3.70988; CLGLUC=1.0; KMETTCOHC=1.90999;
KURNTCAC=0.037587; KMETTCAC=0.29200;
KBILEC=4.79225; KEHRC=1.21240; KURNTCOGC=12.02409;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021271; KKIDBIOACTC=0.0069223;
```



```

BW=0.19; PDOSE=1000.0; TCHNG=0.05; TSTP=73.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cart, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

ResetDoses
RatPost

% Individual posterior parameters for Prout85_Rat (Alderley Park Wistar rats)
QCC=14.08054; VPR=1.09895; DRESPC=2.59115;
QFATC=0.075460; QGUTC=0.16692; QKIDC=0.14114; QLIVC=0.021462; QRAPC=0.28149; QSLWC=0.31352;
VBLDC=0.074074; VFATC=0.072520; VGUTC=0.031773; VKIDC=0.0069566; VLIVC=0.034816;
VPERFC=0.89950; VRAPC=0.087613; VRESPC=0.00049720; VRESPLUMC=0.0046853; VSLWC=0.59125;
FRACPLAS=0.54908;
PB=20.58376; PFAT=30.88396; PGUT=1.23192; PKID=1.22910; PLIV=1.55730; PRAP=1.39147;
PRES=0.95787; PSLW=0.71790;
PRBCPLASTCA=0.48147; PBODTCAC=0.96890; PLIVTCAC=1.48976;
PBODTCOH=1.06553; PLIVTCOH=1.31383;
PBODTCOG=1.37267; PLIVTCOG=10.54197; PEFFDCVG=1.0;
BMAXKDC=1.16409; KDISSOC=267.43087;
KAS=1.13145; KTS=1.79930; KAD=0.35169; KTD=0.0; KASTCA=1.44239; KASTCOH=0.68887;
VMAXC=995.38506; KMC=0.59543; CL=1.0; FRACCTAC=0.084464; FRACOTHERC=0.30605;
VMAXDCVGC=788.91197; KMDCVGC=1.0; CLDCVG=0.094591;
VMAXKIDDCVGC=1.28500; KMKIDDCVGC=1.0; CLKIDDCVG=4.73670;
VMAXLUNGLIV=0.044547; KMCLARA=0.020671; FRACLUNGSYS=1.96168;
VMAXTCOH=2.08945; KMTCOH=22.13146; CLTCOH=1.0;
VMAXGLUC=37.11421; KMGLUC=5.76612; CLGLUC=1.0; KMETTCOH=2.27983;
KURNTCAC=0.038771; KMETTCAC=0.32857;
KBILEC=6.51430; KEHRC=1.50275; KURNTCOG=11.17761;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021186; KKIDBIOACTC=0.0069431;

BW=0.19; PDOSE=10.0; TCHNG=0.05; TSTP=73.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=500.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=1000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

ResetDoses
RatPost

% Individual posterior parameters for Prout85_Rat (Osborne-Mendel rats)
QCC=14.70612; VPR=1.10811; DRESPC=2.57925;
QFATC=0.080920; QGUTC=0.16769; QKIDC=0.14114; QLIVC=0.021441; QRAPC=0.27452; QSLWC=0.31429;
VBLDC=0.074148; VFATC=0.067781; VGUTC=0.031776; VKIDC=0.0069657; VLIVC=0.034102;
VPERFC=0.89950; VRAPC=0.087560; VRESPC=0.00049715; VRESPLUMC=0.0046760; VSLWC=0.59667;
FRACPLAS=0.54961;
PB=20.44611; PFAT=29.68871; PGUT=1.22639; PKID=1.22409; PLIV=1.55599; PRAP=1.39521;
PRES=0.95888; PSLW=0.72164;
PRBCPLASTCA=0.48152; PBODTCAC=0.95121; PLIVTCAC=1.48649;
PBODTCOH=1.07901; PLIVTCOH=1.17218;
PBODTCOG=1.36514; PLIVTCOG=10.14889; PEFFDCVG=1.0;
BMAXKDC=1.15721; KDISSOC=268.78750;
KAS=0.49902; KTS=3.79620; KAD=0.29730; KTD=0.0; KASTCA=1.46580; KASTCOH=0.69004;
VMAXC=770.33821; KMC=0.61787; CL=1.0; FRACTCAC=0.082957; FRACOTHERC=0.16931;
VMAXDCVGC=792.07394; KMDCVGC=1.0; CLDCVG=0.093584;
VMAXKIDDCVGC=1.28243; KMKIDDCVGC=1.0; CLKIDDCVG=4.68957;
VMAXLUNGLIV=0.041953; KMCLARA=0.020817; FRACLUNGSYS=2.00291;
VMAXTCOHC=2.03196; KMTCOH=22.24239; CLTCOH=1.0;
VMAXGLUCC=53.62418; KMGLUC=4.87441; CLGLUC=1.0; KMETTCOHC=1.65616;
KURNTCAC=0.039475; KMETTCAC=0.32368;
KBILEC=5.91801; KEHRC=1.50456; KURNTCOG=11.47203;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021335; KKIDBIOACTC=0.0069640;

BW=0.19; PDOSE=10.0; TCHNG=0.05; TSTP=73.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=500.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=1000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=2000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');

i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Prout85_Rat_Output.txt' @format=ascii

```

Simmons02_Rat.m

```
% Simmons J, Boyes W, Bushnell P, Raymer J, Limsakun T, McDonald A, Sey Y and Evans M. 2002. A
% physiologically based pharmacokinetic model for trichloroethylene in the male Long-Evans rat.
% Toxicol Sci 69: 3-15.
% http://dx.doi.org/10.1093/toxsci/69.1.3.
% Male LE rats (received at ages 60, 65, 90 (+/-2) days)
% Open chamber inhalation of 200, 2000 or 4000 ppm TCE for 1 hour
% OR closed chamber inhalation of 100 ppm TCE for 4 hours or 500, 1000 or 3000 ppm TCE for
% 6 hours
```

```
PlotOutput=[];
ResetDoses
RatPost
```

```
% Individual posterior parameters for Simmons02_Rat open chamber
QCC=14.50660; VPR=1.03899; DRESPC=2.26166;
QFATC=0.066031; QGUTC=0.17289; QKIDC=0.14213; QLIVC=0.021714; QRAPC=0.28264; QSLWC=0.31460;
VBLDC=0.074148; VFATC=0.032683; VGUTC=0.032064; VKIDC=0.0068558; VLIVC=0.033531;
VPERFC=0.89950; VRAPC=0.087754; VRESPC=0.00048700; VRESPLUMC=0.0047413; VSLWC=0.63198;
FRACPLAS=0.55173;
PB=16.78092; PFAT=29.96520; PGUT=1.33435; PKID=1.27752; PLIV=1.59978; PRAP=1.65180;
PRES=0.91581; PSLW=1.00338;
PRBCPLASTCA=0.47752; PBODTCAC=0.95670; PLIVTCAC=1.53405;
PBODTCOH=1.09244; PLIVTCOH=1.28079;
PBODTCOG=1.36788; PLIVTCOG=11.13802; PEFDCVG=1.0;
BMAXKDC=1.17561; KDISSOC=266.71245;
KAS=2.46773; KTS=2.94174; KAD=0.19052; KTD=0.0; KASTCA=1.44687; KASTCOH=0.69274;
VMAXC=529.76296; KMC=1.01870; CL=1.0; FRACTCAC=0.088528; FRACOTHERC=0.33960;
VMAXDCVGC=806.46036; KMDCVGC=1.0; CLDCVG=0.093650;
VMAXKIDDCVGC=1.25453; KMKIDDCVGC=1.0; CLKIDDCVG=4.60131;
VMAXLUNGLIV=0.007095; KMCLARA=0.029276; FRACLUNGSYS=1.96619;
VMAXTCOH=2.01657; KMTCOH=22.42104; CLTCOH=1.0;
VMAXGLUCC=21.69323; KMGLUC=5.94173; CLGLUC=1.0; KMETTCOH=1.90503;
KURNTCAC=0.039043; KMETTCAC=0.32465;
KBILEC=6.91712; KEHRC=1.48290; KURNTCOGC=10.40111;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0020933; KKIDBIOACTC=0.0069849;
```

```
% Open chamber
BW=0.3978625; VFATC=0.08125; VSLWC=0.583413; CONCLIST=[200.0 0.0 0.0]; STRTNEXTLIST=[1.0 10.0];
TSTRT=0.0; TSTP=5.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
BW=0.42014; VFATC=0.0917; VSLWC=0.572963; CONCLIST=[2000.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
BW=0.40651; VFATC=0.0875; VSLWC=0.577163; CONCLIST=[4000.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```

ResetDoses
RatPost

% Individual posterior parameters for Simmons02_Rat closed chamber
QCC=14.50660; VPR=1.03899; DRESPC=2.26166;
QFATC=0.066031; QGUTC=0.17289; QKIDC=0.14213; QLIVC=0.021714; QRAPC=0.28264; QSLWC=0.31460;
VBLDC=0.074148; VFATC=0.032683; VGUTC=0.032064; VKIDC=0.0068558; VLIVC=0.033531;
VPERFC=0.89950; VRAPC=0.087754; VRESPC=0.00048700; VRESPLUMC=0.0047413; VSLWC=0.63198;
FRACPLAS=0.55173;
PB=16.78092; PFAT=29.96520; PGUT=1.33435; PKID=1.27752; PLIV=1.59978; PRAP=1.65180;
PRESF=0.91581; PSLW=1.00338;
PRBCPLASTCA=0.47752; PBODTCAC=0.95670; PLIVTCAC=1.53405;
PBODTCOH=1.09244; PLIVTCOH=1.28079;
PBODTCOG=1.36788; PLIVTCOG=11.13802; PEFFDCVG=1.0;
BMAXKDC=1.17561; KDISSOC=266.71245;
KAS=2.46773; KTSO=2.94174; KAD=0.19052; KTD=0.0; KASTCA=1.44687; KASTCOH=0.69274;
VMAXC=529.76296; KMC=1.01870; CL=1.0; FRACTCAC=0.088528; FRACOTHERC=0.33960;
VMAXDCVGC=806.46036; KMDCVGC=1.0; CLDCVG=0.093650;
VMAXKIDDCVGC=1.25453; KMKIDDCVGC=1.0; CLKIDDCVG=4.60131;
VMAXLUNGLIV=0.007095; KMCLARA=0.029276; FRACLUNGSYS=1.96619;
VMAXTCOHC=2.01657; KMTCOH=22.42104; CLTCOH=1.0;
VMAXGLUCC=21.69323; KMGLUC=5.94173; CLGLUC=1.0; KMETTCOHC=1.90503;
KURNTCAC=0.039043; KMETTCAC=0.32465;
KBILEC=6.91712; KEHRC=1.48290; KURNTCOGC=10.40111;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0020933; KKIDBIOACTC=0.0069849;

BW=0.408907143; CC=1; CONCLIST(1)=108.0; STRTNEXTLIST(1)=10.0; TSTRT=0.0; NRODENTS=1.0;
VCHC=10.4; KLOSSC=exp(-3.912); TSTP=5.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST(1)=506.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST(1)=864.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST(1)=2940.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Simmons02_Rat_Output.txt' @format=ascii

```

Stenner97_Rat.m

```
% Stenner R, Merdink J, Stevens D, Springer D and Bull R. 1997. Enterohepatic recirculation of
% trichloroethanol glucuronide as a significant source of trichloroacetic acid. Metabolites of
% trichloroethylene. Drug Metab Dispos 25: 529-535.
% Male F-344 rats (~300 g)
% Intraduodenal dosing (via duodenal cannula) of 100 mg/kg TCE -- modeled as an oral dose
% OR IV dosing of 100 mg/kg of TCOH without bile cannulated
% OR IV dosing of 5, 20 or 100 mg/kg of TCOH with bile cannulated
```

```
PlotOutput=[];
ResetDoses
RatPost
```

```
% Individual posterior parameters for Stenner97_Rat
QCC=13.76424; VPR=1.63061; DRESPEC=2.50653;
QFATC=0.077000; QGUTC=0.15621; QKIDC=0.14114; QLIVC=0.021231; QRAPC=0.29032; QSLWC=0.31409;
VBLDC=0.074222; VFATC=0.065464; VGUTC=0.031750; VKIDC=0.0069608; VLIVC=0.034986;
VPERFC=0.89950; VRAPC=0.087648; VRESPEC=0.00049665; VRESPLUMC=0.0046900; VSLWC=0.59797;
FRACPLAS=0.56551;
PB=17.40648; PFAT=29.28885; PGUT=1.21601; PKID=1.23031; PLIV=1.55365; PRAP=1.37146;
PRESPEC=0.95934; PSLW=0.69619;
PRBCPLASTCA=0.49741; PBODTCAC=1.04349; PLIVTCAC=1.72102;
PBODTCOH=1.58750; PLIVTCOH=1.07076;
PBODTCOG=1.41944; PLIVTCOG=12.43312; PEFFDCVG=1.0;
BMAXKDC=1.24639; KDISSOC=277.58053;
KAS=14.59969; KTS=2.13721; KAD=0.09404; KTD=0.0; KASTCA=1.44672; KASTCOH=0.68052;
VMAXC=817.80969; KMC=1.95330; CL=1.0; FRACCTAC=0.084887; FRACOTHERC=0.51115;
VMAXDCVGC=788.12345; KMDCVGC=1.0; CLDCVG=0.093781;
VMAXKIDDCVGC=1.29532; KMKIDDCVGC=1.0; CLKIDDCVG=4.68488;
VMAXLUNGLIV=0.034348; KMCLARA=0.023778; FRACLUNGSYS=1.95189;
VMAXTCOHC=1.17175; KMTCOH=34.63969; CLTCOH=1.0;
VMAXGLUCC=57.85848; KMGLUC=18.78390; CLGLUC=1.0; KMETTCOHC=1.57523;
KURNTCAC=0.026567; KMETTCAC=0.34438;
KBILEC=11.47304; KEHRC=3.09875; KURNTCOG=17.28627;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021228; KKIDBIOACTC=0.0069085;
```

```
% TCE dosing
BW=0.3; PDOSE=100.0; TCHNG=0.05; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcog, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
% TCOH dosing without bile cannulated
PDOSE=0.0; IVDOSCTCOH=100.0;
start @NoCallback
plot(_t, _ctcoh)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
% TCOH dosing with bile cannulated
KEHRC=exp(-100.0); IVDOSCTCOH=5.0;
start @NoCallback
plot(_t, _ctcoh)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```

KEHRC=exp(-100.0); IVD0SETCOH=20.0;
start @NoCallback
plot(_t, _ctcoh)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

KEHRC=exp(-100.0); IVD0SETCOH=100.0;
start @NoCallback
plot(_t, _ctcoh)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Stenner97_Rat_Output.txt' @format=ascii

```

Templin95_Rat.m

```

% Templin M, Stevens D, Stenner R, Bonate P, Tuman D and Bull R. 1995. Factors affecting species
% differences in the kinetics of metabolites of trichloroethylene. J Toxicol Environ Health 44:
% 435-447.
% Male F344 rats (250-300 g)
% Oral dosing of 0.15 or 0.76 mmol/kg TCE in 2% polyoxyethylene-sorbitan monooleate (Tween 80)

```

```

PlotOutput=[];
ResetDoses
RatPost

```

```

% Individual posterior parameters for Templin95_Rat
QCC=13.93055; VPR=1.35819; DRESPEC=2.52919;
QFATC=0.077420; QGUTC=0.16998; QKIDC=0.14128; QLIVC=0.021483; QRAPC=0.27433; QSLWC=0.31550;
VBLDC=0.073985; VFATC=0.070560; VGUTC=0.031702; VKIDC=0.0069692; VLIVC=0.033572;
VPERFC=0.89950; VRAPC=0.087613; VRESPEC=0.00049710; VRESPLUMC=0.0046853; VSLWC=0.59460;
FRACPLAS=0.52534;
PB=18.72655; PFAT=30.70535; PGUT=1.20571; PKID=1.23095; PLIV=1.55642; PRAP=1.40247;
PRESPEC=0.96147; PSLW=0.72904;
PRBCPLASTCA=0.50246; PBODTCAC=1.66307; PLIVTCAC=1.32712;
PBODTCOH=1.37007; PLIVTCOH=1.29063;
PBODTCOG=1.36774; PLIVTCOG=11.18266; PEFDCVGC=1.0;
BMAXKDC=1.14677; KDISSOC=263.69974;
KAS=2.28942; KTS=6.24012; KAD=0.21589; KTD=0.0; KASTCA=1.40467; KASTCOH=0.69475;
VMAXC=634.97121; KMC=1.50309; CL=1.0; FRACTCAC=0.089418; FRACOTHERC=0.28365;
VMAXDCVGC=788.12345; KMDCVGC=1.0; CLDCVGC=0.094147;
VMAXKIDDCVGC=1.29662; KMKIDDCVGC=1.0; CLKIDDCVGC=4.68957;
VMAXLUNGLIV=0.034621; KMCLARA=0.023354; FRACLUNGSSYS=1.97763;
VMAXTCOH=1.90066; KMTCOH=23.83130; CLTCOH=1.0;
VMAXGLUCC=34.39805; KMGLUC=7.69061; CLGLUC=1.0; KMETTCOH=2.13785;
KURNTCAC=0.038732; KMETTCAC=0.33121;
KBILEC=6.99363; KEHRC=1.35581; KURNTCOGC=10.51615;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021292; KKIDBIOACTC=0.0069570;

```

```

BW=0.275; PDOSE=100.0; TCHNG=0.05; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

save PlotOutput @file='Templin95_Rat_Output.txt' @format=ascii

```

Yu00_Rat.m

% Yu K, Barton H, Mahle D and Frazier J. 2000. In vivo kinetics of trichloroacetate in male
% Fischer 344 rats. Toxicol Sci 54: 302-311.
% Male Fischer 344 rats (195-235 g)
% IV dosing of 6.1, 61 or 306 mmol/mL TCA ([1-14C] TCA mixed with unlabeled TCA) in physiologic
% saline (6-8 uCi of 14C per rat)

PlotOutput=[];
ResetDoses
RatPost

% Individual posterior parameters for Yu00_Rat

QCC=14.12553; VPR=1.26878; DRESC=2.53071;
QFATC=0.078680; QGUTC=0.16998; QKIDC=0.14142; QLIVC=0.021483; QRAPC=0.27377; QSLWC=0.31466;
VBLDC=0.075850; VFATC=0.068845; VGUTC=0.031754; VKIDC=0.0069685; VLIVC=0.032443;
VPERFC=0.89950; VRAPC=0.087551; VRESC=0.00049735; VRESPLUMC=0.0046760; VSLWC=0.59559;
FRACPLAS=0.54961;
PB=19.30651; PFAT=30.07327; PGUT=1.22749; PKID=1.22716; PLIV=1.55497; PRAP=1.39263;
PRES=0.95759; PSLW=0.71941;
PRBCPLASTCA=0.44337; PBODTCAC=0.71617; PLIVTCAC=1.43292;
PBODTCOH=1.06657; PLIVTCOH=1.25970;
PBODTCOG=1.37776; PLIVTCOG=11.00516; PEFFDCVG=1.0;
BMAXKDC=1.21583; KDISSOC=239.07351;
KAS=2.43854; KTS=2.90665; KAD=0.19515; KTD=0.0; KASTCA=1.43706; KASTCOH=0.69998;
VMAXC=567.88541; KMC=1.54577; CL=1.0; FRACTCAC=0.081477; FRACOTHERC=0.31664;
VMAXDCVGC=792.07394; KMDCVGC=1.0; CLDCVG=0.093472;
VMAXKIDDCVGC=1.28372; KMKIDDCVGC=1.0; CLKIDDCVG=4.68488;
VMAXLUNGLIV=0.035356; KMCLARA=0.023424; FRACLUNGSYSC=1.98139;
VMAXTCOHC=2.02871; KMTCOH=22.42104; CLTCOH=1.0;
VMAXGLUCC=26.44323; KMGLUC=5.69165; CLGLUC=1.0; KMETTCOHC=1.91746;
KURNTCAC=0.041375; KMETTCAC=0.24610;
KBILEC=7.14920; KEHRC=1.44831; KURNTCOGC=10.54775;
KDCVGC=22026.46579; FRACKIDDCVCC=22026.46579;
KNATC=0.0021250; KKIDBIOACTC=0.0069710;

BW=0.215; IVDOSSETCA=1.0; TCHNG=0.05; TSTP=25.0;
start @NoCallback
plot(t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

IVDOSSETCA=10.0;
start @NoCallback
plot(t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

IVDOSSETCA=50.0;
start @NoCallback
plot(t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Yu00_Rat_Output.txt' @format=ascii

APPENDIX K

M Files for Human Validation Figures

The following M files are for generating human output for validation figures in Appendix H.

Bernauer96_Human.m

```
% Bernauer U, Birner G, Dekant W and Henschler D. 1996. Biotransformation of trichloroethene:
% Dose-dependent excretion of 2,2,2-trichloro-metabolites and mercapturic acids in rats and
% humans after inhalation. Arch Toxicol 70: 338-346.
% http://dx.doi.org/10.1007/s002040050283.
% 3 male volunteers, 37-69 years old
% Inhalation of 40, 80 or 160 ppm TCE stabilized with diisopropylamine (40 ppm) for 6 hours
% Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC

PlotOutput=[];
ResetDoses
MalePost

% Individual posterior parameters for Bernauer96_Human male
QCC=12.04427; VPR=1.34552; DRESPC=0.58199;
QFATC=0.039140; QGUTC=0.16581; QKIDC=0.19133; QLIVC=0.045708; QRAPC=0.38744; QSLWC=0.17057;
VLDC=0.077462; VFATC=0.20000; VGUTC=0.019970; VKIDC=0.0043043; VLIVC=0.026625; VPERFC=0.85600;
VRAPC=0.087560; VRESPC=0.00017986; VRESPLUMC=0.0023905; VSLWC=0.43990; FRACPLAS=0.56689;
PB=8.53685; PFAT=59.17461; PGUT=2.70211; PKID=1.59873; PLIV=4.05462; PRAP=2.12020;
PRES=1.31397; PSLW=1.66319;
PRBCPLASTCA=0.34842; PBODTCAC=0.65238; PLIVTCAC=0.76981;
PBODTCOH=1.44526; PLIVTCOH=0.63187;
PBODTCOG=1.14624; PLIVTCOG=5.29291; PEFDCVGC=0.010441;
BMAXKDC=4.09798; KDISSOC=181.01261;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=241.96027; KMC=1.0; CL=1308.52358; FRACCTCAC=0.120846; FRACOTHERC=0.08604;
VMAXDCVGC=1.0; KMDCVGC=1.24360; CLDCVGC=8.54921;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.67858; CLKIDDCVGC=10.44454;
VMAXLUNGLIV=0.074584; KMCLARA=0.85351; FRACLUNGSYS=23.17328;
VMAXTCOH=1.0; KMTCOH=0.90258; CLTCOH=0.12270;
VMAXGLUC=1.0; KMGLUC=137.41424; CLGLUC=0.32661; KMETTCOHC=0.71156;
KURNTCAC=0.0068698; KMETTCAC=0.28650;
KBILEC=6.94485; KEHRC=0.13752; KURNTCOGC=0.94779;
KDCVGC=7.90108; FRACKIDDCVCC=22026.46579;
KNATC=0.00028104; KKIDBIOACTC=0.074274;

CONCLIST=[40.0 0.0 0.0]; STRTNEXTLIST=[6.0 100.0]; TSTRT=0.0; TSTP=55.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[80.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[160.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
```



```

PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Bernauer96_Human_Output.txt' @format=ascii

Chiu07_Human.m
% Chiu W, Micallef S, Monster A and Bois F. 2007. Toxicokinetics of inhaled trichloroethylene and
% tetrachloroethylene in humans at 1 ppm: Empirical results and comparisons with previous
% studies. Toxicol Sci 95: 23-36.
% http://dx.doi.org/10.1093/toxsci/kfl129.
% 7 adult male volunteers
% Inhalation dosing of 1 ppm TCE for 6 hours

% Lines setting different inhalation concentrations were truncated so the values that were there
% are used and the average of the values there were used for the remaining time of exposure

PlotOutput=[];
ResetDoses
MalePost

% Experiment A-TRI
% Individual posterior parameters for Chiu07_Human male Subject A
QCC=14.07202; VPR=1.79855; DRESPC=0.71320;
QFATC=0.017620; QGUTC=0.18175; QKIDC=0.19456; QLIVC=0.055731; QRAPC=0.44104; QSLWC=0.10930;
VBLDC=0.077770; VFATC=0.16563; VGUTC=0.020020; VKIDC=0.0043387; VLIVC=0.025550; VPERFC=0.85600;
VRAPC=0.087850; VRESPC=0.00017996; VRESPLUMC=0.0023953; VSLWC=0.47466; FRACPLAS=0.56984;
PB=9.37046; PFAT=58.52141; PGUT=2.98354; PKID=1.59657; PLIV=4.06399; PRAP=3.40046;
PRES=1.31041; PSLW=4.63037;
PRBCPLASTCA=0.12504; PBODTCAC=0.66569; PLIVTCAC=0.79563;
PBODTCOH=1.28954; PLIVTCOH=0.63008;
PBODTCOG=0.10989; PLIVTCOG=0.96076; PEFDCVGC=0.010275;
BMAXKDC=4.09225; KDISSOC=180.91434;
KAS=1.0; KTSD=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=105.06335; KMC=1.0; CL=432.53132; FRACCTCAC=0.022927; FRACOTHERC=0.27417;
VMAXDCVGC=1.0; KMDCVGC=3.31982; CLDCVGC=77.43501;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.85236; CLKIDDCVGC=47.89827;
VMAXLUNGLIV=0.059993; KMCLARA=1.48453; FRACLUNGSYS=23.24291;
VMAXTCOHC=1.0; KMTCOH=2.24723; CLTCOH=0.06634;
VMAXGLUCC=1.0; KMGLUC=120.30137; CLGLUC=0.64404; KMETTCOHC=0.65869;
KURNTCAC=0.0029392; KMETTCAC=0.27610;
KBILEC=6.34711; KEHRC=0.07273; KURNTCOGC=0.02979;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 310.8
% Start times [0.0 0.283 0.617 1.117 1.367 1.867 2.117 2.367 2.783 2.950 3.700 4.117 4.533 4.950
% 5.533 6.000 6.001];
BW=70.5; VFATC=0.11; VSLWC=0.53029; VPR=0.907784428; TSTRT=0.0; TSTP=125.0; CINT=0.1;
CONCLIST=[1.155 1.185 1.322 1.262 1.357 1.282 1.339 1.33 1.284 1.248 1.077 1.257 1.182 1.175
1.149 1.053 0.0 0.0];
STRTNEXTLIST=[0.283 0.334 0.5 0.25 0.5 0.25 0.25 0.416 0.167 0.75 0.417 0.416 0.417 0.583 0.467
0.001 200.0];
TURN=46.4167; URNMISSLIST=[19.3 9.85 11.1666 8.0 19.3334 7.3333 13.3333 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Start times [0.0 0.300 0.717 1.050 1.383 1.717 2.050 2.383 2.633 3.050 3.383 3.800 4.300 4.467
% 4.800 5.383 5.550 5.800 5.967 6.000 6.001];
TSTP=145.0; CINT=0.1;
CONCLIST=[1.019 0.932 1.085 1.031 1.035 1.165 1.238 1.194 1.200 1.171 1.249 1.194 1.147 1.136
1.234 1.173 1.181 1.300 1.143 1.162 0.0 0.0];
STRTNEXTLIST=[0.3 0.417 0.333 0.333 0.334 0.333 0.333 0.25 0.417 0.333 0.417 0.5 0.167 0.333
0.583 0.167 0.25 0.167 0.033 0.001 200.0];
TURN=47.6333;
URNMISSLIST=[16.3 5.5834 22.9333 4.4 12.6167 11.3833 13.1167 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Experiment B-TRI
% Individual posterior parameters for Chiu07_Human male Subject B
QCC=14.08751; VPR=0.78457; DRESPC=0.52724;
QFATC=0.080250; QGUTC=0.15411; QKIDC=0.18901; QLIVC=0.035451; QRAPC=0.41767; QSLWC=0.12351;
VBLDC=0.078617; VFATC=0.16648; VGUTC=0.020020; VKIDC=0.0042875; VLIVC=0.025250; VPERFC=0.85600;
VRAPC=0.087842; VRESPC=0.00017966; VRESPLUMC=0.0024000; VSLWC=0.47332; FRACPLAS=0.56757;
PB=8.61894; PFAT=59.65587; PGUT=2.93619; PKID=1.60311; PLIV=4.11727; PRAP=2.68788;
PRES=1.31091; PSLW=2.74049;
PRBCPLASTCA=0.12232; PBODTCAC=0.63026; PLIVTCAC=0.78520;
PBODTCOH=1.45192; PLIVTCOH=0.63312;
PBODTCOG=0.12169; PLIVTCOG=1.16529; PEFDCVGC=0.010275;
BMAXKDC=4.08121; KDISSOC=180.96139;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=104.54980; KMC=1.0; CL=189.92984; FRACACTAC=0.039619; FRACOTHERC=0.17605;
VMAXDCVGC=1.0; KMDCVGC=3.36191; CLDCVGC=66.91606;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84641; CLKIDDCVGC=6.13542;
VMAXLUNGLIV=0.058876; KMCLARA=1.62987; FRACLUNGSYSC=23.54704;
VMAXTCOHC=1.0; KMTCOH=2.29768; CLTCOH=0.14602;
VMAXGLUCC=1.0; KMGLUC=121.87550; CLGLUC=0.45140; KMETTCOHC=0.82704;
KURNTCAC=0.0048265; KMETTCAC=0.25976;
KBILEC=6.35982; KEHRC=0.14156; KURNTCOGC=0.09996;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 319.2
% Start times [0.0 0.150 0.317 0.983 1.150 1.483 1.733 2.233 2.483 2.900 3.150 3.400 3.567 3.900
% 4.150 4.317 4.650 4.900 5.567 5.733 5.983 6.000 6.001];
BW=75.6; VFATC=0.204; VSLWC=0.4358; VPR=0.883766019; TSTP=120.0; CINT=0.1;
CONCLIST=[1.117 1.080 1.107 1.060 1.011 1.067 1.114 1.142 1.153 1.116 1.133 1.122 1.196 1.142
1.213 1.159 1.175 1.211 1.111 1.176 1.142 1.142 0.0 0.0];
STRTNEXTLIST=[0.15 0.167 0.666 0.167 0.333 0.25 0.5 0.25 0.417 0.25 0.25 0.167 0.333 0.25 0.167
0.333 0.25 0.667 0.166 0.25 0.017 0.001 200.0];
TURN=47.6333; URNMISSLIST=[15.75 8.5 13.0 7.0 18.0 7.0 15.5 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Start times [0.0 0.133 0.300 0.467 0.717 1.050 1.300 1.383 1.550 1.633 1.717 1.800 1.883 1.967
% 2.100 2.133 2.267 2.333 2.383 2.717 2.967 3.467 3.967 4.050 4.467 4.800 5.133 5.383 5.883
% 6.000 6.001];
TSTP=145.0; CINT=0.1;
CONCLIST=[1.424 1.305 1.367 1.341 1.353 0.492 0.248 0.302 1.594 1.876 1.642 1.583 1.465 0.825
1.259 1.284 1.450 1.386 1.240 1.303 1.315 1.401 1.435 1.381 1.261 1.339 1.436 1.128
1.205 1.166 0.0 0.0];
STRTNEXTLIST=[0.133 0.167 0.167 0.25 0.333 0.25 0.083 0.167 0.083 0.084 0.083 0.083 0.084 0.133
0.033 0.134 0.066 0.05 0.334 0.25 0.5 0.5 0.083 0.417 0.333 0.333 0.25 0.5 0.117
0.001 200.0];
TURN=50.1333; URNMISLIST=[15.0 8.0 14.25 7.25 16.75 6.5834 17.6666 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Experiment C-TRI
% Individual posterior parameters for Chiu07_Human male Subject C
QCC=14.17796; VPR=1.13369; DRESC=0.86226;
QFATC=0.060250; QGUTC=0.19228; QKIDC=0.19665; QLIVC=0.064129; QRAPC=0.39321; QSLWC=0.09348;
VLDC=0.077616; VFATC=0.16632; VGUTC=0.020040; VKIDC=0.0043516; VLIVC=0.025150; VPERFC=0.85600;
VRAPC=0.087639; VRESC=0.00017998; VRESPLUMC=0.0023881; VSLWC=0.47470; FRACPLAS=0.57040;
PB=8.02283; PFAT=45.67690; PGUT=3.17120; PKID=1.60169; PLIV=4.11311; PRAP=3.29732;
PRES=1.31165; PSLW=4.47201;
PRBCPLASTCA=0.15272; PBODTCAC=0.62137; PLIVTCAC=0.77856;
PBODTCOH=1.53172; PLIVTCOH=0.62827;
PBODTCOG=0.08456; PLIVTCOG=0.37590; PEFDCVGC=0.010275;
BMAXKDC=4.23560; KDISSOC=180.88739;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=98.95484; KMC=1.0; CL=512.16905; FRACAC=0.020457; FRACOTHERC=0.36714;
VMAXDCVGC=1.0; KMDCVGC=3.37404; CLDCVGC=94.57933;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84303; CLKIDDCVGC=97.68806;
VMAXLUNGLIV=0.052474; KMCLARA=2.49253; FRACLUNGSYS=23.35941;
VMAXTCOHC=1.0; KMTCOH=2.23893; CLTCOH=0.10445;
VMAXGLUC=1.0; KMGLUC=120.42173; CLGLUC=0.63942; KMETTCOHC=0.46218;
KURNTCAC=0.0022550; KMETTCAC=0.21654;
KBILEC=5.50139; KEHRC=0.20909; KURNTCOGC=0.01632;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 310.8
% Start times [0.0 0.050 0.550 0.883 1.383 1.633 2.133 2.383 2.633 3.050 3.217 3.967 4.383 4.800
% 5.217 5.800 6.000 6.001];
BW=75.2; VFATC=0.204; VSLWC=0.43702; VPR=0.858428016; TSTP=145.0; CINT=0.1;
CONCLIST=[1.218 1.155 1.185 1.322 1.262 1.357 1.282 1.339 1.330 1.284 1.248 1.077 1.257 1.182
1.175 1.149 1.053 0.0 0.0];
STRTNEXTLIST=[0.05 0.5 0.333 0.5 0.25 0.5 0.25 0.417 0.167 0.75 0.416 0.417 0.417 0.583
0.2 0.001 200.0];
TURN=45.6333; URNMISLIST=[16.75 7.5 16.3334 8.25 15.9166 8.0 15.0834 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check

```

```

Output_Check_Reset
% Start times [0.0 0.133 0.467 0.883 1.217 1.550 1.883 2.217 2.550 2.800 3.217 3.550 3.967 4.467
% 4.633 4.967 5.550 5.717 5.967 6.000 6.001];
TSTP=145.0; CINT=0.1;
CONCLIST=[0.965 1.019 0.932 1.085 1.031 1.035 1.165 1.238 1.194 1.200 1.171 1.249 1.194 1.147
1.136 1.234 1.173 1.181 1.300 1.143 0.0 0.0];
STRTNEXTLIST=[0.133 0.334 0.416 0.334 0.333 0.333 0.334 0.333 0.25 0.417 0.333 0.417 0.5 0.166
0.334 0.583 0.167 0.25 0.033 0.001 200.0];
TURN=50.8; URNMISLIST=[13.0 6.3333 16.4167 7.5833 40.6667 1000.0 1000.0 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Experiment D-TRI-1
% Individual posterior parameters for Chiu07_Human male Subject D
QCC=14.21629; VPR=0.94007; DRESPC=0.67740;
QFATC=0.072250; QGUTC=0.16139; QKIDC=0.19076; QLIVC=0.041587; QRAPC=0.35432; QSLWC=0.17970;
VBLDC=0.078078; VFATC=0.16575; VGUTC=0.020060; VKIDC=0.0042824; VLIVC=0.026225; VPERFC=0.85600;
VRAPC=0.087278; VRESPC=0.00018018; VRESPLUMC=0.0023881; VSLWC=0.47415; FRACPLAS=0.56870;
PB=7.16130; PFAT=57.59828; PGUT=2.92593; PKID=1.59394; PLIV=4.06376; PRAP=1.84801;
PRES=1.31228; PSLW=1.21002;
PRBCPLASTCA=0.19962; PBODTCAC=0.63240; PLIVTCAC=0.80984;
PBODTCOH=1.14155; PLIVTCOH=0.66078;
PBODTCOG=0.08881; PLIVTCOG=0.46564; PEFDCVGC=0.010275;
BMAXKDC=4.11811; KDISSOC=180.91000;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=101.34835; KMC=1.0; CL=379.42416; FRACTCAC=0.046308; FRACOTHERC=0.15598;
VMAXDCVGC=1.0; KMDCVGC=3.40999; CLDCVGC=67.85947;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.85066; CLKIDDCVGC=7.96518;
VMAXLUNGLIV=0.053841; KMCLARA=2.47639; FRACLUNGSYSYSC=23.19647;
VMAXTCOH=1.0; KMTCOH=2.27368; CLTCOH=0.15107;
VMAXGLUC=1.0; KMGLUC=121.51042; CLGLUC=0.27253; KMETTCOH=4.37104;
KURNTCAC=0.0036845; KMETTCAC=0.40710;
KBILEC=5.62376; KEHRC=0.16041; KURNTCOGC=0.01078;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 298.2
% Start times [0.0 0.050 0.550 0.717 1.383 1.550 1.883 2.133 2.633 2.883 3.300 3.550 3.800 3.967
% 4.300 4.550 4.717 5.050 5.300 5.967 6.000 6.001];
BW=70.5; VFATC=0.129; VSLWC=0.5109; VPR=0.862143438; TSTP=135.0; CINT=0.1;
CONCLIST=[1.080 1.117 1.080 1.107 1.060 1.011 1.067 1.114 1.142 1.153 1.116 1.133 1.122 1.196
1.142 1.213 1.159 1.175 1.211 1.111 1.176 0.0 0.0];
STRTNEXTLIST=[0.05 0.5 0.167 0.666 0.167 0.333 0.25 0.5 0.25 0.417 0.25 0.25 0.167 0.333 0.25
0.167 0.333 0.25 0.667 0.033 0.001 200.0];
TURN=48.55; URNMISLIST=[12.75 11.0833 12.1167 9.05 14.8333 9.75 12.5 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Experiment F-TRI
% Individual posterior parameters for Chiu07_Human male Subject F
QCC=14.14115; VPR=0.83692; DRESPC=0.74789;
QFATC=0.072700; QGUTC=0.17421; QKIDC=0.19114; QLIVC=0.050986; QRAPC=0.40343; QSLWC=0.10754;
VBLDC=0.077693; VFATC=0.16686; VGUTC=0.020020; VKIDC=0.0043172; VLIVC=0.025750; VPERFC=0.85600;
VRAPC=0.086768; VRESPC=0.00017989; VRESPLUMC=0.0023953; VSLWC=0.47441; FRACPLAS=0.57040;
PB=7.15057; PFAT=57.04227; PGUT=2.90842; PKID=1.60358; PLIV=4.05927; PRAP=1.55848;
PRESP=1.32045; PSLW=2.42162;
PRBCPLASTCA=0.48838; PBODTCAC=0.60036; PLIVTCAC=0.80709;
PBODTCOH=1.32272; PLIVTCOH=0.62857;
PBODTCOG=0.41686; PLIVTCOG=0.36001; PEFDCVGC=0.010275;
BMAXKDC=4.28433; KDISSOC=180.94076;
KAS=1.0; KTSO=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=100.98415; KMC=1.0; CL=439.06819; FRACCTAC=0.023555; FRACOTHERC=0.33994;
VMAXDCVGC=1.0; KMDCVGC=3.32913; CLDCVGC=108.46624;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84641; CLKIDDCVGC=25.92167;
VMAXLUNGLIV=0.054240; KMCLARA=2.38930; FRACLUNGSYS=23.49999;
VMAXTCOH=1.0; KMTCOH=2.31683; CLTCOH=0.12160;
VMAXGLUC=1.0; KMGLUC=120.78354; CLGLUC=0.47502; KMETTCOH=0.58996;
KURNTAC=0.0020383; KMETTCAC=0.34028;
KBILEC=5.36019; KEHRC=0.10894; KURNTCOG=0.04308;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 327.6
% Start times [0.0 0.083 0.333 0.833 1.167 1.667 1.917 2.417 2.667 2.917 3.333 3.500 4.250 4.667
% 5.083 5.500 6.000 6.001];
BW=69.5; VFATC=0.18; VSLWC=0.46127; VPR=0.962433122; TSTP=145.0; CINT=0.1;
CONCLIST=[1.308 1.218 1.155 1.185 1.322 1.262 1.357 1.282 1.339 1.330 1.284 1.248 1.077 1.257
1.182 1.175 1.149 0.0 0.0];
STRTNEXTLIST=[0.083 0.25 0.5 0.334 0.5 0.25 0.5 0.25 0.25 0.416 0.167 0.75 0.417 0.416 0.417
0.5 0.001 200.0];
TURN=48.4167; URNMISLIST=[14.25 9.5 16.5 9.0 15.0 9.5 12.5 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Start times [0.0 0.300 0.383 0.633 0.800 0.967 1.217 1.550 1.800 1.883 2.050 2.133 2.217 2.300
% 2.383 2.467 2.600 2.633 2.767 2.833 2.883 3.217 3.467 3.967 4.467 4.550 4.967 5.300 5.633
% 5.883 6.000 6.001];
TSTP=145.0; CINT=0.1;
CONCLIST=[1.344 1.252 1.424 1.305 1.367 1.341 1.353 0.492 0.248 0.302 1.594 1.876 1.642 1.583
1.465 0.825 1.259 1.284 1.450 1.386 1.240 1.303 1.315 1.401 1.435 1.381 1.261 1.339
1.436 1.128 1.205 0.0 0.0];
STRTNEXTLIST=[0.3 0.083 0.25 0.167 0.167 0.25 0.333 0.25 0.083 0.167 0.083 0.084 0.083 0.083
0.084 0.133 0.033 0.134 0.066 0.05 0.334 0.25 0.5 0.5 0.083 0.417 0.333 0.333
0.25 0.117 0.001 200.0];
TURN=48.6333; URNMISLIST=[15.0 8.5 14.5 7.0 17.0 8.0 16.5 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check

```

```

Output_Check_Reset
% Experiment G-TRI-2
% Individual posterior parameters for Chiu07_Human male Subject G
QCC=14.19215; VPR=1.16787; DRESPC=0.72419;
QFATC=0.074200; QGUTC=0.17336; QKIDC=0.19171; QLIVC=0.051090; QRAPC=0.39326; QSLWC=0.11638;
VBLDC=0.077924; VFATC=0.16670; VGUTC=0.020020; VKIDC=0.0043086; VLIVC=0.025700; VPERFC=0.85600;
VRAPC=0.086636; VRESPC=0.00017953; VRESPLUMC=0.0023881; VSLWC=0.47453; FRACPLAS=0.56927;
PB=8.53856; PFAT=59.32273; PGUT=2.96481; PKID=1.58978; PLIV=4.08540; PRAP=1.57006;
PRES=1.31178; PSLW=4.03997;
PRBCPLASTCA=0.12244; PBODTCAC=0.67650; PLIVTCAC=0.78442;
PBODTCOH=1.25281; PLIVTCOH=0.63286;
PBODTCOG=0.29104; PLIVTCOG=1.63455; PEFDCVGC=0.010275;
BMAXKDC=4.08162; KDISSOC=180.71220;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=100.97405; KMC=1.0; CL=428.22756; FRACCTAC=0.019557; FRACOTHERC=0.27362;
VMAXDCVGC=1.0; KMDCVGC=3.40727; CLDCVGC=82.71814;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84726; CLKIDDCVGC=28.13683;
VMAXLUNGLIV=0.055647; KMCLARA=2.10328; FRACLUNGSYS=23.64141;
VMAXTCOH=1.0; KMTCOH=2.31243; CLTCOH=0.06960;
VMAXGLUCC=1.0; KMGLUC=119.46220; CLGLUC=0.26054; KMETTCOH=0.53665;
KURNTCAC=0.0029926; KMETTCAC=0.24317;
KBILEC=6.65255; KEHRC=0.15614; KURNTCOGC=0.20607;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 302.4
% Start times [0.0 0.050 0.133 0.383 0.550 0.717 0.967 1.300 1.550 1.633 1.800 1.883 1.967 2.050
% 2.133 2.217 2.350 2.383 2.517 2.583 2.633 2.967 3.217 3.717 4.217 4.300 4.717 5.050 5.383
% 5.633 6.000 6.001];
BW=71.0; VFATC=0.096; VSLWC=0.54523; VPR=0.871143765; TSTP=145.0; CINT=0.1;
CONCLIST=[1.344 1.252 1.424 1.305 1.367 1.341 1.353 0.492 0.248 0.302 1.594 1.876 1.642 1.583
1.465 0.825 1.259 1.284 1.450 1.386 1.240 1.303 1.315 1.401 1.435 1.381 1.261 1.339
1.436 1.128 1.205 0.0 0.0];
STRTNEXTLIST=[0.05 0.083 0.25 0.167 0.167 0.25 0.333 0.25 0.083 0.167 0.083 0.084 0.083 0.083
0.084 0.133 0.033 0.134 0.066 0.05 0.334 0.25 0.5 0.5 0.083 0.417 0.333 0.333
0.25 0.367 0.001 200.0];
TURN=29.8833; URNMISSLIST=[33.0 8.25 17.75 7.5 38.0 1000.0 1000.0 1000.0 1000.0 1000.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Chiu07_Human_Output.txt' @format=ascii

```

Fisher98_Human.m

```

% Fisher J, Mahle D and Abbas R. 1998. A human physiologically based pharmacokinetic model for
% trichloroethylene and its metabolites, trichloroacetic acid and free trichloroethanol.
% Toxicol Appl Pharmacol 152: 339-359.
% http://dx.doi.org/10.1006/taap.1998.8486.
% Male and female volunteers, 20-36 years old
% Inhalation dosing of 50 or 100 ppm TCE for 4 hours

```

```

PlotOutput=[];
ResetDoses
MalePost
% Male subject 1
% Individual posterior parameters for Fisher98_Human male Subject 1
QCC=20.72185; VPR=1.93417; DRESPC=0.53983;
QFATC=0.064200; QGUTC=0.13365; QKIDC=0.19076; QLIVC=0.017752; QRAPC=0.41925; QSLWC=0.17439;
VBLDC=0.078540; VFATC=0.16676; VGUTC=0.020060; VKIDC=0.0042729; VLIVC=0.025950; VPERFC=0.85600;
VRAPC=0.087798; VRESPC=0.00018036; VRESPLUMC=0.0023905; VSLWC=0.47244; FRACPLAS=0.56757;

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PB=9.28827; PFAT=54.11939; PGUT=3.14594; PKID=1.60385; PLIV=3.95309; PRAP=2.54801;
PRES=1.31412; PSLW=2.43157;
PRBCPLASTCA=0.07330; PBODTCAC=0.61827; PLIVTCAC=0.81195;
PBODTCOH=1.08523; PLIVTCOH=0.68316;
PBODTCOG=0.27934; PLIVTCOG=9.74123; PEFDCVG=0.010133;
BMAXKDC=3.94045; KDISSOC=180.68383;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=46.58430; KMC=1.0; CL=2093.63013; FRACTCAC=0.042791; FRACOTHERC=0.45249;
VMAXDCVGC=1.0; KMDCVGC=6.03883; CLDCVG=25.00408;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.82882; CLKIDDCVG=4.53615;
VMAXLUNGLIV=0.063006; KMCLARA=0.75014; FRACLUNGSYS=23.38278;
VMAXTCOH=1.0; KMTCOH=6.57977; CLTCOH=0.15961;
VMAXGLUC=1.0; KMGLUC=126.09051; CLGLUC=0.18637; KMETTCOH=1.45281;
KURNTCAC=0.0071501; KMETTCAC=0.20659;
KBILEC=9.69878; KEHRC=0.10383; KURNTCOG=4.08931;
KDCVGC=4.59974; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=71.4; VFATC=0.17; VSLWC=0.4692; PB=11.49; CONCLIST=[105.0 0.0 0.0];
STRNEXTLIST=[4.0 300.0]; TSTRT=0.0; TSTP=265.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 2
% Individual posterior parameters for Fisher98_Human male Subject 2
QCC=9.25615; VPR=1.82902; DRESPC=0.57264;
QFATC=0.033795; QGUTC=0.16228; QKIDC=0.19133; QLIVC=0.041802; QRAPC=0.40164; QSLWC=0.16916;
VBLDC=0.079079; VFATC=0.16632; VGUTC=0.019964; VKIDC=0.0042759; VLIVC=0.027700; VPERFC=0.85600;
VRAPC=0.087595; VRESPC=0.00017975; VRESPLUMC=0.0023929; VSLWC=0.47088; FRACPLAS=0.56984;
PB=9.26109; PFAT=58.45707; PGUT=2.59874; PKID=1.59450; PLIV=4.03291; PRAP=2.13531;
PRES=1.31304; PSLW=1.83921;
PRBCPLASTCA=3.33293; PBODTCAC=0.52789; PLIVTCAC=0.88257;
PBODTCOH=1.95187; PLIVTCOH=0.64761;
PBODTCOG=7.84353; PLIVTCOG=3.42934; PEFDCVG=0.010368;
BMAXKDC=4.46440; KDISSOC=180.78829;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=164.88752; KMC=1.0; CL=432.96407; FRACTCAC=0.030948; FRACOTHERC=0.06607;
VMAXDCVGC=1.0; KMDCVGC=3.27793; CLDCVG=43.34706;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.82965; CLKIDDCVG=4.93859;
VMAXLUNGLIV=0.141730; KMCLARA=0.05399; FRACLUNGSYS=24.11900;
VMAXTCOH=1.0; KMTCOH=4.07145; CLTCOH=0.10635;
VMAXGLUC=1.0; KMGLUC=126.59588; CLGLUC=0.22741; KMETTCOH=9.02501;
KURNTCAC=0.0018352; KMETTCAC=0.19398;
KBILEC=5.64630; KEHRC=0.14142; KURNTCOG=2.94284;
KDCVGC=7.11354; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=69.3; VFATC=0.27; VSLWC=0.3672; PB=10.1; CONCLIST=[49.3 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

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```

% Male subject 3
% Individual posterior parameters for Fisher98_Human male Subject 3
QCC=12.02501; VPR=2.04987; DRESPC=0.36854;
QFATC=0.007100; QGUTC=0.14896; QKIDC=0.19076; QLIVC=0.031967; QRAPC=0.42777; QSLWC=0.19345;
VBLDC=0.078232; VFATC=0.16622; VGUTC=0.019914; VKIDC=0.0042635; VLIVC=0.028025; VPERFC=0.85600;
VRAPC=0.087569; VRESPC=0.00017991; VRESPLUMC=0.0023881; VSLWC=0.47159; FRACPLAS=0.56757;
PB=9.22025; PFAT=59.09183; PGUT=2.35519; PKID=1.59672; PLIV=3.88362; PRAP=1.96838;
PRES=1.31047; PSLW=1.18784;
PRBCPLASTCA=0.46259; PBODTCAC=0.76260; PLIVTCAC=0.88292;
PBODTCOH=1.46432; PLIVTCOH=0.54704;
PBODTCOG=0.15027; PLIVTCOG=4.06075; PEFDCVGC=0.010420;
BMAXKDC=3.93848; KDISSOC=180.81180;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=534.99829; KMC=1.0; CL=33.54054; FRACTCAC=0.045165; FRACOTHERC=0.03515;
VMAXDCVGC=1.0; KMDCVGC=0.07636; CLDCVGC=522.92549;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.80352; CLKIDDCVGC=4.01919;
VMAXLUNGLIV=0.297652; KMCLARA=0.31068; FRACLUNGSYS=24.70486;
VMAXTCOH=1.0; KMTCOH=1.04780; CLTCOH=0.24027;
VMAXGLUCC=1.0; KMGLUC=206.02551; CLGLUC=0.14838; KMETTCOH=0.51217;
KURNTCAC=0.0028466; KMETTCAC=1.36029;
KBILEC=9.39333; KEHRC=0.19731; KURNTCOG=2.67614;
KDCVGC=11.35888; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=71.1; VFATC=0.14; VSLWC=0.49781; PB=11.1; CONCLIST=[55.2 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[101.5 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 4
% Individual posterior parameters for Fisher98_Human male Subject 4
QCC=16.31376; VPR=1.86708; DRESPC=0.60854;
QFATC=0.022745; QGUTC=0.14632; QKIDC=0.19076; QLIVC=0.030056; QRAPC=0.44985; QSLWC=0.16027;
VBLDC=0.076931; VFATC=0.16628; VGUTC=0.020000; VKIDC=0.0042845; VLIVC=0.026975; VPERFC=0.85600;
VRAPC=0.087578; VRESPC=0.00018018; VRESPLUMC=0.0023929; VSLWC=0.47377; FRACPLAS=0.56813;
PB=9.23593; PFAT=59.12729; PGUT=2.84858; PKID=1.60063; PLIV=4.02569; PRAP=2.35321;
PRES=1.31868; PSLW=2.23142;
PRBCPLASTCA=0.07478; PBODTCAC=0.70200; PLIVTCAC=0.76981;
PBODTCOH=1.48615; PLIVTCOH=0.64790;
PBODTCOG=3.15406; PLIVTCOG=3.20710; PEFDCVGC=0.009735;
BMAXKDC=3.88411; KDISSOC=180.95107;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=74.83334; KMC=1.0; CL=1698.76151; FRACTCAC=0.047102; FRACOTHERC=0.66239;
VMAXDCVGC=1.0; KMDCVGC=5.77080; CLDCVGC=97.45970;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83799; CLKIDDCVGC=5.73782;
VMAXLUNGLIV=0.058092; KMCLARA=1.00740; FRACLUNGSYS=23.21968;
VMAXTCOH=1.0; KMTCOH=0.95045; CLTCOH=0.28224;

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VMAXGLUCC=1.0; KMGLUC=175.21258; CLGLUC=0.12707; KMETTCOHC=1.06582;
KURNTCAC=0.0068150; KMETTCAC=0.14705;
KBILEC=5.86499; KEHRC=0.12556; KURNTCOGC=2.75213;
KDCVGC=5.36019; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=52.3; VFATC=0.1; VSLWC=0.54005; PB=12.1; CONCLIST=[53.1 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[97.8 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 5
% Individual posterior parameters for Fisher98_Human male Subject 5
QCC=19.80806; VPR=1.82445; DRESPC=0.55856;
QFATC=0.012690; QGUTC=0.14142; QKIDC=0.19076; QLIVC=0.025220; QRAPC=0.41779; QSLWC=0.21212;
VBLDC=0.076507; VFATC=0.16593; VGUTC=0.020080; VKIDC=0.0042807; VLIVC=0.026000; VPERFC=0.85600;
VRAPC=0.088176; VRESPC=0.00018018; VRESPLUMC=0.0023929; VSLWC=0.47485; FRACPLAS=0.56677;
PB=9.24915; PFAT=58.39280; PGUT=3.15223; PKID=1.59661; PLIV=4.23590; PRAP=3.02591;
PRES=1.31738; PSLW=2.06266;
PRBCPLASTCA=0.14498; PBODTCAC=0.55694; PLIVTCAC=0.80379;
PBODTCOH=0.89292; PLIVTCOH=0.66923;
PBODTCOG=6.51228; PLIVTCOG=4.56020; PEFDCVG=0.009992;
BMAXKDC=4.07469; KDISSOC=180.92610;
KAS=1.0; KTSD=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=88.87790; KMC=1.0; CL=135.53837; FRACTCAC=0.078596; FRACOTHERC=0.25183;
VMAXDCVGC=1.0; KMDCVGC=9.57074; CLDCVG=41.94834;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.82717; CLKIDDCVG=5.18142;
VMAXLUNGLIV=0.052459; KMCLARA=1.53972; FRACLUNGSYS=23.47650;
VMAXTCOHC=1.0; KMTCOH=1.97882; CLTCOH=0.21503;
VMAXGLUCC=1.0; KMGLUC=117.21384; CLGLUC=0.11544; KMETTCOHC=1.12064;
KURNTCAC=0.0075167; KMETTCAC=0.49406;
KBILEC=6.71941; KEHRC=0.14573; KURNTCOGC=1.13131;
KDCVGC=10.27794; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=82.3; VFATC=0.14; VSLWC=0.50078; PB=11.91; CONCLIST=[105.5 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check

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Output_Check_Reset
% Male subject 6
% Individual posterior parameters for Fisher98_Human male Subject 6
QCC=19.88944; VPR=1.66859; DRESC=0.58252;
QFATC=0.008335; QGUTC=0.15607; QKIDC=0.19095; QLIVC=0.037954; QRAPC=0.39734; QSLWC=0.20935;
VBLDC=0.077462; VFATC=0.16622; VGUTC=0.020020; VKIDC=0.0042862; VLIVC=0.025375; VPERFC=0.85600;
VRAPC=0.087842; VRESC=0.00017977; VRESPLUMC=0.0023905; VSLWC=0.47461; FRACPLAS=0.56870;
PB=9.26035; PFAT=59.68571; PGUT=2.87118; PKID=1.60171; PLIV=4.06188; PRAP=2.60456;
PRES=1.31905; PSLW=1.73089;
PRBCPLASTCA=0.14985; PBODTCAC=0.55390; PLIVTCAC=0.81880;
PBODTCOH=1.18683; PLIVTCOH=0.62829;
PBODTCOG=0.34300; PLIVTCOG=0.57419; PEFDCVGC=0.010245;
BMAXKDC=4.19148; KDISSOC=180.98709;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=82.70363; KMC=1.0; CL=141.45119; FRACTCAC=0.059699; FRACOTHERC=0.09808;
VMAXDCVGC=1.0; KMDCVGC=5.68261; CLDCVG=59.17144;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.82469; CLKIDDCVG=6.18471;
VMAXLUNGLIV=0.060215; KMCLARA=0.59102; FRACLUNGSYS=23.49999;
VMAXTCOHC=1.0; KMTCOH=3.31680; CLTCOH=0.11203;
VMAXGLUCC=1.0; KMGLUC=130.32092; CLGLUC=0.23716; KMETTCOHC=0.61079;
KURNTCAC=0.0044244; KMETTCAC=0.49559;
KBILEC=5.84157; KEHRC=0.16235; KURNTCOGC=8.24310;
KDCVGC=9.27201; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=82.7; VFATC=0.14; VSLWC=0.50083; PB=10.85; CONCLIST=[102.6 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 7
% Individual posterior parameters for Fisher98_Human male Subject 7
QCC=18.65079; VPR=0.97885; DRESC=0.68997;
QFATC=0.012135; QGUTC=0.17332; QKIDC=0.19095; QLIVC=0.049868; QRAPC=0.42598; QSLWC=0.14775;
VBLDC=0.079079; VFATC=0.16591; VGUTC=0.020100; VKIDC=0.0043043; VLIVC=0.027225; VPERFC=0.85600;
VRAPC=0.087657; VRESC=0.00018000; VRESPLUMC=0.0023881; VSLWC=0.47155; FRACPLAS=0.56757;
PB=9.25572; PFAT=60.13504; PGUT=3.20949; PKID=1.59921; PLIV=4.17881; PRAP=2.23650;
PRES=1.30947; PSLW=1.77418;
PRBCPLASTCA=0.05924; PBODTCAC=0.76818; PLIVTCAC=0.76942;
PBODTCOH=1.21190; PLIVTCOH=0.64090;
PBODTCOG=0.37280; PLIVTCOG=11.89796; PEFDCVGC=0.010133;
BMAXKDC=3.74865; KDISSOC=180.85194;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=91.31030; KMC=1.0; CL=287.91196; FRACTCAC=0.041278; FRACOTHERC=0.10872;
VMAXDCVGC=1.0; KMDCVGC=4.95556; CLDCVG=163.11231;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.86092; CLKIDDCVG=14.58625;
VMAXLUNGLIV=0.058040; KMCLARA=0.57973; FRACLUNGSYS=23.31274;
VMAXTCOHC=1.0; KMTCOH=2.28188; CLTCOH=0.21056;
VMAXGLUCC=1.0; KMGLUC=129.80067; CLGLUC=0.22180; KMETTCOHC=0.59315;
KURNTCAC=0.0079100; KMETTCAC=0.13305;
KBILEC=8.45705; KEHRC=0.14987; KURNTCOGC=3.89376;
KDCVGC=7.65225; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;
BW=73.2; VFATC=0.18; VSLWC=0.45746; PB=10.47; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');

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PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 8
% Individual posterior parameters for Fisher98_Human male Subject 8
QCC=17.52343; VPR=1.39791; DRESC=0.60963;
QFATC=0.055200; QGUTC=0.16557; QKIDC=0.19152; QLIVC=0.044239; QRAPC=0.41731; QSLWC=0.12617;
VBLDC=0.078078; VFATC=0.16682; VGUTC=0.019966; VKIDC=0.0042970; VLIVC=0.025575; VPERFC=0.85600;
VRAPC=0.087270; VRESC=0.00018018; VRESPLUMC=0.0023905; VSLWC=0.47381; FRACPLAS=0.56927;
PB=8.60017; PFAT=61.21563; PGUT=2.65014; PKID=1.59572; PLIV=3.88816; PRAP=1.84027;
PRES=1.31335; PSLW=1.69374;
PRBCPLASTCA=0.10075; PBODTCAC=0.85059; PLIVTCAC=0.72539;
PBODTCOH=1.38609; PLIVTCOH=0.64318;
PBODTCOG=0.25607; PLIVTCOG=2.81051; PEFDCVG=0.010275;
BMAXKDC=3.88994; KDISSOC=180.65058;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=44.26807; KMC=1.0; CL=2871.68643; FRACTCAC=0.087472; FRACOTHERC=0.16563;
VMAXDCVGC=1.0; KMDCVGC=6.43023; CLDCVG=60.54815;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.87656; CLKIDDCVG=26.15602;
VMAXLUNGLIV=0.073768; KMCLARA=0.38872; FRACLUNGSYS=23.47650;
VMAXTCOH=1.0; KMTCOH=3.58228; CLTCOH=0.24268;
VMAXGLUC=1.0; KMGLUC=130.71247; CLGLUC=0.27915; KMETTCOH=0.89521;
KURNTCAC=0.0036151; KMETTCAC=0.10689;
KBILEC=7.95659; KEHRC=0.14299; KURNTCOG=8.58809;
KDCVGC=3.85357; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=60.9; VFATC=0.1; VSLWC=0.54063; CONCLIST=[101.1 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 9
% Individual posterior parameters for Fisher98_Human male Subject 9
QCC=29.58267; VPR=1.91014; DRESC=0.54865;
QFATC=0.068350; QGUTC=0.14522; QKIDC=0.19114; QLIVC=0.027885; QRAPC=0.41132; QSLWC=0.15609;
VBLDC=0.078540; VFATC=0.16788; VGUTC=0.020020; VKIDC=0.0042798; VLIVC=0.028125; VPERFC=0.85600;
VRAPC=0.087578; VRESC=0.00018000; VRESPLUMC=0.0023881; VSLWC=0.46940; FRACPLAS=0.56456;
PB=14.18510; PFAT=63.57006; PGUT=2.97461; PKID=1.60376; PLIV=3.92744; PRAP=2.38682;
PRES=1.31359; PSLW=3.02992;
PRBCPLASTCA=0.06240; PBODTCAC=0.64686; PLIVTCAC=0.75660;
PBODTCOH=1.54850; PLIVTCOH=0.62663;
PBODTCOG=22.30229; PLIVTCOG=35.35243; PEFDCVG=0.010358;
BMAXKDC=3.78518; KDISSOC=180.80113;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=57.70037; KMC=1.0; CL=2635.04290; FRACTCAC=0.060966; FRACOTHERC=0.05313;
VMAXDCVGC=1.0; KMDCVGC=7.36111; CLDCVG=12.95185;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.81976; CLKIDDCVG=4.23795;
VMAXLUNGLIV=0.070876; KMCLARA=0.41135; FRACLUNGSYS=23.52350;
VMAXTCOH=1.0; KMTCOH=1.74438; CLTCOH=0.40943;
VMAXGLUC=1.0; KMGLUC=133.75369; CLGLUC=1.06422; KMETTCOH=0.21632;
KURNTCAC=0.0240981; KMETTCAC=0.13738;
KBILEC=6.98664; KEHRC=0.09376; KURNTCOG=0.20155;
KDCVGC=4.44153; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

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BW=70.9; VFATC=0.18; VSLWC=0.45728; CONCLIST=[103.4 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
save PlotOutput @file='Fisher98_MHuman_Output.txt' @format=ascii

ResetDoses
FemalePost

% Female subject 1
% Individual posterior parameters for Fisher98_Human female Subject 1
QCC=10.22963; VPR=1.98949; DRESC=0.46329;
QGUTC=0.017034; QGUTC=0.17050; QKIDC=0.17085; QLIVC=0.035763; QRAPC=0.45081; QSLWC=0.15504;
VBLDC=0.070244; VFATC=0.26802; VGUTC=0.021894; VKIDC=0.0045825; VLIVC=0.026404; VPERFC=0.85778;
VRAPC=0.092572; VRESC=0.00017986; VRESPLUMC=0.0023857; VSLWC=0.37388; FRACPLAS=0.61746;
PB=9.24582; PFAT=58.46876; PGUT=2.22958; PKID=1.59568; PLIV=3.87334; PRAP=2.10247;
PRES=1.31576; PSLW=1.46219;
PRBCPLASTCA=0.10947; PBODTCAC=0.53256; PLIVTCAC=0.98944;
PBODTCOH=1.70163; PLIVTCOH=0.58771;
PBODTCOG=0.37254; PLIVTCOG=10.36430; PEFDCVGC=0.010652;
BMAXKDC=3.93887; KDISSOC=180.85104;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=337.93837; KMC=1.0; CL=142.43058; FRACTCAC=0.037052; FRACOTHERC=0.05156;
VMAXDCVGC=1.0; KMDCVGC=0.72449; CLDCVGC=75.82583;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.81241; CLKIDDCVGC=6.29704;
VMAXLUNGLIV=0.085617; KMCLARA=1.55737; FRACLUNGSYS=23.75992;
VMAXTCOH=1.0; KMTCOH=0.24268; CLTCOH=0.66312;
VMAXGLUC=1.0; KMGLUC=163.69419; CLGLUC=0.42511; KMETTCOH=0.33421;
KURNTCAC=0.0039398; KMETTCAC=2.23782;
KBILEC=7.45586; KEHRC=0.18957; KURNTCOGC=6.74213;
KDCVGC=11.84612; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=66.5; VFATC=0.32; VSLWC=0.3219; PB=9.88; CONCLIST=[55.1 0.0 0.0]; STRTNEXTLIST=[4.0 300.0];
TSTR=0.0; TSTP=265.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[101.4 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check

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Output_Check_Reset
% Female subject 2
% Individual posterior parameters for Fisher98_Human female Subject 2
QCC=11.06170; VPR=1.92337; DRESPC=0.56933;
QFATC=0.056874; QGUTC=0.15815; QKIDC=0.17102; QLIVC=0.027957; QRAPC=0.43701; QSLWC=0.14899;
VBLDC=0.067198; VFATC=0.26368; VGUTC=0.021912; VKIDC=0.0045830; VLIVC=0.024426; VPERFC=0.85778;
VRAPC=0.092721; VRESPC=0.00017986; VRESPLUMC=0.0023929; VSLWC=0.38308; FRACPLAS=0.61685;
PB=9.24286; PFAT=57.24227; PGUT=2.41575; PKID=1.59892; PLIV=3.97437; PRAP=2.27234;
PRES=1.31284; PSLW=1.56273;
PRBCPLASTCA=0.15211; PBODTCAC=0.49096; PLIVTCAC=0.83217;
PBODTCOH=2.08150; PLIVTCOH=0.61573;
PBODTCOG=9.87187; PLIVTCOG=3.12167; PEFDCVGC=0.009922;
BMAXKDC=4.18654; KDISSOC=181.17034;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=0.01896; KMC=1.0; CL=1033.44663; FRACCTAC=0.101425; FRACOTHERC=0.28111;
VMAXDCVGC=1.0; KMDCVGC=4.87983; CLDCVGC=79.07834;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.81976; CLKIDDCVGC=5.50733;
VMAXLUNGLIV=0.060672; KMCLARA=2.14277; FRACLUNGSYS=23.31274;
VMAXTCOH=1.0; KMTCOH=1.50802; CLTCOH=0.28737;
VMAXGLUCC=1.0; KMGLUC=170.54514; CLGLUC=0.22492; KMETTCOH=0.79279;
KURNTCAC=0.0061850; KMETTCAC=0.47688;
KBILEC=7.81465; KEHRC=0.13305; KURNTCOGC=3.05377;
KDCVGC=7.02166; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=62.3; VFATC=0.24; VSLWC=0.40676; PB=9.45; CONCLIST=[53.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[97.7 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 3
% Individual posterior parameters for Fisher98_Human female Subject 3
QCC=18.28331; VPR=1.38844; DRESPC=0.60671;
QFATC=0.018114; QGUTC=0.14549; QKIDC=0.17034; QLIVC=0.017752; QRAPC=0.45043; QSLWC=0.19788;
VBLDC=0.067470; VFATC=0.26733; VGUTC=0.022396; VKIDC=0.0045664; VLIVC=0.024587; VPERFC=0.85778;
VRAPC=0.094302; VRESPC=0.00017977; VRESPLUMC=0.0023953; VSLWC=0.37695; FRACPLAS=0.61623;
PB=9.23464; PFAT=58.51556; PGUT=4.65067; PKID=1.60548; PLIV=4.56075; PRAP=4.68334;
PRES=1.31006; PSLW=1.77329;
PRBCPLASTCA=0.20983; PBODTCAC=0.56206; PLIVTCAC=0.74549;
PBODTCOH=1.34459; PLIVTCOH=0.65874;
PBODTCOG=0.24309; PLIVTCOG=6.23618; PEFDCVGC=0.009962;
BMAXKDC=4.26292; KDISSOC=180.87654;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=133.60177; KMC=1.0; CL=246.81887; FRACCTAC=0.027725; FRACOTHERC=0.05255;
VMAXDCVGC=1.0; KMDCVGC=4.93430; CLDCVGC=40.40037;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.81404; CLKIDDCVGC=4.86020;
VMAXLUNGLIV=0.049357; KMCLARA=2.19241; FRACLUNGSYS=23.21968;

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VMAXTCOHC=1.0; KMTCOH=5.14487; CLTCOH=0.14428;
VMAXGLUCC=1.0; KMGLUC=145.76562; CLGLUC=0.35523; KMETTCOHC=0.26821;
KURNTCAC=0.0047594; KMETTCAC=0.22335;
KBILEC=9.76691; KEHRC=0.13279; KURNTCOGC=12.16273;
KDCVGC=9.07933; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=57.5; VFATC=0.21; VSLWC=0.43428; PB=6.47; CONCLIST=[102.5 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 4
% Individual posterior parameters for Fisher98_Human female Subject 4
QCC=11.37126; VPR=1.55890; DRESPC=0.59185;
QFATC=0.061115; QGUTC=0.18722; QKIDC=0.17085; QLIVC=0.046800; QRAPC=0.39816; QSLWC=0.13586;
VBLDC=0.068544; VFATC=0.26378; VGUTC=0.021952; VKIDC=0.0045756; VLIVC=0.022699; VPERFC=0.85778;
VRAPC=0.092526; VRESPC=0.00018000; VRESPLUMC=0.0023953; VSLWC=0.38353; FRACPLAS=0.61623;
PB=9.22246; PFAT=58.89126; PGUT=2.54989; PKID=1.59656; PLIV=3.92964; PRAP=2.14623;
PRES=1.31374; PSLW=1.85863;
PRBCPLASTCA=0.23171; PBODTCAC=0.61451; PLIVTCAC=0.77089;
PBODTCOH=1.79551; PLIVTCOH=0.62697;
PBODTCOG=0.92088; PLIVTCOG=9.65395; PEFDCVGC=0.010462;
BMAXKDC=4.19799; KDISSOC=180.89209;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=48.24362; KMC=1.0; CL=1353.77835; FRACACTC=0.066841; FRACOTHERC=0.16763;
VMAXDCVGC=1.0; KMDCVGC=4.59565; CLDCVGC=52.63804;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84896; CLKIDDCVGC=8.99869;
VMAXLUNGLIV=0.076164; KMCLARA=0.48418; FRACLUNGSYS=23.40618;
VMAXTCOHC=1.0; KMTCOH=3.39736; CLTCOH=0.22091;
VMAXGLUCC=1.0; KMGLUC=122.85441; CLGLUC=0.28451; KMETTCOHC=0.87084;
KURNTCAC=0.0037030; KMETTCAC=0.27472;
KBILEC=7.41126; KEHRC=0.17033; KURNTCOGC=3.35810;
KDCVGC=6.37893; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=55.5; VFATC=0.23; VSLWC=0.41731; PB=7.63; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 5
% Individual posterior parameters for Fisher98_Human female Subject 5
QCC=10.60567; VPR=1.59485; DRESPC=0.63616;
QFATC=0.088145; QGUTC=0.18329; QKIDC=0.17102; QLIVC=0.044740; QRAPC=0.39167; QSLWC=0.12114;
VBLDC=0.068884; VFATC=0.26371; VGUTC=0.021934; VKIDC=0.0045945; VLIVC=0.022080; VPERFC=0.85778;
VRAPC=0.092284; VRESPC=0.00018000; VRESPLUMC=0.0023905; VSLWC=0.38411; FRACPLAS=0.61359;
PB=9.28084; PFAT=58.37529; PGUT=2.49571; PKID=1.59920; PLIV=3.94791; PRAP=1.92671;
PRES=1.31080; PSLW=2.03580;
PRBCPLASTCA=0.09171; PBODTCAC=0.65147; PLIVTCAC=0.77166;
PBODTCOH=1.78049; PLIVTCOH=0.63405;
PBODTCOG=0.29870; PLIVTCOG=17.74968; PEFDCVGC=0.010441;

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BMAXKDC=3.91022; KDISSOC=180.45667;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=43.95927; KMC=1.0; CL=1444.69679; FRACCTAC=0.040258; FRACOTHERC=0.32595;
VMAXDCVGC=1.0; KMDCVGC=4.49340; CLDCVG=52.53287;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.85236; CLKIDDCVG=10.10549;
VMAXLUNGLIV=0.085532; KMCLARA=0.31632; FRACLUNGSYS=23.01164;
VMAXTCOH=1.0; KMTCOH=2.21533; CLTCOH=0.34404;
VMAXGLUC=1.0; KMGLUC=123.47022; CLGLUC=0.29671; KMETTCOH=1.04980;
KURNTCAC=0.0097780; KMETTCAC=0.25717;
KBILEC=9.47825; KEHRC=0.15107; KURNTCOGC=4.29897;
KDCVGC=6.54695; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=67.3; VFATC=0.35; VSLWC=0.29782; PB=11.0; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 6
% Individual posterior parameters for Fisher98_Human female Subject 6
QCC=14.73873; VPR=1.38885; DRESPEC=0.60617;
QFATC=0.048059; QGUTC=0.17128; QKIDC=0.17085; QLIVC=0.037791; QRAPC=0.40760; QSLWC=0.16442;
VBLDC=0.069496; VFATC=0.26609; VGUTC=0.022000; VKIDC=0.0045880; VLIVC=0.023506; VPERFC=0.85778;
VRAPC=0.092916; VRESPC=0.00018018; VRESPLUMC=0.0023905; VSLWC=0.37900; FRACPLAS=0.61445;
PB=9.09034; PFAT=59.92493; PGUT=2.87603; PKID=1.59760; PLIV=4.07547; PRAP=2.58458;
PRESPEC=1.31604; PSLW=1.58619;
PRBCPLASTCA=0.08323; PBODTCAC=0.75599; PLIVTCAC=0.75110;
PBODTCOH=1.95891; PLIVTCOH=0.62208;
PBODTCOG=0.32100; PLIVTCOG=8.84071; PEFDCVGC=0.010368;
BMAXKDC=3.84047; KDISSOC=180.68599;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=77.49888; KMC=1.0; CL=932.30008; FRACCTAC=0.081559; FRACOTHERC=0.08054;
VMAXDCVGC=1.0; KMDCVGC=4.31765; CLDCVG=64.42096;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84219; CLKIDDCVG=7.30880;
VMAXLUNGLIV=0.072182; KMCLARA=0.46996; FRACLUNGSYS=23.61778;
VMAXTCOH=1.0; KMTCOH=2.44856; CLTCOH=0.33421;
VMAXGLUC=1.0; KMGLUC=125.21096; CLGLUC=0.43771; KMETTCOH=0.44428;
KURNTCAC=0.0100155; KMETTCAC=0.14646;
KBILEC=8.75828; KEHRC=0.14764; KURNTCOGC=8.60528;
KDCVGC=7.44841; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=63.2; VFATC=0.26; VSLWC=0.38509; CONCLIST=[101.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Female subject 7
% Individual posterior parameters for Fisher98_Human female Subject 7
QCC=16.95595; VPR=1.73651; DRESPC=0.57247;
QFATC=0.067966; QGUTC=0.16080; QKIDC=0.17085; QLIVC=0.029946; QRAPC=0.41933; QSLWC=0.15111;
VLDC=0.069904; VFATC=0.26599; VGUTC=0.022044; VKIDC=0.0045756; VLIVC=0.023966; VPERFC=0.85778;
VRAPC=0.092935; VRESPC=0.00017957; VRESPLUMC=0.0023848; VSLWC=0.37818; FRACPLAS=0.61346;
PB=11.27730; PFAT=58.77947; PGUT=2.96658; PKID=1.59898; PLIV=4.08284; PRAP=2.75653;
PRESP=1.31612; PSLW=2.52625;
PRBCPLASTCA=0.06620; PBODTCAC=0.71033; PLIVTCAC=0.77630;
PBODTCOH=1.39012; PLIVTCOH=0.62545;
PBODTCOG=1.77605; PLIVTCOG=21.72291; PEFDCVG=0.010410;
BMAXKDC=3.73929; KDISSOC=180.80004;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=55.93910; KMC=1.0; CL=1211.54871; FRACTCAC=0.042919; FRACOTHERC=0.08399;
VMAXDCVGC=1.0; KMDCVGC=4.92740; CLDCVG=18.58768;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.82551; CLKIDDCVG=5.06867;
VMAXLUNGLIV=0.075030; KMCLARA=0.50248; FRACLUNGSYS=23.31274;
VMAXTCOHC=1.0; KMTCOH=4.08369; CLTCOH=0.22025;
VMAXGLUCC=1.0; KMGLUC=123.10037; CLGLUC=0.57018; KMETTCOHC=0.37738;
KURNTCAC=0.0150312; KMETTCAC=0.16480;
KBILEC=10.58037; KEHRC=0.12100; KURNTCOGC=2.14765;
KDCVGC=7.10643; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=48.6; VFATC=0.23; VSLWC=0.41417; CONCLIST=[103.3 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 8
% Individual posterior parameters for Fisher98_Human female Subject 8
QCC=15.32720; VPR=1.23575; DRESPC=0.60890;
QFATC=0.059891; QGUTC=0.18344; QKIDC=0.17068; QLIVC=0.044434; QRAPC=0.38803; QSLWC=0.15353;
VLDC=0.069156; VFATC=0.26539; VGUTC=0.022000; VKIDC=0.0045908; VLIVC=0.023115; VPERFC=0.85778;
VRAPC=0.092851; VRESPC=0.00018054; VRESPLUMC=0.0023881; VSLWC=0.38049; FRACPLAS=0.61494;
PB=9.25091; PFAT=59.37021; PGUT=2.77073; PKID=1.59715; PLIV=4.01135; PRAP=2.53730;
PRESP=1.30875; PSLW=1.97597;
PRBCPLASTCA=0.10454; PBODTCAC=0.59421; PLIVTCAC=0.75200;
PBODTCOH=1.69298; PLIVTCOH=0.61861;
PBODTCOG=1.45396; PLIVTCOG=18.41871; PEFDCVG=0.010620;
BMAXKDC=4.05437; KDISSOC=180.68094;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=61.57547; KMC=1.0; CL=856.32908; FRACTCAC=0.118087; FRACOTHERC=0.16057;
VMAXDCVGC=1.0; KMDCVGC=4.55448; CLDCVG=46.43433;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84726; CLKIDDCVG=8.49162;
VMAXLUNGLIV=0.072030; KMCLARA=0.49012; FRACLUNGSYS=23.47650;
VMAXTCOHC=1.0; KMTCOH=2.95944; CLTCOH=0.26106;
VMAXGLUCC=1.0; KMGLUC=112.50526; CLGLUC=0.46921; KMETTCOHC=0.45172;
KURNTCAC=0.0080860; KMETTCAC=0.18105;
KBILEC=9.23499; KEHRC=0.20888; KURNTCOGC=1.64769;
KDCVGC=7.75238; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=61.8; VFATC=0.33; VSLWC=0.31588; PB=10.37; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');

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PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher98_FHuman_Output.txt' @format=ascii

```

Kimmerle73_Human.m

```

% Kimmerle G and Eben A. 1973. Metabolism, excretion and toxicology of trichloroethylene after
% inhalation: 2. Experimental human exposure. Arch Toxicol 30: 127-138.
% http://dx.doi.org/10.1007/BF02425930.
% Male and female subjects, age 20-50 yrs (total of 4 subjects)
% Single inhalation dosing of 40 or 44 ppm TCE (+/- 4 ppm) over 4 hours
% OR repeated inhalation dosing of 48 ppm TCE (+/- 3 ppm) over 4 hours/day for 5 days

PlotOutput=[];
ResetDoses
FemalePost

% Individual posterior parameters for Kimmerle73_Human female Subject A
QCC=9.18332; VPR=1.40520; DRESPC=0.62939;
QFATC=0.101405; QGUTC=0.17046; QKIDC=0.17085; QLIVC=0.037011; QRAPC=0.38127; QSLWC=0.13901;
VBLDC=0.068068; VFATC=0.23794; VGUTC=0.021971; VKIDC=0.0045917; VLIVC=0.023736; VPERFC=0.85778;
VRAPC=0.092582; VRESPC=0.00018036; VRESPLUMC=0.0023976; VSLWC=0.40871; FRACPLAS=0.61402;
PB=9.39974; PFAT=57.65590; PGUT=2.68600; PKID=1.60127; PLIV=4.05421; PRAP=2.38036;
PRES=1.31250; PSLW=2.56649;
PRBCPLASTCA=0.16087; PBODTCAC=0.61636; PLIVTCAC=0.75766;
PBODTCOH=2.21885; PLIVTCOH=0.60781;
PBODTCOG=0.17705; PLIVTCOG=6.19887; PEFDCVG=0.0;
BMAXKDC=4.06614; KDISSOC=180.88992;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=174.40210; KMC=1.0; CL=668.91349; FRACCTAC=0.147735; FRACOTHERC=0.06601;
VMAXDCVGC=1.0; KMDCVGC=3.32547; CLDCVG=46.19811;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.85321; CLKIDDCVG=6.56058;
VMAXLUNGLIV=0.158204; KMCLARA=0.04750; FRACLUNGSYSC=23.95076;
VMAXTCOHC=1.0; KMTCOH=1.51150; CLTCOH=0.07547;
VMAXGLUCC=1.0; KMGLUC=126.34295; CLGLUC=0.34576; KMETTCOHC=0.27720;
KURNTCAC=0.0093384; KMETTCAC=0.22537;
KBILEC=10.18586; KEHRC=0.19770; KURNTCOGC=4.25620;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[40.0 0.0 0.0]; STRTNEXTLIST=[4.0 200.0]; TSTRT=0.0; TSTP=200.0; CINT=0.1;
TURN=0.0; URNMISSLIST=[168.0 24.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Kimmerle73_Human female Subject B
QCC=12.64028; VPR=1.52589; DRESPC=0.58784;
QFATC=0.070465; QGUTC=0.17604; QKIDC=0.17085; QLIVC=0.040651; QRAPC=0.39674; QSLWC=0.14525;
VBLDC=0.068544; VFATC=0.23388; VGUTC=0.022000; VKIDC=0.0045848; VLIVC=0.023874; VPERFC=0.85778;
VRAPC=0.092749; VRESPC=0.00017995; VRESPLUMC=0.0023953; VSLWC=0.41197; FRACPLAS=0.61562;
PB=9.65728; PFAT=57.45446; PGUT=2.80651; PKID=1.59822; PLIV=4.06561; PRAP=2.53309;
PRES=1.31820; PSLW=2.54196;
PRBCPLASTCA=0.18156; PBODTCAC=0.60561; PLIVTCAC=0.78128;
PBODTCOH=1.43002; PLIVTCOH=0.62519;
PBODTCOG=0.28300; PLIVTCOG=4.39456; PEFDCVG=0.0;

