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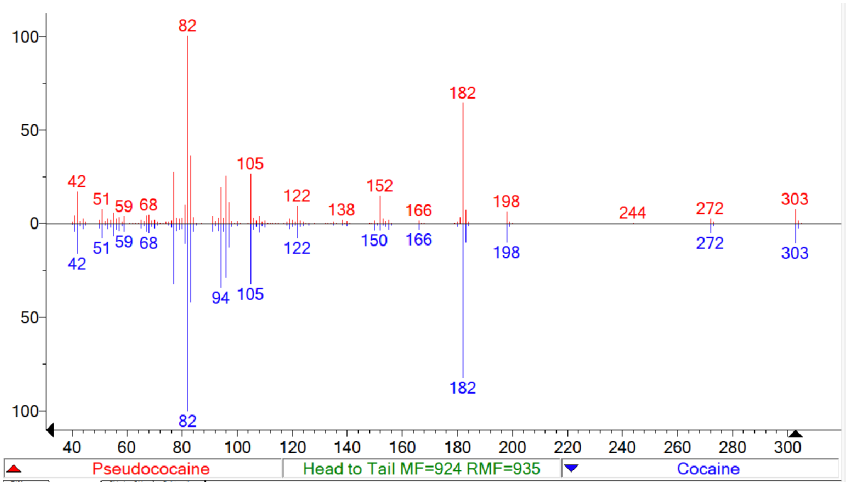
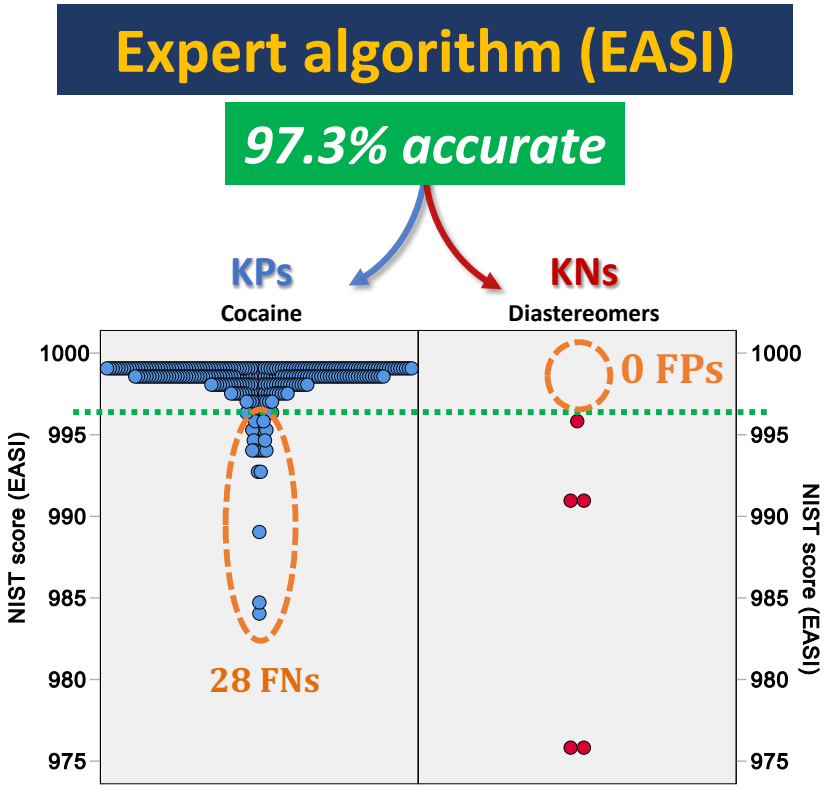
Expert Algorithm for Substance Identification (EASI)





Technical Summary

Glen P. Jackson, PhD

Project Title: Expert Algorithm for Substance Identification (EASI)

Recipient Organization: West Virginia University,
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Award Amount: $327,405

Project Summary

1) Goals and objectives

The major goal of this project was to develop an expert algorithm for substance identification (EASI) that would address several defined needs of the Forensic Science Research and Development Technical Working Group (TWG), including:[1] 1) "solutions to challenges identifying NPS, including…opioids"; 2) "error rate studies on qualitative analysis"; 3) "ability to identify NPS by comparison to spectra from a different instrument rather than reference standard"; and 4) "Continued advancement of practical forensic application/development of emerging or current instrumentation and software (e.g., …GC-MS …) [and] how new technology either may do something that current technology cannot, or may be an improvement over current technology (more sensitive, faster, more cost effective, etc.)"

