



**U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND  
CHEMICAL BIOLOGICAL CENTER**

**ABERDEEN PROVING GROUND, MD 21010-5424**

**DEVCOM CBC-TR-1768**

**Random Forest Permutation Feature Importance  
for Feature Selection in Ion Mobility  
Spectrometry**

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**September 2022**

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# REPORT DOCUMENTATION PAGE

Form Approved  
OMB No. 0704-0188

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<b>1. REPORT DATE (DD-MM-YYYY)</b> XX-09-2022		<b>2. REPORT TYPE</b> Final		<b>3. DATES COVERED (From - To)</b> Oct 2019–Sep 2021	
<b>4. TITLE AND SUBTITLE</b> Random Forest Permutation Feature Importance for Feature Selection in Ion Mobility Spectrometry				<b>5a. CONTRACT NUMBER</b>	
				<b>5b. GRANT NUMBER</b>	
				<b>5c. PROGRAM ELEMENT NUMBER</b>	
<b>6. AUTHOR(S)</b> Riley, Patrick C.; Deshpande, Samir V.; Ince, Brian S.; Wade, Mary M. (DEVCOM CBC); O'Donnell, Kyle P.; Dereje, Ruth; Hauck, Brian C. (STC)				<b>5d. PROJECT NUMBER</b> CB10874; ILIR: PE 0601101A Project 91A	
				<b>5e. TASK NUMBER</b>	
				<b>5f. WORK UNIT NUMBER</b>	
<b>7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)</b> Director, DEVCOM CBC, ATTN: FCDD-CBR-ID, APG, MD 21010-5424 Science and Technology Corporation (STC); 111 C Bata Blvd., Belcamp, MD 21017-1427				<b>8. PERFORMING ORGANIZATION REPORT NUMBER</b> DEVCOM CBC-TR-1768	
<b>9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)</b> Defense Threat Reduction Agency; 8725 John J. Kingman Road, MSC 6201, Fort Belvoir, VA 22060-6201 In-house Laboratory Independent Research Program, U.S. Army Combat Capabilities Development Command Chemical Biological Center; Aberdeen Proving Ground, MD 21010-5424				<b>10. SPONSOR/MONITOR'S ACRONYM(S)</b> DTRA; ILIR, DEVCOM CBC	
				<b>11. SPONSOR/MONITOR'S REPORT NUMBER(S)</b>	
<b>12. DISTRIBUTION / AVAILABILITY STATEMENT</b> Approved for public release: distribution unlimited.					
<b>13. SUPPLEMENTARY NOTES</b>					
<b>14. ABSTRACT: (Limit 200 words)</b> Machine learning (ML) can be used to classify the spectra generated in ion mobility spectrometry (IMS)-based chemical detectors when they are used in the detection of explosives, chemical warfare agents, and other volatile hazardous compounds. The spectra of an IMS detector are composed of drift time bins ( $x$ axis) and their corresponding amplitudes ( $y$ axis). These values represent the peaks that are present in each spectrum and can be used as features to train ML algorithms. When training on the spectrum, the total number of features can exceed 1000 and are of high cardinality. This work demonstrates a method of using random forest (RF) classification and permutation feature importance to downselect the most important spectral bins. These features are representative of common peak locations in the training data. The use of the most important features determined by RF to reduce the dimensions of the training data set greatly enhanced the accuracy of a dense neural network.					
<b>15. SUBJECT TERMS</b>					
Ion mobility spectrometry (IMS) Classification		Machine learning (ML) False alarm		Random forest (RF) Feature selection	
				Neural network (NN) Supervised learning	
<b>16. SECURITY CLASSIFICATION OF:</b>			<b>17. LIMITATION OF ABSTRACT</b>	<b>18. NUMBER OF PAGES</b>	<b>19a. NAME OF RESPONSIBLE PERSON</b>
<b>a. REPORT</b>	<b>b. ABSTRACT</b>	<b>c. THIS PAGE</b>			<b>19b. TELEPHONE NUMBER (include area code)</b>
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## PREFACE

The work described in this report was authorized under Defense Threat Reduction Agency (DTRA), Research and Development Directorate, Chemical and Biological Technologies Department (Fort Belvoir, VA) project number CB10874. In addition, this work was funded by the In-house Laboratory Independent Research Program (PE 0601101A Project 91A) at the U.S. Army Combat Capabilities Development Command Chemical Biological Center (DEVCOM CBC; Aberdeen Proving Ground, MD). The work was started in October 2019 and completed in September 2021.

