



Cylindrical Ion Trap Mass Spectrometer for Chemical Warfare Agent Detection and Identification

**M. Todd Griffin, Jack E. Fulton, Jr., Robert F. McAtee,
Norm Popkie, Michael A. Eagan, Mike Jahn**

**Night Vision/Electro Optics and Chemical/Biological/Explosives Detection Group
Naval Surface Warfare Center, Crane Division
Crane, IN 47522**

**Rong Gao, Lefteri H. Tsoukalas, R. Graham Cooks
Purdue University
W. Lafayette, IN 47907-1290**

Distribution Statement A - Approved for public release; distribution unlimited.



Report Documentation Page				Form Approved OMB No. 0704-0188	
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE 01 OCT 2005		2. REPORT TYPE N/A		3. DATES COVERED -	
4. TITLE AND SUBTITLE Cylindrical Ion Trap Mass Spectrometer for Chemical Warfare Agent Detection and Identification				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Night Vision/Electro Optics and Chemical/Biological/Explosives Detection Group Naval Surface Warfare Center, Crane Division Crane, IN 47522				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release, distribution unlimited					
13. SUPPLEMENTARY NOTES See also ADM001851, Proceedings of the 2003 Joint Service Scientific Conference on Chemical & Biological Defense Research, 17-20 November 2003. , The original document contains color images.					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 17	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

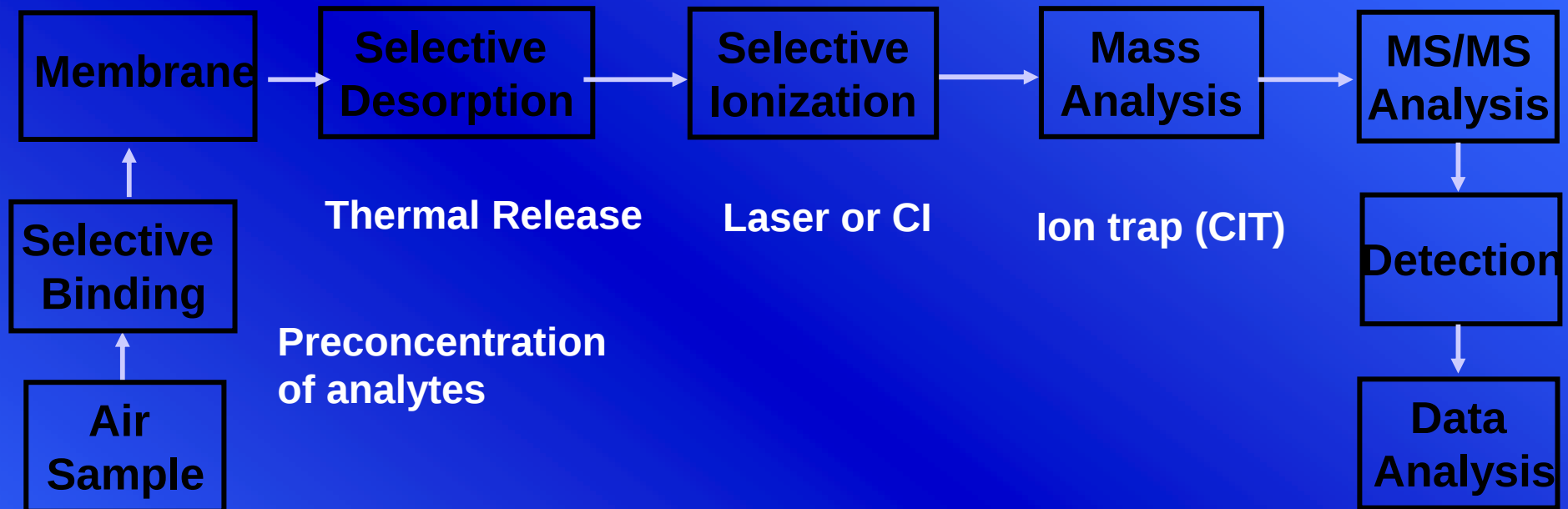
Selective, Rapid Detection of Chemical Warfare Agents in Air by Ion Trap Mass Spectrometry

- Requirements, field portable plus
 - **Speed of analysis:** < 10 seconds
 - **Sensitivity:** LOD < 1 part per trillion by volume
 - **Selectivity:** samples are complex mixtures of organics
- The Solution
 - Miniature mass spectrometer
 - Ion trap with simple cylindrical electrodes
 - Rapid, selective membrane introduction of samples
- Basis for Effort
 - Detailed simulations of ion motion in ion traps
 - Decade-long study of ion trap performance
 - Collaboration between Purdue, Crane, and Griffin, a start-up company who will manufacture instruments



Methodology

*m**



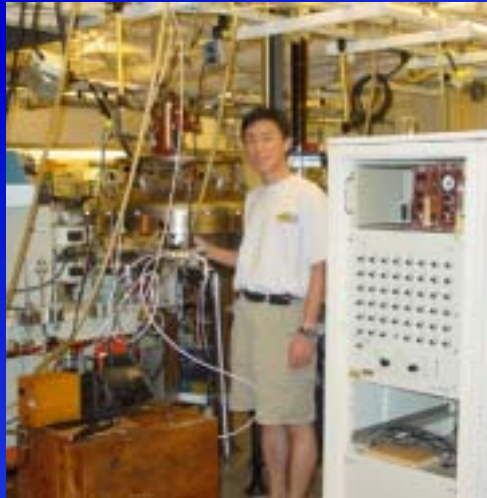
Multiple Stages of Selectivity

- Selective Adsorption/Desorption
- Selective Ionization
- Selective Mass Analysis
- Selective Dissociation and MS/MS Analysis