As described in the original proposal, we identified three objectives to help meet the overall goal of the project. ***The key objectives were: 1) database generation, 2) model development, and 3) performance characterization.*** In accomplishing objective #1, we built five different databases to accomplish the performance characterization of EASI in a variety of applications. These included: 1) a gas chromatography-electron ionization-mass spectrometry (GC-EI-MS) database containing 303 cocaine spectra from more than a dozen crime labs, 10 spectra of cocaine diastereomers from the NIST archive, and 706 replicate spectra of five other common drugs from two different crime labs; 2) A total of ~47,000 GC-EI-MS fentanyl analog spectra from ~10 different labs; 3) a total of 3,888 GC-EI-MS spectra of synthetic cathinones from two different labs; 4) a total of 3,253 GC-EI-MS n-alkane spectra from two different labs, and 5) a total of 137 direct analysis in real time tandem mass spectrometry (DART-MS/MS) spectra of four isomeric cannabinoids (including delta-9-tetrahydrocannabinol (THC) and delta-9-tetrahydrocannabidiol (CBD), 196 DART-MS/MS spectra of four fentanyl analogs, and 284 DART-MS/MS spectra of four opioids (including isobars norhydrocodone and hydrocodone). In accomplishing objective #2, we published a manuscript summarizing the statistical foundations of the algorithm and the basis for multivariate linear modeling. We accomplished objective #3 for cocaine identification by publishing a manuscript that summarized a variety of ways of assessing the performance of the algorithm. These included: 1) assessing the skew and kurtosis of residual of the models; 2) confirming the lack of correlation among residuals of the models, 3) confirming the superior accuracy of EASI model predictions versus conventional model predictions, and 4) establishing the error rate for identifying cocaine on spectra from more than a dozen instruments. These published results apply to database #1. On more than a dozen occasions, we have presented the validity and effectiveness of the new algorithm to compound identification involving databases #2-5, above. We are still completing manuscripts on these additional applications.

2) Research questions.

Several research questions were addressed through this work, including the following:

1) How many replicate spectra are necessary for reliable algorithm development?
2) How many fragment ions should be modeled to resolve a drug from its nearest spectral neighbor?
3) What are the fewest number of variables that need to be defined by a human in the development of a reliable algorithm?
4) Is the algorithm applicable to all substances?
5) Is the algorithm applicable to spectra derived from tandem mass spectrometry (MS/MS) instruments?

3) Summary of project design and methods.

The following paragraphs summarize the findings in seven different publications that resulted from this work.

4) Summary of results.

Manuscript #1. Expert Algorithm for Substance Identification (EASI) using Mass Spectrometry: Part I. Statistical Foundations in Unimolecular Reaction Rate Theory," *J. Am. Soc. Mass Spectrom.* **2023**, 34(7), 1248-1262. (Open Access). https://doi.org/10.1021/jasms.3c00089

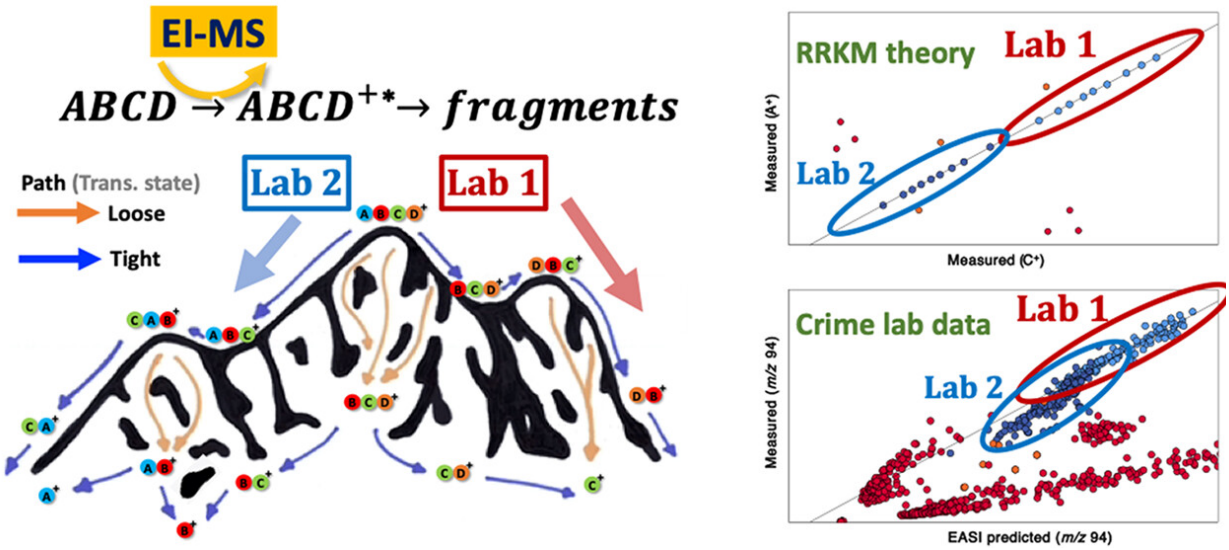


Figure 1. *Table-of-contents graphic to show the relationship between theory and practice for the algorithm at the heart of EASI.*