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This report has been approved for public release.

### Acknowledgments

The authors acknowledge the following individuals for their hard work and assistance with the execution of this technical program:

- Dr. Charles "Steve" Harden (Science and Technology Corporation; Belcamp, MD) for his subject matter expertise in ion mobility spectrometry;
- Vince M. McHugh (DEVCOM CBC, retired) for his support and guidance;
- Dr. Trish P. McDaniel (DEVCOM CBC) for her program and technical support of this project; and
- Dr. Chia-Wei Tsai (DTRA) for her technical guidance of this program.

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# RANDOM FOREST PERMUTATION FEATURE IMPORTANCE FOR FEATURE SELECTION IN ION MOBILITY SPECTROMETRY

## 1. INTRODUCTION

Machine learning (ML) is a field of science that can drastically improve false alarm rates of chemical detectors. ML provides a set of tools for curating data sets. The tools are used to train powerful algorithms to learn from data and thereby make more accurate predictions as compared with traditional techniques. One important factor of curating data sets is feature selection, which is used to reduce the size of a data set to the most relevant inputs, thus increasing model accuracy and performance. Features can be selected by manual or automated methods. The overall goal is to eliminate irrelevant features that provide less differentiating capabilities.<sup>1,2</sup> Ion mobility spectrometry (IMS) is an analytical technique for separating and detecting ions that can be used to identify chemical vapors in the air, such as those due to explosives or chemical warfare agents.<sup>3,4</sup> Although fielded IMS detectors have a small form factor and rapid response, research has shown that without calibration, IMS is prone to high false alarm rates because of interferent peaks that appear within detection windows.<sup>5</sup>

IMS detectors rely on the calculated reduced mobility ( $K_0$ ) of an ion peak to identify unknown compounds.  $K_0$  is determined from the relationship between ion drift time ( $t_d$ ) along a path length ( $L$ ), and the temperature ( $T$ ) and pressure ( $P$ ) of the drift gas:

$$K_0 = \frac{L^2}{vt_d} \left( \frac{273.15}{T} \right) \left( \frac{P}{760} \right) \quad (1)$$

However, the location and shape of a particular peak is dependent upon factors such as concentration of the analyte, water content of the drift gas, and resolving power of the detector.<sup>6</sup> As a result, many fielded IMS systems do not produce a sharp peak in a consistent location easily identifiable by a single  $K_0$  value; instead, they produce a Gaussian curve for which a  $K_0$  value is calculated. Figure 1 provides a typical IMS spectrum of a fielded system and shows the Gaussian shape of three typical IMS peaks: the reactant ion peak (RIP), the monomer peak, and the dimer peak (i.e., peaks 1, 2, and 3, respectively).

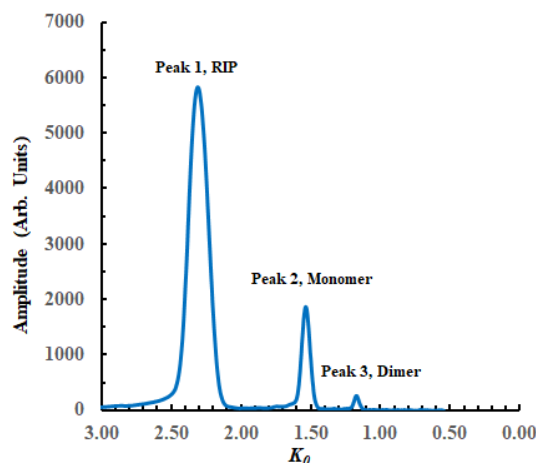


Figure 1. Example IMS spectrum for fielded system showing RIP, monomer, and dimer peaks.