Miniaturization of the Mass Spectrometer

BEEQ –
Research grade
laboratory
Instrument
Size: Big
Weight : 4 tons
Power : 15,000 W



Modified ITS-40
Rugged
Transportable
Size: 200x 200x 100 cm
Weight: 800 lbs
Power: 4500 W



Mini-CIT Ver. 5.0
Size: 45 x 60 x 71 cm
Weight: 140 lbs
Power: 200 - 300 W



Mini-CIT Ver. 7.0
• **Size 18cm x 28cm x 65cm**
• **Weight: 60 lbs**
• **Power 120W**



Current Commercial System



Griffin Analytical Technologies

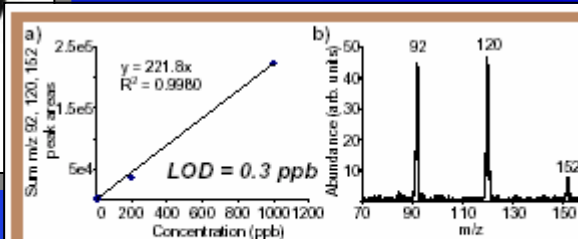
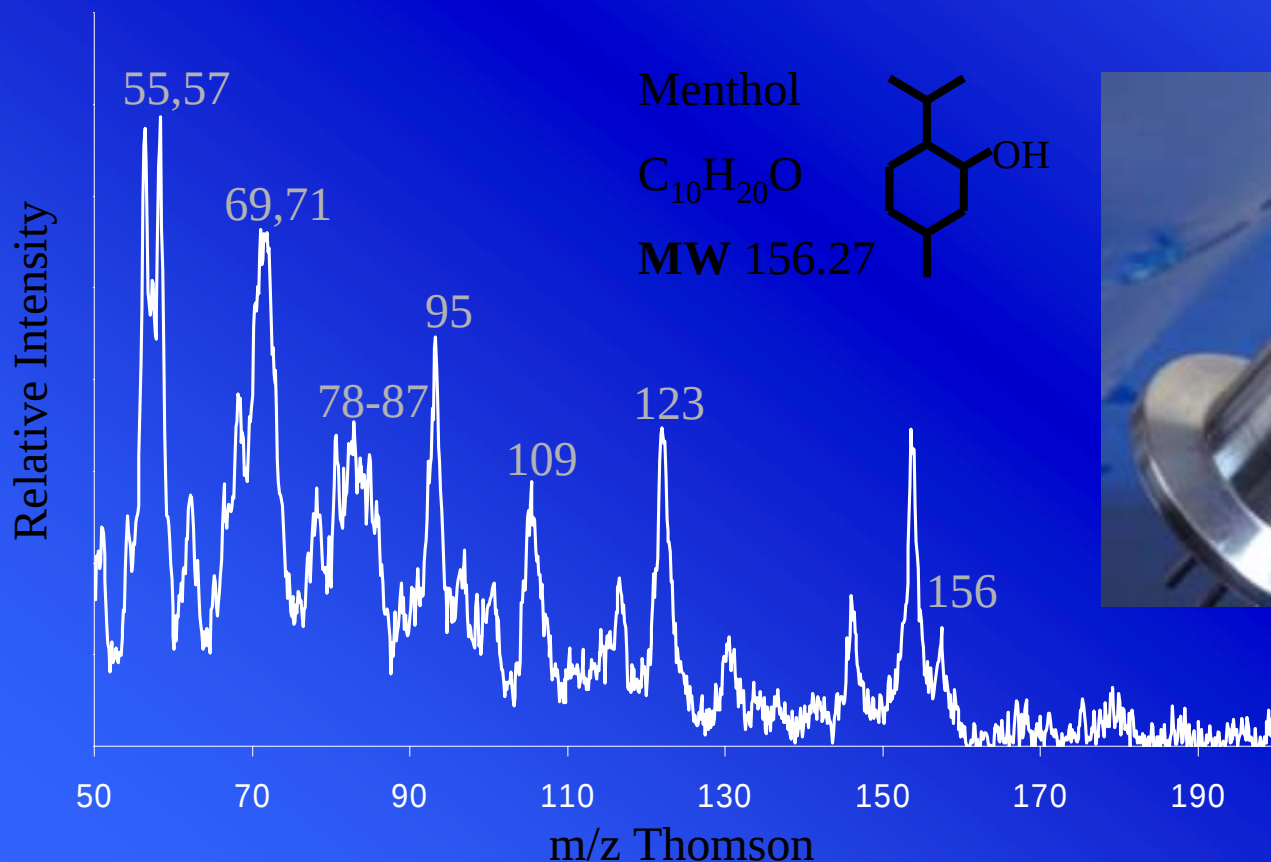


Figure 3: a) Calibration curve for methyl salicylate using direct air sampling onto the membrane. b) Mass spectrum of methyl salicylate from an 8 ppb gas-phase standard.



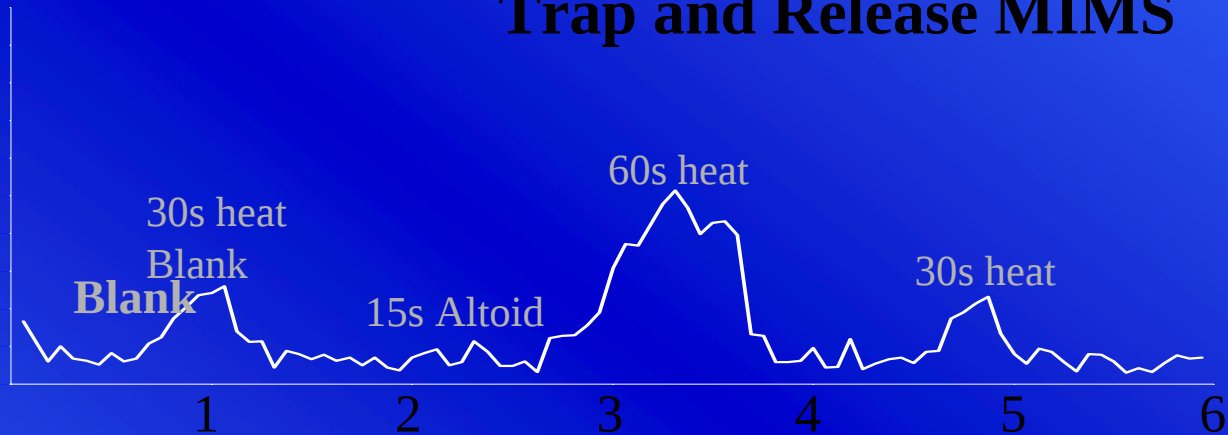
Mini Mass Spec Monitoring of Menthol from Cough Drops in Air