As quoted from the published abstract (**Figure 1**): "This study aims to resolve one of the longest-standing problems in mass spectrometry, which is how to accurately identify an organic substance from its mass spectrum when a spectrum of the suspected substance has

not been analyzed contemporaneously on the same instrument. Part one of this two-part report describes how Rice–Ramsperger–Kassel–Marcus (RRKM) theory predicts that many branching ratios in replicate electron–ionization mass spectra will provide approximately linear correlations when analysis conditions change within or between instruments. Here, proof-of-concept general linear modeling is based on the 20 most abundant fragments in a database of 128 training spectra of cocaine collected over 6 months in an operational crime laboratory. The statistical validity of the approach is confirmed through both analysis of variance (ANOVA) of the regression models and assessment of the distributions of the residuals of the models. General linear modeling models typically explain more than 90% of the variance in normalized abundances. When the linear models from the training set are applied to 175 additional known positive cocaine spectra from more than 20 different laboratories, the linear models enabled ion abundances to be predicted with an accuracy of <2% relative to the base peak, even though the measured abundances vary by more than 30%. The same models were also applied to 716 known negative spectra, including the diastereomers of cocaine: allococaine, pseudococaine, and pseudoallococaine, and the residual errors were larger for the known negatives than for known positives. The second part of the manuscript describes how general linear regression modeling can serve as the basis for binary classification and reliable identification of cocaine from its diastereomers and all other known negatives."

This manuscript is one of the most highly viewed/downloaded manuscripts in this journal in the last year. In the first 7 months of being published, the manuscript has been viewed more than 1600 times (**Figure 2**).

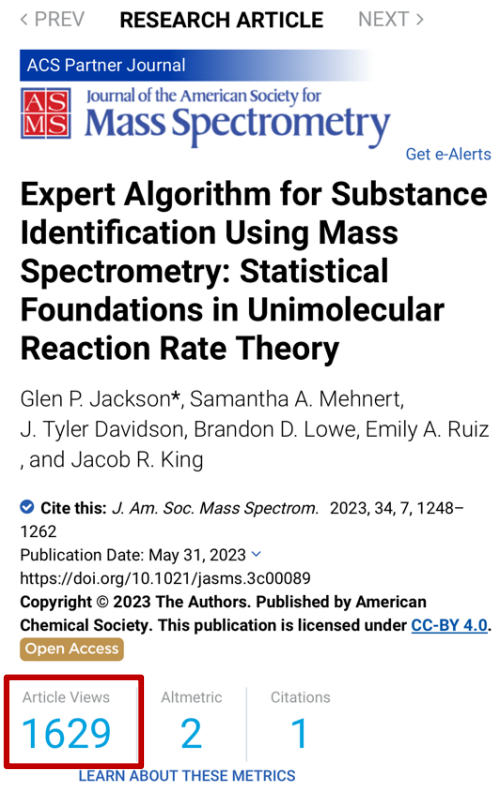


Figure 2. *Screenshot of article metrics for part 1 of the 2-part manuscript.*

Manuscript #2. Expert Algorithm for Substance Identification Using Mass Spectrometry: Application to the Identification of Cocaine on Different Instruments Using Binary Classification Models. *J. Am. Soc. Mass Spectrom.* **2023**, 34(7), 1235-1247. (Open Access).
https://doi.org/10.1021/jasms.3c00090

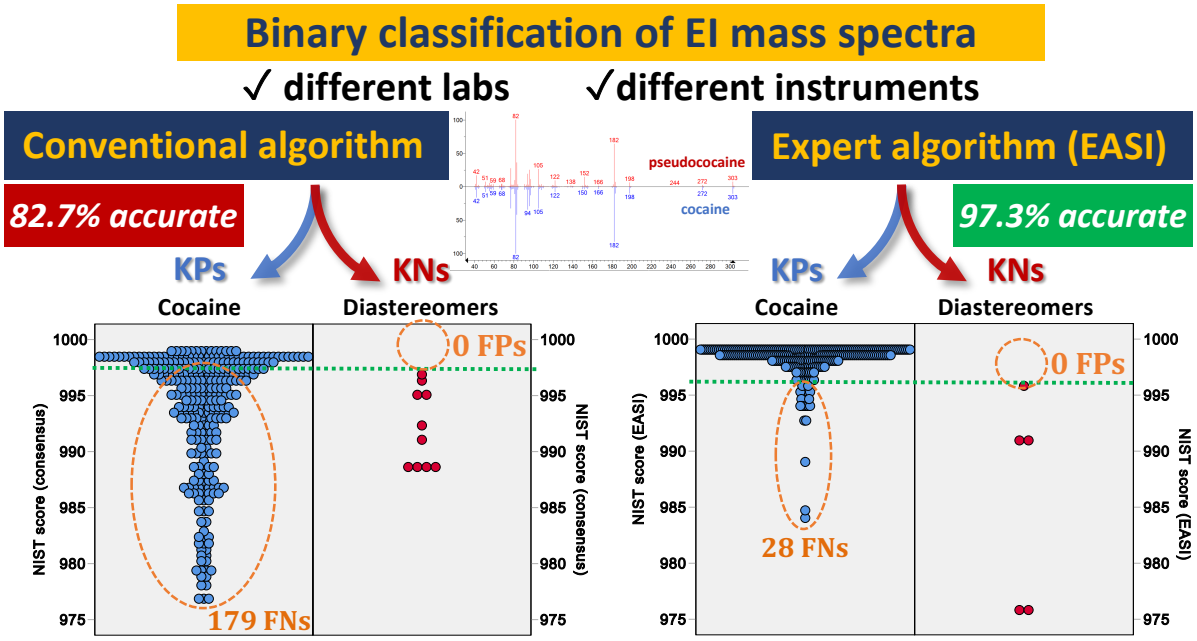


Figure 3. *Table-of-contents graphic to show the improvement in identification accuracy of EASI relative to the traditional approach.*