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BMAXKDC=4.10495; KDISSOC=180.74238;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=129.42008; KMC=1.0; CL=620.58013; FRACTCAC=0.063518; FRACOTHERC=0.08102;
VMAXDCVGC=1.0; KMDCVGC=3.25864; CLDCVG=44.22716;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84388; CLKIDDCVG=6.12929;
VMAXLUNGLIV=0.092470; KMCLARA=0.23955; FRACLUNGSYS=23.52350;
VMAXTCOHC=1.0; KMTCOH=2.91247; CLTCOH=0.14284;
VMAXGLUC=1.0; KMGLUC=124.46194; CLGLUC=0.16965; KMETTCOHC=0.73001;
KURNTCAC=0.0051250; KMETTCAC=0.28536;
KBILEC=7.93275; KEHRC=0.16763; KURNTCOGC=3.30480;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[44.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Kimmerle73_Human female Subject C
QCC=9.38853; VPR=1.58975; DRESPC=0.62195;
QFATC=0.068808; QGUTC=0.16760; QKIDC=0.17085; QLIVC=0.034775; QRAPC=0.40187; QSLWC=0.15609;
VBLDC=0.068476; VFATC=0.25807; VGUTC=0.021976; VKIDC=0.0045724; VLIVC=0.024357; VPERFC=0.85778;
VRAPC=0.092879; VRESPC=0.00017969; VRESPLUMC=0.0023905; VSLWC=0.38727; FRACPLAS=0.61562;
PB=9.67361; PFAT=58.42785; PGUT=2.72073; PKID=1.59841; PLIV=4.08106; PRAP=2.66929;
PRES=1.31926; PSLW=2.57008;
PRBCPLASTCA=0.15150; PBODTCAC=0.57394; PLIVTCAC=0.79301;
PBODTCOH=1.65697; PLIVTCOH=0.61864;
PBODTCOG=0.16691; PLIVTCOG=0.89250; PEFDCVGC=0.0;
BMAXKDC=4.11029; KDISSOC=180.90421;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=210.60062; KMC=1.0; CL=567.16754; FRACTCAC=0.029705; FRACOTHERC=0.06406;
VMAXDCVGC=1.0; KMDCVGC=3.29600; CLDCVG=44.16528;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83548; CLKIDDCVG=5.94814;
VMAXLUNGLIV=0.188084; KMCLARA=0.04154; FRACLUNGSYS=24.43460;
VMAXTCOHC=1.0; KMTCOH=2.47119; CLTCOH=0.18268;
VMAXGLUC=1.0; KMGLUC=125.46163; CLGLUC=0.15536; KMETTCOHC=0.61195;
KURNTCAC=0.0063226; KMETTCAC=0.35772;
KBILEC=7.09933; KEHRC=0.16398; KURNTCOGC=6.05192;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[44.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');

i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Kimmerle73_Human female Subject D
QCC=14.09456; VPR=1.52086; DRESPC=0.59738;
QFATC=0.088400; QGUTC=0.17934; QKIDC=0.17051; QLIVC=0.042406; QRAPC=0.37075; QSLWC=0.14860;
VBLDC=0.068136; VFATC=0.21781; VGUTC=0.022000; VKIDC=0.0045839; VLIVC=0.023851; VPERFC=0.85778;
VRAPC=0.092758; VRESPC=0.00017957; VRESPLUMC=0.0023905; VSLWC=0.42846; FRACPLAS=0.61402;

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PB=9.88612; PFAT=57.36834; PGUT=2.79332; PKID=1.59845; PLIV=4.06338; PRAP=2.59587;
PRES=1.30385; PSLW=2.71893;
PRBCPLASTCA=0.12667; PBODTCAC=0.56225; PLIVTCAC=0.77266;
PBODTCOH=1.88606; PLIVTCOH=0.61275;
PBODTCOG=0.32781; PLIVTCOG=2.67344; PEFDCVG=0.0;
BMAXKDC=4.07754; KDISSOC=180.90530;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=148.20012; KMC=1.0; CL=788.12345; FRACTCAC=0.106306; FRACOTHERC=0.06057;
VMAXDCVGC=1.0; KMDCVGC=3.24596; CLDCVG=39.06547;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83715; CLKIDDCVG=5.72636;
VMAXLUNGLIV=0.108841; KMCLARA=0.13480; FRACLUNGSYS=23.61778;
VMAXTCOHC=1.0; KMTCOH=2.30389; CLTCOH=0.10861;
VMAXGLUC=1.0; KMGLUC=129.02420; CLGLUC=0.23039; KMETTCOHC=0.38293;
KURNTCAC=0.0112024; KMETTCAC=0.25564;
KBILEC=7.18503; KEHRC=0.16663; KURNTCOGC=3.45346;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[44.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

ResetDoses
MalePost

% Individual posterior parameters for Kimmerle73_Human male Subject E
QCC=9.29883; VPR=1.33426; DRESPC=0.60756;
QATC=0.045455; QGUTC=0.15417; QKIDC=0.19095; QLIVC=0.036673; QRAPC=0.39464; QSLWC=0.17811;
VBLDC=0.077308; VFATC=0.17225; VGUTC=0.019992; VKIDC=0.0042897; VLIVC=0.026450; VPERFC=0.85600;
VRAPC=0.087604; VRESPC=0.00018054; VRESPLUMC=0.0023881; VSLWC=0.46792; FRACPLAS=0.56694;
PB=9.16802; PFAT=58.46876; PGUT=2.72414; PKID=1.59685; PLIV=4.04668; PRAP=2.35117;
PRES=1.31422; PSLW=2.29754;
PRBCPLASTCA=0.15927; PBODTCAC=0.58209; PLIVTCAC=0.79540;
PBODTCOH=1.88248; PLIVTCOH=0.61870;
PBODTCOG=0.22871; PLIVTCOG=9.02833; PEFDCVG=0.010275;
BMAXKDC=4.07306; KDISSOC=180.82807;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=143.33199; KMC=1.0; CL=595.05554; FRACTCAC=0.070198; FRACOTHERC=0.08046;
VMAXDCVGC=1.0; KMDCVGC=3.21720; CLDCVG=47.50044;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84726; CLKIDDCVG=7.43411;
VMAXLUNGLIV=0.106903; KMCLARA=0.10477; FRACLUNGSYS=23.59418;
VMAXTCOHC=1.0; KMTCOH=2.51658; CLTCOH=0.10404;
VMAXGLUC=1.0; KMGLUC=127.48516; CLGLUC=0.26714; KMETTCOHC=0.64455;
KURNTCAC=0.0069458; KMETTCAC=0.41674;
KBILEC=8.88176; KEHRC=0.11789; KURNTCOGC=3.38846;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[40.0 0.0 0.0]; STRTNEXTLIST=[4.0 200.0]; TSTRT=0.0; TSTP=200.0; CINT=0.1;
TURN=0.0; URNMISSLIST=[168.0 24.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Individual posterior parameters for Kimmerle73_Human male Subject F
QCC=12.34423; VPR=1.17890; DRESPC=0.61269;
QFATC=0.052250; QGUTC=0.16741; QKIDC=0.19114; QLIVC=0.045312; QRAPC=0.36571; QSLWC=0.17818;
VBLDC=0.077924; VFATC=0.17824; VGUTC=0.019990; VKIDC=0.0043000; VLIVC=0.024898; VPERFC=0.85600;
VRAPC=0.087745; VRESPC=0.00017960; VRESPLUMC=0.0023953; VSLWC=0.46272; FRACPLAS=0.56757;
PB=9.41298; PFAT=59.42961; PGUT=2.81308; PKID=1.60034; PLIV=4.04033; PRAP=2.49730;
PRESP=1.30959; PSLW=2.76389;
PRBCPLASTCA=0.14112; PBODTCAC=0.60888; PLIVTCAC=0.74870;
PBODTCOH=2.00449; PLIVTCOH=0.61525;
PBODTCOG=0.26839; PLIVTCOG=2.43116; PEFDCVG=0.010275;
BMAXKDC=4.15534; KDISSOC=180.79552;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=109.41670; KMC=1.0; CL=699.00280; FRACCTAC=0.024961; FRACOTHERC=0.08442;
VMAXDCVGC=1.0; KMDCVGC=3.29238; CLDCVG=42.71879;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84051; CLKIDDCVGC=6.74013;
VMAXLUNGLIV=0.069057; KMCLARA=0.50606; FRACLUNGSYSYSC=23.54704;
VMAXTCOHC=1.0; KMTCOH=1.72530; CLTCOH=0.20972;
VMAXGLUCC=1.0; KMGLUC=122.24167; CLGLUC=0.31349; KMETTCOHC=0.34164;
KURNTCAC=0.0047357; KMETTCAC=0.16009;
KBILEC=7.29362; KEHRC=0.17136; KURNTCOGC=3.56932;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[40.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Kimmerle73_Human male Subject G
QCC=11.47406; VPR=1.28773; DRESPC=0.60550;
QFATC=0.054000; QGUTC=0.16494; QKIDC=0.19114; QLIVC=0.044883; QRAPC=0.37267; QSLWC=0.17237;
VBLDC=0.077462; VFATC=0.15122; VGUTC=0.019984; VKIDC=0.0042794; VLIVC=0.025525; VPERFC=0.85600;
VRAPC=0.087586; VRESPC=0.00017978; VRESPLUMC=0.0023953; VSLWC=0.48976; FRACPLAS=0.56757;
PB=9.20974; PFAT=56.97386; PGUT=2.72926; PKID=1.60138; PLIV=4.07170; PRAP=2.36028;
PRESP=1.30677; PSLW=2.53258;
PRBCPLASTCA=0.15690; PBODTCAC=0.60470; PLIVTCAC=0.75873;
PBODTCOH=2.01796; PLIVTCOH=0.61447;
PBODTCOG=0.22440; PLIVTCOG=3.24257; PEFDCVG=0.010275;
BMAXKDC=4.12471; KDISSOC=180.59513;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=136.87438; KMC=1.0; CL=687.90775; FRACCTAC=0.058576; FRACOTHERC=0.07855;
VMAXDCVGC=1.0; KMDCVGC=3.33713; CLDCVG=45.20641;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84219; CLKIDDCVGC=7.47885;
VMAXLUNGLIV=0.101385; KMCLARA=0.14242; FRACLUNGSYSYSC=23.64141;
VMAXTCOHC=1.0; KMTCOH=2.41186; CLTCOH=0.12381;
VMAXGLUCC=1.0; KMGLUC=123.10037; CLGLUC=0.30882; KMETTCOHC=0.34994;
KURNTCAC=0.0063989; KMETTCAC=0.21140;
KBILEC=8.53350; KEHRC=0.19205; KURNTCOGC=3.80523;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[40.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check

```

```

Output_Check_Reset
% Individual posterior parameters for Kimmerle73_Human male Subject H
QCC=15.60371; VPR=1.15198; DRESPC=0.61269;
QFATC=0.056650; QGUTC=0.16851; QKIDC=0.19095; QLIVC=0.046787; QRAPC=0.35848; QSLWC=0.17862;
VBLDC=0.077693; VFATC=0.13757; VGUTC=0.020020; VKIDC=0.0042841; VLIVC=0.025750; VPERFC=0.85600;
VRAPC=0.087745; VRESPC=0.00017996; VRESPLUMC=0.0023953; VSLWC=0.50276; FRACPLAS=0.56813;
PB=9.29430; PFAT=56.72940; PGUT=2.83171; PKID=1.59885; PLIV=4.07056; PRAP=2.54208;
PRES=1.31300; PSLW=2.75643;
PRBCPLASTCA=0.18622; PBODTCAC=0.61809; PLIVTCAC=0.78293;
PBODTCOH=1.61283; PLIVTCOH=0.61753;
PBODTCOG=0.66384; PLIVTCOG=3.87044; PEFDCVGC=0.010275;
BMAXKDC=4.13793; KDISSOC=180.70226;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=117.09242; KMC=1.0; CL=707.44136; FRACTCAC=0.034755; FRACOTHERC=0.07895;
VMAXDCVGC=1.0; KMDCVGC=3.38722; CLDCVGC=45.72014;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84557; CLKIDDCVGC=7.75300;
VMAXLUNGLIV=0.074435; KMCLARA=0.34889; FRACLUNGSYSYSC=23.38278;
VMAXTCOH=1.0; KMTCOH=2.15351; CLTCOH=0.09956;
VMAXGLUCC=1.0; KMGLUC=126.97624; CLGLUC=0.26874; KMETTCOH=0.39972;
KURNTCAC=0.0042594; KMETTCAC=0.27555;
KBILEC=6.57319; KEHRC=0.18378; KURNTCOGC=1.76716;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[44.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Repeated dosing
ResetDoses
MalePost

% Individual posterior parameters for Kimmerle73_Human male Subject J
QCC=10.89374; VPR=1.44423; DRESPC=0.59393;
QFATC=0.044495; QGUTC=0.16017; QKIDC=0.19114; QLIVC=0.040879; QRAPC=0.39317; QSLWC=0.17015;
VBLDC=0.077539; VFATC=0.16236; VGUTC=0.020020; VKIDC=0.0042733; VLIVC=0.025875; VPERFC=0.85600;
VRAPC=0.087490; VRESPC=0.00017973; VRESPLUMC=0.0023929; VSLWC=0.47826; FRACPLAS=0.56813;
PB=9.88108; PFAT=59.32273; PGUT=2.78724; PKID=1.59822; PLIV=4.02928; PRAP=2.41607;
PRES=1.32226; PSLW=3.44642;
PRBCPLASTCA=0.18869; PBODTCAC=0.59689; PLIVTCAC=0.79460;
PBODTCOH=1.26300; PLIVTCOH=0.62681;
PBODTCOG=0.46125; PLIVTCOG=2.52785; PEFDCVGC=0.010275;
BMAXKDC=4.14041; KDISSOC=180.82301;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=117.13927; KMC=1.0; CL=579.78349; FRACTCAC=0.035993; FRACOTHERC=0.08647;
VMAXDCVGC=1.0; KMDCVGC=3.38960; CLDCVGC=42.89859;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83883; CLKIDDCVGC=5.04339;
VMAXLUNGLIV=0.075787; KMCLARA=0.31286; FRACLUNGSYSYSC=23.42960;
VMAXTCOH=1.0; KMTCOH=4.42823; CLTCOH=0.09518;
VMAXGLUCC=1.0; KMGLUC=120.78354; CLGLUC=0.11248; KMETTCOH=0.61681;
KURNTCAC=0.0042765; KMETTCAC=0.37054;
KBILEC=6.99363; KEHRC=0.14719; KURNTCOGC=2.37115;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

CONCLIST=[48.0 0.0 48.0 0.0 48.0 0.0 48.0 0.0 48.0 0.0 0.0];
STRTNEXTLIST=[4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 500.0];
TSTRT=0.0; TSTP=410.0; CINT=0.1;
TURN=0.0; URNMISSLIST=[384.0 24.0];

```

```

start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Kimmerle73_Human male Subject K
QCC=12.20797; VPR=1.36558; DRESC=0.60447;
QFATC=0.037285; QGUTC=0.16678; QKIDC=0.19133; QLIVC=0.044733; QRAPC=0.36121; QSLWC=0.19866;
VBLDC=0.077616; VFATC=0.12929; VGUTC=0.020020; VKIDC=0.0042807; VLIVC=0.025425; VPERFC=0.85600;
VRAPC=0.087701; VRESC=0.00017998; VRESPLUMC=0.0023905; VSLWC=0.51149; FRACPLAS=0.56757;
PB=9.47623; PFAT=57.16790; PGUT=2.81272; PKID=1.60079; PLIV=4.05069; PRAP=2.66737;
PRES=1.31738; PSLW=3.31096;
PRBCPLASTCA=0.14717; PBODTCAC=0.59492; PLIVTCAC=0.76116;
PBODTCOH=1.64739; PLIVTCOH=0.61699;
PBODTCOG=0.44074; PLIVTCOG=0.99827; PEFDCVG=0.010275;
BMAXKDC=4.15742; KDISSOC=180.79010;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=148.54138; KMC=1.0; CL=684.47679; FRACCTAC=0.037052; FRACOTHERC=0.06775;
VMAXDCVGC=1.0; KMDCVGC=3.27858; CLDCVG=43.72146;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84557; CLKIDDCVG=6.12929;
VMAXLUNGLIV=0.098981; KMCLARA=0.13213; FRACLUNGSYS=23.49999;
VMAXTCOH=1.0; KMTCOH=4.08777; CLTCOH=0.14428;
VMAXGLUC=1.0; KMGLUC=121.51042; CLGLUC=0.17658; KMETTCOH=0.42130;
KURNTCAC=0.0047452; KMETTCAC=0.21937;
KBILEC=6.44304; KEHRC=0.18582; KURNTCOG=3.48817;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Kimmerle73_Human male Subject L
QCC=11.06281; VPR=1.35077; DRESC=0.60254;
QFATC=0.051700; QGUTC=0.16353; QKIDC=0.19114; QLIVC=0.043661; QRAPC=0.31853; QSLWC=0.23144;
VBLDC=0.078078; VFATC=0.15452; VGUTC=0.020000; VKIDC=0.0042712; VLIVC=0.025000; VPERFC=0.85600;
VRAPC=0.088176; VRESC=0.00018036; VRESPLUMC=0.0023905; VSLWC=0.48577; FRACPLAS=0.56813;
PB=9.83435; PFAT=57.96229; PGUT=2.76144; PKID=1.60258; PLIV=4.06025; PRAP=3.19348;
PRES=1.30362; PSLW=2.98571;
PRBCPLASTCA=0.14585; PBODTCAC=0.60283; PLIVTCAC=0.75426;
PBODTCOH=1.62839; PLIVTCOH=0.61996;
PBODTCOG=0.44784; PLIVTCOG=1.27324; PEFDCVG=0.010275;
BMAXKDC=4.18369; KDISSOC=180.73605;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=124.55701; KMC=1.0; CL=672.26643; FRACCTAC=0.035921; FRACOTHERC=0.07030;
VMAXDCVGC=1.0; KMDCVGC=3.26060; CLDCVG=42.18391;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83632; CLKIDDCVG=5.59056;
VMAXLUNGLIV=0.083841; KMCLARA=0.27063; FRACLUNGSYS=23.45304;
VMAXTCOH=1.0; KMTCOH=4.76358; CLTCOH=0.18214;
VMAXGLUC=1.0; KMGLUC=121.51042; CLGLUC=0.18123; KMETTCOH=0.49184;
KURNTCAC=0.0038005; KMETTCAC=0.18014;
KBILEC=6.54041; KEHRC=0.16914; KURNTCOG=2.95759;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;

```

```

KNATC=0.00034950; KKIDBIOACTC=0.062787;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh_coll, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Kimmerle73_Human male Subject M
QCC=15.69526; VPR=1.05602; DRESPC=0.61576;
QFATC=0.053050; QGUTC=0.17201; QKIDC=0.19095; QLIVC=0.050057; QRAPC=0.33992; QSLWC=0.19402;
VBLDC=0.078232; VFATC=0.09441; VGUTC=0.020040; VKIDC=0.0042807; VLIVC=0.025425; VPERFC=0.85600;
VRAPC=0.087701; VRESPC=0.00018000; VRESPLUMC=0.0023953; VSLWC=0.54574; FRACPLAS=0.56927;
PB=9.18822; PFAT=55.69512; PGUT=2.84343; PKID=1.59929; PLIV=4.05024; PRAP=2.64619;
PRESP=1.31103; PSLW=3.15452;
PRBCPLASTCA=0.24649; PBODTCAC=0.66231; PLIVTCAC=0.74274;
PBODTCOH=1.10229; PLIVTCOH=0.62622;
PBODTCOG=0.40661; PLIVTCOG=0.67312; PEFDCVGC=0.010275;
BMAXKDC=4.23314; KDISSOC=180.65980;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=139.76515; KMC=1.0; CL=841.89453; FRACATC=0.031072; FRACOTHERC=0.07129;
VMAXDCVGC=1.0; KMDCVGC=3.45703; CLDCVG=45.10256;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.85321; CLKIDDCVG=8.60273;
VMAXLUNGLIV=0.088582; KMCLARA=0.17084; FRACLUNGSYS=23.59418;
VMAXTCOHC=1.0; KMTCOH=4.97786; CLTCOH=0.12003;
VMAXGLUCC=1.0; KMGLUC=121.02535; CLGLUC=0.13876; KMETTCOHC=0.66898;
KURNTCAC=0.0024185; KMETTCAC=0.16613;
KBILEC=6.23389; KEHRC=0.18881; KURNTCOGC=3.85502;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca_coll, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Kimmerle73_Human_Output.txt' @format=ascii

```

Monster76_Human.m

```

% Monster A, Boersma G and Duba W. 1976. Pharmacokinetics of trichloroethylene in volunteers,
% influence of workload and exposure concentration. Int Arch Occup Environ Health 38: 87-102.
% http://dx.doi.org/10.1007/BF00378619.
% Four male volunteers
% Inhalation dosing of 70 or 140 ppm TCE for 4 hours

```

```

PlotOutput=[];
ResetDoses
MalePost

```

```

% Subject A
% Individual posterior parameters for Monster76_Human male Subject A
QCC=14.19215; VPR=1.06171; DRESPC=0.77585;
QFATC=0.040010; QGUTC=0.16460; QKIDC=0.19095; QLIVC=0.043128; QRAPC=0.37506; QSLWC=0.18625;
VBLDC=0.077231; VFATC=0.16489; VGUTC=0.020020; VKIDC=0.0042643; VLIVC=0.024923; VPERFC=0.85600;
VRAPC=0.088000; VRESPC=0.00018054; VRESPLUMC=0.0023953; VSLWC=0.47649; FRACPLAS=0.56638;
PB=8.79754; PFAT=53.14333; PGUT=2.85081; PKID=1.60029; PLIV=4.06019; PRAP=2.81742;
PRESP=1.31729; PSLW=2.82565;
PRBCPLASTCA=3.37317; PBODTCAC=0.47942; PLIVTCAC=0.75245;

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PBODTCOH=0.88244; PLIVTCOH=0.60264;
PBODTCOG=19.00476; PLIVTCOG=0.31238; PEFFDCVG=0.010275;
BMAXKDC=4.49981; KDISSOC=180.85791;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=147.32832; KMC=1.0; CL=577.46899; FRACTCAC=0.036355; FRACOTHERC=0.03412;
VMAXDCVGC=1.0; KMDCVGC=3.77730; CLDCVG=42.51849;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83215; CLKIDDCVGC=3.53983;
VMAXLUNGLIV=0.199922; KMCLARA=0.00637; FRACLUNGSYS=27.57749;
VMAXTCOH=1.0; KMTCOH=1.28711; CLTCOH=0.12258;
VMAXGLUC=1.0; KMGLUC=92.48070; CLGLUC=0.13561; KMETTCOH=0.19301;
KURNTCAC=0.0035118; KMETTCAC=0.22358;
KBILEC=5.21219; KEHRC=0.17907; KURNTCOG=0.78457;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 210.0
BW=70.0; VFATC=0.12; VSLWC=0.52138; VPR=0.611431166; CONCLIST=[65.0 0.0 0.0];
STRTNEXTLIST=[4.0 600.0]; TSTR=0.0; TSTP=505.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Measured QP of 282.0
VPR=0.821064709; CONCLIST=[140.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Subject B
% Individual posterior parameters for Monster76_Human male Subject B
QCC=14.15105; VPR=0.73505; DRESPEC=0.64102;
QFATC=0.077000; QGUTC=0.16726; QKIDC=0.19190; QLIVC=0.046475; QRAPC=0.36838; QSLWC=0.14898;
VBLDC=0.076061; VFATC=0.16513; VGUTC=0.020020; VKIDC=0.0042837; VLIVC=0.026825; VPERFC=0.85600;
VRAPC=0.087199; VRESPEC=0.00018054; VRESPLUMC=0.0023845; VSLWC=0.47630; FRACPLAS=0.56757;
PB=9.59576; PFAT=48.90074; PGUT=2.79785; PKID=1.59423; PLIV=4.05758; PRAP=2.06620;
PRESPEC=1.31220; PSLW=3.37582;
PRBCPLASTCA=0.79386; PBODTCAC=0.47841; PLIVTCAC=0.84138;
PBODTCOH=1.22298; PLIVTCOH=0.62167;
PBODTCOG=23.89548; PLIVTCOG=1.41194; PEFFDCVG=0.010275;
BMAXKDC=4.32791; KDISSOC=180.80511;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=120.56193; KMC=1.0; CL=872.75488; FRACTCAC=0.027780; FRACOTHERC=0.06660;
VMAXDCVGC=1.0; KMDCVGC=3.51244; CLDCVG=45.91257;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83715; CLKIDDCVGC=5.77235;
VMAXLUNGLIV=0.071373; KMCLARA=0.27117; FRACLUNGSYS=23.71244;
VMAXTCOH=1.0; KMTCOH=0.89530; CLTCOH=0.34232;
VMAXGLUC=1.0; KMGLUC=122.73162; CLGLUC=0.22335; KMETTCOH=0.49544;
KURNTCAC=0.0035436; KMETTCAC=0.83027;
KBILEC=6.27140; KEHRC=0.22628; KURNTCOG=1.19169;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

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% Measured QP of 390.0
BW=80.0; VFATC=0.26; VSLWC=0.38143; VPR=1.030287549; CONCLIST=[68.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Measured QP of 372.0
VPR=0.982735816; CONCLIST=[138.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Subject C
% Individual posterior parameters for Monster76_Human male Subject C
QCC=14.18363; VPR=0.76926; DRESPC=0.51397;
QFATC=0.049895; QGUTC=0.16802; QKIDC=0.19152; QLIVC=0.049706; QRAPC=0.35083; QSLWC=0.19004;
VBLDC=0.076192; VFATC=0.16618; VGUTC=0.019896; VKIDC=0.0042527; VLIVC=0.022250; VPERFC=0.85600;
VRAPC=0.088528; VRESPC=0.00018108; VRESPLUMC=0.0023905; VSLWC=0.47852; FRACPLAS=0.56399;
PB=9.13161; PFAT=48.29329; PGUT=2.76486; PKID=1.59634; PLIV=4.16192; PRAP=2.60092;
PRES=1.31802; PSLW=2.21448;
PRBCPLASTCA=0.77620; PBODTCAC=0.47675; PLIVTCAC=0.77490;
PBODTCOH=0.94141; PLIVTCOH=0.64910;
PBODTCOG=19.87951; PLIVTCOG=0.42791; PEFDCVGC=0.010275;
BMAXKDC=4.47907; KDISSOC=180.32534;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=44.93709; KMC=1.0; CL=1210.33776; FRACTCAC=0.031605; FRACOTHERC=0.03932;
VMAXDCVGC=1.0; KMDCVGC=6.45471; CLDCVGC=98.04622;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.84811; CLKIDDCVGC=4.07178;
VMAXLUNGLIV=0.149594; KMCLARA=0.04755; FRACLUNGSYS=24.55707;
VMAXTCOHC=1.0; KMTCOH=0.95670; CLTCOH=0.19849;
VMAXGLUC=1.0; KMGLUC=87.61919; CLGLUC=0.17395; KMETTCOHC=0.37236;
KURNTCAC=0.0035613; KMETTCAC=0.43270;
KBILEC=5.88849; KEHRC=0.16629; KURNTCOGC=1.08804;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 258.0
BW=62.0; VFATC=0.14; VSLWC=0.5047; VPR=0.823262901; CONCLIST=[70.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

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% Measured QP of 336.0
VPR=1.072156337; CONCLIST=[142.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Subject D
% Individual posterior parameters for Monster76_Human male Subject D
QCC=14.19924; VPR=1.05710; DRESC=0.71591;
QFATC=0.040645; QGUTC=0.17412; QKIDC=0.19057; QLIVC=0.050434; QRAPC=0.39646; QSLWC=0.14777;
VBLDC=0.077693; VFATC=0.16650; VGUTC=0.020020; VKIDC=0.0042910; VLIVC=0.025475; VPERFC=0.85600;
VRAPC=0.087648; VRESC=0.00017960; VRESPLUMC=0.0023905; VSLWC=0.47419; FRACPLAS=0.56870;
PB=8.63593; PFAT=54.51591; PGUT=2.80163; PKID=1.60195; PLIV=4.05316; PRAP=2.20982;
PRES=1.30976; PSLW=2.42550;
PRBCPLASTCA=0.20559; PBODTCAC=0.58677; PLIVTCAC=0.77700;
PBODTCOH=1.27276; PLIVTCOH=0.62545;
PBODTCOG=23.65772; PLIVTCOG=0.61147; PEFFDCVG=0.010275;
BMAXKDC=4.23924; KDISSOC=180.80655;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=93.15489; KMC=1.0; CL=728.98616; FRACTCAC=0.028144; FRACOTHERC=0.08492;
VMAXDCVGC=1.0; KMDCVGC=3.60532; CLDCVG=53.11392;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83465; CLKIDDCVG=7.26508;
VMAXLUNGLIV=0.065912; KMCLARA=0.27887; FRACLUNGSYS=23.52350;
VMAXTCOHC=1.0; KMTCOH=1.33790; CLTCOH=0.22202;
VMAXGLUCC=1.0; KMGLUC=104.06337; CLGLUC=0.20495; KMETTCOHC=0.47152;
KURNTCAC=0.0031713; KMETTCAC=0.27144;
KBILEC=5.67460; KEHRC=0.17605; KURNTCOGC=1.29612;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

% Measured QP of 444.0
BW=67.0; VFATC=0.09; VSLWC=0.55069; VPR=1.335247484; CONCLIST=[76.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Measured QP of 486.0
VPR=1.461554678; CONCLIST=[140.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

save PlotOutput @file='Monster76_Human_Output.txt' @format=ascii
Muller74_Human.m
% Muller G, Spassovski M and Henschler D. 1974. Metabolism of trichloroethylene in man: II.
% Pharmacokinetics of metabolites. Arch Toxicol 32: 283-295.
% http://dx.doi.org/10.1007/BF00330110.
% Male students, 20 to 30 years
% Oral dosing with 3 mg/kg NaTCA or 10 mg/kg TCOH drunk over 0.01 hours (36 seconds)
% (3 mg/kg NaTCA is equivalent to 2.646 mg/kg TCA (NaTCA MW = 185.4 and 1 mg NaTCA equiv to
% 0.8819 mg TCA))

PlotOutput=[];
ResetDoses
MalePost

% Individual posterior parameters for Muller74_Human male
QCC=10.22963; VPR=1.24356; DRESPC=1.00000;
QFATC=0.044980; QGUTC=0.15658; QKIDC=0.19095; QLIVC=0.038227; QRAPC=0.38803; QSLWC=0.18124;
VBLDC=0.077770; VFATC=0.16595; VGUTC=0.019990; VKIDC=0.0043043; VLIVC=0.028225; VPERFC=0.85600;
VRAPC=0.087701; VRESPC=0.00018018; VRESPLUMC=0.0023905; VSLWC=0.47188; FRACPLAS=0.56927;
PB=9.21416; PFAT=57.04798; PGUT=2.83403; PKID=1.59940; PLIV=4.05470; PRAP=2.40664;
PRESP=1.31422; PSLW=2.43522;
PRBCPLASTCA=4.49899; PBODTCAC=0.63310; PLIVTCAC=0.83234;
PBODTCOH=2.17927; PLIVTCOH=0.70749;
PBODTCOG=0.44065; PLIVTCOG=17.82082; PEFFDCVG=0.010275;
BMAXKDC=3.84816; KDISSOC=180.57184;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=6.59294; KASTCOH=8.73205;
VMAXC=94.69522; KMC=1.0; CL=861.48250; FRACTCAC=0.040908; FRACOTHERC=0.10721;
VMAXDCVGC=1.0; KMDCVGC=3.61760; CLDCVG=52.79619;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83632; CLKIDDCVG=7.94132;
VMAXLUNGLIV=0.087525; KMCLARA=0.24341; FRACLUNGSYS=23.57060;
VMAXTCOHC=1.0; KMTCOH=6.38531; CLTCOH=1.05991;
VMAXGLUC=1.0; KMGLUC=194.22164; CLGLUC=1.94138; KMETTCOHC=51.93537;
KURNTCAC=0.0047357; KMETTCAC=0.86537;
KBILEC=10.15534; KEHRC=0.27117; KURNTCOG=0.15572;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

PODOSETCA=2.646; TCHNG=0.01; TSTP=170.0;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PODOSETCA=0.0; PODOSETCOH=10.0;
start @NoCallback
plot(_t, _ctcoh)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Muller74_Human_Output.txt' @format=ascii

```

Paykoc45_Human.m

% Paykoc Z and Powell J. 1945. The excretion of sodium trichloroacetate. J Pharmacol Exp Ther 85:
% 289-293.
% 6 subjects
% IV dosing with 1.7, 1.8 or 2.9 g sodium trichloroacetate in 3% aqueous solution (approximately
% isotonic) given over 1 hour
% (BWs of 45.6, 48.2 or 64.0 kg so doses of 0.03728, 0.06016 or 0.028125 g sodium TCA/kg which
% convert to 37.2, 60.16 or 28.125 mg NaTCA/kg and to 32.9, 53.06 or 24.80 mg TCA/kg
% (NaTCA MW = 185.4, 1 mg NaTCA equiv to 0.8819 mg TCA)

PlotOutput=[];
ResetDoses
MalePost

% Individual posterior parameters for Paykoc45_Human male Subject 1

QCC=13.93758; VPR=1.24680; DRESPEC=0.60799;
QFATC=0.045145; QGUTC=0.16488; QKIDC=0.19114; QLIVC=0.044395; QRAPC=0.37289; QSLWC=0.18154;
VBLDC=0.078848; VFATC=0.16804; VGUTC=0.020040; VKIDC=0.0042832; VLIVC=0.024778; VPERFC=0.85600;
VRAPC=0.087815; VRESPC=0.00017946; VRESPLUMC=0.0023953; VSLWC=0.47202; FRACPLAS=0.56813;
PB=9.21416; PFAT=57.04798; PGUT=2.83403; PKID=1.59940; PLIV=4.05470; PRAP=2.40664;
PRESPEC=1.31422; PSLW=2.43522;
PRBCPLASTCA=0.03287; PBODTCAC=0.87081; PLIVTCAC=0.72174;
PBODTCOH=1.56375; PLIVTCOH=0.62940;
PBODTCOG=0.62057; PLIVTCOG=3.84344; PEFDCVGC=0.010275;
BMAXKDC=3.68988; KDISSOC=179.35672;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=94.69522; KMC=1.0; CL=861.48250; FRACCTAC=0.040908; FRACOTHERC=0.10721;
VMAXDCVGC=1.0; KMDCVGC=3.61760; CLDCVGC=52.79619;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83632; CLKIDDCVGC=7.94132;
VMAXLUNGLIV=0.087525; KMCLARA=0.24341; FRACLUNGSYS=23.57060;
VMAXTCOH=1.0; KMTCOH=2.27073; CLTCOH=0.17658;
VMAXGLUCC=1.0; KMGLUC=129.28251; CLGLUC=0.28111; KMETTCOH=0.69907;
KURNTCAC=0.0066401; KMETTCAC=0.09739;
KBILEC=7.24274; KEHRC=0.15614; KURNTCOGC=1.82828;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=45.6; FRACPLAS=0.61; IVDOSSETCA=32.9; TCHNG=1.0; TSTP=203.0;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Paykoc45_Human male Subject 2

QCC=14.15105; VPR=1.23464; DRESPEC=0.60799;
QFATC=0.045000; QGUTC=0.16446; QKIDC=0.19095; QLIVC=0.043927; QRAPC=0.37429; QSLWC=0.18137;
VBLDC=0.078001; VFATC=0.16684; VGUTC=0.020000; VKIDC=0.0042914; VLIVC=0.025525; VPERFC=0.85600;
VRAPC=0.087798; VRESPC=0.00018018; VRESPLUMC=0.0023976; VSLWC=0.47336; FRACPLAS=0.56757;
PB=9.21416; PFAT=57.04798; PGUT=2.83403; PKID=1.59940; PLIV=4.05470; PRAP=2.40664;
PRESPEC=1.31422; PSLW=2.43522;
PRBCPLASTCA=0.03912; PBODTCAC=0.61741; PLIVTCAC=0.75223;
PBODTCOH=1.56375; PLIVTCOH=0.62940;
PBODTCOG=0.62057; PLIVTCOG=3.84344; PEFDCVGC=0.010275;
BMAXKDC=4.17742; KDISSOC=180.66738;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=94.69522; KMC=1.0; CL=861.48250; FRACCTAC=0.040908; FRACOTHERC=0.10721;
VMAXDCVGC=1.0; KMDCVGC=3.61760; CLDCVGC=52.79619;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83632; CLKIDDCVGC=7.94132;
VMAXLUNGLIV=0.087525; KMCLARA=0.24341; FRACLUNGSYS=23.57060;
VMAXTCOH=1.0; KMTCOH=2.27073; CLTCOH=0.17658;
VMAXGLUCC=1.0; KMGLUC=129.28251; CLGLUC=0.28111; KMETTCOH=0.69907;
KURNTCAC=0.0050538; KMETTCAC=0.20311;
KBILEC=7.24274; KEHRC=0.15614; KURNTCOGC=1.82828;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;

```

KNATC=0.00034950; KKIDBIOACTC=0.062787;
BW=48.2; FRACPLAS=0.60; IVD0SETCA=53.06;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Individual posterior parameters for Paykoc45_Human male Subject 3
QCC=14.12701; VPR=1.24294; DRESPC=0.60799;
QFATC=0.044900; QGUTC=0.16488; QKIDC=0.19133; QLIVC=0.044259; QRAPC=0.37225; QSLWC=0.18238;
VBLDC=0.077770; VFATC=0.16509; VGUTC=0.020000; VKIDC=0.0042897; VLIVC=0.025650; VPERFC=0.85600;
VRAPC=0.087718; VRESPC=0.00018036; VRESPLUMC=0.0023953; VSLWC=0.47530; FRACPLAS=0.56700;
PB=9.21416; PFAT=57.04798; PGUT=2.83403; PKID=1.59940; PLIV=4.05470; PRAP=2.40664;
PRES=1.31422; PSLW=2.43522;
PRBCPLASTCA=0.04154; PBODTCAC=0.60066; PLIVTCAC=0.76245;
PBODTCOH=1.56375; PLIVTCOH=0.62940;
PBODTCOG=0.62057; PLIVTCOG=3.84344; PEFDCVG=0.010275;
BMAXKDC=4.22232; KDISSOC=180.88450;
KAS=1.0; KTS=1.0; KAD=1.0; KTD=0.0; KASTCA=5.26984; KASTCOH=7.30092;
VMAXC=94.69522; KMC=1.0; CL=861.48250; FRACTCAC=0.040908; FRACOTHERC=0.10721;
VMAXDCVGC=1.0; KMDCVGC=3.61760; CLDCVG=52.79619;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.83632; CLKIDDCVG=7.94132;
VMAXLUNGLIV=0.087525; KMCLARA=0.24341; FRACLUNGSYS=23.57060;
VMAXTCOHC=1.0; KMTCOH=2.27073; CLTCOH=0.17658;
VMAXGLUCC=1.0; KMGLUC=129.28251; CLGLUC=0.28111; KMETTCOHC=0.69907;
KURNTCAC=0.0035471; KMETTCAC=0.21353;
KBILEC=7.24274; KEHRC=0.15614; KURNTCOGC=1.82828;
KDCVGC=7.17068; FRACKIDDCVCC=22026.46579;
KNATC=0.00034950; KKIDBIOACTC=0.062787;