The raw spectral features are represented by a measurement of current, which is expressed as amplitude ( $y$  axis) at given intersecting coordinates of drift time or  $K_0$  ( $x$  axis), as shown in Figure 1. The spectrum of a fielded IMS detector contains thousands of high-cardinality drift time bins with amplitudes in the range of 0 to 8000 counts. To develop an accurate classification model, this large number of features must be downselected to eliminate raw spectral features where amplitude values mainly represent noise and provide no differentiation between chemical vapors of interest. In addition, fielded IMS systems are typically used for detecting a specific range of hazardous compounds such as explosives in an airport. By reducing the total number of drift time bins to analyze and focus on features in regions where peaks are likely to occur, computational resources can be conserved, and the time to classification can be improved. Presented here is a semi-automated feature-selection technique that uses random forest (RF) classification and permutation feature importance for downselecting the most important drift time bins in an IMS data set. This reduced feature set is then used to train a simple neural network (NN) classification model, which is used to evaluate the resulting change on the train/test accuracy of the model across feature sets of 300, 600, and 1676 spectral features.

## 2. METHODS

### 2.1 Data Set

The IMS training data set consisted of 30,530 positive and negative detection mode spectra. Each detection mode spectrum was composed of 1021 spectral bins and represented the features for training the various models described in this study. Initially, 183 spectral bins were dropped to remove spectral noise that can occur before the RIP. This left a total of 838 spectral bins from each detection mode, and the final dimensions of the combined data set were 30,530 rows  $\times$  1676 columns. Each spectral bin had an identifier ( $p_$  or  $n_$ , respectively) assigned to it to differentiate between bins from the positive and negative detection modes. This allowed for training of the RF classifiers on only the positive or negative detection mode data. The labels of the data set were equally distributed across 10 chemical compounds

consisting of RIP only (none); dimethyl methylphosphonate; 2,6-di-*tert*-butylpyridine; triethyl phosphate (TEPO); di(propylene glycol) monomethyl ether (DPM); 1-chloro-2-[(2-chloroethyl)sulfanyl]ethane; methyl salicylate; (RS)-propan-2-yl methylphosphonofluoridate; 3,3-dimethylbutan-2-yl methylphosphonofluoridate; and cyclohexyl methylphosphonofluoridate. These labels were processed using the Panda's `get_dummies` function<sup>i</sup> to create a multi-hot vector for each label in the data set. Finally, the data set was split using the scikit-learn `train_test_split` function:<sup>ii</sup> 80% for training and 20% for testing of the model. The split was performed using a random seed of 42, and it was stratified to ensure labels were equally split across the data sets.<sup>7,8</sup>

## 2.2 RF Model Design

RF classification is a ML technique that fits an ensemble of decision tree classifiers. Each decision tree is fit to a different subset of the data set, and the decision scores are averaged to improve accuracy and prevent overfitting.<sup>9,10</sup> The RF algorithm is well suited to large data sets and multiclass classification problems, and outputs feature importance, giving model interpretation. It has been demonstrated that RF classification is useful in a number of applications to include detection and identification of peaks for IMS detectors.<sup>11,12</sup>

Two RF classifiers were optimized to produce the highest accuracy classification on IMS spectra of positive and negative detection mode data, thus ensuring that the output feature importance would show the spectral bin corresponding to the peaks from the two separate detection modes. To optimize the RF classifiers, out-of-the-box (OOB) error was calculated using a variable number of decision trees in a forest. The parameter for the number of trees (`n_estimators`) ranged from 75 to 500, and OOB error was calculated using three different variations of the maximum number of features RF is allowed to try in an individual tree (`max_features`) as shown in Figure 2.

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<sup>i</sup> [https://pandas.pydata.org/docs/reference/api/pandas.get\\_dummies.html](https://pandas.pydata.org/docs/reference/api/pandas.get_dummies.html) (accessed 7 June 2022).

<sup>ii</sup> [https://scikit-learn.org/stable/modules/generated/sklearn.model\\_selection.train\\_test\\_split.html](https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.train_test_split.html) (accessed 7 June 2022).