Halls cough drops (12 mg menthol per drop) in air
mini 5.0 with internal unheated membrane

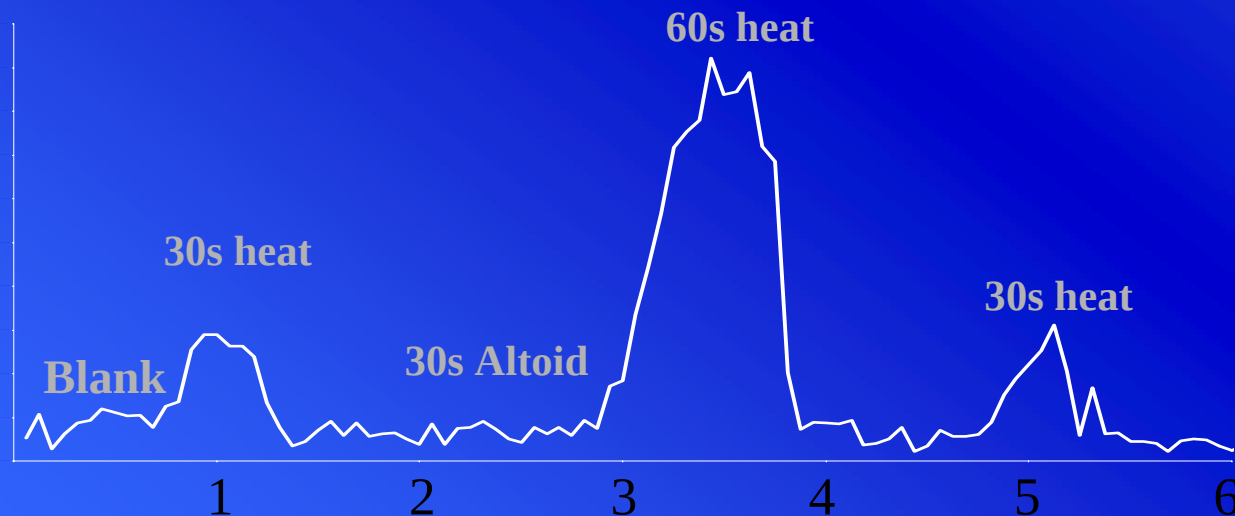
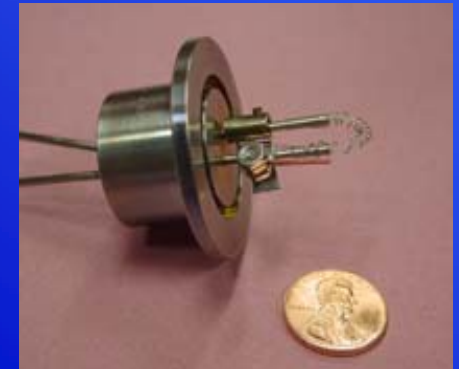