BW=64.0; FRACPLAS=0.55; IVD0SETCA=24.8;
start @NoCallback
plot(_t, _cplastca)
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Paykoc45_Human_Output.txt' @format=ascii

```

APPENDIX L

Data for Mouse Validation Figures

The following data are for generating mouse validation figures in Appendix F.

Abbas and Fisher, 1997a

TCE Oral Gavage 300.0 mg/kg

Hours, AurnTCOGTCOH, CBldTCA, CFat, CKid, CLiv, CLivTCA, CLivTCOH, CTCOGTCOH, CTCOH, Cven, AurnTCA

0.25	nan	26.7	60.13	90.4	70.0	18.9	39.8	15.92	14.54	26.11	nan
0.5	nan	20.4	125.4	21.4	42.1	nan	66.2	21.31	19.66	12.99	nan
1.0	nan	nan	189.9	25.8	16.98	nan	41.52	31.27	37.54	6.67	nan
2.0	nan	42.6	72.58	7.92	8.81	35.8	18.82	10.58	9.85	0.68	nan
4.0	nan	53.4	40.32	6.69	4.17	45.6	20.69	13.57	4.78	0.61	nan
8.0	nan	47.6	18.12	3.4	1.89	48.0	14.68	9.51	2.23	nan	nan
16.0	nan	43.2	31.3	6.7	0.945	35.3	5.06	1.82	1.48	nan	nan
24.0	1.912	35.9	0.65	3.26	nan	8.16	nan	nan	nan	nan	0.707
30.0	nan	25.0	nan	nan	nan	10.4	nan	nan	nan	nan	nan
48.0	3.555	nan	nan	nan	nan	1.229	nan	nan	nan	nan	1.176
72.0	3.76	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.292
96.0	3.803	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.304
120.0	3.84	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.307
144.0	3.855	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.308

TCE Oral Gavage 600.0 mg/kg

Hours, AurnTCOGTCOH, CBldTCA, CFat, CKid, CLiv, CLivTCA, CLivTCOGTCOH, CLivTCOH, CTCOGTCOH, CTCOH, Cven, AurnTCA

0.25	nan	11.18	278.5	83.08	213.5	11.2	18.45	50.25	10.51	18.8	81.9	nan
0.5	nan	14.26	659.0	135.5	163.8	22.9	20.07	46.83	39.66	26.76	71.3	nan
2.0	nan	26.98	468.91	15.98	19.43	33.5	39.44	36.29	27.01	24.01	5.71	nan
4.0	nan	31.73	46.76	10.89	10.63	39.9	19.59	21.06	23.55	8.23	1.94	nan
8.0	nan	31.87	9.48	5.4	0.71	54.99	46.06	11.24	14.76	2.16	0.965	nan
12.0	nan	nan	nan	nan	nan	nan	nan	4.29	6.89	1.02	nan	nan
16.0	nan	29.48	0.71	nan	nan	39.06	nan	nan	nan	nan	nan	nan
24.0	6.892	24.81	0.32	0.42	0.339	28.2	nan	nan	nan	nan	nan	0.762
30.0	nan	nan	nan	nan	nan	15.2	nan	nan	nan	nan	nan	nan
40.0	nan	21.1	nan	nan	nan	7.6	nan	nan	nan	nan	nan	nan
48.0	9.072	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.683
72.0	9.593	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.867
96.0	9.716	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.904
120.0	9.829	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.927
144.0	9.895	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.941

TCE Oral Gavage 1200.0 mg/kg

Hours, AurnTCOGTCOH, CBldTCA, CFat, CKid, CLiv, CLivTCA, CLivTCOGTCOH, CLivTCOH, CTCOGTCOH, CTCOH, Cven, AurnTCA

0.083	nan	nan	61.53	144.9	522.6	nan	nan	nan	nan	nan	165.87	nan
0.17	nan	nan	156.7	171.3	585.3	nan	nan	nan	nan	nan	191.31	nan
0.25	nan	16.5	567.2	265.6	499.4	11.09	23.67	65.35	62.12	18.83	123.52	nan
0.5	nan	23.1	826.0	282.6	408.0	16.95	23.3	75.33	63.13	27.73	86.9	nan
0.75	nan	29.2	865.3	1095.6	289.8	20.09	19.03	98.28	67.59	31.36	70.9	nan
1.0	nan	36.1	nan	690.1	228.8	26.02	34.89	105.3	50.86	35.42	43.08	nan
1.5	nan	41.8	1199.9	303.8	63.04	29.44	54.87	88.25	64.31	28.26	35.17	nan
2.0	nan	59.1	1050.5	109.8	38.97	35.65	62.31	92.24	95.02	41.86	20.36	nan
3.0	nan	64.0	550.2	32.4	nan	37.76	74.66	55.03	41.5	21.54	8.97	nan
4.0	nan	70.2	485.0	nan	26.5	42.07	76.92	57.64	46.7	24.64	7.5	nan
6.0	nan	94.1	219.2	40.2	15.37	43.92	26.66	35.96	51.86	4.589	nan	nan
8.0	nan	90.8	293.7	17.3	14.97	57.83	55.43	37.45	40.88	nan	1.64	nan
12.0	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.487	0.72	nan
16.0	nan	65.2	4.4	3.6	12.86	27.71	nan	10.12	10.11	nan	0.47	nan
24.0	8.23	43.86	1.446	2.2	1.79	18.801	nan	nan	nan	nan	0.52	2.294
30.0	nan	41.48	nan	nan	nan	22.67	nan	nan	nan	nan	nan	nan
40.0	nan	9.15	nan	nan	nan	6.34	nan	nan	nan	nan	nan	nan
48.0	11.263	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.731
72.0	12.195	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.579
96.0	12.409	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.796
120.0	12.641	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.848
144.0	12.709	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.87

TCE Oral Gavage 2000.0 mg/kg
Hours, AurnTCOGTCOH, CBldTCA, CFat, CKid, CLiv, CLivTCA, CLivTCOGTCOH, CLivTCOH, CTCOGTCOH, CTCOH, CVen, AurnTCA

0.25	nan	11.22	1152.0	636.0	1498.0	15.18	17.3	64.69	16.2	21.41	208.3	nan
0.5	nan	20.57	1993.0	652.0	335.0	27.58	14.47	73.45	22.88	32.94	162.0	nan
1.0	nan	30.34	4279.0	542.0	379.7	37.49	205.3	nan	41.84	140.1	nan	nan
2.0	nan	43.51	2015.0	176.0	116.2	49.46	237.98	nan	36.4	64.8	nan	nan
4.0	nan	63.43	1991.0	nan	114.5	65.32	66.23	114.88	61.1	29.14	48.6	nan
8.0	nan	nan	1503.0	139.4	105.1	105.65	23.04	73.96	40.88	nan	17.48	nan
16.0	nan	131.85	75.5	55.0	9.2	59.0	13.08	30.8	21.68	4.21	1.15	nan
24.0	15.28	51.38	7.4	1.3	2.0	44.6	nan	nan	nan	nan	nan	1.423
30.0	nan	54.57	nan	nan	nan	36.35	nan	nan	nan	nan	nan	nan
48.0	21.19	8.74	nan	nan	nan	9.98	nan	nan	nan	nan	nan	2.486
72.0	23.92	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.122
96.0	24.79	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.294
120.0	25.51	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.395
144.0	25.94	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.426
168.0	25.95	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.438
192.0	25.98	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.45

Abbas et al., 1997b

TCA IV 100.0 mg/kg
Hours, CBldTCA, AurnTCA

0.1	281.9	nan
0.15	380.3	nan
0.35	374.4	nan
0.65	207.0	nan
1.0	204.6	nan
2.0	94.3	nan
4.0	83.1	nan
8.0	48.97	nan
24.0	9.37	0.937
30.0	3.91	nan
48.0	nan	1.744
72.0	nan	1.801
96.0	nan	1.828
120.0	nan	1.843
144.0	nan	1.849
168.0	nan	1.853

TCOH IV 100.0 mg/kg
Hours, AurnTCOGTCOH, CBldTCA, CTCOH

0.05	nan	0.83	77.34
0.1	nan	2.05	44.75
0.5	nan	2.21	19.11
1.0	nan	7.45	7.17
2.0	nan	21.1	0.163
24.0	1.093	nan	nan
48.0	1.859	nan	nan
72.0	1.986	nan	nan
96.0	2.097	nan	nan
120.0	2.061	nan	nan
144.0	2.071	nan	nan
168.0	2.1	nan	nan

Fisher et al., 1991

TCE Inhalation 42.0 ppm for 4 hours -- females

Hours, CPlasTCA, CVen

2.0	17.69	0.306666667
3.83	23.94	0.34
4.167	29.92	nan
4.333	35.03	nan
4.5	24.33	nan
4.67	29.72	nan
6.0	25.18	nan
9.0	7.86	nan

TCE Inhalation 236.0 ppm for 4 hours -- females

Hours, CPlasTCA, CVen

2.0	50.8	4.58
3.83	57.2	4.95
4.5	nan	0.88
5.0	58.4	0.45
6.0	43.2	nan
7.0	24.0	nan
9.0	14.4	nan

TCE Inhalation 368.0 ppm for 4 hours -- females

Hours, CPlasTCA, CVen

2.0	58.5	5.9
3.83	59.8	6.3
4.33	61.7	1.03
4.67	69.9	0.8
5.0	59.7	0.22
5.33	57.7	nan
7.0	35.9	nan
10.0	24.5	nan
30.0	0.32	nan

TCE Inhalation 889.0 ppm for 4 hours -- females

Hours, CPlasTCA, CVen

2.0	51.1	3.9
3.83	83.2	3.6
4.167	90.9	2.0
4.333	92.3	1.4
4.5	94.1	0.72
5.0	94.3	0.55
6.0	76.7	nan
8.0	28.6	nan
26.0	0.46	nan

TCE Closed Chamber Inhalation 300.0 ppm for
4 hours -- females

Hours, CInhPPM	
0.05	228.4977169
0.5	101.0376712
0.64	72.01027397
0.84	53.21689498
1.0	37.95890411
1.2	28.65525114
1.3	21.956621
1.5	17.11872146
1.7	12.28082192
1.8	9.489726027
2.0	7.070776256

TCE Closed Chamber Inhalation 700.0 ppm for
4 hours -- females

Hours, CInhPPM	
0.03	645.673516
0.14	503.3276256
0.31	379.0308219
0.49	261.0605023
0.64	182.9098174
0.83	137.880137
0.97	111.4577626
1.13	86.89611872
1.32	65.49771689
1.49	52.10045662
1.65	41.30821918
1.83	33.49315068
1.97	28.46917808
2.20	21.58447489
2.33	16.18835616
2.48	14.32762557
2.69	11.72260274

TCE Closed Chamber Inhalation 1100.0 ppm for
4 hours -- females

Hours, CInhPPM	
0.05	975.3949772
0.15	816.6746575
0.29	603.8070776
0.47	479.8824201
0.66	395.4052511
0.82	325.6278539
0.97	277.8070776
1.14	250.2682648
1.32	206.1689498
1.49	160.9531963
1.65	144.9509132
1.81	119.2728311
1.98	101.9680365
2.14	88.57077626
2.32	72.94063927
2.50	60.10159817
2.67	51.35616438
2.83	42.23858447
2.98	35.35388128
3.17	28.65525114
3.32	22.32876712
3.49	19.72374429
3.65	16.37442922
3.83	13.39726027

TCE Closed Chamber Inhalation 3700.0 ppm for
4 hours -- females

Hours, CInhPPM	
0.04	3673.082192
0.12	2913.90411
0.30	2316.609589
0.47	1907.248858
0.63	1570.456621
0.81	1317.39726
0.95	1250.410959
1.14	1168.538813
1.29	1110.856164
1.49	1001.073059
1.63	950.8333333
1.80	971.3013699
1.98	891.2899543
2.14	876.4041096
2.32	848.4931507
2.48	835.4680365
2.65	794.5319635
2.98	744.2922374
3.14	720.1027397
3.32	697.7739726
3.48	686.609589
3.65	664.2808219
3.82	619.6232877
4.0	612.1803653
4.14	580.5479452
4.32	552.6369863
4.48	524.7260274
4.65	507.9794521
4.82	474.4863014
5.0	442.8538813
5.14	435.4109589
5.33	400.0570776
5.48	366.5639269
5.64	347.956621
5.99	288.413242

TCE Closed Chamber Inhalation 7000.0 ppm for 4 hours -- females

Hours, CInhPPM	
0.03	6514.417808
0.12	5455.6621
0.29	4182.922374
0.46	3323.26484
0.62	2887.853881
0.79	2744.577626
0.97	2472.910959
1.14	2309.166667
1.30	2232.876712
1.46	2123.093607
1.63	2091.461187
1.79	2022.614155
1.96	1994.703196
2.14	2000.285388
2.30	1970.513699
2.47	1907.248858
2.64	1845.844749
2.80	1817.93379
2.95	1790.022831
3.12	1732.340183
3.30	1737.922374
3.49	1713.732877
3.64	1657.910959
3.83	1693.26484
3.95	1607.671233
4.15	1585.342466
4.30	1561.152968
4.46	1536.96347
4.98	1551.849315
5.15	1529.520548
5.33	1453.230594
5.48	1380.6621
5.63	1360.194064
5.81	1317.39726
5.97	1274.600457

TCE Inhalation 110.0 ppm for 4 hours -- males

Hours, CPlasTCA, CVen		
2.0	17.76	1.5
3.75	46.18	nan
3.9	49.81	1.51
4.2	38.99	0.38
4.4	nan	0.38
5.0	70.53	nan
6.0	54.29	nan
8.0	41.02	nan
21.0	7.06	nan

TCE Inhalation 297.0 ppm for 4 hours -- males

Hours, CPlasTCA, CVen		
2.0	nan	1.48
2.5	58.0	nan
3.9	nan	1.2
4.2	101.7	0.88
4.4	88.5	0.37
4.8	109.6	nan
4.9	114.7	nan
5.3	85.8	nan
5.5	80.6	nan
6.3	83.0	nan
24.0	5.7	nan

TCE Inhalation 368.0 ppm for 4 hours -- males

Hours, CPlasTCA, CVen		
2.0	61.8	3.82
3.9	94.2	3.72
4.2	103.1	1.24
4.4	103.0	0.51
4.75	97.0	0.22
5.0	101.4	nan
5.5	71.6	nan
6.5	58.8	nan
24.0	9.8	nan

TCE Inhalation 748.0 ppm for 4 hours -- males

Hours, CPlasTCA, CVen		
2.0	88.6	7.18
3.9	127.4	7.2
4.2	123.6	1.5
4.4	nan	0.88
4.5	123.6	0.49
4.75	125.5	nan
5.0	106.2	nan
7.75	82.1	nan
9.0	58.0	nan
24.0	9.4	nan

TCE Closed Chamber Inhalation 1020.0 ppm for 4 hours -- males

Hours, CInhPPM	
0.07	838.4452055
0.16	609.7614155
0.33	384.9851598
0.50	222.543379
0.66	156.3013699
0.84	100.293379
1.0	64.5673516
1.18	41.49429224
1.33	28.09703196
1.51	18.42123288
1.69	12.65296804
1.85	8.559360731
2.0	6.512557078
2.16	5.023972603
2.32	4.465753425

TCE Closed Chamber Inhalation 1800.0 ppm for 4 hours -- males

Hours, CInhPPM	
0.16	1352.937215
0.25	1113.833333
0.33	950.0890411
0.48	716.0091324
0.67	600.0856164
0.83	494.2100457
1.0	399.8710046
1.16	312.2305936
1.33	243.7557078
1.49	187.0034247
1.67	128.9486301
1.84	93.78082192
2.01	62.52054795
2.17	40.19178082
2.33	27.16666667
2.50	16.9326484
2.68	11.9086758
2.83	8.373287671

TCE Closed Chamber Inhalation 3800.0 ppm for 4 hours -- males

Hours, CInhPPM	
0.14	2471.050228
0.32	1862.591324
0.51	1507.191781
0.69	1356.472603
0.83	1220.639269
1.0	1116.438356
1.19	1023.401826
1.35	952.6940639
1.49	904.3150685
1.66	857.7968037
1.85	785.2283105
2.01	733.1278539
2.15	682.8881279
2.34	614.0410959
2.52	573.1050228
2.68	534.0296804
2.81	480.0684932
2.99	455.8789954
3.17	403.7785388
3.33	349.8173516
3.49	303.2990868
3.67	249.3378995
3.80	206.5410959
3.98	160.0228311
4.16	117.2260274
4.31	87.4543379
4.50	63.26484018
4.65	48.37899543
4.82	33.49315068
5.01	22.32876712
5.15	16.74657534

TCE Closed Chamber Inhalation 5600.0 ppm for 4 hours -- males

Hours, CInhPPM	
0.07	5384.954338
0.16	4434.121005
0.33	3224.646119
0.48	2608.744292
0.68	2186.358447
0.84	1933.299087
0.97	1769.554795
1.18	1620.696347
1.32	1510.913242
1.51	1434.623288
1.68	1384.383562
1.83	1313.675799
2.0	1246.689498
2.15	1183.424658
2.33	1142.488584
2.48	1103.413242
2.65	1047.591324
2.75	1028.984018
2.92	975.0228311
3.08	943.390411
3.26	909.8972603
3.42	863.3789954
3.58	833.6073059
3.76	790.8105023
3.90	777.7853881
4.08	738.7100457
4.24	712.6598174
4.41	677.3059361
4.56	653.1164384
4.75	630.7876712
4.87	599.1552511
5.04	558.2191781
5.23	530.3082192

TCE Closed Chamber Inhalation 10000.0 ppm for 4 hours -- males

Hours, CInhPPM	
0.08	8384.452055
0.15	7279.178082
0.31	5889.212329
0.47	5204.46347
0.66	4683.458904
0.82	4443.424658
0.97	4069.417808
1.16	3861.015982
1.33	3600.513699
1.50	3475.844749
1.67	3299.075342
1.82	3185.570776
2.01	3131.609589
2.15	2969.726027
2.34	2869.246575
2.51	2820.86758
2.65	2724.109589
2.82	2725.97032
3.01	2631.073059

Fisher and Allen, 1993

TCE Oral Gavage 487.0 mg/kg -- females

Hours, CPlasTCA, CVen		
0.083	3.066666667	38.5
0.17	5.466666667	24.33333333
0.5	14.8	12.9
1.0	25.4	6.233333333
2.0	33.8	2.8
4.0	55.63333333	nan
7.0	56.56666667	nan
24.0	2.2	nan

TCE Oral Gavage 973.0 mg/kg -- females

Hours, CPlasTCA, CVen		
0.083	5.39	22.1
0.17	6.6	16.3
0.25	7.0	35.8
0.5	12.0	12.5
1.0	20.16666667	17.88666667
2.0	41.1	21.4
3.0	41.2	nan
4.0	nan	13.70666667
7.0	43.7	nan
27.0	5.466666667	nan

TCE Oral Gavage 1947.0 mg/kg -- females

Hours, CPlasTCA, CVen		
0.033	2.0	14.3
0.083	5.1	38.6
0.17	16.3	48.9
0.25	15.2	42.5
0.5	28.6	50.0
1.0	33.0	27.9
2.0	54.1	136.0
3.0	nan	167.5
4.0	89.3	119.8
6.0	86.0	48.6
8.0	nan	2.233333333
9.0	nan	10.37333333
24.0	14.6	nan
30.0	4.0	nan

TCE Oral Gavage 487.0 mg/kg -- males
 Hours, CPlasTCA, CVen
 0.083 5.8 50.9
 0.17 6.9 39.0
 0.5 17.9 nan
 1.0 32.0 6.9
 2.0 54.9 1.5
 7.0 82.2 nan
 24.0 13.8 nan
 30.0 4.1 nan

TCE Oral Gavage 973.0 mg/kg -- males
 Hours, CPlasTCA, CVen
 0.033 8.933333333 9.7
 0.083 12.1 29.9
 0.17 11.8 50.9
 0.25 17.9 69.3
 0.5 27.4 66.4
 1.0 49.2 48.2
 2.0 76.6 12.68666667
 3.0 85.3 4.8
 4.0 48.6 16.86666667
 5.0 80.9 nan
 6.0 86.4 nan
 7.0 91.4 5.9
 30.0 12.56666667 nan
 48.0 2.0 nan

TCE Oral Gavage 1947.0 mg/kg -- males
 Hours, CPlasTCA, CVen
 0.033 1.2 20.0
 0.083 3.9 30.7
 0.17 11.9 45.1
 0.25 16.3 64.7
 0.5 32.7 71.7
 1.0 61.6 127.3
 2.0 41.3 33.26666667
 3.0 56.1 106.7
 4.0 54.9 75.7
 5.0 61.1 103.4
 6.0 91.0 47.9
 7.0 94.4 23.9
 24.0 47.5 nan
 30.0 29.4 nan
 48.0 28.5 nan
 72.0 1.9 nan
 72.0 1.9 nan

Green and Prout, 1985

TCE Oral Gavage 10.0 mg/kg
 Hours, AUrnTCOGTCOH, AExhPost, AUrnTCA
 24.0 0.151246897 0.011115 0.023867144
 72.0 nan 0.011115 nan

TCE Oral Gavage 500.0 mg/kg
 Hours, AUrnTCOGTCOH, AExhPost, AUrnTCA
 24.0 8.743811279 0.855 0.755310904
 72.0 nan 0.855 nan

TCE Oral Gavage 1000.0 mg/kg
 Hours, AUrnTCOGTCOH, AExhPost, AUrnTCA
 24.0 11.99527586 4.9875 1.036993105
 72.0 nan 4.9875 nan

TCE Oral Gavage 2000.0 mg/kg
 Hours, AUrnTCOGTCOH, AExhPost, AUrnTCA
 24.0 27.90858197 7.752 2.230208548
 72.0 nan 7.752 nan

Greenberg et al., 1999

TCE Inhalation 100.0 ppm for 4 hours
 Hours, CBldTCA, CFat, CKid, CLiv, CLivTCA, CLivTCOGTCOH, CLivTCOH, CTCOGTCOH, CTCOH, CVen
 2.0 18.23 19.35 3.473 0.5719 12.84 18.52 4.134 4.51 2.041 0.6651
 4.0 29.86 44.46 4.91 0.7577 21.17 22.91 4.446 6.222 1.847 0.8605
 4.25 33.72 nan nan 0.1673 21.81 13.73 1.162 2.733 1.778 0.1387
 4.5 25.03 27.68 0.1341 0.051 16.32 5.328 5.099 1.97 0.7934 0.1497
 4.75 31.63 nan nan nan 20.74 6.365 0.5918 2.09 0.3029 nan
 6.0 27.06 nan nan nan 17.04 0.8768 0.4164 0.1985 0.0899 nan
 12.0 6.798 nan nan nan 5.15 nan nan nan nan nan
 18.0 3.992 nan nan nan 2.732 nan nan nan nan nan
 28.0 1.908 nan nan nan 1.404 nan nan nan nan nan

TCE Inhalation 600.0 ppm for 4 hours
 Hours, CBldTCA, CFat, CKid, CLiv, CLivTCA, CLivTCOGTCOH, CLivTCOH, CTCOGTCOH, CTCOH, CVen
 2.0 56.1 244.48 22.85 10.19 33.72 36.6 28.93 16.17 16.53 6.851
 4.0 96.66 233.7 22.04 12.62 52.12 62.08 24.7 25.1 13.37 7.325
 4.25 74.62 198.4 6.167 3.013 45.67 49.31 17.65 17.87 10.89 1.534
 4.5 99.03 167.5 4.714 1.074 54.97 19.37 5.476 6.746 3.979 0.5987
 4.75 77.74 142.2 2.855 0.6447 48.54 30.51 6.282 8.252 3.201 0.4649
 6.0 107.67 104.1 0.6404 0.2754 48.74 4.313 2.647 2.028 1.007 0.1699
 12.0 25.82 nan nan nan 13.01 nan nan 0.3544 nan nan
 18.0 13.34 nan nan nan 7.952 nan nan nan nan nan
 28.0 7.191 nan nan nan 4.405 0.1568 nan nan nan nan
 47.0 0.8069 nan nan nan 0.7298 0.1025 nan nan nan nan

Larson and Bull, 1992a

TCE Oral Gavage 197.25 mg/kg

Hours, CBldMix, CBldTCA, CTCOH

0.25	44.8074	22.876	28.24055
0.75	20.8926	35.131	19.4051
2.0	nan	24.3466	nan
8.0	nan	20.5884	nan
24.0	nan	2.451	nan

TCE Oral Gavage 591.75 mg/kg

Hours, CBldMix, CBldTCA, CTCOH

0.25	151.11	14.0524	25.415
0.75	74.03076	36.4382	32.89
2.0	30.11688	63.0724	37.375
8.0	nan	100.8178	nan
24.0	nan	6.6994	nan

TCE Oral Gavage 1972.5 mg/kg

Hours, CBldMix, CBldTCA, CTCOH

0.25	436.3794	22.876	38.3617
0.75	292.8906	42.9742	34.8634
2.0	154.9206	68.4646	59.8897
8.0	4.0734	122.3866	17.98485
24.0	nan	28.2682	nan
48.0	nan	4.7386	nan

Larson and Bull, 1992b

TCA Oral Gavage 20.0 mg/kg

Hours, CPlasTCA

0.25	35.131
1.0	33.6604
3.0	33.6604
5.0	23.5296
10.0	9.1504
16.0	4.085

TCA Oral Gavage 100.0 mg/kg

Hours, CPlasTCA

0.25	104.576
1.0	119.9356
3.0	109.8048
5.0	89.7066
10.0	49.02
16.0	7.6798
24.0	5.2288

Merdink et al., 1998

TCE IV 100.0 mg/kg

Hours, CBldTCA, TotCTCOH

0.18	6.0458	7.13115
0.359	9.5589	5.8006
0.525	9.86936	3.6179
0.65	12.69618	2.40695
0.76	13.10468	2.6013
1.02	16.34	2.3322
1.26	18.791	0.79534
1.52	16.07856	0.617435
2.99	18.3008	0.192855
6.01	15.09816	nan

Prout et al., 1985

TCE Oral Gavage 1000 mg/kg

Hours, CBldMix, CBldTCA, TotCTCOH, AExhPost

0.25	10.3	nan	nan	nan
0.3	nan	nan	9.6	nan
0.5	18.0	nan	21.7	0.74
0.75	13.6	39.0	29.4	nan
1.0	8.0	106.0	27.8	1.34
1.5	10.5	nan	30.6	1.78
2.0	6.2	69.0	27.6	2.18
2.5	nan	146.0	20.3	2.59
3.0	6.3	121.0	nan	nan
3.5	1.5	nan	9.5	2.88
4.0	1.7	157.0	10.7	3.04
4.5	1.8	133.0	14.3	3.09
5.0	2.2	149.0	2.8	3.1
5.5	2.3	101.0	7.4	3.15
6.0	2.9	121.0	6.6	3.17
6.5	3.3	nan	5.5	3.19
7.0	4.3	162.0	2.6	3.17
7.5	1.9	196.0	1.5	3.24
8.0	nan	211.0	0.7	3.24
8.5	nan	nan	nan	3.25
9.0	nan	201.0	nan	3.27
10.0	nan	190.0	nan	nan
11.0	nan	189.0	nan	nan
12.0	nan	170.0	nan	nan
13.0	nan	260.0	nan	nan
14.0	nan	242.0	nan	nan
15.0	nan	216.0	nan	nan
16.0	nan	179.0	nan	nan
17.0	nan	118.0	nan	nan
18.0	nan	59.0	nan	nan
19.0	nan	124.0	nan	nan
20.0	nan	197.0	nan	nan
21.0	nan	170.0	nan	nan
22.0	nan	146.0	nan	nan
24.0	nan	238.0	nan	nan
25.0	nan	224.0	nan	nan
27.0	nan	158.0	nan	nan
28.0	nan	150.0	nan	nan
29.0	nan	267.0	nan	nan
30.0	nan	285.0	nan	nan
32.0	nan	70.0	nan	nan
33.0	nan	56.0	nan	nan
34.0	nan	29.0	nan	nan
36.0	nan	40.0	nan	nan
38.0	nan	29.0	nan	nan
41.0	nan	20.0	nan	nan
44.0	nan	7.0	nan	nan

Templin et al., 1993

TCE Oral Gavage 500 mg/kg

Hours, CBldMix, CBldTCA, CTCOH

0.25	28.3824	10.7844	17.9101
0.5	24.7032	18.791	27.7771
0.75	21.9438	25.0002	35.5511
1.0	11.826	41.667	40.2454
1.5	3.8106	46.569	30.199
2.0	1.7082	43.4644	8.56635
3.0	nan	57.19	0.73255
4.0	nan	64.8698	nan
6.0	nan	39.7062	nan
9.0	nan	37.2552	nan
12.0	nan	30.8826	nan
18.0	nan	10.7844	nan
24.0	nan	8.8236	nan
36.0	nan	1.9608	nan

APPENDIX M

Data for Rat Validation Figures

The following data are for generating rat validation figures in Appendix G.

Bernauer et al., 1996

TCE Inhalation 40.0 ppm for 6 hours
Hours, AurnTCOGTCOH, AurnNDCVC, AurnTCA

12.0	0.851813835	0.000462562	0.055668023
24.0	0.973501526	0.001002218	0.055668023
36.0	1.095189217	0.001561147	0.055668023
48.0	1.156033062	0.00213935	0.055668023

TCE Inhalation 80.0 ppm for 6 hours
Hours, AurnTCOGTCOH, AurnNDCVC, AurnTCA

12.0	1.703627671	0.000510746	0.111336045
24.0	2.068690743	0.000992581	0.167004068
36.0	2.312066124	0.00149369	0.167004068
48.0	2.433753815	0.002033346	0.167004068

TCE Inhalation 160.0 ppm for 6 hours
Hours, AurnTCOGTCOH, AurnNDCVC, AurnTCA

12.0	2.798816887	0.000636023	0.334008135
24.0	3.16387996	0.001618968	0.556680225
36.0	3.468099186	0.002775373	0.668016271
48.0	3.711474568	0.00360413	0.723684293

Dallas et al., 1991

TCE Inhalation 50.0 ppm for 2 hours
Hours, CArT, CExhResp

0.023166667	nan	0.127
0.027166667	0.203	nan
0.057333333	nan	0.146
0.064666667	0.261	nan
0.089333333	nan	0.161
0.100833333	0.335	nan
0.1335	0.443	nan
0.163833333	0.402	nan
0.175	nan	0.155
0.253333333	0.452	nan
0.26	nan	0.177
0.336666667	0.491	nan
0.343333333	nan	0.176
0.42	0.349	nan
0.501666667	0.49	nan
0.506666667	nan	0.176
0.671666667	nan	0.18
0.756666667	0.429	nan
0.843333333	nan	0.173
1.008333333	nan	0.179
1.01	0.55	nan
1.176666667	nan	0.187
1.253333333	0.508	nan
1.335	nan	0.183
1.501666667	nan	0.192
1.505	0.639	nan
1.666666667	nan	0.185
1.75	0.59	nan
1.816666667	nan	0.182
2.0	0.601	0.178
2.016666667	nan	0.0601
2.033333333	0.339	nan
2.05	nan	0.0315
2.066666667	0.268	nan
2.083333333	nan	0.0271
2.1	0.259	0.00352
2.133333333	0.158	nan
2.166666667	0.219	0.0129
2.25	0.148	0.00946
2.333333333	0.158	nan
2.416666667	0.0864	nan
2.5	0.119	0.0063
2.75	0.0797	0.0025
3.0	0.0685	0.00445
3.25	0.0492	0.00128
3.516666667	0.039	nan
3.766666667	0.0278	nan
4.016666667	0.0202	nan
4.5	0.0141	nan

TCE Inhalation 500.0 ppm for 2 hours
Hours, Cart, CExhResp

0.012966667	nan	1.26
0.039833333	2.88	nan
0.058166667	nan	1.44
0.0695	4.43	nan
0.092666667	nan	1.49
0.107666667	4.7	nan
0.129333333	6.92	nan
0.173333333	7.23	1.56
0.255	7.64	nan
0.258333333	nan	1.63
0.341666667	10.2	1.61
0.421666667	11.2	nan
0.495	12.2	nan
0.508333333	nan	1.73
0.675	nan	1.73
0.748333333	13.5	nan
0.835	nan	1.78
1.003333333	nan	1.82
1.005	15.2	nan
1.173333333	nan	1.84
1.253333333	14.5	nan
1.338333333	nan	1.73
1.503333333	15.4	nan
1.506666667	nan	1.83
1.666666667	nan	1.82
1.75	15.3	nan
1.85	nan	1.91
2.016666667	17.3	1.79
2.033333333	12.9	0.702
2.05	nan	0.513
2.066666667	12.6	nan
2.083333333	nan	0.465
2.1	11.5	nan
2.116666667	nan	0.406
2.133333333	10.5	nan
2.166666667	10.3	0.382
2.25	8.92	0.362
2.333333333	7.55	nan
2.416666667	7.46	nan
2.516666667	6.69	0.222
2.766666667	5.63	0.153
3.0	3.46	nan
3.016666667	nan	0.0991
3.266666667	2.58	0.0806
3.5	1.91	nan
3.516666667	nan	0.0621
3.75	1.6	nan
3.766666667	nan	0.0258
4.0	1.28	nan
4.016666667	nan	0.0324
4.516666667	1.0	0.0312
5.016666667	0.729	0.0121

TCE Closed Chamber Inhalation 1100.0 ppm
Hours, CinhPPM

0.083	921.0
0.167	760.0
0.333	553.0
0.5	423.0
0.667	327.0
0.833	267.0
1.0	221.0
1.167	185.0
1.333	156.0
1.5	133.0
1.667	115.0
1.833	100.0
2.0	84.0
2.167	70.0
2.333	58.0
2.5	47.0
2.667	37.0

TCE Closed Chamber Inhalation 2200.0 ppm
Hours, CinhPPM

0.083	1918.0
0.167	1629.0
0.333	1331.0
0.5	1092.0
0.667	944.0
0.833	802.0
1.0	693.0
1.167	607.0
1.333	544.0
1.5	492.0
1.667	447.0
1.833	418.0
2.0	389.0
2.167	363.0
2.333	339.0
2.5	314.0
2.667	292.0
2.833	274.0
3.0	257.0
3.167	241.0
3.333	227.0
3.5	214.0
3.667	201.0
3.833	189.0
4.0	176.0
4.167	164.0
4.333	151.0
4.5	137.0
4.667	124.0
4.833	113.0
5.0	102.0

Fisher et al., 1989

TCE Closed Chamber Inhalation 300.0 ppm
Hours, CinhPPM

0.083	214.0
0.5	99.0
0.667	70.3
0.833	52.3
1.0	38.1
1.167	14.0
1.333	11.0
1.5	8.0

TCE Closed Chamber Inhalation 5100.0 ppm

Hours, CInhPPM
 0.083 4507.0
 0.167 3951.0
 0.333 3079.0
 0.5 2553.0
 0.667 2152.0
 0.833 1797.0
 1.0 1544.0
 1.167 1373.0
 1.333 1214.0
 1.5 1093.0
 1.667 1004.0
 1.833 934.0
 2.0 872.0
 2.167 826.0
 2.333 781.0
 2.5 743.0
 2.667 716.0
 2.833 695.0
 3.0 674.0
 3.167 651.0
 3.333 634.0
 3.5 619.0
 3.667 603.0
 3.833 589.0
 4.0 571.0
 4.167 561.0
 4.333 547.0
 4.5 536.0
 4.667 528.0
 4.833 515.0
 5.0 507.0
 5.167 502.0
 5.333 492.0
 5.5 480.0
 5.667 468.0
 5.833 457.0
 6.0 448.0

Fisher et al., 1991

TCE Inhalation 600.0 ppm for 4 hours -- females

Hours, CBldTCA, CPlasTCA, CVen
 0.6 1.672 2.2 9.3
 3.75 15.656 20.6 26.4
 4.25 14.972 19.7 19.7
 5.0 24.016 31.6 6.9
 6.0 25.232 33.2 3.5
 8.75 29.564 38.9 nan
 26.0 8.284 10.9 nan
 32.0 4.484 5.9 nan
 48.0 0.988 1.3 nan

TCE Inhalation 505.0 ppm for 4 hours -- males

Hours, CBldTCA, CPlasTCA
 2.0 4.94 6.5
 3.75 8.284 10.9
 6.0 16.948 22.3
 8.0 16.34 21.5
 10.0 15.352 20.2
 12.0 13.3 17.5
 26.0 4.788 6.3
 32.0 3.42 4.5

Green and Prout, 1985

TCA IV 10.0 mg/kg
 Hours, AurnTCOT_mMole
 24.0 0.004011628

TCA Oral Gavage 75.0 mg/kg
 Hours, AurnTCOT_mMole
 24.0 0.05119186

TCE Oral Gavage 500.0 mg/kg
 Hours, AurnTCOGTCOH, AurnTCA
 24.0 44.7973223 3.423565753

TCE Oral Gavage 500.0 mg/kg with bile cannulation
 Hours, AurnTCOT_mMole, ABileTCOG
 24.0 0.187975647 18.35018265

Hissink et al., 2002

TCE IV 10.0 mg/kg
 Hours, AurnTCOT_mMole, CVen
 0.25 nan 3.4821
 0.5 nan 1.99728
 1.0 nan 0.588672
 1.5 nan 0.274626
 2.0 nan 0.165564
 3.0 nan 0.0614952
 4.0 nan 0.0218124
 6.0 0.010066591 0.00953964
 8.0 nan 0.0026937
 12.0 0.011866438 nan
 24.0 0.012808219 nan
 48.0 0.013164003 nan
 72.0 0.013247717 nan
 96.0 0.013331431 nan
 120.0 0.013331431 nan
 144.0 0.013415145 nan
 168.0 0.013436073 nan

TCE IV 75.0 mg/kg

Hours, AurnTCOT_mMole, CVen
 0.25 nan 48.618
 0.5 nan 32.0616
 1.0 nan 14.5854
 1.5 nan 6.67512
 2.0 nan 3.83688
 3.0 nan 1.60308
 4.0 nan 0.697734
 6.0 0.05744863 0.278568
 8.0 nan 0.1013094
 12.0 0.075185502 nan
 24.0 0.083818493 nan
 48.0 0.086015982 nan
 72.0 0.086486872 nan
 96.0 0.086957763 nan
 120.0 0.086957763 nan
 144.0 0.08774258 nan
 168.0 0.08774258 nan

TCE Oral Gavage 100.0 mg/kg

0.25	nan	5.70276
0.5	nan	6.75396
1.0	nan	5.54508
1.5	nan	4.69098
2.0	nan	3.6135
3.0	nan	1.73448
4.0	nan	0.67671
6.0	0.080993151	0.140598
8.0	nan	0.0865926
12.0	0.144197108	nan
24.0	0.165334855	nan
48.0	0.169520548	nan
72.0	0.171194825	nan
96.0	0.171822679	nan
120.0	0.172450533	nan
144.0	0.172869102	nan
168.0	0.172869102	nan

TCE Oral Gavage 1000.0 mg/kg
Hours, AurnTCOTCOH, Cven

0.25	nan	69.7734
0.5	nan	54.6624
1.0	nan	44.8074
1.5	nan	42.8364
2.0	nan	38.6316
3.0	nan	44.9388
4.0	nan	54.9252
6.0	0.073877473	66.0942
8.0	nan	55.188
12.0	0.274162861	nan
24.0	0.655060883	0.178704
48.0	0.763888889	nan
72.0	0.778538813	nan
96.0	0.782724505	nan
120.0	0.780631659	nan
144.0	0.784817352	nan
168.0	0.789003044	nan

Keys et al., 2003

TCE Intra-arterial 8.0 mg/kg
Hours, CFat, CGut, CKid, CLiv, CMus, Cven

0.083	12.92166667	1.928333333	3.177333333
0.167	28.3185	1.332666667	2.351666667
0.333	35.25533333	0.428833333	0.639333333
0.5	28.5052	0.3312	0.3044
0.75	18.1114	0.0706	0.219
1.0	19.24	0.0342	0.077666667
1.5	12.351	0.0488	0.071
2.0	14.3292	0.045166667	0.0436
2.5	8.593666667	0.024	0.024166667
4.0	4.881875	nan	nan
6.0	3.50475	nan	nan
8.0	2.228166667	nan	nan
12.0	0.734	nan	nan
16.0	0.1924	nan	nan
18.0	0.009	nan	nan
24.0	0.007833333	nan	nan

Kaneko et al., 1994

TCE Inhalation 50.0 ppm for 6 hours
Hours, AurnTCOTCOH, Cven, AurnTCA

6.0	0.37375	0.385002	0.00893798
8.0	nan	0.0902718	nan
10.0	nan	0.0254916	nan
12.0	0.743015	nan	0.0339872
24.0	0.84916	nan	0.0619286
48.0	0.89102	nan	0.1379096

TCE Inhalation 100.0 ppm for 6 hours
Hours, AurnTCOTCOH, Cven, AurnTCA

6.0	0.781885	0.772632	0.01550666
8.0	nan	0.248346	nan
10.0	nan	0.054531	nan
12.0	1.36643	nan	0.0861118
24.0	1.48902	nan	0.189544
48.0	1.50995	nan	0.29412

TCE Inhalation 500.0 ppm for 6 hours
Hours, AurnTCOTCOH, Cven, AurnTCA

6.0	1.5249	5.11146	0.062909
8.0	nan	1.21545	nan
10.0	nan	0.337698	nan
12.0	3.72255	nan	0.328434
24.0	4.23085	nan	0.617652
48.0	4.3654	nan	0.861118

TCE Inhalation 1000.0 ppm for 6 hours
Hours, AurnTCOTCOH, Cven, AurnTCA

6.0	1.8239	29.565	0.0856216
8.0	nan	11.60262	nan
10.0	nan	4.6647	nan
12.0	4.23085	1.78704	0.4902
24.0	5.5913	nan	1.197722
48.0	5.96505	nan	1.62583

TCE Inhalation 50.0 ppm for 2 hours

Hours, CFat, CGut, CKid, CLiv, CCMus, CVen

0.083	1.6636	0.7058	1.392	0.5934	0.5354	1.7216
0.333	5.5892	0.9556	1.2434	0.4838	0.6714	0.8474
0.667	10.3988	1.082	1.548	0.5636	0.9312	0.8866
1.0	16.2034	1.4052	1.759	0.7816	1.3028	1.1678
1.5	12.0516	0.9892	1.272	0.4514	0.759	0.9346
2.0	10.9364	0.9814	0.9038	0.3976	0.5388	1.0914
2.083	13.4514	0.6324	0.4354	0.1056	0.5352	0.4452
2.167	14.3444	0.60975	0.3874	0.1678	0.3982	0.427
2.25	11.9392	0.364	0.2428	0.1006	0.3098	0.333
2.5	12.2154	0.3128	0.1656	0.0782	0.241	0.2264
2.75	10.5036	0.3016	0.1756	0.0414	0.2424	0.108
3.0	8.4308	0.1674	0.1236	0.0692	0.1405	0.1068
3.5	10.26	0.11	0.056	0.0435	0.127	0.025
4.0	3.61	0.15	0.062	0.0436	0.128	0.048
5.0	5.92	nan	nan	nan	nan	0.05

TCE Inhalation 500.0 ppm for 2 hours

Hours, CFat, CGut, CKid, CLiv, CCMus, CVen

0.083	19.111	nan	14.408	18.211	5.956	6.25
0.333	66.285	nan	18.915	23.888	10.084	10.276
1.0	186.123	nan	20.26	27.611	15.028	11.503
2.0	323.977	nan	24.907	31.538	17.4	17.679
2.083	266.279	14.987	11.504	13.564	9.141	11.806
2.25	493.956	16.831	11.176	13.184	8.868	8.571
2.75	269.573	7.856	5.177	4.335	4.547	3.118
3.5	298.914	3.803	3.474	2.079	1.589	2.211
5.0	150.91	0.876	0.846	0.251	1.113	0.608

TCE Oral Gavage 8.0 mg/kg

Hours, CFat, CGut, CKid, CLiv, CCMus, CVen

0.083	14.97966667	2.360833333	3.730833333	6.362666667	2.8555	3.934833333
0.167	33.653	1.687833333	2.7075	3.914833333	2.4565	2.695666667
0.333	36.5155	0.796666667	1.015333333	1.468333333	1.3795	1.061
0.5	28.9104	0.4382	0.3888	0.5634	0.3588	0.5296
0.75	18.803	0.2488	0.3106	0.4128	0.5798	0.235
1.0	18.88566667	0.112833333	0.1375	0.197833333	0.318	0.128
1.5	24.3598	0.0958	0.0926	0.144	0.1614	0.0934
2.0	13.99866667	0.062166667	0.042833333	0.057166667	0.061	0.030166667
3.0	8.718833333	0.029833333	0.026833333	0.037333333	0.072833333	0.023
4.0	5.178875	nan	nan	nan	nan	nan
6.0	3.604625	nan	nan	nan	nan	nan
8.0	2.348333333	nan	nan	nan	nan	nan
12.0	0.784	nan	nan	nan	nan	nan
18.0	0.0306	nan	nan	nan	nan	nan
24.0	0.0297	nan	nan	nan	nan	nan

Kimmerle73_Rat.m

TCE Inhalation 49.0 ppm for 4 hours

Hours, AurnTCOGTCOH, AExhPost, AurnTCA

5.0	nan	0.0511	nan
6.0	nan	0.0635	nan
7.0	nan	0.0738	nan
8.0	nan	0.0827	nan
28.0	0.848	nan	0.3425
52.0	0.8591	nan	0.4252

TCE Inhalation 54.0 ppm for 4 hours

Hours, CTCOH

4.083333333	0.8
4.5	0.3
5.0	0.2

TCE Inhalation 175.0 ppm for 4 hours

Hours, AurnTCOGTCOH, AExhPost, AurnTCA

5.0	nan	0.3941	nan
6.0	nan	0.5094	nan
7.0	nan	0.5551	nan
8.0	nan	0.5777	nan
9.0	nan	0.5923	nan
10.0	nan	0.5995	nan
11.0	nan	0.6055	nan
12.0	nan	0.6113	nan
28.0	2.2852	nan	0.8618
52.0	2.306	nan	1.0076
76.0	2.3092	nan	1.0373

TCE Inhalation 330.0 ppm for 4 hours
Hours, AurnTCOGTCOH, AExhPost, AurnTCA

5.0	nan	3.87	nan
6.0	nan	4.445	nan
7.0	nan	4.624	nan
8.0	nan	4.711	nan
9.0	nan	4.757	nan
10.0	nan	4.783	nan
11.0	nan	4.807	nan
12.0	nan	4.824	nan
28.0	4.0664	nan	1.0291
52.0	4.0828	nan	1.2373
76.0	4.0851	nan	1.2713

TCE Inhalation 3160.0 ppm for 4 hours
Hours, CTCOH, CVen

4.083333333	1.74	89.2
4.5	1.68	35.4
5.0	1.75	19.4

Larson and Bull, 1992a

TCA Oral Gavage 20.0 mg/kg

0.25	17.3204
1.0	36.765
3.0	36.1114
5.0	30.229
10.0	16.8302
16.0	8.0066
24.0	4.4118

TCA Oral Gavage 100.0 mg/kg
Hours, CPlasTCA

0.25	85.1314
1.0	202.2892
3.0	147.5502
5.0	107.6806
10.0	57.3534
16.0	26.144
24.0	10.621
32.0	4.4118

Larson and Bull, 1992b

TCE Oral Gavage 197.25 mg/kg
Hours, CBldTCA, CTCOH, CVen

1.0	6.0458	1.196	11.18214
2.0	8.17	2.37705	6.42546
4.0	12.7452	2.392	2.50974
8.0	13.2354	0.61295	1.14318
12.0	10.621	0.1495	nan
24.0	2.1242	nan	nan

TCE Oral Gavage 591.75 mg/kg
Hours, CBldTCA, CTCOH, CVen

1.0	2.7778	1.30065	25.8201
2.0	6.76476	1.59965	34.40052
4.0	9.08504	2.43685	20.1699
8.0	20.16356	4.44015	6.74082
12.0	24.49366	1.92855	3.23244
24.0	17.18968	0.43355	nan
48.0	1.53596	nan	nan

TCE Oral Gavage 3024.0 mg/kg
Hours, CBldTCA, CTCOH, CVen

1.0	4.2484	1.794	61.6266
2.0	9.804	2.99	164.5128
4.0	11.1112	2.99	101.178
8.0	23.5296	3.289	88.1694
12.0	36.6016	5.083	46.2528
24.0	60.6214	3.4385	6.4386
48.0	5.5556	nan	nan

Lee et al., 2000

TCE IV 16.0 mg/kg

Hours, CBldMix, Cliv

0.011111111	16.0	20.0
0.019444444	25.0	22.0
0.036111111	20.0	41.0
0.086111111	11.0	17.0

TCE Portal vein injection 16.0 mg/kg

Hours, CBldMix, Cliv

0.011111111	19.0	82.0
0.019444444	25.0	209.0
0.036111111	15.0	44.0
0.086111111	8.0	14.0

Merdink et al., 1999

TCOH IV 100.0 mg/kg

Hours, CTCOH

3.274	182.39
3.509	130.5135
4.01	72.059
4.99	41.86
6.0	28.2555
8.01	14.4417

Prout et al., 1985

TCE Oral Gavage 1000.0 mg/kg - rats not specified

Hours, CArt, CBldTCA, CTCOH, AExhPost

0.25	5.77	nan	nan	nan
0.5	14.6	nan	nan	3.4
0.75	20.1	nan	nan	nan
1.0	25.4	nan	0.81	6.0
1.5	20.2	nan	1.17	9.1
2.0	24.0	nan	1.08	11.7
2.5	42.4	3.4	0.9	15.7
3.0	61.8	nan	0.81	20.8
3.5	nan	nan	0.9	27.0
4.0	43.7	4.4	1.17	35.5
4.5	41.1	nan	1.35	41.1
5.0	29.6	10.7	0.9	46.7
5.5	28.9	nan	1.17	50.8
6.0	28.8	10.7	0.99	55.2
6.5	nan	nan	1.26	59.9
7.0	21.2	15.2	0.72	63.5
7.5	nan	nan	nan	67.3
8.0	19.1	15.7	1.17	71.0
8.5	nan	nan	nan	74.7
9.0	13.4	27.7	1.62	nan
10.0	12.0	19.7	7.39	83.3
10.5	nan	nan	nan	86.0
11.0	8.25	47.1	2.07	88.6
11.5	nan	nan	nan	90.5
12.0	nan	37.9	2.34	nan
13.0	nan	48.8	1.35	nan
14.0	nan	nan	0.81	nan
15.0	nan	nan	1.98	nan
16.0	nan	29.2	0.81	nan
17.0	nan	34.9	1.17	nan
18.0	nan	nan	0.81	nan
19.0	nan	44.5	nan	nan
20.0	nan	40.5	nan	nan
22.0	nan	23.8	nan	nan
23.0	nan	18.7	nan	nan
25.0	nan	14.6	nan	nan
26.0	nan	14.5	nan	nan
28.0	nan	22.5	nan	nan
29.0	nan	33.3	nan	nan
30.0	nan	39.0	nan	nan
32.0	nan	32.7	nan	nan
33.0	nan	18.9	nan	nan
35.0	nan	20.5	nan	nan
36.0	nan	24.5	nan	nan
37.0	nan	21.6	nan	nan
40.0	nan	7.2	nan	nan

TCE Oral Gavage 10.0 mg/kg - Alderley Park Wistar

Hours, AurnTCTot_mMole, AExhPost

24.0	0.007894977	0.019
48.0	0.008314307	0.019
72.0	0.008429985	nan

TCE Oral Gavage 500.0 mg/kg - Alderley Park Wistar

Hours, AurnTCTot_mMole, AExhPost

24.0	0.180022831	47.405
48.0	0.18869863	47.405
72.0	0.191590563	nan

TCE Oral Gavage 1000.0 mg/kg - Alderley Park Wistar

Hours, AurnTCTot_mMole, AExhPost

24.0	0.247260274	98.99
48.0	0.264611872	98.99
72.0	0.270395738	nan

TCE Oral Gavage 10.0 mg/kg - Osborne-Mendel

Hours, AurnTCTot_mMole, AExhPost

24.0	0.009586758	0.0247
72.0	0.010035008	0.0247

TCE Oral Gavage 500.0 mg/kg - Osborne-Mendel

Hours, AurnTCTot_mMole, AExhPost

24.0	0.297869102	40.565
72.0	0.3152207	40.565

TCE Oral Gavage 1000.0 mg/kg - Osborne-Mendel

Hours, AurnTCTot_mMole, AExhPost

24.0	0.422222222	106.78
72.0	0.449695586	106.78

TCE Oral Gavage 2000.0 mg/kg - Osborne-Mendel

Hours, AurnTCTot_mMole, AExhPost

24.0	0.38173516	295.64
72.0	0.404870624	295.64

Simmons et al., 2002

TCE Inhalation 200.0 ppm for 5 hours

Hours, CFat, CLiv, CVen

0.083	1.6	0.875	0.79
0.333	4.875	1.275	1.29
1.0	23.0	1.5	1.2
2.0	11.1	0.015	0.14

TCE Inhalation 2000.0 ppm for 5 hours

Hours, CFat, CLiv, CVen

0.083	13.5	24.0	9.35
0.333	8.45	42.0	12.15
1.0	256.6666667	79.0	40.75
2.0	245.0	8.4	4.75

TCE Inhalation 4000.0 ppm for 5 hours

Hours, CFat, CLiv, CVen

0.083	20.4	69.0	31.5
0.333	200.0	140.0	70.75
1.0	595.875	189.025	57.05
2.0	670.0	55.0	31.75

TCE Closed Chamber Inhalation 108.0 ppm
Hours, CInhPPM

0.00598	108.0
0.161	94.8
0.316	85.1
0.489	76.4
0.661	70.1
0.816	64.3
0.989	59.0
1.16	54.1
1.32	50.7
1.49	47.5
1.64	44.5
1.82	40.9
1.97	38.3
2.14	35.9
2.32	33.6
2.47	31.5
2.66	29.5
2.82	27.1
2.99	25.4
3.14	23.3
3.32	22.3
3.49	20.9
3.66	20.0
3.82	18.4
3.99	17.6
4.16	16.8
4.31	16.1

TCE Closed Chamber Inhalation 506.0 ppm
Hours, CInhPPM

0.00598	506.0
0.17	454.0
0.325	408.0
0.481	366.0
0.653	343.0
0.825	315.0
0.998	282.0
1.15	265.0
1.31	243.0
1.48	228.0
1.65	209.0
1.81	191.0
1.98	176.0
2.15	165.0
2.33	154.0
2.48	142.0
2.65	135.0
2.81	127.0
3.0	116.0
3.14	109.0
3.31	102.0
3.48	95.9
3.65	89.9
3.82	84.2
4.0	77.2
4.17	74.0
4.32	67.8
4.5	63.6
4.67	58.3
4.82	52.4
5.0	48.0
5.17	45.0
5.32	43.1
5.5	41.3
5.67	37.9
5.82	35.5

TCE Closed Chamber Inhalation 864.0 ppm
Hours, CInhPPM

0.00598	864.0
0.167	793.0
0.323	697.0
0.495	639.0
0.667	599.0
0.823	549.0
0.995	504.0
1.17	483.0
1.32	462.0
1.49	433.0
1.65	415.0
1.8	397.0
1.98	372.0
2.15	364.0
2.3	341.0
2.49	320.0
2.65	313.0
2.8	293.0
2.98	281.0
3.15	275.0
3.3	263.0
3.48	252.0
3.66	241.0
3.82	231.0
3.97	216.0
4.15	207.0
4.32	198.0
4.49	190.0
4.66	182.0
4.82	170.0
4.99	163.0
5.16	153.0
5.34	143.0
5.51	137.0
5.66	129.0
5.84	123.0

TCE Closed Chamber Inhalation 2940.0 ppm
Hours, CInhPPM

0.00598	2940.0
0.161	2810.0
0.316	2520.0
0.489	2320.0
0.661	2170.0
0.816	1950.0
0.989	1870.0
1.16	1790.0
1.32	1710.0
1.49	1600.0
1.66	1570.0
1.82	1470.0
1.97	1440.0
2.16	1350.0
2.33	1350.0
2.49	1290.0
2.66	1260.0
2.81	1230.0
2.99	1180.0
3.14	1160.0
3.31	1130.0
3.49	1110.0
3.64	1080.0
3.81	1060.0
3.97	1040.0
4.16	1010.0
4.31	1010.0
4.48	991.0
4.66	949.0
4.81	948.0
4.98	927.0
5.15	907.0
5.33	907.0
5.5	887.0
5.67	887.0
5.83	867.0

Stenner et al., 1997

TCE Oral Gavage 100.0 mg/kg
Hours, CBldTCA, CTCOG, CTCOH

0.251	0.727	0.412	2.02
0.439	1.64	0.727	2.77
0.966	2.11	0.791	2.93
1.43	2.46	0.886	3.12
2.42	3.34	0.668	2.4
3.41	3.97	0.166	2.43
4.47	4.07	0.105	2.28
5.41	4.07	nan	1.96
6.66	nan	0.0462	nan
8.4	4.61	nan	0.364
16.8	3.77	nan	nan

Yu et al., 2000

TCA IV 1.0 mg/kg
Hours, CBldTCA, CLivTCA, CPlasTCA, AUrnTCA

0.083	3.42323	1.86276	4.67324	nan
0.5	2.5835991	1.034322	3.4314	nan
1.0	2.2724038	0.9804	2.97388	nan
3.0	2.0143135	1.245108	2.82682	nan
6.0	1.6624316	1.367658	2.27126	0.066218422
9.0	1.2100587	1.099682	1.66668	0.075218984
24.0	0.3230418	0.545756	0.450984	0.101792073

TCOH IV 100.0 mg/kg without bile cannulation
Hours, AUrnTCOGTCOH, CBldTCA, TotCTCOH, AUrnTCA

0.534	nan	2.04	nan	nan
0.979	nan	3.7	72.8	nan
2.05	nan	5.21	41.3	nan
3.03	nan	5.5	27.5	nan
4.99	nan	6.47	14.3	nan
8.01	nan	7.1	6.89	nan
11.0	nan	5.4	1.97	nan
16.0	nan	4.57	nan	nan
24.0	nan	2.63	nan	nan
48.0	7.9	nan	nan	0.46

TCOH IV 5.0 mg/kg with bile cannulation
Hours, AUrnTCOGTCOH, AUrnTCA

48.0	0.5	0.01

TCOH IV 20.0 mg/kg with bile cannulation
Hours, AUrnTCOGTCOH, AUrnTCA

48.0	3.1	0.03

TCOH IV 100.0 mg/kg with bile cannulation
Hours, AUrnTCOGTCOH, CBldTCA, TotCTCOH, AUrnTCA

0.534	nan	0.389	nan	nan
1.07	nan	0.973	45.7	nan
2.05	nan	1.65	9.84	nan
3.03	nan	2.38	2.95	nan
4.99	nan	1.99	0.984	nan
8.01	nan	1.8	nan	nan
11.0	nan	1.17	nan	nan
16.0	nan	0.827	nan	nan
24.0	nan	0.584	nan	nan
48.0	8.1	nan	nan	0.09

Templin et al., 1995

TCE Oral Gavage 100.0 mg/kg
Hours, CBldTCA, CTCOH, CVen

0.25	0.94772	0.91195	5.67648
0.5	1.42158	1.56975	9.21114
0.75	1.91178	1.9435	10.52514
1.0	1.61766	2.0033	6.79338
1.5	2.23858	2.04815	2.32578
2.0	4.2484	2.70595	1.55052
2.5	3.80722	3.39365	0.94608
3.0	4.9837	2.67605	nan
4.0	6.06214	2.4817	nan
5.0	6.74842	2.2126	nan
6.0	6.92816	2.04815	nan
9.0	7.64712	0.9867	nan
12.0	7.30398	nan	nan
24.0	4.28108	nan	nan
48.0	1.43792	nan	nan

TCA IV 10.0 mg/kg
Hours, CBldTCA, CLivTCA, CPlasTCA, AUrnTCA

0.083	35.35159	18.3008	46.8958	nan
0.5	29.26494	14.6243	38.2356	nan
1.0	25.210986	14.10142	34.314	nan
3.0	21.347393	15.78444	29.5754	nan
6.0	13.804849	11.7648	17.974	0.762904796
9.0	10.840773	9.10138	13.33344	0.919343139
24.0	3.0365439	5.89874	4.31376	1.43580397

TCA IV 50.0 mg/kg
Hours, CBldTCA, CLivTCA, CPlasTCA, AUrnTCA

0.083	143.30997	78.9222	176.472	nan
0.5	103.89789	69.2816	130.8834	nan
1.0	104.38809	68.1378	128.4324	nan
3.0	70.13945	57.6802	90.3602	nan
6.0	42.68825	44.4448	57.0266	6.407051256
9.0	35.05747	45.4252	48.3664	6.278050224
24.0	8.812162	20.2616	12.8269	9.08382267

APPENDIX N

Data for Human Validation Figures

The following data are for generating human validation figures in Appendix H.

Bernauer et al., 1996

TCE Inhalation 40.0 ppm for 6 hours (Human #43)

Hours, AurnTCOGTCOH, AurnNDCVC, AurnTCA

6.0	13.63675325	0.005309749	1.557452405
11.0	33.61944879	0.012434097	3.14839841
16.0	51.78263372	0.019694974	5.681351918
23.0	61.25685742	0.025776734	8.719500561
30.0	71.08859899	0.035646562	11.70391989
35.0	81.97374145	0.042820557	14.45667515
40.0	91.93316798	0.05376152	16.84309415
47.0	98.27911027	0.060468832	19.6760945
54.0	103.3290503	0.0647	21.54196714

TCE Inhalation 80.0 ppm for 6 hours (Human #43)

Hours, AurnTCOGTCOH, AurnNDCVC, AurnTCA

6.0	36.6438435	0.007553303	1.941365664
11.0	86.08691135	0.013224905	4.874486405
16.0	124.9572477	0.027986974	7.841594641
23.0	151.426392	0.036437397	11.14857782
30.0	174.630428	0.057308365	16.28748693
35.0	192.4174939	0.068022128	21.28364856
40.0	208.1833023	0.078623254	27.26544753
47.0	220.8519223	0.088400143	31.66206976
54.0	231.5179426	0.095756	36.99130884

TCE Inhalation 160.0 ppm for 6 hours (Human #43)

Hours, AurnTCOGTCOH, AurnNDCVC, AurnTCA

6.0	62.99517723	0.01122279	2.838297949
11.0	150.9920375	0.026161736	8.369594126
16.0	229.5471746	0.053723225	16.2537551
23.0	284.5357705	0.064310553	24.5176767
30.0	305.7381042	0.073536529	35.0353951
35.0	334.9696792	0.078057851	44.90091589
40.0	359.5181595	0.091739498	55.13794165
47.0	375.6974964	0.102725693	63.40186326
54.0	393.3572955	0.111284	73.34168504

Chiu et al., 2007

TCE Inhalation -- Experiment A-TRI-1 (Human #37)

Hours, AurnTCOGTCOH_Coll, CALVPPM, CBldTCA, CTCOH, CVen, TotCTCOH, AurnTCA_Coll

0.3333	nan	0.259221	nan	nan	nan	nan	nan
0.3343	nan	0.26847	nan	nan	nan	nan	nan
0.6667	nan	0.34737	nan	nan	nan	nan	nan
0.6677	nan	0.389423	nan	nan	nan	nan	nan
1.0	nan	0.351313	0.002	0.005	0.0045	0.007	nan
1.001	nan	0.417967	nan	nan	nan	nan	nan
1.3333	nan	0.495419	nan	nan	nan	nan	nan
1.3343	nan	0.424781	nan	nan	nan	nan	nan
1.6667	nan	0.437765	nan	nan	nan	nan	nan
1.6677	nan	0.452817	nan	nan	nan	nan	nan
1.6687	nan	0.49446	nan	nan	nan	nan	nan
1.6697	nan	0.446217	nan	nan	nan	nan	nan
2.0	nan	0.493601	0.004	0.007	0.0045	0.048	nan
2.001	nan	0.409691	nan	nan	nan	nan	nan
2.6667	nan	0.474658	nan	nan	nan	nan	nan
2.6677	nan	0.451876	nan	nan	nan	nan	nan
3.0	nan	0.416239	nan	nan	nan	nan	nan
3.6667	nan	0.389068	nan	nan	nan	nan	nan
3.6677	nan	0.390245	nan	nan	nan	nan	nan
4.0	nan	0.444807	0.01	0.011	0.005	0.066	nan
4.001	nan	0.398569	nan	nan	nan	nan	nan
4.3333	nan	0.326154	nan	nan	nan	nan	nan

4.3343	nan	0.300993	nan	nan	nan	nan	nan
4.6667	nan	0.412284	nan	nan	nan	nan	nan
4.6677	nan	0.420992	nan	nan	nan	nan	nan
5.0	nan	0.267463	nan	nan	nan	nan	nan
5.001	nan	0.302049	nan	nan	nan	nan	nan
5.3333	nan	0.353893	nan	nan	nan	nan	nan
5.3343	nan	0.244604	nan	nan	nan	nan	nan
5.6667	nan	0.261695	nan	nan	nan	nan	nan
5.6677	nan	0.294977	nan	nan	nan	nan	nan
5.7833	nan	nan	0.019	0.027	0.004	0.0995	nan
5.8333	nan	0.366387	nan	nan	nan	nan	nan
5.8343	nan	0.290711	nan	nan	nan	nan	nan
6.0333	nan	0.142397	nan	nan	nan	nan	nan
6.0667	nan	0.118484	nan	nan	nan	nan	nan
6.1	nan	0.104238	nan	nan	nan	nan	nan
6.1167	nan	nan	0.0265	0.0165	0.002	0.088	nan
6.1333	nan	0.099659	nan	nan	nan	nan	nan
6.1667	nan	0.097115	nan	nan	nan	nan	nan
6.2833	nan	0.123063	nan	nan	nan	nan	nan
6.3333	nan	0.080043	nan	nan	nan	nan	nan
6.4167	nan	0.053037	nan	nan	nan	nan	nan
6.5	nan	0.054674	nan	nan	nan	nan	nan
6.6667	nan	0.062257	nan	nan	nan	nan	nan
6.8333	nan	0.056389	nan	nan	nan	nan	nan
7.0	nan	0.043814	nan	nan	nan	nan	nan
7.0333	nan	nan	0.0275	0.0195	0.002	0.104	nan
7.5	nan	0.04124	nan	nan	nan	nan	nan
8.0	nan	0.02635	nan	nan	nan	nan	nan
8.0333	nan	nan	0.0375	0.02	0.001	0.037	nan
9.0	nan	0.018905	nan	nan	nan	nan	nan
10.0	nan	0.017538	nan	nan	nan	nan	nan
11.0	nan	0.014803	nan	nan	nan	nan	nan
14.3833	nan	0.01106	nan	nan	nan	nan	nan
15.4167	nan	0.006724	nan	nan	nan	nan	nan
22.8667	nan	0.007639	nan	nan	nan	nan	nan
22.9167	0.5003	nan	nan	nan	nan	nan	nan
27.1167	nan	0.003938	nan	nan	nan	nan	nan
29.7	0.6866	nan	nan	nan	nan	nan	nan
31.2333	0.7662	nan	nan	nan	nan	nan	0.0101
36.3667	1.0048	nan	nan	nan	nan	nan	nan
38.6167	1.0342	nan	nan	nan	nan	nan	0.0165
39.4	1.0736	nan	nan	nan	nan	nan	0.0277
40.7833	nan	nan	0.047	0.002	nan	0.0035	nan
46.4167	1.1472	nan	nan	nan	nan	nan	nan
46.45	nan	0.001551	nan	nan	nan	nan	nan
46.6167	nan	0.002001	nan	nan	nan	nan	nan
51.1167	nan	0.000819	nan	nan	nan	nan	nan
58.3667	nan	0.000466	nan	nan	nan	nan	nan
71.9833	nan	0.000741	nan	nan	nan	nan	nan
75.4	nan	0.000246	nan	nan	nan	nan	nan
75.5667	1.1793	nan	nan	nan	nan	nan	nan
77.6167	nan	nan	nan	nan	nan	0.0015	nan
94.7333	1.1995	nan	nan	nan	nan	nan	nan
94.8333	nan	0.000318	nan	nan	nan	nan	nan
98.2833	nan	nan	0.024	nan	nan	0.003	nan
103.9167	nan	0.000148	nan	nan	nan	nan	nan
121.4	1.2039	nan	nan	nan	nan	nan	0.0465
122.55	nan	nan	0.0175	nan	nan	nan	nan

TCE Inhalation -- Experiment A-TRI-2 (Human #37)

Hours, AurnTCOGTCOH_Coll, CALvPPM, CBldTCA, CTCOH, CVen, TotCTCOH, AurnTCA_Coll

0.3333	nan	0.249519	nan	nan	nan	nan	nan
0.3343	nan	0.262734	nan	nan	nan	nan	nan
0.6667	nan	0.378056	nan	nan	nan	nan	nan
0.6677	nan	0.382217	nan	nan	nan	nan	nan
0.8	nan	nan	0.001	nan	0.003	0.007	nan
1.0	nan	0.350707	nan	nan	nan	nan	nan
1.001	nan	0.385927	nan	nan	nan	nan	nan
1.3333	nan	0.354557	nan	nan	nan	nan	nan
1.3343	nan	0.314386	nan	nan	nan	nan	nan
1.6667	nan	0.307842	nan	nan	nan	nan	nan

1.6677	nan	0.387507	nan	nan	nan	nan	nan
2.0	nan	0.33907	nan	nan	nan	nan	nan
2.001	nan	0.34747	nan	nan	nan	nan	nan
2.05	nan	nan	0.002	nan	0.003	0.011	nan
2.3333	nan	0.357612	nan	nan	nan	nan	nan
2.3343	nan	0.427078	nan	nan	nan	nan	nan
2.6667	nan	0.414282	nan	nan	nan	nan	nan
2.6677	nan	0.231707	nan	nan	nan	nan	nan
3.0	nan	0.437608	nan	nan	nan	nan	nan
3.3333	nan	0.472409	nan	nan	nan	nan	nan
3.3343	nan	0.499564	nan	nan	nan	nan	nan
3.6667	nan	0.470648	nan	nan	nan	nan	nan
3.6677	nan	0.427958	nan	nan	nan	nan	nan
4.0	nan	0.391077	nan	nan	nan	nan	nan
4.05	nan	nan	nan	nan	nan	0.041	nan
4.3333	nan	0.395443	nan	nan	nan	nan	nan
4.3343	nan	0.412294	nan	nan	nan	nan	nan
4.6667	nan	0.378057	nan	nan	nan	nan	nan
4.6677	nan	0.474724	nan	nan	nan	nan	nan
5.0	nan	0.479064	nan	nan	nan	nan	nan
5.001	nan	0.406866	nan	nan	nan	nan	nan
5.3333	nan	0.476614	nan	nan	nan	nan	nan
5.3343	nan	0.492051	nan	nan	nan	nan	nan
5.6667	nan	0.580758	nan	nan	nan	nan	nan
5.6677	nan	0.463621	nan	nan	nan	nan	nan
5.8333	nan	0.47456	0.0105	0.0025	0.006	0.057	nan
6.0333	nan	0.173685	nan	nan	nan	nan	nan
6.0667	nan	0.157038	nan	nan	nan	nan	nan
6.1	nan	0.132661	nan	nan	nan	nan	nan
6.1333	nan	0.124388	nan	nan	nan	nan	nan
6.1667	nan	0.095374	nan	nan	nan	nan	nan
6.2167	nan	nan	0.0115	0.003	0.0015	0.0595	0.017
6.25	nan	0.146307	nan	nan	nan	nan	nan
6.3333	nan	0.108293	nan	nan	nan	nan	nan
6.5	nan	0.033362	nan	nan	nan	nan	nan
6.501	nan	0.036	nan	nan	nan	nan	nan
6.6667	nan	0.063939	nan	nan	nan	nan	nan
6.6677	nan	0.063	nan	nan	nan	nan	nan
6.8333	nan	0.054916	nan	nan	nan	nan	nan
6.8343	nan	0.061	nan	nan	nan	nan	nan
7.0	nan	0.050446	nan	nan	nan	nan	nan
7.001	nan	0.047	nan	nan	nan	nan	nan
7.5	nan	0.035078	nan	nan	nan	nan	nan
7.501	nan	0.039	nan	nan	nan	nan	nan
8.0	nan	0.024738	nan	nan	nan	nan	nan
8.001	nan	0.032	nan	nan	nan	nan	nan
8.05	nan	nan	0.0125	0.0025	0.0005	0.044	nan
14.3667	0.5175	nan	nan	nan	nan	nan	nan
14.3667	nan	nan	nan	nan	nan	nan	0.0336
23.7167	0.9178	nan	nan	nan	nan	nan	nan
25.6333	nan	nan	0.0205	nan	nan	0.01	nan
30.4667	nan	0.004378	nan	nan	nan	nan	nan
31.4667	0.9796	nan	nan	nan	nan	nan	0.039
34.4667	nan	0.001287	nan	nan	nan	nan	nan
34.4677	nan	0.002111	nan	nan	nan	nan	nan
37.2167	1.0985	nan	nan	nan	nan	nan	nan
39.0667	1.1677	nan	nan	nan	nan	nan	nan
39.1167	nan	0.003002	nan	nan	nan	nan	nan
42.0167	1.2565	nan	nan	nan	nan	nan	0.0491
46.7167	nan	0.001518	nan	nan	nan	nan	nan
46.7177	nan	0.001805	nan	nan	nan	nan	nan
47.6333	1.3254	nan	nan	nan	nan	nan	nan
51.7167	nan	0.000979	nan	nan	nan	nan	nan
51.7177	nan	0.001069	nan	nan	nan	nan	nan
56.4667	nan	0.000348	nan	nan	nan	nan	nan
56.4677	nan	0.000465	nan	nan	nan	nan	nan
56.4687	nan	0.000458	nan	nan	nan	nan	nan
69.5167	1.3535	nan	nan	nan	nan	nan	0.062
70.9167	nan	0.000189	nan	nan	nan	nan	nan
73.8	nan	nan	0.0325	nan	nan	nan	nan
79.2167	nan	0.000313	nan	nan	nan	nan	nan

79.2177	nan	0.000196	nan	nan	nan	nan	nan
86.8	nan	0.000667	nan	nan	nan	nan	nan
86.801	nan	0.000864	nan	nan	nan	nan	nan
86.9667	nan	0.000388	nan	nan	nan	nan	nan
96.8167	nan	0.000097	nan	nan	nan	nan	nan
96.8177	nan	0.000164	nan	nan	nan	nan	nan
96.8187	nan	0.000246	nan	nan	nan	nan	nan
96.85	1.3605	nan	nan	nan	nan	nan	0.0709
98.7167	nan	nan	0.024	nan	nan	nan	nan
120.85	1.365	nan	nan	nan	nan	nan	0.0847
122.9667	nan	nan	0.0285	nan	nan	nan	nan
122.9677	nan	nan	0.024	0.0055	0.001	nan	nan
142.5	1.3664	nan	nan	nan	nan	nan	0.0962

TCE Inhalation -- Experiment B-TRI-1 (Human #38)

Hours,	AurnTCOGTCOH_Coll,	CalvPPM,	CBldTCA,	CTCOH,	CVen,	TotCTCOH
0.3333	nan	0.297425	nan	nan	nan	nan
0.3343	nan	0.284702	nan	nan	nan	nan
0.3353	nan	0.27631	nan	nan	nan	nan
0.6667	nan	0.280924	nan	nan	nan	nan
0.6677	nan	0.269558	nan	nan	nan	nan
0.6687	nan	0.28923	nan	nan	nan	nan
1.0	nan	0.254859	0.002	0.003	0.002	0.0055
1.001	nan	0.28093	nan	nan	nan	nan
1.3667	nan	0.29746	nan	nan	nan	nan
1.3677	nan	0.343662	nan	nan	nan	nan
1.6667	nan	0.361015	nan	nan	nan	nan
2.0	nan	nan	0.005	0.006	0.0045	0.011
2.3333	nan	0.381184	nan	nan	nan	nan
2.3343	nan	0.384937	nan	nan	nan	nan
2.3353	nan	0.340788	nan	nan	nan	nan
2.6667	nan	0.324214	nan	nan	nan	nan
2.6677	nan	0.337734	nan	nan	nan	nan
3.0	nan	0.298919	nan	nan	nan	nan
3.3333	nan	0.32549	nan	nan	nan	nan
3.3343	nan	0.36164	nan	nan	nan	nan
3.6667	nan	0.342242	nan	nan	nan	nan
4.0	nan	0.310441	0.12	0.008	0.003	0.034
4.001	nan	0.329029	nan	nan	nan	nan
4.3333	nan	0.334923	nan	nan	nan	nan
4.3343	nan	0.296386	nan	nan	nan	nan
4.6667	nan	0.329482	nan	nan	nan	nan
4.6677	nan	0.350791	nan	nan	nan	nan
5.0	nan	0.313065	nan	nan	nan	nan
5.001	nan	0.353667	nan	nan	nan	nan
5.3333	nan	0.355003	nan	nan	nan	nan
5.3343	nan	0.336777	nan	nan	nan	nan
5.6667	nan	0.344067	nan	nan	nan	nan
5.6677	nan	0.348624	nan	nan	nan	nan
5.8333	nan	0.343156	0.031	0.011	0.004	nan
5.8343	nan	0.332677	nan	nan	nan	nan
6.0333	nan	0.225231	nan	nan	nan	nan
6.0667	nan	0.157472	nan	nan	nan	nan
6.1	nan	0.149624	nan	nan	nan	nan
6.1333	nan	0.150308	nan	nan	nan	nan
6.1667	nan	0.129402	nan	nan	nan	0.053
6.25	nan	0.134187	nan	nan	nan	nan
6.3333	nan	0.125676	nan	nan	nan	nan
6.4167	nan	0.075	nan	nan	nan	nan
6.4833	0.6936	nan	nan	nan	nan	nan
6.5	nan	0.086772	nan	nan	nan	nan
6.7167	nan	0.078	nan	nan	nan	nan
6.8333	nan	0.065	nan	nan	nan	nan
7.0	nan	0.05	0.035	0.026	0.001	0.04
7.5	nan	0.035353	nan	nan	nan	nan
7.501	nan	0.044	nan	nan	nan	nan
8.0	nan	0.044	0.0425	0.0135	0.001	0.04
9.0	nan	0.024978	nan	nan	nan	nan
10.5	nan	0.019178	nan	nan	nan	nan
11.0	nan	0.016161	nan	nan	nan	nan
14.2333	nan	0.011541	nan	nan	nan	nan

20.4833	1.1404	nan	nan	nan	nan	nan
22.9833	1.3606	nan	nan	nan	nan	nan
24.2333	nan	0.006049	nan	nan	nan	nan
26.2333	1.4823	nan	nan	nan	nan	nan
26.4833	nan	0.005569	nan	nan	nan	nan
26.5	nan	nan	0.0725	0.0055	nan	0.007
29.4833	1.6973	nan	nan	nan	nan	nan
34.4833	1.8812	nan	nan	nan	nan	nan
38.4833	nan	0.003943	nan	nan	nan	nan
39.4833	2.0137	nan	nan	nan	nan	nan
47.2333	2.1577	nan	nan	nan	nan	nan
47.2333	nan	0.002919	nan	nan	nan	nan
47.2343	nan	0.003068	nan	nan	nan	nan
47.75	nan	nan	0.0685	0.0025	nan	0.0025
62.9167	nan	0.002467	nan	nan	nan	nan
71.4833	2.1792	nan	nan	nan	nan	nan
71.9833	nan	0.002008	nan	nan	nan	nan
72.8333	nan	nan	0.0485	nan	nan	0.001
77.9833	nan	0.001714	nan	nan	nan	nan
84.4833	nan	0.001331	nan	nan	nan	nan
91.4833	2.2126	nan	nan	nan	nan	nan
93.2333	nan	0.000976	nan	nan	nan	nan
93.2343	nan	0.001209	nan	nan	nan	nan
98.5	nan	nan	nan	nan	nan	0.0015
105.4833	nan	0.000651	nan	nan	nan	nan
116.4833	2.2329	nan	nan	nan	nan	nan

TCE Inhalation -- Experiment B-TRI-2 (Human #38)
Hours, AurnTCOGTCOH_Coll, CALvPPM, CBldTCA, CTCOH, Cven, TotCTCOH
Chiu07_B_2 = [...

0.3333	nan	0.292512	nan	nan	nan	nan
0.3343	nan	0.230086	nan	nan	nan	nan
0.6667	nan	0.25225	nan	nan	nan	nan
0.6677	nan	0.233197	nan	nan	nan	nan
0.95	nan	nan	0.002	nan	0.0025	nan
1.0	nan	0.195014	nan	nan	nan	nan
1.001	nan	0.249061	nan	nan	nan	nan
1.3333	nan	0.073272	nan	nan	nan	nan
1.6667	nan	0.0486764	nan	nan	nan	nan
1.6677	nan	0.0822443	nan	nan	nan	nan
2.3333	nan	0.238585	nan	nan	nan	nan
2.3343	nan	0.250825	nan	nan	nan	nan
2.6667	nan	0.29416	nan	nan	nan	nan
2.6677	nan	0.341965	nan	nan	nan	nan
3.0	nan	0.335391	nan	nan	nan	nan
3.001	nan	0.36076	nan	nan	nan	nan
3.3333	nan	0.273437	nan	nan	nan	nan
3.3343	nan	0.271976	nan	nan	nan	nan
3.6667	nan	0.393574	nan	nan	nan	nan
3.6677	nan	0.343947	nan	nan	nan	nan
4.0	nan	0.358395	nan	nan	nan	nan
4.001	nan	0.412402	nan	nan	nan	nan
4.3333	nan	0.358135	nan	nan	nan	nan
4.3343	nan	0.334281	nan	nan	nan	nan
4.6667	nan	0.407889	nan	nan	nan	nan
4.6677	nan	0.404538	nan	nan	nan	nan
5.0	nan	0.458073	nan	nan	nan	nan
5.001	nan	0.377995	nan	nan	nan	nan
5.3333	nan	0.376453	nan	nan	nan	nan
5.3343	nan	0.324713	nan	nan	nan	nan
5.6667	nan	0.348042	nan	nan	nan	nan
5.7833	nan	nan	0.041	0.011	0.006	0.0425
5.8333	nan	0.372123	nan	nan	nan	nan
6.0333	nan	0.166853	nan	nan	nan	nan
6.0667	nan	0.111252	nan	nan	nan	nan
6.1	nan	0.129059	nan	nan	nan	nan
6.1167	nan	nan	0.034	0.0075	0.003	0.037
6.1333	nan	0.101955	nan	nan	nan	nan
6.1667	nan	0.100765	nan	nan	nan	nan
6.25	nan	0.098608	nan	nan	nan	nan
6.3333	nan	0.090289	nan	nan	nan	nan

6.45	nan	0.058627	nan	nan	nan	nan
6.8333	nan	0.061	nan	nan	nan	nan
6.95	nan	nan	0.0325	0.0065	0.001	0.036
7.0	nan	0.05	nan	nan	nan	nan
7.5	nan	0.037	nan	nan	nan	nan
7.95	nan	nan	0.042	0.008	0.001	0.0325
8.0	nan	0.034	nan	nan	nan	nan
11.1333	nan	0.030738	nan	nan	nan	nan
14.1333	nan	0.019318	nan	nan	nan	nan
15.1333	0.2776	nan	nan	nan	nan	nan
24.1333	nan	0.008817	nan	nan	nan	nan
25.6333	nan	0.009376	nan	nan	nan	nan
25.6343	nan	0.009201	nan	nan	nan	nan
26.1333	0.8985	nan	nan	nan	nan	nan
26.4667	nan	nan	0.057	nan	nan	0.011
32.1333	1.1068	nan	nan	nan	nan	nan
35.1333	nan	0.006491	nan	nan	nan	nan
36.1333	1.3213	nan	nan	nan	nan	nan
40.6333	nan	0.007261	nan	nan	nan	nan
41.6333	1.4584	nan	nan	nan	nan	nan
49.6333	nan	0.004046	nan	nan	nan	nan
50.1333	1.6555	nan	nan	nan	nan	nan
50.2167	nan	nan	0.06	nan	nan	0.004
53.6333	nan	0.005629	nan	nan	nan	nan
62.3833	nan	0.003618	nan	nan	nan	nan
72.6333	nan	0.003276	nan	nan	nan	nan
73.1333	1.7119	nan	nan	nan	nan	nan
74.1333	nan	nan	0.068	nan	nan	0.0025
76.3833	nan	0.002677	nan	nan	nan	nan
86.3833	nan	0.002406	nan	nan	nan	nan
94.6333	1.7378	nan	nan	nan	nan	nan
94.6333	nan	0.000952	nan	nan	nan	nan
99.6333	nan	0.000978	nan	nan	nan	0.001
117.9667	1.7532	nan	nan	nan	nan	nan
144.6667	nan	nan	0.0405	nan	nan	nan

TCE Inhalation -- Experiment C-TRI-1 (Human #39)

Hours, AurnTCOGTCOH_Coll, CALVPPM, CBldTCA, CTCOH, CVen, TotCTCOH, AurnTCA_Coll

0.3333	nan	0.401675	nan	nan	nan	nan	nan
0.3343	nan	0.330756	nan	nan	nan	nan	nan
0.6667	nan	0.377474	nan	nan	nan	nan	nan
0.6677	nan	0.356618	nan	nan	nan	nan	nan
1.0	nan	0.403155	0.001	0.003	0.001	0.005	nan
1.001	nan	0.375551	nan	nan	nan	nan	nan
1.3333	nan	0.331179	nan	nan	nan	nan	nan
1.3343	nan	0.328483	nan	nan	nan	nan	nan
1.6667	nan	0.309511	nan	nan	nan	nan	nan
1.6677	nan	0.319748	nan	nan	nan	nan	nan
2.0	nan	0.385379	0.004	0.006	0.004	0.0165	nan
2.001	nan	0.388993	nan	nan	nan	nan	nan
2.3333	nan	0.460043	nan	nan	nan	nan	nan
2.3343	nan	0.44499	nan	nan	nan	nan	nan
2.6667	nan	0.480806	nan	nan	nan	nan	nan
2.6677	nan	0.422521	nan	nan	nan	nan	nan
3.0	nan	0.406884	nan	nan	nan	nan	nan
3.001	nan	0.394325	nan	nan	nan	nan	nan
3.3333	nan	0.322196	nan	nan	nan	nan	nan
3.3343	nan	0.355099	nan	nan	nan	nan	nan
3.6667	nan	0.330437	nan	nan	nan	nan	nan
3.6677	nan	0.320814	nan	nan	nan	nan	nan
4.0	nan	0.379121	0.014	0.02	0.004	0.213	nan
4.3333	nan	0.233554	nan	nan	nan	nan	nan
4.3343	nan	0.3079	nan	nan	nan	nan	nan
4.6667	nan	0.307107	nan	nan	nan	nan	nan
5.0	nan	0.224368	nan	nan	nan	nan	nan
5.001	nan	0.255573	nan	nan	nan	nan	nan
5.3333	nan	0.27075	nan	nan	nan	nan	nan
5.6667	nan	0.259446	nan	nan	nan	nan	nan
5.6677	nan	0.291828	nan	nan	nan	nan	nan
5.8333	nan	0.268891	0.015	0.016	0.0025	0.094	nan
5.8343	nan	0.225715	nan	nan	nan	nan	nan

6.0333	nan	0.105026	nan	nan	nan	nan	nan
6.0667	nan	0.078629	nan	nan	nan	nan	nan
6.1	nan	0.073664	nan	nan	nan	nan	nan
6.1333	nan	0.083212	nan	nan	nan	nan	nan
6.1667	nan	0.075192	nan	nan	nan	0.095	nan
6.2833	nan	0.063266	nan	nan	nan	nan	nan
6.3333	nan	0.066949	nan	nan	nan	nan	nan
6.4167	nan	0.054265	nan	nan	nan	nan	nan
6.5333	nan	0.049763	nan	nan	nan	nan	nan
6.6667	nan	0.050582	nan	nan	nan	nan	nan
6.8333	nan	0.049355	nan	nan	nan	nan	nan
7.0	nan	0.045262	nan	nan	nan	nan	nan
7.05	nan	nan	0.035	0.024	0.001	0.088	nan
7.2167	0.5381	nan	nan	nan	nan	nan	nan
7.2167	nan	nan	nan	nan	nan	nan	0.0106
7.5	nan	0.024803	nan	nan	nan	nan	nan
8.0	nan	0.032	nan	nan	nan	nan	nan
8.1333	nan	0.032289	nan	nan	nan	nan	nan
8.3833	nan	nan	nan	nan	nan	0.075	nan
9.25	nan	0.021	nan	nan	nan	nan	nan
9.251	nan	0.023554	nan	nan	nan	nan	nan
10.25	nan	0.015935	nan	nan	nan	nan	nan
11.0	nan	0.012913	nan	nan	nan	nan	nan
14.05	nan	0.020003	nan	nan	nan	nan	nan
14.051	nan	0.01928	nan	nan	nan	nan	nan
22.8833	nan	0.007244	nan	nan	nan	nan	nan
27.05	nan	0.007512	nan	nan	nan	nan	nan
28.3833	0.9118	nan	nan	nan	nan	nan	nan
28.3833	nan	nan	nan	nan	nan	nan	0.0213
28.55	nan	nan	0.055	0.006	nan	0.012	nan
33.2167	nan	0.003531	nan	nan	nan	nan	nan
38.3833	1.1632	nan	nan	nan	nan	nan	nan
38.3833	nan	0.003104	nan	nan	nan	nan	nan
45.6333	1.3584	nan	nan	nan	nan	nan	nan
45.6333	nan	nan	nan	nan	nan	nan	0.0333
45.8	nan	0.003364	nan	nan	nan	nan	nan
51.8833	nan	0.001355	0.053	0.0015	0.0005	0.014	nan
62.3833	nan	0.003528	nan	nan	nan	nan	nan
69.8	nan	0.001538	nan	nan	nan	nan	nan
69.8833	1.4847	nan	nan	nan	nan	nan	nan
69.8833	nan	nan	nan	nan	nan	nan	0.0527
74.9667	nan	nan	0.045	0.001	nan	0.012	nan
75.0	nan	0.000655	nan	nan	nan	nan	nan
80.7167	nan	0.000321	nan	nan	nan	nan	nan
86.2167	nan	0.001165	nan	nan	nan	nan	nan
93.6333	nan	0.00036	nan	nan	nan	nan	nan
94.3833	nan	0.000689	nan	nan	nan	nan	nan
94.3843	nan	0.000681	nan	nan	nan	nan	nan
94.4667	1.5212	nan	nan	nan	nan	nan	nan
94.4667	nan	nan	nan	nan	nan	nan	0.067
98.6	nan	nan	0.033	nan	nan	nan	nan
103.6333	nan	0.000388	nan	nan	nan	nan	nan
103.6343	nan	0.000452	nan	nan	nan	nan	nan
118.3833	1.5427	nan	nan	nan	nan	nan	nan
118.3833	nan	nan	nan	nan	nan	nan	0.0823
120.8833	nan	nan	0.027	nan	nan	0.001	nan
141.3833	1.5485	nan	nan	nan	nan	nan	nan
141.3833	nan	nan	nan	nan	nan	nan	0.0951

TCE Inhalation -- Experiment C-TRI-2 (Human #39)

Hours, AurnTCOGTCOH_Coll, CALvPPM, CBldTCA, CTCOH, CVen, TotCTCOH, AurnTCA_Coll

0.3833	nan	0.253178	nan	nan	nan	nan	nan
0.3843	nan	0.257009	nan	nan	nan	nan	nan
0.6667	nan	0.254465	nan	nan	nan	nan	nan
0.6677	nan	0.29185	nan	nan	nan	nan	nan
0.95	nan	0.301115	nan	nan	nan	nan	nan
0.951	nan	0.312384	nan	nan	nan	nan	nan
1.0	nan	nan	0.001	nan	0.002	0.006	nan
1.3667	nan	0.340338	nan	nan	nan	nan	nan
1.3677	nan	0.287822	nan	nan	nan	nan	nan
1.65	nan	0.370802	nan	nan	nan	nan	nan

1.651	nan	0.30183	nan	nan	nan	nan	nan
1.9	nan	nan	0.004	nan	0.002	0.013	nan
2.0	nan	0.251879	nan	nan	nan	nan	nan
2.001	nan	0.247645	nan	nan	nan	nan	nan
2.3333	nan	0.288842	nan	nan	nan	nan	nan
2.3343	nan	0.256194	nan	nan	nan	nan	nan
2.75	nan	0.347955	nan	nan	nan	nan	nan
2.751	nan	0.343899	nan	nan	nan	nan	nan
3.3833	nan	0.381599	nan	nan	nan	nan	nan
3.3843	nan	0.354656	nan	nan	nan	nan	nan
3.6667	nan	0.302258	nan	nan	nan	nan	nan
3.6677	nan	0.282438	nan	nan	nan	nan	nan
3.9833	nan	nan	0.0065	0.002	0.003	0.055	nan
4.0	nan	0.333418	nan	nan	nan	nan	nan
4.001	nan	0.279138	nan	nan	nan	nan	nan
4.3333	nan	0.248589	nan	nan	nan	nan	nan
4.3343	nan	0.280191	nan	nan	nan	nan	nan
4.6667	nan	0.262212	nan	nan	nan	nan	nan
4.6677	nan	0.238468	nan	nan	nan	nan	nan
5.3333	nan	0.314908	nan	nan	nan	nan	nan
5.3343	nan	0.320199	nan	nan	nan	nan	nan
5.6667	nan	0.23351	nan	nan	nan	nan	nan
5.6677	nan	0.273286	nan	nan	nan	nan	nan
5.8333	nan	0.293398	nan	nan	nan	nan	nan
5.8343	nan	0.31403	nan	nan	nan	nan	nan
5.8833	nan	nan	0.012	0.003	0.003	0.097	nan
6.0333	nan	0.104011	nan	nan	nan	nan	nan
6.0667	nan	0.08682	nan	nan	nan	nan	nan
6.1	nan	0.07929	nan	nan	nan	nan	nan
6.1333	nan	0.077221	nan	nan	nan	nan	nan
6.1667	nan	0.050574	nan	nan	nan	nan	nan
6.2167	nan	nan	0.0135	0.004	0.001	0.066	nan
6.25	nan	0.050266	nan	nan	nan	nan	nan
6.3333	nan	0.044009	nan	nan	nan	nan	nan
6.4167	nan	0.041885	nan	nan	nan	nan	nan
6.5	nan	0.04326	nan	nan	nan	nan	nan
6.6667	nan	0.03298	nan	nan	nan	nan	nan
6.8333	nan	0.027589	nan	nan	nan	nan	nan
7.0667	nan	0.035016	0.018	0.003	0.0005	0.069	nan
7.5167	nan	0.011413	nan	nan	nan	nan	nan
7.9667	nan	nan	nan	nan	nan	nan	0.0133
8.0667	nan	0.000367	0.0155	0.003	0.001	0.079	nan
9.1333	nan	0.018218	nan	nan	nan	nan	nan
10.3333	nan	0.011661	nan	nan	nan	nan	nan
22.1333	0.5968	nan	nan	nan	nan	nan	nan
22.3	nan	0.004863	nan	nan	nan	nan	nan
22.301	nan	0.004727	nan	nan	nan	nan	nan
22.302	nan	0.005205	nan	nan	nan	nan	nan
25.6333	nan	nan	0.048	0.002	nan	0.013	nan
27.8833	nan	0.001923	nan	nan	nan	nan	nan
27.9667	nan	0.002692	nan	nan	nan	nan	nan
29.1333	0.9005	nan	nan	nan	nan	nan	nan
29.1333	nan	nan	nan	nan	nan	nan	0.0232
33.4667	1.0882	nan	nan	nan	nan	nan	nan
33.4667	nan	0.002092	nan	nan	nan	nan	nan
33.4677	nan	0.002603	nan	nan	nan	nan	nan
33.4687	nan	0.002335	nan	nan	nan	nan	nan
33.8833	nan	0.001203	nan	nan	nan	nan	nan
33.8843	nan	0.000656	nan	nan	nan	nan	nan
37.6333	1.2845	nan	nan	nan	nan	nan	nan
37.6333	nan	nan	nan	nan	nan	nan	0.0315
37.7167	nan	0.002035	nan	nan	nan	nan	nan
46.1333	1.556	nan	nan	nan	nan	nan	nan
46.1333	nan	0.002554	nan	nan	nan	nan	nan
46.1343	nan	0.002702	nan	nan	nan	nan	nan
50.8	1.6346	nan	nan	nan	nan	nan	nan
50.8	nan	nan	nan	nan	nan	nan	0.0454
52.6333	nan	nan	0.058	nan	nan	0.0095	nan
53.1333	nan	0.001537	nan	nan	nan	nan	nan
53.1343	nan	0.001002	nan	nan	nan	nan	nan
70.1333	1.6844	nan	nan	nan	nan	nan	nan

70.6333	nan	0.000237	nan	nan	nan	nan	nan
70.6343	nan	0.000666	nan	nan	nan	nan	nan
74.8	nan	0.000391	0.051	nan	nan	0.004	nan
74.801	nan	0.001138	nan	nan	nan	nan	nan
74.802	nan	0.00068	nan	nan	nan	nan	nan
80.9167	nan	0.000141	nan	nan	nan	nan	nan
80.9177	nan	0.000181	nan	nan	nan	nan	nan
86.5833	nan	0.000631	nan	nan	nan	nan	nan
86.5843	nan	0.000813	nan	nan	nan	nan	nan
94.1333	1.706	nan	nan	nan	nan	nan	nan
94.1333	nan	0.000729	nan	nan	nan	nan	0.0542
97.8	nan	nan	0.038	nan	nan	nan	nan
109.8833	nan	0.000656	nan	nan	nan	nan	nan
124.1333	nan	nan	0.036	nan	nan	nan	nan
141.6333	1.7109	nan	nan	nan	nan	nan	nan
141.6333	nan	nan	nan	nan	nan	nan	0.0575

TCE Inhalation -- Experiment D-TRI-1 (Human #40)

Hours, AurnTCOGTCOH_Coll, CalvPPM, CBldTCA, CTCOH, Cven, TotCTCOH, AurnTCA_Coll

0.3333	nan	0.339106	nan	nan	nan	nan	nan
0.3343	nan	0.340422	nan	nan	nan	nan	nan
0.6667	nan	0.424221	nan	nan	nan	nan	nan
0.6677	nan	0.398335	nan	nan	nan	nan	nan
1.0	nan	0.393694	0.003	0.0025	0.004	0.006	nan
1.001	nan	0.396775	nan	nan	nan	nan	nan
1.3333	nan	0.309778	nan	nan	nan	nan	nan
1.3343	nan	0.348686	nan	nan	nan	nan	nan
1.6667	nan	0.301157	nan	nan	nan	nan	nan
1.6677	nan	0.313293	nan	nan	nan	nan	nan
2.0	nan	0.481734	nan	nan	nan	0.011	nan
2.001	nan	0.436713	nan	nan	nan	nan	nan
2.3333	nan	0.386535	nan	nan	nan	nan	nan
2.3343	nan	0.373559	nan	nan	nan	nan	nan
2.6667	nan	0.399467	nan	nan	nan	nan	nan
2.6677	nan	0.377011	nan	nan	nan	nan	nan
3.0	nan	0.428886	nan	nan	nan	nan	nan
3.001	nan	0.441738	nan	nan	nan	nan	nan
3.3333	nan	0.285831	nan	nan	nan	nan	nan
3.3343	nan	0.31491	nan	nan	nan	nan	nan
3.6667	nan	0.336511	nan	nan	nan	nan	nan
3.6677	nan	0.33477	nan	nan	nan	nan	nan
4.0	nan	0.355122	0.032	0.016	0.0035	0.035	nan
4.001	nan	0.337867	nan	nan	nan	nan	nan
4.3333	nan	0.35645	nan	nan	nan	nan	nan
4.3343	nan	0.356892	nan	nan	nan	nan	nan
4.6667	nan	0.377994	nan	nan	nan	nan	nan
4.6677	nan	0.345809	nan	nan	nan	nan	nan
5.0	nan	0.460963	nan	nan	nan	nan	nan
5.001	nan	0.434667	nan	nan	nan	nan	nan
5.3333	nan	0.335875	nan	nan	nan	nan	nan
5.3343	nan	0.378302	nan	nan	nan	nan	nan
5.6667	nan	0.421981	nan	nan	nan	nan	nan
5.6677	nan	0.404211	nan	nan	nan	nan	nan
5.8333	nan	0.658911	0.056	0.022	0.007	0.073	nan
5.8343	nan	0.525865	nan	nan	nan	nan	nan
6.0333	nan	0.243293	nan	nan	nan	nan	nan
6.0667	nan	0.164947	nan	nan	nan	nan	nan
6.1	nan	0.150146	nan	nan	nan	nan	nan
6.1333	nan	0.079	nan	nan	nan	nan	nan
6.1667	nan	0.128442	0.047	0.014	0.0025	0.104	nan
6.25	nan	0.108595	nan	nan	nan	nan	nan
6.3	nan	nan	nan	nan	nan	nan	0.0141
6.3333	nan	0.101212	nan	nan	nan	nan	nan
6.4167	nan	0.062	nan	nan	nan	nan	nan
6.5	nan	0.076	nan	nan	nan	nan	nan
6.6667	nan	0.075	nan	nan	nan	nan	nan
6.8333	nan	0.066	nan	nan	nan	nan	nan
7.0	nan	0.081382	nan	nan	nan	0.366	nan
7.5	nan	0.045	nan	nan	nan	nan	nan
7.501	nan	0.032546	nan	nan	nan	nan	nan
8.0	nan	0.031561	0.072	0.0095	0.001	0.133	nan

8.001	nan	0.052	nan	nan	nan	nan	nan
9.0	nan	0.009309	nan	nan	nan	nan	nan
9.001	nan	0.014	nan	nan	nan	nan	nan
11.0	nan	0.011843	nan	nan	nan	nan	nan
22.7167	nan	0.007562	nan	nan	nan	nan	nan
25.2167	nan	nan	0.0595	0.005	nan	0.01	nan
25.9667	0.2368	nan	nan	nan	nan	nan	nan
26.8833	nan	0.006445	nan	nan	nan	nan	nan
26.8843	nan	0.014	nan	nan	nan	nan	nan
31.8833	0.3721	nan	nan	nan	nan	nan	nan
33.3833	0.3835	nan	nan	nan	nan	nan	nan
35.55	0.4405	nan	nan	nan	nan	nan	nan
40.4167	0.4633	nan	nan	nan	nan	nan	nan
40.4167	nan	nan	nan	nan	nan	nan	0.0171
48.55	0.6079	nan	nan	nan	nan	nan	nan
49.8833	nan	nan	0.0875	0.003	nan	nan	nan
71.8833	nan	0.000948	nan	nan	nan	nan	nan
71.8843	nan	0.000915	nan	nan	nan	nan	nan
72.3833	0.6947	nan	nan	nan	nan	nan	nan
73.7333	nan	nan	0.052	nan	nan	0.0025	nan
74.3833	nan	0.001914	nan	nan	nan	nan	nan
80.8833	nan	0.000675	nan	nan	nan	nan	nan
93.55	0.7139	nan	nan	nan	nan	nan	nan
99.6333	nan	nan	nan	nan	nan	0.001	nan
99.8833	nan	0.000462	nan	nan	nan	nan	nan
118.1333	0.728	nan	nan	nan	nan	nan	nan
132.8833	0.7312	nan	nan	nan	nan	nan	nan

TCE Inhalation -- Experiment F-TRI-1 (Human #41)

Hours, AurnTCOGTCOH_Coll, CALvPPM, CBldTCA, CTCOH, CVen, TotCTCOH, AurnTCA_Coll

0.3333	nan	0.214147	nan	nan	nan	nan	nan
0.3343	nan	0.446694	nan	nan	nan	nan	nan
0.6667	nan	0.166763	nan	nan	nan	nan	nan
0.6677	nan	0.188716	nan	nan	nan	nan	nan
1.0	nan	0.43794	0.002	0.002	0.0025	0.014	nan
1.001	nan	0.41233	nan	nan	nan	nan	nan
1.3333	nan	0.330501	nan	nan	nan	nan	nan
1.3343	nan	0.20073	nan	nan	nan	nan	nan
1.6667	nan	0.312345	nan	nan	nan	nan	nan
1.6677	nan	0.670053	nan	nan	nan	nan	nan
2.0	nan	0.306643	nan	nan	nan	0.0115	nan
2.001	nan	0.546148	nan	nan	nan	nan	nan
2.3333	nan	0.409665	nan	nan	nan	nan	nan
2.3343	nan	0.348649	nan	nan	nan	nan	nan
2.6667	nan	0.482744	nan	nan	nan	nan	nan
2.6677	nan	0.33319	nan	nan	nan	nan	nan
3.0	nan	0.377029	nan	nan	nan	nan	nan
3.001	nan	0.310925	nan	nan	nan	nan	nan
3.3333	nan	0.285336	nan	nan	nan	nan	nan
3.3343	nan	0.26259	nan	nan	nan	nan	nan
3.6667	nan	0.315737	nan	nan	nan	nan	nan
3.6677	nan	0.52209	nan	nan	nan	nan	nan
4.0	nan	0.37886	0.018	0.008	0.004	0.022	nan
4.001	nan	0.441677	nan	nan	nan	nan	nan
4.3333	nan	0.477375	nan	nan	nan	nan	nan
4.3343	nan	0.369961	nan	nan	nan	nan	nan
4.6667	nan	0.335101	nan	nan	nan	nan	nan
4.6677	nan	0.260754	nan	nan	nan	nan	nan
5.0	nan	0.528222	nan	nan	nan	nan	nan
5.001	nan	0.467475	nan	nan	nan	nan	nan
5.3333	nan	0.331078	nan	nan	nan	nan	nan
5.3343	nan	0.43603	nan	nan	nan	nan	nan
5.6667	nan	0.34399	nan	nan	nan	nan	nan
5.6677	nan	0.340704	nan	nan	nan	nan	nan
5.8333	nan	nan	0.029	0.0095	0.005	0.05	nan
6.0	nan	0.278839	nan	nan	nan	nan	nan
6.001	nan	0.317781	nan	nan	nan	nan	nan
6.0333	nan	0.137457	nan	nan	nan	nan	nan
6.0667	nan	0.113505	nan	nan	nan	nan	nan
6.1	nan	0.092436	nan	nan	nan	nan	nan
6.1333	nan	0.07859	nan	nan	nan	nan	nan

6.1667	nan	0.073743	0.0445	0.0175	0.002	0.05	nan
6.25	nan	0.07154	nan	nan	nan	nan	nan
6.3	0.0063	nan	nan	nan	nan	nan	nan
6.4167	nan	0.063609	nan	nan	nan	nan	nan
6.5	nan	0.052152	nan	nan	nan	nan	nan
6.6667	nan	0.049949	nan	nan	nan	nan	nan
6.8333	nan	0.04334	nan	nan	nan	nan	nan
7.0	nan	0.039814	0.041	0.01	0.001	0.141	nan
7.5	nan	0.031	nan	nan	nan	nan	nan
7.501	nan	0.040115	nan	nan	nan	nan	nan
8.0	nan	0.030142	0.048	0.01	0.001	0.044	nan
8.001	nan	0.023	nan	nan	nan	nan	nan
8.1667	0.2254	nan	nan	nan	nan	nan	nan
9.0	nan	0.017	nan	nan	nan	nan	nan
9.001	nan	0.021898	nan	nan	nan	nan	nan
10.0	nan	0.019181	nan	nan	nan	nan	nan
11.0	nan	0.015861	nan	nan	nan	nan	nan
12.6667	0.4775	nan	nan	nan	nan	nan	nan
14.6667	0.6152	nan	nan	nan	nan	nan	nan
14.6667	nan	0.004786	nan	nan	nan	nan	nan
24.6667	0.9452	nan	nan	nan	nan	nan	nan
25.6667	nan	nan	0.067	0.003	nan	0.0075	nan
28.1667	nan	0.003477	nan	nan	nan	nan	nan
29.6667	1.0952	nan	nan	nan	nan	nan	nan
31.6667	1.143	nan	nan	nan	nan	nan	0.0088
35.6667	nan	0.0047	nan	nan	nan	nan	nan
36.6667	1.2548	nan	nan	nan	nan	nan	nan
39.1667	1.3098	nan	nan	nan	nan	nan	nan
41.6667	1.3584	nan	nan	nan	nan	nan	nan
48.4167	1.3788	nan	nan	nan	nan	nan	nan
48.4167	nan	0.002362	nan	nan	nan	nan	nan
49.8333	nan	nan	0.073	0.001	0.0005	nan	nan
51.6667	nan	0.001782	nan	nan	nan	nan	nan
51.6677	nan	0.001578	nan	nan	nan	nan	nan
59.6667	nan	0.001653	nan	nan	nan	nan	nan
72.1667	1.4181	nan	nan	nan	nan	nan	nan
72.1667	nan	0.001031	nan	nan	nan	nan	nan
73.8333	nan	nan	0.07	0.001	nan	0.003	nan
82.6667	nan	0.000647	nan	nan	nan	nan	nan
97.6667	1.4272	0.000536	nan	nan	nan	nan	nan
100.4167	nan	0.000368	nan	nan	nan	nan	nan
100.9667	nan	nan	0.0505	nan	nan	nan	nan
122.1667	1.4363	nan	nan	nan	nan	nan	nan
122.6333	nan	nan	0.039	nan	nan	0.001	nan
143.4167	1.4402	nan	nan	nan	nan	nan	nan

TCE Inhalation -- Experiment F-TRI-2 (Human #41)