As quoted from the published abstract (**Figure 3**): "This is the second of two manuscripts describing how general linear modeling (GLM) of a selection of the most abundant normalized fragment ion abundances of replicate mass spectra from one laboratory can be used in conjunction with binary classifiers to enable specific and selective identifications with reportable error rates of spectra from other laboratories. Here, the proof-of-concept uses a training set of 128 replicate cocaine spectra from one crime laboratory as the basis of GLM modeling. GLM models for the 20 most abundant fragments of cocaine were then applied to 175 additional test/validation cocaine spectra collected in more than a dozen crime laboratories and 716 known negative spectra, which included 10 spectra of three diastereomers of cocaine. Spectral similarity and dissimilarity between the measured and predicted abundances were assessed using a variety of conventional measures, including the mean absolute residual and NIST's spectral similarity score. For each spectral measure, GLM predictions were compared to the traditional exemplar approach, which used the average of the cocaine training set as the consensus spectrum for comparisons. In unsupervised models, EASI provided better than a 95% true positive rate for cocaine with a 0% false positive rate. A supervised binary logistic regression model provided 100% accuracy and no errors using EASI-predicted

abundances of only four peaks at m/z 152, 198, 272, and 303. Regardless of the measure of spectral similarity, error rates for identifications using EASI were superior to the traditional exemplar/consensus approach. As a supervised binary classifier, EASI was more reliable than using Mahalanobis distances.

This manuscript is also one of the most highly viewed/downloaded manuscripts in this journal in the last year. In the first 7 months of being published, the manuscript has been viewed almost 1300 times (**Figure 4**).

Figure 4. *Screenshot of article metrics for part 1 of the 2-part manuscript.*

Manuscript #3. G. P. Jackson, M. A. Barkett, "Forensic Mass Spectrometry: Scientific and Legal Precedents," *J. Am. Soc. Mass Spectrom.* **2023**, 34(7), 1210-1224. (Open Access)
https://doi.org/10.1021/jasms.3c00124

During the extensive literature review for the first two manuscripts listed above, we discovered many historical examples of forensic applications of mass spectrometry that had not been adequately summarized or contextualized in the history of forensic mass spectrometry. As part of our broader effort to help disseminate the historical relevance and importance of mass spectrometry in forensic sciences, we therefore wrote and published this

extensive “Accounts and Perspectives” article, which has also received huge interest from the community and has already been read more than 3400 times (**Figure 5**).

Figure 5. *Screenshot of article metrics for a review on forensic applications of mass spectrometry.*

As quoted from the published abstract (**Figure 6**): “Mass Mass spectrometry has made profound contributions to the criminal justice system by providing an instrumental method of analysis that delivers exquisite analytical figures of merit for a wide variety of samples and analytes. Applications include the characterization of trace metal impurities in hair and glass to the identification of drugs, explosives, polymers, and ignitable liquids. This review describes major historical developments and, where possible, relates the developed capabilities to casework and legal precedents. This review also provides insight into how historical applications have evolved into, and out of, modern consensus standards. Unlike many pattern-based techniques and physical-matching methods, mass spectrometry has strong scientific foundations and a long history of successful applications that have made it one of the most reliable and respected sources of scientific evidence in criminal and civil cases. That said, in several appellate decisions in which mass spectrometric evidence was challenged but admitted, decisions