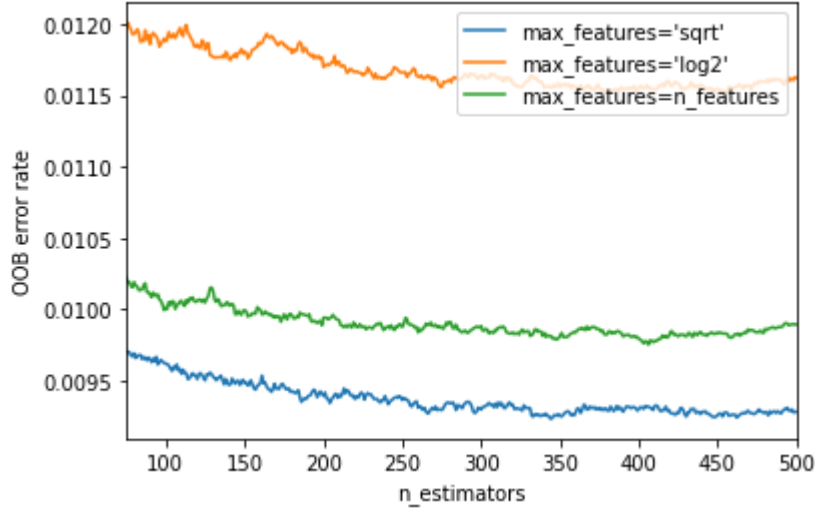


Figure 2. OOB error rate for positive detection mode data for three different values of max\_features, given variable number of decision trees (n\_estimators).

OOB error provides a measurement of prediction error for the model by removing several rows of data from training and predicting the result of these rows given a subset of the training data. OOB error should eventually converge to equal the cross-validation error when it stabilizes. Figure 2 shows that a minimum value resulted in the error at approximately 325 n\_estimators, and when max\_features was set to “sqrt”, these hyperparameter settings were used to build the RF classifier model to determine important features.

### 2.3 RF Model Feature Importance Calculation

A significant aspect of the RF classifier is the calculation of feature importance, which can be used to rank a particular feature when the model makes a classification providing interpretability of the model. The default measurement of feature importance in RF classification is mean decrease impurity or Gini importance. Gini importance is calculated by the frequency ( $f_i$ ) of a label ( $i$ ) at a node given a number of unique labels ( $C$ ):

$$\sum_{i=1}^C f_i(1 - f_i) \quad (2)$$

However, when features of high cardinality are used in training a RF classifier, Gini importance has often incorrectly assigned importance to features based on domain knowledge.<sup>13,14</sup> When dealing with features of high cardinality for a time-series data set, permutation feature importance should be used to obtain a more accurate representation of true feature importance. Permutation feature importance in scikit-learn is defined as the relationship between the decrease in a model’s score and the shuffling of a random feature value. Permutation feature importance provides a more accurate estimation of feature importance. However, due to the costly computation time of permutation, feature importance must be predetermined and hard-coded when a model is deployed.

## 2.4 NNs for Classification

Deep NNs have been adapted to a number of classification tasks that include IMS data.<sup>15,16</sup> The popularity of deep neural techniques such as NNs, convolutional NNs, and long short-term memory have been used in the classification of chemical data.<sup>17,18</sup> In particular, these techniques have been shown to be extremely accurate when classifying from raw, spectral data.<sup>19,20</sup>

To test how the downselected IMS spectral features impact a model's accuracy, a classification NN was built using TensorFlow (Google Brain Team; Seattle, WA) and trained on data sets consisting of positive and negative mode data where the number of features ( $n$ ) was equal to 300, 600, or 1676 spectral bins.<sup>21,22</sup> These values represent an equal quantity of features from the positive and negative detection modes. Thus, each detection mode had 150, 300, and 838 features, which first included the RIP and the monomer, then the dimer, and subsequently, all other features, respectively. The optimizer chosen for NN was root-mean-square propagation or RMSprop, and the loss was calculated with categorical cross entropy. The NNs were composed of four fully connected layers, where the input layer, dense layer 1, dense layer 2, and output layer consisted of  $n_{\text{units}}=n_{\text{features}}$ ,  $n_{\text{units}}=n_{\text{features}}/2$ ,  $n_{\text{units}}=n_{\text{features}}/4$ , and  $n_{\text{units}}=n_{\text{labels}}$ , respectively. The activation functions for the first three layers were all sigmoid, and the output layer was a softmax function. An example of this fully connected NN is shown in Figure 3.