Hours, AurnTCOHTCOH_Coll, CALVPPM, CBldTCA, CTCOH, CVen, TotCTCOH, AurnTCA_Coll

0.3333	nan	0.42561	nan	nan	nan	nan	nan
0.3343	nan	0.351669	nan	nan	nan	nan	nan
0.6667	nan	0.416291	nan	nan	nan	nan	nan
0.6677	nan	0.294322	nan	nan	nan	nan	nan
1.0	nan	0.39137	0.002	nan	0.0035	0.0065	nan
1.001	nan	0.543459	nan	nan	nan	nan	nan
1.3333	nan	0.347941	nan	nan	nan	nan	nan
1.3343	nan	0.392029	nan	nan	nan	nan	nan
1.6667	nan	0.072125	nan	nan	nan	nan	nan
1.6677	nan	0.074234	nan	nan	nan	nan	nan
2.0	nan	0.059767	0.0035	nan	0.001	0.018	nan
2.001	nan	0.054379	nan	nan	nan	nan	nan
2.3333	nan	0.159857	nan	nan	nan	nan	nan
2.3343	nan	0.492105	nan	nan	nan	nan	nan
2.6667	nan	0.386478	nan	nan	nan	nan	nan
2.6677	nan	0.344507	nan	nan	nan	nan	nan
3.0	nan	0.530141	nan	nan	nan	nan	nan
3.001	nan	0.497122	nan	nan	nan	nan	nan
3.3333	nan	0.545553	nan	nan	nan	nan	nan
3.3343	nan	0.544988	nan	nan	nan	nan	nan
3.6667	nan	0.445338	nan	nan	nan	nan	nan
3.6677	nan	0.413655	nan	nan	nan	nan	nan
4.0	nan	0.331208	0.02	0.008	0.005	0.038	nan

4.001	nan	0.544767	nan	nan	nan	nan	nan
4.4667	nan	0.505634	nan	nan	nan	nan	nan
4.4677	nan	0.529838	nan	nan	nan	nan	nan
4.6667	nan	0.417287	nan	nan	nan	nan	nan
4.6677	nan	0.327814	nan	nan	nan	nan	nan
5.0	nan	0.440222	nan	nan	nan	nan	nan
5.001	nan	0.511302	nan	nan	nan	nan	nan
5.3333	nan	0.317899	nan	nan	nan	nan	nan
5.3343	nan	0.312976	nan	nan	nan	nan	nan
5.6667	nan	0.308524	nan	nan	nan	nan	nan
5.6677	nan	0.478391	nan	nan	nan	nan	nan
5.8333	nan	0.412262	0.039	0.009	0.006	0.065	nan
6.0333	nan	0.179332	nan	nan	nan	nan	nan
6.0667	nan	0.134678	nan	nan	nan	nan	nan
6.1	nan	0.092383	nan	nan	nan	nan	nan
6.1333	0.5917	nan	nan	nan	nan	nan	nan
6.1333	nan	0.059	nan	nan	nan	nan	nan
6.1667	nan	0.09907	nan	nan	nan	nan	nan
6.2333	nan	nan	0.0425	0.009	0.002	0.043	nan
6.25	nan	0.050897	nan	nan	nan	nan	nan
6.3333	nan	0.059	nan	nan	nan	nan	nan
6.4167	nan	0.051	nan	nan	nan	nan	nan
6.5	nan	0.045315	nan	nan	nan	nan	nan
6.6667	nan	0.045715	nan	nan	nan	nan	nan
6.8333	nan	0.043	nan	nan	nan	nan	nan
7.0	nan	0.038	nan	nan	nan	0.041	nan
7.5	nan	0.03	nan	nan	nan	nan	nan
8.0	nan	0.015	0.048	0.007	0.001	0.036	nan
9.6333	1.0628	nan	nan	nan	nan	nan	nan
15.6333	1.4811	nan	nan	nan	nan	nan	nan
16.15	nan	0.010247	nan	nan	nan	nan	nan
22.8	1.9016	nan	nan	nan	nan	nan	nan
22.8833	nan	0.007517	nan	nan	nan	nan	nan
26.6333	2.0542	nan	0.074	0.002	nan	0.012	nan
27.6333	nan	0.00535	nan	nan	nan	nan	nan
30.3833	2.1926	nan	nan	nan	nan	nan	nan
34.1333	2.3728	nan	nan	nan	nan	nan	nan
34.1333	nan	0.00279	nan	nan	nan	nan	nan
35.6333	nan	0.006341	nan	nan	nan	nan	nan
39.3833	2.4387	0.003194	nan	nan	nan	nan	nan
40.6333	2.4618	nan	nan	nan	nan	nan	0.0198
48.6333	2.5126	nan	nan	nan	nan	nan	nan
48.6333	nan	0.001592	nan	nan	nan	nan	nan
50.55	nan	nan	nan	nan	nan	0.0025	nan
51.6333	nan	0.001841	nan	nan	nan	nan	nan
58.6333	nan	0.001643	nan	nan	nan	nan	nan
58.6343	nan	0.002178	nan	nan	nan	nan	nan
58.6353	nan	0.002056	nan	nan	nan	nan	nan
72.1333	2.5518	nan	nan	nan	nan	nan	nan
72.3833	nan	0.001587	nan	nan	nan	nan	nan
73.3833	nan	nan	0.067	nan	nan	0.001	nan
75.6333	nan	0.001208	nan	nan	nan	nan	nan
75.6343	nan	0.000874	nan	nan	nan	nan	nan
82.6333	nan	0.00112	nan	nan	nan	nan	nan
92.8833	nan	0.000748	nan	nan	nan	nan	nan
93.6333	2.566	nan	nan	nan	nan	nan	nan
94.3833	nan	nan	0.0545	nan	nan	nan	nan
99.6333	nan	0.00031	nan	nan	nan	nan	nan
99.6343	nan	0.000223	nan	nan	nan	nan	nan
99.6353	nan	0.000584	nan	nan	nan	nan	nan
118.6333	2.5684	nan	nan	nan	nan	nan	0.024
128.6333	nan	nan	0.036	nan	nan	nan	nan
143.1333	2.5711	nan	nan	nan	nan	nan	nan

TCE Inhalation -- Experiment G-TRI-1 (Human #42)

Hours,	AurnTCOGTCOH_Coll,	CALvPPM,	CBldTCA,	CTCOH,	CVen,	TotCTCOH,	AurnTCA_Coll
0.3333	nan	0.313836	nan	nan	nan	nan	nan
0.3343	nan	0.289407	nan	nan	nan	nan	nan
0.6667	nan	0.358654	nan	nan	nan	nan	nan
0.6677	nan	0.330007	nan	nan	nan	nan	nan
1.0	nan	0.286794	0.001	nan	0.002	0.008	nan
1.001	nan	0.351549	nan	nan	nan	nan	nan
1.3333	nan	0.098419	nan	nan	nan	nan	nan
1.3343	nan	0.111763	nan	nan	nan	nan	nan
1.6667	nan	0.055313	nan	nan	nan	nan	nan
1.6677	nan	0.056352	nan	nan	nan	nan	nan
2.0	nan	0.477732	0.002	nan	0.004	nan	nan
2.001	nan	0.560644	nan	nan	nan	nan	nan
2.3333	nan	0.280315	nan	nan	nan	nan	nan
2.3343	nan	0.307747	nan	nan	nan	nan	nan
2.6667	nan	0.420583	nan	nan	nan	nan	nan
2.6677	nan	0.32215	nan	nan	nan	nan	nan
3.0	nan	0.494522	nan	nan	nan	nan	nan
3.001	nan	0.568965	nan	nan	nan	nan	nan
3.3833	nan	0.38854	nan	nan	nan	nan	nan
3.3843	nan	0.352325	nan	nan	nan	nan	nan
3.6667	nan	0.383471	nan	nan	nan	nan	nan
3.6677	nan	0.353154	nan	nan	nan	nan	nan
4.0	nan	0.401385	0.0135	0.008	0.004	0.024	nan
4.001	nan	0.384194	nan	nan	nan	nan	nan
4.3333	nan	0.449241	nan	nan	nan	nan	nan
4.3343	nan	0.413776	nan	nan	nan	nan	nan
4.6667	nan	0.421671	nan	nan	nan	nan	nan
4.6677	nan	0.405174	nan	nan	nan	nan	nan
5.0	nan	0.510643	nan	nan	nan	nan	nan
5.001	nan	0.454817	nan	nan	nan	nan	nan
5.3333	nan	0.47175	nan	nan	nan	nan	nan
5.3343	nan	0.523048	nan	nan	nan	nan	nan
5.6667	nan	0.392709	nan	nan	nan	nan	nan
5.6677	nan	0.37841	nan	nan	nan	nan	nan
5.8333	nan	0.416564	0.0255	0.011	0.005	0.0455	nan
6.0667	nan	0.09573	nan	nan	nan	nan	nan
6.1	nan	0.104838	nan	nan	nan	nan	nan
6.1333	nan	0.082287	nan	nan	nan	nan	nan
6.1667	nan	0.075879	nan	nan	nan	nan	nan
6.2	nan	nan	0.027	0.013	0.001	0.049	nan
6.3333	nan	0.076577	nan	nan	nan	nan	nan
6.4167	nan	0.046446	nan	nan	nan	nan	nan
6.5	nan	0.039067	nan	nan	nan	nan	nan
6.6667	nan	0.027451	nan	nan	nan	nan	nan
6.8333	nan	0.023355	nan	nan	nan	nan	nan
7.0	nan	0.051239	nan	nan	nan	0.049	nan
7.5	nan	0.0165	nan	nan	nan	nan	nan
8.05	nan	nan	nan	nan	nan	0.041	nan
9.4	nan	0.042249	nan	nan	nan	nan	nan
10.7167	nan	0.027713	nan	nan	nan	nan	nan
12.8833	nan	0.025106	nan	nan	nan	nan	nan
13.3833	nan	nan	nan	nan	nan	nan	0.0037
24.3833	0.778	0.011491	nan	nan	nan	nan	nan
24.3843	nan	0.010796	nan	nan	nan	nan	nan
27.1333	nan	0.006405	nan	nan	nan	nan	nan
27.1343	nan	0.007495	nan	nan	nan	nan	nan
27.3833	nan	nan	nan	nan	nan	0.009	nan
29.8833	0.9906	nan	nan	nan	nan	nan	nan
32.3833	nan	0.003457	nan	nan	nan	nan	nan
32.3843	nan	0.003741	nan	nan	nan	nan	nan
37.3833	nan	0.005975	nan	nan	nan	nan	nan
48.3833	nan	0.002303	nan	nan	nan	nan	nan
48.3843	nan	0.001115	nan	nan	nan	nan	nan
51.1333	nan	nan	0.0665	nan	nan	0.006	nan
51.3833	nan	0.001783	nan	nan	nan	nan	nan
51.3843	nan	0.001744	nan	nan	nan	nan	nan
57.3833	nan	0.003287	nan	nan	nan	nan	nan
57.3843	nan	0.002935	nan	nan	nan	nan	nan
71.1333	1.0389	0.001309	nan	nan	nan	nan	nan

71.1343	nan	0.003156	nan	nan	nan	nan	nan
71.8833	nan	nan	0.0635	nan	nan	nan	nan
81.3833	nan	0.000455	nan	nan	nan	nan	nan
81.3843	nan	0.000346	nan	nan	nan	nan	nan
85.3833	nan	0.000209	nan	nan	nan	nan	nan
85.3843	nan	0.001095	nan	nan	nan	nan	nan
96.3833	1.0529	0.000518	nan	nan	nan	nan	nan
98.55	nan	nan	0.0445	nan	nan	nan	nan
101.3833	nan	0.000259	nan	nan	nan	nan	nan
143.75	nan	nan	0.0385	nan	nan	nan	nan

Fisher et al., 1998

TCE Inhalation 105.5 ppm for 4 hours -- Male subject 1 (Human #1)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.52	nan	0.15	nan	nan	1.98	nan	nan
0.579	nan	nan	0.00886	nan	nan	nan	nan
1.0	nan	0.5	nan	0.39	2.69	0.39	nan
1.01	nan	nan	0.0349	nan	nan	nan	nan
2.0	nan	1.07	0.0461	1.3	3.38	1.3	nan
3.0	nan	2.11	0.0337	2.18	3.76	2.18	nan
4.0	nan	3.12	nan	2.83	3.95	2.83	nan
4.02	nan	nan	0.0313	nan	nan	nan	nan
4.24	nan	nan	0.0241	nan	nan	nan	nan
4.25	nan	2.87	nan	2.94	3.26	2.94	nan
4.5	13.94	3.39	0.0132	3.21	2.54	3.21	1.47
5.0	nan	4.0	nan	2.78	1.12	2.78	nan
5.01	nan	nan	0.00552	nan	nan	nan	nan
6.0	nan	4.09	nan	2.84	0.72	2.84	nan
6.1	23.22	nan	nan	nan	nan	nan	2.82
6.02	nan	nan	0.00417	nan	nan	nan	nan
8.0	30.95	4.76	nan	2.52	0.52	2.52	5.02
8.01	nan	nan	0.000671	nan	nan	nan	nan
10.0	nan	5.52	nan	2.03	0.31	2.03	nan
10.1	37.58	nan	nan	nan	nan	nan	7.1
11.4	43.49	nan	nan	nan	nan	nan	8.87
12.0	nan	6.16	nan	1.56	0.28	1.56	nan
12.1	46.17	nan	nan	nan	nan	nan	10.22
14.0	nan	6.48	nan	1.56	0.23	1.56	nan
14.1	50.32	nan	nan	nan	nan	nan	12.67
16.0	56.69	8.12	nan	1.31	0.17	1.31	15.33
18.0	61.37	7.18	nan	1.21	0.15	1.21	16.85
20.03	nan	8.56	nan	1.15	nan	1.15	nan
20.23	65.35	nan	nan	nan	nan	nan	22.83
21.97	68.94	nan	nan	nan	nan	nan	25.23
22.02	nan	8.14	nan	nan	nan	nan	nan
26.0	74.63	nan	nan	nan	nan	nan	30.03
31.5	79.76	nan	nan	nan	nan	nan	33.1
34.25	82.89	nan	nan	nan	nan	nan	39.59
35.5	84.29	nan	nan	nan	nan	nan	42.21
36.75	86.91	nan	nan	nan	nan	nan	48.47
44.75	90.23	nan	nan	nan	nan	nan	52.39
45.83	nan	9.3	nan	nan	nan	nan	nan
52.0	91.8	nan	nan	nan	nan	nan	55.28
54.5	93.75	nan	nan	nan	nan	nan	58.64
56.5	94.88	nan	nan	nan	nan	nan	59.8
59.5	96.1	nan	nan	nan	nan	nan	62.4
60.5	96.99	nan	nan	nan	nan	nan	65.0
68.5	99.59	nan	nan	nan	nan	nan	79.17
69.74	nan	7.37	nan	nan	nan	nan	nan
70.25	100.64	nan	nan	nan	nan	nan	83.51
73.0	102.16	nan	nan	nan	nan	nan	88.15
79.5	104.07	nan	nan	nan	nan	nan	99.19
81.5	104.74	nan	nan	nan	nan	nan	100.11
84.67	104.94	nan	nan	nan	nan	nan	100.62
93.75	nan	6.97	nan	nan	nan	nan	nan

TCE Inhalation 49.3 ppm for 4 hours -- Male subject 2 (Human #2)

Hours, AurnTCOGTCOH, CBldTCA, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	0.29	0.44	0.61	0.44	nan
1.0	nan	0.65	0.55	0.74	0.55	nan
2.0	nan	1.47	0.83	1.11	0.83	nan
3.0	nan	2.27	1.08	1.01	1.08	nan
4.0	nan	2.91	1.35	1.05	1.35	nan
4.25	nan	2.99	1.26	0.81	1.26	nan
4.5	nan	3.12	1.34	0.46	1.34	nan
4.55	8.45	nan	nan	nan	nan	0.041
5.0	nan	3.49	1.11	nan	1.11	nan
5.08	15.2	nan	nan	nan	nan	0.062
6.0	nan	3.66	1.01	nan	1.01	nan
6.06	21.6	nan	nan	nan	nan	0.15
8.0	nan	4.29	0.9	nan	0.9	nan
8.08	28.09	nan	nan	nan	nan	0.26
10.0	nan	4.69	0.76	nan	0.76	nan
10.06	35.67	nan	nan	nan	nan	0.41
12.0	nan	5.11	nan	nan	nan	nan
12.08	39.98	nan	nan	nan	nan	0.53
14.0	nan	5.17	0.66	nan	0.66	nan
14.08	43.78	nan	nan	nan	nan	0.65
16.0	nan	5.26	0.63	nan	0.63	nan
16.08	47.68	nan	nan	nan	nan	0.8
18.0	nan	5.66	0.56	nan	0.56	nan
18.08	50.54	nan	nan	nan	nan	0.92
20.0	nan	5.18	0.51	nan	0.51	nan
20.08	53.03	nan	nan	nan	nan	1.05
22.0	nan	5.69	nan	nan	nan	nan
22.17	55.3	nan	nan	nan	nan	1.18
31.33	60.62	nan	nan	nan	nan	1.46
49.0	69.8	nan	nan	nan	nan	2.2
49.08	nan	6.67	nan	nan	nan	nan
64.33	73.15	nan	nan	nan	nan	3.61
71.72	nan	6.49	nan	nan	nan	nan
77.0	74.82	nan	nan	nan	nan	4.36
86.25	76.02	nan	nan	nan	nan	5.03
97.47	nan	6.01	nan	nan	nan	nan

TCE Inhalation 55.2 ppm for 4 hours -- Male subject 3 (Human #3)

Hours, AurnTCOGTCOH, CBldTCA, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	nan	nan	nan	0.002
0.58	nan	0.43	0.63	1.89	0.63	nan
0.98	nan	0.55	1.07	1.36	1.07	nan
2.02	nan	1.07	1.57	2.68	1.57	nan
3.02	nan	1.57	1.9	2.67	1.9	nan
3.12	8.24	nan	nan	nan	nan	0.082
4.02	nan	1.96	1.94	2.79	1.94	nan
4.25	nan	2.01	2.02	2.42	2.02	nan
4.44	nan	2.19	2.26	1.52	2.26	nan
4.63	11.6	nan	nan	nan	nan	0.184
5.02	nan	2.28	1.02	0.82	1.02	nan
5.45	13.64	nan	nan	nan	nan	0.249
5.83	nan	2.52	0.96	0.37	0.96	nan
6.45	15.64	nan	nan	nan	nan	0.307
8.0	nan	2.92	1.65	0.29	1.65	nan
8.13	19.73	nan	nan	nan	nan	0.539
10.0	nan	3.2	1.38	nan	1.38	nan
10.17	23.26	nan	nan	nan	nan	0.852
12.0	nan	3.56	1.26	nan	1.26	nan
12.15	28.95	nan	nan	nan	nan	1.35
14.17	nan	4.19	1.13	nan	1.13	nan
14.27	28.95	nan	nan	nan	nan	1.78
16.02	nan	3.9	1.03	nan	1.03	nan
16.13	29.79	nan	nan	nan	nan	2.12
18.02	nan	4.95	1.05	nan	1.05	nan
18.15	32.07	nan	nan	nan	nan	2.48
20.0	nan	5.04	0.9	nan	0.9	nan
20.2	34.21	nan	nan	nan	nan	2.89
22.0	nan	5.08	nan	nan	nan	nan
22.22	38.49	nan	nan	nan	nan	3.48

24.22	43.06	nan	nan	nan	nan	4.28
32.85	47.48	nan	nan	nan	nan	5.35
34.22	48.6	nan	nan	nan	nan	5.66
39.85	52.15	nan	nan	nan	nan	6.72
44.25	53.88	nan	nan	nan	nan	7.42
44.83	nan	5.51	nan	nan	nan	nan
47.25	55.21	nan	nan	nan	nan	8.14
52.13	57.21	nan	nan	nan	nan	8.93
58.59	59.15	nan	nan	nan	nan	10.17
67.75	60.89	nan	nan	nan	nan	11.19
68.72	nan	9.45	nan	nan	nan	nan
72.37	61.46	nan	nan	nan	nan	12.56
77.15	61.84	nan	nan	nan	nan	13.78
82.92	62.2	nan	nan	nan	nan	14.44
91.83	62.56	nan	nan	nan	nan	15.63
93.12	nan	4.27	nan	nan	nan	nan

TCE Inhalation 101.5 ppm for 4 hours -- Male subject 3 (Human #3)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	0.3	nan	0.56	3.1	0.56	nan
0.579	nan	nan	0.00886	nan	nan	nan	nan
1.0	nan	0.75	nan	1.12	3.76	1.12	nan
1.01	nan	nan	0.0349	nan	nan	nan	nan
2.0	nan	1.42	0.0461	1.75	3.46	1.75	nan
3.0	nan	2.34	0.0337	2.55	3.83	2.55	nan
4.02	nan	3.01	0.0313	3.48	3.78	3.48	nan
4.24	nan	nan	0.0241	nan	nan	nan	nan
4.25	nan	2.58	nan	3.73	2.9	3.73	nan
4.35	28.92	nan	nan	nan	2.11	nan	0.98
4.5	nan	3.1	0.0132	3.52	1.09	3.52	nan
5.0	nan	3.26	nan	3.78	nan	3.78	nan
5.01	nan	nan	0.00552	nan	nan	nan	nan
5.03	31.85	nan	nan	nan	nan	nan	1.21
6.0	nan	4.21	nan	3.79	nan	3.79	nan
6.02	nan	nan	0.00417	nan	nan	nan	nan
6.07	40.01	nan	nan	nan	nan	nan	1.42
8.0	nan	4.99	nan	3.3	nan	3.3	nan
8.01	nan	nan	0.000671	nan	nan	nan	nan
8.07	56.31	nan	nan	nan	nan	nan	2.05
10.0	nan	5.46	nan	2.96	nan	2.96	nan
10.04	68.48	nan	nan	nan	nan	nan	3.12
12.05	nan	5.74	nan	2.71	nan	2.71	nan
12.07	78.8	nan	nan	nan	nan	nan	3.6
14.0	nan	6.69	nan	2.38	nan	2.38	nan
14.06	89.82	nan	nan	nan	nan	nan	4.09
16.0	nan	6.85	nan	2.04	nan	2.04	nan
16.03	98.66	nan	nan	nan	nan	nan	4.57
18.0	nan	7.14	nan	1.89	nan	1.89	nan
18.02	105.25	nan	nan	nan	nan	nan	4.86
20.0	nan	9.85	nan	1.57	nan	1.57	nan
20.04	112.29	nan	nan	nan	nan	nan	5.28
22.05	nan	9.32	nan	1.4	nan	1.4	nan
22.13	122.73	nan	nan	nan	nan	nan	5.98
25.5	141.62	nan	nan	nan	nan	nan	8.14
36.5	150.29	nan	nan	nan	nan	nan	8.94
44.1	162.32	nan	nan	nan	nan	nan	10.97
47.0	165.74	nan	nan	nan	nan	nan	11.58
50.52	nan	8.87	nan	nan	nan	nan	nan
54.0	173.84	nan	nan	nan	nan	nan	13.48
61.45	178.3	nan	nan	nan	nan	nan	15.33
69.3	182.24	nan	nan	nan	nan	nan	17.47
74.03	nan	8.08	nan	nan	nan	nan	nan
85.0	185.01	nan	nan	nan	nan	nan	21.65
93.55	186.89	nan	nan	nan	nan	nan	21.65
98.58	nan	3.82	nan	nan	nan	nan	nan

TCE Inhalation 53.1 ppm for 4 hours -- Male subject 4 (Human #4)

Hours, AurnTCOGTCOH, CBldTCA, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	nan	0.67	nan	nan
1.0	nan	0.29	0.43	1.37	0.43	nan
2.03	nan	0.77	1.2	1.96	1.2	nan
3.0	nan	1.33	1.26	1.92	1.26	nan
4.02	nan	1.84	1.69	2.08	1.69	nan
4.25	nan	1.93	1.66	1.13	1.66	nan
4.5	nan	2.07	1.6	0.76	1.6	nan
5.02	nan	2.27	1.58	0.42	1.58	nan
5.25	5.26	nan	nan	nan	nan	1.0
5.97	8.23	nan	nan	nan	nan	1.53
6.02	nan	2.94	1.51	0.3	1.51	nan
8.0	13.05	nan	nan	nan	nan	3.34
8.08	nan	3.58	1.44	0.21	1.44	nan
10.0	nan	3.72	1.52	0.15	1.52	nan
10.17	16.3	nan	nan	nan	nan	6.01
12.0	nan	3.98	1.14	nan	1.14	nan
12.17	19.05	nan	nan	nan	nan	7.6
14.0	nan	4.4	1.05	nan	1.05	nan
14.17	24.62	nan	nan	nan	nan	13.02
16.0	nan	4.58	1.04	nan	1.04	nan
16.17	26.97	nan	nan	nan	nan	14.83
18.0	nan	4.86	1.06	nan	1.06	nan
18.17	29.06	nan	nan	nan	nan	16.67
20.0	nan	5.73	0.45	nan	0.45	nan
20.17	30.62	nan	nan	nan	nan	18.69
22.0	nan	4.22	0.75	nan	0.75	nan
22.17	32.53	nan	nan	nan	nan	21.3
25.0	33.35	nan	nan	nan	nan	21.95
29.83	35.43	nan	nan	nan	nan	26.24
37.83	37.99	nan	nan	nan	nan	31.79
44.78	nan	5.0	nan	nan	nan	nan
44.83	38.21	nan	nan	nan	nan	40.44
45.67	39.06	nan	nan	nan	nan	40.86
49.67	39.63	nan	nan	nan	nan	42.64
53.33	39.7	nan	nan	nan	nan	42.94
61.23	39.9	nan	nan	nan	nan	43.8
62.83	40.23	nan	nan	nan	nan	44.54
68.72	nan	4.72	nan	nan	nan	nan
79.1	40.67	nan	nan	nan	nan	48.73
100.4	nan	4.47	nan	nan	nan	nan

TCE Inhalation 97.8 ppm for 4 hours -- Male subject 4 (Human #4)

Hours, AurnTCOGTCOH, CALvPPM, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	0.21	nan	0.64	nan	nan	nan
0.579	nan	nan	nan	nan	nan	nan	nan	0.00886
1.0	nan	nan	0.49	0.47	0.94	0.47	nan	nan
1.01	nan	nan	nan	nan	nan	nan	nan	0.0349
2.0	nan	nan	nan	nan	nan	nan	nan	0.0461
2.02	nan	nan	1.1	1.1	1.35	1.1	nan	nan
3.0	nan	nan	1.67	1.58	1.62	1.58	nan	0.0337
4.02	nan	24.679	2.52	2.1	1.56	2.1	nan	0.0313
4.24	nan	nan	nan	nan	nan	nan	nan	0.0241
4.25	nan	6.422	2.44	2.21	1.16	2.21	nan	nan
4.5	nan	4.394	2.71	2.2	0.77	2.2	nan	0.0132
4.55	11.6	nan	nan	nan	nan	nan	0.32	nan
5.0	nan	2.691	3.18	2.15	0.37	2.15	nan	nan
5.01	nan	nan	nan	nan	nan	nan	nan	0.00552
5.12	13.64	nan	nan	nan	nan	nan	0.41	nan
6.0	nan	1.388	3.46	1.94	0.23	1.94	nan	nan
6.02	nan	nan	nan	nan	nan	nan	nan	0.00417
6.08	18.54	nan	nan	nan	nan	nan	1.04	nan
8.0	nan	1.198	4.26	1.88	0.19	1.88	nan	nan
8.01	nan	nan	nan	nan	nan	nan	nan	0.000671
8.13	25.0	nan	nan	nan	nan	nan	1.32	nan
10.03	nan	0.592	4.93	1.61	0.17	1.61	2.51	nan
10.13	33.99	nan	nan	nan	nan	nan	nan	nan
12.02	nan	0.47	5.43	1.39	nan	1.39	nan	nan
12.1	42.1	nan	nan	nan	nan	nan	4.77	nan
14.03	nan	0.369	5.85	1.26	nan	1.26	nan	nan

14.1	50.19	nan	nan	nan	nan	nan	7.29	nan
16.0	nan	0.351	6.02	1.06	nan	1.06	nan	nan
16.1	60.58	nan	nan	nan	nan	nan	10.23	nan
18.0	nan	nan	6.18	0.95	nan	0.95	nan	nan
18.12	64.73	nan	nan	nan	nan	nan	11.5	nan
19.97	nan	nan	6.35	0.88	nan	0.88	nan	nan
20.08	70.85	nan	nan	nan	nan	nan	13.03	nan
22.07	nan	nan	6.52	0.77	nan	0.77	nan	nan
22.3	77.69	nan	nan	nan	nan	nan	14.26	nan
30.42	79.75	nan	nan	nan	nan	nan	17.65	nan
35.67	80.14	nan	nan	nan	nan	nan	18.58	nan
48.0	nan	nan	12.88	nan	nan	nan	nan	nan
51.83	80.23	nan	nan	nan	nan	nan	18.58	nan
56.67	80.32	nan	nan	nan	nan	nan	18.58	nan
61.5	80.66	nan	nan	nan	nan	nan	18.95	nan
70.17	81.44	nan	nan	nan	nan	nan	20.95	nan
71.83	nan	nan	6.25	nan	nan	nan	nan	nan
72.67	82.38	nan	nan	nan	nan	nan	22.77	nan
76.92	82.74	nan	nan	nan	nan	nan	25.76	nan
82.67	83.28	nan	nan	nan	nan	nan	30.01	nan
85.75	83.35	nan	nan	nan	nan	nan	30.7	nan
93.67	83.79	nan	nan	nan	nan	nan	34.88	nan
101.08	nan	nan	5.07	nan	nan	nan	nan	nan

TCE Inhalation 105.5 ppm for 4 hours -- Male subject 5 (Human #5)

Hours, AurntCOGTCOH, CbltTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.52	nan	0.24	nan	nan	1.69	nan	nan
0.579	nan	nan	0.00886	nan	nan	nan	nan
1.0	nan	0.6	nan	0.37	2.5	0.37	nan
1.01	nan	nan	0.0349	nan	nan	nan	nan
2.0	nan	nan	0.0461	nan	nan	nan	nan
2.02	nan	1.24	nan	1.41	3.5	1.41	nan
3.0	nan	nan	0.0337	nan	nan	nan	nan
3.02	nan	2.71	nan	2.4	4.24	2.4	nan
4.02	nan	nan	0.0313	3.59	4.75	3.59	nan
4.24	nan	nan	0.0241	nan	nan	nan	nan
4.27	nan	4.23	nan	4.16	3.76	4.16	nan
4.38	nan	nan	nan	nan	nan	nan	1.74
4.5	nan	nan	0.0132	nan	nan	nan	nan
4.52	nan	3.86	nan	3.73	2.2	3.73	nan
5.01	nan	nan	0.00552	nan	nan	nan	nan
5.02	nan	3.92	nan	3.65	0.96	3.65	nan
6.0	8.69	nan	nan	nan	nan	nan	2.77
6.02	nan	nan	0.00417	nan	nan	nan	nan
6.42	nan	4.54	nan	3.63	0.53	3.63	nan
8.0	18.39	5.71	nan	2.6	0.26	2.6	3.94
8.01	nan	nan	0.000671	nan	nan	nan	nan
10.0	27.48	6.21	nan	2.82	0.17	2.82	5.52
12.0	37.49	nan	nan	1.84	0.17	1.84	7.66
14.0	44.58	7.96	nan	1.55	nan	1.55	9.62
16.0	51.78	9.08	nan	1.59	nan	1.59	11.69
18.0	56.11	8.3	nan	1.06	nan	1.06	13.57
20.0	60.47	8.43	nan	1.23	nan	1.23	20.39
22.0	64.77	nan	nan	nan	nan	nan	26.25
22.03	nan	8.95	nan	0.75	nan	0.75	nan
24.42	66.98	nan	nan	nan	nan	nan	30.32
31.0	75.49	nan	nan	nan	nan	nan	40.91
35.42	79.43	nan	nan	nan	nan	nan	50.7
44.9	82.13	nan	nan	nan	nan	nan	65.02
49.75	85.29	nan	nan	nan	nan	nan	65.02
53.75	88.15	nan	nan	nan	nan	nan	78.15
54.76	88.66	nan	nan	nan	nan	nan	79.79
59.42	89.44	nan	nan	nan	nan	nan	83.82
68.9	90.6	nan	nan	nan	nan	nan	93.09
69.72	nan	5.51	nan	nan	nan	nan	nan
70.83	91.71	nan	nan	nan	nan	nan	98.82
72.0	91.84	nan	nan	nan	nan	nan	100.66
74.58	92.37	nan	nan	nan	nan	nan	112.13
77.0	93.07	nan	nan	nan	nan	nan	117.83
83.92	93.79	nan	nan	nan	nan	nan	118.82
86.0	94.17	nan	nan	nan	nan	nan	119.3

92.67	94.55	nan	nan	nan	nan	nan	120.02
93.61	nan	3.55	nan	nan	nan	nan	nan

TCE Inhalation 102.6 ppm for 4 hours -- Male subject 6 (Human #6)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, Cven, TotCTCOH, AurntTCA

0.5	nan	0.23	nan	0.45	1.93	0.45	nan
0.579	nan	nan	0.00886	nan	nan	nan	nan
1.01	nan	nan	0.0349	nan	nan	nan	nan
1.07	nan	0.49	nan	0.77	2.34	0.77	nan
2.0	nan	1.07	0.0461	1.51	2.84	1.51	nan
3.0	nan	1.89	0.0337	2.41	3.4	2.41	nan
3.03	32.7	nan	nan	nan	nan	nan	0.488
3.98	nan	2.87	nan	3.3	3.41	3.3	nan
4.02	nan	nan	0.0313	nan	nan	nan	nan
4.24	nan	nan	0.0241	nan	nan	nan	nan
4.25	nan	3.69	nan	3.64	2.2	3.64	nan
4.5	nan	3.87	0.0132	3.67	1.66	3.67	nan
4.75	60.26	nan	nan	nan	nan	nan	0.961
5.0	nan	3.59	nan	3.48	0.89	3.48	nan
5.01	nan	nan	0.00552	nan	nan	nan	nan
6.0	nan	4.18	nan	3.05	0.38	3.05	nan
6.02	nan	nan	0.00417	nan	nan	nan	nan
6.7	97.98	nan	nan	nan	nan	nan	2.09
8.0	nan	4.71	nan	2.52	nan	2.52	nan
8.01	nan	nan	0.000671	nan	nan	nan	nan
8.25	130.67	nan	nan	nan	nan	nan	2.96
10.02	nan	5.46	nan	2.38	nan	2.38	nan
10.17	182.9	nan	nan	nan	nan	nan	5.56
12.0	nan	5.67	nan	2.16	nan	2.16	nan
12.08	204.64	nan	nan	nan	nan	nan	7.17
14.0	nan	5.97	nan	1.73	nan	1.73	nan
14.19	224.53	nan	nan	nan	nan	nan	8.37
15.58	233.79	nan	nan	nan	nan	nan	9.09
16.02	nan	6.05	nan	1.48	nan	1.48	nan
17.6	240.99	nan	nan	nan	nan	nan	9.7
17.6	nan	nan	nan	nan	nan	nan	nan
18.07	nan	6.22	nan	1.12	nan	1.12	nan
18.23	245.36	nan	nan	nan	nan	nan	10.13
19.58	253.46	nan	nan	nan	nan	nan	10.99
20.0	nan	7.54	nan	1.01	nan	1.01	nan
20.05	255.9	nan	nan	nan	nan	nan	11.24
21.33	261.17	nan	nan	nan	nan	nan	11.88
22.0	nan	7.26	nan	0.85	nan	0.85	nan
22.17	265.4	nan	nan	nan	nan	nan	12.36
23.2	269.76	nan	nan	nan	nan	nan	13.03
35.42	271.64	nan	nan	nan	nan	nan	14.18
40.67	276.15	nan	nan	nan	nan	nan	16.14
46.67	277.54	nan	nan	nan	nan	nan	18.07
46.85	nan	8.43	nan	nan	nan	nan	nan
47.17	277.83	nan	nan	nan	nan	nan	19.06
52.33	278.12	nan	nan	nan	nan	nan	20.35
55.25	278.81	nan	nan	nan	nan	nan	23.68
68.17	278.88	nan	nan	nan	nan	nan	24.71
69.75	279.07	nan	nan	nan	nan	nan	27.02
71.47	nan	3.86	nan	nan	nan	nan	nan
95.5	nan	3.55	nan	nan	nan	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Male subject 7 (Human #7)

Hours, AurnTCOGTCOH, CALvPPM, CBldTCA, CDCVG_mMole, CTCOH, Cven, TotCTCOH, AurntTCA

0.5	nan	nan	0.11	nan	nan	0.76	nan	nan
0.579	nan	nan	nan	0.00886	nan	nan	nan	nan
1.0	nan	nan	0.36	nan	0.52	0.86	0.52	nan
1.01	nan	nan	nan	0.0349	nan	nan	nan	nan
2.0	nan	nan	1.07	0.0461	1.35	1.15	1.35	nan
3.0	nan	nan	1.55	0.0337	1.87	1.15	1.87	nan
4.0	nan	12.386	2.31	nan	2.5	1.23	2.5	nan
4.02	nan	nan	nan	0.0313	nan	nan	nan	nan
4.24	nan	nan	nan	0.0241	nan	nan	nan	nan
4.25	nan	3.305	2.03	nan	2.59	0.77	2.59	nan
4.5	nan	nan	nan	0.0132	nan	nan	nan	nan
4.53	nan	2.478	2.16	nan	2.58	0.46	2.58	nan

4.67	16.05	nan	nan	nan	nan	nan	nan	1.36
5.0	nan	1.567	2.35	nan	2.25	0.34	2.25	nan
5.01	nan	nan	nan	0.00552	nan	nan	nan	nan
5.05	18.22	nan	nan	nan	nan	nan	nan	1.66
6.0	nan	0.577	2.53	nan	2.15	0.21	2.15	nan
6.02	nan	nan	nan	0.00417	nan	nan	nan	nan
6.3	25.28	nan	nan	nan	nan	nan	nan	2.7
8.0	nan	0.317	3.61	nan	1.98	0.15	1.98	nan
8.01	nan	nan	nan	0.000671	nan	nan	nan	nan
8.05	34.46	nan	nan	nan	nan	nan	nan	4.22
10.0	nan	0.286	3.93	nan	1.56	nan	1.56	nan
10.07	43.49	nan	nan	nan	nan	nan	nan	6.04
12.0	nan	nan	4.57	nan	1.02	nan	1.02	nan
12.07	49.91	nan	nan	nan	nan	nan	nan	8.04
14.0	nan	nan	4.5	nan	1.26	nan	1.26	nan
14.07	55.78	nan	nan	nan	nan	nan	nan	10.37
16.03	nan	nan	5.02	nan	0.89	nan	0.89	nan
16.15	59.33	nan	nan	nan	nan	nan	nan	13.33
18.0	nan	nan	5.1	nan	0.79	nan	0.79	nan
18.08	65.07	nan	nan	nan	nan	nan	nan	16.55
20.0	nan	nan	5.07	nan	0.73	nan	0.73	nan
20.05	68.36	nan	nan	nan	nan	nan	nan	20.04
22.0	nan	nan	5.91	nan	0.7	nan	0.7	nan
22.15	71.48	nan	nan	nan	nan	nan	nan	23.89
25.33	76.1	nan	nan	nan	nan	nan	nan	30.02
31.92	81.25	nan	nan	nan	nan	nan	nan	35.07
35.33	83.82	nan	nan	nan	nan	nan	nan	38.42
43.58	86.11	nan	nan	nan	nan	nan	nan	43.06
51.0	nan	nan	6.38	nan	nan	nan	nan	nan
51.08	87.66	nan	nan	nan	nan	nan	nan	46.65
53.25	88.38	nan	nan	nan	nan	nan	nan	48.88
56.92	89.39	nan	nan	nan	nan	nan	nan	54.83
58.33	89.71	nan	nan	nan	nan	nan	nan	57.31
59.67	89.92	nan	nan	nan	nan	nan	nan	59.49
63.75	89.92	nan	nan	nan	nan	nan	nan	62.36
67.42	90.38	nan	nan	nan	nan	nan	nan	66.44
73.08	91.07	nan	nan	nan	nan	nan	nan	70.15
78.0	91.55	nan	nan	nan	nan	nan	nan	73.57
78.08	nan	nan	5.33	nan	nan	nan	nan	nan
80.58	91.79	nan	nan	nan	nan	nan	nan	75.42
82.75	91.94	nan	nan	nan	nan	nan	nan	77.73
84.25	92.03	nan	nan	nan	nan	nan	nan	78.87
84.92	92.22	nan	nan	nan	nan	nan	nan	80.37
87.58	92.37	nan	nan	nan	nan	nan	nan	83.6
91.83	92.55	nan	nan	nan	nan	nan	nan	86.81
100.83	nan	nan	4.01	nan	nan	nan	nan	nan

TCE Inhalation 101.1 ppm for 4 hours -- Male subject 8 (Human #8)
Hours, AurnTCOGTCOH, CALvPPM, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	0.36	nan	0.28	0.59	0.28	nan
0.579	nan	nan	nan	0.00886	nan	nan	nan	nan
1.0	nan	nan	0.84	nan	0.76	0.85	0.76	nan
1.01	nan	nan	nan	0.0349	nan	nan	nan	nan
2.0	nan	nan	1.73	0.0461	1.92	1.1	1.92	nan
3.0	nan	nan	2.6	0.0337	1.69	1.04	1.69	nan
4.0	nan	21.575	3.42	nan	2.34	1.18	2.34	nan
4.02	nan	nan	nan	0.0313	nan	nan	nan	nan
4.03	nan	14.272	nan	nan	nan	nan	nan	nan
4.05	nan	10.77	nan	nan	nan	nan	nan	nan
4.08	nan	7.056	nan	nan	nan	nan	nan	nan
4.167	nan	5.876	nan	nan	nan	nan	nan	nan
4.24	nan	nan	nan	0.0241	nan	nan	nan	nan
4.3	nan	5.773	3.9	nan	2.34	0.64	2.34	nan
4.5	nan	5.01	3.67	0.0132	2.16	0.42	2.16	nan
4.75	40.71	nan	nan	nan	nan	nan	nan	0.93
5.0	nan	2.498	4.47	nan	2.13	0.19	2.13	nan
5.01	nan	nan	nan	0.00552	nan	nan	nan	nan
6.0	nan	1.713	5.0	nan	1.95	nan	1.95	nan
6.02	nan	nan	nan	0.00417	nan	nan	nan	nan
7.95	69.81	nan	nan	nan	nan	nan	nan	3.02
8.0	nan	1.263	5.95	nan	1.61	nan	1.61	nan

8.01	nan	nan	nan	0.000671	nan	nan	nan	nan
10.0	nan	1.029	6.74	nan	1.33	nan	1.33	nan
12.0	nan	0.936	7.12	nan	1.58	nan	1.58	nan
14.0	nan	0.809	7.75	nan	0.84	nan	0.84	nan
14.08	89.76	nan	nan	nan	nan	nan	nan	5.95
16.0	nan	0.738	8.22	nan	0.77	nan	0.77	nan
16.08	96.8	nan	nan	nan	nan	nan	nan	7.07
18.0	nan	0.683	8.17	nan	0.57	nan	0.57	nan
18.1	102.69	nan	nan	nan	nan	nan	nan	8.28
20.03	nan	nan	9.01	nan	0.76	nan	0.76	nan
20.25	107.93	nan	nan	nan	nan	nan	nan	9.63
24.67	121.3	nan	nan	nan	nan	nan	nan	13.46
29.17	128.51	nan	nan	nan	nan	nan	nan	15.73
32.67	135.51	nan	nan	nan	nan	nan	nan	20.11
35.33	138.05	nan	nan	nan	nan	nan	nan	22.71
38.83	140.2	nan	nan	nan	nan	nan	nan	24.07
44.25	142.48	nan	nan	nan	nan	nan	nan	25.6
49.67	144.47	nan	nan	nan	nan	nan	nan	27.51
49.75	nan	nan	10.66	nan	nan	nan	nan	nan
55.92	144.96	nan	nan	nan	nan	nan	nan	29.6
58.75	145.55	nan	nan	nan	nan	nan	nan	33.36
68.25	146.67	nan	nan	nan	nan	nan	nan	39.61
73.8	nan	nan	8.6	nan	nan	nan	nan	nan
73.83	147.09	nan	nan	nan	nan	nan	nan	43.7
75.92	147.25	nan	nan	nan	nan	nan	nan	45.78
77.92	147.38	nan	nan	nan	nan	nan	nan	48.52
81.17	147.5	nan	nan	nan	nan	nan	nan	51.21
82.58	147.62	nan	nan	nan	nan	nan	nan	53.54
92.17	147.98	nan	nan	nan	nan	nan	nan	60.72
95.24	nan	nan	7.46	nan	nan	nan	nan	nan
264.0	nan	nan	3.13	nan	nan	nan	nan	nan

TCE Inhalation 103.4 ppm for 4 hours -- Male subject 9 (Human #9)
Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, Cven, TotCTCOH, AurntTCA

0.5	nan	0.43	nan	0.47	2.69	0.47	nan
0.579	nan	nan	0.00886	nan	nan	nan	nan
1.0	nan	1.0	nan	0.68	2.98	0.68	nan
1.01	nan	nan	0.0349	nan	nan	nan	nan
2.0	nan	2.15	0.0461	1.51	3.51	1.51	nan
3.0	nan	3.4	0.0337	3.58	3.58	3.58	nan
4.0	nan	4.94	nan	2.72	2.88	2.72	nan
4.02	nan	nan	0.0313	nan	nan	nan	nan
4.24	nan	nan	0.0241	nan	nan	nan	nan
4.25	nan	5.42	nan	2.87	1.96	2.87	nan
4.5	nan	5.67	0.0132	2.77	1.53	2.77	nan
4.58	0.935	nan	nan	nan	nan	nan	40.02
5.01	nan	nan	0.00552	nan	nan	nan	nan
5.03	1.34	nan	nan	nan	nan	nan	40.67
5.75	nan	5.83	nan	2.63	0.81	2.63	nan
6.0	nan	5.99	nan	2.3	0.52	2.3	nan
6.02	nan	nan	0.00417	nan	nan	nan	nan
6.03	4.1	nan	nan	nan	nan	nan	57.48
8.0	nan	7.23	nan	1.9	0.32	1.9	nan
8.01	nan	nan	0.000671	nan	nan	nan	nan
8.05	6.1	nan	nan	nan	nan	nan	76.6
10.0	nan	7.96	nan	1.59	0.27	1.59	nan
10.03	9.74	nan	nan	nan	nan	nan	99.19
12.0	nan	8.14	nan	1.28	0.24	1.28	nan
12.03	13.29	nan	nan	nan	nan	nan	115.98
14.0	nan	8.39	nan	1.23	0.22	1.23	nan
14.07	16.29	nan	nan	nan	nan	nan	126.0
16.0	nan	8.36	nan	1.06	0.22	1.06	nan
16.05	20.29	nan	nan	nan	nan	nan	136.55
18.0	nan	8.83	nan	0.98	0.2	0.98	nan
18.03	22.87	nan	nan	nan	nan	nan	143.51
20.0	nan	8.96	nan	0.72	0.16	0.72	nan
20.02	24.83	nan	nan	nan	nan	nan	150.54
22.0	nan	9.51	nan	0.71	0.16	0.71	nan
22.08	29.98	nan	nan	nan	nan	nan	163.57
44.98	nan	10.75	nan	nan	nan	nan	nan
45.42	56.81	nan	nan	nan	nan	nan	196.37

47.42	61.82	nan	nan	nan	nan	nan	197.62
48.92	64.84	nan	nan	nan	nan	nan	198.48
50.42	67.02	nan	nan	nan	nan	nan	199.33
53.92	74.27	nan	nan	nan	nan	nan	201.12
57.33	76.87	nan	nan	nan	nan	nan	201.12
59.17	78.68	nan	nan	nan	nan	nan	201.73
60.92	61.05	nan	nan	nan	nan	nan	202.15
63.92	88.53	nan	nan	nan	nan	nan	202.88
67.92	90.31	nan	nan	nan	nan	nan	203.6
68.9	nan	9.21	nan	nan	nan	nan	nan
74.58	92.43	nan	nan	nan	nan	nan	204.11
80.25	95.17	nan	nan	nan	nan	nan	204.47
82.42	97.12	nan	nan	nan	nan	nan	204.92
84.33	100.02	nan	nan	nan	nan	nan	205.07
85.58	100.76	nan	nan	nan	nan	nan	205.15
86.92	103.23	nan	nan	nan	nan	nan	205.3
93.08	nan	7.94	nan	nan	nan	nan	nan
264.0	nan	1.94	nan	nan	nan	nan	nan

TCE Inhalation 55.1 ppm for 4 hours -- Female subject 1 (Human #10)
Hours, AurnTCOGTCOH, CBldTCA, CTCOH, CVen, TotCTCOH, AurntTCA

0.58	nan	0.16	0.32	1.0	0.32	nan
1.02	nan	0.46	0.49	1.29	0.49	nan
2.0	nan	1.15	0.85	1.38	0.85	nan
3.0	nan	1.53	0.97	1.7	0.97	nan
4.0	nan	1.9	1.2	1.72	1.2	nan
4.25	nan	2.1	1.14	1.08	1.14	nan
4.47	nan	2.18	1.18	1.17	1.18	nan
4.58	20.08	nan	nan	nan	nan	0.64
5.0	nan	2.13	1.13	0.55	1.13	nan
5.26	22.91	nan	nan	nan	nan	0.76
6.0	nan	2.56	nan	0.39	nan	nan
6.12	24.87	nan	nan	nan	nan	0.85
8.03	nan	3.32	nan	0.22	nan	nan
8.12	28.94	nan	nan	nan	nan	1.83
9.98	nan	2.83	0.7	nan	0.7	nan
10.18	36.46	nan	nan	nan	nan	2.57
12.0	nan	2.98	0.6	nan	0.6	nan
12.18	39.14	nan	nan	nan	nan	3.36
14.02	nan	3.42	0.52	nan	0.52	nan
14.32	42.64	nan	nan	nan	nan	3.94
16.0	nan	3.44	0.55	nan	0.55	nan
16.18	45.16	nan	nan	nan	nan	5.12
18.03	nan	3.31	0.54	nan	0.54	nan
18.16	53.64	nan	nan	nan	nan	6.03
20.0	nan	4.15	0.45	nan	0.45	nan
20.25	56.34	nan	nan	nan	nan	6.67
22.0	nan	4.07	0.35	nan	0.35	nan
22.53	57.08	nan	nan	nan	nan	7.3
23.25	57.64	nan	nan	nan	nan	7.6
25.25	58.45	nan	nan	nan	nan	7.96
27.58	60.33	nan	nan	nan	nan	8.6
29.5	61.44	nan	nan	nan	nan	8.89
30.92	62.83	nan	nan	nan	nan	9.21
32.92	67.36	nan	nan	nan	nan	9.86
35.0	68.3	nan	nan	nan	nan	9.66
39.83	69.92	nan	nan	nan	nan	11.19
42.0	70.88	nan	nan	nan	nan	11.85
43.08	71.09	nan	nan	nan	nan	12.35
44.33	nan	3.7	nan	nan	nan	nan
44.72	71.59	nan	nan	nan	nan	12.73
46.5	71.99	nan	nan	nan	nan	13.49
49.83	72.6	nan	nan	nan	nan	14.31
52.0	73.6	nan	nan	nan	nan	15.73
53.59	73.93	nan	nan	nan	nan	16.12
54.53	74.27	nan	nan	nan	nan	16.34
56.83	74.26	nan	nan	nan	nan	16.93
58.5	74.56	nan	nan	nan	nan	17.24
59.25	74.71	nan	nan	nan	nan	17.85
63.83	74.77	nan	nan	nan	nan	18.13
68.28	75.16	nan	nan	nan	nan	18.53

68.32	nan	nan	nan	nan	nan	nan
70.67	75.34	nan	nan	nan	nan	19.18
72.78	75.52	nan	nan	nan	nan	19.42
74.75	75.75	nan	nan	nan	nan	20.0
76.92	75.81	nan	nan	nan	nan	20.58
80.33	76.05	nan	nan	nan	nan	20.79
81.5	76.06	nan	nan	nan	nan	20.93
82.42	76.12	nan	nan	nan	nan	21.82
83.5	76.15	nan	nan	nan	nan	21.37
90.25	76.3	nan	nan	nan	nan	21.56
91.42	76.34	nan	nan	nan	nan	21.69
92.33	76.39	nan	nan	nan	nan	21.87
93.38	nan	1.02	nan	nan	nan	nan

TCE Inhalation 101.4 ppm for 4 hours -- Female subject 1 (Human #10)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	nan	nan	1.18	nan	nan
0.51	nan	nan	0.0032	nan	nan	nan	nan
0.985	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	nan	nan	0.74	2.17	0.74	nan
1.99	nan	nan	0.0106	nan	nan	nan	nan
2.0	nan	0.91	nan	1.38	2.3	1.38	nan
2.96	nan	nan	0.0127	nan	nan	nan	nan
3.0	nan	1.75	nan	1.93	2.41	1.93	nan
4.0	nan	2.65	nan	2.41	2.65	2.41	nan
4.02	nan	nan	0.0133	nan	nan	nan	nan
4.23	nan	2.54	0.0087	2.4	1.84	2.4	nan
4.37	35.78	nan	nan	nan	nan	nan	0.31
4.5	nan	2.65	nan	2.33	1.17	2.33	nan
4.52	nan	nan	0.00508	nan	nan	nan	nan
5.0	nan	2.73	nan	2.17	0.62	2.17	nan
5.01	nan	nan	0.00229	nan	nan	nan	nan
5.03	44.4	nan	nan	nan	nan	nan	0.39
6.0	nan	3.26	nan	1.94	0.38	1.94	nan
6.03	nan	nan	0.00074	nan	nan	nan	nan
6.1	54.4	nan	nan	nan	nan	nan	0.64
8.05	nan	3.58	nan	1.81	nan	1.81	nan
8.1	72.58	nan	nan	nan	nan	nan	1.21
10.0	nan	4.5	nan	1.38	nan	1.38	nan
10.07	90.61	nan	nan	nan	nan	nan	1.66
12.0	nan	4.02	nan	1.17	nan	1.17	nan
12.03	104.44	nan	nan	nan	nan	nan	2.16
14.02	nan	4.17	nan	1.25	nan	1.25	nan
14.1	116.9	nan	nan	nan	nan	nan	2.96
16.0	nan	4.45	nan	1.01	nan	1.01	nan
16.05	127.49	nan	nan	nan	nan	nan	3.66
18.0	nan	4.9	nan	0.88	nan	0.88	nan
18.05	127.49	nan	nan	nan	nan	nan	4.37
20.0	nan	5.26	nan	0.74	nan	0.74	nan
20.06	136.49	nan	nan	nan	nan	nan	5.44
22.02	nan	5.94	nan	0.7	nan	0.7	nan
22.15	144.45	nan	nan	nan	nan	nan	6.66
24.32	147.89	nan	nan	nan	nan	nan	7.63
27.05	150.61	nan	nan	nan	nan	nan	8.16
28.3	154.52	nan	nan	nan	nan	nan	8.71
30.1	157.72	nan	nan	nan	nan	nan	10.3
32.45	160.74	nan	nan	nan	nan	nan	10.92
34.2	163.47	nan	nan	nan	nan	nan	11.77
36.1	165.86	nan	nan	nan	nan	nan	12.45
43.2	167.54	nan	nan	nan	nan	nan	13.71
45.4	168.21	nan	nan	nan	nan	nan	14.04
46.7	nan	6.68	nan	nan	nan	nan	nan
48.0	169.24	nan	nan	nan	nan	nan	15.07
51.4	170.26	nan	nan	nan	nan	nan	15.98
54.05	171.66	nan	nan	nan	nan	nan	16.51
56.4	172.85	nan	nan	nan	nan	nan	17.0
58.2	173.7	nan	nan	nan	nan	nan	17.6
59.55	175.02	nan	nan	nan	nan	nan	19.57
67.55	175.31	nan	nan	nan	nan	nan	19.76
70.2	175.67	nan	nan	nan	nan	nan	20.25
70.25	nan	5.2	nan	nan	nan	nan	nan

72.2	176.21	nan	nan	nan	nan	nan	21.31
75.0	176.6	nan	nan	nan	nan	nan	22.08
77.55	177.07	nan	nan	nan	nan	nan	22.65
81.55	178.04	nan	nan	nan	nan	nan	24.79
84.1	178.43	nan	nan	nan	nan	nan	30.86
89.1	178.65	nan	nan	nan	nan	nan	31.05
91.35	178.94	nan	nan	nan	nan	nan	31.06
93.72	nan	3.6	nan	nan	nan	nan	nan

TCE Inhalation 53.0 ppm for 4 hours -- Female subject 2 (Human #11)
Hours, AurnTCOGTCOH, CBldTCA, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	nan	0.93	nan	nan	
1.0	nan	0.38	0.33	1.33	0.33	nan	
2.0	nan	1.23	0.63	1.65	0.63	nan	
3.0	nan	1.96	0.79	1.85	0.79	nan	
4.0	nan	2.8	0.98	1.45	0.98	nan	
4.27	nan	2.81	0.83	0.94	0.83	nan	
4.55	nan	3.23	0.83	0.63	0.83	nan	
5.1	nan	3.34	0.9	0.32	0.9	nan	
5.25	4.42	nan	nan	nan	nan	1.35	
5.97	6.71	nan	nan	nan	nan	4.49	
6.0	nan	3.72	0.89	0.18	0.89	nan	
8.0	12.0	4.88	0.76	nan	0.76	7.17	
10.0	nan	4.93	0.66	nan	0.66	nan	
10.17	15.4	nan	nan	nan	nan	9.38	
12.0	nan	5.28	0.67	nan	0.67	nan	
12.17	16.73	nan	nan	nan	nan	10.36	
14.0	nan	5.18	0.54	nan	0.54	nan	
14.17	20.35	nan	nan	nan	nan	11.91	
16.05	nan	5.37	0.48	nan	0.48	nan	
16.17	23.49	nan	nan	nan	nan	13.46	
18.0	nan	6.03	0.47	nan	0.47	nan	
18.17	25.44	nan	nan	nan	nan	14.7	
20.02	nan	4.87	nan	nan	0.35	nan	
20.17	25.44	nan	nan	nan	nan	15.64	
22.0	nan	6.66	0.35	nan	nan	nan	
22.17	26.96	nan	nan	nan	nan	16.49	
25.0	30.55	nan	nan	nan	nan	22.11	
29.83	32.71	nan	nan	nan	nan	23.27	
37.83	34.38	nan	nan	nan	nan	26.03	
44.83	34.88	nan	nan	nan	nan	27.35	
44.92	nan	6.66	nan	nan	nan	nan	
49.67	37.25	nan	nan	nan	nan	33.94	
53.33	38.53	nan	nan	nan	nan	35.83	
61.23	41.16	nan	nan	nan	nan	42.58	
62.83	41.38	nan	nan	nan	nan	43.36	
67.92	43.01	nan	nan	nan	nan	50.68	
68.86	nan	5.27	nan	nan	nan	nan	
75.75	43.29	nan	nan	nan	nan	52.36	
79.63	43.53	nan	nan	nan	nan	53.79	
96.67	43.66	nan	nan	nan	nan	54.16	
96.92	43.85	nan	nan	nan	nan	55.93	
100.44	nan	2.27	nan	nan	nan	nan	

TCE Inhalation 97.7 ppm for 4 hours -- Female subject 2 (Human #11)

Hours, AurnTCOGTCOH, CALVPPM, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	0.44	nan	nan	0.83	nan	nan
0.51	nan	nan	nan	0.0032	nan	nan	nan	nan
0.985	nan	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	nan	0.97	nan	nan	0.99	nan	nan
1.99	nan	nan	nan	0.0106	nan	nan	nan	nan
2.03	nan	nan	2.16	nan	0.53	1.2	0.53	nan
2.96	nan	nan	nan	0.0127	nan	nan	nan	nan
3.0	nan	nan	3.79	nan	0.83	1.59	0.83	nan
4.02	nan	nan	nan	0.0133	nan	nan	nan	nan
4.03	nan	22.398	5.12	nan	1.27	2.03	1.27	nan
4.23	nan	nan	nan	0.0087	nan	nan	nan	nan
4.25	nan	7.317	5.35	nan	0.92	1.33	0.92	nan
4.5	nan	5.917	5.6	nan	0.85	0.87	0.85	nan
4.52	nan	nan	nan	0.00508	nan	nan	nan	nan
4.55	11.67	nan	nan	nan	nan	nan	nan	0.3

5.0	nan	2.903	5.88	nan	1.17	0.42	1.17	nan
5.01	nan	nan	nan	0.00229	nan	nan	nan	nan
5.12	14.56	nan	nan	nan	nan	nan	nan	0.56
6.0	nan	1.382	6.55	nan	1.03	0.21	1.03	nan
6.03	nan	nan	nan	0.00074	nan	nan	nan	nan
6.08	20.78	nan	nan	nan	nan	nan	nan	1.75
8.0	nan	0.982	7.3	nan	0.86	0.22	0.86	nan
8.19	25.55	nan	nan	nan	nan	nan	nan	1.97
10.0	nan	0.691	7.66	nan	0.8	0.15	0.8	nan
10.19	34.83	nan	nan	nan	nan	nan	nan	3.75
12.0	nan	0.524	8.61	nan	0.71	nan	0.71	nan
12.17	45.33	nan	nan	nan	nan	nan	nan	6.58
14.03	nan	0.428	8.73	nan	0.62	nan	0.62	nan
14.33	45.98	nan	nan	nan	nan	nan	nan	6.81
16.03	nan	nan	9.65	nan	0.55	nan	0.55	nan
16.23	54.21	nan	nan	nan	nan	nan	nan	8.64
18.07	nan	nan	8.29	nan	0.48	nan	0.48	nan
18.19	60.91	nan	nan	nan	nan	nan	nan	10.3
20.0	nan	nan	8.6	nan	0.41	nan	0.41	nan
20.13	68.01	nan	nan	nan	nan	nan	nan	12.13
22.0	nan	nan	10.2	nan	nan	nan	nan	nan
22.38	73.35	nan	nan	nan	nan	nan	nan	13.64
31.92	75.14	nan	nan	nan	nan	nan	nan	15.77
34.25	79.52	nan	nan	nan	nan	nan	nan	18.03
36.92	79.97	nan	nan	nan	nan	nan	nan	18.16
47.95	nan	nan	6.15	nan	nan	nan	nan	nan
48.67	85.95	nan	nan	nan	nan	nan	nan	22.69
55.83	90.84	nan	nan	nan	nan	nan	nan	28.52
59.0	91.82	nan	nan	nan	nan	nan	nan	30.85
63.5	92.13	nan	nan	nan	nan	nan	nan	31.36
70.8	92.13	nan	nan	nan	nan	nan	nan	33.88
71.98	nan	nan	7.11	nan	nan	nan	nan	nan
76.0	95.09	nan	nan	nan	nan	nan	nan	37.2
85.5	96.05	nan	nan	nan	nan	nan	nan	41.32
87.25	96.34	nan	nan	nan	nan	nan	nan	42.86
88.08	96.45	nan	nan	nan	nan	nan	nan	49.42
94.75	97.45	nan	nan	nan	nan	nan	nan	54.14
101.22	nan	nan	6.73	nan	nan	nan	nan	nan

TCE Inhalation 102.5 ppm for 4 hours -- Female subject 3 (Human #12)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	0.21	nan	0.22	1.11	0.22	nan
0.51	nan	nan	0.0032	nan	nan	nan	nan
0.985	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	0.39	nan	0.46	1.36	0.46	nan
1.99	nan	nan	0.0106	nan	nan	nan	nan
2.0	nan	1.05	nan	1.18	2.11	1.18	nan
2.96	nan	nan	0.0127	nan	nan	nan	nan
3.0	nan	1.86	nan	2.18	1.92	2.18	nan
4.0	nan	3.46	nan	3.03	2.3	3.03	nan
4.02	nan	nan	0.0133	nan	nan	nan	nan
4.23	nan	nan	0.0087	nan	nan	nan	nan
4.25	nan	3.78	nan	3.29	1.56	3.29	nan
4.5	nan	3.91	nan	3.67	1.26	3.67	nan
4.52	nan	nan	0.00508	nan	nan	nan	nan
4.62	44.83	nan	nan	nan	nan	nan	0.51
5.0	nan	4.22	nan	3.13	0.73	3.13	nan
5.01	nan	nan	0.00229	nan	nan	nan	nan
5.08	52.08	nan	nan	nan	nan	nan	0.65
6.0	nan	4.67	nan	2.57	0.42	2.57	nan
6.03	nan	nan	0.00074	nan	nan	nan	nan
6.86	77.84	nan	nan	nan	nan	nan	1.26
8.0	nan	5.71	nan	2.46	nan	2.46	nan
8.33	89.76	nan	nan	nan	nan	nan	1.85
10.0	nan	6.29	nan	1.93	nan	1.93	nan
10.25	108.58	nan	nan	nan	nan	nan	2.92
12.0	nan	7.76	nan	1.57	nan	1.57	nan
12.13	122.65	nan	nan	nan	nan	nan	3.91
14.0	nan	7.78	nan	1.3	nan	1.3	nan
14.08	133.38	nan	nan	nan	nan	nan	4.92
16.05	nan	8.11	nan	1.08	nan	1.08	nan

16.15	140.85	nan	nan	nan	nan	nan	5.91
18.0	147.19	8.79	nan	0.89	nan	0.89	5.91
20.02	nan	9.05	nan	0.56	nan	0.56	nan
20.05	151.76	nan	nan	nan	nan	nan	7.12
22.02	nan	9.34	nan	0.65	nan	0.65	nan
22.17	155.86	nan	nan	nan	nan	nan	9.55
30.67	169.38	nan	nan	nan	nan	nan	15.22
33.67	174.67	nan	nan	nan	nan	nan	17.85
35.42	175.78	nan	nan	nan	nan	nan	19.66
40.67	179.31	nan	nan	nan	nan	nan	24.08
46.17	nan	9.58	nan	0.3	nan	0.3	nan
46.67	179.77	nan	nan	nan	nan	nan	26.68
47.17	179.97	nan	nan	nan	nan	nan	27.91
52.33	180.44	nan	nan	nan	nan	nan	30.49
55.25	181.52	nan	nan	nan	nan	nan	35.74
68.17	184.09	nan	nan	nan	nan	nan	35.75
69.75	184.16	nan	nan	nan	nan	nan	36.78
69.83	nan	7.93	nan	nan	nan	nan	nan
73.92	184.26	nan	nan	nan	nan	nan	37.71
76.0	184.7	nan	nan	nan	nan	nan	41.25
78.17	185.2	nan	nan	nan	nan	nan	45.21
80.33	185.35	nan	nan	nan	nan	nan	46.43
81.5	185.42	nan	nan	nan	nan	nan	47.22
82.25	185.51	nan	nan	nan	nan	nan	47.91
92.58	185.81	nan	nan	nan	nan	nan	49.66
93.67	185.91	nan	nan	nan	nan	nan	50.98
94.17	185.95	nan	nan	nan	nan	nan	51.67
94.67	nan	6.69	nan	nan	nan	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Female subject 4 (Human #13)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.51	nan	nan	0.0032	nan	nan	nan	nan
0.58	nan	0.4	nan	0.33	0.81	0.33	nan
0.985	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	0.97	nan	0.57	0.88	0.57	nan
1.99	nan	nan	0.0106	nan	nan	nan	nan
2.0	nan	1.72	nan	1.01	1.09	1.01	nan
2.96	nan	nan	0.0127	nan	nan	nan	nan
3.0	nan	2.64	nan	1.25	1.03	1.25	nan
4.0	nan	3.41	nan	1.79	1.13	1.79	nan
4.02	nan	nan	0.0133	nan	nan	nan	nan
4.17	nan	3.62	nan	1.64	0.59	1.64	nan
4.23	nan	nan	0.0087	nan	nan	nan	nan
4.5	nan	3.86	nan	1.54	0.47	1.54	nan
4.52	nan	nan	0.00508	nan	nan	nan	nan
4.58	12.63	nan	nan	nan	nan	nan	0.44
5.0	nan	4.39	nan	1.43	0.3	1.43	nan
5.01	nan	nan	0.00229	nan	nan	nan	nan
6.0	nan	4.8	nan	1.27	0.18	1.27	nan
6.03	17.83	nan	0.00074	nan	nan	nan	0.71
8.02	nan	5.73	nan	0.95	0.15	0.95	nan
8.12	26.05	nan	nan	nan	nan	nan	1.31
10.02	nan	6.79	nan	1.01	nan	1.01	nan
10.08	30.4	nan	nan	nan	nan	nan	2.28
12.02	nan	7.55	nan	0.9	nan	0.9	nan
12.1	36.72	nan	nan	nan	nan	nan	3.48
14.03	nan	7.68	nan	0.88	nan	0.88	nan
14.1	41.26	nan	nan	nan	nan	nan	4.64
16.0	nan	7.98	nan	0.74	nan	0.74	nan
16.05	44.27	nan	nan	nan	nan	nan	5.64
18.0	nan	9.27	nan	0.69	nan	0.69	nan
18.1	47.94	nan	nan	nan	nan	nan	6.76
20.0	nan	8.91	nan	0.63	nan	0.63	nan
20.05	50.31	nan	nan	nan	nan	nan	7.66
21.92	53.17	nan	nan	nan	nan	nan	8.89
22.0	nan	9.12	nan	0.61	nan	0.61	nan
26.17	57.9	nan	nan	nan	nan	nan	10.64
33.25	65.27	nan	nan	nan	nan	nan	13.81
37.92	65.8	nan	nan	nan	nan	nan	14.11
44.92	69.74	nan	nan	nan	nan	nan	15.44
46.08	nan	11.31	nan	nan	nan	nan	nan

49.0	69.74	nan	nan	nan	nan	nan	16.0
54.92	72.07	nan	nan	nan	nan	nan	23.2
58.42	73.58	nan	nan	nan	nan	nan	22.4
61.42	75.39	nan	nan	nan	nan	nan	24.1
66.42	76.98	nan	nan	nan	nan	nan	29.1
70.67	79.89	nan	nan	nan	nan	nan	32.6
74.75	80.98	nan	nan	nan	nan	nan	36.2
75.67	nan	10.49	nan	nan	nan	nan	nan
80.42	82.2	nan	nan	nan	nan	nan	36.8
82.42	82.57	nan	nan	nan	nan	nan	37.5
84.92	82.74	nan	nan	nan	nan	nan	37.79
93.42	83.41	nan	nan	nan	nan	nan	45.72
94.25	nan	8.47	nan	nan	nan	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Female subject 5 (Human #14)

Hours, AurnTCOGTCOH, CALvPPM, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	nan	0.25	nan	nan	0.74	nan	nan
0.51	nan	nan	nan	0.0032	nan	nan	nan	nan
0.985	nan	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	nan	0.76	nan	0.41	1.0	0.41	nan
1.99	nan	nan	nan	0.0106	nan	nan	nan	nan
2.0	nan	nan	1.48	nan	0.78	1.27	0.78	nan
2.96	nan	nan	nan	0.0127	nan	nan	nan	nan
3.0	nan	nan	2.21	nan	1.04	1.45	1.04	nan
4.0	nan	nan	2.79	nan	1.18	1.19	1.18	nan
4.02	nan	nan	nan	0.0133	nan	nan	nan	nan
4.23	nan	nan	nan	0.0087	nan	nan	nan	nan
4.25	nan	4.243	2.78	nan	1.17	0.81	1.17	nan
4.52	nan	nan	nan	0.00508	nan	nan	nan	nan
4.55	nan	2.798	3.12	nan	1.18	0.66	1.18	nan
4.67	9.98	nan	nan	nan	nan	nan	nan	0.69
5.0	9.98	nan	nan	nan	nan	nan	nan	0.8
5.0	nan	1.849	3.23	nan	1.18	0.46	1.18	nan
5.01	nan	nan	nan	0.00229	nan	nan	nan	nan
6.02	nan	1.467	3.52	nan	nan	0.25	nan	nan
6.03	nan	nan	nan	0.00074	nan	nan	nan	nan
6.3	12.41	nan	nan	nan	nan	nan	nan	1.64
8.02	nan	0.681	4.76	nan	0.84	0.19	0.84	nan
8.08	16.09	nan	nan	nan	nan	nan	nan	3.16
10.0	nan	0.452	4.95	nan	0.72	nan	0.72	nan
10.08	18.99	nan	nan	nan	nan	nan	nan	4.95
12.0	nan	0.409	5.29	nan	0.82	nan	0.82	nan
12.07	20.96	nan	nan	nan	nan	nan	nan	7.19
14.0	nan	0.356	5.33	nan	0.56	nan	0.56	nan
14.08	23.08	nan	nan	nan	nan	nan	nan	9.89
16.12	24.46	nan	nan	nan	nan	nan	nan	13.14
18.02	nan	nan	6.46	nan	0.49	nan	0.49	nan
18.11	26.22	nan	nan	nan	nan	nan	nan	17.46
20.0	nan	nan	6.91	nan	0.41	nan	0.41	nan
20.1	27.92	nan	nan	nan	nan	nan	nan	21.67
22.0	nan	nan	7.1	nan	nan	nan	nan	nan
22.12	29.05	nan	nan	nan	nan	nan	nan	26.4
22.67	29.64	nan	nan	nan	nan	nan	nan	29.05
26.5	32.31	nan	nan	nan	nan	nan	nan	35.18
29.67	34.4	nan	nan	nan	nan	nan	nan	41.73
34.17	36.58	nan	nan	nan	nan	nan	nan	49.36
35.67	37.14	nan	nan	nan	nan	nan	nan	50.76
40.67	38.8	nan	nan	nan	nan	nan	nan	56.47
43.67	39.86	nan	nan	nan	nan	nan	nan	60.68
46.58	nan	nan	6.63	nan	nan	nan	nan	nan
47.17	40.61	nan	nan	nan	nan	nan	nan	69.0
49.67	41.58	nan	nan	nan	nan	nan	nan	73.32
53.42	42.31	nan	nan	nan	nan	nan	nan	76.81
56.17	42.94	nan	nan	nan	nan	nan	nan	79.16
58.0	43.3	nan	nan	nan	nan	nan	nan	81.7
59.67	43.53	nan	nan	nan	nan	nan	nan	83.84
60.17	43.6	nan	nan	nan	nan	nan	nan	84.56
61.67	43.78	nan	nan	nan	nan	nan	nan	86.11
67.67	44.79	nan	nan	nan	nan	nan	nan	91.59
70.5	nan	nan	5.28	nan	nan	nan	nan	nan
72.67	45.19	nan	nan	nan	nan	nan	nan	95.63

76.67	45.69	nan	nan	nan	nan	nan	nan	100.35
82.67	46.42	nan	nan	nan	nan	nan	nan	110.14
84.17	46.54	nan	nan	nan	nan	nan	nan	111.45
85.67	46.6	nan	nan	nan	nan	nan	nan	112.62
91.67	47.13	nan	nan	nan	nan	nan	nan	115.92

TCE Inhalation 101.0 ppm for 4 hours -- Female subject 6 (Human #15)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.51	nan	nan	0.0032	nan	nan	nan	nan
0.52	nan	0.39	nan	0.35	0.53	0.35	nan
0.985	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	1.08	nan	0.58	1.0	0.58	nan
1.99	nan	nan	0.0106	nan	nan	nan	nan
2.0	nan	1.9	nan	0.86	0.97	0.86	nan
2.96	nan	nan	0.0127	nan	nan	nan	nan
3.0	nan	3.83	nan	1.6	1.31	1.6	nan
4.0	nan	4.48	nan	2.03	1.48	2.03	nan
4.02	nan	nan	0.0133	nan	nan	nan	nan
4.23	nan	nan	0.0087	nan	nan	nan	nan
4.28	nan	4.65	nan	2.04	0.84	2.04	nan
4.5	nan	4.8	nan	1.93	0.58	1.93	nan
4.52	nan	nan	0.00508	nan	nan	nan	nan
4.67	37.76	nan	nan	nan	nan	nan	2.51
5.0	nan	4.73	nan	1.95	0.39	1.95	nan
5.01	nan	nan	0.00229	nan	nan	nan	nan
5.17	42.18	nan	nan	nan	nan	nan	3.07
6.03	nan	nan	0.00074	nan	nan	nan	nan
6.05	nan	6.02	nan	1.79	nan	1.79	nan
6.25	48.68	nan	nan	nan	nan	nan	6.21
8.0	nan	6.02	nan	1.29	nan	1.29	nan
8.08	60.91	nan	nan	nan	nan	nan	9.97
10.0	nan	7.12	nan	1.14	nan	1.14	nan
10.13	72.32	nan	nan	nan	nan	nan	13.01
12.0	nan	7.13	nan	1.03	nan	1.03	nan
12.08	81.05	nan	nan	nan	nan	nan	16.35
14.12	86.76	nan	nan	nan	nan	nan	20.65
16.02	94.78	nan	nan	nan	nan	nan	23.23
18.02	100.92	nan	nan	nan	nan	nan	26.31
20.17	105.91	nan	nan	nan	nan	nan	26.31
25.27	115.12	nan	nan	nan	nan	nan	34.28
25.75	116.22	nan	nan	nan	nan	nan	34.84
30.0	125.29	nan	nan	nan	nan	nan	42.19
34.5	131.36	nan	nan	nan	nan	nan	51.62
37.92	135.91	nan	nan	nan	nan	nan	61.19
45.08	143.62	nan	nan	nan	nan	nan	75.52
46.75	nan	9.1	nan	nan	nan	nan	nan
49.33	146.34	nan	nan	nan	nan	nan	81.43
56.92	149.7	nan	nan	nan	nan	nan	92.21
60.42	151.17	nan	nan	nan	nan	nan	104.12
68.33	153.38	nan	nan	nan	nan	nan	116.32
72.58	154.28	nan	nan	nan	nan	nan	121.17
73.97	nan	6.92	nan	nan	nan	nan	nan
80.5	155.7	nan	nan	nan	nan	nan	131.94
84.33	155.93	nan	nan	nan	nan	nan	134.71
86.17	156.09	nan	nan	nan	nan	nan	136.09
93.5	156.7	nan	nan	nan	nan	nan	142.3
95.42	nan	6.14	nan	nan	nan	nan	nan

TCE Inhalation 103.3 ppm for 4 hours -- Female subject 7 (Human #16)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, CVen, TotCTCOH, AurntTCA

0.5	nan	0.27	nan	0.47	1.32	0.47	nan
0.51	nan	nan	0.0032	nan	nan	nan	nan
0.985	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	0.7	nan	0.68	1.68	0.68	nan
1.99	nan	nan	0.0106	nan	nan	nan	nan
2.0	nan	1.48	nan	1.51	1.86	1.51	nan
2.96	nan	nan	0.0127	nan	nan	nan	nan
3.0	nan	2.8	nan	2.15	2.37	2.15	nan
4.0	nan	3.92	nan	2.72	2.66	2.72	nan
4.02	nan	nan	0.0133	nan	nan	nan	nan
4.23	nan	nan	0.0087	nan	nan	nan	nan

4.25	nan	3.86	nan	2.87	2.1	2.87	nan
4.5	nan	3.98	nan	2.77	1.23	2.77	nan
4.52	nan	nan	0.00508	nan	nan	nan	nan
4.58	15.54	nan	nan	nan	nan	nan	2.34
5.0	nan	4.55	nan	2.63	0.83	2.63	nan
5.01	nan	nan	0.00229	nan	nan	nan	nan
5.05	18.22	nan	nan	nan	nan	nan	2.92
6.0	nan	4.8	nan	2.3	0.42	2.3	nan
6.03	nan	nan	0.00074	nan	nan	nan	nan
6.05	24.58	nan	nan	nan	nan	nan	5.27
8.05	nan	5.96	nan	1.9	0.33	1.9	nan
8.08	33.76	nan	nan	nan	nan	nan	8.33
10.03	nan	6.09	nan	1.59	0.3	1.59	nan
10.07	41.25	nan	nan	nan	nan	nan	12.15
12.05	nan	6.41	nan	1.28	nan	1.28	nan
12.08	47.8	nan	nan	nan	nan	nan	17.02
14.02	nan	7.01	nan	1.23	nan	1.23	nan
14.31	54.36	nan	nan	nan	nan	nan	21.46
16.0	nan	7.23	nan	1.1	nan	1.1	nan
16.05	59.99	nan	nan	nan	nan	nan	26.02
18.0	nan	7.57	nan	0.98	nan	0.98	nan
18.05	63.23	nan	nan	nan	nan	nan	28.88
20.0	nan	7.68	nan	0.72	nan	0.72	nan
20.03	68.23	nan	nan	nan	nan	nan	32.6
22.0	nan	8.46	nan	0.71	nan	0.71	nan
22.08	73.9	nan	nan	nan	nan	nan	37.96
43.33	110.18	nan	nan	nan	nan	nan	80.45
45.03	nan	8.75	nan	nan	nan	nan	nan
45.58	112.61	nan	nan	nan	nan	nan	85.25
47.58	113.7	nan	nan	nan	nan	nan	87.93
49.17	115.14	nan	nan	nan	nan	nan	91.55
53.58	118.2	nan	nan	nan	nan	nan	99.63
61.33	122.07	nan	nan	nan	nan	nan	110.21
67.33	124.3	nan	nan	nan	nan	nan	114.43
69.03	nan	7.73	nan	nan	nan	nan	nan
70.58	125.29	nan	nan	nan	nan	nan	118.52
74.58	126.29	nan	nan	nan	nan	nan	123.23
77.25	127.48	nan	nan	nan	nan	nan	128.78
83.25	128.07	nan	nan	nan	nan	nan	133.51
84.25	128.31	nan	nan	nan	nan	nan	134.95
85.17	128.49	nan	nan	nan	nan	nan	136.29
90.5	129.56	nan	nan	nan	nan	nan	143.83
93.13	nan	5.72	nan	nan	nan	nan	nan
264.0	nan	0.53	nan	nan	nan	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Female subject 8 (Human #17)

Hours, AurnTCOGTCOH, CBldTCA, CDCVG_mMole, CTCOH, Cven, TotCTCOH, AurntTCA

0.51	nan	nan	0.0032	nan	nan	nan	nan
0.55	nan	0.47	nan	nan	0.55	nan	nan
0.985	nan	nan	0.00868	nan	nan	nan	nan
1.0	nan	1.05	nan	0.39	0.81	0.39	nan
1.99	nan	nan	0.0106	nan	nan	nan	nan
2.12	nan	2.73	nan	1.2	1.3	1.2	nan
2.33	4.52	nan	nan	nan	nan	nan	0.29
2.96	nan	nan	0.0127	nan	nan	nan	nan
3.05	nan	3.85	nan	1.59	1.37	1.59	nan
4.0	nan	4.82	nan	1.93	1.43	1.93	nan
4.02	nan	nan	0.0133	nan	nan	nan	nan
4.23	nan	nan	0.0087	nan	nan	nan	nan
4.25	nan	5.02	nan	1.97	0.81	1.97	nan
4.5	nan	5.29	nan	1.75	0.54	1.75	nan
4.52	nan	nan	0.00508	nan	nan	nan	nan
4.57	8.37	nan	nan	nan	nan	nan	1.62
5.0	nan	5.37	nan	1.63	0.35	1.63	nan
5.01	nan	nan	0.00229	nan	nan	nan	nan
5.12	12.49	nan	nan	nan	nan	nan	2.09
6.0	nan	6.01	nan	1.32	0.18	1.32	nan
6.03	nan	nan	0.00074	nan	nan	nan	nan
6.12	19.46	nan	nan	nan	nan	nan	4.01
8.05	nan	7.6	nan	1.1	nan	1.1	nan
8.12	29.26	nan	nan	nan	nan	nan	5.81

10.08	nan	6.77	nan	0.91	nan	0.91	nan
10.33	35.93	nan	nan	nan	nan	nan	8.27
12.08	40.21	nan	nan	nan	nan	nan	10.21
14.03	nan	8.65	nan	0.83	nan	0.83	nan
14.12	44.9	nan	nan	nan	nan	nan	13.06
16.0	48.15	nan	nan	nan	nan	nan	16.29
18.02	nan	9.49	nan	0.69	nan	0.69	nan
18.08	51.04	nan	nan	nan	nan	nan	19.09
20.0	55.72	nan	nan	nan	nan	nan	21.96
21.92	58.76	nan	nan	nan	nan	nan	24.17
22.02	nan	10.64	nan	0.54	nan	0.54	nan
25.08	60.75	nan	nan	nan	nan	nan	27.09
29.25	62.24	nan	nan	nan	nan	nan	29.05
32.58	72.07	nan	nan	nan	nan	nan	35.13
35.83	76.15	nan	nan	nan	nan	nan	45.84
38.33	79.24	nan	nan	nan	nan	nan	56.12
41.0	81.48	nan	nan	nan	nan	nan	65.21
45.0	83.84	nan	nan	nan	nan	nan	75.98
46.08	nan	9.58	nan	nan	nan	nan	nan
48.83	86.37	nan	nan	nan	nan	nan	81.05
50.33	87.44	nan	nan	nan	nan	nan	83.74
53.67	88.84	nan	nan	nan	nan	nan	87.89
56.33	90.9	nan	nan	nan	nan	nan	91.72
59.33	92.91	nan	nan	nan	nan	nan	97.13
66.83	94.07	nan	nan	nan	nan	nan	100.34
73.25	94.96	nan	nan	nan	nan	nan	102.88
75.67	nan	8.55	nan	nan	nan	nan	nan
80.58	96.17	nan	nan	nan	nan	nan	106.5
83.5	96.82	nan	nan	nan	nan	nan	110.02
86.0	97.41	nan	nan	nan	nan	nan	113.61
93.0	98.54	nan	nan	nan	nan	nan	117.51
94.25	nan	7.82	nan	nan	nan	nan	nan

Kimmerle and Eben, 1973

TCE Inhalation 40.0 ppm for 4 hours - female #1 (Human #21)

Hours, AurnTCOGTCOH, AurnTCOGTCOH_Coll, CTCOH, CVen, AurnTCA, AurnTCA_Coll

4.0	12.046	nan	0.706	0.196	1.32	nan
5.0	nan	nan	0.693	0.104	nan	nan
6.0	nan	nan	0.614	0.078	nan	nan
7.0	nan	nan	0.574	nan	nan	nan
8.0	15.644	nan	0.602	nan	1.645	nan
24.0	41.741	nan	0.473	nan	5.803	nan
48.0	61.959	nan	0.244	nan	18.403	nan
72.0	75.097	nan	0.2	nan	32.335	nan
96.0	81.615	nan	nan	nan	40.805	nan
120.0	85.263	nan	nan	nan	48.605	nan
192.0	nan	1.297	nan	nan	nan	2.322

TCE Inhalation 44.0 ppm for 4 hours - female #2 (Human #22)

Hours, AurnTCOGTCOH, AurnTCOGTCOH_Coll, CTCOH, CVen, AurnTCA, AurnTCA_Coll

4.0	8.816	nan	1.636	0.479	0.294	nan
5.0	nan	nan	1.621	0.151	nan	nan
6.0	nan	nan	1.335	0.109	nan	nan
7.0	nan	nan	1.195	0.077	nan	nan
8.0	24.94	nan	1.302	nan	1.842	nan
24.0	44.218	nan	0.525	nan	7.027	nan
32.0	nan	nan	0.659	nan	nan	nan
48.0	60.919	nan	0.134	nan	19.845	nan
72.0	68.921	nan	0.096	nan	31.698	nan
96.0	70.903	nan	nan	nan	38.408	nan
192.0	nan	0.239	nan	nan	nan	3.682

TCE Inhalation 44.0 ppm for 4 hours - female #3 (Human #23)

Hours, AurnTCOGTCOH, AurnTCOGTCOH_Coll, CTCOH, CVen, AurnTCA, AurnTCA_Coll

4.0	23.797	nan	1.776	0.277	0.467	nan
5.0	nan	nan	1.712	0.216	nan	nan
6.0	nan	nan	1.465	0.113	nan	nan
7.0	nan	nan	1.32	0.077	nan	nan
8.0	28.703	nan	1.545	nan	1.333	nan
24.0	58.809	nan	0.521	nan	14.093	nan
32.0	nan	nan	0.543	nan	nan	nan
48.0	85.586	nan	0.108	nan	30.235	nan
72.0	93.276	nan	0.05	nan	42.643	nan
96.0	95.967	nan	nan	nan	51.288	nan
192.0	nan	0.268	nan	nan	nan	1.518

TCE Inhalation 44.0 ppm for 4 hours - female #4 (Human #24)

Hours, AurnTCOGTCOH, CTCOH, CVen, AurnTCA

4.0	14.848	1.49	0.256	1.273
5.0	nan	1.335	0.194	nan
6.0	nan	1.239	0.097	nan
7.0	nan	1.172	0.077	nan
8.0	44.609	1.356	nan	3.715
24.0	82.283	0.696	nan	18.435
32.0	nan	0.668	nan	nan
48.0	113.34	0.232	nan	40.529
72.0	126.783	0.129	nan	57.932
96.0	131.251	nan	nan	69.431

TCE Inhalation 40.0 ppm for 4 hours - male #1 (Human #25)

Hours, AurnTCOGTCOH, AurnTCOGTCOH_Coll, CTCOH, CVen, AurnTCA, AurnTCA_Coll

4.0	6.262	nan	0.775	0.322	0.426	nan
5.0	nan	nan	0.66	0.117	nan	nan
6.0	nan	nan	0.638	0.117	nan	nan
7.0	nan	nan	0.585	nan	nan	nan
8.0	15.15	nan	0.574	nan	1.195	nan
24.0	29.19	nan	0.438	nan	6.565	nan
48.0	36.782	nan	0.2	nan	11.965	nan
72.0	42.539	nan	0.141	nan	23.235	nan
96.0	44.553	nan	nan	nan	32.775	nan
120.0	46.221	nan	nan	nan	37.96	nan
192.0	nan	1.126	nan	nan	nan	1.280

TCE Inhalation 40.0 ppm for 4 hours - male #2 (Human #26)

Hours, AurnTCOGTCOH, AurnTCOGTCOH_Coll, CTCOH, CVen, AurnTCA, AurnTCA_Coll

4.0	12.878	nan	0.806	0.252	0.205	nan
5.0	nan	nan	0.681	0.132	nan	nan
6.0	nan	nan	0.614	0.08	nan	nan
7.0	nan	nan	0.551	nan	nan	nan
8.0	24.712	nan	0.504	nan	0.489	nan
24.0	58.083	nan	0.243	nan	4.818	nan
48.0	72.72	nan	0.08	nan	17.241	nan
72.0	76.4	nan	nan	nan	28.511	nan
96.0	77.744	nan	nan	nan	38.051	nan
120.0	78.599	nan	nan	nan	43.199	nan
192.0	nan	0.297	nan	nan	nan	2.695

TCE Inhalation 40.0 ppm for 4 hours - male #3 (Human #27)

Hours, AurnTCOGTCOH, AurnTCOGTCOH_Coll, CTCOH, CVen, AurnTCA, AurnTCA_Coll

4.0	15.053	nan	0.939	0.266	0.462	nan
5.0	nan	nan	0.69	0.127	nan	nan
6.0	nan	nan	0.812	0.078	nan	nan
7.0	nan	nan	0.696	nan	nan	nan
8.0	21.897	nan	0.658	nan	0.822	nan
24.0	62.789	nan	0.339	nan	8.42	nan
48.0	85.28	nan	0.128	nan	19.045	nan
72.0	93.302	nan	0.09	nan	27.681	nan
96.0	95.789	nan	nan	nan	33.457	nan
120.0	97.177	nan	nan	nan	39.762	nan
192.0	nan	0.324	nan	nan	nan	3.610

TCE Inhalation 44.0 ppm for 4 hours - male #4 (Human #28)

Hours,	AUrntCOGTCOH,	AUrntCOGTCOH_Coll,	CTCOH,	CVen,	AUrntTCA,	AUrntTCA_Coll
4.0	11.722	nan	1.323	0.246	nan	nan
5.0	nan	nan	1.283	0.131	nan	nan
6.0	nan	nan	1.191	0.077	nan	nan
7.0	nan	nan	1.035	0.077	nan	nan
8.0	37.419	nan	1.093	nan	0.585	nan
24.0	92.855	nan	0.551	nan	4.673	nan
32.0	nan	nan	0.403	nan	nan	nan
48.0	114.296	nan	0.155	nan	11.492	nan
72.0	121.185	nan	0.098	nan	18.063	nan
96.0	123.768	nan	0.044	nan	23.734	nan
192.0	nan	0.234	nan	nan	nan	2.108

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days - subject #1 (Human #29)

Hours,	AUrntCOGTCOH,	AUrntCOGTCOH_Coll,	CTCOH,	CVen,	AUrntTCA,	AUrntTCA_Coll
4.0	nan	nan	2.047	0.42	nan	nan
5.0	nan	nan	1.672	0.13	nan	nan
8.0	nan	nan	1.596	0.085	nan	nan
9.0	nan	nan	1.406	nan	nan	nan
10.0	nan	nan	1.26	nan	nan	nan
24.0	46.14	nan	1.174	nan	4.175	nan
28.0	nan	nan	2.002	0.51	nan	nan
33.0	nan	nan	1.801	0.17	nan	nan
48.0	121.6	nan	0.917	nan	19.16	nan
52.0	nan	nan	2.38	0.408	nan	nan
57.0	nan	nan	1.72	nan	nan	nan
72.0	175.55	nan	0.946	nan	46.72	nan
76.0	nan	nan	2.58	0.51	nan	nan
81.0	nan	nan	2.064	nan	nan	nan
96.0	238.17	nan	1.267	nan	72.82	nan
100.0	nan	nan	2.509	0.85	nan	nan
104.0	nan	nan	2.142	nan	nan	nan
105.0	nan	nan	2.113	nan	nan	nan
120.0	358.26	nan	2.11	nan	124.285	nan
144.0	378.55	nan	0.507	nan	153.321	nan
168.0	396.33	nan	0.272	nan	168.271	nan
192.0	nan	nan	0.138	nan	nan	nan
216.0	nan	nan	0.08	nan	nan	nan
240.0	nan	nan	0.054	nan	nan	nan
264.0	nan	nan	0.03	nan	nan	nan
408.0	nan	0.20	nan	nan	nan	1.365

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days - subject #2 (Human #30)

Hours,	AUrntCOGTCOH,	AUrntCOGTCOH_Coll,	CTCOH,	CVen,	AUrntTCA,	AUrntTCA_Coll
4.0	nan	nan	1.958	0.34	nan	nan
5.0	nan	nan	1.596	0.23	nan	nan
8.0	nan	nan	1.368	0.13	nan	nan
9.0	nan	nan	1.204	nan	nan	nan
10.0	nan	nan	1.152	nan	nan	nan
24.0	88.46	nan	1.036	nan	6.613	nan
28.0	nan	nan	1.82	0.34	nan	nan
33.0	nan	nan	1.674	nan	nan	nan
48.0	214.54	nan	0.812	nan	25.399	nan
52.0	nan	nan	2.01	0.476	nan	nan
57.0	nan	nan	1.87	nan	nan	nan
72.0	335.72	nan	0.591	nan	75.391	nan
76.0	nan	nan	2.322	0.272	nan	nan
81.0	nan	nan	1.909	nan	nan	nan
96.0	453.37	nan	0.845	nan	139.375	nan
100.0	nan	nan	2.509	0.782	nan	nan
104.0	nan	nan	2.016	nan	nan	nan
105.0	nan	nan	2.016	nan	nan	nan
120.0	557.89	nan	1.01	nan	229.037	nan
144.0	600.5	nan	0.386	nan	271.661	nan
168.0	638.16	nan	0.102	nan	304.179	nan
192.0	643.27	nan	nan	nan	328.651	nan
216.0	647.1	nan	0.04	nan	346.571	nan
240.0	649.13	nan	nan	nan	360.221	nan
264.0	650.17	nan	nan	nan	371.781	nan
408.0	nan	0.08	nan	nan	nan	2.1

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days - subject #3 (Human #31)

Hours, AurnTCOGTCOH, AurnTCOGTCOH_Coll, CTCOH, Cven, AurnTCA, AurnTCA_Coll

4.0	nan	nan	1.275	0.28	nan	nan
5.0	nan	nan	1.014	1.18	nan	nan
8.0	nan	nan	0.9	0.09	nan	nan
9.0	nan	nan	0.803	nan	nan	nan
10.0	nan	nan	0.72	nan	nan	nan
24.0	63.33	nan	0.567	nan	5.341	nan
28.0	nan	nan	1.44	0.34	nan	nan
33.0	nan	nan	1.85	nan	nan	nan
48.0	149.89	nan	0.55	nan	17.631	nan
52.0	nan	nan	2.09	0.34	nan	nan
57.0	nan	nan	1.4	nan	nan	nan
72.0	234.33	nan	0.676	nan	49.311	nan
76.0	nan	nan	1.565	0.34	nan	nan
81.0	nan	nan	1.248	nan	nan	nan
96.0	320.33	nan	0.507	nan	110.463	nan
100.0	nan	nan	1.974	0.51	nan	nan
104.0	nan	nan	1.638	nan	nan	nan
105.0	nan	nan	1.323	nan	nan	nan
120.0	409.94	nan	0.51	nan	187.167	nan
144.0	434.46	nan	0.179	nan	234.983	nan
168.0	440.59	nan	nan	nan	283.309	nan
192.0	444.02	nan	0.045	nan	319.077	nan
216.0	446.58	nan	0.028	nan	337.788	nan
240.0	447.9	nan	nan	nan	356.118	nan
264.0	448.61	nan	nan	nan	372.468	nan
408.0	nan	0.07	nan	nan	nan	2.184

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days - subject #4 (Human #32)

Hours, AurnTCOGTCOH, CTCOH, Cven, AurnTCA, AurnTCA_Coll

4.0	nan	2.849	0.17	nan	nan
5.0	nan	2.394	0.17	nan	nan
8.0	nan	2.28	0.09	nan	nan
9.0	nan	2.052	nan	nan	nan
10.0	nan	1.976	nan	nan	nan
24.0	116.1	1.296	nan	2.928	nan
28.0	nan	2.912	0.34	nan	nan
33.0	nan	2.429	nan	nan	nan
48.0	246.68	0.825	nan	12.19	nan
52.0	nan	2.53	0.272	nan	nan
57.0	nan	2.26	nan	nan	nan
72.0	363.79	0.473	nan	29.482	nan
76.0	nan	2.322	nan	nan	nan
81.0	nan	2.418	nan	nan	nan
96.0	458.92	0.76	nan	48.094	nan
100.0	nan	2.87	nan	nan	nan
104.0	nan	2.52	nan	nan	nan
105.0	nan	2.293	nan	nan	nan
120.0	556.48	1.01	nan	111.934	nan
144.0	597.53	0.198	nan	169.81	nan
168.0	638.45	0.034	nan	186.895	nan
192.0	641.52	nan	nan	206.764	nan
216.0	642.45	nan	nan	218.839	nan
240.0	642.84	nan	nan	230.578	nan
264.0	642.97	nan	nan	239.119	nan
408.0	nan	nan	nan	nan	3.564

Monster et al., 1976

TCE Inhalation 65.0 ppm for 4 hours - subject 1 (Human #33)

Hours	AurnTCOGTCOH	CALvPPM	CBldTCA	CVen	RetDose	TotCTCOH	AURnTCA
3.5	nan	nan	3.6	1.2	nan	4.3	nan
4.0	nan	nan	nan	nan	320.0	nan	nan
4.5	nan	3.766118721	nan	nan	nan	nan	nan
6.0	nan	1.842123288	5.7	0.13	nan	4.4	nan
16.0	31.5445	nan	nan	nan	nan	nan	1.1445
23.75	nan	0.122808219	10.1	0.01	nan	1.1	nan
24.0	84.4675	nan	nan	nan	nan	nan	3.27
32.0	119.4505	nan	nan	nan	nan	nan	5.232
40.0	146.3605	nan	nan	nan	nan	nan	8.502
48.0	157.573	0.034795662	11.4	nan	nan	nan	9.9735
56.0	163.553	nan	nan	nan	nan	nan	10.791
64.0	169.0845	nan	nan	nan	nan	nan	12.099
72.0	176.709	0.020877397	11.8	nan	nan	nan	14.388
80.0	179.699	nan	nan	nan	nan	nan	15.5325
88.0	182.5395	nan	nan	nan	nan	nan	16.8405

TCE Inhalation 140.0 ppm for 4 hours - subject 1 (Human #33)

Hours	AurnTCOGTCOH	CALvPPM	CBldTCA	CVen	RetDose	TotCTCOH	AURnTCA
3.99	nan	nan	5.2	nan	nan	6.1	nan
4.0	nan	nan	nan	nan	740.0	nan	nan
4.5	nan	5.989968911	nan	nan	nan	nan	nan
6.5	nan	2.572163121	9.0	0.28	nan	7.2	nan
16.0	58.305	nan	nan	nan	nan	nan	0.8175
23.5	nan	0.28188089	15.0	0.014	nan	2.9	nan
24.0	164.5995	nan	nan	nan	nan	nan	3.597
32.0	246.675	nan	nan	nan	nan	nan	5.559
40.0	295.113	nan	nan	nan	nan	nan	9.81
48.0	326.209	0.070470222	20.0	0.005	nan	0.72	13.8975
56.0	340.561	nan	nan	nan	nan	nan	17.1675
64.0	353.418	nan	nan	nan	nan	nan	22.563
72.0	360.594	nan	17.5	0.0025	nan	0.15	26.9775
80.0	364.481	nan	nan	nan	nan	nan	28.9395
142.0	nan	nan	12.5	nan	nan	nan	nan
214.0	nan	nan	7.4	nan	nan	nan	nan
479.0	nan	nan	1.5	nan	nan	nan	nan

TCE Inhalation 68.0 ppm for 4 hours - subject 2 (Human #34)

Hours	AurnTCOGTCOH	CALvPPM	CBldTCA	CVen	RetDose	TotCTCOH	AURnTCA
3.5	nan	nan	4.0	1.5	nan	2.9	nan
4.0	nan	nan	nan	nan	430.0	nan	nan
4.083	nan	3.675658588	nan	nan	nan	nan	nan
4.5	nan	1.531524412	nan	nan	nan	nan	nan
6.0	nan	nan	6.6	0.16	nan	2.5	nan
8.0	nan	nan	nan	nan	nan	nan	0.4905
16.0	41.86	nan	nan	nan	nan	nan	2.1255
22.0	nan	0.245043906	nan	nan	nan	nan	nan
22.833	nan	nan	9.1	0.0156	nan	0.45	nan
24.0	92.391	nan	nan	nan	nan	nan	7.0305
32.0	117.507	nan	nan	nan	nan	nan	11.9355
40.0	136.4935	nan	nan	nan	nan	nan	19.7835
47.0	nan	nan	8.9	0.0065	nan	0.15	nan
48.0	148.1545	0.110269758	nan	nan	nan	nan	25.3425
56.0	155.6295	nan	nan	nan	nan	nan	29.103
64.0	162.5065	nan	nan	nan	nan	nan	34.989
72.0	167.2905	nan	8.8	0.0034	nan	nan	41.856
80.0	170.729	0.076882525	nan	nan	nan	nan	46.2705
88.0	176.8585	nan	nan	nan	nan	nan	51.5025
142.0	nan	nan	4.5	nan	nan	nan	nan
214.0	nan	nan	2.4	nan	nan	nan	nan

TCE Inhalation 138.0 ppm for 4 hours - subject 2 (Human #34)

Hours	AurnTCOGTCOH	CalvPPM	CBldTCA	CVen	RetDose	TotCTCOH	AurnTCA
3.99	nan	nan	4.0	nan	nan	4.5	nan
4.0	nan	nan	nan	nan	790.0	nan	nan
4.083	nan	4.993960819	nan	nan	nan	nan	nan
6.0	nan	3.433348063	nan	nan	nan	nan	nan
6.5	nan	nan	6.6	0.22	nan	3.9	nan
16.0	74.75	nan	nan	nan	nan	nan	1.7985
23.0	nan	nan	12.0	0.028	nan	1.2	nan
24.0	181.493	0.343334806	nan	nan	nan	nan	8.829
32.0	232.7715	nan	nan	nan	nan	nan	14.715
40.0	272.09	nan	nan	nan	nan	nan	26.487
47.333	nan	nan	13.0	0.0085	nan	0.35	nan
48.0	301.99	nan	nan	nan	nan	nan	39.24
56.0	315.445	0.103000442	nan	nan	nan	nan	47.415
64.0	324.415	nan	nan	nan	nan	nan	55.59
72.0	331.292	nan	nan	nan	nan	nan	64.419
72.333	nan	nan	11.0	0.0048	nan	0.11	nan
80.0	336.076	nan	nan	nan	nan	nan	71.1225
94.5	nan	nan	10.0	0.0011	nan	0.03	nan
95.0	nan	0.043697157	nan	nan	nan	nan	nan
164.0	nan	nan	5.4	nan	nan	nan	nan
260.0	nan	nan	1.6	nan	nan	nan	nan
404.0	nan	nan	0.04	nan	nan	nan	nan

TCE Inhalation 70.0 ppm for 4 hours - subject 3 (Human #35)

Hours	AurnTCOGTCOH	CalvPPM	CBldTCA	CVen	RetDose	TotCTCOH	AurnTCA
3.583	nan	nan	3.1	1.6	nan	2.8	nan
4.0	nan	nan	nan	nan	330.0	nan	nan
4.5	nan	5.517282574	nan	nan	nan	nan	nan
6.0	nan	3.678188383	5.2	0.18	nan	2.7	nan
16.0	35.88	nan	nan	nan	nan	nan	1.4715
22.5	nan	0.239082245	7.8	0.011	nan	0.51	nan
24.0	91.6435	nan	nan	nan	nan	nan	4.7415
32.0	116.909	nan	nan	nan	nan	nan	7.521
40.0	134.849	nan	nan	nan	nan	nan	14.715
47.75	nan	0.062529203	8.1	0.0023	nan	nan	nan
48.0	145.1645	nan	nan	nan	nan	nan	20.4375
56.0	149.6495	nan	nan	nan	nan	nan	22.563
64.0	153.088	nan	nan	nan	nan	nan	26.814
70.5	nan	0.018390942	6.2	nan	nan	nan	nan
72.0	155.48	nan	nan	nan	nan	nan	31.2285
80.0	156.676	nan	nan	nan	nan	nan	33.354
88.0	157.1245	nan	nan	nan	nan	nan	36.1335
134.0	nan	nan	4.1	nan	nan	nan	nan
214.0	nan	nan	2.1	nan	nan	nan	nan
454.0	nan	nan	0.04	nan	nan	nan	nan

TCE Inhalation 142.0 ppm for 4 hours - subject 3 (Human #35)

Hours,	AurnTCOGTCOH,	CALvPPM,	CBldTCA,	CVen,	RetDose,	TotCTCOH,	AurnTCA
3.99	nan	nan	3.6	nan	nan	5.2	nan
4.0	nan	nan	nan	nan	710.0	nan	nan
4.5	nan	4.884417808	nan	nan	nan	nan	nan
6.0	nan	2.767836758	6.5	0.25	nan	5.1	nan
16.0	49.933	nan	nan	nan	nan	nan	0.654
23.333	nan	0.325627854	12.0	0.022	nan	1.6	nan
24.0	132.457	nan	nan	nan	nan	nan	2.4525
32.0	178.204	nan	nan	nan	nan	nan	4.251
40.0	210.3465	nan	nan	nan	nan	nan	11.118
48.0	226.7915	nan	nan	nan	nan	nan	15.696
48.167	nan	0.11071347	11.0	0.0054	nan	0.34	nan
56.0	239.499	nan	nan	nan	nan	nan	22.7265
64.0	242.19	nan	nan	nan	nan	nan	25.3425
71.5	nan	0.035819064	10.0	0.0025	nan	0.06	nan
72.0	247.871	nan	nan	nan	nan	nan	31.2285
80.0	250.861	nan	nan	nan	nan	nan	36.297
88.0	251.758	nan	nan	nan	nan	nan	41.202
96.0	251.9075	nan	nan	nan	nan	nan	45.6165
104.0	252.5055	nan	nan	nan	nan	nan	48.069
191.0	nan	nan	5.8	nan	nan	nan	nan
263.0	nan	nan	3.8	nan	nan	nan	nan
407.0	nan	nan	1.5	nan	nan	nan	nan

TCE Inhalation 76.0 ppm for 4 hours - subject 4 (Human #36)

Hours,	AurnTCOGTCOH,	CALvPPM,	CBldTCA,	CVen,	RetDose,	TotCTCOH,	AurnTCA
3.417	nan	nan	2.4	nan	nan	3.2	nan
4.0	nan	nan	nan	nan	470.0	nan	nan
4.5	nan	4.666913489	nan	nan	nan	nan	nan
6.0	nan	2.10011107	4.5	0.175	nan	3.2	nan
16.0	49.7835	nan	nan	nan	nan	nan	1.308
24.0	121.5435	nan	nan	nan	nan	nan	3.27
24.083	nan	0.204177465	9.0	0.0088	nan	0.6	nan
32.0	153.088	nan	nan	nan	nan	nan	5.886
40.0	179.5495	nan	nan	nan	nan	nan	12.9165
48.0	192.257	nan	nan	nan	nan	nan	21.582
48.167	nan	0.06125324	11.6	0.0025	nan	0.11	nan
56.0	198.237	nan	nan	nan	nan	nan	25.6695
64.0	202.124	nan	nan	nan	nan	nan	30.2475
72.0	207.3565	0.020417747	9.8	nan	nan	nan	35.316
80.0	209.4495	nan	nan	nan	nan	nan	39.4035
88.0	211.2435	nan	nan	nan	nan	nan	44.799
96.0	212.29	nan	nan	nan	nan	nan	51.339
142.0	nan	nan	5.4	nan	nan	nan	nan
214.0	nan	nan	2.6	nan	nan	nan	nan
504.0	nan	nan	0.25	nan	nan	nan	nan

TCE Inhalation 140.0 ppm for 4 hours - subject 4 (Human #36)

Hours,	AurnTCOGTCOH,	CALvPPM,	CBldTCA,	CVen,	RetDose,	TotCTCOH,	AurnTCA
3.99	nan	nan	3.3	3.1	nan	5.0	nan
4.0	nan	nan	nan	nan	790.0	nan	nan
4.5	nan	4.520886183	nan	nan	nan	nan	nan
6.417	nan	2.542998478	6.4	0.26	nan	5.5	nan
16.0	74.75	nan	nan	nan	nan	nan	1.635
23.25	nan	0.268427617	11.0	0.019	nan	1.7	nan
24.0	222.755	nan	nan	nan	nan	nan	8.829
32.0	290.7775	nan	nan	nan	nan	nan	17.004
40.0	332.6375	nan	nan	nan	nan	nan	25.6695
48.0	355.0625	nan	nan	nan	nan	nan	40.548
48.917	nan	0.062162185	14.0	0.004	nan	0.35	nan
56.0	366.1255	nan	nan	nan	nan	nan	49.8675
64.0	374.4975	nan	nan	nan	nan	nan	60.168
72.0	380.029	nan	nan	nan	nan	nan	74.229
72.667	nan	0.025429985	12.5	0.002	nan	0.06	nan
80.0	382.421	nan	nan	nan	nan	nan	80.9325
88.0	383.7665	nan	nan	nan	nan	nan	89.271
96.0	384.215	nan	nan	nan	nan	nan	100.5525
104.0	384.6635	nan	nan	nan	nan	nan	106.1115
144.0	nan	nan	5.3	nan	nan	nan	nan
216.0	nan	nan	3.4	nan	nan	nan	nan

Muller et al., 1974

TCA Oral Gavage 2.646 mg/kg (Human #44)

Hours	CPlasTCA	AurnTCA
0.496	22.7	nan
0.993	29.4	nan
2.98	23.0	nan
5.46	24.4	nan
9.93	21.8	nan
23.8	17.2	nan
24.0	nan	43.4
34.2	15.6	nan
48.0	nan	59.7
48.9	14.0	nan
58.8	11.4	nan
72.0	8.95	75.0
81.6	8.48	nan
95.8	5.4	nan
96.0	nan	88.7
106.0	5.82	nan
120.0	5.0	98.58
144.0	nan	107.98
148.0	3.38	nan
168.0	2.42	113.03

TCOH Oral Gavage 10.0 mg/kg (Human #44)

Hours, AurnTCOGTCOH, CPlasTCA, CTCOH, AurnTCA

0.402	nan	nan	5.79	nan
0.415	nan	nan	4.93	nan
0.496	nan	4.8	nan	nan
0.807	nan	nan	4.1	nan
0.993	nan	3.88	nan	nan
1.49	nan	6.57	nan	nan
1.57	nan	nan	3.76	nan
3.11	nan	nan	2.58	nan
3.47	nan	6.86	nan	nan
5.96	nan	11.5	nan	nan
5.97	nan	nan	1.91	nan
10.9	nan	18.7	1.22	nan
23.8	nan	24.2	nan	nan
24.0	84.2	nan	0.498	27.8
34.7	nan	20.8	nan	nan
35.2	nan	nan	0.276	nan
47.6	nan	17.1	nan	nan
47.9	nan	nan	0.163	nan
48.0	100.9	nan	nan	70.2
71.7	nan	12.1	nan	nan
72.0	109.26	nan	nan	101.0
72.2	nan	nan	0.0487	nan
95.5	nan	9.28	nan	nan
96.0	113.16	nan	nan	125.8
96.2	nan	nan	0.0196	nan
120.0	115.39	nan	nan	147.9
122.0	nan	8.72	nan	nan
144.0	nan	nan	nan	156.74
146.0	nan	5.73	nan	nan
168.0	nan	nan	nan	161.23
170.0	nan	5.3	nan	nan

Paykoc and Powell, 1945

TCA IV 24.8 mg/kg (Human #18)

Hours, CBldTCA, CPlasTCA

34.0	65.0	119.0
58.0	50.0	95.0
82.0	44.0	83.0
106.0	32.0	61.0

TCA IV 32.9 mg/kg (Human #19)

Hours, CBldTCA, CPlasTCA, AUrnTCA

10.0	80.0	140.0	189.0
34.0	57.0	100.0	453.0
58.0	44.0	77.0	703.0
82.0	35.0	61.0	928.0
106.0	28.0	50.0	1075.0
130.0	24.0	42.0	1148.0
154.0	21.0	37.0	1224.0
178.0	nan	nan	1284.0
202.0	nan	nan	1332.0

TCA Oral Gavage 53.06 mg/kg (Human #20)

Hours, CBldTCA, CPlasTCA, AUrnTCA

34.0	102.0	179.0	900.0
58.0	78.0	136.0	1260.0
82.0	62.0	108.0	1500.0
106.0	48.0	84.0	1690.0
130.0	40.0	70.0	1816.0
154.0	nan	nan	1856.0
178.0	nan	nan	1878.0
202.0	nan	nan	1932.0

APPENDIX O

M Files for Sensitivity Analyses

The following are M files for generating output for the sensitivity analyses.

Mouse_SARun.m