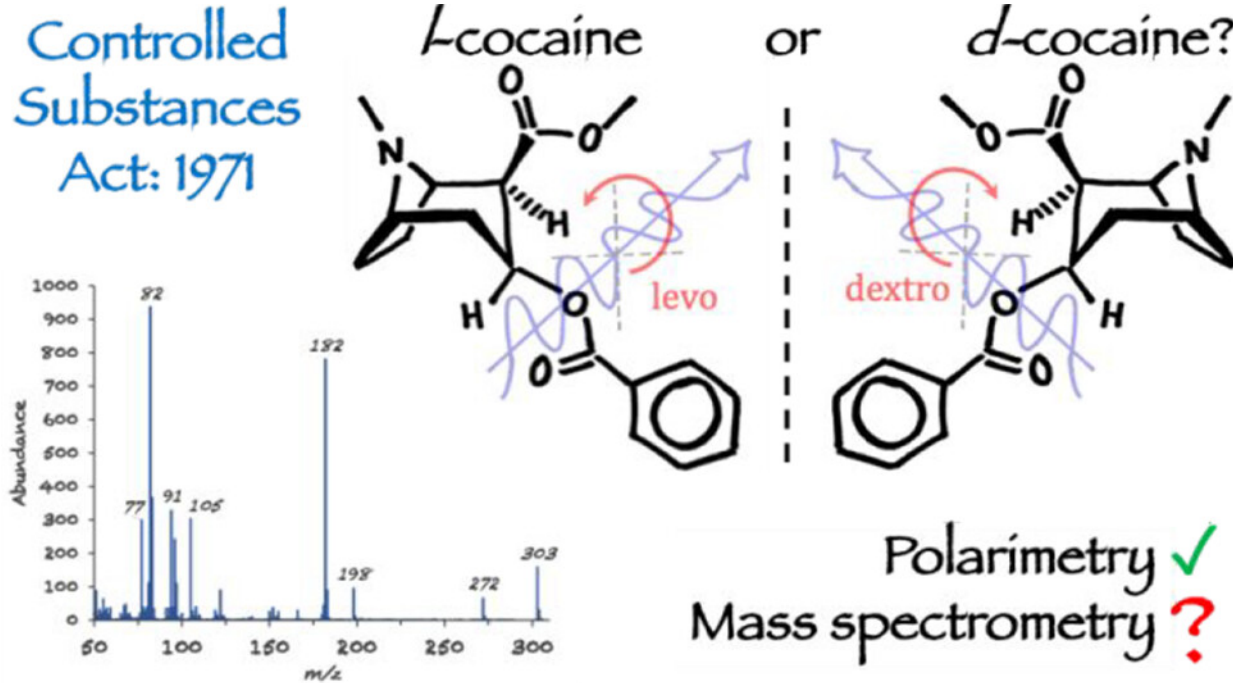


Figure 6. *Table-of-contents graphic to show the improvement in identification accuracy of EASI relative to the traditional approach.*

sometimes still went against the mass spectrometric data anyway, which goes to show that mass spectrometric evidence is always just one piece of the larger legal puzzle."

Unpublished results.

Regarding work that we have presented but not yet published, these results relate to databases #2-5 listed in the goals section.

Database #2. This project involved the creation of a database of ~47,000 EI-MS spectra of fentanyl analogs from ~10 different labs. Most of the replicate spectra were from 2 labs. This project formed the basis of an MS thesis for Alexandra Adeoye. The difficulty of spectral identification is demonstrated by the head-to-tail plot of valerylfentanyl and isovalerylfentanyl, below.

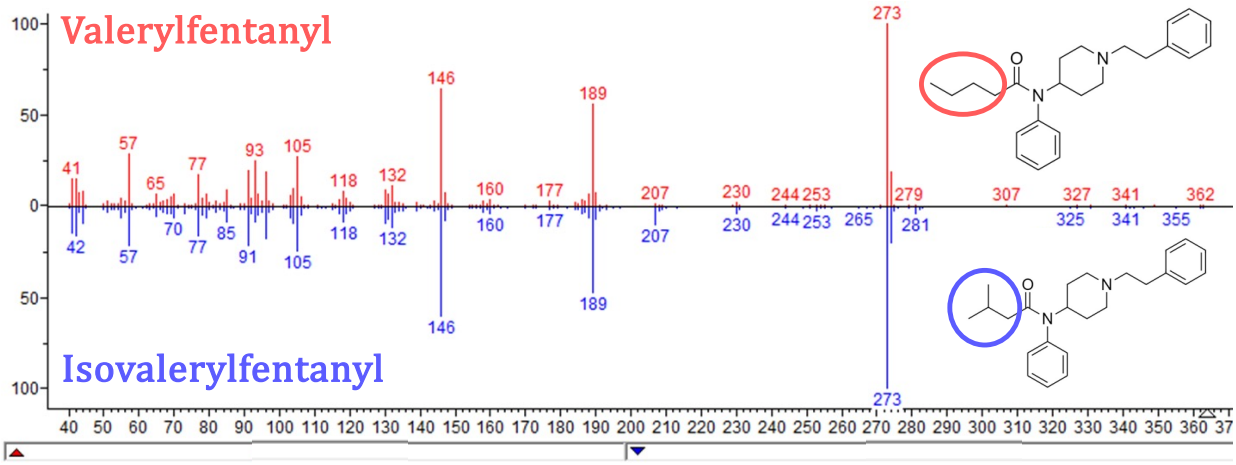


Figure 7. *Head-to-tail plot to show the difficulty in distinguishing valerylfentanyl and isovalerylfentanyl from the EI mass spectra.*

Other positional isomers and regio-isomers are equally difficult to distinguish. The mean absolute residual (MAR) of 20 abundance predictions was computed for each query spectrum relative to 1) the consensus spectrum (mean of the training set) or 2) the EASI models. **Figure 8** show population plots for different sets of data. For the consensus approach, the frequency distribution of MAR values for known negatives overlaps the frequency distribution for known positives, so it is not possible to establish a threshold for binary classification that is without error. A MAR threshold of, say 2.2% would provide no false positives, but many false negatives. In contrast, using EASI, all spectra of o-MMAF were well described by the models, so provided MARS that were smaller than 1.8%. Therefore, a MAR threshold of 1.8%, for example, provides errorless identifications for *o*-MMAF, even when tested against 4600 known negative regio-isomers *m*- and *p*-MMAF.