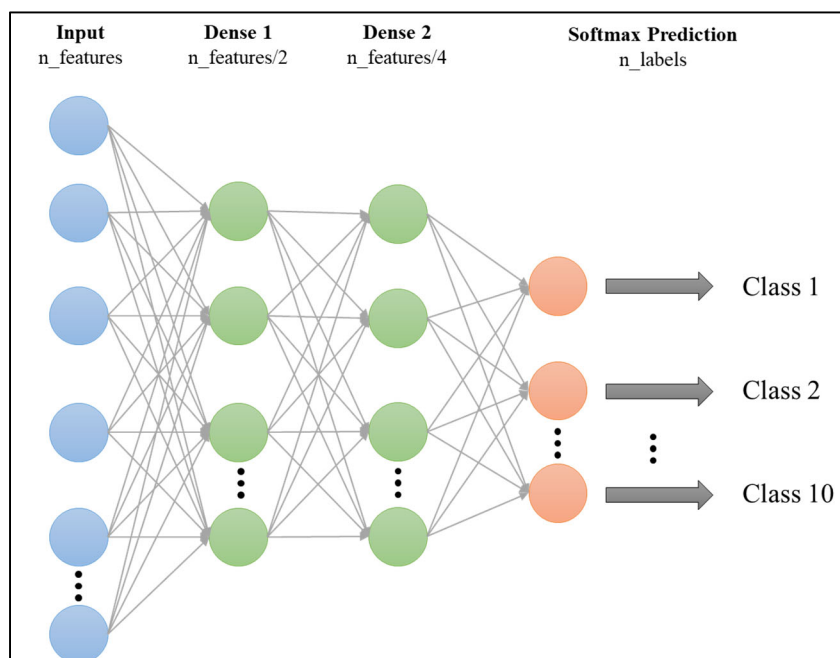


Figure 3. Densely connected NN schematic.

### 3. RESULTS

#### 3.1 RF Feature Selection

The trained RF classifier for the positive and negative detection data sets had validation scores of 0.93 and 0.87, respectively. Figure 4a shows the top 25 most important features as selected by Gini importance for the positive and negative detection modes. The selected features are shown to be the most important, in descending order of spectral bin. Our results confirm that Gini importance was not suitable for feature selection due to the high cardinality of the data.

Figure 4b shows the top 25 most important features as selected by permutation feature importance for the positive and negative detection modes. The selected features are shown to be a mixture of spectral bins focused on a specific span of bins.