```
load @format=model @file=New_EPA
Init

ResetDoses
MousePost
TSTRT=0.0; TCHNG=1700.0; DOSEINT=1700.0; DMINT=168.0; TSTP=1680.0;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=100.0;
    STRTNEXTLIST(i1)=7.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=17.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=65.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='mouse_hours_100inh.txt' @format=ascii
save SA_All @file='mouse_sareresults_100inh.txt' @format=ascii

ResetDoses
MousePost
TSTRT=0.0; DOSEINT=1700.0; DMINT=168.0; TSTP=1680.0;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=600.0;
    STRTNEXTLIST(i1)=7.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=17.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=65.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='mouse_hours_600inh.txt' @format=ascii
save SA_All @file='mouse_sareresults_600inh.txt' @format=ascii

ResetDoses
MousePost
PDOSE=300.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; DOSEINT=24.0; DMINT=168.0; TSTP=1680.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='mouse_hours_300oral.txt' @format=ascii
save SA_All @file='mouse_sareresults_300oral.txt' @format=ascii

ResetDoses
MousePost
PDOSE=1000.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; DOSEINT=24.0; DMINT=168.0; TSTP=1680.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='mouse_hours_1000oral.txt' @format=ascii
save SA_All @file='mouse_sareresults_1000oral.txt' @format=ascii
```

Rat_SARun.m

```
load @format=model @file=New_EPA
Init

ResetDoses
RatPost
TSTRT=0.0; DOSEINT=1700.0; DMINT=168.0; TSTP=1680.0;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=100.0;
    STRTNEXTLIST(i1)=7.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=17.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=65.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='rat_hours_100inh.txt' @format=ascii
save SA_All @file='rat_sareresults_100inh.txt' @format=ascii

ResetDoses
RatPost
TSTRT=0.0; DOSEINT=1700.0; DMINT=168.0; TSTP=1680.0;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=600.0;
    STRTNEXTLIST(i1)=7.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=17.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=65.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='rat_hours_600inh.txt' @format=ascii
save SA_All @file='rat_sareresults_600inh.txt' @format=ascii

ResetDoses
RatPost
PDOSE=300.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; DOSEINT=24.0; DMINT=168.0; TSTP=1680.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='rat_hours_300oral.txt' @format=ascii
save SA_All @file='rat_sareresults_300oral.txt' @format=ascii

ResetDoses
RatPost
PDOSE=1000.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; DOSEINT=24.0; DMINT=168.0; TSTP=1680.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='rat_hours_1000oral.txt' @format=ascii
save SA_All @file='rat_sareresults_1000oral.txt' @format=ascii
```

Female SARun.m

```
load @format=model @file=New_EPA
Init

ResetDoses
FemalePost
CONCLIST=[0.001 0.0]; STRTNEXTLIST=[17000.0]; TSTRT=0.0; DOSEINT=17000.0; DMINT=24.0;
TSTP=16800.0; CINT=0.1;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='female_hours_inh.txt' @format=ascii
save SA_All @file='female_sareresults_inh.txt' @format=ascii

ResetDoses
FemalePost
DRINK=0.001; TSTP=16800.0; DOSEINT=100000.0; DMINT=24.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='female_hours_oral.txt' @format=ascii
save SA_All @file='female_sareresults_oral.txt' @format=ascii
```

Male SARun.m

```
load @format=model @file=New_EPA
Init

ResetDoses
MalePost
CONCLIST=[0.001 0.0]; STRTNEXTLIST=[17000.0]; TSTRT=0.0; DOSEINT=17000.0; DMINT=24.0;
TSTP=16800.0; CINT=0.1;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='male_hours_inh.txt' @format=ascii
save SA_All @file='male_sareresults_inh.txt' @format=ascii

ResetDoses
MalePost
DRINK=0.001; TSTP=16800.0; DOSEINT=100000.0; DMINT=24.0;
SA_Hours=[]; SA_All=[]; delta=0.1/2.0;
SA
save SA_Hours @file='male_hours_oral.txt' @format=ascii
save SA_All @file='male_sareresults_oral.txt' @format=ascii
```

SA.m

```
i = 0;
FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
qccs=[]; cenQCC=QCC; for QCC=[cenQCC*(1.0-delta) cenQCC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACOXMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; qccs=[qccs QCC]; end;
Calc_SCs
QCC=cenQCC;
disp("-----finished QCC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vprs=[]; cenVPR=VPR; for VPR=[cenVPR*(1.0-delta) cenVPR*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACOXMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; vprs=[vprs VPR]; end;
Calc_SCs
```

```

VPR=cenVPR;
disp("-----finished VPR");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
qfatcs=[]; cenQFATC=QFATC; for QFATC=[cenQFATC*(1.0-delta) cenQFATC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; qfatcs=[qfatcs QFATC]; end;
    Calc_SCs
    QFATC=cenQFATC;
    disp("-----finished QFATC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
qgutcs=[]; cenQGUTC=QGUTC; for QGUTC=[cenQGUTC*(1.0-delta) cenQGUTC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; qgutcs=[qgutcs QGUTC]; end;
    Calc_SCs
    QGUTC=cenQGUTC;
    disp("-----finished QGUTC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
qlivcs=[]; cenQLIVC=QLIVC; for QLIVC=[cenQLIVC*(1.0-delta) cenQLIVC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; qlivcs=[qlivcs QLIVC]; end;
    Calc_SCs
    QLIVC=cenQLIVC;
    disp("-----finished QLIVC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
qslwcs=[]; cenQSLWC=QSLWC; for QSLWC=[cenQSLWC*(1.0-delta) cenQSLWC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; qslwcs=[qslwcs QSLWC]; end;
    Calc_SCs
    QSLWC=cenQSLWC;
    disp("-----finished QSLWC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
drespcs=[]; cenDRESPC=DRESPC; for DRESPC=[cenDRESPC*(1.0-delta) cenDRESPC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];

```



```

AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; drespcs=[drespcs DRESPC]; end;
Calc_SCs
DRESPC=cenDRESPC;
disp("-----finished DRESPC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
qkidcs=[]; cenQKIDC=QKIDC; for QKIDC=[cenQKIDC*(1.0-delta) cenQKIDC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; qkidcs=[qkidcs QKIDC]; end;
Calc_SCs
QKIDC=cenQKIDC;
disp("-----finished QKIDC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
fracplass=[]; cenFRACPLAS=FRACPLAS;
for FRACPLAS=[cenFRACPLAS*(1.0-delta) cenFRACPLAS*(1.0+delta)]; start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; fracplass=[fracplass FRACPLAS]; end;
Calc_SCs
FRACPLAS=cenFRACPLAS;
disp("-----finished FRACPLAS");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vfatcs=[]; cenVFATC=VFATC; for VFATC=[cenVFATC*(1.0-delta) cenVFATC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vfatcs=[vfatcs VFATC]; end;
Calc_SCs
VFATC=cenVFATC;
disp("-----finished VFATC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vgutcs=[]; cenVGUTC=VGUTC; for VGUTC=[cenVGUTC*(1.0-delta) cenVGUTC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vgutcs=[vgutcs VGUTC]; end;
Calc_SCs
VGUTC=cenVGUTC;
disp("-----finished VGUTC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vlivcs=[]; cenVLIVC=VLIVC; for VLIVC=[cenVLIVC*(1.0-delta) cenVLIVC*(1.0+delta)];
start @NoCallback;

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FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vlivcs=[vlivcs VLIVC]; end;
Calc_SCs
VLIVC=cenVLIVC;
disp("-----finished VLIVC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vrapcs=[]; cenVRAPC=VRAPC; for VRAPC=[cenVRAPC*(1.0-delta) cenVRAPC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vrapcs=[vrapcs VRAPC]; end;
Calc_SCs
VRAPC=cenVRAPC;
disp("-----finished VRAPC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vresplumcs=[]; cenVRESPLUMC=VRESPLUMC;
for VRESPLUMC=[cenVRESPLUMC*(1.0-delta) cenVRESPLUMC*(1.0+delta)]; start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vresplumcs=[vresplumcs VRESPLUMC]; end;
Calc_SCs
VRESPLUMC=cenVRESPLUMC;
disp("-----finished VRESPLUMC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vrespc=[]; cenVRESPC=VRESPC; for VRESPC=[cenVRESPC*(1.0-delta) cenVRESPC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vrespc=[vrespc VRESPC]; end;
Calc_SCs
VRESPC=cenVRESPC;
disp("-----finished VRESPC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
vkidcs=[]; cenVKIDC=VKIDC; for VKIDC=[cenVKIDC*(1.0-delta) cenVKIDC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vkidcs=[vkidcs VKIDC]; end;
Calc_SCs
VKIDC=cenVKIDC;
disp("-----finished VKIDC");

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FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
vblcds=[]; cenVBLDC=VBLDC; for VBLDC=[cenVBLDC*(1.0-delta) cenVBLDC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; vblcds=[vblcds VBLDC]; end;
    Calc_SCs
    VBLDC=cenVBLDC;
    disp("-----finished VBLDC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
pbs=[]; cenPB=PB; for PB=[cenPB*(1.0-delta) cenPB*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; pbs=[pbs PB]; end;
    Calc_SCs
    PB=cenPB;
    disp("-----finished PB");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
pfats=[]; cenPFAT=PFAT; for PFAT=[cenPFAT*(1.0-delta) cenPFAT*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; pfats=[pfats PFAT]; end;
    Calc_SCs
    PFAT=cenPFAT;
    disp("-----finished PFAT");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
pguts=[]; cenPGUT=PGUT; for PGUT=[cenPGUT*(1.0-delta) cenPGUT*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; pguts=[pguts PGUT]; end;
    Calc_SCs
    PGUT=cenPGUT;
    disp("-----finished PGUT");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
plivs=[]; cenPLIV=PLIV; for PLIV=[cenPLIV*(1.0-delta) cenPLIV*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; plivs=[plivs PLIV]; end;
    Calc_SCs

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PLIV=cenPLIV;
disp("-----finished PLIV");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
praps=[]; cenPRAP=PRAP; for PRAP=[cenPRAP*(1.0-delta) cenPRAP*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCLBDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; praps=[praps PRAP]; end;
    Calc_SCs
    PRAP=cenPRAP;
    disp("-----finished PRAP");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
presps=[]; cenPRES=PRES; for PRES=[cenPRES*(1.0-delta) cenPRES*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCLBDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; presps=[presps PRES]; end;
    Calc_SCs
    PRES=cenPRES;
    disp("-----finished PRES");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
pkids=[]; cenPKID=PKID; for PKID=[cenPKID*(1.0-delta) cenPKID*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCLBDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; pkids=[pkids PKID]; end;
    Calc_SCs
    PKID=cenPKID;
    disp("-----finished PKID");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
pslws=[]; cenPSLW=PSLW; for PSLW=[cenPSLW*(1.0-delta) cenPSLW*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCLBDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; pslws=[pslws PSLW]; end;
    Calc_SCs
    PSLW=cenPSLW;
    disp("-----finished PSLW");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
prbcplastcas=[]; cenPRBCPLASTCA=PRBCPLASTCA;
for PRBCPLASTCA=[cenPRBCPLASTCA*(1.0-delta) cenPRBCPLASTCA*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];

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AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; prbcplastcas=[prbcplastcas PRBCPLASTCA]; end;
Calc_SCs
PRBCPLASTCA=cenPRBCPLASTCA;
disp("-----finished PRBCPLASTCA");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
pbodtcacs=[]; cenPBODTCAC=PBODTCAC;
for PBODTCAC=[cenPBODTCAC*(1.0-delta) cenPBODTCAC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; pbodtcacs=[pbodtcacs PBODTCAC]; end;
Calc_SCs
PBODTCAC=cenPBODTCAC;
disp("-----finished PBODTCAC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
plivtcacs=[]; cenPLIVTCAC=PLIVTCAC;
for PLIVTCAC=[cenPLIVTCAC*(1.0-delta) cenPLIVTCAC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; plivtcacs=[plivtcacs PLIVTCAC]; end;
Calc_SCs
PLIVTCAC=cenPLIVTCAC;
disp("-----finished PLIVTCAC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
kdissoCs=[]; cenKDISSOC=KDISSOC;
for KDISSOC=[cenKDISSOC*(1.0-delta) cenKDISSOC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kdissoCs=[kdissoCs KDISSOC]; end;
Calc_SCs
KDISSOC=cenKDISSOC;
disp("-----finished KDISSOC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
bmaxkdcS=[]; cenBMAXKDC=BMAXKDC; for BMAXKDC=[cenBMAXKDC*(1.0-delta) cenBMAXKDC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; bmaxkdcS=[bmaxkdcS BMAXKDC]; end;
Calc_SCs
BMAXKDC=cenBMAXKDC;
disp("-----finished BMAXKDC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
pbodtcohs=[]; cenPBODTCOH=PBODTCOH;
for PBODTCOH=[cenPBODTCOH*(1.0-delta) cenPBODTCOH*(1.0+delta)]; start @NoCallback;

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FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
SA_Hours=[SA_Hours HOURS]; pbodtcohs=[pbodtcohs PBODTCOH]; end;
Calc_SCs
PBODTCOH=cenPBODTCOH;
disp("-----finished PBODTCOH");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
plivtcohs=[]; cenPLIVTCOH=PLIVTCOH;
for PLIVTCOH=[cenPLIVTCOH*(1.0-delta) cenPLIVTCOH*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; plivtcohs=[plivtcohs PLIVTCOH]; end;
    Calc_SCs
    PLIVTCOH=cenPLIVTCOH;
    disp("-----finished PLIVTCOH");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
pbodtcogs=[]; cenPBODTCOG=PBODTCOG;
for PBODTCOG=[cenPBODTCOG*(1.0-delta) cenPBODTCOG*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; pbodtcogs=[pbodtcogs PBODTCOG]; end;
    Calc_SCs
    PBODTCOG=cenPBODTCOG;
    disp("-----finished PBODTCOG");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
plivtcogs=[]; cenPLIVTCOG=PLIVTCOG;
for PLIVTCOG=[cenPLIVTCOG*(1.0-delta) cenPLIVTCOG*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; plivtcogs=[plivtcogs PLIVTCOG]; end;
    Calc_SCs
    PLIVTCOG=cenPLIVTCOG;
    disp("-----finished PLIVTCOG");

if (SPECIES == 1)
    FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
    FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
    peffdcvgs=[]; cenPEFFDCVG=PEFFDCVG;
    for PEFFDCVG=[cenPEFFDCVG*(1.0-delta) cenPEFFDCVG*(1.0+delta)]; start @NoCallback;
        FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
        FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
        FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
        FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
        FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCBLDDM];
        AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
        SA_Hours=[SA_Hours HOURS]; peffdcvgs=[peffdcvgs PEFFDCVG]; end;
        Calc_SCs
        PEFFDCVG=cenPEFFDCVG;
        disp("-----finished PEFFDCVG");

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end

if (SPECIES > 1)
  FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
  FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
  ktsds=[]; cenKTSD=KTSD; for KTSD=[cenKTSD*(1.0-delta) cenKTSD*(1.0+delta)];
  start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
    FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCLDDM];
    AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; ktsds=[ktsds KTSD]; end;
  Calc_SCs
  KTSD=cenKTSD;
  disp("-----finished KTSD");

  FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
  FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
  kass=[]; cenKAS=KAS; for KAS=[cenKAS*(1.0-delta) cenKAS*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
    FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCLDDM];
    AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kass=[kass KAS]; end;
  Calc_SCs
  KAS=cenKAS;
  disp("-----finished KAS");

  FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
  FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
  kads=[]; cenKAD=KAD; for KAD=[cenKAD*(1.0-delta) cenKAD*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
    FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCLDDM];
    AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kads=[kads KAD]; end;
  Calc_SCs
  KAD=cenKAD;
  disp("-----finished KAD");

end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
kastcas=[]; cenKASTCA=KASTCA; for KASTCA=[cenKASTCA*(1.0-delta) cenKASTCA*(1.0+delta)];
start @NoCallback;
  FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
  FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
  FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
  FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
  AUCCBldDMS=[AUCCBldDMS AUCCLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
  AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
  SA_Hours=[SA_Hours HOURS]; kastcas=[kastcas KASTCA]; end;
  Calc_SCs
  KASTCA=cenKASTCA;
  disp("-----finished KASTCA");

if (SPECIES == 1)
  FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
  FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
  kastcoh=[]; cenKASTCOH=KASTCOH;
  for KASTCOH=[cenKASTCOH*(1.0-delta) cenKASTCOH*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];

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FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; kastcohs=[kastcohs KASTCOH]; end;
Calc_SCs
KASTCOH=cenKASTCOH;
disp("-----finished KASTCOH");
end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
vmaxcs=[]; cenVMAXC=VMAXC; for VMAXC=[cenVMAXC*(1.0-delta) cenVMAXC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vmaxcs=[vmaxcs VMAXC]; end;
Calc_SCs
VMAXC=cenVMAXC;
disp("-----finished VMAXC");

if (SPECIES == 1)
FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
cls=[]; cenCL=CL; for CL=[cenCL*(1.0-delta) cenCL*(1.0+delta)]; start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; cls=[cls CL]; end;
Calc_SCs
CL=cenCL;
disp("-----finished CL");
else
FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[];
AUCLlivTCADMS=[];
kmcs=[]; cenKMC=KMC; for KMC=[cenKMC*(1.0-delta) cenKMC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH];
FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; kmcs=[kmcs KMC]; end;
Calc_SCs
KMC=cenKMC;
disp("-----finished KMC");
end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
fracothercs=[]; cenFRACOTHERC=FRACOTHERC;
for FRACOTHERC=[cenFRACOTHERC*(1.0-delta) cenFRACOTHERC*(1.0+delta)]; start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; fracothercs=[fracothercs FRACOTHERC]; end;
Calc_SCs
FRACOTHERC=cenFRACOTHERC;
disp("-----finished FRACOTHERC");

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FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
fractcacs=[]; cenFRACTCAC=FRACTCAC;
for FRACTCAC=[cenFRACTCAC*(1.0-delta) cenFRACTCAC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; fractcacs=[fractcacs FRACTCAC]; end;
    Calc_SCs
    FRACTCAC=cenFRACTCAC;
    disp("-----finished FRACTCAC");

if (SPECIES > 1)
    FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
    FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
    vmaxdcvgcs=[]; cenVMAXDCVGC=VMAXDCVGC;
    for VMAXDCVGC=[cenVMAXDCVGC*(1.0-delta) cenVMAXDCVGC*(1.0+delta)]; start @NoCallback;
        FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
        FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
        FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
        FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
        FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM];
        AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
        SA_Hours=[SA_Hours HOURS]; vmaxdcvgcs=[vmaxdcvgcs VMAXDCVGC]; end;
        Calc_SCs
        VMAXDCVGC=cenVMAXDCVGC;
        disp("-----finished VMAXDCVGC");
    end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
cldcvgs=[]; cenCLDCVG=CLDCVG; for CLDCVG=[cenCLDCVG*(1.0-delta) cenCLDCVG*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; cldcvgs=[cldcvgs CLDCVG]; end;
    Calc_SCs
    CLDCVG=cenCLDCVG;
    disp("-----finished CLDCVG");

if (SPECIES == 1)
    FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
    FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
    kmdcvgcs=[]; cenKMDCVGC=KMDCVGC;
    for KMDCVGC=[cenKMDCVGC*(1.0-delta) cenKMDCVGC*(1.0+delta)]; start @NoCallback;
        FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
        FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
        FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
        FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
        FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM];
        AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
        SA_Hours=[SA_Hours HOURS]; kmdcvgcs=[kmdcvgcs KMDCVGC]; end;
        Calc_SCs
        KMDCVGC=cenKMDCVGC;
        disp("-----finished KMDCVGC");
    else
        FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
        FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[];
        AUCLlivTCADMS=[];
        vmaxkiddcvgs=[]; cenVMAXKIDDCVGC=VMAXKIDDCVGC;
        for VMAXKIDDCVGC=[cenVMAXKIDDCVGC*(1.0-delta) cenVMAXKIDDCVGC*(1.0+delta)];
        start @NoCallback;
            FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
            FracMetGSHS=[FracMetGSHS FRACMETGSH];

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FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vmaxkiddcvgs=[vmaxkiddcvgs VMAXKIDDCVGC]; end;
Calc_SCs
VMAXKIDDCVGC=cenVMAXKIDDCVGC;
disp("-----finished VMAXKIDDCVGC");
end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
clkiddcvgs=[]; cenCLKIDDCVG=CLKIDDCVG;
for CLKIDDCVG=[cenCLKIDDCVG*(1.0-delta) cenCLKIDDCVG*(1.0+delta)]; start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; clkiddcvgs=[clkiddcvgs CLKIDDCVG]; end;
Calc_SCs
CLKIDDCVG=cenCLKIDDCVG;
disp("-----finished CLKIDDCVG");

if (SPECIES == 1)
FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kmkiddcvgs=[]; cenKMKIDDCVGC=KMKIDDCVGC;
for KMKIDDCVGC=[cenKMKIDDCVGC*(1.0-delta) cenKMKIDDCVGC*(1.0+delta)]; start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; kmkiddcvgs=[kmkiddcvgs KMKIDDCVGC]; end;
Calc_SCs
KMKIDDCVGC=cenKMKIDDCVGC;
disp("-----finished KMKIDDCVGC");
end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
vmaxlunglives=[]; cenVMAXLUNGLIV=VMAXLUNGLIV;
for VMAXLUNGLIV=[cenVMAXLUNGLIV*(1.0-delta) cenVMAXLUNGLIV*(1.0+delta)]; start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; vmaxlunglives=[vmaxlunglives VMAXLUNGLIV]; end;
Calc_SCs
VMAXLUNGLIV=cenVMAXLUNGLIV;
disp("-----finished VMAXLUNGLIV");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kmclaras=[]; cenKMCLARA=KMCLARA; for KMCLARA=[cenKMCLARA*(1.0-delta) cenKMCLARA*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; kmclaras=[kmclaras KMCLARA]; end;
Calc_SCs

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KMCLARA=cenKMCLARA;
disp("-----finished KMCLARA");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
fraclungsyscs=[]; cenFRACLUNGSYSC=FRACLUNGSYSC;
for FRACLUNGSYSC=[cenFRACLUNGSYSC*(1.0-delta) cenFRACLUNGSYSC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCBldDMS=[AUCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; fraclungsyscs=[fraclungsyscs FRACLUNGSYSC]; end;
    Calc_SCs
    FRACLUNGSYSC=cenFRACLUNGSYSC;
    disp("-----finished FRACLUNGSYSC");

if (SPECIES == 1)
    FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
    FracMetLivOtherS=[]; FracMetLngS=[]; AUCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
    cltcohs=[]; cenCLTCOH=CLTCOH; for CLTCOH=[cenCLTCOH*(1.0-delta) cenCLTCOH*(1.0+delta)];
    start @NoCallback;
        FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
        FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
        FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
        FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
        FracMetLngS=[FracMetLngS FRACMETLNG]; AUCBldDMS=[AUCBldDMS AUCCBLDDM];
        AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
        SA_Hours=[SA_Hours HOURS]; cltcohs=[cltcohs CLTCOH]; end;
        Calc_SCs
        CLTCOH=cenCLTCOH;
        disp("-----finished CLTCOH");
    else
        FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
        FracMetLivOtherS=[]; FracMetLngS=[]; AUCBldDMS=[]; AUCCTCOHDMS=[];
        AUCCLivTCADMS=[];
        vmxtcohc=[]; cenVMAXTCOHC=VMAXTCOHC;
        for VMAXTCOHC=[cenVMAXTCOHC*(1.0-delta) cenVMAXTCOHC*(1.0+delta)]; start @NoCallback;
            FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
            FracMetGSHS=[FracMetGSHS FRACMETGSH];
            FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
            FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
            FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
            FracMetLngS=[FracMetLngS FRACMETLNG]; AUCBldDMS=[AUCBldDMS AUCCBLDDM];
            AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
            SA_Hours=[SA_Hours HOURS]; vmxtcohc=[vmxtcohc VMAXTCOHC]; end;
            Calc_SCs
            VMAXTCOHC=cenVMAXTCOHC;
            disp("-----finished VMAXTCOHC");
        end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
kmtcohs=[]; cenKMTCOH=KMTCOH; for KMTCOH=[cenKMTCOH*(1.0-delta) cenKMTCOH*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCBldDMS=[AUCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kmtcohs=[kmtcohs KMTCOH]; end;
    Calc_SCs
    KMTCOH=cenKMTCOH;
    disp("-----finished KMTCOH");

if (SPECIES == 1)
    FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
    FracMetLivOtherS=[]; FracMetLngS=[]; AUCBldDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];

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    clglucs=[]; cenCLGLUC=CLGLUC; for CLGLUC=[cenCLGLUC*(1.0-delta) cenCLGLUC*(1.0+delta)];
    start @NoCallback;
        FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
        FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
        FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
        FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
        FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM];
        AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
        SA_Hours=[SA_Hours HOURS]; clglucs=[clglucs CLGLUC]; end;
        Calc_SCs
        CLGLUC=cenCLGLUC;
        disp("-----finished CLGLUC");
else
    FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
    FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[];
    AUCCLivTCADMS=[];
    vmaxglucss=[]; cenVMAXGLUCC=VMAXGLUCC;
    for VMAXGLUCC=[cenVMAXGLUCC*(1.0-delta) cenVMAXGLUCC*(1.0+delta)]; start @NoCallback;
        FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
        FracMetGSHS=[FracMetGSHS FRACMETGSH];
        FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
        FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
        FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
        FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM];
        AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
        SA_Hours=[SA_Hours HOURS]; vmaxglucss=[vmaxglucss VMAXGLUCC]; end;
        Calc_SCs
        VMAXGLUCC=cenVMAXGLUCC;
        disp("-----finished VMAXGLUCC");
end

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
kmgLucs=[]; cenKMGLUC=KMGLUC; for KMGLUC=[cenKMGLUC*(1.0-delta) cenKMGLUC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kmgLucs=[kmgLucs KMGLUC]; end;
    Calc_SCs
    KMGLUC=cenKMGLUC;
    disp("-----finished KMGLUC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
kmettcohcS=[]; cenKMETTCOHC=KMETTCOHC;
for KMETTCOHC=[cenKMETTCOHC*(1.0-delta) cenKMETTCOHC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kmettcohcS=[kmettcohcS KMETTCOHC]; end;
    Calc_SCs
    KMETTCOHC=cenKMETTCOHC;
    disp("-----finished KMETTCOHC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBLdDMS=[]; AUCCTCOHDMS=[]; AUCCLivTCADMS=[];
kurntcacS=[]; cenKURNTCAC=KURNTCAC;
for KURNTCAC=[cenKURNTCAC*(1.0-delta) cenKURNTCAC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBLdDMS=[AUCCBLdDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCCLivTCADMS=[AUCCLivTCADMS AUCCLIVTCADM];

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SA_Hours=[SA_Hours HOURS]; kurntcacs=[kurntcacs KURNTCAC]; end;
Calc_SCs
KURNTCAC=cenKURNTCAC;
disp("-----finished KURNTCAC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kmettcacs=[]; cenKMETTCAC=KMETTCAC;
for KMETTCAC=[cenKMETTCAC*(1.0-delta) cenKMETTCAC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kmettcacs=[kmettcacs KMETTCAC]; end;
    Calc_SCs
    KMETTCAC=cenKMETTCAC;
    disp("-----finished KMETTCAC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kbilecs=[]; cenKBILEC=KBILEC; for KBILEC=[cenKBILEC*(1.0-delta) cenKBILEC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kbilecs=[kbilecs KBILEC]; end;
    Calc_SCs
    KBILEC=cenKBILEC;
    disp("-----finished KBILEC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kehracs=[]; cenKEHRC=KEHRC; for KEHRC=[cenKEHRC*(1.0-delta) cenKEHRC*(1.0+delta)];
start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kehracs=[kehracs KEHRC]; end;
    Calc_SCs
    KEHRC=cenKEHRC;
    disp("-----finished KEHRC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kurntcogcs=[]; cenKURNTCOGC=KURNTCOGC;
for KURNTCOGC=[cenKURNTCOGC*(1.0-delta) cenKURNTCOGC*(1.0+delta)]; start @NoCallback;
    FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
    FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
    FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
    FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER]; FracMetLngS=[FracMetLngS FRACMETLNG];
    AUCCBldDMS=[AUCCBldDMS AUCCBLDDM]; AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM];
    AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
    SA_Hours=[SA_Hours HOURS]; kurntcogcs=[kurntcogcs KURNTCOGC]; end;
    Calc_SCs
    KURNTCOGC=cenKURNTCOGC;
    disp("-----finished KURNTCOGC");

if (SPECIES == 1)
    FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
    FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
    kdcvgcs=[]; cenKDCVGC=KDCVGC; for KDCVGC=[cenKDCVGC*(1.0-delta) cenKDCVGC*(1.0+delta)];

```

```

start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; kdcvgcs=[kdcvgcs KDCVGC]; end;
Calc_SCs
KDCVGC=cenKDCVGC;
disp("-----finished KDCVGC");
end

if (SPECIES < 3)
FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kntacs=[]; cenKNATC=KNATC; for KNATC=[cenKNATC*(1.0-delta) cenKNATC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; kntacs=[kntacs KNATC]; end;
Calc_SCs
KNATC=cenKNATC;
disp("-----finished KNATC");

FracMetabS=[]; FracOxMetabS=[]; FracMetGSHS=[]; FracBioactKidS=[]; FracMetLiv1S=[];
FracMetLivOtherS=[]; FracMetLngS=[]; AUCCBldDMS=[]; AUCCTCOHDMS=[]; AUCLlivTCADMS=[];
kkidbioactcs=[]; cenKKIDBIOACTC=KKIDBIOACTC;
for KKIDBIOACTC=[cenKKIDBIOACTC*(1.0-delta) cenKKIDBIOACTC*(1.0+delta)];
start @NoCallback;
FracMetabS=[FracMetabS FRACMETAB]; FracOxMetabS=[FracOxMetabS FRACMETAB];
FracMetGSHS=[FracMetGSHS FRACMETGSH]; FracBioactKidS=[FracBioactKidS FRACBIOACTKID];
FracMetLiv1S=[FracMetLiv1S FRACMETLIV1];
FracMetLivOtherS=[FracMetLivOtherS FRACMETLIVOTHER];
FracMetLngS=[FracMetLngS FRACMETLNG]; AUCCBldDMS=[AUCCBldDMS AUCCBLDDM];
AUCCTCOHDMS=[AUCCTCOHDMS AUCCTCOHDM]; AUCLlivTCADMS=[AUCLlivTCADMS AUCLLIVTCADM];
SA_Hours=[SA_Hours HOURS]; kkidbioactcs=[kkidbioactcs KKIDBIOACTC]; end;
Calc_SCs
KKIDBIOACTC=cenKKIDBIOACTC;
disp("-----finished KKIDBIOACTC");
end
end

```

Calc_SCs.m

```

% SA_*2 is using equation in EPA report
% SA_* uses equation I'm used to using (fractional change in output over fractional change in
% input)

i = i + 1;
SA_FracMetab=((FracMetabS(:,2)-FracMetabS(:,1))/(delta*2.0)./FracMetabS(:,1))*(1.0-delta);
SA_FracOxMetab=((FracOxMetabS(:,2)-FracOxMetabS(:,1))/(delta*2.0)./FracOxMetabS(:,1))*(1-delta);
SA_FracMetGSH=((FracMetGSHS(:,2)-FracMetGSHS(:,1))/(delta*2.0)./FracMetGSHS(:,1))*(1.0-delta);
SA_FracBioactKid=((FracBioactKidS(:,2)-FracBioactKidS(:,1))/(delta*2.0)./FracBioactKidS(:,1))
*(1.0-delta);
SA_FracMetLiv1=((FracMetLiv1S(:,2)-FracMetLiv1S(:,1))/(delta*2.0)./FracMetLiv1S(:,1))*(1-delta);

SA_FracMetLivOther=((FracMetLivOtherS(:,2)-
FracMetLivOtherS(:,1))/(delta*2.0)./FracMetLivOtherS(:,1))*(1.0-delta);

SA_FracMetLng=((FracMetLngS(:,2)-FracMetLngS(:,1))/(delta*2.0)./FracMetLngS(:,1))*(1.0-delta);
SA_AUCCBldDM=((AUCCBldDMS(:,2)-AUCCBldDMS(:,1))/(delta*2.0)./AUCCBldDMS(:,1))*(1.0-delta);
SA_AUCCTCOHDM=((AUCCTCOHDMS(:,2)-AUCCTCOHDMS(:,1))/(delta*2.0)./AUCCTCOHDMS(:,1))*(1.0-delta);
SA_AUCLlivTCADM=((AUCLlivTCADMS(:,2)-AUCLlivTCADMS(:,1))/(delta*2.0)./AUCLlivTCADMS(:,1))
*(1.0-delta);
SA_FracMetab2=20.0*((FracMetabS(:,2)-FracMetabS(:,1))./(FracMetabS(:,2)+FracMetabS(:,1)));

```

```

SA_FracOxMetab2=20.0*((FracOxMetabS(:,2)-
FracOxMetabS(:,1))./(FracOxMetabS(:,2)+FracOxMetabS(:,1))));

SA_FracMetGSH2=20.0*((FracMetGSHS(:,2)-FracMetGSHS(:,1))./(FracMetGSHS(:,2)+FracMetGSHS(:,1))));

SA_FracBioactKid2=20.0*((FracBioactKidS(:,2)-
FracBioactKidS(:,1))./(FracBioactKidS(:,2)+FracBioactKidS(:,1))));

SA_FracMetLiv12=20.0*((FracMetLiv1S(:,2)-
FracMetLiv1S(:,1))./(FracMetLiv1S(:,2)+FracMetLiv1S(:,1))));

SA_FracMetLivOther2=20.0*((FracMetLivOtherS(:,2)-
FracMetLivOtherS(:,1))./(FracMetLivOtherS(:,2)+FracMetLivOtherS(:,1))));

SA_FracMetLng2=20.0*((FracMetLngS(:,2)-FracMetLngS(:,1))./(FracMetLngS(:,2)+FracMetLngS(:,1))));
SA_AUCCBldDM2=20.0*((AUCCBldDMS(:,2)-AUCCBldDMS(:,1))./(AUCCBldDMS(:,2)+AUCCBldDMS(:,1))));
SA_AUCCTCOHDM2=20.0*((AUCCTCOHDMs(:,2)-AUCCTCOHDMs(:,1))./(AUCCTCOHDMs(:,2)+AUCCTCOHDMs(:,1))));

SA_AUCCLivTCADM2=20.0*((AUCCLivTCADMS(:,2)-
AUCCLivTCADMS(:,1))./(AUCCLivTCADMS(:,2)+AUCCLivTCADMS(:,1))));

SA_All(i,1)=SA_FracMetab;
SA_All(i,2)=SA_FracOxMetab;
SA_All(i,3)=SA_FracMetGSH;
SA_All(i,4)=SA_FracBioactKid;
SA_All(i,5)=SA_FracMetLiv1;
SA_All(i,6)=SA_FracMetLivOther;
SA_All(i,7)=SA_FracMetLng;
SA_All(i,8)=SA_AUCCBldDM;
SA_All(i,9)=SA_AUCCTCOHDM;
SA_All(i,10)=SA_AUCCLivTCADM;

SA_All(i,11)=SA_FracMetab2;
SA_All(i,12)=SA_FracOxMetab2;
SA_All(i,13)=SA_FracMetGSH2;
SA_All(i,14)=SA_FracBioactKid2;
SA_All(i,15)=SA_FracMetLiv12;
SA_All(i,16)=SA_FracMetLivOther2;
SA_All(i,17)=SA_FracMetLng2;
SA_All(i,18)=SA_AUCCBldDM2;
SA_All(i,19)=SA_AUCCTCOHDM2;
SA_All(i,20)=SA_AUCCLivTCADM2;

```

APPENDIX P

M Files for Mouse Dose Metrics

The following are M files for generating mouse dose metric values.

Cosby92_MouseDM.m

```
% Cosby NC, Dukelow WR. Toxicology of maternally ingested trichloroethylene
%      (TCE) on embryonal and fetal development in mice and of TCE metabolites on
%      in vitro fertilization. Fundam Appl Toxicol. 1992 Aug;19(2):268-74.

% C57BL/6 X DBA/2 (B6D2F1) mice, female, n = 11 with litters
% Oral gavage of 240.2 mg/kg TCE (NOAEL, POD) daily for 5 dy (GD1-5, GD6-10, or GD11-15)
%      Doses assumed to take 1 minute (0.017 hr)
% Doses based upon 1/10 and 1/100 of the LD50 value of 2402 mg/kg body weight
% Critical Effect: Litter size/viability, pup size/gross development
% Also tested: 0, 24.02 mg/kg

% Females were 6-8 wk at study start. Mean values for weight of female litter-bearing
% mice were not significantly different across treatment doses for any treatment
% group (data not shown).
% Mice are 8-10 wk at the end of the study. Since the mice are dosed by bw, size of
% mouse does not change the dose. As there are no adverse effects recorded, no
% particular exposure time is more important than another.
% The mice will be ~20-23 g during pregnancy (using the high end of the female curve due
% to pregnancy). The simulation will be run for 22 g.
% https://www.criver.com/products-services/find-model/b6d2f1-bdf1-mouse?region=3611

ResetDoses
MousePost
BW=0.022; PDOSE=240.2; TCHNG=0.017; DAYS=5.0; TMAX=120.0; DOSEINT=24.0; DMINT=24.0; TSTP=120.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

George85_MouseDM.m

```
% George JD, Reel JR, Myers CB, Lawton AD, Lamb JC. 1985. Trichloroethylene: Reproduction and
% Fertility Assessment in CD-1 Mice When Administered in the Feed. Research Triangle
% Park NC: National Toxicology Program, National Institute of Environmental Health
% Sciences. NTP-86-068

% CD-1 mice, male and female, n = 8/sex
% 0.3% TCE in diet or 375 mg/kg-dy TCE (NOAEL, POD) for 15 wk
% LOAEL: 0.6% or 750 mg/kg-dy
% Critical Effect: Decreased sperm motility
% Continuous breeding study (1 wk pre-dosing, 14 wks breeding, 3 wk segregation)
% Also tested: 0, 0.15% TCE in food (0, 187.5 mg/kg) (page 20)

% Male mouse weight in the 750 mg/kg-dy dose group was 37.79 +/- 0.62 g and was not
% different from controls (39.19 +/- 0.55) (Table 6); it is assumed that the
% 375 mg/kg-dy group would be similar in weight (assuming 38 g)
% Assume it takes them 10 hours to consume their food (dark hours) as lights were on 0500
% to 1900 hours

% Run until weekly AUC dosemetrics aren't changing
ResetDoses
MousePost
BW=0.038; PDOSE=750.0; TCHNG=10.0; DAYS=7.0; TMAX=1008.0; DOSEINT=24.0; DMINT=168.0;
TSTP=1008.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```


Griffin00_MouseDM.m

% Griffin JM, Gilbert KM, Lamps LW, Pumford NR. 2000. CD4+ T-cell activation and induction
% of autoimmune hepatitis following trichloroethylene treatment in MRL+/+ mice.
% Toxicological Sciences 57: 345-52.

% MRL+/+ autoimmune prone mice, female, n = 8
% 0.1 mg/mL TCE in drinking water or 21 mg/kg-dy TCE (NOAEL, POD) for 32 wk
% LOAEL: 0.5 mg/mL or 100 mg/kg-dy
% Critical Effect: Liver lymphocyte infiltration (Table 2)
% Also tested: 0, 2.5 mg/mL (400 mg/kg-dy) TCE in drinking water

% Body weights were not different between groups
% Mice were 4 wk old at purchase; assuming a 2 wk acclimation period, mice were 38
% wk at study end
% A growth chart for MRL mice was not found. A comparison was found (10-week-old
% female C57BL/6 weighed 20.1+/-0.5 g, MRL/MpJ weighed an average of 31.7+/-0.4 g)
% Thuret S, Thallmair M, Horky LL, Gage FH. 2012. Enhanced Functional Recovery in
% MRL/MpJ Mice after Spinal Cord Dorsal Hemisection. PLoS ONE 7(2):
% e30904. doi:10.1371/journal.pone.0030904
% At 270 days, female C57BL/6 weigh 27 g (Hilltop Labs), so the MRL females may
% weigh 43 g
% <http://www.hilltoplabs.com/public/c57growth.html>

% Run until daily AUC dosemetrics aren't changing
ResetDoses
MousePost
BW=0.043; DRINK=13.4; DMINT=24.0; TSTP=288.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check

Kaneko00_MouseDM.m

% Kaneko T, Saegusa M, Tasaka K, Sato A. 2000. Immunotoxicity of Trichloroethylene:
% a Study with MRL-lpr/lpr Mice. J. Appl. Toxicol. 20, 471-475

% MRL-lpr/lpr male mice, n = 5
% Inhalation of 500 ppm TCE (LOAEL, POD) for 4 hr/dy, 6 dy/wk, 8 wk
% Effect: B cell function in MRL mice was used b/c the histology was not quantified
% and the T cell staining lacks clear relevance and shows an effect at only one dose.
% Also tested: 0, 1000, 2000 ppm

% Mice were ~46-48 g at study finish (not statistically different between groups)
% (Figure 1) - Using middle number (47 g)

% Run until weekly AUC dosemetrics aren't changing
ResetDoses
MousePost
BW=0.047; TSTRT=0.0; DMINT=168.0; TSTP=840.0;
CONCLIST=[500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0
0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0
500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0
0.0 500.0 0.0 500.0 0.0 500.0 0.0 500.0 0.0 0.0];
STRTNEXTLIST=[4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 44.0 4.0 20.0 4.0 20.0 4.0 20.0
4.0 20.0 4.0 20.0 4.0 44.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 44.0
4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 44.0 4.0 20.0 4.0 20.0 4.0 20.0
4.0 20.0 4.0 20.0 4.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check

Kjellstrand83_MouseDM.m

```
% Kjellstrand P, Holmquist B, Aim P, Kanje M, Romare S, Jonsson I, Mansson L, Bjerkemo M.
%      1983. Trichloroethylene: Further Studies of the Effects on Body and Organ
%      Weights and Plasma Butyrylcholinesterase Activity in Mice. Acta pharmacol. et
%      toxicol. 1983, 53, 375-384.

% White NMRI mice, 20 male and 20 female (see Table 1)
% Inhalation of 37 ppm TCE (LOAEL, POD) for 24 hr/dy, 7 dy/wk, 30 dy
%      Critical effect: Relative liver weight increase (see Table 3)
%
% Also tested: 75, 150, 300 ppm continuous; intermittent exposures also tested

% Female ending BW = 35.0 +/- 1.3 g (Table 2)
ResetDoses
MousePost
BW=0.035; CONCLIST(1)=37.0; STRTNEXTLIST(1)=800.0; TSTRT=0.0; DMINT=24.0; TSTP=720.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check

% Male ending BW = 36.2 +/- 1.0 g (Table 2)
ResetDoses
MousePost
BW=0.0362; CONCLIST(1)=37.0; STRTNEXTLIST(1)=800.0; TSTRT=0.0; DMINT=24.0; TSTP=720.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

Land81_MouseDM.m

```
% Land PC, Owen EL, Linde HW. 1981. Morphologic Changes in Mouse Spermatozoa after
%      Exposure to Inhalational Anesthetics during Early Spermatogenesis

% (C57B1 x C3H)F1 mice (n = 5)
% Inhalation of 200 ppm TCE (NOAEL, POD) for 4 hr/dy, 5 dy
% LOAEL (abnormal epididymal sperm, euthanized 28 dy after 1st exposure) 2000 ppm (n = 10)
% Also tested: 0 ppm

% Mice obtained at 8-10 wk old and exposed at 11 wk old; should be about 26 g
%      RAO GN, HASEMAN JK, GRUMBEIN S, CRAWFORD DD, EUSTIS SL. 1990. Growth, Body Weight,
%      Survival, and Tumor Trends in (C57BL/6 X C3H/HeN) F1 (B6C3Fl) Mice During a
%      Nine-Year Period. TOXICOLOGIC PATHOLOGY. 18(1): 71-77.
```

```
ResetDoses
MousePost
BW=0.026; TSTRT=0.0; DMINT=24.0; TSTP=120.0; CINT=0.1;
CONCLIST=[575.0 0.0 575.0 0.0 575.0 0.0 575.0 0.0 575.0 0.0 0.0];
STRTNEXTLIST=[4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

Ramadhan10_MouseDM.m

```
% Ramadhan DH, Kamijima M, Wang D, Ito Y, Naito H, Yanagiba Y, Hayashi Y, Tanaka N,  
% Aoyama T, Gonzalez FJ, Nakajima T. 2010. Differential Response to  
% Trichloroethylene-Induced Hepatosteatosi in Wild-Type and PPAR $\alpha$ -Humanized Mice.  
% Environ Health Perspect 118:1557-1563
```

```
% Wild type PPAR $\alpha$  mice, male (n = 6)  
% Inhalation of 1000 ppm TCE (LOAEL, POD) for 8 hr/dy, 7 dy  
% Critical Effect: increased ALT  
% Also tested: 0, 2000 ppm
```

```
% NOTE: Ppar $\alpha$ -null and hPPAR $\alpha$  mice were also tested; only wild type results were  
% highlighted in the journal article copies received for this project so only  
% HEC from wild type data are predicted
```

```
% BW for wild type mice exposed to 1000 ppm was listed as 25.0 +/- 2.3 g in Table 1
```

```
ResetDoses  
MousePost  
BW=0.025; TSTRT=0.0; DMINT=24.0; TSTP=168.0;  
CONCLIST=[546.0 0.0 546.0 0.0 546.0 0.0 546.0 0.0 546.0 0.0 546.0 0.0 546.0 0.0 0.0];  
STRTNEXTLIST=[8.0 16.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 100.0];  
start @NoCallback  
plot(_t, _cart);  
i = i + 1;  
SaveDMS  
Output_Check
```

Sanders82_MouseDM.m

```
% Sanders VM, Tucker AN, White KL, Kauffmann BM, Hallett P, Carchman RA, Borzelleca JF,  
% Munson AE. 1982. Humoral and cell-mediated immune status in mice exposed to  
% trichloroethylene in the drinking water. Toxicol. Appl. Pharmacol. 62: 358-68.
```

```
% CD-1 mice, female and male, n = 12-20 for each sex  
% 0.1 mg/mL TCE in drinking water or 18.4 mg/kg-dy TCE (LOAEL, POD) for 4 mo  
% NOTE: A second group was exposed for 6 mo but the cell mediated response at the  
% LOAEL was only significant in the 4 mo group (Table 6)  
% Critical Effect: Cell-mediated SRBC response (Table 6) and bone marrow stem cells  
% (Table 8)  
% Also tested: 0, 1.0, 2.5, 5.0 mg/mL (0, 216.7, 393, 660.2 mg/kg-dy) TCE in drinking  
% water for 4 or 6 months
```

```
% Simulation is for last week of study  
% Effects on BW and starting ages or BW were not mentioned  
% Assuming the mice are approximately 5 mo old for the 4 mo exposures  
% At 15 wk, female CD-1 rats would be 40 g at the top of the range and may indicate  
% their size at 20 wk  
% At 15 wk, male CD-1 rats would be 49 g at the top of the range and may indicate  
% their size at 20 wk  
% https://www.criver.com/products-services/find-model/cd-1-igs-mouse?region=3611
```

```
% Females  
% Run until daily AUC dosemetrics aren't changing  
ResetDoses  
MousePost  
BW=0.040; DRINK=18.4; DMINT=24.0; TSTP=312.0; CINT=0.1;  
start @NoCallback  
plot(_t, _cart);  
i = i + 1;  
SaveDMS  
Output_Check
```

```
% Males
% Run until daily AUC dosemetrics aren't changing
ResetDoses
MousePost
BW=0.049; DRINK=18.4; DMINT=24.0; TSTP=312.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

Schwetz75_MouseDM.m

```
% Schwetz BA, Leong BKJ, Gehring PJ. 1975. The effect of maternally inhaled
% trichloroethylene, perchloroethylene, methyl chloroform, and methylene
% chloride on embryonal and fetal development in mice and rats. Toxicology
% and Applied Pharmacology. 32:84-96.

% Swiss-Webster female mice, n = 12
% Inhalation of 306 ppm TCE (NOAEL, POD) for 7 hr/dy, GD 6-15 (10 days)
% No effect on fetal development
% Tables 5-6
% Also tested: 0 ppm, also tested mice (see additional m file)

% Mice were 25-30 g prior to pregnancy; Mice exposed to TCE did not have decreased body
% weight as the rats did
% Ending mouse weights are not given but liver weight was 2.8 +/- 0.3 g in TCE group and
% relative liver weight was 0.052 +/- 0.006 g LW/g BW (Table 2)
% Therefore BW was ~54 g in this group

ResetDoses
MousePost
BW=0.054; TSTRT=0.0; DMINT=24.0; TSTP=240.0;
CONCLIST=[306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0
0.0 306.0 0.0 0.0];
STRTNEXTLIST=[7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

APPENDIX Q

M Files for Rat Dose Metrics

The following are M files for generating rat dose metric values.

Adams51_RatDM.m

% Adams EM, Spencer HC, Rowe VK, McCollister DD, Irish DD. 1951. Vapor toxicity of
% trichloroethylene determined by experiments on laboratory animals. AMA Archives of
% Industrial Hygiene and Occupational Medicine 4:469-481.

```
% Wistar origin rats, 15 male and 15 female
% Inhalation of 200 ppm TCE (NOAEL, POD) for 7 hr/dy, ~5 dy/wk,
%   as many as 151 exposures in 205 days (29.3 wk, 6.7 mo) (Table 5)
% LOAEL (increased relative liver & kidney wt) 400 ppm, 7 hr/dy, ~5 dy/wk,
%   as many as 173 exposures in 242 days (34.6 wk, 8 mo) (Table 3)
% Also tested: 100 ppm
```

```
% Female ending BW = 207 g (Table 5)
% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.207; TSTRT=0.0; DMINT=168.0; TSTP=1008.0; CINT=0.1;
CONCLIST=[200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0
0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0
200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0
0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0];
STRTNEXTLIST=[7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0
7.0 17.0 7.0 17.0 7.0 100.0];

start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output Check
```

```
% Male ending BW = 349 g (Table 5)
% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.349; TSTRT=0.0; DMINT=168.0; TSTP=1008.0; CINT=0.1;
CONCLIST=[200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0
0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0
200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0
0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0 200.0 0.0];
STRTNEXTLIST=[7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0
7.0 17.0 7.0 17.0 7.0 100.0];

start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output Check
```

Albee06_RatDM.m

```
% Albee RR, Spencer PJ, Johnson KA, Bradley GJ, Marable BR. 2006. Lack of trigeminal
% nerve toxicity in rats exposed to trichloroethylene vapor for 13 weeks.
% International Journal of Toxicology 25:531-540.

% Fischer-344 rats, 10 male and 10 female
% Inhalation of 800 ppm TCE (NOAEL, POD) for 6 hr/dy, 5 dy/wk, 13 wk
% LOAEL (hearing loss, loss of hair cells) 2500 ppm
% Also tested: 250 ppm

% Body weights are not specified; only that they were not different between groups
% Rats were 14 wk at receipt, 16 wk (most likely) at study start, and 29 wk at end
% Rats would be about 275 g (M) and 175 g (F) at study start
% Based on 2018 Charles River catalog
% Estimated 29 wk weight is 400 g (M) and 200 g (F)
% (4 wk F344 rats, 25 wk on feeding study, Fig 1)
% Rao GN, Morris RW, Seely JC. 2001 Beneficial effects of NTP-2000 diet on growth,
% survival, and kidney and heart diseases of Fischer 344 rats in chronic studies
% Toxicological Sciences 63:245-255.

% Female ending BW = 200 g (estimated from Rao et al. 2001)
% Run for 13 weeks
ResetDoses
RatPost
BW=0.2; TSTRT=0.0; DMINT=168.0; TSTP=2184.0; CINT=0.1;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=800.0;
    STRTNEXTLIST(i1)=6.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=18.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=66.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check

% Male ending BW = 400 g (estimated from Rao et al. 2001)
% Run for 13 weeks
ResetDoses
RatPost
BW=0.4; TSTRT=0.0; DMINT=168.0; TSTP=2184.0; CINT=0.1;
for iter = [1 : 65]
    i1 = (2 * iter) - 1;
    CONCLIST(i1)=800.0;
    STRTNEXTLIST(i1)=6.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=18.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=66.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

Arito94_RatDM.m

```
% Arito H, Takahashi M, Ishikawa T. 1994. Effect of subchronic inhalation exposure
%   to low-level trichloroethylene on heart rate and wakefulness-sleep in freely
%   moving rats. Japanese Journal of Industrial Health 36:1-8.

% JCL-Wistar rats, 20 male (4 groups of 5 exposed to each concentration)
% Inhalation of 50 ppm TCE (LOAEL, POD) for 8 hr/dy, 5 dy/wk, 2,4,6 wk
%   Critical effect: Decreased wakefulness
% Also tested: 100 & 300 ppm

% Body weights are not specified
% Rats were 4 wk at receipt, 9 wk at EEG/EMG/ECG implant, 11 wk (most likely) at
%   study start, and 17 wk at end
% Rats would be about 375 g (M) at 17 weeks
%   Estimate based on website growth curve:
%   http://www.clea-japan.com/en/animals/animal_e/e_03.html

% Male ending BW = 375 g
% Run for 6 weeks
ResetDoses
RatPost
BW=0.375; TSTRT=0.0; DMINT=168.0; TSTP=1008.0; CINT=0.1;
CONCLIST=[18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4
          0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0
          18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4 0.0 18.4
          0.0 18.4 0.0 0.0];
STRTNEXTLIST=[8.0 16.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 64.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 16.0
              8.0 64.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 64.0 8.0 16.0 8.0 16.0 8.0 16.0
              8.0 16.0 8.0 64.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 16.0 8.0 64.0 8.0 16.0 8.0 16.0
              8.0 16.0 8.0 16.0 8.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

Bushnell197_RatDM.m

```
% Bushnell PJ. 1997. Concentration-time relationships for the effects of inhaled
%   trichloroethylene on signal detection behavior in rats. Fundamental and Applied
%   Toxicology 36:30-38.

% Long-Evans rats, 11 male
% Inhalation of 800 ppm TCE (NOAEL, POD) for 1 hr/dy
%   see Figure 1 of article
% LOAEL (sensitivity to light stimulus, visual learning) 1200 ppm
% Also tested: 400, 1600, 2000, 2400 ppm

% The spreadsheet "Studies to Run PBPK" indicates that the animals are exposed 3 times
%   a week. All animals are exposed to air, then 3 different concentrations on 4
%   consecutive days of a week (0, 400, 600, 1200 ppm). The following week, the
%   same rats are exposed to 0, 800, 1200, 2400 ppm.

% Ending BW = 350 g (controlled by measured diet)
% Simulation for 1 day of exposure
ResetDoses
RatPost
BW=0.35; TSTRT=0.0; DMINT=24.0; TSTP=24.0;
CONCLIST=[1366.0 0.0 0.0];
STRTNEXTLIST=[1.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
```

```
% Simulation for 3 days per week for 2 weeks
```

```
ResetDoses
RatPost
BW=0.35; TSTR=24.0; DMINT=168.0; TSTP=336.0;
CONCLIST=[1366.0 0.0 1366.0 0.0 1366.0 0.0 1366.0 0.0 1366.0 0.0 1366.0 0.0 0.0];
STRTNEXTLIST=[1.0 23.0 1.0 23.0 1.0 119.0 1.0 23.0 1.0 23.0 1.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
```

Carney06_RatDM.m

```
% Carney, E.W., Thorsrud, B.A., Dugard, P.H. and Zablony, C.L. 2006. Developmental toxicity
% studies in Crl:CD (SD) rats following inhalation exposure to trichloroethylene and
% perchloroethylene. Birth Defects Res B Dev Reprod Toxicol 77(5): 405-12.
```

```
% Crl:CD rats (Sprague-Dawley), 27 female
% Developmental study to look for cardiac defects
% Inhalation of 600 ppm TCE (NOAEL, POD) for 6 hr/dy, 7 dy/wk, GD6-20 (15 days)
% Also tested: 50, 150 ppm
```

```
% Body weights are not specified; According to the Charles River 2018 catalog,
% young adult female SD rats are about 200 g with the high end of the range
% at 225 g. Since these are pregnant, 225 g was chosen.
```

```
% Timed pregnant female ending BW = 225 g (estimated from CRL catalog)
```

```
ResetDoses
RatPost
BW=0.225; TSTR=0.0; DMINT=24.0; TSTP=360.0;
CONCLIST=[600.0 0.0 600.0 0.0 600.0 0.0 600.0 0.0 600.0 0.0 600.0 0.0 600.0 0.0 600.0
0.0 600.0 0.0 600.0 0.0 600.0 0.0 600.0 0.0 600.0 0.0 600.0 0.0 0.0];
STRTNEXTLIST=[6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0
6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
```

Crofton97_RatDM.m

```
% Crofton KM and Zhao X. 1997. The Ototoxicity of Trichloroethylene: Extrapolation and
% Relevance of High-Concentration, Short-Duration Animal Exposure Data. FUNDAMENTAL
% AND APPLIED TOXICOLOGY 38, 101-106
```

```
% Long Evan rats, 10-12 male
% Inhalation of 1600 ppm TCE (NOAEL, POD) for 6 hr/dy, 5 dy/wk, 13 wk
% LOAEL (shift in auditory threshold, 13 wk group) 2400 ppm
% Also tested: 800, 3200 ppm; All concentrations tested for 1 dy, 1 wk, 4 wk, 13 wk
```

```
% Rats were received at 60 dy of age (8.5 wk) and would have been 23 wks at study
% finish, including a 2 wk quarantine/acclimation period
% Rats would be about 300 g at 8 wk and 700 g at 23 wk (675 g at 21 wk, no acclimation)
% Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
% 17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.
```

```
% Run for 13 weeks
```

```
ResetDoses
RatPost
BW=0.700; TSTR=0.0; DMINT=168.0; TSTP=2184.0; CINT=0.1;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=1367.0;
    STRTNEXTLIST(i1)=6.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=18.0;
end
```



```

for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=66.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check

```

Fisher01_RatDM.m

```

% Fisher JW, Channel SR, Eggers JS, Johnson PD, MacMahon KL, Goodyear CD, Sudberry GL,
% Warren DA, Latendresse JR, Graeter LJ. 2001. Trichloroethylene, Trichloroacetic
% Acid, and Dichloroacetic Acid: Do They Affect Fetal Rat Heart Development?
% International Journal of Toxicology, 20:257-267.

```

```

% Sprague Dawley rats, female, n = 20 litters
% Oral gavage of 500 mg/kg TCE (NOAEL, POD) daily for 10 dy (GD6-15)
% Doses assumed to take 1 minute (0.017 hr)
% Critical Effect: Cardiovascular malformation
% Also tested: 0 mg/kg TCE (2 groups, water or soybean oil); 300 mg/kg TCA, 300 mg/kg DCA
% or 15 mg/kg retinoic acid groups were included in the study

```

```

% Males and females were purchased at 9 wk and 200-300 g at study start. They were 11 wk
% at study start
% Rats were approximately 13 wk at study end.
% Maternal body weight gain for TCE- and RA-treated rats during gestation was not
% significantly different from the control soybean oil vehicle; TCE rats had gained
% almost 20 g at study end
% SD females should weigh about 225 g at this age (middle of range), making them 245-250 g
% when pregnant and at the top end of the weight range for this strain (250 g)
% From: Charles River 2018 catalog

```

```

ResetDoses
RatPost
BW=0.250; PDOSE=500.0; TCHNG=0.017; DAYS=7.0; TMAX=240.0; DOSEINT=24.0; DMINT=24.0; TSTP=240.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check

```

Healy82_RatDM.m

```

% Healy TEJ, Poole TR and Hopper A. 1982. Rat fetal development and maternal exposure to
% trichloroethylene 100 ppm. Br. J. Anaesth. 54, 337-341.

```

```

% Wistar origin rats, 32 female (31 control), GD 8-21
% Inhalation of 100 ppm TCE (LOAEL, POD) for 4 hr/dy, 7 dy/wk, 14 dy
% Increased resorptions, decreased fetal weight
% Also tested: 0 ppm

```

```

% Body weights were 200-300 g at breeding. These rats are approximately 11 weeks old
% according to the Charles River 2018 catalog. Three weeks later (14 wk) they
% would weigh 210-330 g. Taking the middle value at start (250 g) and adding 20 g
% growth and 30 g of babies, you get 300 g at study end.

```

```

ResetDoses
RatPost
BW=0.300; TSTRT=0.0; DMINT=24.0; TSTP=336.0;
CONCLIST=[100.0 0.0 100.0 0.0 100.0 0.0 100.0 0.0 100.0 0.0 100.0 0.0 100.0 0.0 100.0 0.0 100.0];
STRTNEXTLIST=[4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0];
start @NoCallback

```

```

plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check

```

Jaspers93 RatDM.m

```

% Jaspers RMA, Muijser H, Lammers JHCM and Kulig BM. 1993. Mid-frequency hearing loss and
% reduction of acoustic startle responding in rats following trichloroethylene exposure.
% Neurotoxicology and Teratology, Vol. 15, pp. 407-412.

```

```

% Wistar-derived Wag-Rij/MBL strain rats, 12, assumed male but not specified
% Inhalation of 1500 ppm TCE (NOAEL, POD) for 18 hr/dy, 5 dy/wk, 3 wk
% LOAEL (auditory threshold shift) 3000 ppm
% Also tested: 0 ppm

```

```

% BW = 180 +/- 10 g (about 11 weeks old) at receipt
% Figure 1 shows BW change over time; At last week of exposure, rats weighed
% ~250, ~240, ~225 for exposure groups 0, 1500, 3000 ppm, respectively. BW
% differences were significant. 240 g was used for the NOAEL POD simulation

```

```

ResetDoses
RatPost
BW=0.240; TSTRT=0.0; DMINT=168.0; TSTP=504.0; CINT=0.1;
CONCLIST=[1500.0 0.0 1500.0 0.0 1500.0 0.0 1500.0 0.0 1500.0 0.0 1500.0 0.0 1500.0
0.0 1500.0 0.0 1500.0 0.0 1500.0 0.0 1500.0 0.0 1500.0 0.0 1500.0 0.0
0.0];
STRTNEXTLIST=[18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 54.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0
18.0 54.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check

```

Kumar00a 01a RatDM.m

```

% Kumar P, Prasad AK, Dutta KK. 2000. Steroidogenic alterations in testes and sera of
% rats exposed to trichloroethylene (TCE) by inhalation. Human & Experimental
% Toxicology (2000) 19, 117-121
% Wistar origin rats, 12-13 male
% Inhalation of 376 ppm TCE (LOAEL, POD) for 4 hr/dy, 5 dy/wk, 12 or 24 wk
% Critical effect: Decreased sperm count & motility
% Also tested: 0 ppm

```

```

% A smaller rat would inhale a relatively higher total amount of TCE. Therefore
% the simulation will model the last week of the 12 wk exposure.
% BW at receipt: 50 +/- 5 g
% The Charles River Laboratory 2018 catalog indicates that these rats would be just
% weaned and about 3 weeks old
% Rats were bred in house; they would not have needed quarantine and there was no mention
% of acclimation. The rats would be 15 weeks of age
% The rats would be approximately 500 g according to Tordoff et al. 2008
% Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
% 17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.

```

```

% Kumar P, Prasad AK, Maji BK, Mani U, Dutta KK. 2001. Hepatotoxic alterations induced
% by inhalation of trichloroethylene (TCE) in rats. Biomedical and Environmental
% Sciences 14, 325-332.
% Wistar rats, 6 male
% Inhalation of 376 +/- 1.76 ppm TCE (LOAEL, POD) for 4 hr/dy, 5 dy/wk,
% 8, 12, or 24 wk
% Critical effect: Liver weight (significant increase but data not shown), enlarged
% fatty hepatocytes (via histology but no statistics); All effects evident at 8 wk
% and more progressive at 12 and 24 wk
% Also tested: 0 ppm

```

```
% Simulating the last week of the 8 wk exposure; Younger rats will inhale comparatively
% more TCE than larger due to higher respiratory rates
% BW was 130 +/- 10 g at study start; Animals bred in-house, so no quarantine was
% necessary; Acclimation was not mentioned in the study
% Rats were about 5 weeks at study start (Charles River Laboratories 2018 catalog)
% Rats would be 13 weeks at study end and approximately 400 g according to Tordoff et al.
% Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
% 17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.

% Ending BW = 530 g
% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.5; TSTRT=0.0; DMINT=168.0; TSTP=1176.0; CINT=0.1;
CONCLIST=[376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0
0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0
376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0
0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0 376.0 0.0
376.0 0.0 0.0];
STRTNEXTLIST=[4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 68.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0
4.0 68.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 68.0 4.0 20.0 4.0 20.0 4.0 20.0
4.0 20.0 4.0 68.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 68.0 4.0 20.0 4.0 20.0
4.0 20.0 4.0 20.0 4.0 68.0 4.0 20.0 4.0 20.0 4.0 20.0 4.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
```

Maltoni88_RatDM.m

```
% Maltoni C, Lefemine G, Coiti G, Perino G. 1988. Long-term carcinogenicity bioassays
% on trichloroethylene administered by inhalation to sprague-dawley rats and swiss
% and B6C3F1 mice. Annals of the New York Academy of Sciences. 534: 316-342.

% Sprague-Dawley rats, 15 male and 15 female
% Inhalation of 300 ppm TCE (NOAEL, POD) for 7 hr/dy, 5 dy/wk, 104 wk
% LOAEL (meganucleocytosis of kidney, Table 20) 600 ppm
% Also tested: 100 ppm

% Rats were 12-13 wk at start of experiment; this strain of male rat appears to max out
% at 850 g
% Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
% 17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.
% Simulating the last week of exposures

% NOTE: These POD simulations for HEC predictions are for non-cancer endpoints. This
% study contains cancer endpoints as well. Further, the study was performed in two
% strains of mice also. However, the non-cancer POD for this study was found
% in the male rats only.

% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.85; TSTRT=0.0; DMINT=168.0; TSTP=840.0; CINT=0.1;
CONCLIST=[221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0
0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0
221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0 0.0 221.0
0.0];
STRTNEXTLIST=[7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 17.0 7.0 65.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
```

Manson84_RatDM.m

% Manson JM, Murphy M, Richdale N, Smith MK. 1984. Effects of oral exposure to
% trichloroethylene on female reproductive function. Toxicology. 32: 229-42.

% Long-Evans rats, female, n = 23
% Oral gavage of 100 mg/kg TCE (NOAEL, POD) 5 dy/wk for 3 wk, 7 dy/wk for 3 wk
% Doses assumed to take 1 minute (0.017 hr)
% Simulating last week of gestation (7 dy/wk)
% LOAEL: 1000 mg/kg-dy
% Critical Effect: Neonatal+Postnatal death
% Also tested: 0, 10 mg/kg-dy TCE (corn oil)

% Males and females were purchased at 80-100 dy. There was a 2 wk quarantine.
% Body weights in the 100 mg/kg-dy group on GD22 were 405 +/- 7.4 g (Table 1).
% NOTE: BW were significantly decreased in the 1000 mg/kg-dy group.

% Run until weekly AUC dosemetrics aren't changing

ResetDoses

RatPost

BW=0.405; PDOSE=100.0; TCHNG=0.017; DAYS=7.0; TMAX=504.0; DOSEINT=24.0; DMINT=168.0;

TSTP=504.0; CINT=0.1;

start @NoCallback

plot(_t, _cart);

i = i + 1;

SaveDMS

Output_Check

Narotsky95_RatDM.m

% Narotsky MG, Weller EA, Chinchilli VM, Kavlock RJ. Nonadditive Developmental Toxicity
% in Mixtures of Trichloroethylene, Di(2-ethylhexyl) Phthalate, and Heptachlor
% in a 5 x 5 x 5 Design. Fundam. Appl. Toxicol. 27, 203-216.

% F-344 rats, female, n = 7-12

% Oral gavage of 844 mg/kg TCE (NOAEL, POD) daily on GD6-15 (10 dy)

% Doses assumed to take 1 minute (0.017 hr)

% LOAEL: 1125 mg/kg-dy

% Critical Effect: Litter resorptions (Table 3a)

% Also tested: 0, 475, 633 mg/kg-dy TCE (corn oil)

% Timed pregnant females were purchased at 90 dy old

% Doses were the same daily and were based on GD6 BW (~96 dy or ~14 wk)

% Weight gain data were given (Table 5) but no data were presented on actual BW

% F-344 females at 14 wk weigh ~175 g at 14 wk (high end of range due to pregnancy);

% This weight is what the dose was calculated on, not the ending pregnancy wt

% Charles River Laboratories 2018 Catalog

ResetDoses

RatPost

BW=0.175; PDOSE=36.0; TCHNG=0.017; DAYS=7.0; TMAX=240.0; DOSEINT=24.0; DMINT=24.0; TSTP=240.0;

start @NoCallback

plot(_t, _cart);

i = i + 1;

SaveDMS

Output_Check

Schwetz75_RatDM.m

```
% Schwetz BA, Leong BKJ, Gehring PJ. 1975. The effect of maternally inhaled
%   trichloroethylene, perchloroethylene, methyl chloroform, and methylene
%   chloride on embryonal and fetal development in mice and rats. Toxicology
%   and Applied Pharmacology. 32:84-96.