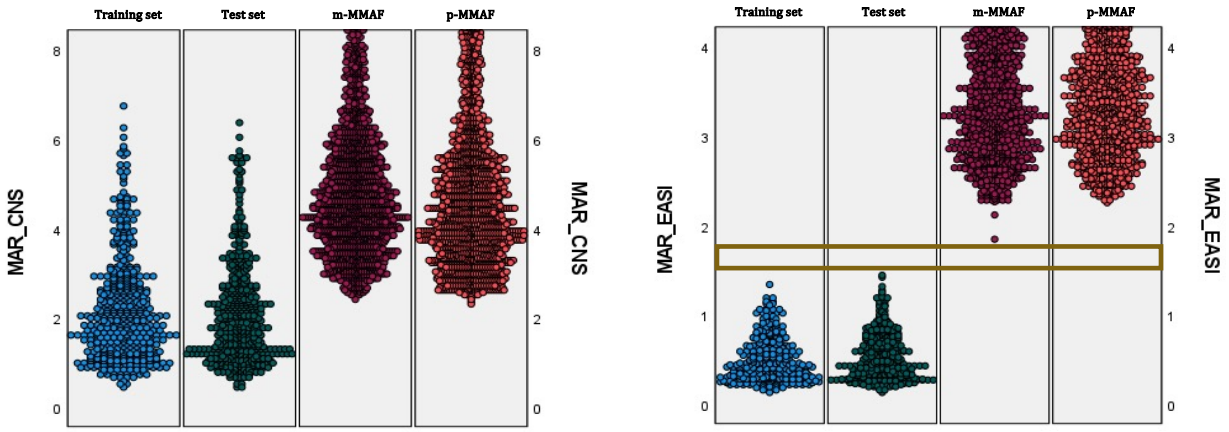


Figure 8. *Population plots to the spectral similarity between different query spectra and the training set of ortho-methoxymethylacetylfentanyl (o-MMAF). There are a total of 978 known positives in the training set and test set of o-MMAF and 4600 known negatives in the m-MMAF and p-MMAF sets.*

Figure 9 provides a receiver-operating characteristic (ROC) curve of the true positive rate (TPR, sensitivity) versus false positive rate (1-specificity) to show the effectiveness of the binary classification models. The areas under the ROC curves (AUROC) are 0.94 and 1 for the consensus and EASI approaches, respectively, which means that whereas the consensus approach will always make some mistakes, EASI is capable of errorless identifications in this dataset.

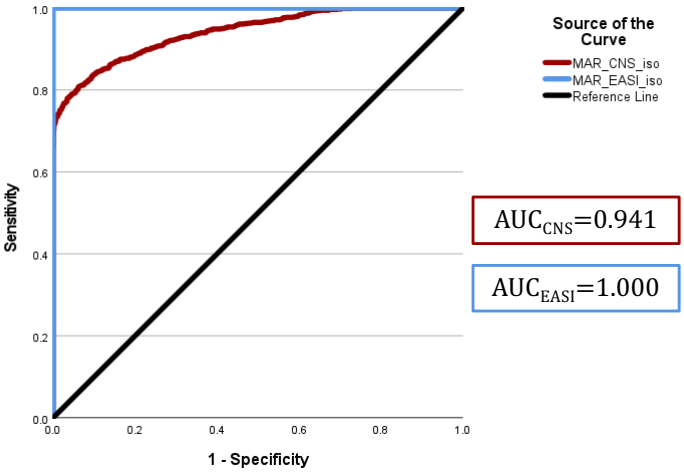


Figure 9. *Receiver-operative characteristic (ROC) curves for the binary classification of o-MMAF based on the MAR relative to the o-MMAF model. CNS=consensus approach, which is relative to the mean spectrum of the database.*

Alex's thesis, and the draft manuscripts explain the effectiveness of EASI modeling for inter-laboratory comparison of three different types of fentanyl analogs: 1) valerylfentanyl and isovalerylfentanyl; 2) *o*-, *m*-, and *p*-methoxymethylacetylfentanyl; and 3) *cis*- and *trans*-3-methyl thiofentanyl.

Database #3. This database was initiated through a collaboration with Stephen Hokanson at the Virginia Department of Forensic Science in Roanoke, VA. His lab collected dozens of

spectra on three different instruments over a period of several weeks (**Figure 10**). We also collected replicates in our lab at WVU to produce a database of 3,888 GC-EI-MS spectra of synthetic cathinones. A summary of the results is provided in **Figure 11**.