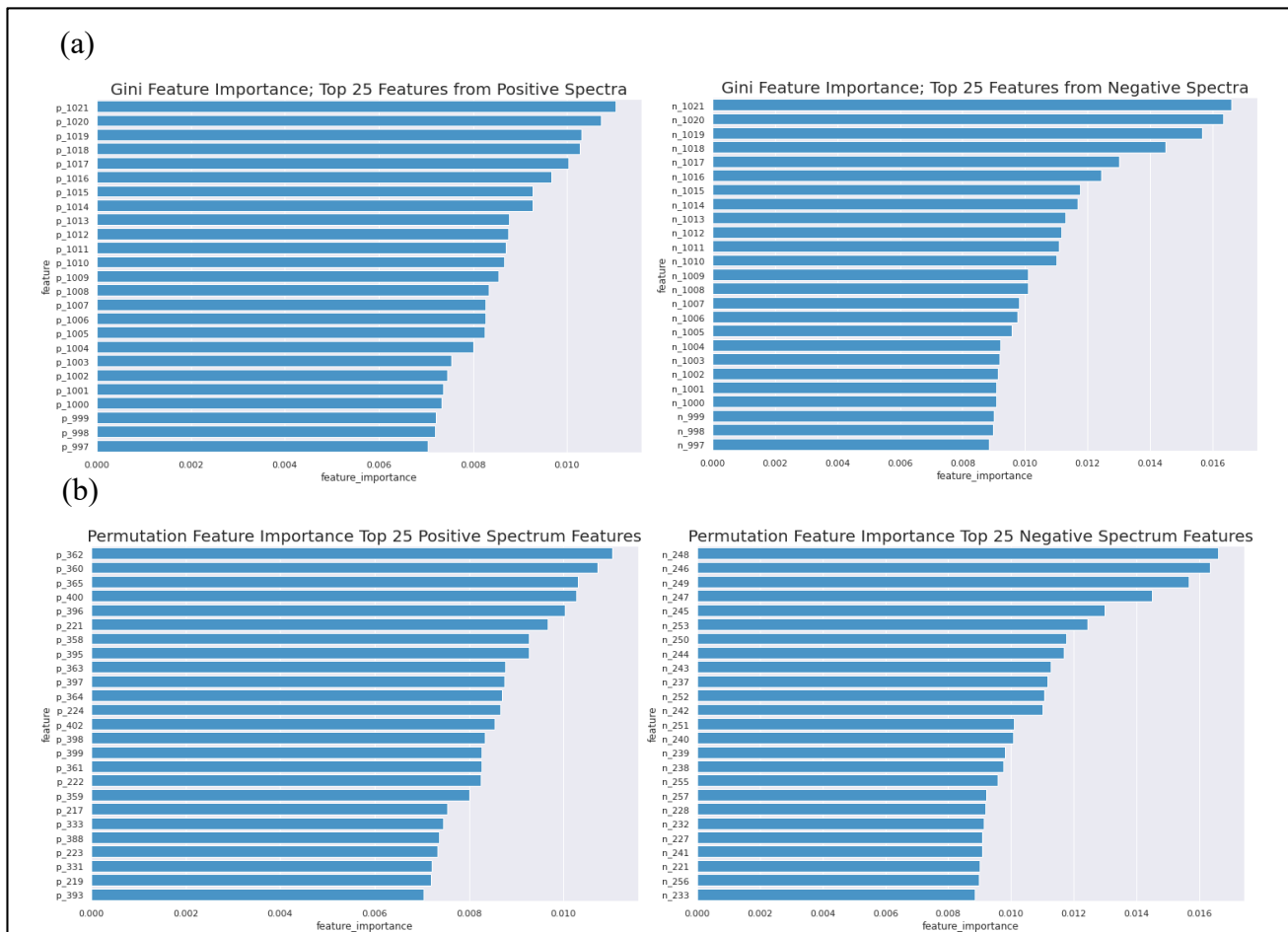


Figure 4. Gini (a) and permutation (b) feature importance for the top 25 features from the positive and negative detection modes.

Figure 5a,b shows the span of important features as selected by permutation importance and plotted in groups of 100 onto a positive and negative detection mode spectrum of TEPO and DPM, where feature 1 is most important and feature 500 is least important. The positive mode spectrum for the two chemicals shows that the top 200 most important features are for the monomer peak and the RIP. The dimer and trimer spectral bins are selected between the top 300 and 400 most important features. The negative detection mode selected feature shows that the RIP is in the first 100 most important features, and the monomer peak region is in the top 200 most important features.