Altoid in Air: Mini Mass Spec

Trap and Release MIMS

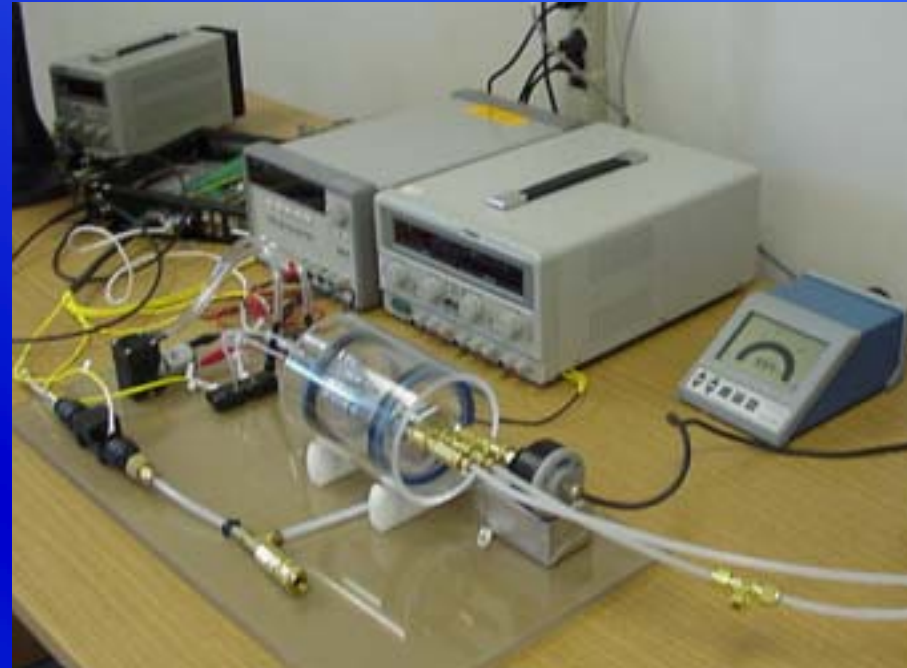


0.45 V peak height
Rise :26 sec.
Fall: 26 sec.



0.9 V peak height
Rise :30 sec.
Fall: 30 sec.

Membrane Introduction Test Set



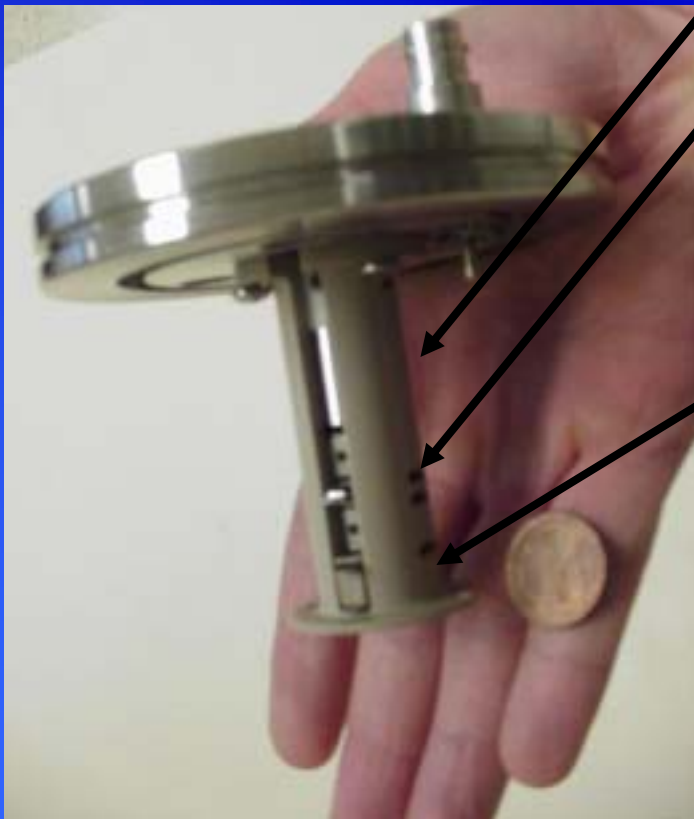
- Flow-Bench with mass flow meters
- RTDs/Humidity sensors
- Variable membrane heater
- Vacuum chamber with variable pump
- Dual chamber vapor generator
- Automated testing



Mini-Mass Spectrometer

m^*

New Design



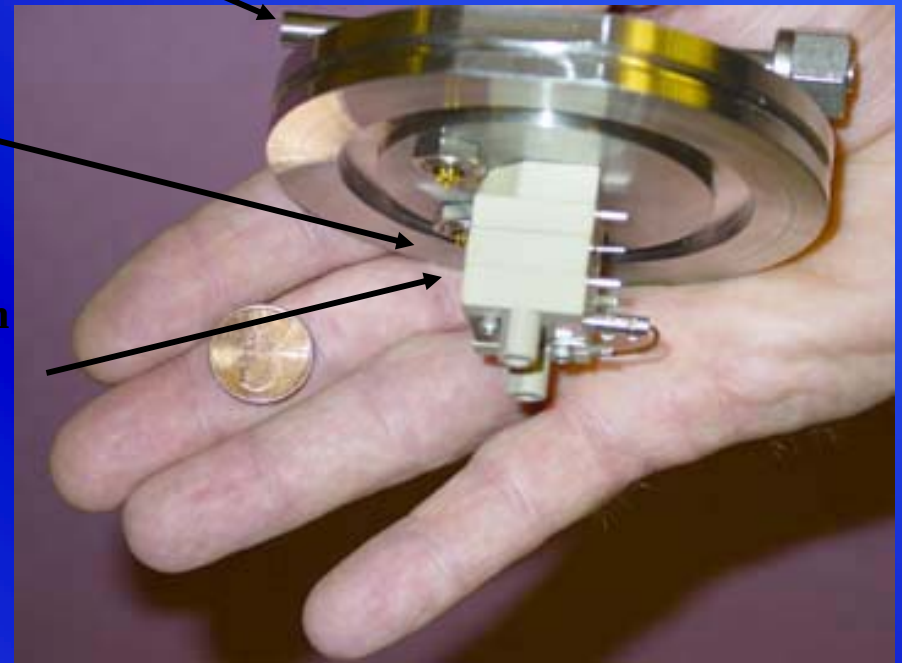
Sample Inlet

Filament

Ion Lenses

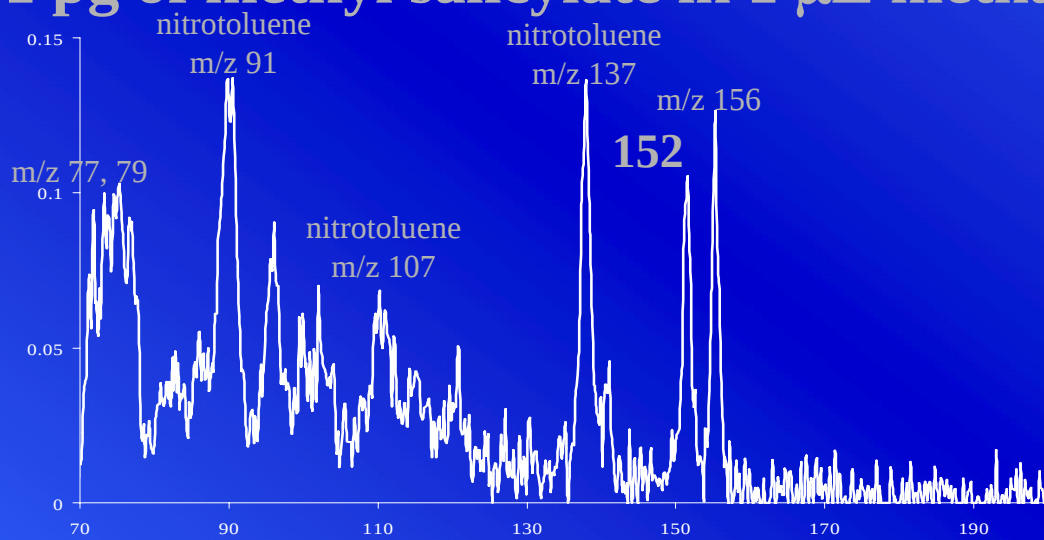
Cylindrical Ion
Trap
 $r_0 = 2.5 \text{ mm}$