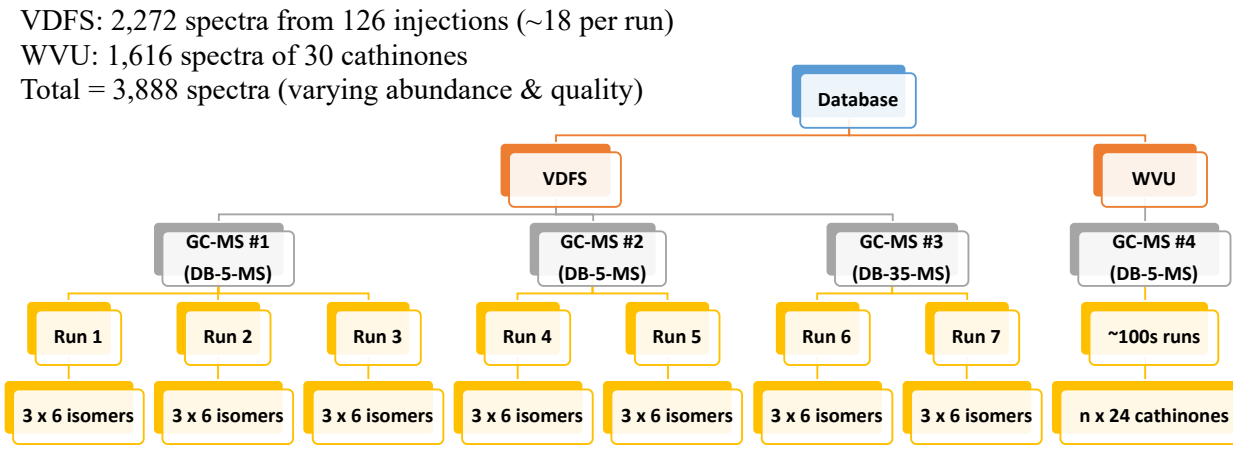


Figure 10. *Flow chart for database generation for cathinone analogs for database #3.*

EASI modelling was conducted in the manner described in the first two publications (for cocaine), and ROC curves were again generated to assess the overall separation of the cumulative distribution functions for known positives and known negatives for each model. An example of a frequency distribution plot is provided in **Figure 11** for the MAR or 20 general linear models for N-isopropylbutylone (NIPB).

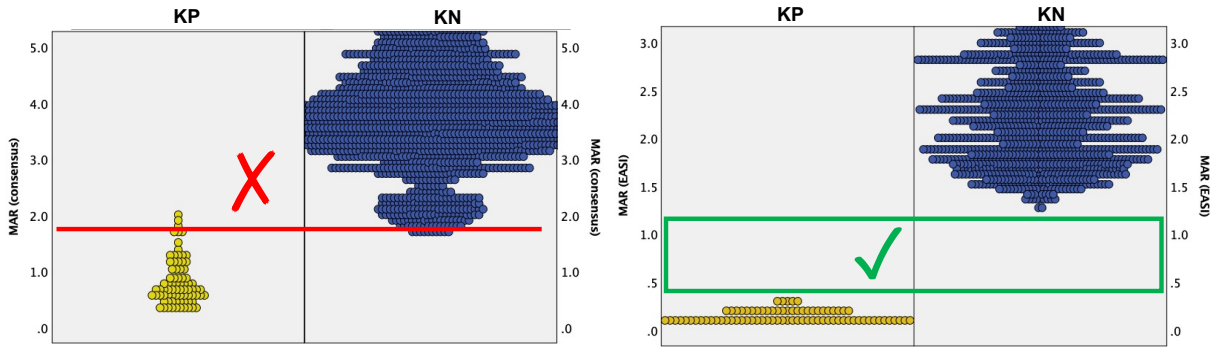


Figure 11. *Population plots for the MARs using the consensus spectrum approach or EASI for predicting 20 ion abundances in the spectra of 311 known positives (KPs) of N-isopropylbutylone (NIPB) and 3351 known negative spectra (KN) of related cathinones. The red line and green box indicate potential thresholds for binary classification.*

The AUROCs for five different cathinones are provided in **Table 1**. The table also compares the consensus approach and EASI for the same training/test sets. Unlike the consensus approach, EASI can make errorless identifications for all five constitutional isomers. Other

measures of spectral similarity provided similar results, which demonstrates that the success of EASI is not related to the chosen method of spectral comparison. The success of EASI is related to the ability to model and make use of the correlated changes in branching ratios in replicate spectra.

Table 1. Area under the ROC curve (AUROC) for binary classification of five different cathinones using the mean absolute residual (MAR) of 20 fragment ion abundances as the measure of spectral dissimilarity. CNS = consensus approach, which measures each query spectrum to the mean of the training set. EASI = expert algorithm for substance identification.

Compound	CNS	EASI
NENMB	0.9998	1.0000
NEP	0.9980	1.0000
NIPB	0.9976	1.0000
NMH	1.0000	1.0000
NNDP	1.0000	1.0000

Database #4. This database consists of a total of 3,253 GC-EI-MS spectra of n-alkanes from two different labs. One was our own in-house replicates of n-alkane standards and the other was n-alkane spectra from data files made available by the ignitable liquid reference collection (ILRC) at the National Center for Forensic Science (NCFS) at the University of Central Florida (UCF). The larger n-alkanes, like nC20 and nC21, are notoriously difficult to resolve from one another because the base peak is often missing and the branching ratios of the majority of fragments is almost indistinguishable. We modeled the branching ratios for three sets of n-alkanes, nC8, nC20 and nC21.