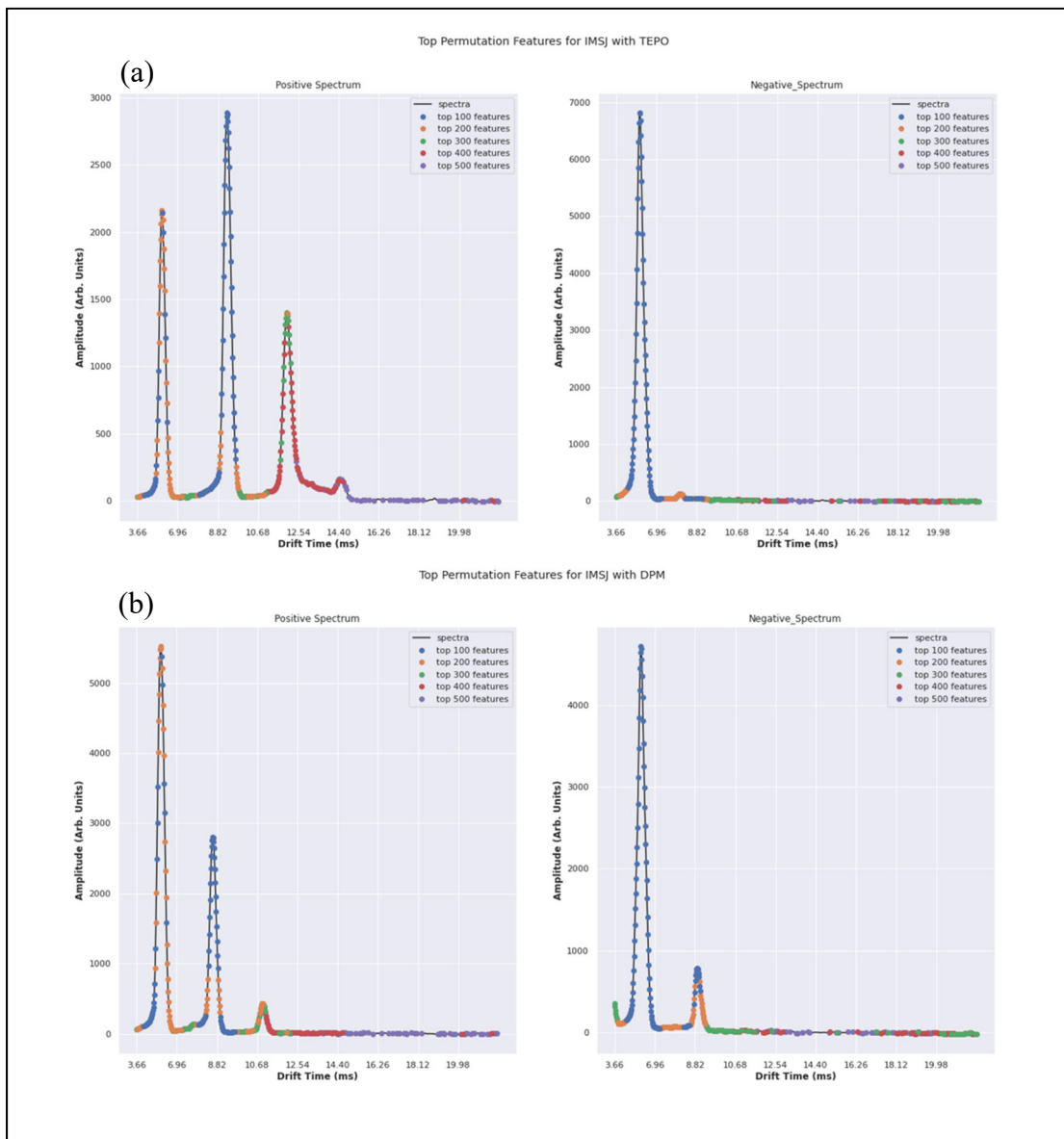


Figure 5. (a) TEPO and (b) DPM positive and negative mode spectra displaying the RF permutation-based drift time bin selection for the first 100, 200, 300, 400, and 500 features (shown in blue, orange, green, red, and purple, respectively).

The selected features in order of importance were not unexpected and match the domain knowledge used when designing traditional IMS alarm algorithms. The RIP is always present, representing the ions, which are available to cluster around other chemicals, whereas the monomer peak will almost always be present across a range of concentrations when a chemical of interest is within the detector. In a traditional detection algorithm, the monomer peak is often the focus of the alarm design and is critical in determining the presence of any chemical compound. On the other hand, the dimer and trimer peaks only occur at high concentrations and are typically not reliable for use in traditional alarm algorithm designs.