Current Design

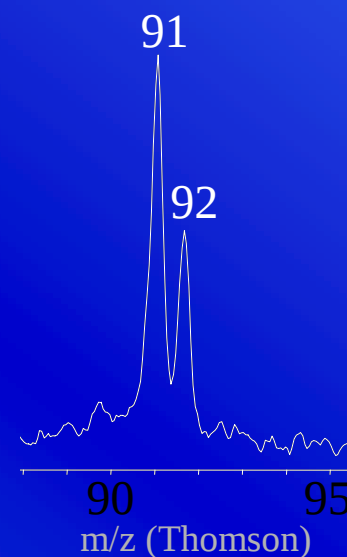


Performance Characteristics: Sensitivity and Resolution

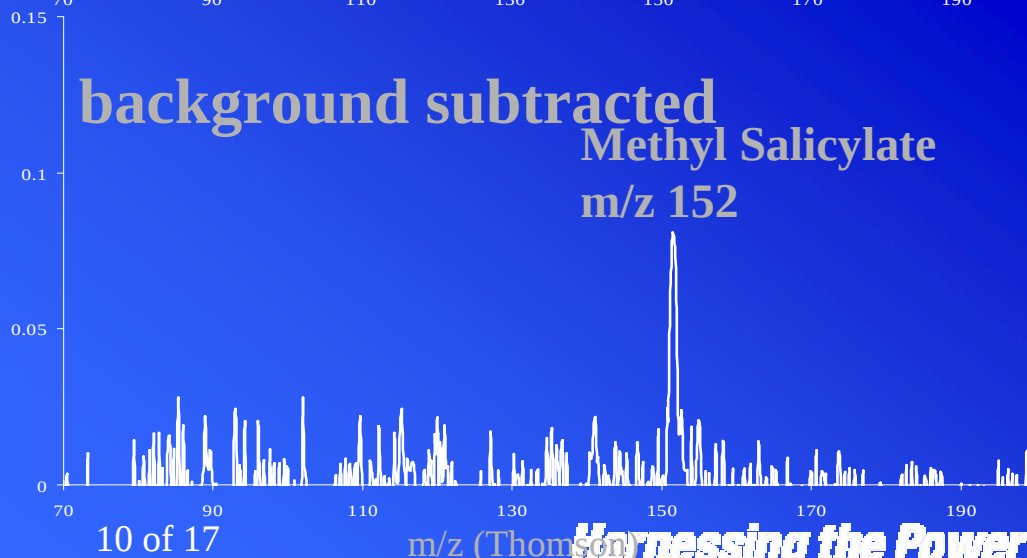
1 pg of methyl salicylate in 1 μ L methanol