% Sprague-Dawley female rats, n = 18
% Inhalation of 306 ppm TCE (NOAEL, POD) for 7 hr/dy, GD 6-15 (10 days)
% No effect on fetal development
%   Tables 5-6
% Also tested: 0 ppm, also tested mice (see additional m file)

% Rats were ~250 g prior to pregnancy; Rats exposed to TCE weighed 4-5% less than
%   controls (statistically significant; not really biologically significant)
% Ending rat weights are not given but liver weight was 13.7 +/- 1.4 g in TCE group and
%   relative liver weight was 0.037 +/- 0.004 g LW/g BW (Table 2)
%   Therefore BW was ~370 g in this group
```

```
ResetDoses
RatPost
BW=0.370; TSTRT=0.0; DMINT=24.0; TSTP=240.0;
CONCLIST=[306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0 0.0 306.0
0.0 306.0 0.0 0.0];
STRTNEXTLIST=[7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0 7.0 17.0
7.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
```

Woolhiser06_RatDM.m

```
% Woolhiser MR, Krieger SM, Thomas J., Hotchkiss JA. 2006. Trichloroethylene (TCE):
%   immunotoxicity potential in CD rats following a 4-week vapor inhalation exposure.
%   Midland, MI: The Dow Chemical Company. Study ID: 031020
```

```
% Sprague-Dawley rats, female, n =
% Inhalation of 300 ppm TCE (NOAEL, POD) for 6 hr/dy, 5 dy/wk, 4 wk
%   LOAEL 1000 ppm
% Increased relative kidney & liver weight; Decreased PFC response (plaque
%   forming cell assay) - Tables 10, 19
% Also tested: 100 ppm
```

```
% Rats were 214.6 g at end (300 ppm group, Table 6)
%   Simulations are for the final week of exposure
```

```
% Immune effects
ResetDoses
RatPost
BW=0.2146; TSTRT=0.0; DMINT=168.0; TSTP=672.0; CINT=0.1;
CONCLIST=[243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0
0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0 243.0 0.0
243.0 0.0 243.0 0.0 243.0 0.0 0.0];
STRTNEXTLIST=[6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 66.0 6.0 18.0 6.0 18.0 6.0 18.0
6.0 66.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 18.0 6.0 66.0 6.0 18.0 6.0 18.0 6.0 18.0
6.0 18.0 6.0 100.0];
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
```


APPENDIX R

M Files for Human Equivalent Concentrations (HECs) Predictions

The following are M files for generating the HECs to correspond to the mouse and rat dose metrics. Values for “Target” in FitHumanDMs.m are the mouse or rat dose metric values from running the RunDMs.m file.

Female_Fit_DMs_ContInh.m

```
% Fit female human continuous inhalation doses to animal internal dosemetrics

load @format=model @file=New_EPA
Init
CheckOutput=[]; DMOutput=[]; Params=[]; i = 0;

% Set parameters for simulations
FitDoses = []; j = 0; Sex = 'Female';
ResetDoses
FemalePost
ConcFit = 'ContInh';
CONCLIST=[10.0 0.0]; STRTNEXTLIST=[10000.0]; TSTRT=0.0; DMINT=24.0; TSTP=1344.0; CINT=0.1;

FitHumanDMs

% Save the results of the dose fitting
save FitDoses @file='FitDoses_Female_ContInh_DMs.txt' @format=ascii
save CheckOutput @file='CheckOutput_FemaleContDMs.txt' @format=ascii
```

Female_Fit_DMs_OccInh.m

```
% Fit female human occupational (8 hr/d, 5 d/w) Occupational inhalation doses to animal internal
% dosemetrics

load @format=model @file=New_EPA
Init
CheckOutput=[]; DMOutput=[]; Params=[]; i = 0;

% Set parameters for simulations
FitDoses = []; j = 0; Sex = 'Female';
ResetDoses
FemalePost
ConcFit = 'OccInh ';
TSTRT=0.0; DMINT=168.0; TSTP=2184.0; CINT=0.1;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=10.0;
    STRTNEXTLIST(i1)=8.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=16.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=64.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;

FitHumanDMs

% Save the results of the dose fitting
save FitDoses @file='FitDoses_Female_OccInh_DMs.txt' @format=ascii
save CheckOutput @file='CheckOutput_FemaleOccDMs.txt' @format=ascii
```

Male_Fit_DMs_ContInh.m

```
% Fit male human continuous inhalation doses to animal internal dosemetrics

load @format=model @file=New_EPA
Init
CheckOutput=[]; DMOutput=[]; Params=[]; i = 0;

% Set parameters for simulations
FitDoses = []; j = 0; Sex = 'Male ';
ResetDoses
MalePost
ConcFit = 'ContInh';
CONCLIST=[10.0 0.0]; STRTNEXTLIST=[10000.0]; TSTRT=0.0; DMINT=24.0; TSTP=1344.0; CINT=0.1;

FitHumanDMS

% Save the results of the dose fitting
save FitDoses @file='FitDoses_Male_ContInh_DMs.txt' @format=ascii
save CheckOutput @file='CheckOutput_MaleContDMS.txt' @format=ascii
```

Male_Fit_DMs_OccInh.m

```
% Fit male human occupational (8 hr/d, 5 d/w) Occupational inhalation doses to animal internal
% dosemetrics

load @format=model @file=New_EPA
Init
CheckOutput=[]; DMOutput=[]; Params=[]; i = 0;

% Set parameters for simulations
FitDoses = []; j = 0; Sex = 'Male ';
ResetDoses
MalePost
ConcFit = 'OccInh ';
TSTRT=0.0; DMINT=168.0; TSTP=2184.0; CINT=0.1;
for iter = [1 : 65]
    i1=(2 * iter) - 1;
    CONCLIST(i1)=10.0;
    STRTNEXTLIST(i1)=8.0;
    CONCLIST(i1+1) = 0.0;
    STRTNEXTLIST(i1+1)=16.0;
end
for iter = [1 : 12]
    j1=iter*10;
    STRTNEXTLIST(j1)=64.0;
end
CONCLIST(131) = 0.0;
STRTNEXTLIST(130)=100.0;

FitHumanDMS

% Save the results of the dose fitting
save FitDoses @file='FitDoses_Male_OccInh_DMs.txt' @format=ascii
save CheckOutput @file='CheckOutput_MaleOccDMS.txt' @format=ascii
```


FitHumanDMS.m

```
% Cosby92 -- Mouse
% max(_cart)
    TargetParam='MaxCArt      '; Target=14.38; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM    '; Target=10.04; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=79.98; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=79.79; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% George85 -- Mouse
% max(_cart)
    TargetParam='MaxCArt      '; Target=3.205; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM    '; Target=26.28; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=300.7; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check
```

```

%% This block is commented out because metabolism was saturated and dose, if fit, would be larger
%% than 30,000 ppm
%% TotOxMetBW34DM
% TargetParam='TotOxMetBW34DM'; Target=300.1; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,10) = CONCLIST(1);
% FitDoses(i,11) = Target;
% FitDoses(i,12) = TOTOXMETBW34DM;
% Output_Check

% Griffin00 -- Mouse
% max(_cart)
% TargetParam='MaxCART'; Target=0.009553; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% i = i + 1;
% FitDoses(i,1) = CONCLIST(1);
% FitDoses(i,2) = Target;
% FitDoses(i,3) = max(_cart);
% Output_Check

% AUCCBLDDM
% TargetParam='AUCCBLDDM'; Target=0.2293; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,4) = CONCLIST(1);
% FitDoses(i,5) = Target;
% FitDoses(i,6) = AUCCBLDDM;
% Output_Check

% TotMetabBW34DM
% TargetParam='TotMetabBW34DM'; Target=5.840; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,7) = CONCLIST(1);
% FitDoses(i,8) = Target;
% FitDoses(i,9) = TOTMETABBW34DM;
% Output_Check

% TotOxMetBW34DM
% TargetParam='TotOxMetBW34DM'; Target=5.834; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,10) = CONCLIST(1);
% FitDoses(i,11) = Target;
% FitDoses(i,12) = TOTOXMETBW34DM;
% Output_Check

% Kaneko00 -- Mouse
% max(_cart)
% TargetParam='MaxCART'; Target=17.91; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% i = i + 1;
% FitDoses(i,1) = CONCLIST(1);
% FitDoses(i,2) = Target;
% FitDoses(i,3) = max(_cart);
% Output_Check

% AUCCBLDDM
% TargetParam='AUCCBLDDM'; Target=60.62; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,4) = CONCLIST(1);
% FitDoses(i,5) = Target;
% FitDoses(i,6) = AUCCBLDDM;
% Output_Check

```

```

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=135.1; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=134.7; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Kjellstrand83b -- Mouse -- Female
% max(_cart)
    TargetParam='MaxCArt          '; Target=0.7902; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM        '; Target=18.96; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=146.4; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=146.3; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% max(_cliv)
    TargetParam='MaxCLiv          '; Target=0.3001; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,13) = CONCLIST(1);
    FitDoses(i,14) = Target;
    FitDoses(i,15) = max(_cliv);
    Output_Check

```

```

% AUCCLivDM
    TargetParam='AUCCLivDM      '; Target=7.202; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,16) = CONCLIST(1);
    FitDoses(i,17) = Target;
    FitDoses(i,18) = AUCCLIVDM;
    Output_Check

% AMetLiv1BW34DM
    TargetParam='AMetLiv1BW34DM'; Target=41.62; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,19) = CONCLIST(1);
    FitDoses(i,20) = Target;
    FitDoses(i,21) = AMETLIV1BW34DM;
    Output_Check

% Kjellstrand83b -- Mouse -- Male
% max(_cart)
    TargetParam='MaxCArt      '; Target=0.7885; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLdDM
    TargetParam='AUCCBLdDM      '; Target=18.92; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=146.7; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=146.6; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% max(_cliv)
    TargetParam='MaxCLiv      '; Target=0.2973; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,13) = CONCLIST(1);
    FitDoses(i,14) = Target;
    FitDoses(i,15) = max(_cliv);
    Output_Check

```

```

% AUCCLivDM
    TargetParam='AUCCLivDM      '; Target=7.134; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,16) = CONCLIST(1);
    FitDoses(i,17) = Target;
    FitDoses(i,18) = AUCCLIVDM;
    Output_Check

% AMetLiv1BW34DM
    TargetParam='AMetLiv1BW34DM'; Target=41.60; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,19) = CONCLIST(1);
    FitDoses(i,20) = Target;
    FitDoses(i,21) = AMETLIV1BW34DM;
    Output_Check

% Land81 -- Mouse
% max(_cart)
    TargetParam='MaxCART      '; Target=23.90; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM      '; Target=92.08; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=157.6; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=156.9; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Ramdhan10 -- Mouse
% max(_cart)
    TargetParam='MaxCART      '; Target=23.50; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

```

```

% AUCCBLDDM
    TargetParam='AUCCBLDDM      '; Target=179.9; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=287.6; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

%% This block is commented out because metabolism was saturated and dose, if fit, would be larger
%% than 30,000 ppm
%% TotOxMetBW34DM
% TargetParam='TotOxMetBW34DM'; Target=286.2; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,10) = CONCLIST(1);
% FitDoses(i,11) = Target;
% FitDoses(i,12) = TOTOXMETBW34DM;
% Output_Check

% max(_cliv)
    TargetParam='MaxCLiv      '; Target=29.21; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,13) = CONCLIST(1);
    FitDoses(i,14) = Target;
    FitDoses(i,15) = max(_cliv);
    Output_Check

% AUCCLivDM
    TargetParam='AUCCLivDM      '; Target=204.7; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,16) = CONCLIST(1);
    FitDoses(i,17) = Target;
    FitDoses(i,18) = AUCCLIVDM;
    Output_Check

%% This block is commented out because metabolism was saturated and dose, if fit, would be larger
%% than 30,000 ppm
%% AMetLiv1BW34DM
% TargetParam='AMetLiv1BW34DM'; Target=228.0; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,19) = CONCLIST(1);
% FitDoses(i,20) = Target;
% FitDoses(i,21) = AMETLIV1BW34DM;
% Output_Check

% Sanders82 -- Mouse -- Female
% max(_cart)
    TargetParam='MaxCART      '; Target=0.01313; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

```

```

% AUCCBLDDM
    TargetParam='AUCCBLDDM      '; Target=0.3151; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=7.868; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=7.861; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Sanders82 -- Mouse -- Male
% max(_cart)
    TargetParam='MaxCART      '; Target=0.01318; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM      '; Target=0.3163; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=8.295; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=8.288; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

```

```

% Schwetz75 -- Mouse
% max(_cart)
    TargetParam='MaxCART          '; Target=9.794; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM        '; Target=67.89; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=193.4; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

%% This block is commented out because metabolism was saturated and dose, if fit, would be larger
%% than 30,000 ppm
%% TotOxMetBW34DM
% TargetParam='TotOxMetBW34DM'; Target=193.0; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,10) = CONCLIST(1);
% FitDoses(i,11) = Target;
% FitDoses(i,12) = TOTOXMETBW34DM;
% Output_Check

% Adams51 -- Rat -- Female
% max(_cart)
    TargetParam='MaxCART          '; Target=6.034; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM        '; Target=28.36; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=56.65; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

```



```

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=56.59; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% max(_cliv)
    TargetParam='MaxCLiv      '; Target=4.331; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,13) = CONCLIST(1);
    FitDoses(i,14) = Target;
    FitDoses(i,15) = max(_cliv);
    Output_Check

% AUCCLivDM
    TargetParam='AUCCLivDM    '; Target=17.77; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,16) = CONCLIST(1);
    FitDoses(i,17) = Target;
    FitDoses(i,18) = AUCCLIVDM;
    Output_Check

% AMetLiv1BW34DM
    TargetParam='AMetLiv1BW34DM'; Target=53.07; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,19) = CONCLIST(1);
    FitDoses(i,20) = Target;
    FitDoses(i,21) = AMETLIV1BW34DM;
    Output_Check

% max(_ckid)
    TargetParam='MaxCKid      '; Target=7.369; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,22) = CONCLIST(1);
    FitDoses(i,23) = Target;
    FitDoses(i,24) = max(_ckid);
    Output_Check

% AUCCKidDM
    TargetParam='AUCCKidDM    '; Target=34.62; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,25) = CONCLIST(1);
    FitDoses(i,26) = Target;
    FitDoses(i,27) = AUCCKIDDM;
    Output_Check

% AMetKidBW34DM
    TargetParam='AMetKidBW34DM '; Target=0.04146; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,28) = CONCLIST(1);
    FitDoses(i,29) = Target;
    FitDoses(i,30) = AMETKIDBW34DM;
    Output_Check

```

```

% Adams51 -- Rat -- Male
% max(_cart)
    TargetParam='MaxCART          '; Target=5.360; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM        '; Target=25.73; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=58.92; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=58.85; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% max(_cliv)
    TargetParam='MaxCLiv          '; Target=3.042; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,13) = CONCLIST(1);
    FitDoses(i,14) = Target;
    FitDoses(i,15) = max(_cliv);
    Output_Check

% AUCCLivDM
    TargetParam='AUCCLivDM        '; Target=12.76; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,16) = CONCLIST(1);
    FitDoses(i,17) = Target;
    FitDoses(i,18) = AUCCLIVDM;
    Output_Check

% AMetLiv1BW34DM
    TargetParam='AMetLiv1BW34DM'; Target=54.86; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,19) = CONCLIST(1);
    FitDoses(i,20) = Target;
    FitDoses(i,21) = AMETLIV1BW34DM;
    Output_Check

```

```

% max(_ckid)
    TargetParam='MaxCKid      '; Target=6.545; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,22) = CONCLIST(1);
    FitDoses(i,23) = Target;
    FitDoses(i,24) = max(_ckid);
    Output_Check

% AUCCKidDM
    TargetParam='AUCCKidDM    '; Target=31.41; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,25) = CONCLIST(1);
    FitDoses(i,26) = Target;
    FitDoses(i,27) = AUCCKIDDM;
    Output_Check

% AMetKidBW34DM
    TargetParam='AMetKidBW34DM '; Target=0.04805; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,28) = CONCLIST(1);
    FitDoses(i,29) = Target;
    FitDoses(i,30) = AMETKIDBW34DM;
    Output_Check

% Albee06 -- Rat -- Female
% max(_cart)
    TargetParam='MaxCART      '; Target=55.80; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBlDDM
    TargetParam='AUCCBlDDM    '; Target=222.8; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=95.52; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=95.07; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

```

```

% Albee06 -- Rat -- Male
% max(_cart)
    TargetParam='MaxCart          '; Target=50.59; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM        '; Target=200.4; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=112.9; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=112.5; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Arito94 -- Rat
% max(_cart)
    TargetParam='MaxCart          '; Target=0.3464; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM        '; Target=1.979; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=8.287; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

```

```

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=8.262; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Bushnell97 -- Rat -- One day
% max(_cart)
    TargetParam='MaxCArt      '; Target=50.88; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM    '; Target=65.22; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=56.55; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=56.39; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Bushnell97 -- Rat -- Two weeks
% max(_cart)
    TargetParam='MaxCArt      '; Target=50.88; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM    '; Target=27.95; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

```

```

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=24.24; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=24.17; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Carney06 -- Rat
% max(_cart)
    TargetParam='MaxCArt          '; Target=37.54; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM        '; Target=203.5; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=124.0; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=123.5; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Crofton97 -- Rat
% max(_cart)
    TargetParam='MaxCArt          '; Target=91.63; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

```

```

% AUCCBLDDM
    TargetParam='AUCCBLDDM'; Target=386.8; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=158.6; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=157.6; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Fisher01 -- Rat
% max(_cart)
    TargetParam='MaxCART'; Target=124.1; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM'; Target=250.1; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=170.2; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    if (Sex == 'Male ')
        TargetParam='TotOxMetBW34DM'; Target=169.4; Tolerance=Target/1000000.0;
        start @NoCallback
        Fit_Dose
        FitDoses(i,10) = CONCLIST(1);
        FitDoses(i,11) = Target;
        FitDoses(i,12) = TOTOXMETBW34DM;
        Output_Check
        save FitDoses @file='FitDoses_DMs.txt' @format=ascii
    end

```

```

% Healy82 -- Rat
% max(_cart)
    TargetParam='MaxCart          '; Target=2.200; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM        '; Target=8.918; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=25.39; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=25.35; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Jaspers93 -- Rat
% max(_cart)
    TargetParam='MaxCart          '; Target=132.5; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM        '; Target=1635.0; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=241.2; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

```



```

%% This block is commented out because metabolism was saturated and dose, if fit, would be larger
%% than 30,000 ppm
%% TotOxMetBW34DM
% TargetParam='TotOxMetBW34DM'; Target=237.7; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,10) = CONCLIST(1);
% FitDoses(i,11) = Target;
% FitDoses(i,12) = TOTOXMETBW34DM;
% Output_Check

% Kumar00a & Kumar01a -- Rat
% max(_cart)
% TargetParam='MaxCART'; Target=13.25; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% i = i + 1;
% FitDoses(i,1) = CONCLIST(1);
% FitDoses(i,2) = Target;
% FitDoses(i,3) = max(_cart);
% Output_Check

% AUCCBLDDM
% TargetParam='AUCCBLDDM'; Target=34.88; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,4) = CONCLIST(1);
% FitDoses(i,5) = Target;
% FitDoses(i,6) = AUCCBLDDM;
% Output_Check

% TotMetabBW34DM
% TargetParam='TotMetabBW34DM'; Target=57.29; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,7) = CONCLIST(1);
% FitDoses(i,8) = Target;
% FitDoses(i,9) = TOTMETABBW34DM;
% Output_Check

% TotOxMetBW34DM
% TargetParam='TotOxMetBW34DM'; Target=57.20; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,10) = CONCLIST(1);
% FitDoses(i,11) = Target;
% FitDoses(i,12) = TOTOXMETBW34DM;
% Output_Check

% max(_cliv)
% TargetParam='MaxCLiv'; Target=13.26; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,13) = CONCLIST(1);
% FitDoses(i,14) = Target;
% FitDoses(i,15) = max(_cliv);
% Output_Check

% AUCCLIVDM
% TargetParam='AUCCLIVDM'; Target=27.56; Tolerance=Target/1000000.0;
% start @NoCallback
% Fit_Dose
% FitDoses(i,16) = CONCLIST(1);
% FitDoses(i,17) = Target;
% FitDoses(i,18) = AUCCLIVDM;
% Output_Check

```

```

% AMetLiv1BW34DM
    TargetParam='AMetLiv1BW34DM'; Target=53.85; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,19) = CONCLIST(1);
    FitDoses(i,20) = Target;
    FitDoses(i,21) = AMETLIV1BW34DM;
    Output_Check

% Maltoni88 -- Rat
% max(_cart)
    TargetParam='MaxCART'; Target=5.308; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBldDM
    TargetParam='AUCCBldDM'; Target=26.00; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=67.33; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=67.24; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% max(_ckid)
    TargetParam='MaxCKid'; Target=6.480; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,22) = CONCLIST(1);
    FitDoses(i,23) = Target;
    FitDoses(i,24) = max(_ckid);
    Output_Check

% AUCCKidDM
    TargetParam='AUCCKidDM'; Target=31.73; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,25) = CONCLIST(1);
    FitDoses(i,26) = Target;
    FitDoses(i,27) = AUCCKIDDM;
    Output_Check

```

```

% AMetKidBW34DM
    TargetParam='AMetKidBW34DM '; Target=0.06425; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,28) = CONCLIST(1);
    FitDoses(i,29) = Target;
    FitDoses(i,30) = AMETKIDBW34DM;
    Output_Check

% Manson84 -- Rat
% max(_cart)
    TargetParam='MaxCart      '; Target=23.13; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM    '; Target=20.12; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=66.10; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=65.98; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Narotsky95 -- Rat
% max(_cart)
    TargetParam='MaxCart      '; Target=5.966; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM    '; Target=3.550; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

```

```

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=21.02; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=20.99; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Schwetz75 -- Rat
% max(_cart)
    TargetParam='MaxCART'; Target=11.35; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM'; Target=71.04; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=112.9; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=112.7; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Woolhiser06 -- Rat -- Immuno
% max(_cart)
    TargetParam='MaxCART'; Target=8.387; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check
    save FitDoses @file='FitDoses_DMs.txt' @format=ascii

```

```

% AUCCBLDDM
    TargetParam='AUCCBLDDM      '; Target=32.73; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=56.36; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=56.29; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

% Woolhiser06 -- Rat -- kidney
% max(_cart)
    TargetParam='MaxCART      '; Target=2.057; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLDDM
    TargetParam='AUCCBLDDM      '; Target=8.757; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=24.32; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=24.28; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

```

```

% max(_ckid)
    TargetParam='MaxCKid      '; Target=2.510; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,22) = CONCLIST(1);
    FitDoses(i,23) = Target;
    FitDoses(i,24) = max(_ckid);
    Output_Check

% AUCCKidDM
    TargetParam='AUCCKidDM    '; Target=10.68; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,25) = CONCLIST(1);
    FitDoses(i,26) = Target;
    FitDoses(i,27) = AUCCKIDDM;
    Output_Check

% AMetKidBW34DM
    TargetParam='AMetKidBW34DM '; Target=0.03028; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,28) = CONCLIST(1);
    FitDoses(i,29) = Target;
    FitDoses(i,30) = AMETKIDBW34DM;
    Output_Check

% Woolhiser06 -- Rat -- liver
% max(_cart)
    TargetParam='MaxCART      '; Target=2.539; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBlDDM
    TargetParam='AUCCBlDDM    '; Target=10.76; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=28.70; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=28.66; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

```

```

% max(_cliv)
    TargetParam='MaxCLiv      '; Target=0.9786; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,13) = CONCLIST(1);
    FitDoses(i,14) = Target;
    FitDoses(i,15) = max(_cliv);
    Output_Check

% AUCCLivDM
    TargetParam='AUCCLivDM    '; Target=3.879; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,16) = CONCLIST(1);
    FitDoses(i,17) = Target;
    FitDoses(i,18) = AUCCLIVDM;
    Output_Check

% AMetLiv1BW34DM
    TargetParam='AMetLiv1BW34DM'; Target=25.88; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,19) = CONCLIST(1);
    FitDoses(i,20) = Target;
    FitDoses(i,21) = AMETLIV1BW34DM;
    Output_Check

% Wu07 -- Rat
% max(_cart)
    TargetParam='MaxCART      '; Target=0.09164; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    i = i + 1;
    FitDoses(i,1) = CONCLIST(1);
    FitDoses(i,2) = Target;
    FitDoses(i,3) = max(_cart);
    Output_Check

% AUCCBLdDM
    TargetParam='AUCCBLdDM    '; Target=2.199; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,4) = CONCLIST(1);
    FitDoses(i,5) = Target;
    FitDoses(i,6) = AUCCBLDDM;
    Output_Check

% TotMetabBW34DM
    TargetParam='TotMetabBW34DM'; Target=42.90; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,7) = CONCLIST(1);
    FitDoses(i,8) = Target;
    FitDoses(i,9) = TOTMETABBW34DM;
    Output_Check

% TotOxMetBW34DM
    TargetParam='TotOxMetBW34DM'; Target=42.85; Tolerance=Target/1000000.0;
    start @NoCallback
    Fit_Dose
    FitDoses(i,10) = CONCLIST(1);
    FitDoses(i,11) = Target;
    FitDoses(i,12) = TOTOXMETBW34DM;
    Output_Check

```

Fit_Dose.m

```
% Dose fitting algorithm -- uses ratios

if (TargetParam == 'MaxCART      ')
    EndPt = max(_cart);
else
    if (TargetParam == 'AUCCBldDM  ')
        EndPt = AUCCBLDDM;
    else
        if (TargetParam == 'MaxCLiv      ')
            EndPt = max(_cliv);
        else
            if (TargetParam == 'AUCCLivDM  ')
                EndPt = AUCCLIVDM;
            else
                if (TargetParam == 'TotMetabBW34DM')
                    EndPt = TOTMETABBW34DM;
                else
                    if (TargetParam == 'TotOxMetBW34DM')
                        EndPt = TOTOXMETBW34DM;
                    else
                        if (TargetParam == 'AMetLiv1BW34DM')
                            EndPt = AMETLIV1BW34DM;
                        else
                            if (TargetParam == 'MaxCKid      ')
                                EndPt = max(_ckid);
                            else
                                if (TargetParam == 'AUCCKidDM      ')
                                    EndPt = AUCCKIDDM;
                                else
                                    if (TargetParam == 'AMetKidBW34DM ')
                                        EndPt = AMETKIDBW34DM;
                                    end
                                end
                            end
                        end
                    end
                end
            end
        end
    end
end

NumAttempt = 0;
while abs(EndPt-Target) > Tolerance
    if (ConcFit == 'ContInh')
        CONCLIST(1) = CONCLIST(1) * (Target / EndPt);
    else
        TmpConc = CONCLIST(1) * (Target / EndPt);
        for iter = [1 : 65]
            i1 = (2 * iter) - 1;
            CONCLIST(i1) = TmpConc;
        end
    end

    start @NoCallback
    NumAttempt = NumAttempt + 1;
    CONCLIST(1)

    if (TargetParam == 'MaxCART      ')
        max(_cart)
        EndPt = max(_cart);
    else
        if (TargetParam == 'AUCCBldDM  ')
            AUCCBLDDM
            EndPt = AUCCBLDDM;
        else
            if (TargetParam == 'MaxCLiv      ')
                max(_cliv)
                EndPt = max(_cliv);
            end
        end
    end
end
```


end

APPENDIX S

Comparison of Predictions from the EPA and Harmonized Models

In the course of executing the acslX version of the USEPA (2011) model, questions arose as to how the model predictions compared to those that might be obtained from the harmonized model (Covington *et al.*, 2006; Hack *et al.*, 2006). In an effort to assess the differences between predictions of the two models, each model was executed for data sets which were common to the development of both models. These predictions were then plotted along with the study data for comparison. In some cases, data which appeared to be from the same source varied somewhat, and there were a few instances where data from the same source were in the harmonized model files more than once and varied slightly.

The figures of the comparisons are shown below for mouse (Figure S1), rat (Figure S2) and human (Figure S3). Some figures have predictions from only one of the models. In these cases, the other model did not include calculation of the given endpoint. Some figures also have data from the model files for only one model.

For further comparison, the harmonized model was also run to predict the internal animal dose metrics and to estimate the corresponding HECs (Tables S1 to S3). Note that since the harmonized model did not include a kidney compartment, dose metrics and HECs based on kidney endpoints are not included.

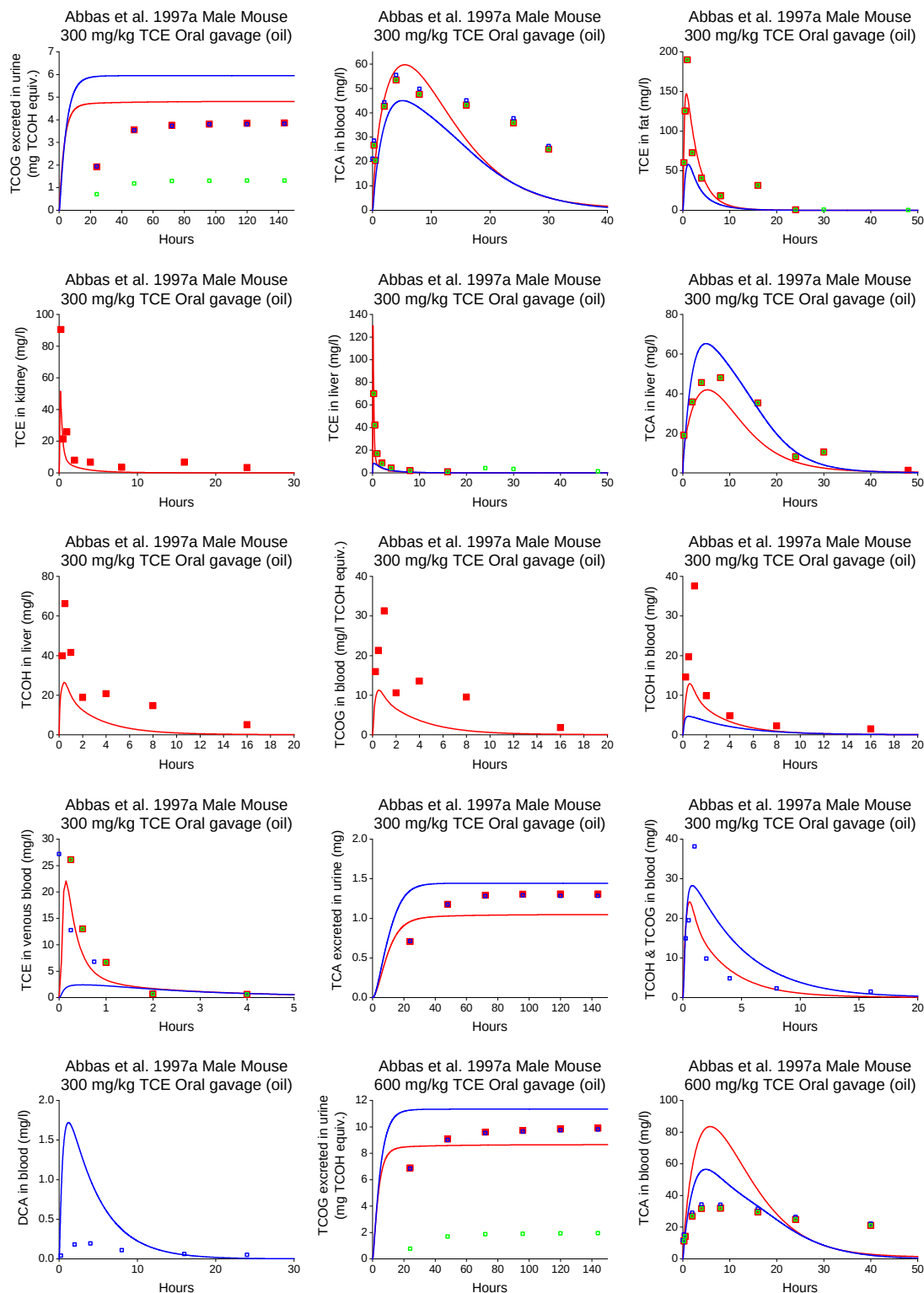


Figure S1. Comparison of Mouse Predictions. Red lines and symbols represent predictions from the acslX version of the USEPA (2011) model. Blue lines and symbols are for the harmonized model. Green symbols are duplicate data from the harmonized model files.

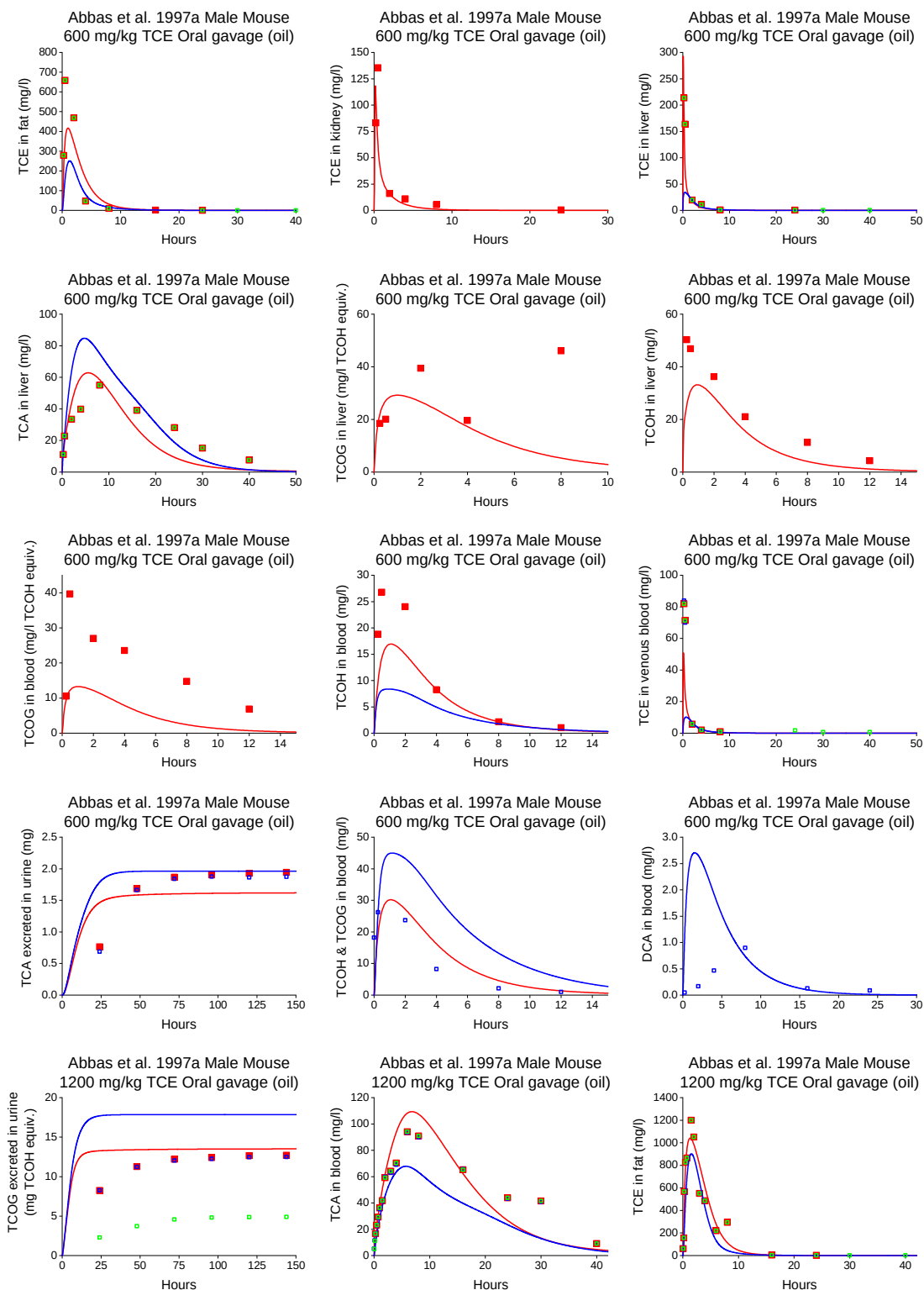


Figure S1. Comparison of Mouse Predictions (continued).

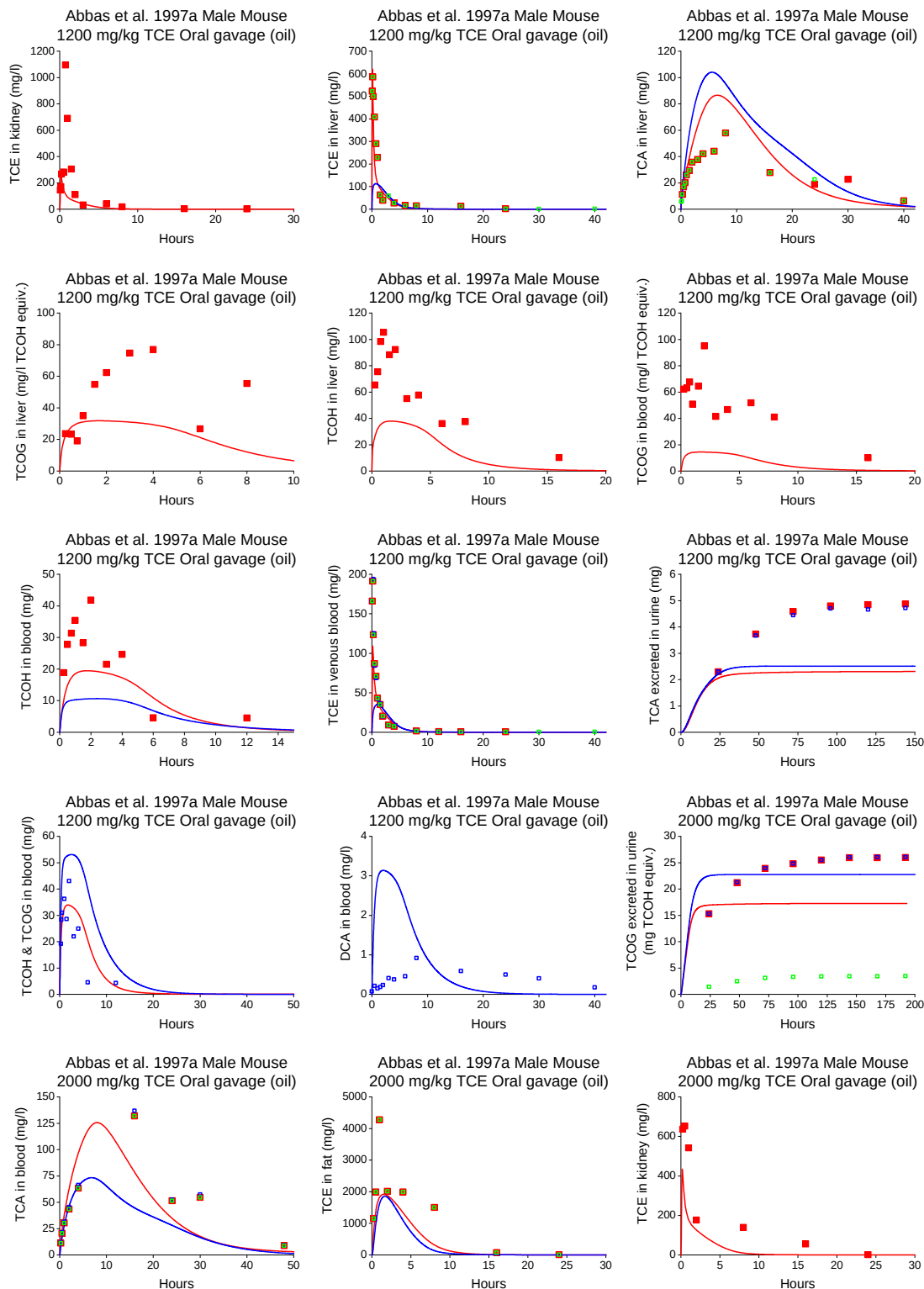


Figure S1. Comparison of Mouse Predictions (continued).

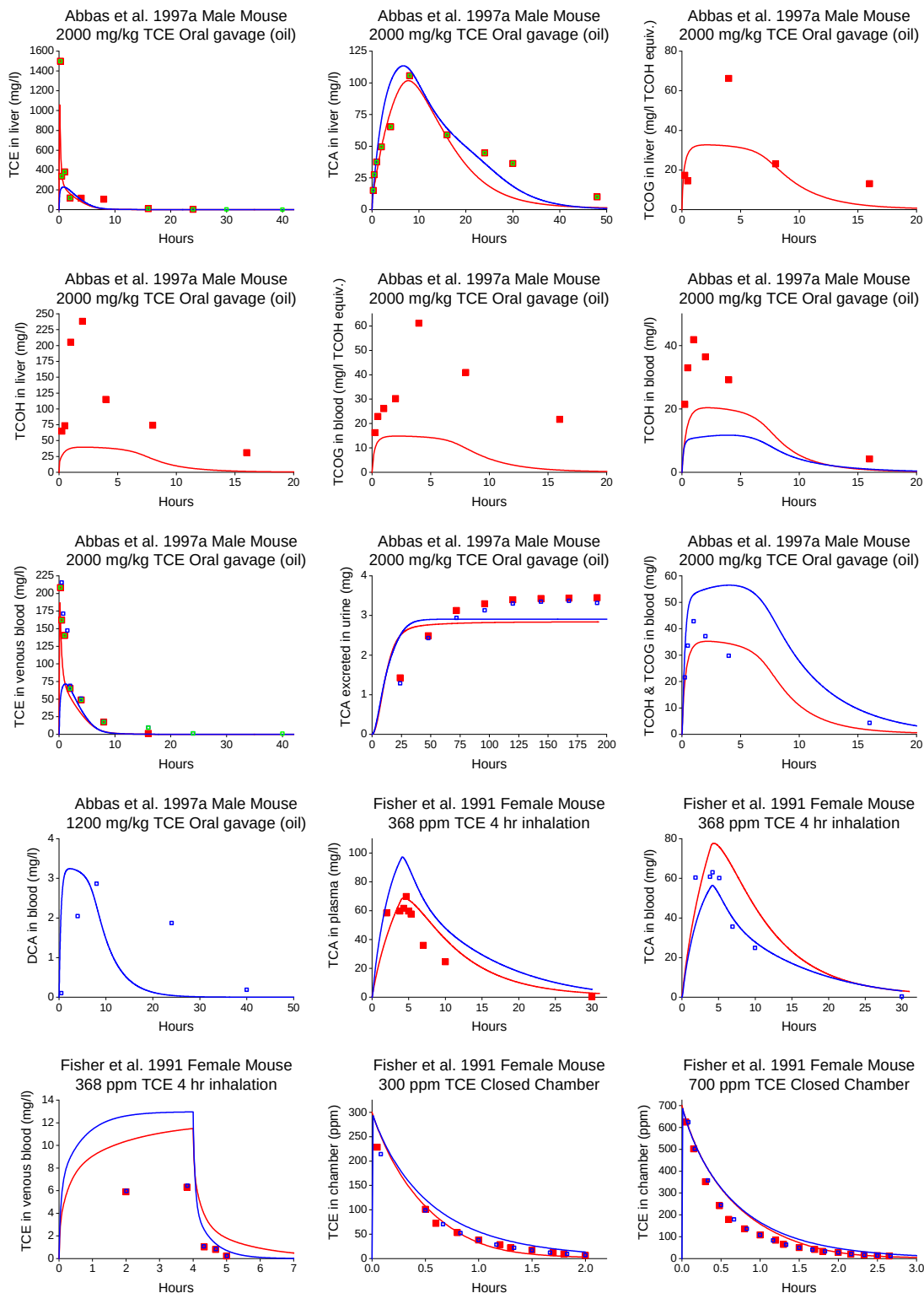


Figure S1. Comparison of Mouse Predictions (continued).

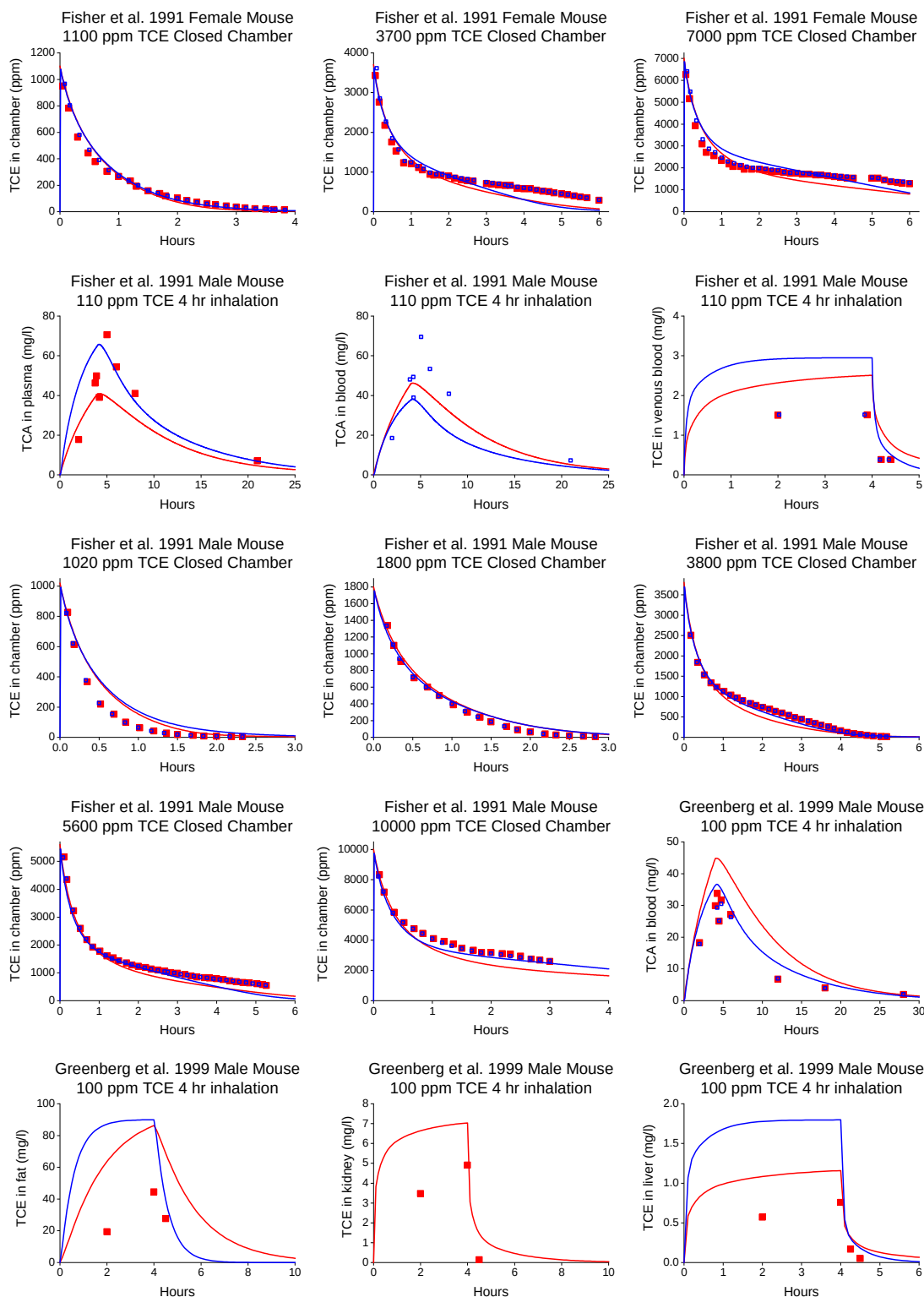


Figure S1. Comparison of Mouse Predictions (continued).

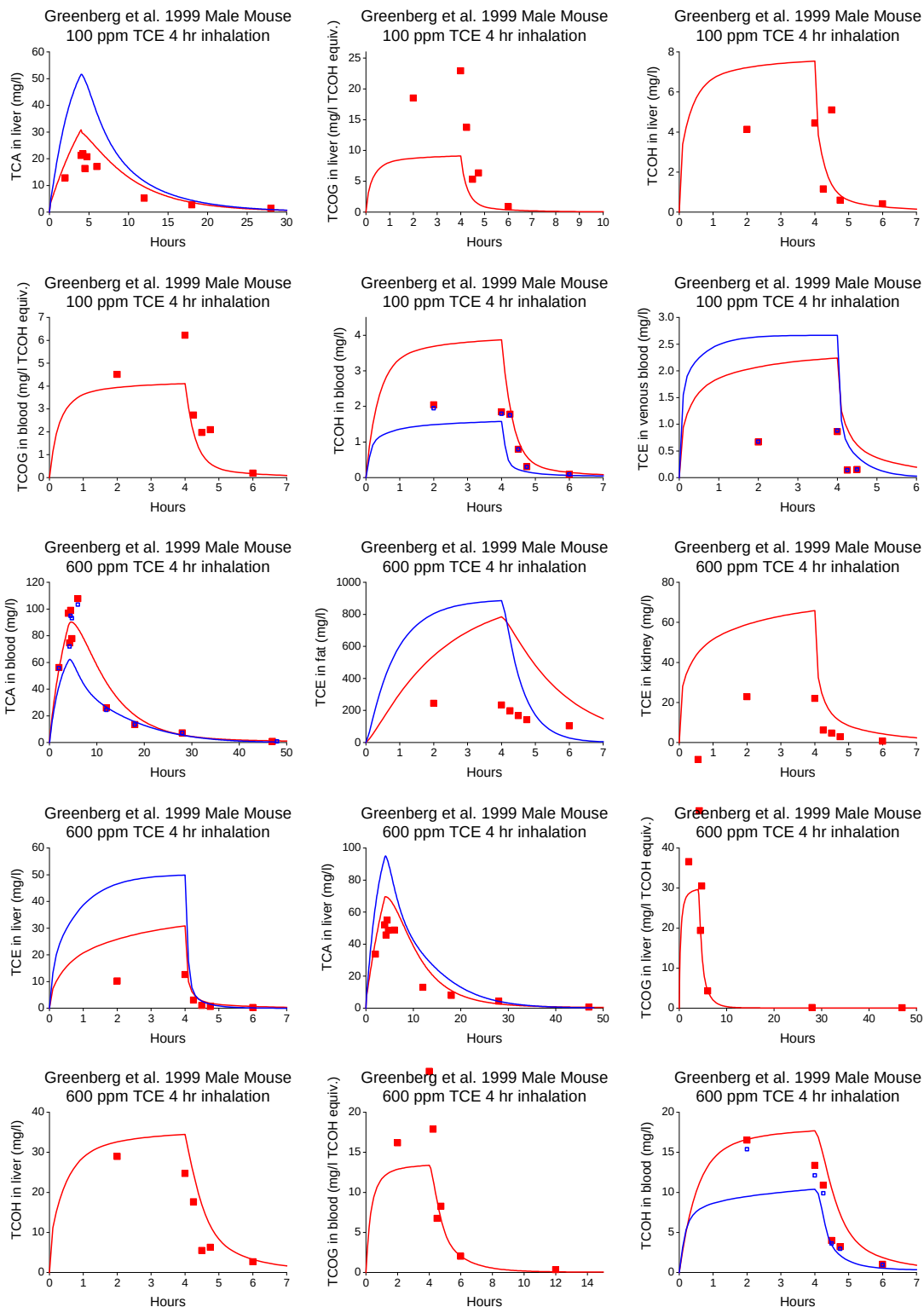


Figure S1. Comparison of Mouse Predictions (continued).

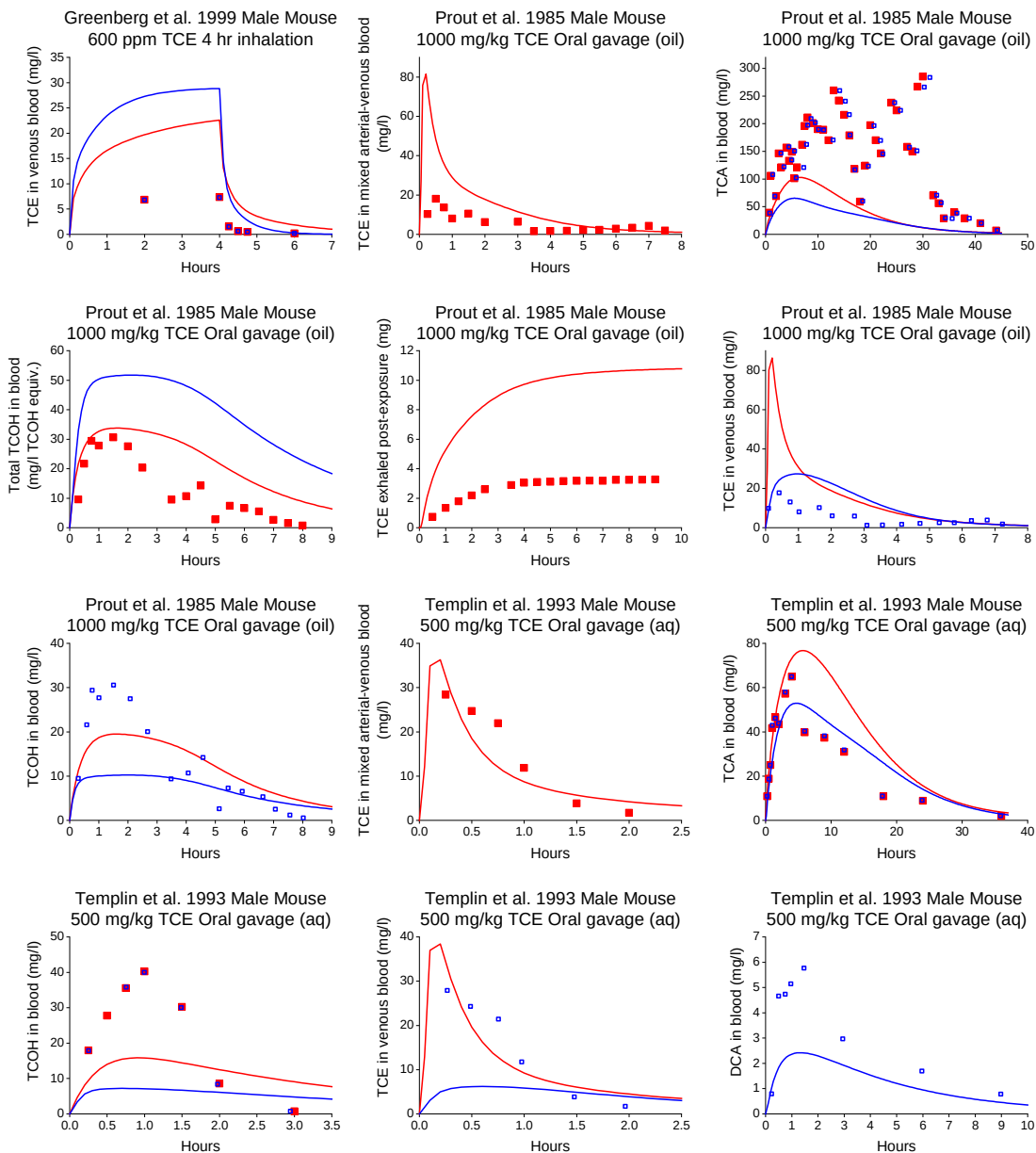


Figure S1. Comparison of Mouse Predictions (continued).

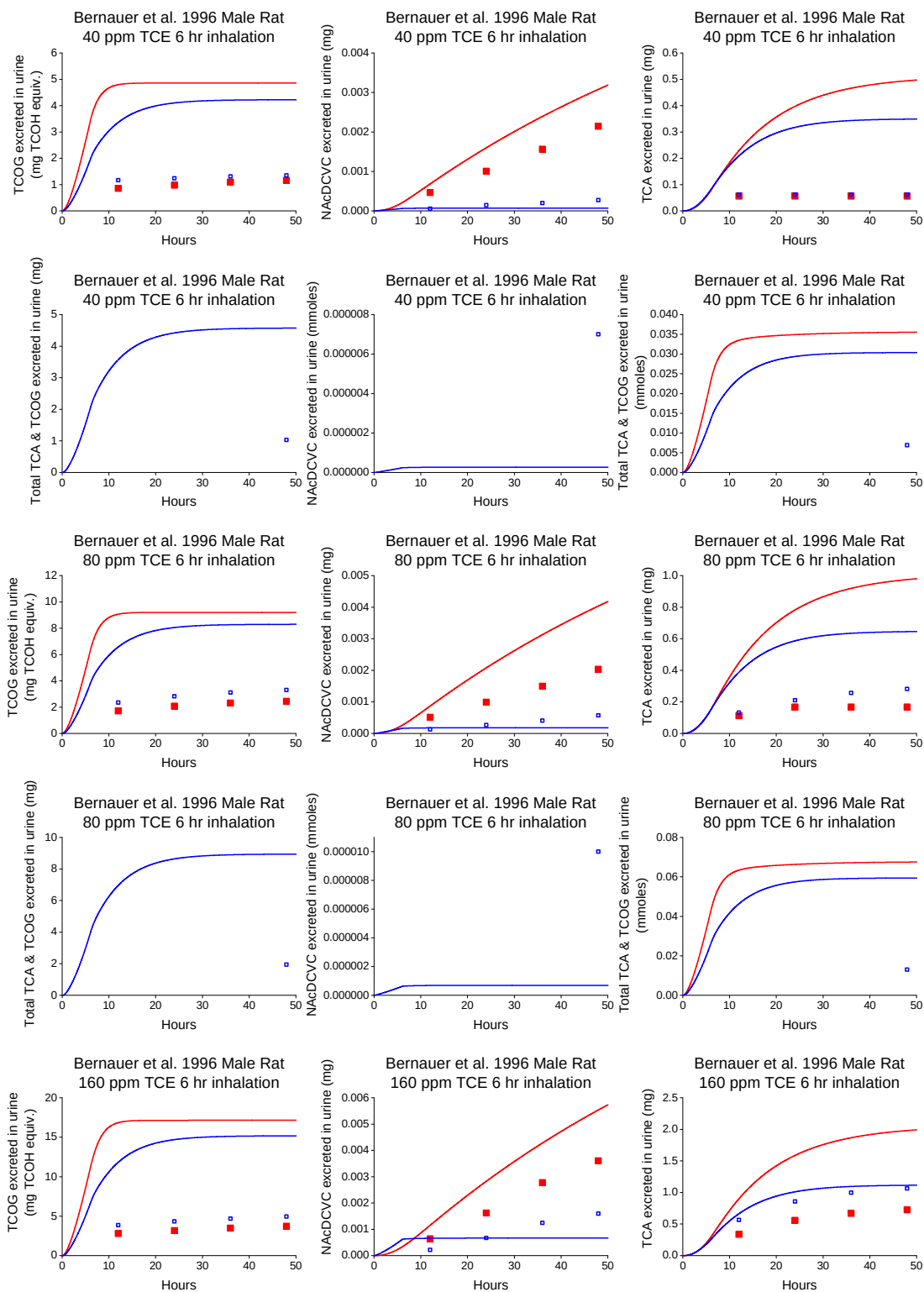


Figure S2. Comparison of Rat Predictions. Red lines and symbols represent predictions from the acslX version of the USEPA (2011) model. Blue lines and symbols are for the harmonized model.

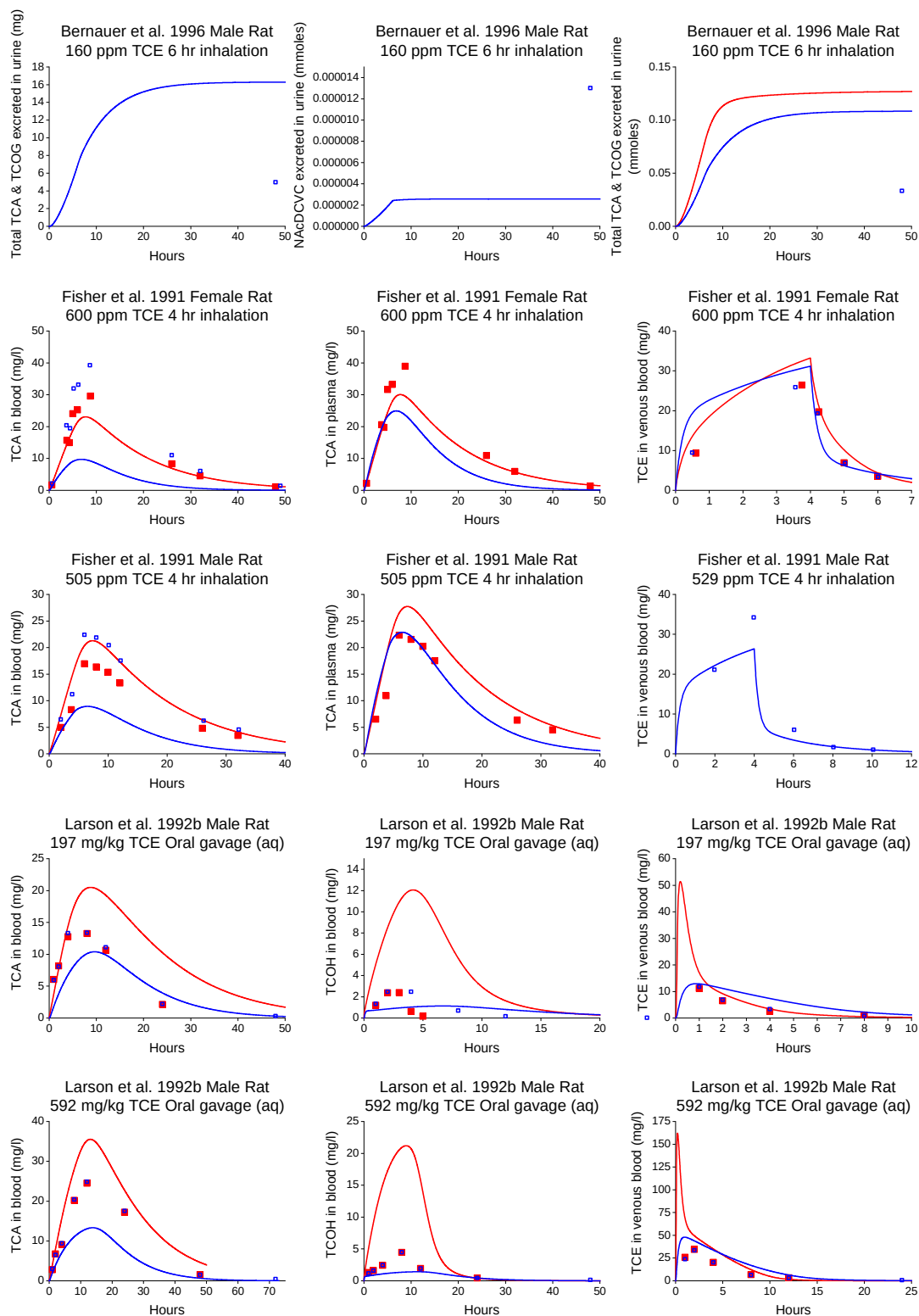


Figure S2. Comparison of Rat Predictions (continued).

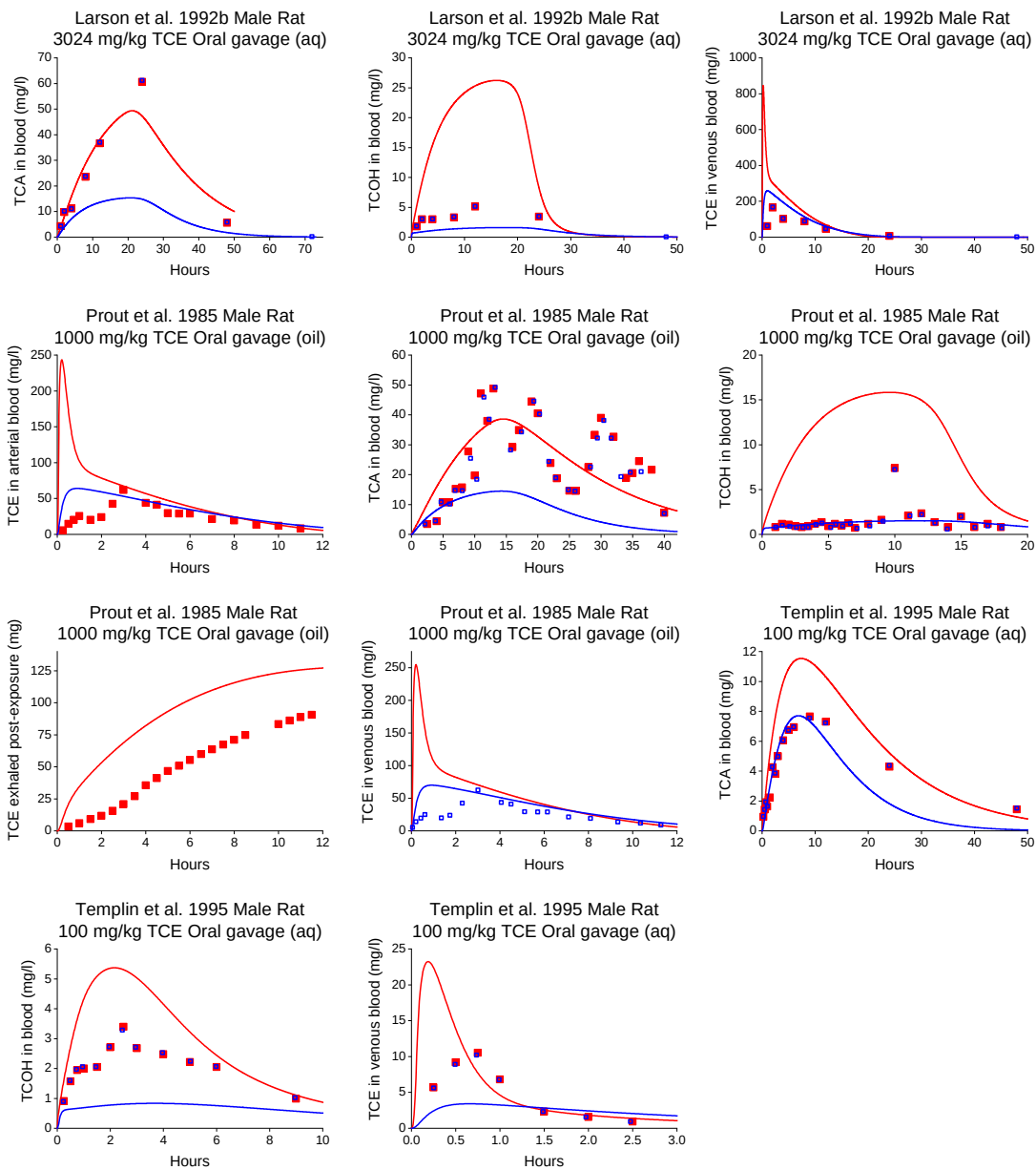


Figure S2. Comparison of Rat Predictions (continued).

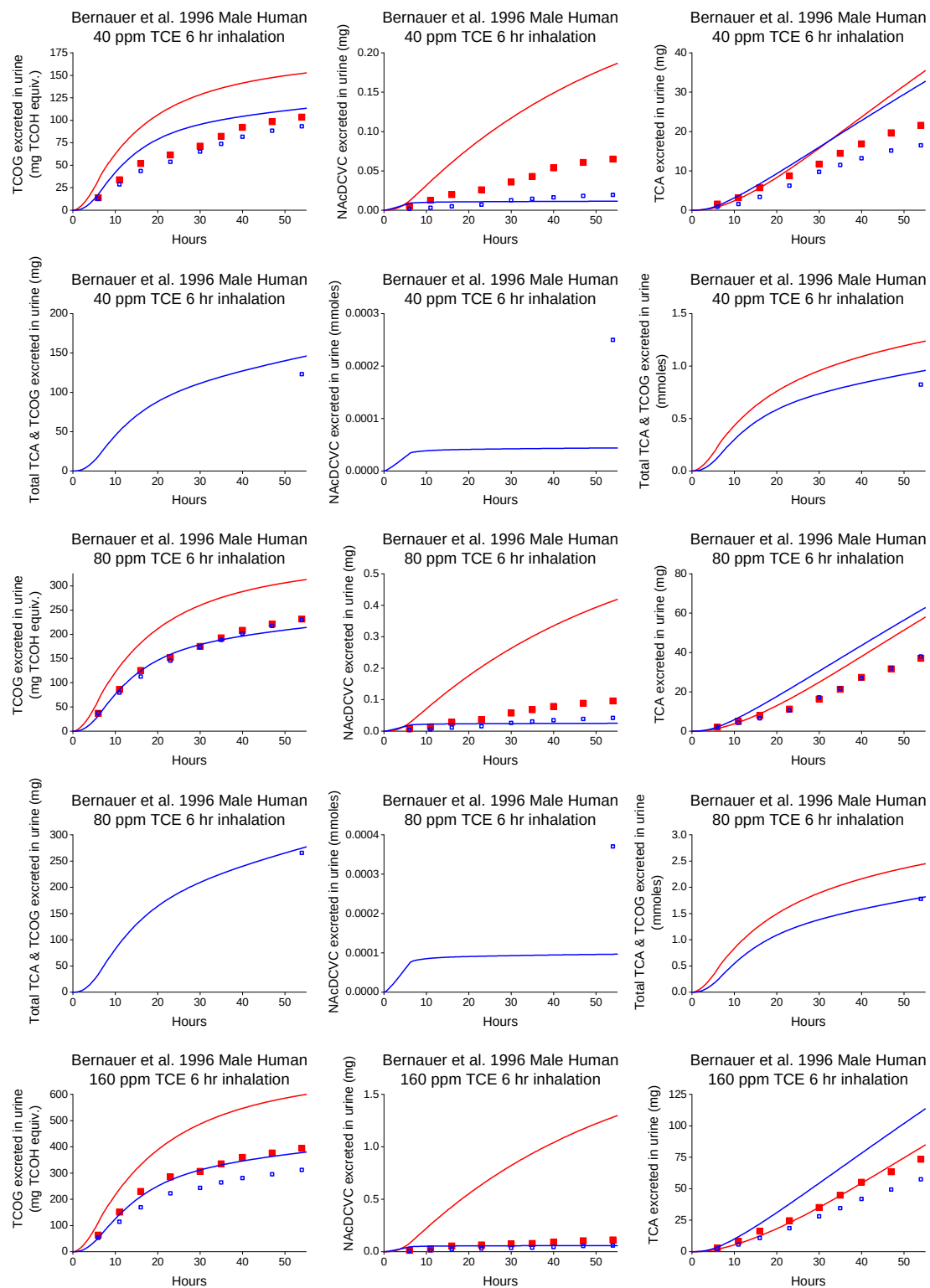


Figure S3. Comparison of Human Predictions. Red lines and symbols represent predictions from the acslX version of the USEPA (2011) model. Blue lines and symbols are for the harmonized model.

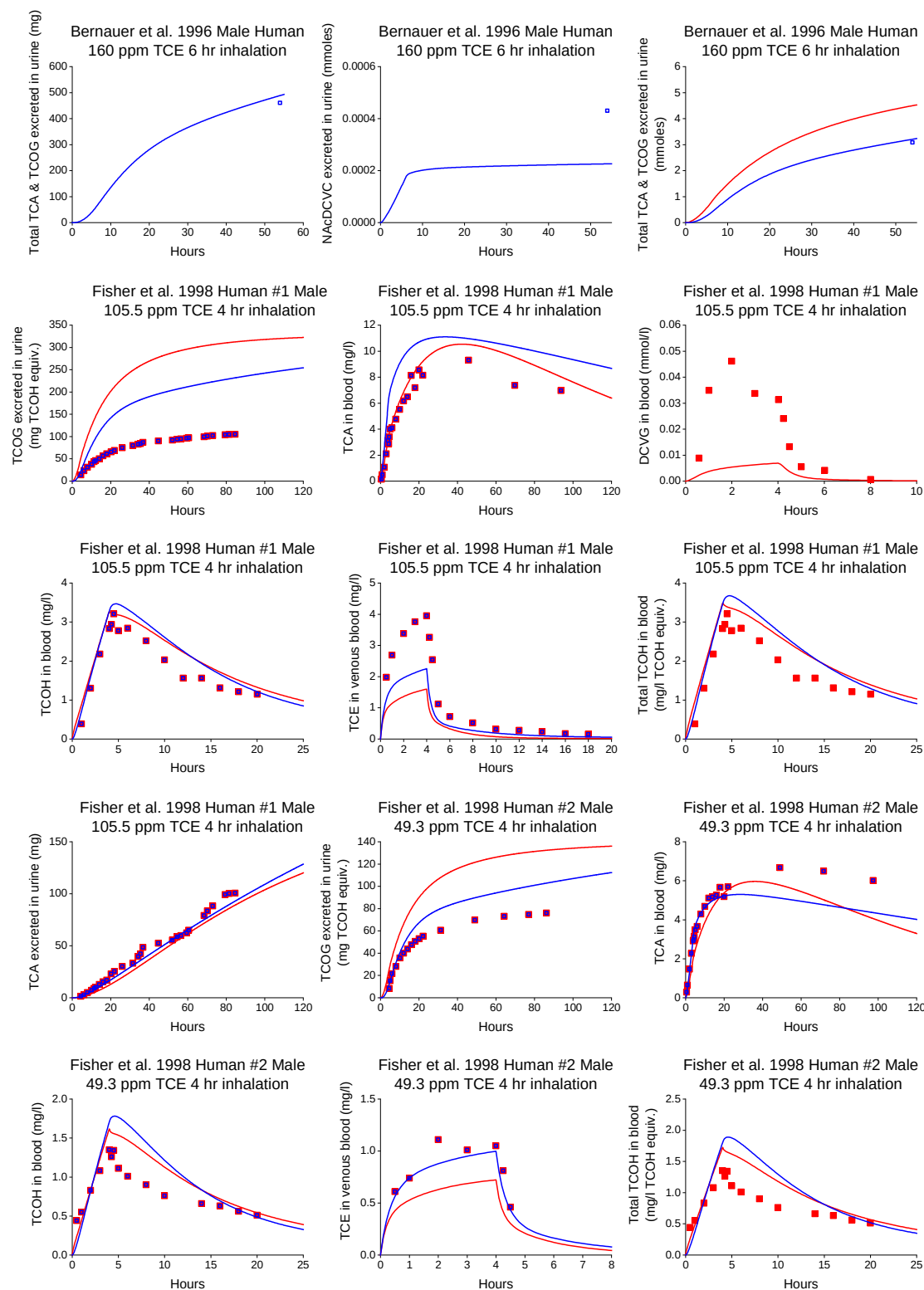


Figure S3. Comparison of Human Predictions (continued).

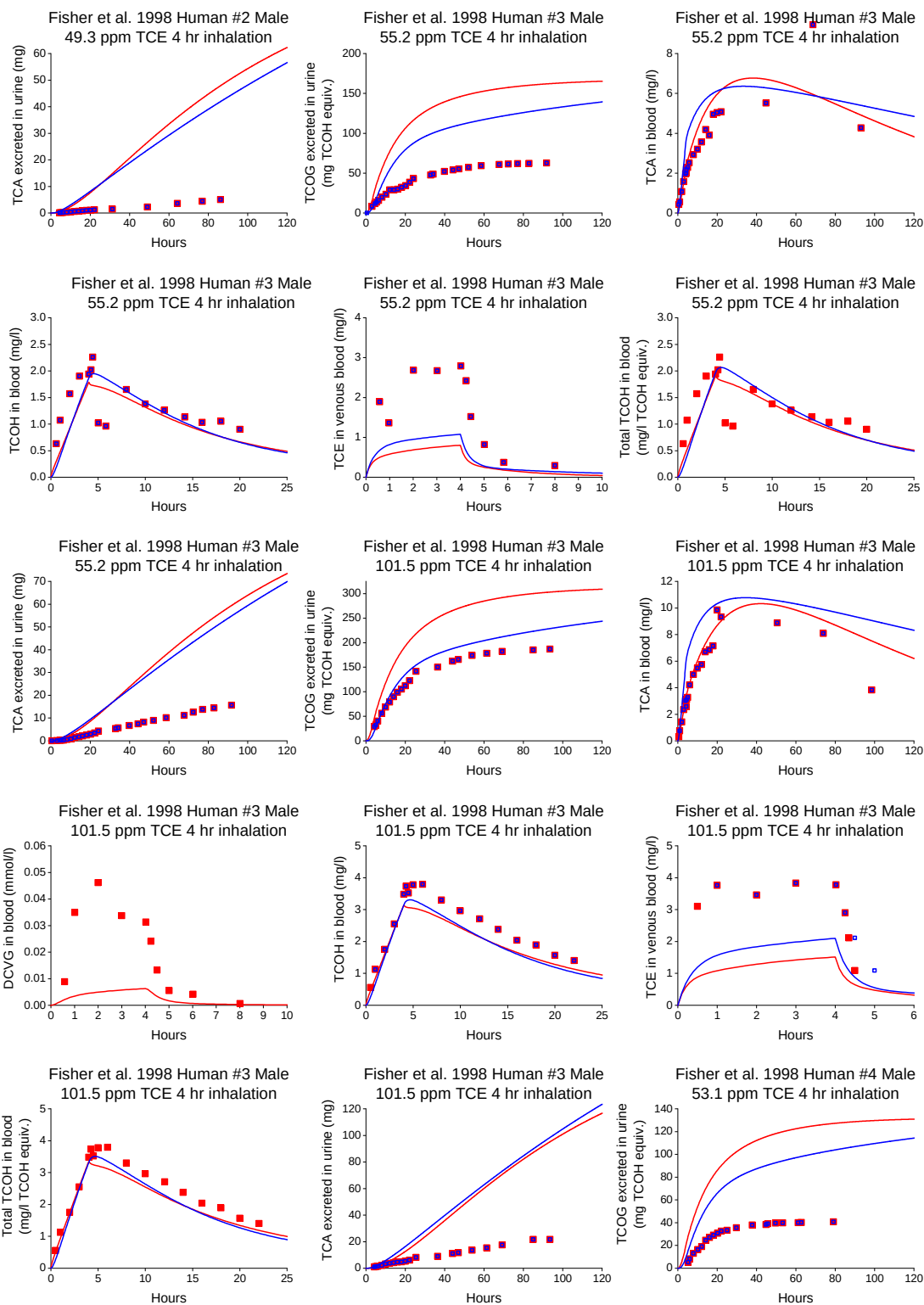


Figure S3. Comparison of Human Predictions (continued).

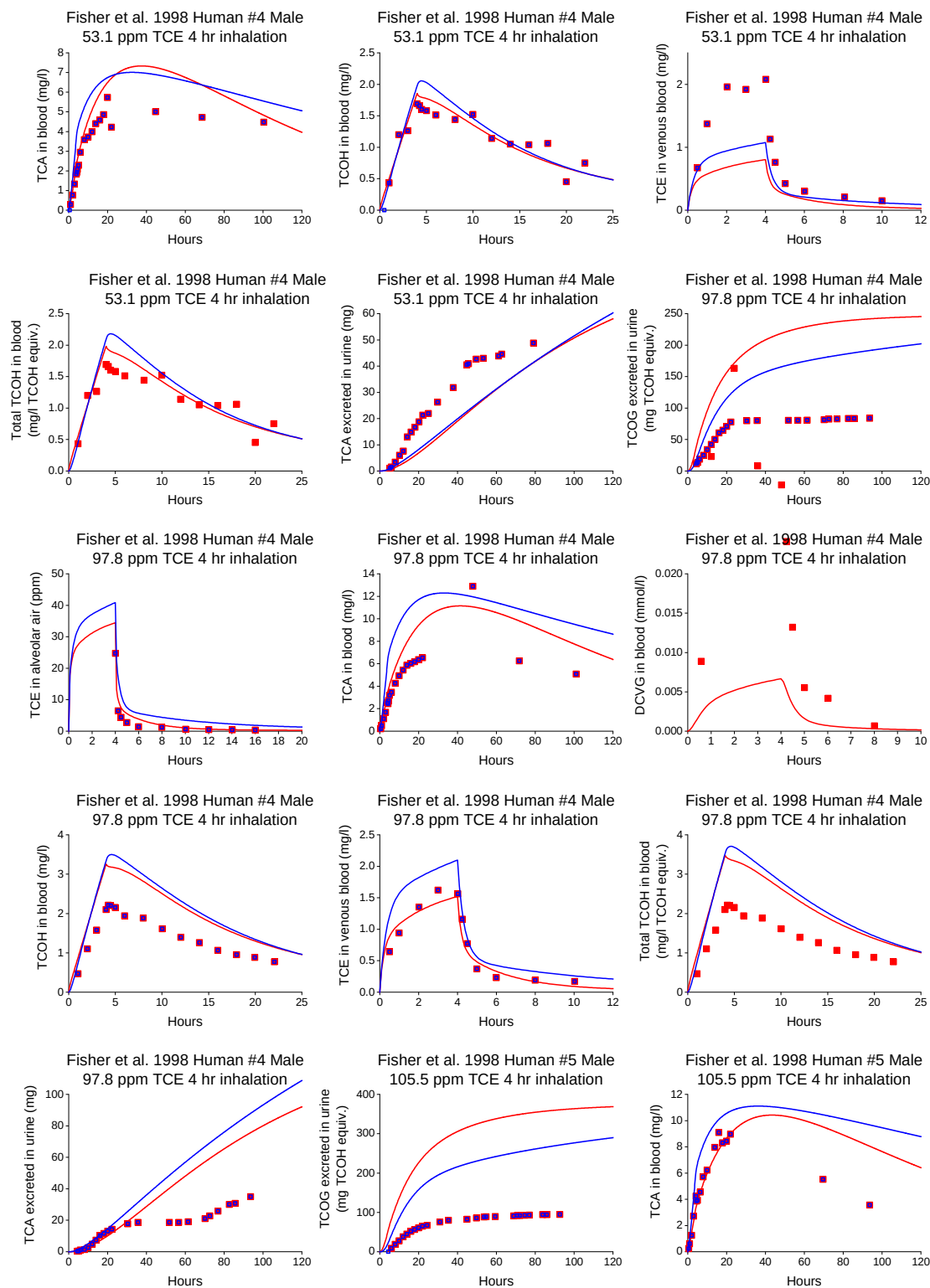


Figure S3. Comparison of Human Predictions (continued).

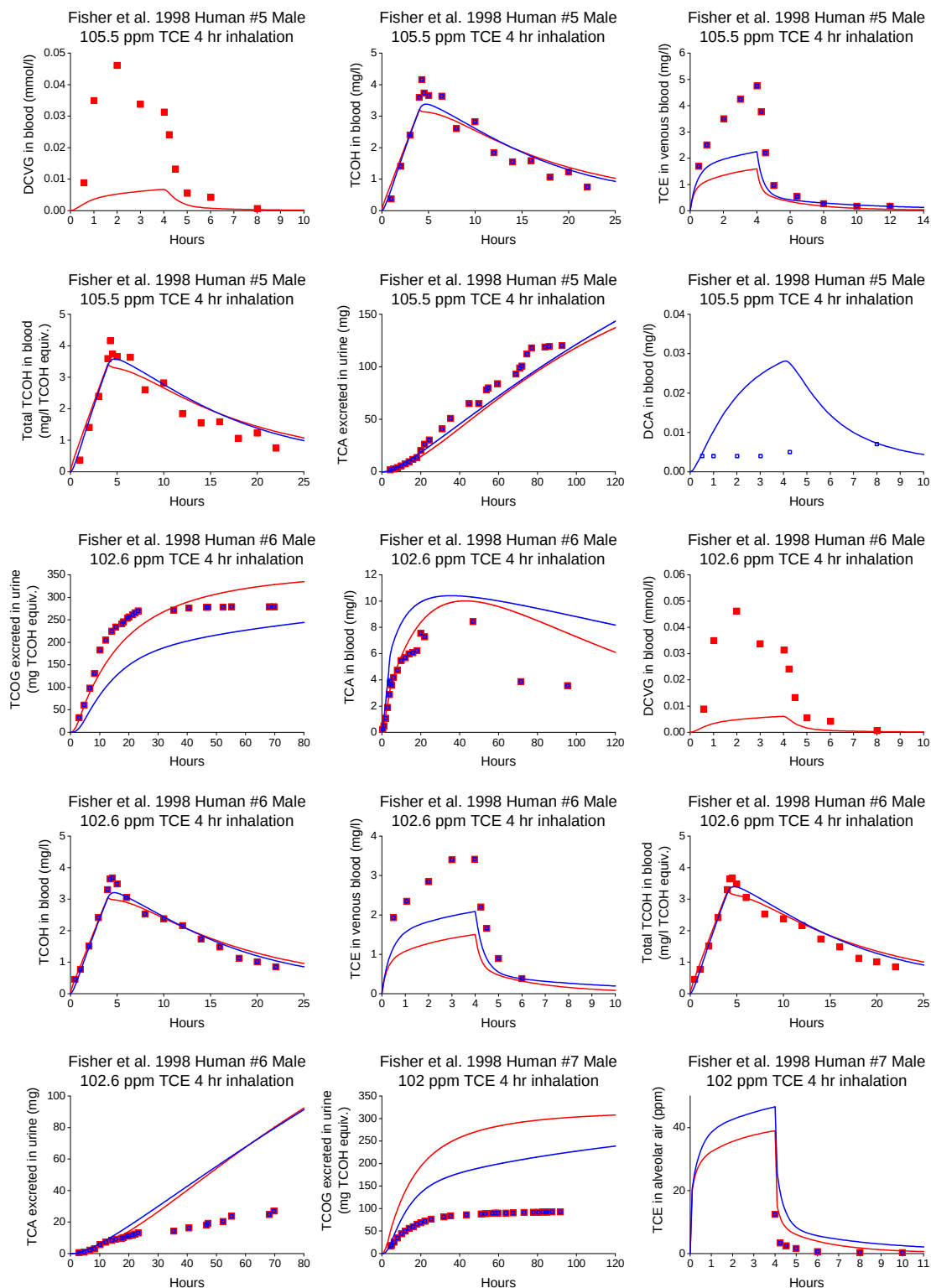


Figure S3. Comparison of Human Predictions (continued).

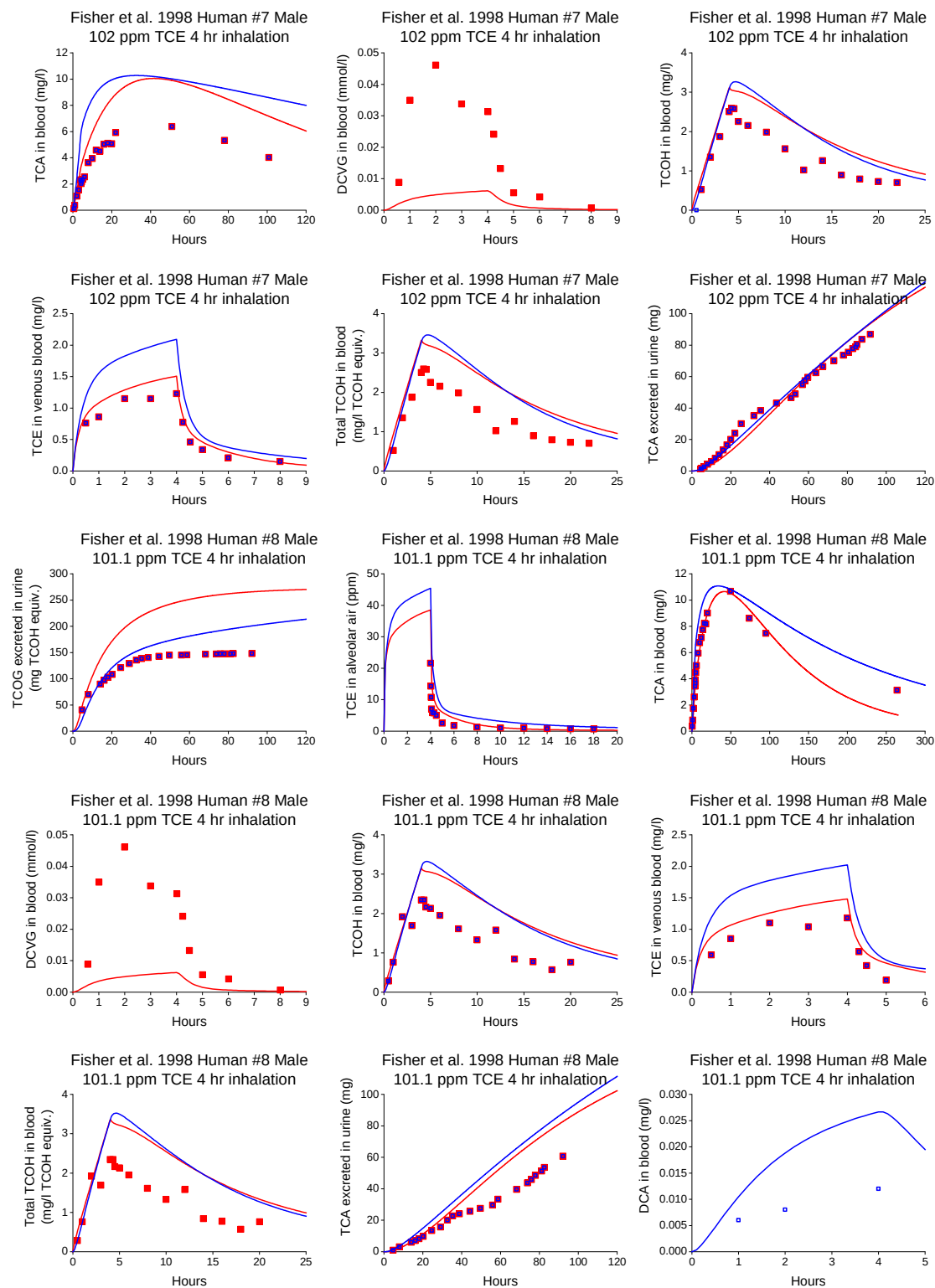


Figure S3. Comparison of Human Predictions (continued).

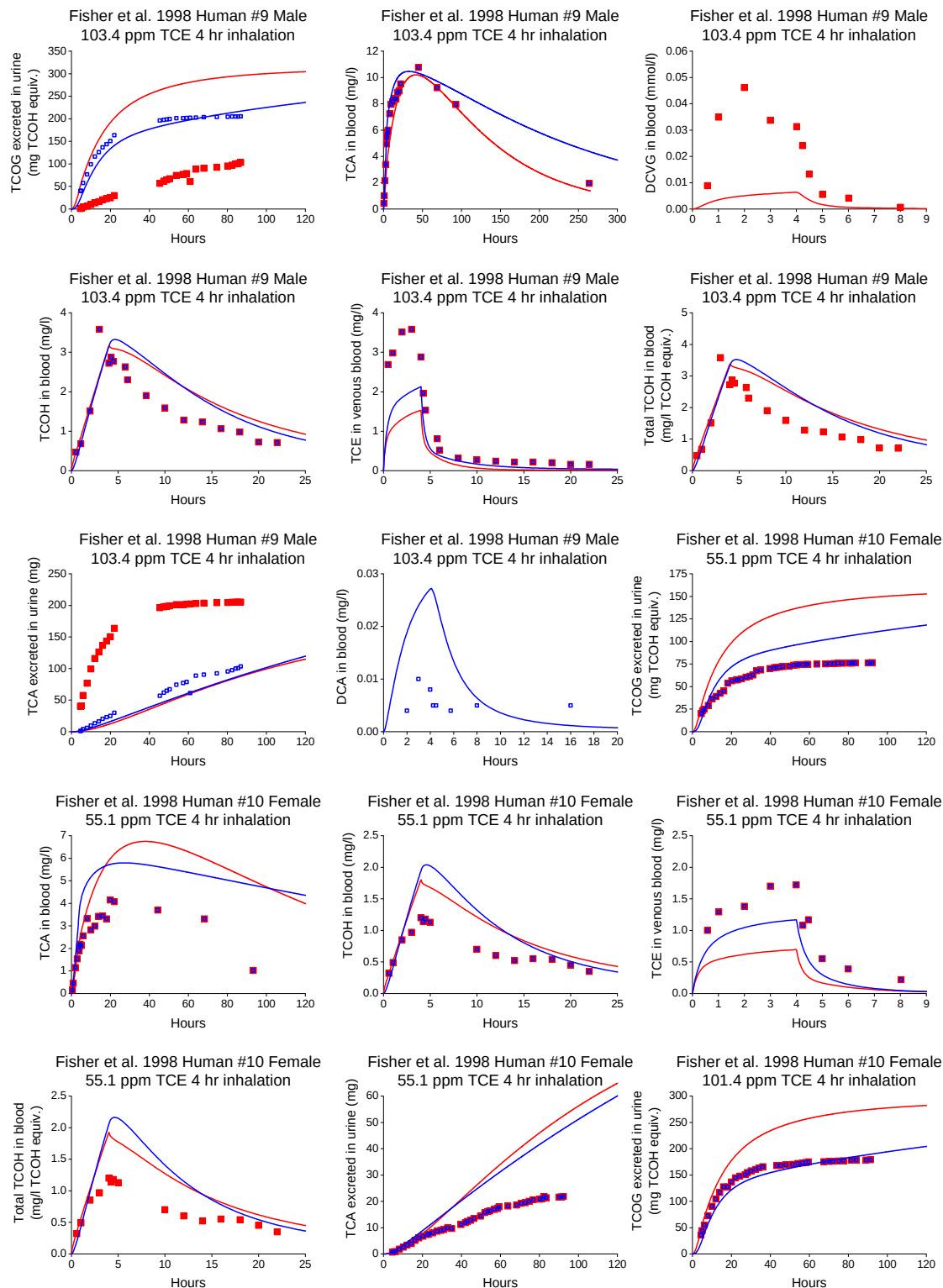


Figure S3. Comparison of Human Predictions (continued).

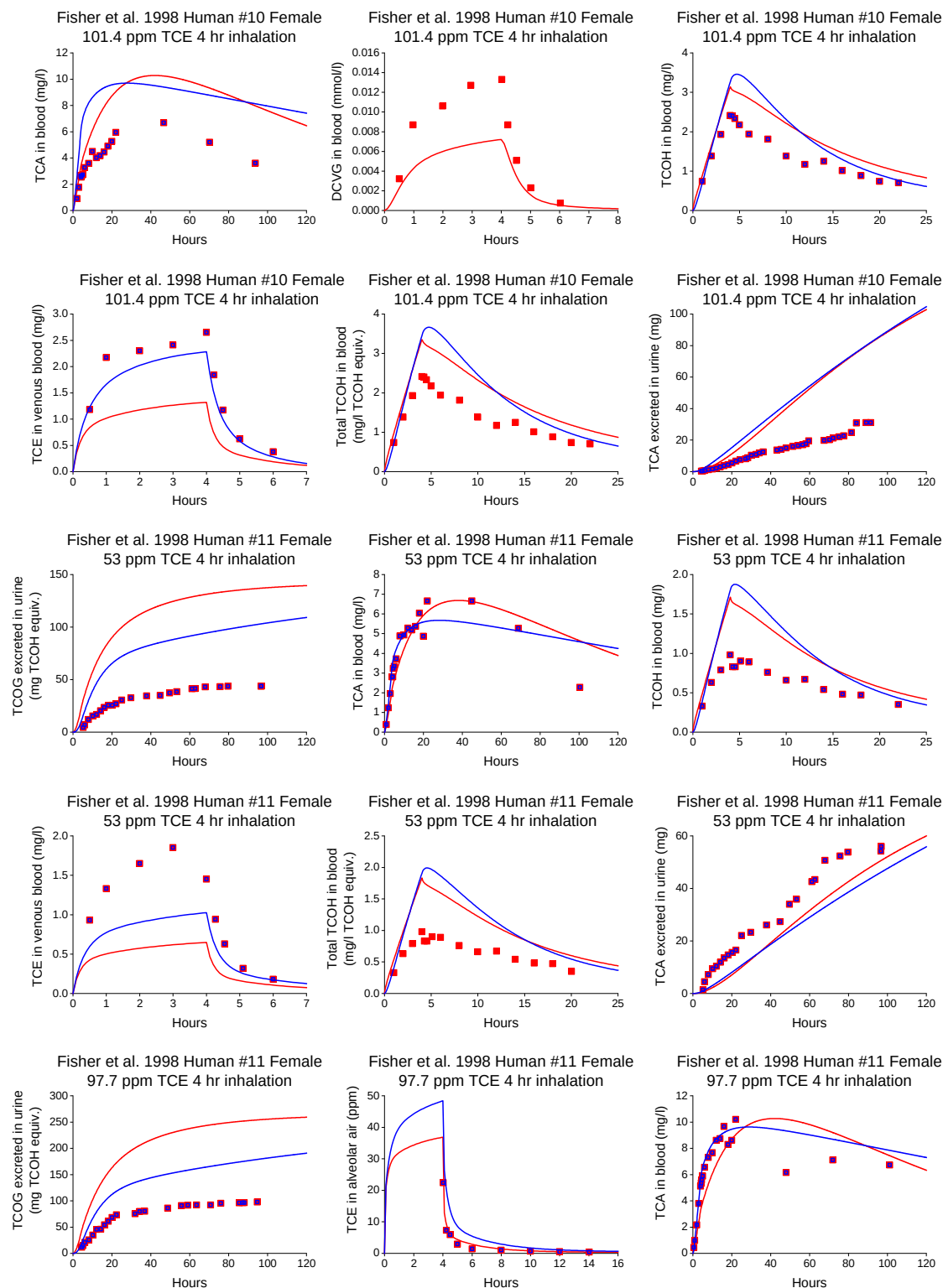


Figure S3. Comparison of Human Predictions (continued).

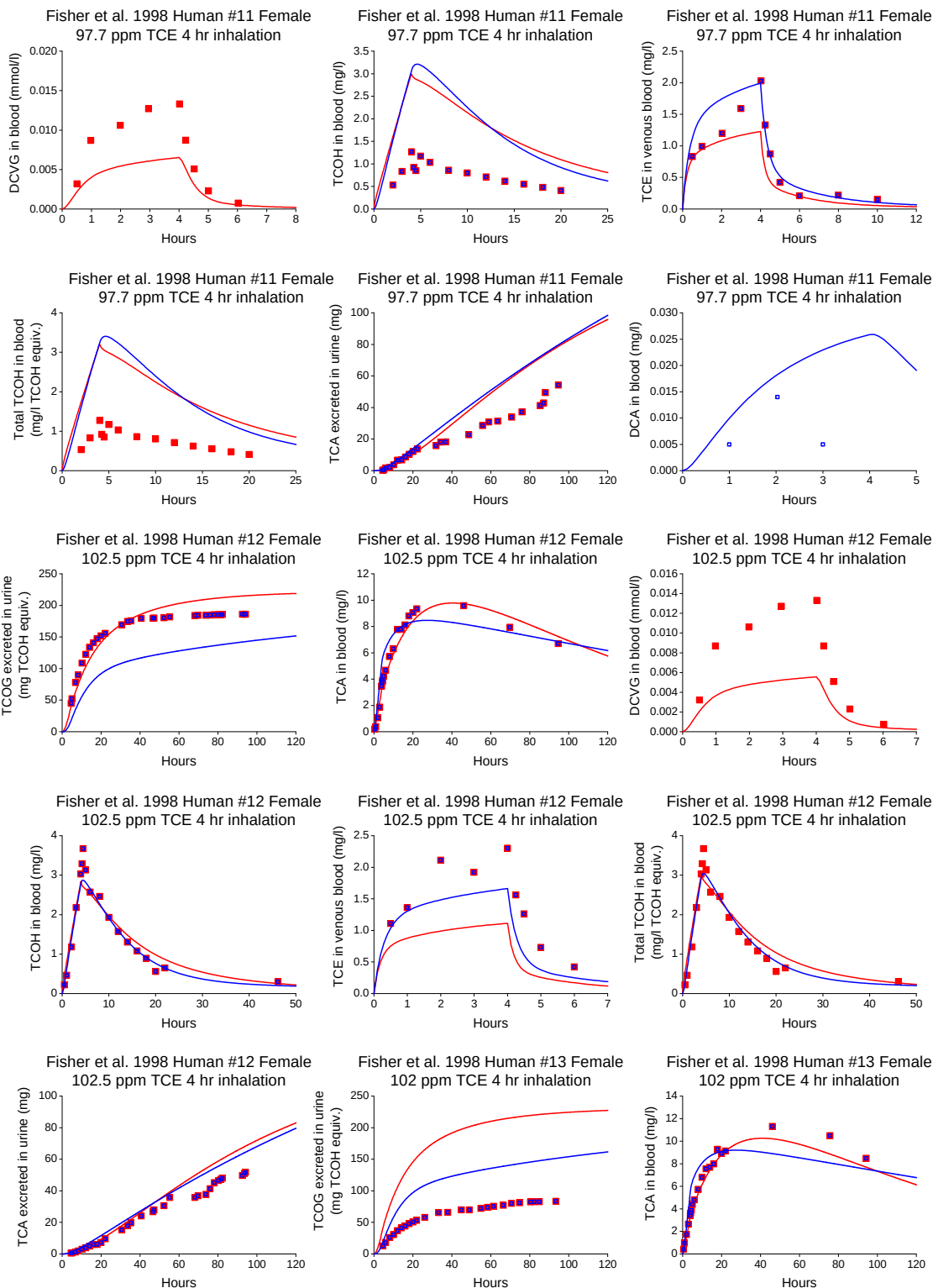


Figure S3. Comparison of Human Predictions (continued).

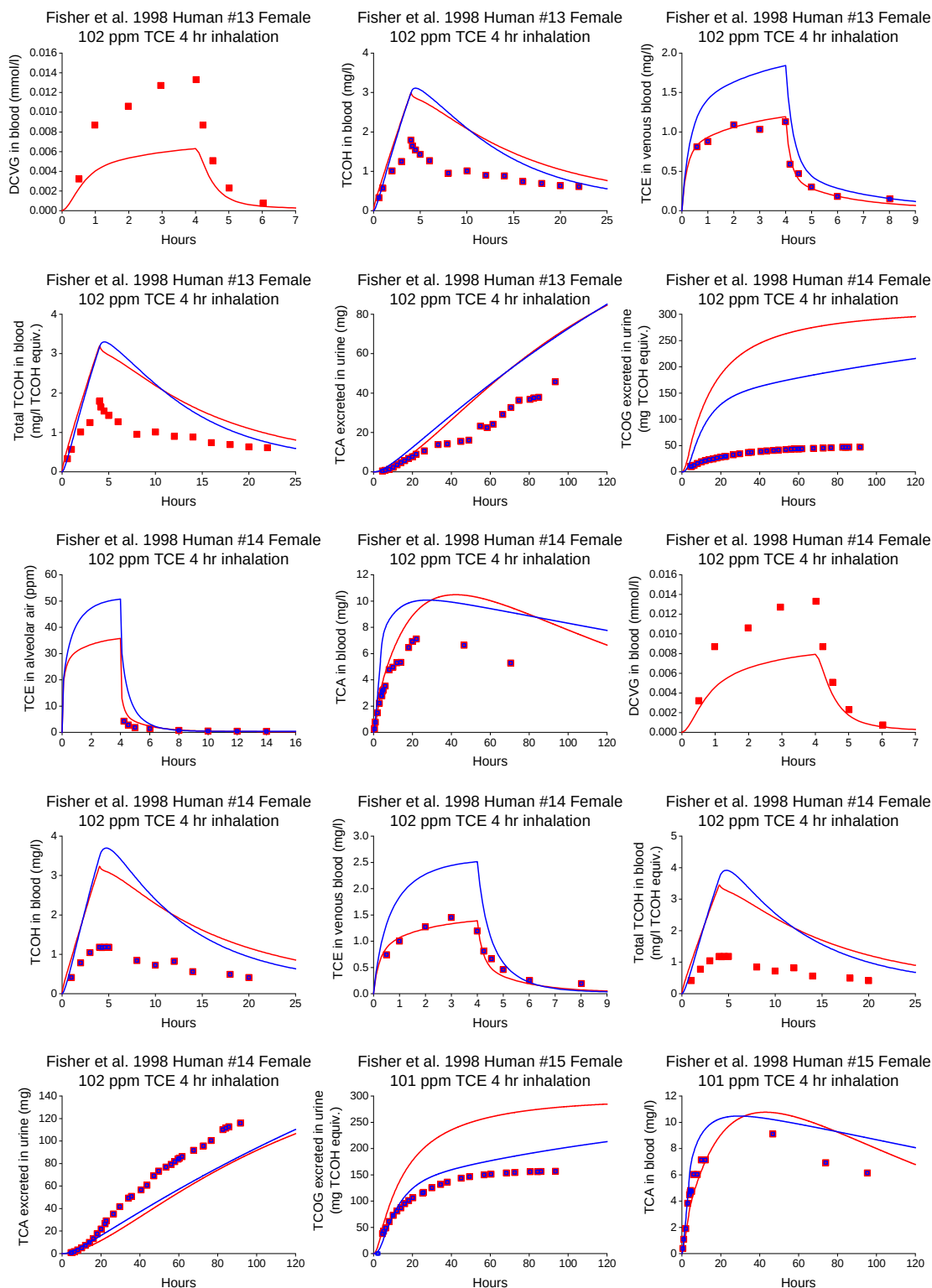


Figure S3. Comparison of Human Predictions (continued).

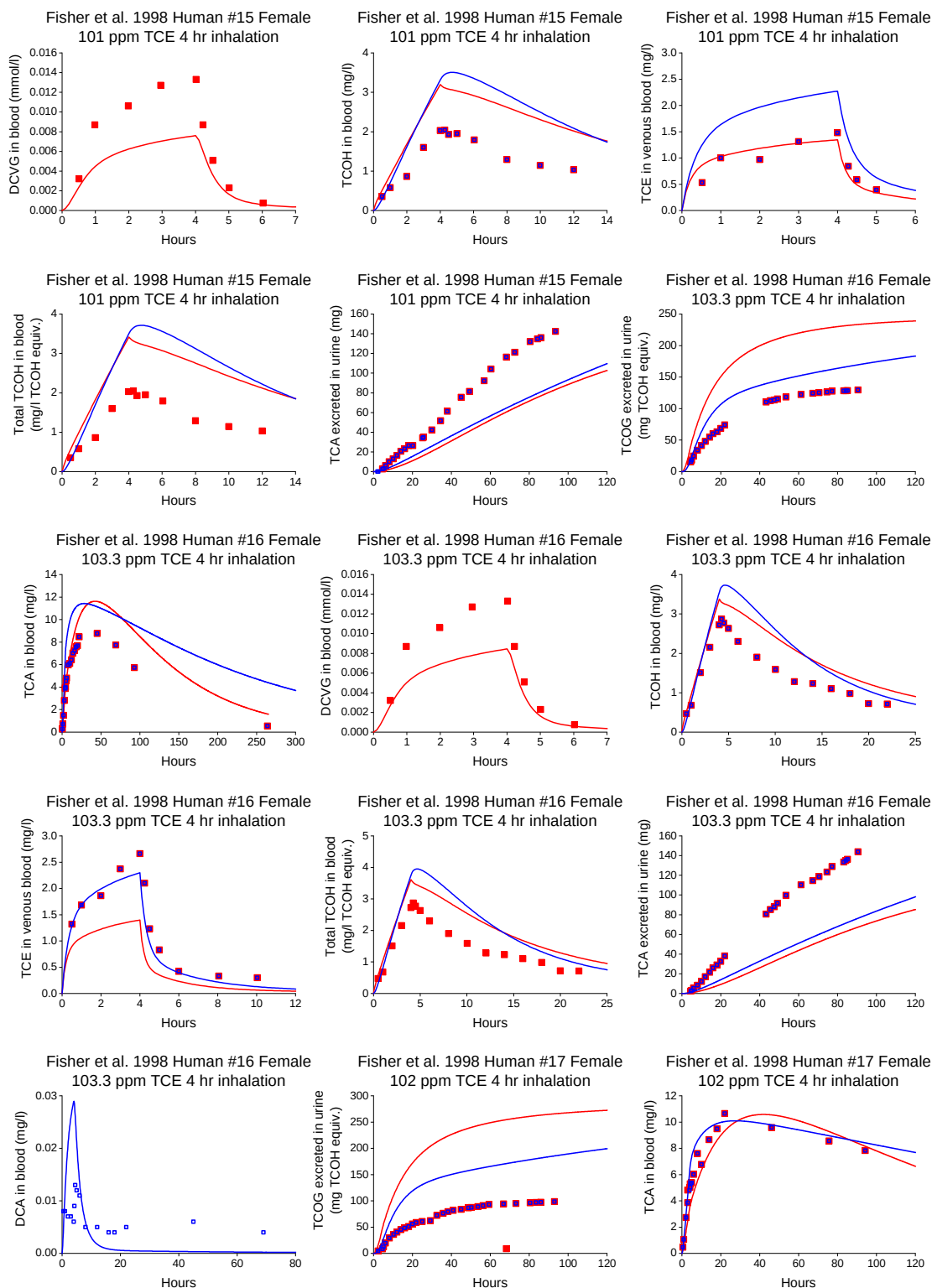


Figure S3. Comparison of Human Predictions (continued).

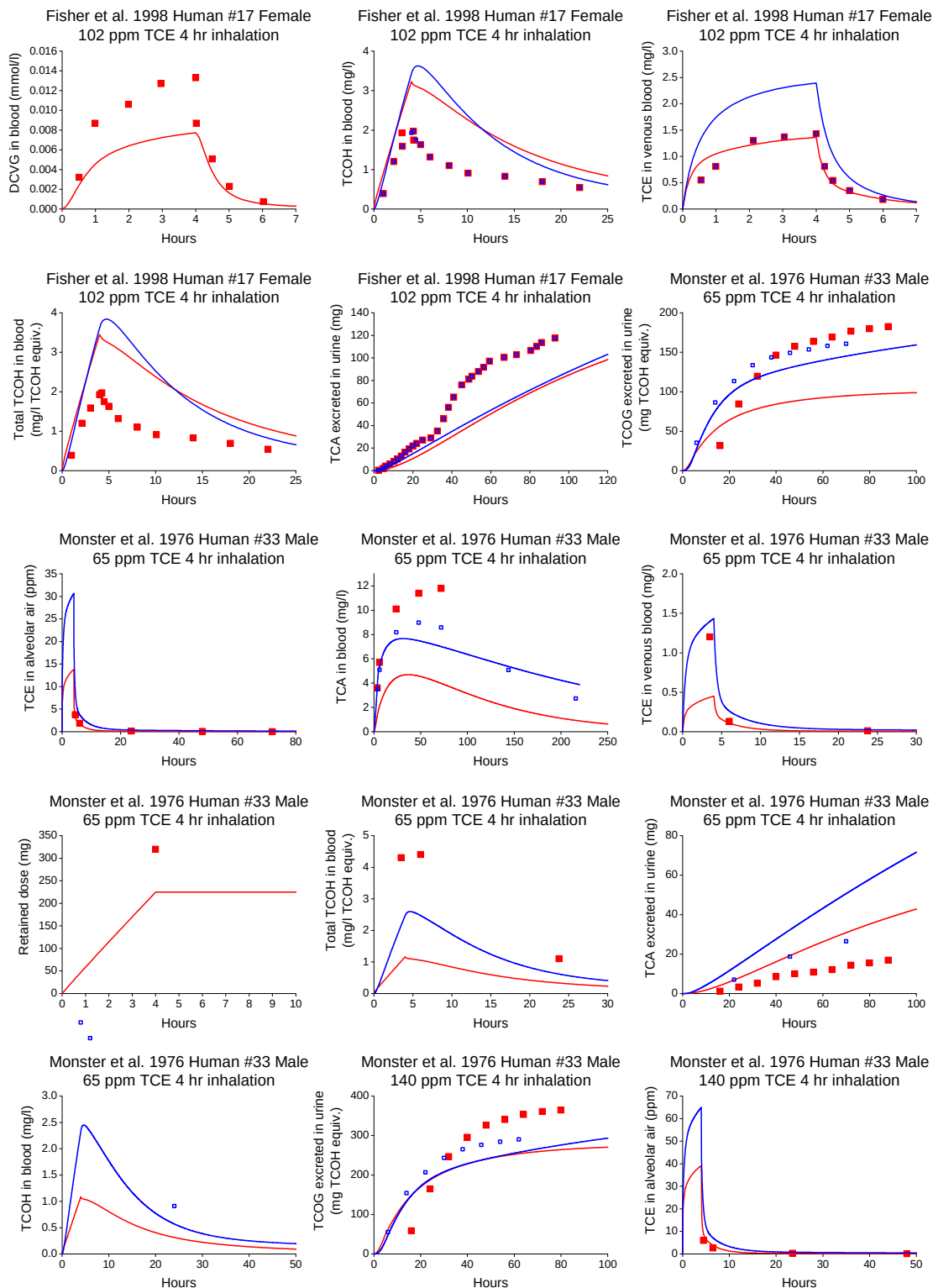


Figure S3. Comparison of Human Predictions (continued).

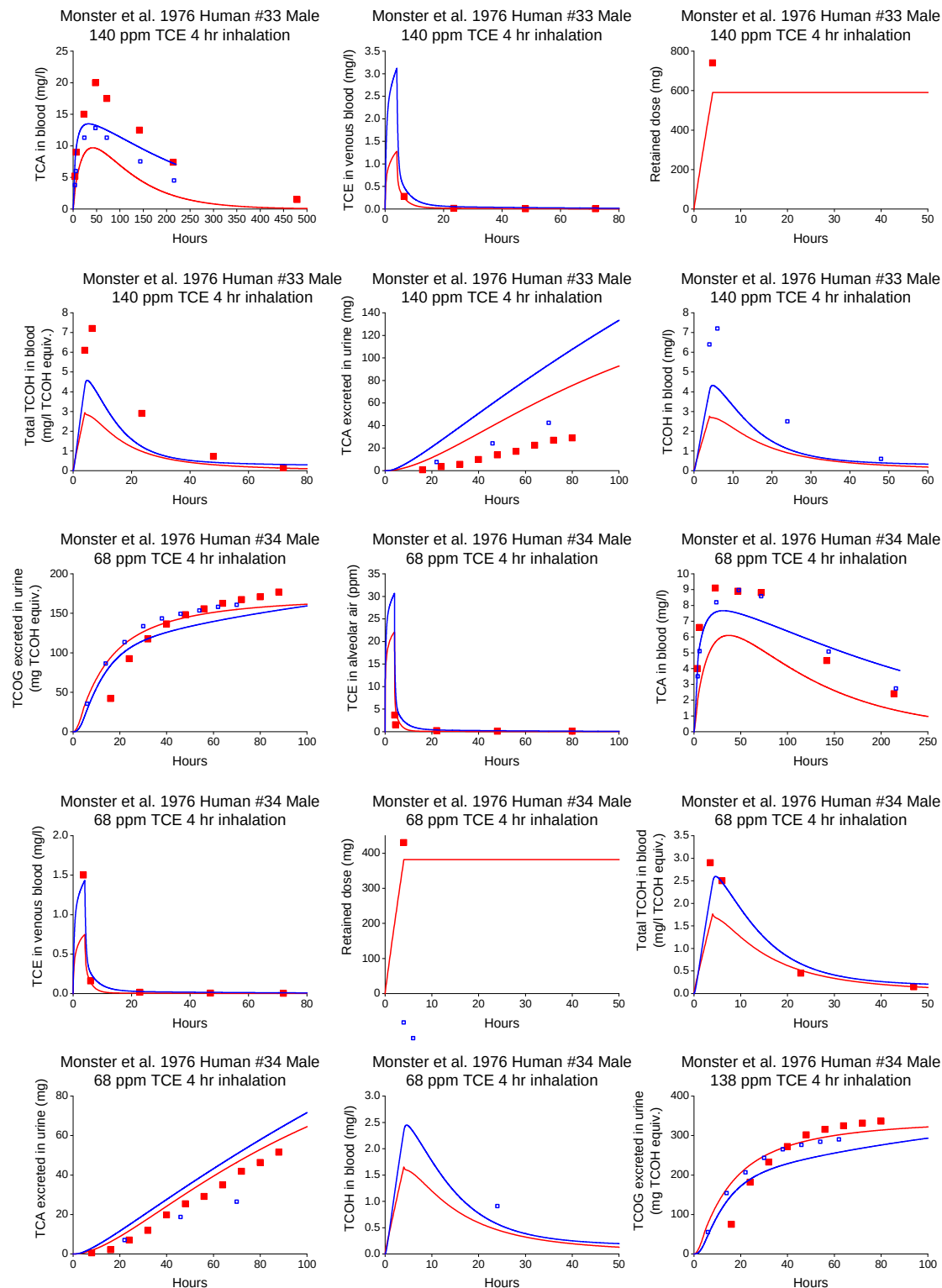


Figure S3. Comparison of Human Predictions (continued).

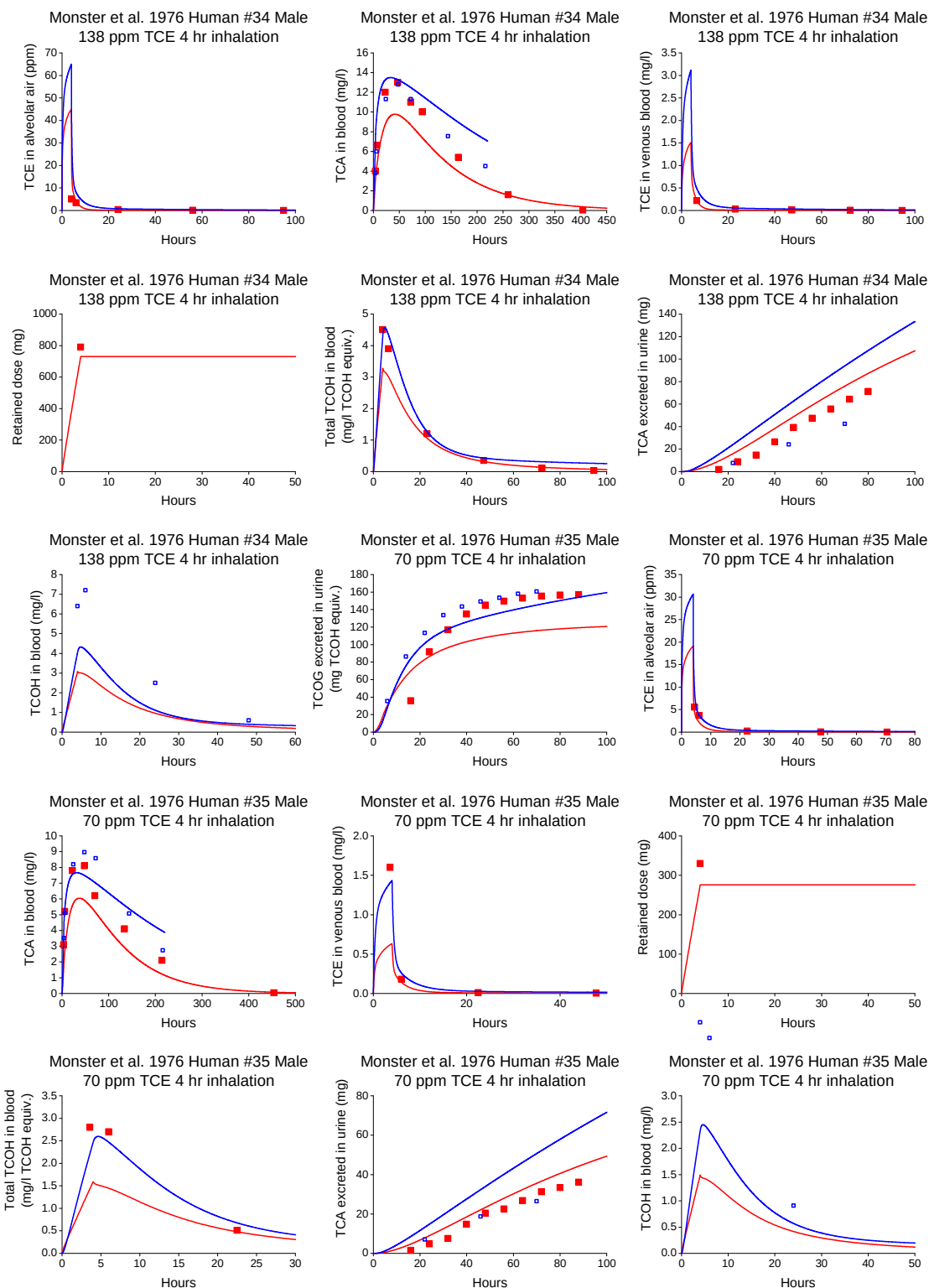


Figure S3. Comparison of Human Predictions (continued).

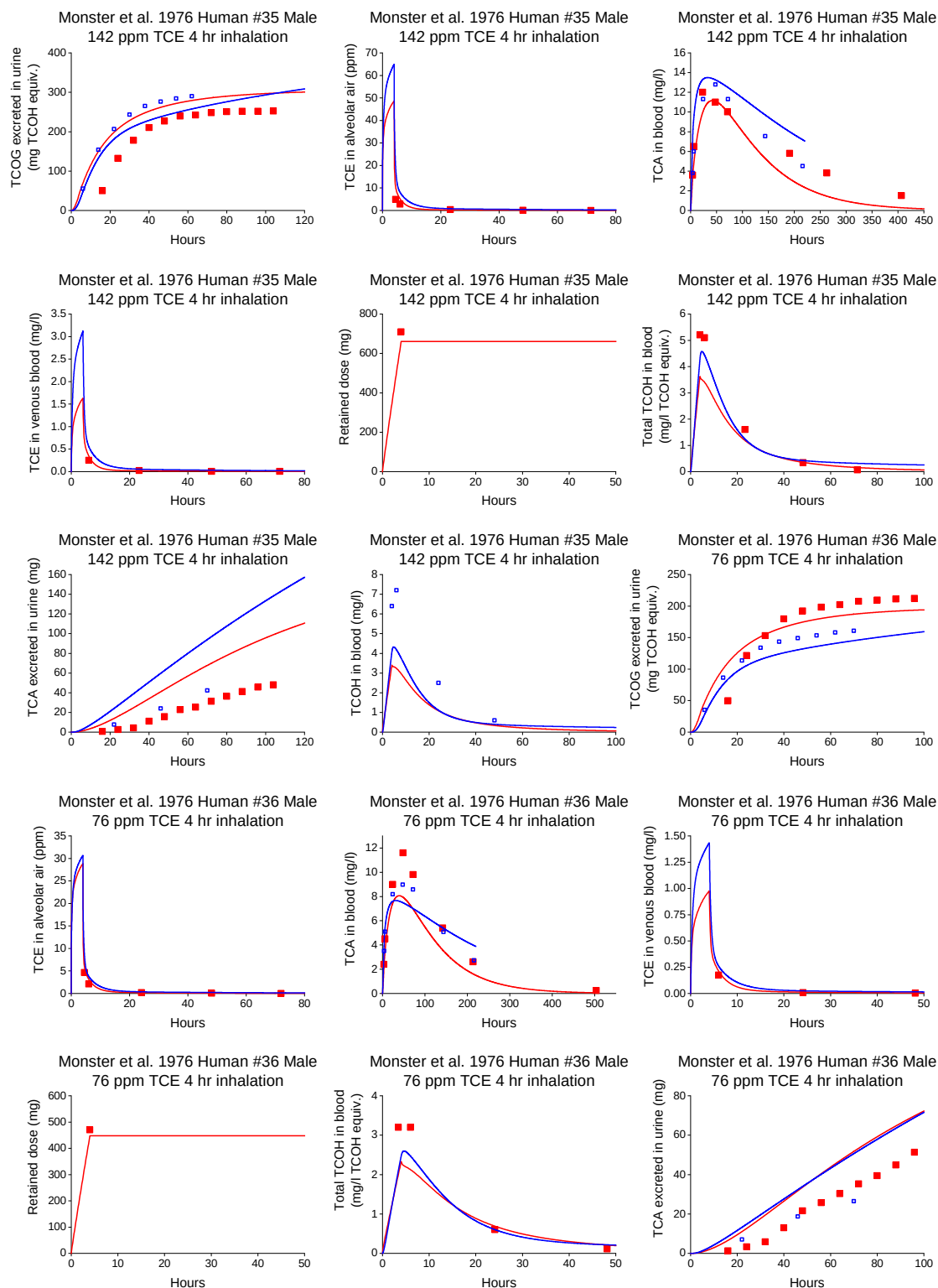


Figure S3. Comparison of Human Predictions (continued).

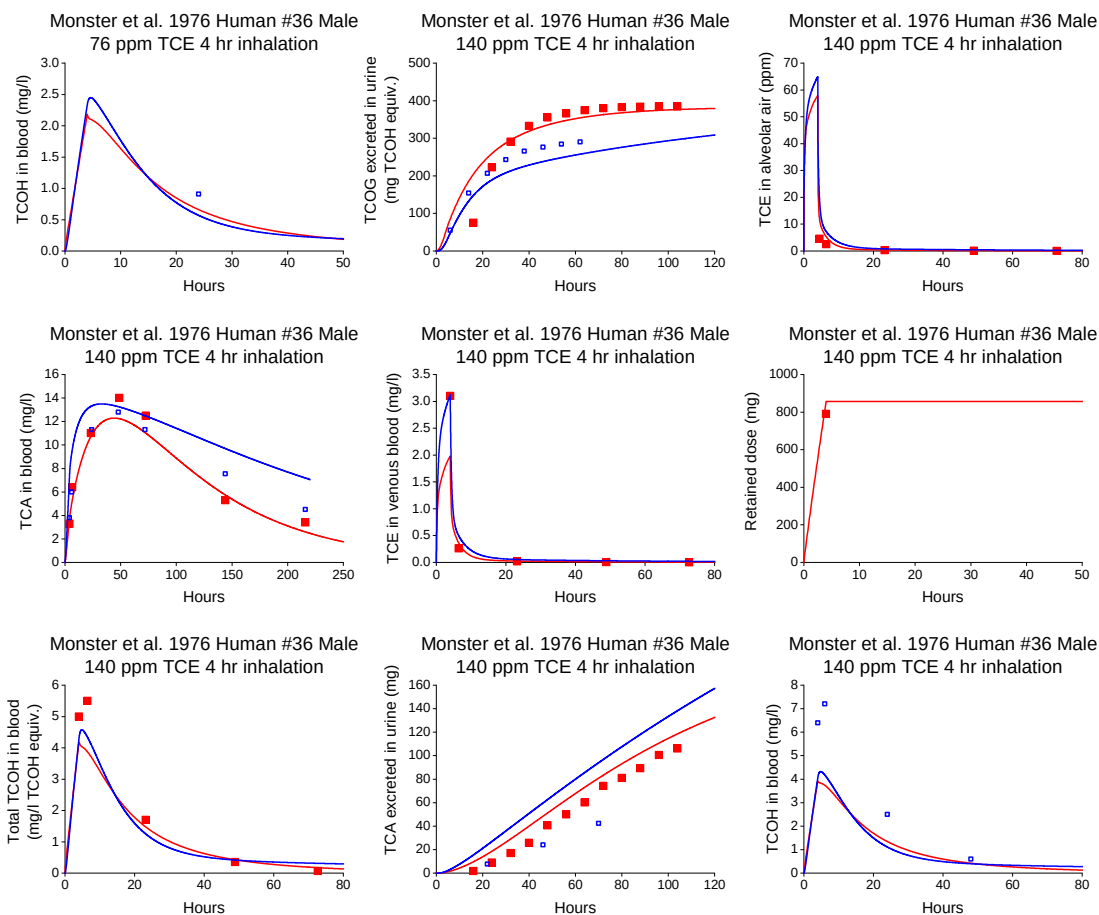


Figure S3. Comparison of Human Predictions (continued).

Table S1. Animal Internal Dose Metric Values

Study Name	Species	Route	Sex	Domain	Peak TCE in Blood (mg/L)	TCE AUC in Blood (mg-h/L/d)	Total Metabolized (mg/kg ^{0.75} /d)	Total Amount Metabolized by Oxidation (mg/kg ^{0.75} /d)	Peak TCE in Liver (mg/L)	TCE AUC in Liver (mg-h/L/d)	TCE Metabolized in Liver (mg/kg ^{0.75} /d)
Adams <i>et al.</i> , [1] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	8.503 & 8.328	41.01 & 40.58	44.43 & 44.91	44.41 & 44.89	6.795 & 6.586	28.32 & 27.51	39.43 & 39.83
Albee <i>et al.</i> [2]	Rat	Inhalation	Female & Male	Neuro	49.37 & 47.68	212.5 & 208.8	71.82 & 75.93	71.70 & 75.82			
Arito <i>et al.</i> [3]	Rat	Inhalation	Male	Neuro	0.5328	3.129	5.996	5.995			
Bushnell [4] ^b	Rat	Inhalation	Male	Neuro	60.53 & 60.55	75.04 & 32.18	39.28 & 16.85	39.24 & 16.84			
Carney <i>et al.</i> [5]	Rat	Inhalation	Female	Develop	35.24	209.5	90.64	90.53			
Cosby & Dukelow [6]	Mouse	Gavage	Female	Develop	1.459	5.760	84.44	84.44			
Crofton & Zhao [7]	Rat	Inhalation	Male	Neuro	83.45	385.4	97.67	97.45			
Fisher <i>et al.</i> [8]	Rat	Gavage	Female	Develop	32.15	202.6	126.6	126.4			
George <i>et al.</i> [9]	Mouse	Diet	Male	Repro	3.483	28.91	290.7	290.6			
Griffin <i>et al.</i> [10]	Mouse	Drinking water	MRL female	Immuno	0.01158	0.2778	5.713	5.713			
Healy <i>et al.</i> [11]	Rat	Inhalation	Female	Develop	3.028	12.91	21.68	21.68			
Jaspers <i>et al.</i> [12]	Rat	Inhalation	Male	Neuro	112.3	1421	151.5	150.7			
Kaneko <i>et al.</i> [13]	Mouse	Inhalation	MRL male	Immuno	22.97	74.46	128.1	128.1			
Kjellstrand <i>et al.</i> [14]	Mouse	Inhalation	Female & Male	Liver	1.119	26.85	82.76	82.75	0.5679	13.63	79.10
Kumar <i>et al.</i> [15, 16]	Rat	Inhalation	Male	Liver & Repro	17.45	51.71	39.15	39.13	17.99	45.23	34.69

Study Name	Species	Route	Sex	Domain	Peak TCE in Blood (mg/L)	TCE AUC in Blood (mg-h/L/d)	Total Metabolized (mg/kg ^{0.75} /d)	Total Amount Metabolized by Oxidation (mg/kg ^{0.75} /d)	Peak TCE in Liver (mg/L)	TCE AUC in Liver (mg-h/L/d)	TCE Metabolized in Liver (mg/kg ^{0.75} /d)
Land <i>et al.</i> [17]	Mouse	Inhalation	Male	Repro	28.72	108.4	160.0	159.9			
Maltoni <i>et al.</i> [18]	Rat	Inhalation	Male	Kidney	9.267	45.90	48.44	48.42			
Manson <i>et al.</i> [19]	Rat	Gavage	Female	Develop	4.186	17.22	60.49	60.47			
Narotsky <i>et al.</i> [20]	Rat	Gavage	Female	Develop	0.4187	1.952	21.10	21.10			
Ramdhan <i>et al.</i> [21]	Mouse	Inhalation	Male	Liver	26.58	206.5	302.9	302.7	40.96	307.8	274.7
Sanders <i>et al.</i> [22]	Mouse	Drinking water	Female & Male	Immuno	0.01564 & 0.01646	0.3754 & 0.3951	7.703 & 8.104	7.703 & 8.103			
Schwetz <i>et al.</i> [23]	Mouse & Rat	Inhalation	Female	Develop	11.12 & 15.21	76.69 & 103.0	182.9 & 78.20	182.9 & 78.15			
Woolhiser <i>et al.</i> [24]	Rat	Inhalation	Female	Immuno, Kidney & Liver	10.98, 2.830 & 3.528	45.67, 12.40 & 15.35	42.95, 20.96 & 24.63	42.93, 20.96 & 24.63	1.636 ^c	6.366 ^c	21.45 ^c
Wu & Berger [25]	Rat	Drinking water	Female	Repro	0.1357	3.258	40.49	40.48			

^aFirst number is the value for the female rats, and the second is for male rats.

^bFirst number is the value for the single dose scenario, and the second is for the 2 week scenario.

^cValue is for liver effects. Rat internal dose metric was from simulating inhalation exposure at 108.0 ppm.

Table S2. Estimated HECs for Human Male Continuous Inhalation

Study Name	Species	Route	Sex	Domain	Endpoint						
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver
Adams <i>et al.</i> , [1] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	197.2 & 193.9	49.33 & 48.86	31.65 & 32.02	31.64 & 32.01	61.77 & 60.25	13.19 & 12.83	27.90 & 28.20
Albee <i>et al.</i> [2]	Rat	Inhalation	Female & Male	Neuro	906.2 & 877.5	203.9 & 201.0	53.84 & 57.42	53.74 & 57.33			
Arito <i>et al.</i> [3]	Rat	Inhalation	Male	Neuro	16.24	4.050	4.043	4.043			
Bushnell [4] ^b	Rat	Inhalation	Male	Neuro	1096 & 1096	85.00 & 39.36	27.75 & 11.52	27.72 & 11.52			
Carney <i>et al.</i> [5]	Rat	Inhalation	Female	Develop	665.7	201.5	70.95	70.85			
Cosby & Dukelow [6]	Mouse	Gavage	Female	Develop	42.60	7.417	65.10	65.11			
Crofton & Zhao [7]	Rat	Inhalation	Male	Neuro	1484	334.6	77.87	77.66			
Fisher <i>et al.</i> [8]	Rat	Gavage	Female	Develop	612.9	196.1	110.7	110.5			
George <i>et al.</i> [9]	Mouse	Diet	Male	Repro	93.37	35.59	-- ^c	-- ^c			
Griffin <i>et al.</i> [10]	Mouse	Drinking water	MRL female	Immuno	0.3617	0.3616	3.851	3.852			
Healy <i>et al.</i> [11]	Rat	Inhalation	Female	Develop	82.64	16.39	14.92	14.92			
Jaspers <i>et al.</i> [12]	Rat	Inhalation	Male	Neuro	1972	1073	148.3	146.9			
Kaneko <i>et al.</i> [13]	Mouse	Inhalation	MRL male	Immuno	455.1	84.42	112.7	112.7			
Kjellstrand <i>et al.</i> [14]	Mouse	Inhalation	Female & Male	Liver	33.19	33.18	63.56	63.56	6.533	6.533	60.31
Kumar <i>et al.</i> [15, 16]	Rat	Inhalation	Male	Liver & Repro	359.1	60.99	27.65	27.64	128.0	20.42	24.37
Land <i>et al.</i> [17]	Mouse	Inhalation	Male	Repro	554.1	116.6	164.4	164.3			
Maltoni <i>et al.</i> [18]	Rat	Inhalation	Male	Kidney	211.7	54.72	34.74	34.73			
Manson <i>et al.</i> [19]	Rat	Gavage	Female	Develop	109.3	21.68	44.34	44.32			
Narotsky <i>et al.</i> [20]	Rat	Gavage	Female	Develop	12.83	2.532	14.51	14.51			
Ramdhan <i>et al.</i> [21]	Mouse	Inhalation	Male	Liver	517.4	199.2	-- ^c	-- ^c	228.8	100.3	-- ^c
Sanders <i>et al.</i> [22]	Mouse	Drinking water	Female & Male	Immuno	0.4885 & 0.5141	0.4885 & 0.5141	5.206 & 5.479	5.206 & 5.479			

Study Name	Species	Route	Sex	Domain	Endpoint						
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver
Schwetz <i>et al.</i> [23]	Mouse & Rat	Inhalation	Female	Develop	246.1 & 319.6	86.63 & 111.7	223.9 & 59.44	224.0 & 59.40			
Woolhiser <i>et al.</i> [24]	Rat	Inhalation	Female	Immuno, Kidney & Liver	243.5, 77.86 & 94.42	54.47, 15.76 & 19.40	30.52, 14.41 & 17.02	30.51, 14.41 & 17.03	17.92 ^d	3.097 ^d	14.78 ^d
Wu & Berger [25]	Rat	Drinking water	Female	Repro	4.214	4.216	28.66	28.66			

^aFirst number is the value based on female rats, and the second is for male rats.

^bFirst number is the HEC for the single dose scenario, and the second is for the 2 week scenario.

^cDue to saturation of metabolism, the HEC could not be estimated.

^dHEC is for liver effects. HEC is from simulating inhalation exposure at 94.42 ppm.

^eHEC is for kidney effects. HEC is from simulating inhalation exposure at 77.86 ppm.

Table S3. Estimated HECs for Human Male Occupational Inhalation

Study Name	Species	Route	Sex	Domain	Endpoint						
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver
Adams <i>et al.</i> , [1] ^a	Rat	Inhalation	Female & Male	Kidney & Liver	242.3 & 238.0	187.8 & 186.1	154.2 & 156.4	154.1 & 156.3	72.96 & 71.13	51.12 & 49.82	132.7 & 134.4
Albee <i>et al.</i> [2]	Rat	Inhalation	Female & Male	Neuro	1168 & 1131	784.6 & 772.5	307.1 & 336.1	306.4 & 335.4			
Arito <i>et al.</i> [3]	Rat	Inhalation	Male	Neuro	18.90	16.84	17.20	17.20			
Bushnell [4] ^b	Rat	Inhalation	Male	Neuro	1416 & 1416	316.4 & 151.9	131.9 & 50.39	131.8 & 50.36			
Carney <i>et al.</i> [5]	Rat	Inhalation	Female	Develop	853.7	774.8	454.8	454.0			
Cosby & Dukelow [6]	Mouse	Gavage	Female	Develop	49.97	30.58	401.8	401.9			
Crofton & Zhao [7]	Rat	Inhalation	Male	Neuro	1923	1339	520.5	518.6			
Fisher <i>et al.</i> [8]	Rat	Gavage	Female	Develop	1923	1339	520.5	518.6			
George <i>et al.</i> [9]	Mouse	Diet	Male	Repro	111.3	138.1	-- ^c	-- ^c			
Griffin <i>et al.</i> [10]	Mouse	Drinking water	MRL female	Immuno	0.4193	1.517	16.37	16.37			
Healy <i>et al.</i> [11]	Rat	Inhalation	Female	Develop	98.18	66.15	66.24	66.24			
Jaspers <i>et al.</i> [12]	Rat	Inhalation	Male	Neuro	2559	4482	1289	1274			
Kaneko <i>et al.</i> [13]	Mouse	Inhalation	MRL male	Immuno	578.1	314.3	885.2	885.9			
Kjellstrand <i>et al.</i> [14]	Mouse	Inhalation	Female & Male	Liver	38.82	129.3	388.2	388.2	7.589	26.28	360.2
Kumar <i>et al.</i> [15, 16]	Rat	Inhalation	Male	Liver & Repro	452.5	229.6	131.4	131.3	154.5	76.47	113.5
Land <i>et al.</i> [17]	Mouse	Inhalation	Male	Repro	707.6	434.7	1477	1476			
Maltoni <i>et al.</i> [18]	Rat	Inhalation	Male	Kidney	260.9	207.1	172.8	172.7			
Manson <i>et al.</i> [19]	Rat	Gavage	Female	Develop	131.0	86.46	235.9	235.9			
Narotsky <i>et al.</i> [20]	Rat	Gavage	Female	Develop	14.92	10.57	64.29	64.30			
Ramdhan <i>et al.</i> [21]	Mouse	Inhalation	Male	Liver	659.5	764.9	-- ^c	-- ^c	283.3	337.5	-- ^c
Sanders <i>et al.</i> [22]	Mouse	Drinking water	Female & Male	Immuno	0.5662 & 0.5958	2.049 & 2.157	22.23 & 23.42	22.23 & 23.42			

Study Name	Species	Route	Sex	Domain	Endpoint						
					Peak TCE in Blood	TCE AUC in Blood	Total Metabolized	Total Amount Metabolized by Oxidation	Peak TCE in Liver	TCE AUC in Liver	TCE Metabolized in Liver
Schwetz <i>et al.</i> [23]	Mouse & Rat	Inhalation	Female	Develop	305.3 & 400.9	322.4 & 415.9	2166 & 352.8	2171 & 352.6			
Woolhiser <i>et al.</i> [24]	Rat	Inhalation	Female	Immuno, Kidney & Liver	302.0, 92.36 & 112.6	206.2, 63.69 & 77.74	147.6, 63.83 & 76.31	147.6, 63.83 & 76.31	20.88 ^d	12.73 ^d	65.55 ^d
Wu & Berger [25]	Rat	Drinking water	Female	Repro	4.889	17.52	137.0	137.0			

^aFirst number is the value based on female rats, and the second is for male rats.

^bFirst number is the HEC for the single dose scenario, and the second is for the 2 week scenario.

^cDue to saturation of metabolism, the HEC could not be estimated.

^dHEC is for liver effects. HEC is from simulating inhalation exposure at 112.6 ppm.

^eHEC is for kidney effects. HEC is from simulating inhalation exposure at 92.36 ppm.

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APPENDIX T

M Files for Mouse Comparison Predictions from the USEPA [1] Model

The following M files are for generating mouse output for the comparison figures in Appendix S. They are essentially the same as the M files from Appendix I with the lines setting the study-specific parameters removed.

Abbas97a_Mouse.m