### 3.2 Testing Features in an NN Model

The F1 scores and losses of the three resulting NN models were compared to evaluate the impact of the various quantities of features that were used to train an NN classification model. The Table shows the NN train and validation results. The resulting accuracy, loss, and the harmonic mean between precision and recall (F1 score) corresponding to each set of features are compared.

Table. Variable NN Classification Accuracy, Loss, and F1 Score Using 300 and 600 RF Permutation-Selected Features and All 1676 Available Features

Number of Features	NN Results					
	Train			Validation		
	Accuracy	Loss	F1 Score	Accuracy	Loss	F1 Score
300	0.9807	0.0601	0.9806	0.9744	0.0873	0.9743
600	0.9742	0.0823	0.9741	0.9652	0.1268	0.9649
1676	0.9593	0.1237	0.9594	0.9085	0.4159	0.9083

Although they are close, the resulting accuracies and F1 scores demonstrate that reducing the feature set through RF permutation feature importance can reduce the spectral features to a more focused data set, and thereby improve training accuracy over the use of all IMS spectral features. The loss, as displayed in Figure 6, shows improved generalization of the model over fewer epochs for the reduced feature set.

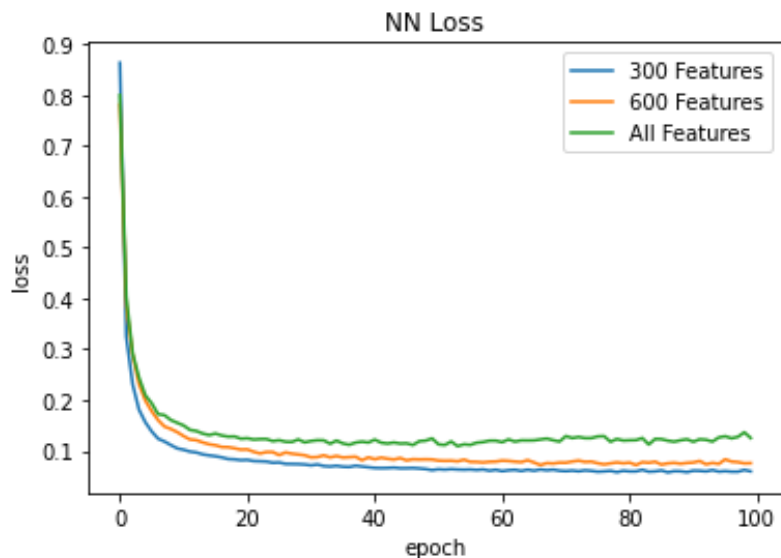


Figure 6. Loss comparison of NNs trained for 100 epochs. Reducing the number of features improved the generalization of the trained model.

#### 4. CONCLUSIONS

Typically, classification from IMS spectra is impacted by the number of features in a data set. These features represent data of high cardinality, which leads to poor feature selection by impurity-based methods, and all features for classification training time and classification accuracy are negatively affected. However, our study shows that an RF classification model can be trained to downselect features with permutation-based feature importance. The drift time bins selected by permutation feature importance match the intuitive knowledge of IMS corresponding to the monomer, RIP, dimer, and trimer, in that order of importance. These downselected features were used to train an NN with higher accuracy over the use of all features. The result is a deployable model that requires less data for making predictions. Furthermore, we show that individuals without IMS domain knowledge could train an RF classifier to machine select features and thereby improve downstream model performance. The impact of total features on model accuracy may vary across various NN techniques, and future work will examine an optimized classification pipeline of IMS data.

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## ACRONYMS AND ABBREVIATIONS

$C$	number of unique labels
DPM	di(propylene glycol) monomethyl ether
$f_i$	frequency of a label at a node
F1 score	harmonic mean between precision and recall
$i$	label at a node
IMS	ion mobility spectrometry
$K_0$	reduced mobility
$L$	path length
max_features	maximum number of features random forest is allowed to try in an individual tree
ML	machine learning
$n$	number of features
n_estimators	parameter for number of trees
NN	neural network
OOB	out-of-the-box
$P$	pressure
RIP	reactant ion peak
RF	random forest
RMSprop	root-mean-square propagation
$T$	temperature
$t_d$	drift time
TEPO	triethyl phosphate



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