Resolution ~100
Toluene with membrane inlet



background subtracted
Methyl Salicylate
m/z 152

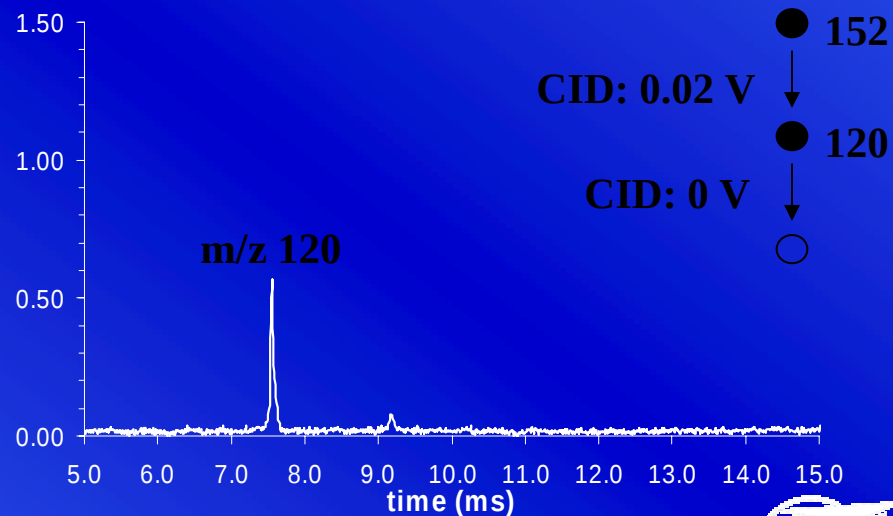
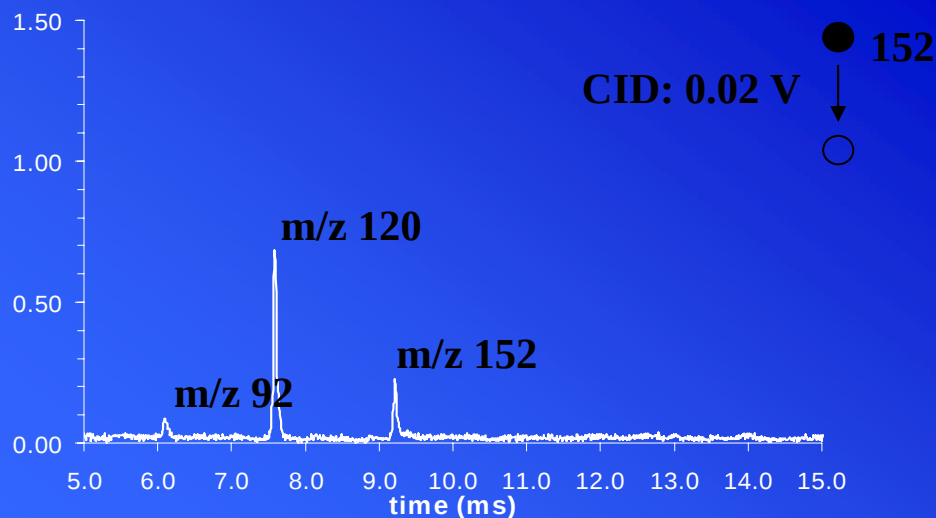
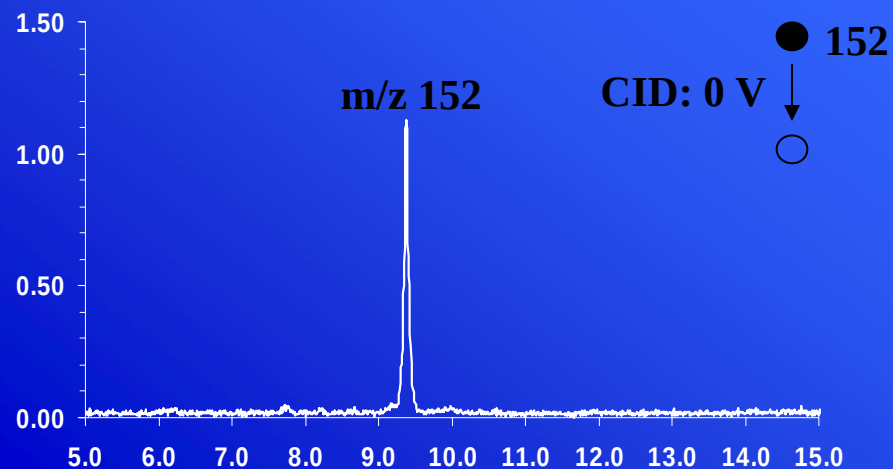
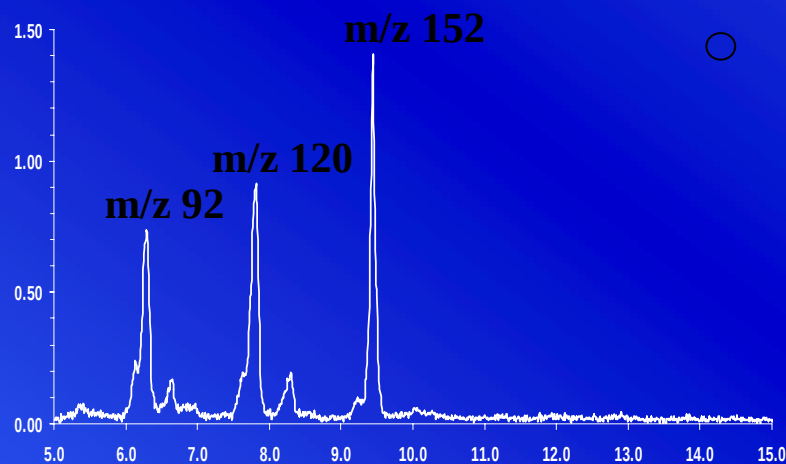


Harnessing the Power of Technology for the Warfighter



MSⁿ of Methyl Salicylate

*m**



Wavelets

- Wavelet transform
 - Definition

$$WT_x(a, \tau) = \frac{1}{\sqrt{a}} \int x(t) \psi^* \left(\frac{t - \tau}{a} \right) dt$$