```
% Abbas R and Fisher J. 1997. A physiologically based pharmacokinetic model for trichloroethylene
% and its metabolites, chloral hydrate, trichloroacetate, dichloroacetate, trichloroethanol,
% and trichloroethanol glucuronide in B6C3F1 mice. Toxicol Appl Pharmacol 147: 15-30.
% Male B6C3F1 mice, 25-30 grams
% Oral dosing of 300, 600, 1200 or 2000 mg/kg TCE in corn oil (dose volume of 0.5 mL, 20 mL corn
% oil/kg BW)
```

```
PlotOutput=[];
ResetDoses
MousePost
```

```
BW=0.0275; PDOSE=300.0; TCHNG=0.05; TSTP=193.0; CINT=0.05;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
Output_Check
Output_Check_Reset
```

```
PDOSE=600.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
PDOSE=1200.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
```

```

PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

PDOSE=2000.0;
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PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Abbas97a_Mouse_Output.txt' @format=ascii

```

Fisher91_Mouse.m

```

% Fisher J, Gargas M, Allen B and Andersen M. 1991. Physiologically based pharmacokinetic
% modeling with trichloroethylene and its metabolite, trichloroacetic acid, in the rat and
% mouse. Toxicol Appl Pharmacol 109: 183-195.
% B6C3F1 female and male mice
% Open or closed chamber inhalation of various concentrations of TCE for 4 hours

% Female mice -- inhalation of 42, 236, 368 or 889 ppm TCE for 4 hours
PlotOutput=[];
ResetDoses
MousePost

BW=0.024; CONCLIST=[368.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=31.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female mice -- closed chamber inhalation of 300, 700, 1100, 3700 or 7000 ppm TCE
ResetDoses
BW=0.024; CC=1; CONCLIST(1)=300.0; STRTNEXTLIST(1)=10.0; TSTRT=0.0; NRODENTS=14.0; VCHC=9.1;
KLOSSC=exp(-3.912); TSTP=2.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.021; CONCLIST(1)=700.0; STRTNEXTLIST(1)=10.0; TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');

```

```

i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022; CONCLIST(1)=1100.0; STRTNEXTLIST(1)=10.0; TSTP=4.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022; CONCLIST(1)=3700.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022; CONCLIST(1)=7000.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male mice -- inhalation of 110, 297, 368 or 748 ppm TCE for 4 hours
ResetDoses
MousePost

BW=0.031; CONCLIST=[110.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=25.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male mice -- closed chamber inhalation of 1020, 1800, 3800, 5600 or 10000 ppm TCE
ResetDoses
BW=0.03; CC=1; CONCLIST(1)=1020.0; STRTNEXTLIST(1)=10.0; TSTRT=0.0; NRODENTS=14.0; VCHC=9.1;
KLOSSC=exp(-3.912); TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.026; CONCLIST(1)=1800.0; STRTNEXTLIST(1)=10.0; TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.03; CONCLIST(1)=3800.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

BW=0.028; CONCLIST(1)=5600.0; STRTNEXTLIST(1)=10.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.026; CONCLIST(1)=10000.0; STRTNEXTLIST(1)=10.0; TSTP=4.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher91_Mouse_Output.txt' @format=ascii

```

Greenberg99_Mouse.m

```

% Greenberg M, Burton G and Fisher J. 1999. Physiologically based pharmacokinetic modeling of
%   inhaled trichloroethylene and its oxidative metabolites in B6C3F1 mice. Toxicol Appl
%   Pharmacol 154: 264-278.
% Male B6C3F1 mice, 28-32 grams (N=6/time point)
% Inhalation of 100 or 600 ppm TCE for 4 hours

```

```

PlotOutput=[];
ResetDoses
MousePost

BW=0.03; CONCLIST=[100.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTRT=0.0; TSTP=50.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[600.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ckid, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Greenberg99_Mouse_Output.txt' @format=ascii

```

Prout85_Mouse.m

```
% Prout M, Provan W and Green T. 1985. Species differences in response to trichloroethylene: I
% pharmacokinetics in rats and mice. Toxicol Appl Pharmacol 79: 389-400.
% Male B6C3F1 and Swiss-Webster mice, 25-32 grams (N=4 or 2 mice/group
% Oral dosing of 10, 500, 1000 or 2000 mg/kg trichloro[14C]ethylene in corn oil (0.5 mL)
% (containing 10 uCi)
```

```
PlotOutput=[];
ResetDoses
MousePost
```

```
BW=0.0295; PDOSE=1000.0; TCHNG=0.05; TSTP=45.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
save PlotOutput @file='Prout85_Mouse_Output.txt' @format=ascii
```

Templin93_Mouse.m

```
% Templin M, Parker J and Bull R. 1993. Relative formation of dichloroacetate and
% trichloroacetate from trichloroethylene in male B6C3F1 mice. Toxicol Appl Pharmacol 123: 1-8.
% Male B6C3F1 mice, 7 weeks of age (N=4/time point)
% Oral dosing of 3.8 mmol/kg (499.282 mg/kg) trichloroethylene in 2% polyoxyethylcnc-sorbitan
% monooleate (Tween 80)
```

```
PlotOutput=[];
ResetDoses
MousePost
```

```
BW=0.027; PDOSE=500.0; TCHNG=0.05; TSTP=37.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldmix, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
% PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
save PlotOutput @file='Templin93_Mouse_Output.txt' @format=ascii
```

APPENDIX U

M Files for Rat Comparison Predictions from the EPA Model

The following M files are for generating rat output for validation figures in Appendix S. They are essentially the same as the M files from Appendix J with the lines setting the study-specific parameters removed.

Bernauer96_Rat.m

```
% Bernauer U, Birner G, Dekant W and Henschler D. 1996. Biotransformation of trichloroethene:
% Dose-dependent excretion of 2,2,2-trichloro-metabolites and mercapturic acids in rats and
% humans after inhalation. Arch Toxicol 70: 338-346.
% http://dx.doi.org/10.1007/s002040050283.
% 2 male Wistar (300-350 g) and 2 female Wistar (200-250 g) exposed simultaneously with humans
% Inhalation of 40, 80 or 160 ppm TCE stabilized with diisopropylamine (40 ppm) for 6 hours
```

```
PlotOutput=[];
ResetDoses
RatPost

BW=0.325; CONCLIST=[40.0 0.0 0.0]; STRTNEXTLIST=[6.0 50.0]; TSTRT=0.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[80.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[160.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Bernauer96_Rat_Output.txt' @format=ascii
```

Fisher91_Rat.m

% Fisher J, Gargas M, Allen B and Andersen M. 1991. Physiologically based pharmacokinetic
% modeling with trichloroethylene and its metabolite, trichloroacetic acid, in the rat and
% mouse. Toxicol Appl Pharmacol 109: 183-195.
% Female and male Fischer 344 rats
% Inhalation of 600 or 505 ppm TCE for 4 hours

```
PlotOutput=[];  
ResetDoses  
RatPost
```

```
BW=0.186; CONCLIST=[600.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTR=0.0; TSTP=50.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
ResetDoses  
RatPost
```

```
BW=0.236; CONCLIST=[505.0 0.0 0.0]; STRTNEXTLIST=[4.0 50.0]; TSTR=0.0; TSTP=50.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
save PlotOutput @file='Fisher91_Rat_Output.txt' @format=ascii
```

Larson92b_Rat.m

% Larson J and Bull R. 1992. Species differences in the metabolism of trichloroethylene to the
% carcinogenic metabolites trichloroacetate and dichloroacetate. Toxicol Appl Pharmacol 115:
% 278-285. [http://dx.doi.org/10.1016/0041-008X\(92\)90333-N](http://dx.doi.org/10.1016/0041-008X(92)90333-N).
% Male Sprague-Dawley rats (404 +/- 91 g)
% Oral dosing of 1.5, 4.5 or 23 mmol TCE/kg in Tween 80 (constant volume of 3 ml/kg) after
% fasting for 24 hours

```
PlotOutput=[];  
ResetDoses  
RatPost
```

```
BW=0.404; PDOSE=197.25; TCHNG=0.05; TSTP=50.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
PDOSE=591.75;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```

PDOSE=3024.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Larson92b_Rat_Output.txt' @format=ascii

```

Prout85_Rat.m

```

% Prout M, Provan W and Green T. 1985. Species differences in response to trichloroethylene: I
%   pharmacokinetics in rats and mice. Toxicol Appl Pharmacol 79: 389-400.
% Male Alderley Park Wistar OR Osborne-Mendel derived rats, 180-200g
% Oral dosing of 10, 500, 1000 or 2000 mg/kg trichloro[14C]ethylene (10 uCi) in corn oil

```

```

PlotOutput=[];

% Non-specified rats
ResetDoses
RatPost

BW=0.19; PDOSE=1000.0; TCHNG=0.05; TSTP=73.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cart, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aexhpost, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Prout85_Rat_Output.txt' @format=ascii

```

Templin95_Rat.m

```

% Templin M, Stevens D, Stenner R, Bonate P, Tuman D and Bull R. 1995. Factors affecting species
%   differences in the kinetics of metabolites of trichloroethylene. J Toxicol Environ Health 44:
%   435-447.
% Male F344 rats (250-300 g)
% Oral dosing of 0.15 or 0.76 mmol/kg TCE in 2% polyoxyethylene-sorbitan monooleate (Tween 80)

```

```

PlotOutput=[];
ResetDoses
RatPost

BW=0.275; PDOSE=100.0; TCHNG=0.05; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Templin95_Rat_Output.txt' @format=ascii

```


APPENDIX V

M Files for Human Comparison Predictions from the USEPA Model

The following M files are for generating human output for validation figures in Appendix S. They are essentially the same as the M files from Appendix K with the lines setting the study- and subject-specific parameters removed.

Bernauer96_Human.m

```
% Bernauer U, Birner G, Dekant W and Henschler D. 1996. Biotransformation of trichloroethene:  
% Dose-dependent excretion of 2,2,2-trichloro-metabolites and mercapturic acids in rats and  
% humans after inhalation. Arch Toxicol 70: 338-346.  
% http://dx.doi.org/10.1007/s002040050283.  
% 3 male volunteers, 37-69 years old  
% Inhalation of 40, 80 or 160 ppm TCE stabilized with diisopropylamine (40 ppm) for 6 hours  
% Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
```

```
PlotOutput=[];  
ResetDoses  
MalePost
```

```
CONCLIST=[40.0 0.0 0.0]; STRTNEXTLIST=[6.0 100.0]; TSTRT=0.0; TSTP=55.0; CINT=0.1;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurnndcvc, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
CONCLIST=[80.0 0.0 0.0];  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurnndcvc, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
CONCLIST=[160.0 0.0 0.0];  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurnndcvc, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntctot_mmole, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
save PlotOutput @file='Bernauer96_Human_Output.txt' @format=ascii
```

Fisher98_Human.m

```
% Fisher J, Mahle D and Abbas R. 1998. A human physiologically based pharmacokinetic model for
% trichloroethylene and its metabolites, trichloroacetic acid and free trichloroethanol.
% Toxicol Appl Pharmacol 152: 339-359.
% http://dx.doi.org/10.1006/taap.1998.8486.
% Male and female volunteers, 20-36 years old
% Inhalation dosing of 50 or 100 ppm TCE for 4 hours
```

```
PlotOutput=[];
ResetDoses
MalePost
% Male subject 1
BW=71.4; VFATC=0.17; VSLWC=0.4692; PB=11.49; CONCLIST=[105.0 0.0 0.0];
STRTEXTLIST=[4.0 300.0]; TSTRT=0.0; TSTP=265.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 2
BW=69.3; VFATC=0.27; VSLWC=0.3672; PB=10.1; CONCLIST=[49.3 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 3
BW=71.1; VFATC=0.14; VSLWC=0.49781; PB=11.1; CONCLIST=[55.2 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[101.5 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```

% Male subject 4
BW=52.3; VFATC=0.1; VSLWC=0.54005; PB=12.1; CONCLIST=[53.1 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[97.8 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 5
BW=82.3; VFATC=0.14; VSLWC=0.50078; PB=11.91; CONCLIST=[105.5 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 6
BW=82.7; VFATC=0.14; VSLWC=0.50083; PB=10.85; CONCLIST=[102.6 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 7
BW=73.2; VFATC=0.18; VSLWC=0.45746; PB=10.47; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');

```

```

PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 8
BW=60.9; VFATC=0.1; VSLWC=0.54063; CONCLIST=[101.1 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 9
BW=70.9; VFATC=0.18; VSLWC=0.45728; CONCLIST=[103.4 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher98_MHuman_Output.txt' @format=ascii

ResetDoses
FemalePost

% Female subject 1
BW=66.5; VFATC=0.32; VSLWC=0.3219; PB=9.88; CONCLIST=[55.1 0.0 0.0]; STRTNEXTLIST=[4.0 300.0];
TSTRT=0.0; TSTP=265.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[101.4 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');

```

```

PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 2
BW=62.3; VFATC=0.24; VSLWC=0.40676; PB=9.45; CONCLIST=[53.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONCLIST=[97.7 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 3
BW=57.5; VFATC=0.21; VSLWC=0.43428; PB=6.47; CONCLIST=[102.5 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 4
BW=55.5; VFATC=0.23; VSLWC=0.41731; PB=7.63; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Female subject 5
BW=67.3; VFATC=0.35; VSLWC=0.29782; PB=11.0; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 6
BW=63.2; VFATC=0.26; VSLWC=0.38509; CONCLIST=[101.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 7
BW=48.6; VFATC=0.23; VSLWC=0.41417; CONCLIST=[103.3 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 8
BW=61.8; VFATC=0.33; VSLWC=0.31588; PB=10.37; CONCLIST=[102.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher98_FHuman_Output.txt' @format=ascii

```

Monster76_Human.m

```
% Monster A, Boersma G and Duba W. 1976. Pharmacokinetics of trichloroethylene in volunteers,  
% influence of workload and exposure concentration. Int Arch Occup Environ Health 38: 87-102.  
% http://dx.doi.org/10.1007/BF00378619.  
% Four male volunteers  
% Inhalation dosing of 70 or 140 ppm TCE for 4 hours
```

```
PlotOutput=[];  
ResetDoses  
MalePost
```

```
% Subject A
```

```
% Measured QP of 210.0
```

```
BW=70.0; VFATC=0.12; VSLWC=0.52138; VPR=0.611431166; CONCLIST=[65.0 0.0 0.0];  
STRTNEXTLIST=[4.0 600.0]; TSTRT=0.0; TSTP=505.0; CINT=0.1;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _hours, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
% Measured QP of 282.0
```

```
VPR=0.821064709; CONCLIST=[140.0 0.0 0.0];  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
% Subject B
```

```
% Measured QP of 390.0
```

```
BW=80.0; VFATC=0.26; VSLWC=0.38143; VPR=1.030287549; CONCLIST=[68.0 0.0 0.0];  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
% Measured QP of 372.0
```

```
VPR=0.982735816; CONCLIST=[138.0 0.0 0.0];  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
```

```

PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Subject C
% Measured QP of 258.0
BW=62.0; VFATC=0.14; VSLWC=0.5047; VPR=0.823262901; CONCLIST=[70.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Measured QP of 336.0
VPR=1.072156337; CONCLIST=[142.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Subject D
% Measured QP of 444.0
BW=67.0; VFATC=0.09; VSLWC=0.55069; VPR=1.335247484; CONCLIST=[76.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Measured QP of 486.0
VPR=1.461554678; CONCLIST=[140.0 0.0 0.0];
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _retdose, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');

```



```
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Monster76_Human_Output.txt' @format=ascii
```

APPENDIX W

Utility M Files for Simulations with Harmonized Model

The following M files are used in the various M files for the harmonized model.

Init.m

```
prepare @All
```

```
xerror(["Ach", "AUCCBld", "AExh", "ATB", "AMetLng"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["RiskP", "ARap", "ASlw", "AFatBld", "AFat"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ASTom", "ADuod", "AExc", "AO", "AGut", [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ALiv", "AUCCLiv", "AMetLiv1", "AMetLiv2"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["InhDose", "TCEDiff"], [1.0e-9, 1.0e-9])
xerror(["APlastTCA", "ABodTCA", "ALivTCA", "AUrnTCA"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ATCOH", "AUCCTCOH", "AMetTCOHTCA", "AMetTCOHGluc"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["ATCOG", "AUCCTCOG", "ABileTCOG", "ARecircTCOG"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
xerror(["AUrnTCOG"], [1.0e-9])
xerror(["ADCA", "AElimDCA"], [1.0e-9, 1.0e-9])
xerror(["ADCVC", "AUrnDCVC", "AUrnNDCVC", "RiskKid"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])

merror(["Ach", "AUCCBld", "AExh", "ATB", "AMetLng"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
merror(["RiskP", "ARap", "ASlw", "AFatBld", "AFat"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
merror(["ASTom", "ADuod", "AExc", "AO", "AGut"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
merror(["ALiv", "AUCCLiv", "AMetLiv1", "AMetLiv2"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
merror(["InhDose", "TCEDiff"], [1.0e-9, 1.0e-9])
merror(["APlastTCA", "ABodTCA", "ALivTCA", "AUrnTCA"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
merror(["ATCOH", "AUCCTCOH", "AMetTCOHTCA", "AMetTCOHGluc"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])

merror(["ATCOG", "AUCCTCOG", "ABileTCOG", "ARecircTCOG"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
merror(["AUrnTCOG"], [1.0e-9])
merror(["ADCA", "AElimDCA"], [1.0e-9, 1.0e-9])
merror(["ADCVC", "AUrnDCVC", "AUrnNDCVC", "RiskKid"], [1.0e-9, 1.0e-9, 1.0e-9, 1.0e-9])
```

```
HVDPRN=0;
WESITG=0;
```

ResetDoses.m

```
CONC=0.0; IVDOSE=0.0; PDOSE=0.0; DIET=0.0; DRINK=0.0;
CC=0; NRATS=1.0; KLOSSC=0.0; VCHC=1.0;
DAYS=1.0, TMAX=24.0
TSTP=24.0, CINT=0.01
TCHNG=1.0; DOSEINT=100000.0;
```

Mouse.m

```
% Parameter values taken from CMD file for the harmonized model
```

```
BW=0.035;
QCC=18.0; QPC=18.0;
QFATC=0.07; QGUTC=0.141; QLIVC=0.02; QRAPC=0.713; QSLWC=0.287; QTBC=0.005;
VBLDC=0.049; VBODC=0.2; VFATBLDC=0.02; VFATC=0.07; VGUTC=0.042; VKIDC=0.017; VLIVC=0.055;
VRAPC=0.217; VSLWC=0.619; VTBC=0.0007;
VDDCAC=0.5; VDTCOHC=0.65;
PB=14.0; PFAT=36.0; PGUT=1.8; PLIV=1.8; PRAP=1.8; PSLW=0.75; PTB=1.8;
PAFATC1=10.0; PAFATC2=10.0;
PBODTCA=0.76; PLIVTCA=1.14;
VMAXC=32.7; KM=0.25; KDCVCC=0.015; FRACDCA=0.04; FRACTCE=0.035;
VMAXCLARAC=3.0; KMCLARA=0.25;
VMAXCLEARC=250.0; KMCLEAR=250.0;
KDISSOC=46.1; NUMSITES=0.17; PROTCONC=196.0;
VMAXTCOHC=1.0; KMTCOH=0.25;
VMAXGLUCC=100.0; KMGLUC=25.0;
KNATC=0.5; KKIDCYTOC=0.4;
KAS=0.0; KTSO=10.0; KAD=0.6; KTD=0.0;
KBILEC=1.0; KEHRC=0.0;
KCLEARDCAC=1.0; KURNTCAC=0.3; KURNTCOGC=0.5;
FRACPLAS=0.58; TCAPLAS=0.76;
```

MousePost.m

```
% Posterior values from Hack et al. (2006)
% Other values from Eric's MCSim input file for mouse (VKIDC, VDDCAC, VMaxClearC, KMClear, kNATC,
%   kKidCytoC, kAS, kTD and kClearDCAC
% Did not see values for BW, VFatBldC, PAFatC1 and PAFatC2
% Calculated QRapC from (1 - QFatC - QGutC - QLivC - QSLWC)
% QSLWC adjusted to be (QSLWC + QFatC) from posteriors since model calculates QSLW as
%   (QSLWC - QFatC)*QC
% VBodC adjusted to be (VBodC + VBldC + VLivC) from posteriors since model calculates VBod as
%   (VBodC - VBldC - VLivC)*BW
% VRapC adjusted to be (VRapC + VGutC + VLivC + VTBC) from posteriors since model calculates VRap
%   as (VRap - VGutC - VLivC - VTBC)*BW
% Calculated VSLWC as (0.82 - VBldC - VFatBldC - VFatC - VGutC - VLivC - VRapC - VTBC)
% Set PAFatC1 and PAFatC2 to 100.0 to ensure they are larger than QFat since fat diffusion was
%   removed from model for MCMC Hack work
```

```
BW=0.035;
QCC=21.0; QPC=25.2;
QFATC=0.073; QGUTC=0.16; QLIVC=0.02; QRAPC=0.707; QSLWC=0.293; QTBC=0.0065;
VBLDC=0.047; VBODC=0.195; VFATBLDC=0.02; VFATC=0.052; VGUTC=0.042; VKIDC=0.017; VLIVC=0.051;
VRAPC=0.2137; VSLWC=0.5593; VTBC=0.0007;
VDDCAC=0.5; VDTCOHC=0.83;
PB=18.0; PFAT=29.0; PGUT=1.7; PLIV=2.3; PRAP=1.7; PSLW=0.65; PTB=1.8;
PAFATC1=100.0; PAFATC2=100.0;
PBODTCA=0.68; PLIVTCA=0.91;
VMAXC=38.0; KM=2.6; KDCVCC=0.016; FRACDCA=0.045; FRACTCE=0.036;
VMAXCLARAC=9.8; KMCLARA=0.25;
VMAXCLEARC=250.0; KMCLEAR=250.0;
KDISSOC=46.0; NUMSITES=0.17; PROTCONC=490.0;
VMAXTCOHC=1.1; KMTCOH=0.15;
VMAXGLUCC=88.0; KMGLUC=14.0;
KNATC=0.5; KKIDCYTOC=0.4;
KAS=0.0; KTS=36.0; KAD=0.25; KTD=0.0;
KBILEC=0.45; KEHRC=0.074;
KCLEARDCAC=1.0; KURNTCAC=0.86; KURNTCOGC=1.9;
FRACPLAS=0.55; TCAPLAS=0.58;
```

Rat.m

```
% Parameter values taken from CMD file for the harmonized model
```

```
BW=0.35;
QCC=15.0; QPC=24.0;
QFATC=0.07; QGUTC=0.162; QLIVC=0.021; QRAPC=0.594; QSLWC=0.406; QTBC=0.021;
VBLDC=0.074; VBODC=0.2; VFATBLDC=0.02; VFATC=0.07; VGUTC=0.027; VKIDC=0.007; VLIVC=0.034;
VRAPC=0.213; VSLWC=0.664; VTBC=0.0005;
VDDCAC=0.5; VDTCOHC=0.65;
PB=18.5; PFAT=27.5; PGUT=1.3; PLIV=1.3; PRAP=1.3; PSLW=0.5; PTB=1.3;
PAFATC1=10.0; PAFATC2=10.0;
PBODTCA=0.51; PLIVTCA=0.76;
VMAXC=11.2; KM=0.25; KDCVCC=0.015; FRACDCA=0.04; FRACTCE=0.04;
VMAXCLARAC=0.3; KMCLARA=0.25;
VMAXCLEARC=250.0; KMCLEAR=250.0;
KDISSOC=383.6; NUMSITES=1.49; PROTCONC=190.0;
VMAXTCOHC=0.12; KMTCOH=0.25;
VMAXGLUCC=100.0; KMGLUC=25.0;
KNATC=1.1; KKIDCYTOC=17.0;
KAS=0.0; KTS=10.0; KAD=0.3; KTD=0.0;
KBILEC=1.0; KEHRC=0.0;
KCLEARDCAC=1.3; KURNTCAC=0.3; KURNTCOGC=0.5;
FRACPLAS=0.58; TCAPLAS=0.76;
```

RatPost.m

```
% Posterior values from Hack et al. (2006)
% Other values from Eric's MCSim input file for mouse (VKIDC, VDDCAC, VMaxClearC, KMClear, KAS,
%   kTD and kClearDCAC
% Did not see values for BW, VFatBldC, PAFatC1 and PAFatC2
% Calculated QRapC from (1 - QFatC - QGutC - QLivC - QSLWC)
% QSLWC adjusted to be (QSLWC + QFatC) from posteriors since model calculates QSLW as
%   (QSLWC - QFatC)*QC
% VBodC adjusted to be (VBodC + VBldC + VLivC) from posteriors since model calculates VBod as
%   (VBodC - VBldC - VLivC)*BW
% VRapC adjusted to be (VRapC + VGutC + VLivC + VTBC) from posteriors since model calculates VRap
%   as (VRap - VGutC - VLivC - VTBC)*BW
% Calculated VSLWC as (0.82 - VBldC - VFatBldC - VFatC - VGutC - VLivC - VRapC - VTBC)
% Calculated oxidative capacities (VMaxClaraC, VMaxTCOHC, VMaxGlucC) from posterior clearances
%   and oxidative affinities (VM=Cl*KM)
% Set PAFatC1 and PAFatC2 to 100.0 to ensure they are larger than QFat since fat diffusion was
%   removed from model for MCMC Hack work
```

```
BW=0.35;
QCC=12.0; QPC=16.8;
QFATC=0.078; QGUTC=0.15; QLIVC=0.021; QRAPC=0.592; QSLWC=0.408; QTBC=0.026;
VBLDC=0.074; VBODC=0.218; VFATBLDC=0.02; VFATC=0.089; VGUTC=0.027; VKIDC=0.007; VLIVC=0.034;
VRAPC=0.2115; VSLWC=0.5345; VTBC=0.0005;
VDDCAC=0.5; VDTCOHC=0.85;
PB=15.0; PFAT=39.0; PGUT=1.3; PLIV=1.3; PRAP=1.4; PSLW=0.54; PTB=1.3;
PAFATC1=100.0; PAFATC2=100.0;
PBODTCA=0.52; PLIVTCA=0.72;
VMAXC=7.8; KM=0.85; KDCVCC=0.019; FRACDCA=0.096; FRACTCE=0.046;
VMAXCLARAC=0.816; KMCLARA=0.34;
VMAXCLEARC=250.0; KMCLEAR=250.0;
KDISSOC=390.0; NUMSITES=1.5; PROTCONC=130.0;
VMAXTCOHC=0.0462; KMTCOH=0.33;
VMAXGLUCC=253.0; KMGLUC=23.0;
KNATC=1.3; KKIDCYTOC=13.0;
KAS=0.0; KTS=19.0; KAD=0.23; KTD=0.0;
KBILEC=0.87; KEHRC=0.32;
KCLEARDCAC=1.3; KURNTCAC=0.36; KURNTCOGC=0.64;
FRACPLAS=0.57; TCAPLAS=0.39;
```

Human.m

```
% Parameter values taken from CMD file for the harmonized model
```

```
BW=70.0;
QCC=13.0; QPC=18.0;
QFATC=0.052; QGUTC=0.181; QLIVC=0.046; QRAPC=0.699; QSLWC=0.301; QTBC=0.025;
VBLDC=0.079; VBODC=0.2; VFATBLDC=0.02; VFATC=0.214; VGUTC=0.017; VKIDC=0.004; VLIVC=0.026;
VRAPC=0.192; VSLWC=0.651; VTBC=0.0008;
VDDCAC=0.26; VDTCOHC=0.65;
PB=9.2; PFAT=73.0; PGUT=6.8; PLIV=6.8; PRAP=6.8; PSLW=2.3; PTB=6.8;
PAFATC1=10.0; PAFATC2=10.0;
PBODTCA=1.9; PLIVTCA=2.5;
VMAXC=12.0; KM=1.5; KDCVCC=0.015; FRACDCA=0.004; FRACTCE=0.08;
VMAXCLARAC=0.0045; KMCLARA=1.5;
VMAXCLEARC=250.0; KMCLEAR=250.0;
KDISSOC=174.6; NUMSITES=2.97; PROTCONC=239.0;
VMAXTCOHC=25.0; KMTCOH=250.0;
VMAXGLUCC=5.0; KMGLUC=25.0;
KNATC=19.0; KKIDCYTOC=37.0;
KAS=0.0; KTS=10.0; KAD=1.0; KTD=0.0;
KBILEC=1.0; KEHRC=0.0;
KCLEARDCAC=1.9; KURNTCAC=0.2; KURNTCOGC=3.0;
FRACPLAS=0.58; TCAPLAS=0.76;
```

HumanPost.m

```
% Posterior values from Hack et al. (2006)
% Other values from Eric's MCSim input file for mouse (VKidC, VDDCAC, VMaxClearC, KMClear, kAS,
%   kTD and kClearDCAC
% Did not see values for VFatBldC, PAFatC1, PAFatC2, KTSd and kAD
% Calculated QRapC from (1 - QFatC - QGutC - QLivC - QSLwC)
% QSLwC adjusted to be (QSLwC + QFatC) from posteriors since model calculates QSLw as
%   (QSLwC - QFatC)*QC
% VBodC adjusted to be (VBodC + VBldC + VLivC) from posteriors since model calculates VBod as
%   (VBodC - VBldC - VLivC)*BW
% VRapC adjusted to be (VRapC + VGutC + VLivC + VTBC) from posteriors since model calculates VRap
%   as (VRap - VGutC - VLivC - VTBC)*BW
% Calculated VSLwC as (0.82 - VBldC - VFatBldC - VFatC - VGutC - VLivC - VRapC - VTBC)
% Calculated VMaxC and KM from posterior values (VMax = Cl*VLiv*KMC and KM = KMC)/PLiv) -- Cl and
%   KMC are the values from the posterior table
% Calculated oxidative capacities (VMaxClaraC, VMaxTCOHC, VMaxGlucC) from posterior clearances
%   and oxidative affinities (VM=Cl*KM)
% Set PAFatC1 and PAFatC2 to 100.0 to ensure they are larger than QFat since fat diffusion was
%   removed from model for MCMC Hack work
```

```
BW=64.0;
QCC=14.0; QPC=25.2;
QFATC=0.063; QGUTC=0.24; QLIVC=0.061; QRAPC=0.827; QSLWC=0.173; QTBC=0.034;
VBLDC=0.063; VBODC=0.253; VFATBLDC=0.02; VFATC=0.2; VGUTC=0.014; VKIDC=0.004; VLIVC=0.02;
VRAPC=0.15479; VSLWC=0.60221; VTBC=0.00079;
VDDCAC=0.26; VDTCOHC=1.1;
PB=11.0; PFAT=71.0; PGUT=4.0; PLIV=4.9; PRAP=3.4; PSLW=3.7; PTB=6.5;
PAFATC1=100.0; PAFATC2=100.0;
PBODTCA=3.0; PLIVTCA=1.4;
VMAXC=10.30; KM=2.86; KDCVCC=0.011; FRACDCA=0.004; FRACTCE=0.21;
VMAXCLARAC=0.00476; KMCLARA=1.4;
VMAXCLEARC=250.0; KMCLEAR=250.0;
KDISSOC=170.0; NUMSITES=3.0; PROTCONC=240.0;
VMAXTCOHC=14.64; KMTCOH=240.0;
VMAXGLUCC=13.2; KMGLUC=44.0;
KNATC=17.0; KKIDCYTOC=45.0;
KAS=0.0; KTSd=10.0; KAD=1.0; KTD=0.0;
KBILEC=4.8; KEHRC=0.023;
KCLEARDCAC=1.9; KURNTCAC=0.38; KURNTCOGC=4.3;
FRACPLAS=0.54; TCAPLAS=0.61;
```

Output_Check.m

```
% Output parameters to check that all parameters are within range
Params(i,1) = QC;
Params(i,2) = QP;
Params(i,3) = QFAT;
Params(i,4) = QGUT;
Params(i,5) = QLIV;
Params(i,6) = QGUTLIV;
Params(i,7) = QRAP;
Params(i,8) = QSLW;
Params(i,9) = QTB;
Params(i,10) = QCPLAS;
Params(i,11) = QBODPLAS;
Params(i,12) = QLIVPLAS;
Params(i,13) = VBLD;
Params(i,14) = VBOD;
Params(i,15) = VFATBLD;
Params(i,16) = VFAT;
Params(i,17) = VGUT;
Params(i,18) = VKID;
Params(i,19) = VLIV;
Params(i,20) = VPLAS;
Params(i,21) = VRAP;
Params(i,22) = VSLW;
Params(i,23) = VTBC;
Params(i,24) = VDDCA;
Params(i,25) = VDTCOH;
Params(i,26) = PAFAT1;
Params(i,27) = PAFAT2;
```

```

Params(i,28) = VMAX;
Params(i,29) = KM;
Params(i,30) = KDCVC;
Params(i,31) = VMAXCLARA;
Params(i,32) = VMAXCLEAR;
Params(i,33) = TOTCONC;
Params(i,34) = VMAXTCOH;
Params(i,35) = KMTCOH;
Params(i,36) = VMAXGLUC;
Params(i,37) = KMGLUC;
Params(i,38) = KNAT;
Params(i,39) = KKIDCYTO;
Params(i,40) = KBILE;
Params(i,41) = KEHR;
Params(i,42) = KURNTCA;
Params(i,43) = KURNTCOG;
Params(i,44) = KCLEARCA;
Params(i,45) = DOSE;
Params(i,46) = KDIET;
Params(i,47) = KDRINK;
Params(i,48) = CC;
Params(i,49) = RATS;
Params(i,50) = KLOSS;
Params(i,51) = VCH;
Params(i,52) = ACH0;

```

```

TmpCheckOutput = [];
TmpCheckOutput = addcolsj(TmpCheckOutput, _totdose, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottissue, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _totmetab, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tcediff, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltce, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbalabs, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _rinhdose, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ach, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cart, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _calv, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aexh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _atb, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametlng, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _arap, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aslw, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _afatbld, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _afat, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _astom, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aduod, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aexc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ao, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _agut, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aliv, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametliv1, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _ametliv2, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cven, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcain, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcatis, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tcadiff, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aplastca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cplastcafree, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aplastcafree, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cplastcabnd, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _abodtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _alivtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aurntca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcohin, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _totmetabtcOH, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltcoH, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _atcoH, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _amettcohtca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _amettcoHgluc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcogin, @Justification = 'begin');

```

```

TmpCheckOutput = addcolsj(TmpCheckOutput, _tottcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaltcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _atcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _abiletcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _arecirtcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aurntcog, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _totdcain, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaldca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _adca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aelimdca, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _totdcvcin, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _massbaldcvc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _adcvc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _aurndcvc, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _cinh, @Justification = 'begin');
TmpCheckOutput = addcolsj(TmpCheckOutput, _kiv, @Justification = 'begin');

CheckOutput = atrrowsj(CheckOutput, max(TmpCheckOutput), @Justification = 'begin');
CheckOutput = atrrowsj(CheckOutput, min(TmpCheckOutput), @Justification = 'begin');

```

Output_Check_Reset.m

% Output parameters to check that all parameters are reset with each run
ParamsReset=[];

```

ParamsReset(1,1) = BW;
ParamsReset(2,1) = QCC;
ParamsReset(3,1) = QPC;
ParamsReset(4,1) = QFATC;
ParamsReset(5,1) = QGUTC;
ParamsReset(6,1) = QLIVC;
ParamsReset(7,1) = QRAPC;
ParamsReset(8,1) = QSLWC;
ParamsReset(9,1) = QTBC;
ParamsReset(10,1) = VBLDC;
ParamsReset(11,1) = VBODC;
ParamsReset(12,1) = VFATBLDC;
ParamsReset(13,1) = VFATC;
ParamsReset(14,1) = VGUTC;
ParamsReset(15,1) = VLIVC;
ParamsReset(16,1) = VRAPC;
ParamsReset(17,1) = VSLWC;
ParamsReset(18,1) = VTBC;
ParamsReset(19,1) = VDDCAC;
ParamsReset(20,1) = VDTCOHC;
ParamsReset(21,1) = PB;
ParamsReset(22,1) = PFAT;
ParamsReset(23,1) = PGUT;
ParamsReset(24,1) = PLIV;
ParamsReset(25,1) = PRAP;
ParamsReset(26,1) = PSLW;
ParamsReset(27,1) = PTB;
ParamsReset(28,1) = PAFATC1;
ParamsReset(29,1) = PAFATC2;
ParamsReset(30,1) = PBODTCA;
ParamsReset(31,1) = PLIVTCA;
ParamsReset(32,1) = MWTCE;
ParamsReset(33,1) = MWDCA;
ParamsReset(34,1) = MWDCVC;
ParamsReset(35,1) = MWTCA;
ParamsReset(36,1) = MWCHLOR;
ParamsReset(37,1) = MWTCOH;
ParamsReset(38,1) = MWTCOHGLUC;
ParamsReset(39,1) = MWNADCVC;
ParamsReset(40,1) = VMAXC;
ParamsReset(41,1) = KM;
ParamsReset(42,1) = KDCVCC;
ParamsReset(43,1) = FRACDCA;
ParamsReset(44,1) = FRACTCE;
ParamsReset(45,1) = VMAXCLARAC;
ParamsReset(46,1) = KMCLARA;

```

```

ParamsReset(47,1) = VMAXCLEARC;
ParamsReset(48,1) = KMCLEAR;
ParamsReset(49,1) = KDISSOC;
ParamsReset(50,1) = NUMSITES;
ParamsReset(51,1) = PROTCNC;
ParamsReset(52,1) = VMAXTCOHC;
ParamsReset(53,1) = KMTCOH;
ParamsReset(54,1) = VMAXGLUCC;
ParamsReset(55,1) = KMGLUC;
ParamsReset(56,1) = KNATC;
ParamsReset(57,1) = KKIDCYTOC;
ParamsReset(58,1) = KAS;
ParamsReset(59,1) = KTSD;
ParamsReset(60,1) = KAD;
ParamsReset(61,1) = KTD;
ParamsReset(62,1) = KBILEC;
ParamsReset(63,1) = KEHRC;
ParamsReset(64,1) = KCLEARDCAC;
ParamsReset(65,1) = KURNTCAC;
ParamsReset(66,1) = KURNTCOGC;
ParamsReset(67,1) = FRACPLAS;
ParamsReset(68,1) = TCAPLAS;
ParamsReset(69,1) = CONC;
ParamsReset(70,1) = IVDOS;
ParamsReset(71,1) = TCHNG;
ParamsReset(72,1) = PDOS;
ParamsReset(73,1) = DAYS;
ParamsReset(74,1) = TMAX;
ParamsReset(75,1) = DRINK;
ParamsReset(76,1) = CC;
ParamsReset(77,1) = NRATS;
ParamsReset(78,1) = KLOSSC;
ParamsReset(79,1) = VCHC;
ParamsReset(80,1) = TSTP;
ParamsReset(81,1) = CINT;
ParamsReset(82,1) = QC;
ParamsReset(83,1) = QP;
ParamsReset(84,1) = QFAT;
ParamsReset(85,1) = QGUT;
ParamsReset(86,1) = QLIV;
ParamsReset(87,1) = QGUTLIV;
ParamsReset(88,1) = QRAP;
ParamsReset(89,1) = QSLW;
ParamsReset(90,1) = QTB;
ParamsReset(91,1) = QCPLAS;
ParamsReset(92,1) = QBODPLAS;
ParamsReset(93,1) = QLIVPLAS;
ParamsReset(94,1) = VBLD;
ParamsReset(95,1) = VBOD;
ParamsReset(96,1) = VFATBLD;
ParamsReset(97,1) = VFAT;
ParamsReset(98,1) = VGUT;
ParamsReset(99,1) = VKID;
ParamsReset(100,1) = VLIV;
ParamsReset(101,1) = VPLAS;
ParamsReset(102,1) = VRAP;
ParamsReset(103,1) = VSLW;
ParamsReset(104,1) = VTB;
ParamsReset(105,1) = VDDCA;
ParamsReset(106,1) = VDTCH;
ParamsReset(107,1) = PAFAT1;
ParamsReset(108,1) = PAFAT2;
ParamsReset(109,1) = STOCHCHLORTCE;
ParamsReset(110,1) = STOCHTCATCE;
ParamsReset(111,1) = STOCHTCATCOH;
ParamsReset(112,1) = STOCHTCOHTCE;
ParamsReset(113,1) = STOCHGLUCTCOH;
ParamsReset(114,1) = STOCHTCOHLUC;
ParamsReset(115,1) = STOCHTCEGLUC;
ParamsReset(116,1) = STOCHDCVCTCE;
ParamsReset(117,1) = STOCHN;

```



```

ParamsReset(118,1) = STOCHDCATCE;
ParamsReset(119,1) = VMAX;
ParamsReset(120,1) = KDCVC;
ParamsReset(121,1) = VMAXCLARA;
ParamsReset(122,1) = VMAXCLEAR;
ParamsReset(123,1) = TOTCONC;
ParamsReset(124,1) = VMAXTCOH;
ParamsReset(125,1) = VMAXGLUC;
ParamsReset(126,1) = KNAT;
ParamsReset(127,1) = KKIDCYTO;
ParamsReset(128,1) = KBILE;
ParamsReset(129,1) = KEHR;
ParamsReset(130,1) = KURNTCA;
ParamsReset(131,1) = KURNTCOG;
ParamsReset(132,1) = KCLEARDCA;
ParamsReset(133,1) = _dose(1,1);
ParamsReset(134,1) = _kdrink(1,1);
ParamsReset(135,1) = RATS;
ParamsReset(136,1) = KLOSS;
ParamsReset(137,1) = VCH;
ParamsReset(138,1) = _kiv(1,1);
ParamsReset(139,1) = _concon(1,1);
ParamsReset(140,1) = ACH0;
ParamsReset(141,1) = _cinh(1,1);
ParamsReset(142,1) = _total(1,1);
ParamsReset(143,1) = _day(1,1);
ParamsReset(144,1) = _cvtb(1,1);
ParamsReset(145,1) = _paucbld(1,1);
ParamsReset(146,1) = _aucblddm(1,1);
ParamsReset(147,1) = _pauccliv(1,1);
ParamsReset(148,1) = _aucclivdm(1,1);
ParamsReset(149,1) = _pametliv1bw34(1,1);
ParamsReset(150,1) = _ametliv1bw34dm(1,1);
ParamsReset(151,1) = _t(1,1);
ParamsReset(152,1) = _rach(1,1);
ParamsReset(153,1) = _ach(1,1);
ParamsReset(154,1) = _cinh(1,1);
ParamsReset(155,1) = _cinhppm(1,1);
ParamsReset(156,1) = _cart(1,1);
ParamsReset(157,1) = _aucbld(1,1);
ParamsReset(158,1) = _calv(1,1);
ParamsReset(159,1) = _calvppm(1,1);
ParamsReset(160,1) = _raexh(1,1);
ParamsReset(161,1) = _aexh(1,1);
ParamsReset(162,1) = _ratb(1,1);
ParamsReset(163,1) = _cvtb(1,1);
ParamsReset(164,1) = _atb(1,1);
ParamsReset(165,1) = _ctb(1,1);
ParamsReset(166,1) = _rametlng(1,1);
ParamsReset(167,1) = _ametlng(1,1);
ParamsReset(168,1) = _rarap(1,1);
ParamsReset(169,1) = _arap(1,1);
ParamsReset(170,1) = _crap(1,1);
ParamsReset(171,1) = _cvrap(1,1);
ParamsReset(172,1) = _raslw(1,1);
ParamsReset(173,1) = _aslw(1,1);
ParamsReset(174,1) = _cslw(1,1);
ParamsReset(175,1) = _cvslw(1,1);
ParamsReset(176,1) = _rafatbld(1,1);
ParamsReset(177,1) = _afatbld(1,1);
ParamsReset(178,1) = _cvfat(1,1);
ParamsReset(179,1) = _rafat(1,1);
ParamsReset(180,1) = _afat(1,1);
ParamsReset(181,1) = _cfat(1,1);
ParamsReset(182,1) = _rstom(1,1);
ParamsReset(183,1) = _astom(1,1);
ParamsReset(184,1) = _raduod(1,1);
ParamsReset(185,1) = _aduod(1,1);
ParamsReset(186,1) = _raexc(1,1);
ParamsReset(187,1) = _aexc(1,1);
ParamsReset(188,1) = _rao(1,1);

```

```

ParamsReset(189,1) = _ao(1,1);
ParamsReset(190,1) = _ragut(1,1);
ParamsReset(191,1) = _agut(1,1);
ParamsReset(192,1) = _cgut(1,1);
ParamsReset(193,1) = _cvgut(1,1);
ParamsReset(194,1) = _raliv(1,1);
ParamsReset(195,1) = _aliv(1,1);
ParamsReset(196,1) = _cliv(1,1);
ParamsReset(197,1) = _cvliv(1,1);
ParamsReset(198,1) = _auccliv(1,1);
ParamsReset(199,1) = _rametliv1(1,1);
ParamsReset(200,1) = _ametliv1(1,1);
ParamsReset(201,1) = _ametliv1bw34(1,1);
ParamsReset(202,1) = _rametliv2(1,1);
ParamsReset(203,1) = _ametliv2(1,1);
ParamsReset(204,1) = _cven(1,1);
ParamsReset(205,1) = _cvenmole(1,1);
ParamsReset(206,1) = _rinhdose(1,1);
ParamsReset(207,1) = _inhdose(1,1);
ParamsReset(208,1) = _totdose(1,1);
ParamsReset(209,1) = _tottissue(1,1);
ParamsReset(210,1) = _totmetab(1,1);
ParamsReset(211,1) = _tcediff(1,1);
ParamsReset(212,1) = _massbaltce(1,1);
ParamsReset(213,1) = _massbalabs(1,1);
ParamsReset(214,1) = _raplastca(1,1);
ParamsReset(215,1) = _aplastca(1,1);
ParamsReset(216,1) = _cplastca(1,1);
ParamsReset(217,1) = _cplastcamole(1,1);
ParamsReset(218,1) = _cplastcafreemole(1,1);
ParamsReset(219,1) = _aplastcafree(1,1);
ParamsReset(220,1) = _cplastcafree(1,1);
ParamsReset(221,1) = _cplastcabnd(1,1);
ParamsReset(222,1) = _cbldtca(1,1);
ParamsReset(223,1) = _rabodtca(1,1);
ParamsReset(224,1) = _abodtca(1,1);
ParamsReset(225,1) = _cbodtca(1,1);
ParamsReset(226,1) = _cvbodtca(1,1);
ParamsReset(227,1) = _ralivtca(1,1);
ParamsReset(228,1) = _alivtca(1,1);
ParamsReset(229,1) = _clivtca(1,1);
ParamsReset(230,1) = _cvlivtca(1,1);
ParamsReset(231,1) = _raurntca(1,1);
ParamsReset(232,1) = _aurntca(1,1);
ParamsReset(233,1) = _tottcain(1,1);
ParamsReset(234,1) = _tottcatis(1,1);
ParamsReset(235,1) = _tcadiff(1,1);
ParamsReset(236,1) = _massbaltca(1,1);
ParamsReset(237,1) = _ratcoh(1,1);
ParamsReset(238,1) = _atcoh(1,1);
ParamsReset(239,1) = _ctcoh(1,1);
ParamsReset(240,1) = _aucctcoh(1,1);
ParamsReset(241,1) = _ramettcohtca(1,1);
ParamsReset(242,1) = _amettcohtca(1,1);
ParamsReset(243,1) = _ramettcohgluc(1,1);
ParamsReset(244,1) = _amettcohgluc(1,1);
ParamsReset(245,1) = _tottcohin(1,1);
ParamsReset(246,1) = _totmetabtcogh(1,1);
ParamsReset(247,1) = _massbaltcoh(1,1);
ParamsReset(248,1) = _ratcog(1,1);
ParamsReset(249,1) = _atcog(1,1);
ParamsReset(250,1) = _ctcog(1,1);
ParamsReset(251,1) = _aucctcog(1,1);
ParamsReset(252,1) = _rabiletcog(1,1);
ParamsReset(253,1) = _abiletcog(1,1);
ParamsReset(254,1) = _rarecirtcog(1,1);
ParamsReset(255,1) = _arecirtcog(1,1);
ParamsReset(256,1) = _raurntcog(1,1);
ParamsReset(257,1) = _aurntcog(1,1);
ParamsReset(258,1) = _aurntcogtcoh(1,1);
ParamsReset(259,1) = _aurntcogtce(1,1);

```

```

ParamsReset(260,1) = _tottcogin(1,1);
ParamsReset(261,1) = _tottcog(1,1);
ParamsReset(262,1) = _massbaltcog(1,1);
ParamsReset(263,1) = _radca(1,1);
ParamsReset(264,1) = _adca(1,1);
ParamsReset(265,1) = _cdca(1,1);
ParamsReset(266,1) = _raelimdca(1,1);
ParamsReset(267,1) = _aelimdca(1,1);
ParamsReset(268,1) = _totdcain(1,1);
ParamsReset(269,1) = _massbaldca(1,1);
ParamsReset(270,1) = _radcvc(1,1);
ParamsReset(271,1) = _adcvc(1,1);
ParamsReset(272,1) = _cdcvc(1,1);
ParamsReset(273,1) = _aurndcvc(1,1);
ParamsReset(274,1) = _aurndcvc(1,1);
ParamsReset(275,1) = _aurndcvc(1,1);
ParamsReset(276,1) = _aurndcvc(1,1);
ParamsReset(277,1) = _totdcvcin(1,1);
ParamsReset(278,1) = _massbaldcvc(1,1);

```

```

OutputReset = addcolsj(OutputReset, ParamsReset, @Justification = 'begin');

```

RunFigures.m

```

% Mouse
CheckOutput = []; OutputReset=[]; Params=[]; i=0;
Abbas97a_Mouse
Fisher91_Mouse
Greenberg99_Mouse
Prout85_Mouse
Templin93_Mouse
save CheckOutput @file='CheckOutput_MouseFigures.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_MouseFigures.txt' @format=ascii
save Params @file='Params_MouseFigures.txt' @format=ascii

% Rat
CheckOutput = []; OutputReset=[]; Params=[]; i=0;
Bernauer96_Rat
Fisher91_Rat
Larson92b_Rat
Prout85_Rat
Templin95_Rat
save CheckOutput @file='CheckOutput_RatFigures.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_RatFigures.txt' @format=ascii
save Params @file='Params_RatFigures.txt' @format=ascii

% Human
CheckOutput = []; OutputReset=[]; Params=[]; i=0;
Bernauer96_Human
Fisher98_Human
Monster76_Human
save CheckOutput @file='CheckOutput_HumanFigures.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_HumanFigures.txt' @format=ascii
save Params @file='Params_HumanFigures.txt' @format=ascii

```

RunDMs.m

```

load @format=model @file=TCE_BD
Init

% Mouse
CheckOutput=[]; DMOutput=[]; OutputReset=[]; Params=[]; i=0;
Cosby92_MouseDM
George85_MouseDM
Griffin00_MouseDM
Kaneko00_MouseDM
Kjellstrand83_MouseDM
Land81_MouseDM
Ramdhan10_MouseDM
Sanders82_MouseDM
Schwetz75_MouseDM

```

```

save CheckOutput @file='CheckOutput_MouseDMs.txt' @format=ascii
save DMOutput @file='MouseDMs.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_MouseDMs.txt' @format=ascii
save Params @file='Params_MouseDMs.txt' @format=ascii

% Rat
CheckOutput=[]; DMOutput=[]; OutputReset=[]; Params=[]; i=0;
Adams51_RatDM
Albee06_RatDM
Arito94_RatDM
Bushnell97_RatDM
Carney06_RatDM
Crofton97_RatDM
Fisher01_RatDM
Healy82_RatDM
Jaspers93_RatDM
Kumar00a_01a_RatDM
Maltoni88_RatDM
Manson84_RatDM
Narotsky95_RatDM
Schwetz75_RatDM
Woolhiser06_RatDM
Wu07_RatDM
save CheckOutput @file='CheckOutput_RatDMs.txt' @format=ascii
save DMOutput @file='RatDMs.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_RatDMs.txt' @format=ascii
save Params @file='Params_RatDMs.txt' @format=ascii

RunHECs.m
load @format=model @file=TCE_BD
Init

% Human
CheckOutput=[]; DMOutput=[]; OutputReset=[]; Params=[]; i=0;
Human_Fit_DMs_ContInh
save CheckOutput @file='CheckOutput_HumanContDMs.txt' @format=ascii
CheckOutput = []; i=0;

Human_Fit_DMs_OccInh
save CheckOutput @file='CheckOutput_HumanOccDMs.txt' @format=ascii
save OutputReset @file='CheckOutput_Reset_HumanDMDoses.txt' @format=ascii
save Params @file='Params_HumanDMs.txt' @format=ascii

SaveDMs.m

DMOutput(i,1) = max(_cart);
DMOutput(i,2) = AUCCBLDDM;
DMOutput(i,3) = TOTMETABBW34DM;
DMOutput(i,4) = TOTOXMETBW34DM;
DMOutput(i,5) = max(_cliv);
DMOutput(i,6) = AUCCLIVDM;
DMOutput(i,7) = AMETLIV1BW34DM;

```

APPENDIX X

M Files for Mouse Comparison Predictions from the Harmonized Model

The following M files are for generating mouse output for validation figures (Figure S1) and for predicting the internal dose metrics (Table S1) in Appendix S. M files for the validation figures are first.

Abbas97a_Mouse.m

```
% Abbas R and Fisher J. 1997. A physiologically based pharmacokinetic model for trichloroethylene
% and its metabolites, chloral hydrate, trichloroacetate, dichloroacetate, trichloroethanol,
% and trichloroethanol glucuronide in B6C3F1 mice. Toxicol Appl Pharmacol 147: 15-30.
% Male B6C3F1 mice, 25-30 grams
% Oral dosing of 300, 600, 1200 or 2000 mg/kg TCE in corn oil (dose volume of 0.5 mL, 20 mL corn
% oil/kg BW)
```

```
PlotOutput=[];
ResetDoses
MousePost
```

```
% Settings from CMD file (BW from Eric's MCSim input file)
% QPC=20.0; QCC=20.0;
BW=0.025;
PDOSE=300.0; DAYS=1.0; TMAX=48.0; DOSEINT=24.0; CALCINT=1000.0; TSTP=250.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
% Settings from CMD file
% QPC=15.0; QCC=15.0;
```

```
PDOSE=600.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```

% Settings from CMD file
% QPC=12.0; QCC=12.0;

PDOSE=1200.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Settings from CMD file
% QPC=6.0; QCC=6.0;

PDOSE=2000.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Abbas97a_Mouse_Output.txt' @format=ascii

```

Fisher91_Mouse.m

```

% Fisher J, Gargas M, Allen B and Andersen M. 1991. Physiologically based pharmacokinetic
% modeling with trichloroethylene and its metabolite, trichloroacetic acid, in the rat and
% mouse. Toxicol Appl Pharmacol 109: 183-195.
% B6C3Fl female and male mice
% Open or closed chamber inhalation of various concentrations of TCE for 4 hours

```

```

% Female mice -- inhalation of 42, 236, 368 or 889 ppm TCE for 4 hours
PlotOutput=[];
ResetDoses
MousePost

```

```

% Settings from CMD file (BW from Eric's MCSim input file)
% KURNTCAC=0.6;
BW=0.0265;
CONC=368.0; TCHNG=4.0; DAYS=1.0; TMAX=24.0; DOSEINT=24.0; CALCINT=50.0; TSTP=30.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Female mice -- closed chamber inhalation of 300, 700, 1100, 3700 or 7000 ppm TCE
ResetDoses

% Settings from CMD file
% QPC=30.0; VFATC=0.10; VMAXC=23.2;

BW=0.024;
CC=1; NRATS=14.0; KLOSSC=0.02; VCHC=9.1;
CONC=300.0; TCHNG=10.0; DAYS=1.0; TMAX=24.0; DOSEINT=24.0; CALCINT=24.0; TSTP=2.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.021;
CONC=700.0; TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022;
CONC=1100.0; TSTP=4.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022;
CONC=3700.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.022;
CONC=7000.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male mice -- inhalation of 110, 297, 368 or 748 ppm TCE for 4 hours
ResetDoses
MousePost

% BW from Eric's MCSim input file
BW=0.0265;
CONC=110.0; TCHNG=4.0; DAYS=1.0; TMAX=24.0; DOSEINT=24.0; CALCINT=50.0; TSTP=25.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Male mice -- closed chamber inhalation of 1020, 1800, 3800, 5600 or 10000 ppm TCE
ResetDoses

% Settings from CMD file
% QPC=30.0; VFATC=0.05;

BW=0.03;
CC=1; NRATS=14.0; KLOSSC=0.02; VCHC=9.1;
CONC=1020.0; TCHNG=10.0; DAYS=1.0; TMAX=24.0; DOSEINT=24.0; CALCINT=24.0; TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.026;
NRATS=15.0; CONC=1800.0; TSTP=3.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.03;
NRATS=14.0; CONC=3800.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.028;
NRATS=15.0; CONC=5600.0; TSTP=6.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=0.026;
NRATS=15.0; CONC=10000.0; TSTP=4.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cinhppm, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher91_Mouse_Output.txt' @format=ascii

```

Greenberg99_Mouse.m

```

% Greenberg M, Burton G and Fisher J. 1999. Physiologically based pharmacokinetic modeling of
% inhaled trichloroethylene and its oxidative metabolites in B6C3F1 mice. Toxicol Appl
% Pharmacol 154: 264-278.
% Male B6C3F1 mice, 28-32 grams (N=6/time point)
% Inhalation of 100 or 600 ppm TCE for 4 hours

PlotOutput=[];
ResetDoses
MousePost

% BW from Eric's MCSim input file
BW=0.030;
CONC=100.0; TCHNG=4.0; DAYS=1.0; TMAX=48.0; DOSEINT=50.0; CALCINT=50.0; TSTP=48.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)

```



```

PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONC=600.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cfat, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cliv, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _clivtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Greenberg99_Mouse_Output.txt' @format=ascii

```

Prout85_Mouse.m

```

% Prout M, Provan W and Green T. 1985. Species differences in response to trichloroethylene: I
%   pharmacokinetics in rats and mice. Toxicol Appl Pharmacol 79: 389-400.
% Male B6C3F1 and Swiss-Webster mice, 25-32 grams (N=4 or 2 mice/group)
% Oral dosing of 10, 500, 1000 or 2000 mg/kg trichloro[14C]ethylene in corn oil (0.5 mL)
%   (containing 10 uCi)

```

```

PlotOutput=[];
ResetDoses
MousePost

```

```

% Settings from CMD file
% VMAXC=50.0; VMAXTCOHC=2.0; KAD=0.3;

```

```

BW=0.028;
PDOSE=1000.0; DAYS=1.0; TMAX=1.0; DOSEINT=50.0; CALCINT=50.0; TSTP=45.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

save PlotOutput @file='Prout85_Mouse_Output.txt' @format=ascii

```

Templin93_Mouse.m

```

% Templin M, Parker J and Bull R. 1993. Relative formation of dichloroacetate and
%   trichloroacetate from trichloroethylene in male B6C3F1 mice. Toxicol Appl Pharmacol 123: 1-8.
% Male B6C3F1 mice, 7 weeks of age (N=4/time point)
% Oral dosing of 3.8 mmol/kg (499.282 mg/kg) trichloroethylene in 2% polyoxyethylcnc-sorbitan
%   monooleate (Tween 80)

```

```

PlotOutput=[];
ResetDoses
MousePost

```

```

% Settings from CMD file
% VMAXC=60.0; VMAXTCOHC=0.5; KAD=1.0;

```

```

BW=0.02;
PDOSE=500.0; DAYS=1.0; TMAX=1.0; DOSEINT=50.0; CALCINT=50.0; TSTP=37.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Templin93_Mouse_Output.txt' @format=ascii

```

Cosby92_MouseDM.m

```

% Cosby NC, Dukelow WR. Toxicology of maternally ingested trichloroethylene
%      (TCE) on embryonal and fetal development in mice and of TCE metabolites on
%      in vitro fertilization. Fundam Appl Toxicol. 1992 Aug;19(2):268-74.

% C57BL/6 X DBA/2 (B6D2F1) mice, female, n = 11 with litters
% Oral gavage of 240.2 mg/kg TCE (NOAEL, POD) daily for 5 dy (GD1-5, GD6-10, or GD11-15)
%      Doses assumed to take 1 minute (0.017 hr)
% Doses based upon 1/10 and 1/100 of the LD50 value of 2402 mg/kg body weight
% Critical Effect: Litter size/viability, pup size/gross development
% Also tested: 0, 24.02 mg/kg

% Females were 6-8 wk at study start. Mean values for weight of female litter-bearing
%      mice were not significantly different across treatment doses for any treatment
%      group (data not shown).
% Mice are 8-10 wk at the end of the study. Since the mice are dosed by bw, size of
%      mouse does not change the dose. As there are no adverse effects recorded, no
%      particular exposure time is more important than another.
% The mice will be ~20-23 g during pregnancy (using the high end of the female curve due
%      to pregnancy). The simulation will be run for 22 g.
%      https://www.criver.com/products-services/find-model/b6d2f1-bdf1-mouse?region=3611

```

```

ResetDoses
MousePost
BW=0.022; PDOSE=240.2; DAYS=5.0; TMAX=120.0; DOSEINT=24.0; CALCINT=24.0; TSTP=120.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset

```

George85_MouseDM.m

```

% George JD, Reel JR, Myers CB, Lawton AD, Lamb JC. 1985. Trichloroethylene: Reproduction and
%      Fertility Assessment in CD-1 Mice When Administered in the Feed. Research Triangle
%      Park NC: National Toxicology Program, National Institute of Environmental Health
%      Sciences. NTP-86-068

% CD-1 mice, male and female, n = 8/sex
% 0.3% TCE in diet or 375 mg/kg-dy TCE (NOAEL, POD) for 15 wk
%      LOAEL: 0.6% or 750 mg/kg-dy
% Critical Effect: Decreased sperm motility
% Continuous breeding study (1 wk pre-dosing, 14 wks breeding, 3 wk segregation)
% Also tested: 0, 0.15% TCE in food (0, 187.5 mg/kg) (page 20)

% Male mouse weight in the 750 mg/kg-dy dose group was 37.79 +/- 0.62 g and was not
%      different from controls (39.19 +/- 0.55) (Table 6); it is assumed that the
%      375 mg/kg-dy group would be similar in weight (assuming 38 g)
% Assume it takes them 10 hours to consume their food (dark hours) as lights were on 0500
%      to 1900 hours

% Run until weekly AUC dosemetrics aren't changing
ResetDoses
MousePost

```

```

BW=0.038; DIET=750.0; TCHNG=10.0; DAYS=7.0; TMAX=1008.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=1008.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

```

Griffin00_MouseDM.m

```

% Griffin JM, Gilbert KM, Lamps LW, Pumford NR. 2000. CD4+ T-cell activation and induction
%   of autoimmune hepatitis following trichloroethylene treatment in MRL+/+ mice.
%   Toxicological Sciences 57: 345-52.

```

```

% MRL+/+ autoimmune prone mice, female, n = 8
% 0.1 mg/mL TCE in drinking water or 21 mg/kg-dy TCE (NOEL, POD) for 32 wk
%   LOEL: 0.5 mg/mL or 100 mg/kg-dy
% Critical Effect: Liver lymphocyte infiltration (Table 2)
% Also tested: 0, 2.5 mg/mL (400 mg/kg-dy) TCE in drinking water

```

```

% Body weights were not different between groups
%   Mice were 4 wk old at purchase; assuming a 2 wk acclimation period, mice were 38
%   wk at study end
% A growth chart for MRL mice was not found. A comparison was found (10-week-old
%   female C57BL/6 weighed 20.1+/-0.5 g, MRL/MpJ weighed an average of 31.7+/-0.4 g)
%   Thuret S, Thallmair M, Horky LL, Gage FH. 2012. Enhanced Functional Recovery in
%   MRL/MpJ Mice after Spinal Cord Dorsal Hemisection. PLoS ONE 7(2):
%   e30904. doi:10.1371/journal.pone.0030904
%   At 270 days, female C57BL/6 weigh 27 g (Hilltop Labs), so the MRL females may
%   weigh 43 g
%   http://www.hilltoplabs.com/public/c57growth.html

```

```

% Run until daily AUC dosemetrics aren't changing
ResetDoses
MousePost
BW=0.043; DRINK=13.4; CALCINT=24.0; TSTP=288.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

```

Kaneko00_MouseDM.m

```

% Kaneko T, Saegusa M, Tasaka K, Sato A. 2000. Immunotoxicity of Trichloroethylene:
%   a Study with MRL-lpr/lpr Mice. J. Appl. Toxicol. 20, 471-475

```

```

% MRL-lpr/lpr male mice, n = 5
% Inhalation of 500 ppm TCE (LOEL, POD) for 4 hr/dy, 6 dy/wk, 8 wk
% Effect: B cell function in MRL mice was used b/c the histology was not quantified
%   and the T cell staining lacks clear relevance and shows an effect at only one dose.
% Also tested: 0, 1000, 2000 ppm

```

```

% Mice were ~46-48 g at study finish (not statistically different between groups)
%   (Figure 1) - Using middle number (47 g)

```

```

% Run until weekly AUC dosemetrics aren't changing
ResetDoses
MousePost
BW=0.047; CONC=500.0; TCHNG=4.0; DAYS=6.0; TMAX=850.0; DOSEINT=24.0; CALCINT=168.0; TSTP=840.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

```

Kjellstrand83_MouseDM.m

% Kjellstrand P, Holmquist B, Aim P, Kanje M, Romare S, Jonsson I, Mansson L, Bjerkemo M.
% 1983. Trichloroethylene: Further Studies of the Effects on Body and Organ
% Weights and Plasma Butyrylcholinesterase Activity in Mice. Acta pharmacol. et
% toxicol. 1983, 53, 375-384.

% White NMRI mice, 20 male and 20 female (see Table 1)
% Inhalation of 37 ppm TCE (LOAEL, POD) for 24 hr/dy, 7 dy/wk, 30 dy
% Critical effect: Relative liver weight increase (see Table 3)
%
% Also tested: 75, 150, 300 ppm continuous; intermittent exposures also tested

% Female ending BW = 35.0 +/- 1.3 g (Table 2)

```
ResetDoses
MousePost
BW=0.035; CONC=37.0; TCHNG=800.0; DAYS=7.0; TMAX=800.0; DOSEINT=800.0; CALCINT=24.0;
TSTP=720.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset
```

% Male ending BW = 36.2 +/- 1.0 g (Table 2)

```
ResetDoses
MousePost
BW=0.0362; CONC=37.0; TCHNG=800.0; DAYS=7.0; TMAX=800.0; DOSEINT=800.0; CALCINT=24.0;
TSTP=720.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset
```

Land81_MouseDM.m

% Land PC, Owen EL, Linde HW. 1981. Morphologic Changes in Mouse Spermatozoa after
% Exposure to Inhalational Anesthetics during Early Spermatogenesis

% (C57B1 x C3H)F1 mice (n = 5)
% Inhalation of 200 ppm TCE (NOAEL, POD) for 4 hr/dy, 5 dy
% LOAEL (abnormal epididymal sperm, euthanized 28 dy after 1st exposure) 2000 ppm (n = 10)
% Also tested: 0 ppm

% Mice obtained at 8-10 wk old and exposed at 11 wk old; should be about 26 g
% RAO GN, HASEMAN JK, GRUMBEIN S, CRAWFORD DD, EUSTIS SL. 1990. Growth, Body Weight,
% Survival, and Tumor Trends in (C57BL/6 X C3H/HeN) F1 (B6C3F1) Mice During a
% Nine-Year Period. TOXICOLOGIC PATHOLOGY. 18(1): 71-77.

```
ResetDoses
MousePost
BW=0.026; CONC=575.0; TCHNG=4.0; DAYS=5.0; TMAX=130.0; DOSEINT=24.0; CALCINT=24.0; TSTP=120.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset
```

Ramadhan10_MouseDM.m

```
% Ramadhan DH, Kamijima M, Wang D, Ito Y, Naito H, Yanagiba Y, Hayashi Y, Tanaka N,  
% Aoyama T, Gonzalez FJ, Nakajima T. 2010. Differential Response to  
% Trichloroethylene-Induced Hepatosteatosi s in Wild-Type and PPAR $\alpha$ -Humanized Mice.  
% Environ Health Perspect 118:1557-1563  
  
% Wild type PPAR $\alpha$  mice, male (n = 6)  
% Inhalation of 1000 ppm TCE (LOAEL, POD) for 8 hr/dy, 7 dy  
% Critical Effect: increased ALT  
% Also tested: 0, 2000 ppm  
  
% NOTE: Ppar $\alpha$ -null and hPPAR $\alpha$  mice were also tested; only wild type results were  
% highlighted in the journal article copies received for this project so only  
% HEC from wild type data are predicted  
  
% BW for wild type mice exposed to 1000 ppm was listed as 25.0 +/- 2.3 g in Table 1  
  
ResetDoses  
MousePost  
BW=0.025; CONC=546.0; TCHNG=8.0; DAYS=7.0; TMAX=170.0; DOSEINT=24.0; CALCINT=24.0; TSTP=168.0;  
start @NoCallback  
plot(_t, _cart);  
i = i + 1;  
SaveDMS  
Output_Check  
Output_Check_Reset
```

Sanders82_MouseDM.m

```
% Sanders VM, Tucker AN, White KL, Kauffmann BM, Hallett P, Carchman RA, Borzelleca JF,  
% Munson AE. 1982. Humoral and cell-mediated immune status in mice exposed to  
% trichloroethylene in the drinking water. Toxicol. Appl. Pharmacol. 62: 358-68.  
  
% CD-1 mice, female and male, n = 12-20 for each sex  
% 0.1 mg/mL TCE in drinking water or 18.4 mg/kg-dy TCE (LOAEL, POD) for 4 mo  
% NOTE: A second group was exposed for 6 mo but the cell mediated response at the  
% LOAEL was only significant in the 4 mo group (Table 6)  
% Critical Effect: Cell-mediated SRBC response (Table 6) and bone marrow stem cells  
% (Table 8)  
% Also tested: 0, 1.0, 2.5, 5.0 mg/mL (0, 216.7, 393, 660.2 mg/kg-dy) TCE in drinking  
% water for 4 or 6 months  
  
% Simulation is for last week of study  
% Effects on BW and starting ages or BW were not mentioned  
% Assuming the mice are approximately 5 mo old for the 4 mo exposures  
% At 15 wk, female CD-1 rats would be 40 g at the top of the range and may indicate  
% their size at 20 wk  
% At 15 wk, male CD-1 rats would be 49 g at the top of the range and may indicate  
% their size at 20 wk  
% https://www.criver.com/products-services/find-model/cd-1-igs-mouse?region=3611  
  
% Females  
% Run until daily AUC dosemetrics aren't changing  
ResetDoses  
MousePost  
BW=0.040; DRINK=18.4; CALCINT=24.0; TSTP=312.0; CINT=0.1;  
start @NoCallback  
plot(_t, _cart);  
i = i + 1;  
SaveDMS  
Output_Check  
Output_Check_Reset  
  
% Males  
% Run until daily AUC dosemetrics aren't changing  
ResetDoses  
MousePost  
BW=0.049; DRINK=18.4; CALCINT=24.0; TSTP=312.0; CINT=0.1;  
start @NoCallback  
plot(_t, _cart);  
i = i + 1;
```

SaveDMs
Output_Check
Output_Check_Reset

Schwetz75_MouseDM.m

```
% Schwetz BA, Leong BKJ, Gehring PJ. 1975. The effect of maternally inhaled
%   trichloroethylene, perchloroethylene, methyl chloroform, and methylene
%   chloride on embryonal and fetal development in mice and rats. Toxicology
%   and Applied Pharmacology. 32:84-96.

% Swiss-Webster female mice, n = 12
% Inhalation of 306 ppm TCE (NOAEL, POD) for 7 hr/dy, GD 6-15 (10 days)
% No effect on fetal development
%   Tables 5-6
% Also tested: 0 ppm, also tested mice (see additional m file)

% Mice were 25-30 g prior to pregnancy; Mice exposed to TCE did not have decreased body
%   weight as the rats did
% Ending mouse weights are not given but liver weight was 2.8 +/- 0.3 g in TCE group and
%   relative liver weight was 0.052 +/- 0.006 g LW/g BW (Table 2)
%   Therefore BW was ~54 g in this group

ResetDoses
MousePost
BW=0.054; CONC=306.0; TCHNG=7.0; DAYS=7.0; TMAX=250.0; DOSEINT=24.0; CALCINT=24.0; TSTP=240.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset
```

APPENDIX Y

M Files for Rat Comparison Predictions from the Harmonized Model

The following M files are for generating rat output for validation figures (Figure S2) and for predicting the internal dose metrics (Table S1) in Appendix S. M files for the validation figures are first.

Bernauer96_Rat.m

```
% Bernauer U, Birner G, Dekant W and Henschler D. 1996. Biotransformation of trichloroethene:
% Dose-dependent excretion of 2,2,2-trichloro-metabolites and mercapturic acids in rats and
% humans after inhalation. Arch Toxicol 70: 338-346.
% http://dx.doi.org/10.1007/s002040050283.
% 2 male Wistar (300-350 g) and 2 female Wistar (200-250 g) exposed simultaneously with humans
% Inhalation of 40, 80 or 160 ppm TCE stabilized with diisopropylamine (40 ppm) for 6 hours
```

```
PlotOutput=[];
ResetDoses
RatPost
```

```
% Settings from CMD file
% KM=12.0;
```

```
BW=0.275;
CONC=40.0; TCHNG=6.0; DAYS=1.0; TMAX=6.0; DOSEINT=60.0; CALCINT=60.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvcmmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctotmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
CONC=80.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvcmmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctotmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
CONC=160.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvcmmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctotmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
save PlotOutput @file='Bernauer96_Rat_Output.txt' @format=ascii
```

Fisher91_Rat.m

```
% Fisher J, Gargas M, Allen B and Andersen M. 1991. Physiologically based pharmacokinetic
% modeling with trichloroethylene and its metabolite, trichloroacetic acid, in the rat and
% mouse. Toxicol Appl Pharmacol 109: 183-195.
% Female and male Fischer 344 rats
% Inhalation of 600, 505 or 529 ppm TCE for 4 hours
```

```
PlotOutput=[];
```

```
% Fisher91_Rat female
ResetDoses
RatPost
```

```
% Settings from CMD file (BW from Eric's MCSim input file)
% QPC=15.0; VMAXC=20.0;
BW=0.186;
CONC=600.0; TCHNG=4.0; DAYS=1.0; TMAX=24.0; DOSEINT=60.0; CALCINT=60.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
% Fisher91_Rat male
ResetDoses
RatPost
```

```
% BW from Eric's MCSim input file
BW=0.236;
CONC=505.0; TCHNG=4.0; DAYS=1.0; TMAX=24.0; DOSEINT=60.0; CALCINT=60.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cplastca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
% BW from Eric's MCSim input file
BW=0.236;
CONC=529.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
save PlotOutput @file='Fisher91_Rat_Output.txt' @format=ascii
```


Larson92b_Rat.m

% Larson J and Bull R. 1992. Species differences in the metabolism of trichloroethylene to the
% carcinogenic metabolites trichloroacetate and dichloroacetate. Toxicol Appl Pharmacol 115:
% 278-285. [http://dx.doi.org/10.1016/0041-008X\(92\)90333-N](http://dx.doi.org/10.1016/0041-008X(92)90333-N).
% Male Sprague-Dawley rats (404 +/- 91 g)
% Oral dosing of 1.5, 4.5 or 23 mmol TCE/kg in Tween 80 (constant volume of 3 ml/kg) after
% fasting for 24 hours

```
PlotOutput=[];  
ResetDoses  
RatPost
```

% Settings from CMD file (BW from Eric's MCSim input file)

```
% FRACTCE=0.02;  
BW=0.404;  
PDOSE=200.0; DAYS=1.0; TMAX=24.0; DOSEINT=100.0; CALCINT=100.0; TSTP=73.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
PDOSE=600.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
PDOSE=2996.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');  
i = i + 1;  
Output_Check  
Output_Check_Reset
```

```
save PlotOutput @file='Larson92b_Rat_Output.txt' @format=ascii
```

Prout85_Rat.m

% Prout M, Provan W and Green T. 1985. Species differences in response to trichloroethylene: I
% pharmacokinetics in rats and mice. Toxicol Appl Pharmacol 79: 389-400.
% Male Alderley Park Wistar OR Osborne-Mendel derived rats, 180-200g
% Oral dosing of 10, 500, 1000 or 2000 mg/kg trichloro[14C]ethylene (10 uCi) in corn oil

```
PlotOutput=[];
```

% Non-specified rats

```
ResetDoses  
RatPost  
BW=0.19; PDOSE=1000.0; DAYS=1.0; TMAX=1.0; DOSEINT=100.0; CALCINT=100.0; TSTP=73.0;  
start @NoCallback  
plot(_t, _cart)  
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cart, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cbldtca, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');  
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
```

```

i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Prout85_Rat_Output.txt' @format=ascii

Templin95_Rat.m
% Templin M, Stevens D, Stenner R, Bonate P, Tuman D and Bull R. 1995. Factors affecting species
% differences in the kinetics of metabolites of trichloroethylene. J Toxicol Environ Health 44:
% 435-447.
% Male F344 rats (250-300 g)
% Oral dosing of 0.15 or 0.76 mmol/kg TCE in 2% polyoxyethylene-sorbitan monooleate (Tween 80)

PlotOutput=[];
ResetDoses
RatPost

% Settings from CMD file
% FRACTCE=0.01; VMAXTCHOHC=0.06; VMAXGLUCC=150.0; KEHRC=0.3; KAD=0.6;

BW=0.2;
PDOSE=100.0; DAYS=1.0; TMAX=24.0; DOSEINT=60.0; CALCINT=60.0; TSTP=50.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Templin95_Rat_Output.txt' @format=ascii

Adams51_RatDM.m
% Adams EM, Spencer HC, Rowe VK, McCollister DD, Irish DD. 1951. Vapor toxicity of
% trichloroethylene determined by experiments on laboratory animals. AMA Archives of
% Industrial Hygiene and Occupational Medicine 4:469-481.

% Wistar origin rats, 15 male and 15 female
% Inhalation of 200 ppm TCE (NOAEL, POD) for 7 hr/dy, ~5 dy/wk,
% as many as 151 exposures in 205 days (29.3 wk, 6.7 mo) (Table 5)
% LOAEL (increased relative liver & kidney wt) 400 ppm, 7 hr/dy, ~5 dy/wk,
% as many as 173 exposures in 242 days (34.6 wk, 8 mo) (Table 3)
% Also tested: 100 ppm

% Female ending BW = 207 g (Table 5)
% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.207; CONC=200.0; TCHNG=7.0; DAYS=5.0; TMAX=1010.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=1008.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset

% Male ending BW = 349 g (Table 5)
% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.349; CONC=200.0; TCHNG=7.0; DAYS=5.0; TMAX=1010.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=1008.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;

```

SaveDMS
Output_Check
Output_Check_Reset

Albee06_RatDM.m

% Albee RR, Spencer PJ, Johnson KA, Bradley GJ, Marable BR. 2006. Lack of trigeminal
% nerve toxicity in rats exposed to trichloroethylene vapor for 13 weeks.
% International Journal of Toxicology 25:531-540.

% Fischer-344 rats, 10 male and 10 female
% Inhalation of 800 ppm TCE (NOAEL, POD) for 6 hr/dy, 5 dy/wk, 13 wk
% LOAEL (hearing loss, loss of hair cells) 2500 ppm
% Also tested: 250 ppm

% Body weights are not specified; only that they were not different between groups
% Rats were 14 wk at receipt, 16 wk (most likely) at study start, and 29 wk at end
% Rats would be about 275 g (M) and 175 g (F) at study start
% Based on 2018 Charles River catalog
% Estimated 29 wk weight is 400 g (M) and 200 g (F)
% (4 wk F344 rats, 25 wk on feeding study, Fig 1)
% Rao GN, Morris RW, Seely JC. 2001 Beneficial effects of NTP-2000 diet on growth,
% survival, and kidney and heart diseases of Fischer 344 rats in chronic studies
% Toxicological Sciences 63:245-255.

% Female ending BW = 200 g (estimated from Rao et al. 2001)
% Run for 13 weeks
ResetDoses
RatPost
BW=0.2; CONC=800.0; TCHNG=6.0; DAYS=5.0; TMAX=2190.0; DOSEINT=24.0; CALCINT=168.0; TSTP=2184.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

% Male ending BW = 400 g (estimated from Rao et al. 2001)
% Run for 13 weeks
ResetDoses
RatPost
BW=0.4; CONC=800.0; TCHNG=6.0; DAYS=5.0; TMAX=2190.0; DOSEINT=24.0; CALCINT=168.0; TSTP=2184.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

Arito94_RatDM.m

% Arito H, Takahashi M, Ishikawa T. 1994. Effect of subchronic inhalation exposure
% to low-level trichloroethylene on heart rate and wakefulness-sleep in freely
% moving rats. Japanese Journal of Industrial Health 36:1-8.

% JCL-Wistar rats, 20 male (4 groups of 5 exposed to each concentration)
% Inhalation of 50 ppm TCE (LOAEL, POD) for 8 hr/dy, 5 dy/wk, 2,4,6 wk
% Critical effect: Decreased wakefulness
% Also tested: 100 & 300 ppm

% Body weights are not specified
% Rats were 4 wk at receipt, 9 wk at EEG/EMG/ECG implant, 11 wk (most likely) at
% study start, and 17 wk at end
% Rats would be about 375 g (M) at 17 weeks
% Estimate based on website growth curve:
% http://www.clea-japan.com/en/animals/animal_e/e_03.html

% Male ending BW = 375 g
% Run for 6 weeks

```

ResetDoses
RatPost
BW=0.375; CONC=18.4; TCHNG=8.0; DAYS=5.0; TMAX=1010.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=1008.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

```

Bushnell197_RatDM.m

```

% Bushnell PJ. 1997. Concentration-time relationships for the effects of inhaled
%   trichloroethylene on signal detection behavior in rats. Fundamental and Applied
%   Toxicology 36:30-38.

```

```

% Long-Evans rats, 11 male
% Inhalation of 800 ppm TCE (NOAEL, POD) for 1 hr/dy
%   see Figure 1 of article
% LOAEL (sensitivity to light stimulus, visual learning) 1200 ppm
% Also tested: 400, 1600, 2000, 2400 ppm

```

```

% The spreadsheet "Studies to Run PBPK" indicates that the animals are exposed 3 times
%   a week. All animals are exposed to air, then 3 different concentrations on 4
%   consecutive days of a week (0, 400, 600, 1200 ppm). The following week, the
%   same rats are exposed to 0, 800, 1200, 2400 ppm.

```

```

% Ending BW = 350 g (controlled by measured diet)
% Simulation for 1 day of exposure
ResetDoses
RatPost
BW=0.35; CONC=1366.0; TCHNG=1.0; DAYS=1.0; TMAX=25.0; DOSEINT=24.0; CALCINT=24.0; TSTP=24.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

```

```

% Simulation for 3 days per week for 2 weeks
% Says dosed on 2nd, 3rd and 4th day of week but currently running for 1st, 2nd and 3rd so as to
%   not have to change model code
ResetDoses
RatPost
BW=0.35; CONC=1366.0; TCHNG=1.0; DAYS=3.0; TMAX=340.0; DOSEINT=24.0; CALCINT=168.0; TSTP=336.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

```

Carney06_RatDM.m

```

% Carney, E.W., Thorsrud, B.A., Dugard, P.H. and Zablony, C.L. 2006. Developmental toxicity
%   studies in Crl:CD (SD) rats following inhalation exposure to trichloroethylene and
%   perchloroethylene. Birth Defects Res B Dev Reprod Toxicol 77(5): 405-12.

```

```

% Crl:CD rats (Sprague-Dawley), 27 female
% Developmental study to look for cardiac defects
% Inhalation of 600 ppm TCE (NOAEL, POD) for 6 hr/dy, 7 dy/wk, GD6-20 (15 days)
% Also tested: 50, 150 ppm

```

```

% Body weights are not specified; According to the Charles River 2018 catalog,
%   young adult female SD rats are about 200 g with the high end of the range
%   at 225 g. Since these are pregnant, 225 g was chosen.

```

```

% Timed pregnant female ending BW = 225 g (estimated from CRL catalog)
ResetDoses
RatPost

```

```

BW=0.225; CONC=600.0; TCHNG=6.0; DAYS=7.0; TMAX=370.0; DOSEINT=24.0; CALCINT=24.0; TSTP=360.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset

```

Crofton97_RatDM.m

```

% Crofton KM and Zhao X. 1997. The Ototoxicity of Trichloroethylene: Extrapolation and
% Relevance of High-Concentration, Short-Duration Animal Exposure Data. FUNDAMENTAL
% AND APPLIED TOXICOLOGY 38, 101-106

```

```

% Long Evan rats, 10-12 male
% Inhalation of 1600 ppm TCE (NOAEL, POD) for 6 hr/dy, 5 dy/wk, 13 wk
% LOAEL (shift in auditory threshold, 13 wk group) 2400 ppm
% Also tested: 800, 3200 ppm; All concentrations tested for 1 dy, 1 wk, 4 wk, 13 wk

```

```

% Rats were received at 60 dy of age (8.5 wk) and would have been 23 wks at study
% finish, including a 2 wk quarantine/acclimation period
% Rats would be about 300 g at 8 wk and 700 g at 23 wk (675 g at 21 wk, no acclimation)
% Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
% 17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.

```

```

% Run for 13 weeks

```

```

ResetDoses
RatPost
BW=0.700; CONC=1367.0; TCHNG=6.0; DAYS=5.0; TMAX=2190.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=2184.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset

```

Fisher01_RatDM.m

```

% Fisher JW, Channel SR, Eggers JS, Johnson PD, MacMahon KL, Goodyear CD, Sudberry GL,
% Warren DA, Latendresse JR, Graeter LJ. 2001. Trichloroethylene, Trichloroacetic
% Acid, and Dichloroacetic Acid: Do They Affect Fetal Rat Heart Development?
% International Journal of Toxicology, 20:257-267.

```

```

% Sprague Dawley rats, female, n = 20 litters
% Oral gavage of 500 mg/kg TCE (NOAEL, POD) daily for 10 dy (GD6-15)
% Doses assumed to take 1 minute (0.017 hr)
% Critical Effect: Cardiovascular malformation
% Also tested: 0 mg/kg TCE (2 groups, water or soybean oil); 300 mg/kg TCA, 300 mg/kg DCA
% or 15 mg/kg retinoic acid groups were included in the study

```

```

% Males and females were purchased at 9 wk and 200-300 g at study start. They were 11 wk
% at study start
% Rats were approximately 13 wk at study end.
% Maternal body weight gain for TCE- and RA-treated rats during gestation was not
% significantly different from the control soybean oil vehicle; TCE rats had gained
% almost 20 g at study end
% SD females should weigh about 225 g at this age (middle of range), making them 245-250 g
% when pregnant and at the top end of the weight range for this strain (250 g)
% From: Charles River 2018 catalog

```

```

ResetDoses
RatPost
BW=0.250; PDOSE=500.0; TCHNG=0.017; DOSEINT=24.0; DAYS=7.0; TMAX=240.0; CALCINT=24.0;
TSTP=240.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset

```

Healy82_RatDM.m

% Healy TEJ, Poole TR and Hopper A. 1982. Rat fetal development and maternal exposure to
% trichloroethylene 100 ppm. Br. J. Anaesth. 54, 337-341.

% Wistar origin rats, 32 female (31 control), GD 8-21
% Inhalation of 100 ppm TCE (LOAEL, POD) for 4 hr/dy, 7 dy/wk, 14 dy
% Increased resorptions, decreased fetal weight
% Also tested: 0 ppm

% Body weights were 200-300 g at breeding. These rats are approximately 11 weeks old
% according to the Charles River 2018 catalog. Three weeks later (14 wk) they
% would weigh 210-330 g. Taking the middle value at start (250 g) and adding 20 g
% growth and 30 g of babies, you get 300 g at study end.

```
ResetDoses
RatPost
BW=0.300; CONC=100.0; TCHNG=4.0; DAYS=7.0; TMAX=340.0; DOSEINT=24.0; CALCINT=24.0; TSTP=336.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset
```

Jaspers93_RatDM.m

% Jaspers RMA, Muijsers H, Lammers JHCM and Kulig BM. 1993. Mid-frequency hearing loss and
% reduction of acoustic startle responding in rats following trichloroethylene exposure.
% Neurotoxicology and Teratology, Vol. 15, pp. 407-412.

% Wistar-derived Wag-Rij/MBL strain rats, 12, assumed male but not specified
% Inhalation of 1500 ppm TCE (NOAEL, POD) for 18 hr/dy, 5 dy/wk, 3 wk
% LOAEL (auditory threshold shift) 3000 ppm
% Also tested: 0 ppm

% BW = 180 +/- 10 g (about 11 weeks old) at receipt
% Figure 1 shows BW change over time; At last week of exposure, rats weighed
% ~250, ~240, ~225 for exposure groups 0, 1500, 3000 ppm, respectively. BW
% differences were significant. 240 g was used for the NOAEL POD simulation

```
ResetDoses
RatPost
BW=0.240; CONC=1500.0; TCHNG=18.0; DAYS=5.0; TMAX=510.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=504.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset
```

Kumar00a_01a_RatDM.m

% Kumar P, Prasad AK, Dutta KK. 2000. Steroidogenic alterations in testes and sera of
% rats exposed to trichloroethylene (TCE) by inhalation. Human & Experimental
% Toxicology (2000) 19, 117-121

% Wistar origin rats, 12-13 male
% Inhalation of 376 ppm TCE (LOAEL, POD) for 4 hr/dy, 5 dy/wk, 12 or 24 wk
% Critical effect: Decreased sperm count & motility
% Also tested: 0 ppm

% A smaller rat would inhale a relatively higher total amount of TCE. Therefore
% the simulation will model the last week of the 12 wk exposure.
% BW at receipt: 50 +/- 5 g
% The Charles River Laboratory 2018 catalog indicates that these rats would be just
% weaned and about 3 weeks old
% Rats were bred in house; they would not have needed quarantine and there was no mention
% of acclimation. The rats would be 15 weeks of age

```

% The rats would be approximately 500 g according to Tordoff et al. 2008
%   Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
%   17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.

% KUMAR P, PRASAD AK, MAJI BK, MANI U, DUTTA KK. 2001. Hepatotoxic Alterations Induced
%   by Inhalation of Trichloroethylene (TCE) in Rats. BIOMEDICAL AND ENVIRONMENTAL
%   SCIENCES 14, 325-332.

% Wistar rats, 6 male
% Inhalation of 376 +/- 1.76 ppm TCE (LOAEL, POD) for 4 hr/dy, 5 dy/wk,
%   8, 12, or 24 wk
% Critical effect: Liver weight (significant increase but data not shown), enlarged
%   fatty hepatocytes (via histology but no statistics); All effects evident at 8 wk
%   and more progressive at 12 and 24 wk
% Also tested: 0 ppm

% Simulating the last week of the 8 wk exposure; Younger rats will inhale comparatively
%   more TCE than larger due to higher respiratory rates
% BW was 130 +/- 10 g at study start; Animals bred in-house, so no quarantine was
%   necessary; Acclimation was not mentioned in the study
% Rats were about 5 weeks at study start (Charles River Laboratories 2018 catalog)
% Rats would be 13 weeks at study end and approximately 400 g according to Tordoff et al.
%   Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
%   17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.

% Ending BW = 530 g
% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.5; CONC=376.0; TCHNG=4.0; DAYS=5.0; TMAX=1180.0; DOSEINT=24.0; CALCINT=168.0; TSTP=1176.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset

```

Maltoni88_RatDM.m

```

% Maltoni C, Lefemine G, Coiti G, Perino G. 1988. Long-term carcinogenicity bioassays
%   on trichloroethylene administered by inhalation to sprague-dawley rats and swiss
%   and B6C3F1 mice. Annals of the New York Academy of Sciences. 534: 316-342.
% Sprague-Dawley rats, 15 male and 15 female
% Inhalation of 300 ppm TCE (NOAEL, POD) for 7 hr/dy, 5 dy/wk, 104 wk
% LOAEL (meganucleocytosis of kidney, Table 20) 600 ppm
% Also tested: 100 ppm

% Rats were 12-13 wk at start of experiment; this strain of male rat appears to max out
%   at 850 g
%   Tordoff MG, Alarcon LK, Lawler MP. 2008. Preferences of 14 rat strains for
%   17 taste compounds. Physiol Behav. 2008 October 20; 95(3): 308-332.
% Simulating the last week of exposures

% NOTE: These POD simulations for HEC predictions are for non-cancer endpoints. This
%   study contains cancer endpoints as well. Further, the study was performed in two
%   strains of mice also. However, the non-cancer POD for this study was found
%   in the male rats only.

% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.85; CONC=221.0; TCHNG=7.0; DAYS=5.0; TMAX=850.0; DOSEINT=24.0; CALCINT=168.0; TSTP=840.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset

```

Manson84_RatDM.m

```
% Manson JM, Murphy M, Richdale N, Smith MK. 1984. Effects of oral exposure to
%      trichloroethylene on female reproductive function. Toxicology. 32: 229-42.

% Long-Evans rats, female, n = 23
% Oral gavage of 100 mg/kg TCE (NOAEL, POD) 5 dy/wk for 3 wk, 7 dy/wk for 3 wk
%      Doses assumed to take 1 minute (0.017 hr)
%      Simulating last week of gestation (7 dy/wk)
% LOAEL: 1000 mg/kg-dy
% Critical Effect: Neonatal+Postnatal death
% Also tested: 0, 10 mg/kg-dy TCE (corn oil)

% Males and females were purchased at 80-100 dy. There was a 2 wk quarantine.
% Body weights in the 100 mg/kg-dy group on GD22 were 405 +/- 7.4 g (Table 1).
%      NOTE: BW were significantly decreased in the 1000 mg/kg-dy group.

% Run until weekly AUC dosemetrics aren't changing
ResetDoses
RatPost
BW=0.405; PDOSE=100.0; TCHNG=0.017; DOSEINT=24.0; DAYS=7.0; TMAX=504.0; CALCINT=168.0;
TSTP=504.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset
```

Narotsky95_RatDM.m

```
% Narotsky MG, Weller EA, Chinchilli VM, Kavlock RJ. Nonadditive Developmental Toxicity
%      in Mixtures of Trichloroethylene, Di(2-ethylhexyl) Phthalate, and Heptachlor
%      in a 5 x 5 x 5 Design. Fundam. Appl. Toxicol. 27, 203-216.

% F-344 rats, female, n = 7-12
% Oral gavage of 844 mg/kg TCE (NOAEL, POD) daily on GD6-15 (10 dy)
%      Doses assumed to take 1 minute (0.017 hr)
% LOAEL: 1125 mg/kg-dy
% Critical Effect: Litter resorptions (Table 3a)
% Also tested: 0, 475, 633 mg/kg-dy TCE (corn oil)

% Timed pregnant females were purchased at 90 dy old
% Doses were the same daily and were based on GD6 BW (~96 dy or ~14 wk)
% Weight gain data were given (Table 5) but no data were presented on actual BW
% F-344 females at 14 wk weigh ~175 g at 14 wk (high end of range due to pregnancy);
%      This weight is what the dose was calculated on, not the ending pregnancy wt
%      Charles River Laboratories 2018 Catalog

ResetDoses
RatPost
BW=0.175; PDOSE=36.0; TCHNG=0.017; DOSEINT=24.0; DAYS=7.0; TMAX=240.0; CALCINT=24.0;
TSTP=240.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset
```

Schwetz75_RatDM.m

```
% Schwetz BA, Leong BKJ, Gehring PJ. 1975. The effect of maternally inhaled
%      trichloroethylene, perchloroethylene, methyl chloroform, and methylene
%      chloride on embryonal and fetal development in mice and rats. Toxicology
%      and Applied Pharmacology. 32:84-96.

% Sprague-Dawley female rats, n = 18
% Inhalation of 306 ppm TCE (NOAEL, POD) for 7 hr/dy, GD 6-15 (10 days)
% No effect on fetal development
%      Tables 5-6
```



```

% Also tested: 0 ppm, also tested mice (see additional m file)

% Rats were ~250 g prior to pregnancy; Rats exposed to TCE weighed 4-5% less than
%     controls (statistically significant; not really biologically significant)
% Ending rat weights are not given but liver weight was 13.7 +/- 1.4 g in TCE group and
%     relative liver weight was 0.037 +/- 0.004 g LW/g BW (Table 2)
%     Therefore BW was ~370 g in this group

ResetDoses
RatPost
BW=0.370; CONC=306.0; TCHNG=7.0; DAYS=7.0; TMAX=250.0; DOSEINT=24.0; CALCINT=24.0; TSTP=240.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

Woolhiser06_RatDM.m
% Woolhiser MR, Krieger SM, Thomas J., Hotchkiss JA. 2006. Trichloroethylene (TCE):
%     immunotoxicity potential in CD rats following a 4-week vapor inhalation exposure.
%     Midland, MI: The Dow Chemical Company. Study ID: 031020

% Sprague-Dawley rats, female, n =
% Inhalation of 300 ppm TCE (NOAEL, POD) for 6 hr/dy, 5 dy/wk, 4 wk
%     LOAEL 1000 ppm
% Increased relative kidney & liver weight; Decreased PFC response (plaque
%     forming cell assay) - Tables 10, 19
% Also tested: 100 ppm

% Rats were 214.6 g at end (300 ppm group, Table 6)
%     Simulations are for the final week of exposure

% Immune effects
ResetDoses
RatPost
BW=0.2146; CONC=243.0; TCHNG=6.0; DAYS=5.0; TMAX=675.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=672.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

% Kidney effects
BW=0.2146; CONC=90.0; TCHNG=6.0; DAYS=5.0; TMAX=675.0; DOSEINT=24.0; CALCINT=168.0; TSTP=672.0;
CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

% Liver effects
BW=0.2146; CONC=108.0; TCHNG=6.0; DAYS=5.0; TMAX=675.0; DOSEINT=24.0; CALCINT=168.0;
TSTP=672.0; CINT=0.1;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMS
Output_Check
Output_Check_Reset

```

Wu07_RatDM.m

```
% Wu KL, Berger T. 2007. Trichloroethylene metabolism in the rat ovary reduces oocyte
%      fertilizability. Chemico-Biological Interactions 170 (2007) 20-30.

% Simonson albino rats, a Sprague-Dawley derived strain, female, n = 12-20
% 0.45% in drinking water or 66 mg/kg-dy TCE (LOAEL, POD) for 2 wk
% Critical Effect: In vitro fertilization by oocytes from exposed females less successful
% Also tested: 0 mg/kg-dy (3% Tween vehicle control) in drinking
%      water for 4 or 5 dy or 2 wk

% Simulation is for whole study
% Female rats were between 28 and 45 days old at receipt (using 37 dy); Assuming a 2 wk
%      acclimation; Therefore the rats were ~51 dy at start and 65 dy (~9 wk) at finish
%      (in vitro fertilization collection)
% BW was not mentioned in the results but no effect was seen on liver wt
% Growth data on Simonson albino rats were not found; Sprague-Dawley females are
%      approximately 200 g at that age (mid-range)
%      Charles River Laboratories 2018 catalog

ResetDoses
RatPost
BW=0.200; DRINK=66.0; CALCINT=24.0; TSTP=336.0;
start @NoCallback
plot(_t, _cart);
i = i + 1;
SaveDMs
Output_Check
Output_Check_Reset
```

APPENDIX Z

M Files for Human Comparison Predictions from the Harmonized Model

The following M files are for generating human output for validation figures (Figure S3) and for predicting the internal dose metrics (Tables S2 and S3) in Appendix S. M files for the validation figures are first. “FitHumanDMS.m” is the same as for the acslX version of the EPA model except that “CONCLIST(1)” should be changed to “CONC” so it is not repeated here. Note that values for “Target” would also need to be changed based on the results in Table S1. Lines for endpoints for kidney and some additional endpoints might need to be commented out as the harmonized model does not include a kidney compartment and some HECs could not be estimated due to saturation of the metabolic route (see results in Tables S2 and S3 for HECs).

Bernauer96_Human.m

```
% Bernauer U, Birner G, Dekant W and Henschler D. 1996. Biotransformation of trichloroethene:
% Dose-dependent excretion of 2,2,2-trichloro-metabolites and mercapturic acids in rats and
% humans after inhalation. Arch Toxicol 70: 338-346.
% http://dx.doi.org/10.1007/s002040050283.
% 3 male volunteers, 37-69 years old
% Inhalation of 40, 80 or 160 ppm TCE stabilized with diisopropylamine (40 ppm) for 6 hours
% Revised for consistency with molar data, and for 1,1+1,2 isomers for DCVC
```

```
PlotOutput=[];
ResetDoses
HumanPost
```

```
CONC=40.0; TCHNG=6.0; DAYS=1.0; TMAX=6.0; DOSEINT=60.0; CALCINT=60.0; TSTP=55.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvcmmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctotmmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
CONC=80.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvcmmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctotmmole, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
```

```
CONC=160.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvc, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctot, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurndcvcmmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntctotmmole, @Justification = 'begin');
i = i + 1;
```

```

Output_Check
Output_Check_Reset
save PlotOutput @file='Bernauer96_Human_Output.txt' @format=asci

```

Fisher98_Human.m

```

% Fisher J, Mahle D and Abbas R. 1998. A human physiologically based pharmacokinetic model for
% trichloroethylene and its metabolites, trichloroacetic acid and free trichloroethanol.
% Toxicol Appl Pharmacol 152: 339-359.
% http://dx.doi.org/10.1006/taap.1998.8486.
% Male and female volunteers, 20-36 years old
% Inhalation dosing of 50 or 100 ppm TCE for 4 hours

```

```

PlotOutput=[];
ResetDoses
HumanPost

```

```

% Male subject 1
% PB from Eric's MCSim input file
BW=71.4; VFATC=0.17; VSLWC=0.63221; PB=11.47;
CONC=105.5; TCHNG=4.0; DAYS=1.0; TMAX=24.0; DOSEINT=320.0; CALCINT=320.0; TSTP=300.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Male subject 2
% PB from Eric's MCSim input file
BW=69.3; VFATC=0.27; VSLWC=0.53221; PB=10.07;
CONC=49.3;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Male subject 3
% PB from Eric's MCSim input file
BW=71.1; VFATC=0.14; VSLWC=0.66221; PB=11.13;
CONC=55.2;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

CONC=101.5;
start @NoCallback
plot(_t, _cart)

```

```

PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 4
% PB from Eric's MCSim input file
BW=52.3; VFATC=0.10; VSLWC=0.70221; PB=12.06;
CONC=53.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=52.3; VFATC=0.06; VSLWC=0.74221;
CONC=97.8;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 5
% PB from Eric's MCSim input file
BW=82.3; VFATC=0.14; VSLWC=0.66221; PB=11.94;
CONC=105.5;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 6
% PB from Eric's MCSim input file
BW=82.7; VFATC=0.14; VSLWC=0.66221; PB=10.91;
CONC=102.6;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cblدتca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');

```

```

PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 7
% PB from Eric's MCSim input file
BW=73.2; VFATC=0.18; VSLWC=0.62221; PB=10.49;
CONC=102.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 8
% Settings from CMD file
% VMAXC=3.0;

BW=60.9; VFATC=0.1; VSLWC=0.70221;
CONC=101.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Male subject 9
BW=70.9; VFATC=0.18; VSLWC=0.62221;
CONC=103.4;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher98_MHuman_Output.txt' @format=ascii

```

```

PlotOutput=[];
ResetDoses
HumanPost

% Female subject 1
% PB from Eric's MCSim input file
BW=66.5; VFATC=0.32; VSLWC=0.48221; PB=9.87;
CONC=55.1; TCHNG=4.0; DAYS=1.0; TMAX=24.0; DOSEINT=320.0; CALCINT=320.0; TSTP=300.0; CINT=0.1;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

BW=66.6;
CONC=101.4;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 2
% PB from Eric's MCSim input file
BW=62.3; VFATC=0.24; VSLWC=0.56221; PB=9.49;
CONC=53.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Settings from CMD file
% VMAXC=3.0;

CONC=97.7;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

```

```

% Female subject 3
% PB from Eric's MCSim input file
BW=57.5; VFATC=0.21; VSLWC=0.59221; PB=6.49;
CONC=102.5;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 4
% PB from Eric's MCSim input file
BW=55.5; VFATC=0.23; VSLWC=0.57221; PB=7.61;
CONC=102.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 5
% PB from Eric's MCSim input file
BW=67.3; VFATC=0.35; VSLWC=0.45221; PB=11.02;
CONC=102.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 6
BW=63.2; VFATC=0.26; VSLWC=0.54221;
CONC=101.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

% Female subject 7
BW=48.6; VFATC=0.23; VSLWC=0.57221;
CONC=103.3;
start @NoCallback

```



```

plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cdca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset
% Female subject 8
% PB from Eric's MCSim input file
BW=61.8; VFATC=0.33; VSLWC=0.47221; PB=10.38;
CONC=102.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
% PlotOutput = addcolsj(PlotOutput, _cdcvg_mmole, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

save PlotOutput @file='Fisher98_FHuman_Output.txt' @format=ascii

```

Monster76 Human.m

```

% Monster A, Boersma G and Duba W. 1976. Pharmacokinetics of trichloroethylene in volunteers,
% influence of workload and exposure concentration. Int Arch Occup Environ Health 38: 87-102.
% http://dx.doi.org/10.1007/BF00378619.
% Four male volunteers
% Inhalation dosing of 70 or 140 ppm TCE for 4 hours

```

```

PlotOutput=[];
ResetDoses
HumanPost

% Single exposure
BW=69.7;
CONC=70.0; TCHNG=4.0; DAYS=1.0; TMAX=24.0; DOSEINT=230.0; CALCINT=230.0; TSTP=220.0;
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _t, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;
Output_Check
Output_Check_Reset

CONC=140.0
start @NoCallback
plot(_t, _cart)
PlotOutput = addcolsj(PlotOutput, _aurntcogtcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _calvppm, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cbltdtca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _cven, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _totctcoh, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _aurntca, @Justification = 'begin');
PlotOutput = addcolsj(PlotOutput, _ctcoh, @Justification = 'begin');
i = i + 1;

```

```

Output_Check
Output_Check_Reset

save PlotOutput @file='Monster76_Human_Output.txt' @format=ascii

Human_Fit_DMs_ContInh.m
% Fit human continuous inhalation doses to animal internal dosemetrics
load @format=model @file=TCE_BD
Init

% Set parameters for simulations
FitDoses = []; j = 0;
ResetDoses
HumanPost
CONC=10.0; TCHNG=2020.0; DAYS=7.0; TMAX=2020.0; DOSEINT=2020.0; CALCINT=24.0; TSTP=2016.0;
CINT=0.1;

FitHumanDMS

% Save the results of the dose fitting
save FitDoses @file='FitDoses_Human_ContInh_DMS.txt' @format=ascii

Human_Fit_DMs_OccInh.m
% Fit human occupational (8 hr/d, 5 d/w) Occupational inhalation doses to animal internal
% dosemetrics

load @format=model @file=TCE_BD
Init

% Set parameters for simulations
FitDoses = []; j = 0;
ResetDoses
HumanPost
CONC=10.0; TCHNG=8.0; DAYS=5.0; TMAX=2020.0; DOSEINT=24.0; CALCINT=168.0; TSTP=2016.0;
CINT=0.1;

FitHumanDMS

% Save the results of the dose fitting
save FitDoses @file='FitDoses_Human_OccInh_DMS.txt' @format=ascii

Fit_Dose.m
% Dose fitting algorithm -- uses ratios

if (TargetParam == 'MaxCART      ')
    EndPt = max(_cart);
else
    if (TargetParam == 'AUCCBLDDM  ')
        EndPt = AUCCBLDDM;
    else
        if (TargetParam == 'MaxCLiv      ')
            EndPt = max(_cliv);
        else
            if (TargetParam == 'AUCCLIVDM      ')
                EndPt = AUCCLIVDM;
            else
                if (TargetParam == 'TotMetabBW34DM')
                    EndPt = TOTMETABBW34DM;
                else
                    if (TargetParam == 'TotOxMetBW34DM')
                        EndPt = TOTOXMETBW34DM;
                    else
                        if (TargetParam == 'AMetLiv1BW34DM')
                            EndPt = AMETLIV1BW34DM;
                        end
                    end
                end
            end
        end
    end
end
end
end

```

```

        end
    end
end

NumAttempt = 0;
while abs(EndPt-Target) > Tolerance
    CONC = CONC * (Target / EndPt);

    start @NoCallback
    NumAttempt = NumAttempt + 1;
    CONC

    if (TargetParam == 'MaxCart      ')
        max(_cart)
        EndPt = max(_cart);
    else
        if (TargetParam == 'AUCCBLDDM      ')
            AUCCBLDDM
            EndPt = AUCCBLDDM;
        else
            if (TargetParam == 'MaxCLiv      ')
                max(_cliv)
                EndPt = max(_cliv);
            else
                if (TargetParam == 'AUCCLIVDM      ')
                    AUCCLIVDM
                    EndPt = AUCCLIVDM;
                else
                    if (TargetParam == 'TotMetabBW34DM')
                        TOTMETABBW34DM
                        EndPt = TOTMETABBW34DM;
                    else
                        if (TargetParam == 'TotOxMetBW34DM')
                            TOTOXMETBW34DM
                            EndPt = TOTOXMETBW34DM;
                        else
                            if (TargetParam == 'AMetLiv1BW34DM')
                                AMETLIV1BW34DM
                                EndPt = AMETLIV1BW34DM;
                            end
                        end
                    end
                end
            end
        end
    end

    if (NumAttempt > 15)
        Fit_Dose_Alt
        break;
    end
end

```

Fit_Dose_Alt.m

% Alternate dose fitting algorithm -- uses interval halving

% Find doses that bound the target endpoint value

CurrentConc = CONC;

if (EndPt < Target)

while EndPt < Target

PLowConc = CurrentConc;

CurrentConc = 1.1 * CurrentConc;

CONC = CurrentConc;

start @NoCallback

CurrentConc

if (TargetParam == 'MaxCart ')


```

start @NoCallback
CONC

if (TargetParam == 'MaxCART      ')
    max(_cart)
    EndPt = max(_cart);
else
    if (TargetParam == 'AUCCBLDDM      ')
        AUCCBLDDM
        EndPt = AUCCBLDDM;
    else
        if (TargetParam == 'MaxCLiv      ')
            max(_cliv)
            EndPt = max(_cliv);
        else
            if (TargetParam == 'AUCCLivDM      ')
                AUCCLIVDM
                EndPt = AUCCLIVDM;
            else
                if (TargetParam == 'TotMetabBW34DM')
                    TOTMETABBW34DM
                    EndPt = TOTMETABBW34DM;
                else
                    if (TargetParam == 'TotOxMetBW34DM')
                        TOTOXMETBW34DM
                        EndPt = TOTOXMETBW34DM;
                    else
                        if (TargetParam == 'AMetLiv1BW34DM')
                            AMETLIV1BW34DM
                            EndPt = AMETLIV1BW34DM;
                        end
                    end
                end
            end
        end
    end
end
end
end
end
end

% -----
% Repeat simulations until the dose to match the target endpoint value is found
NumAttempt2 = 0;
while abs(EndPt-Target) > Tolerance
    if (EndPt < Target)
        PLowConc = CurrentConc;
    else
        PHighConc = CurrentConc;
    end

    CONC = (PHighConc + PLowConc) / 2.0;
    CurrentConc = CONC;

    start @NoCallback
    NumAttempt2 = NumAttempt2 + 1;
    CONC

    if (TargetParam == 'MaxCART      ')
        max(_cart)
        EndPt = max(_cart);
    else
        if (TargetParam == 'AUCCBLDDM      ')
            AUCCBLDDM
            EndPt = AUCCBLDDM;
        else
            if (TargetParam == 'MaxCLiv      ')
                max(_cliv)
                EndPt = max(_cliv);
            else

```

```

if (TargetParam == 'AUCCLivDM')
    AUCCLIVDM
    EndPt = AUCCLIVDM;

else
    if (TargetParam == 'TotMetabBW34DM')
        TOTMETABBW34DM
        EndPt = TOTMETABBW34DM;
    else
        if (TargetParam == 'TotOxMetBW34DM')
            TOTOXMETBW34DM
            EndPt = TOTOXMETBW34DM;
        else
            if (TargetParam == 'AMetLiv1BW34DM')
                AMETLIV1BW34DM
                EndPt = AMETLIV1BW34DM;
            end
        end
    end
end
end
end
end
end

if (NumAttempt2 > 15)
    break;
end

```

LIST OF ABBREVIATIONS AND ACRONYMS

AFRL	Air Force Research Laboratory
AUC	area under the curve
DoD	Department of Defense
EPA	Environmental Protection Agency
HEC	human equivalent concentration
IRIS	Integrated Risk Information System
OASD EI&E	Office of the Assistant Secretary of Defense (Energy, Installations and Environment)
OEL	occupational exposure limit
PBPK	physiologically-based pharmacokinetic
RfC	reference concentration
SC	sensitivity coefficients
TCE	trichloroethylene
TSTC	TriService Toxicology Consortium