- Admissible condition

$$c_\psi = \int_0^\infty \frac{|\Psi(\omega)|^2}{\omega} d\omega < \infty$$

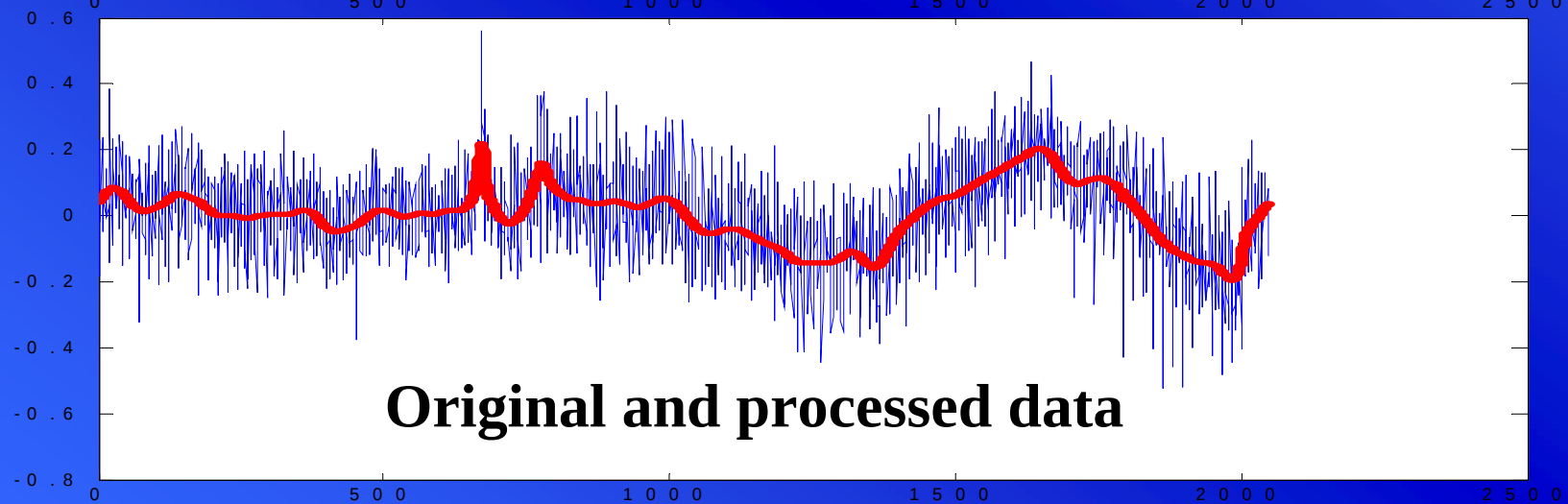
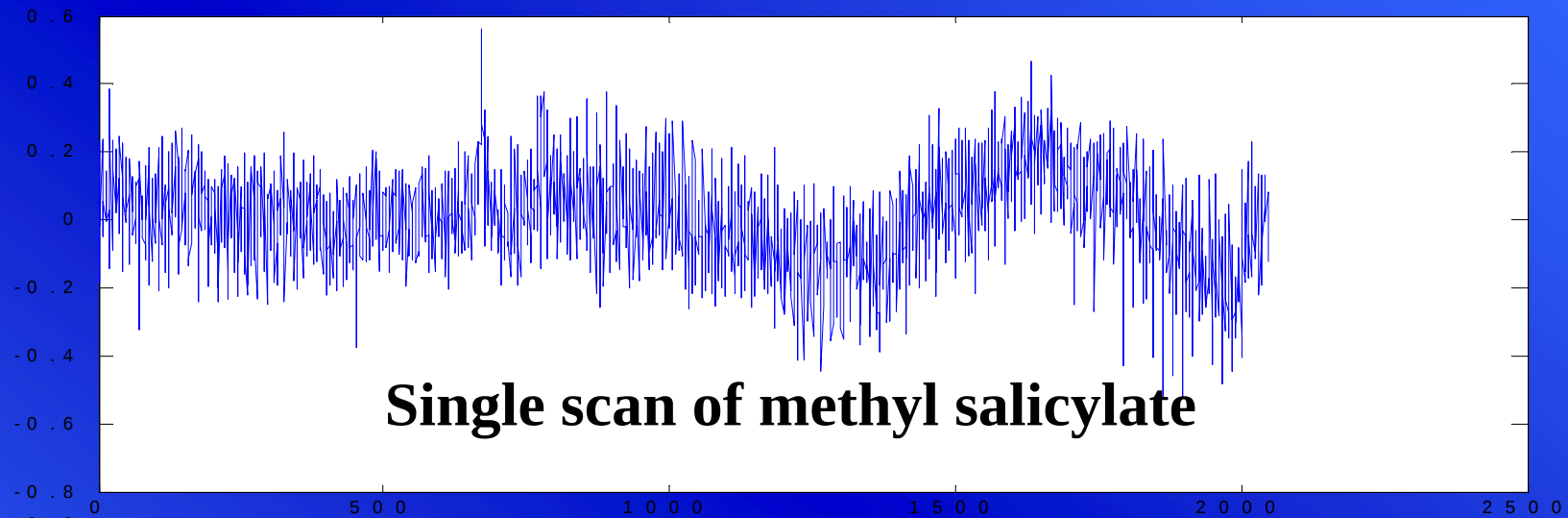
- Inverse transform

$$x(t) = \frac{1}{c_\psi} \int_0^\infty \frac{da}{a^2} \int_{-\infty}^{+\infty} WT_x(a, \tau) \frac{1}{\sqrt{a}} \psi \left(\frac{t - \tau}{a} \right) d\tau$$



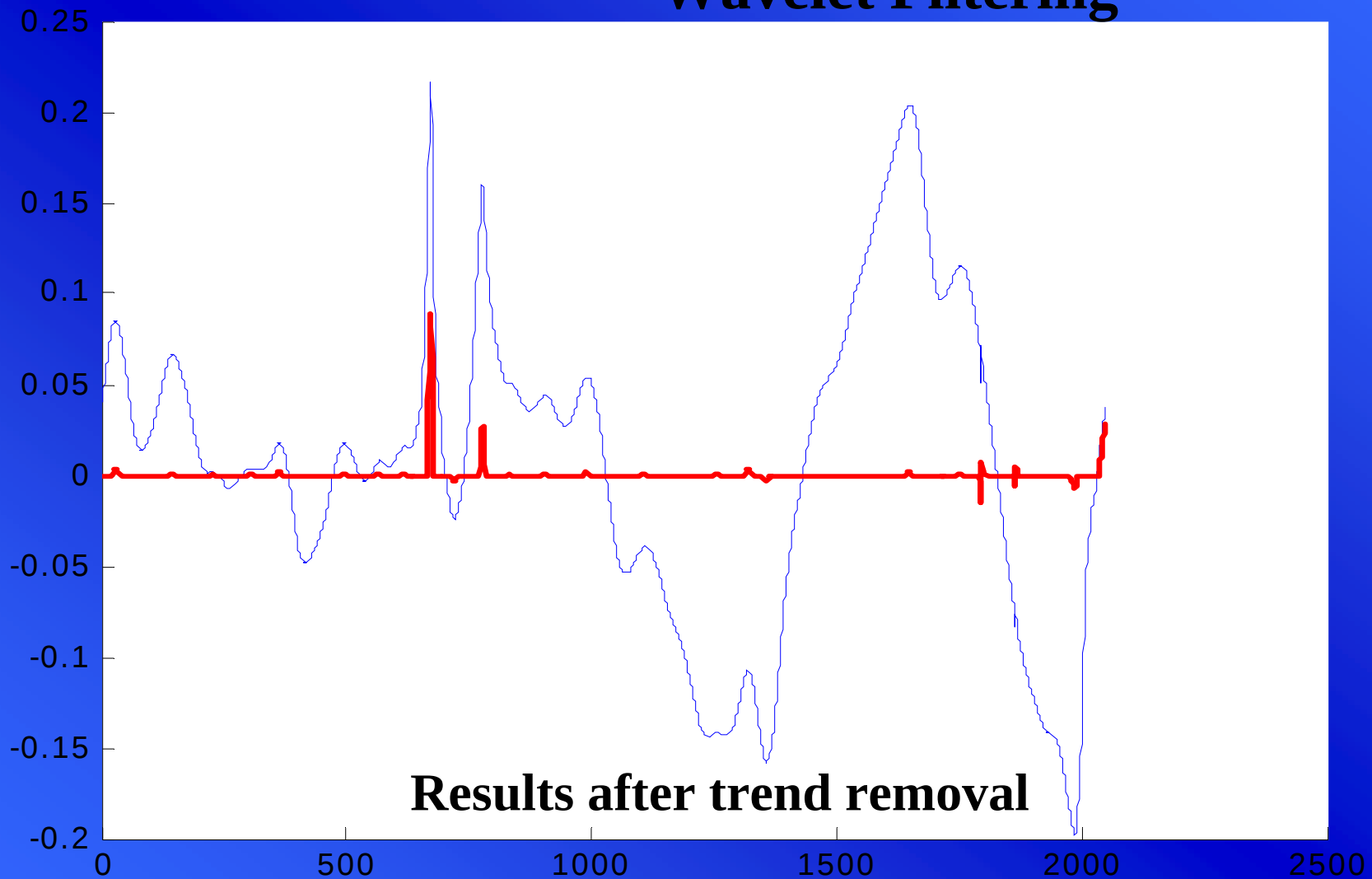
Signal Processing of Data

Wavelet Filtering



Signal Processing of Data

Wavelet Filtering



Results after trend removal



CIT Automated Test Set



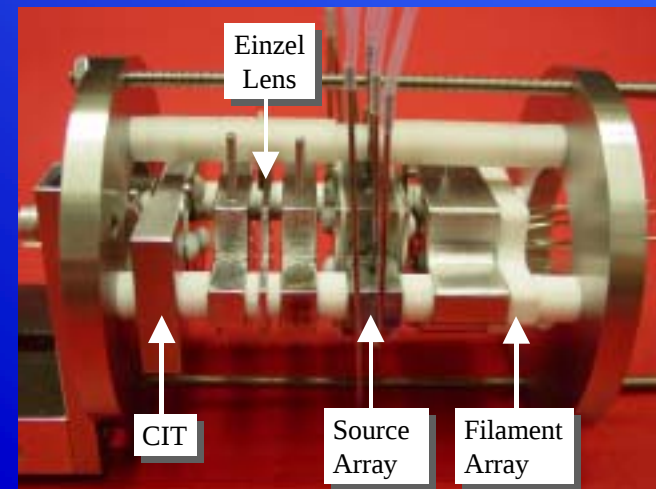
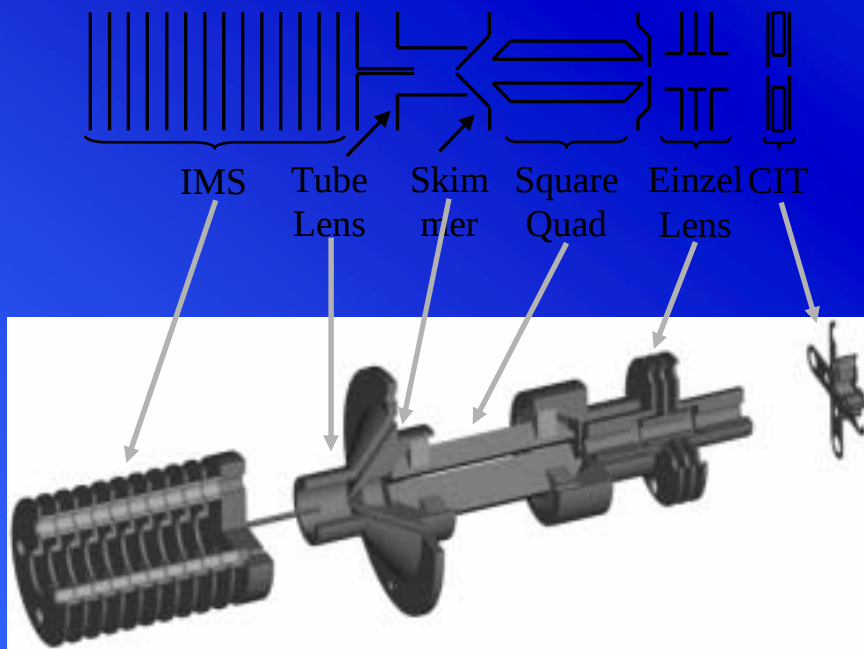
- Fully automated PXI based control system
- Control software written in LabVIEW
- Leak valve and membrane introduction system
- Couple with flow bench and vapor generator



Future Work

Multiplexed CIT

IMS-MS



- System integration
- Performance optimization
- IMS-MS
- Multiplexed CIT
- Biological Capabilities
- Algorithm Development



Acknowledgements

Funding:

Integrated Detection of Hazardous Materials (IDHM) Program, a Department of Defense project managed jointly by Center for Sensing Science and Technology, Purdue University, and Naval Surface Warfare Center, Crane, Indiana

Dr. Cooks acknowledges the technical support of the Army Instrumentation and Dr Robert Santini provided via the Indiana Instrumentation Institute (III).

Robert Santini, Andy Guymon, Chris Doerge, Mark Carlsen, Mike Everly, Jim Zimmerman, Alan Ronemus, Robert Fagan, Randy Rapogle, and Greg Hawkins.