An example of the accuracy of spectral predictions is provided in **Figure 12**. Here, the EASI-predicted values for the model for *m/z* 41 are plotted versus the measured values. Known positives in the training and test sets were collected on Agilent GC-MS instruments and have negligible residual errors. The known positives in the external validation set were collected on a Perkin Elmer instrument and have larger residual errors for this particular model. However, when the absolute residuals of 20 such models are combined in the MAR, the MAR for known positives on the Perkin Elmer are generally smaller than for known negatives. The MAR therefore enables errorless binary classification when any individual model might not (**Figure 13**).

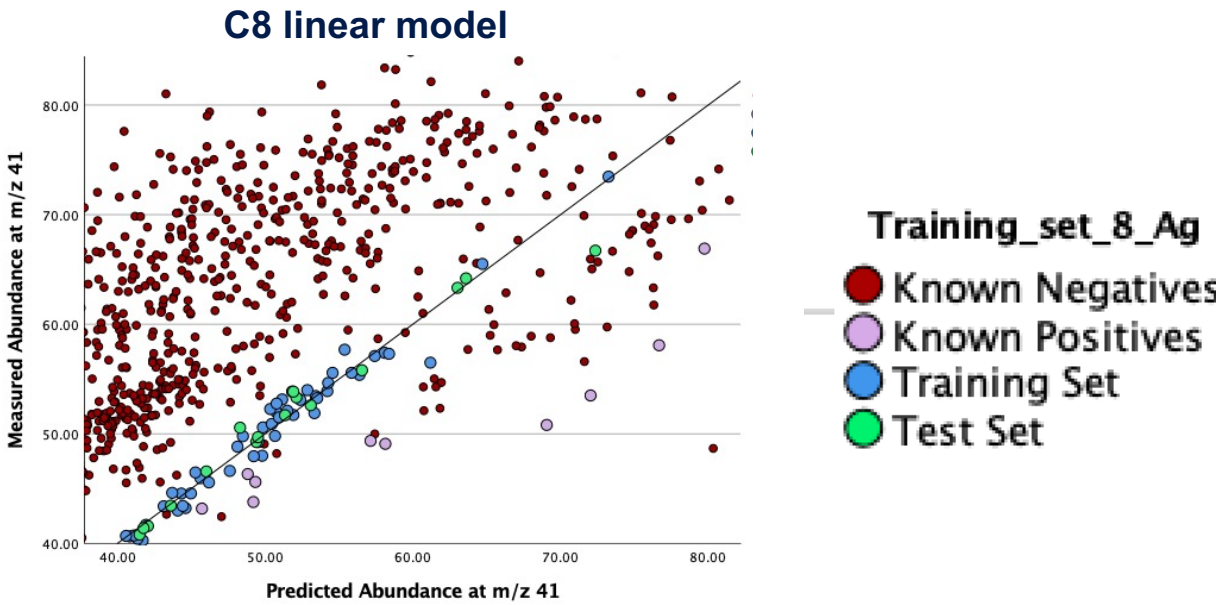


Figure 12. *Scatter plot of predicted abundance versus measured abundance for one general linear model for m/z 41 for nC8. The training set consisted of 17 replicate spectra of nC8. The equation for the model is* $\hat{A}_{m/z\ 41} = 23.12 + 1.89(A_{m/z\ 39}) + 0.1(A_{m/z\ 32}) - 0.72(A_{m/z\ 44})$*. The test- and training set contained data from several Agilent GC-MS instruments, and the pink known positives were collected on a Perkin Elmer GC-MS instrument.*

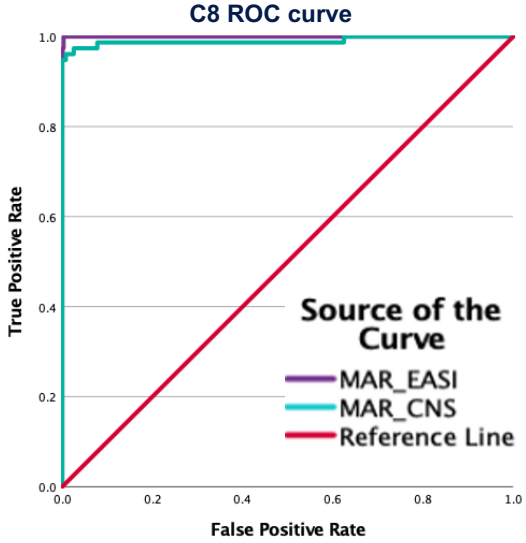


Figure 13. *Receiver-operative characteristic (ROC) curves for the binary classification of various n-alkanes based on the MAR relative to the nC8 models. CNS=consensus approach, which is relative to the mean spectrum of the database.*

As shown in Table 2, EASI made errorless binary classifications for nC8 spectra and "not nC8" spectra, even if the spectra were collected on a different instrument and not part of the training set. For each method of spectral comparison, the consensus approach was not able to make errorless predictions, so there were always some false positives and false negatives, depending on the threshold for binary classification.

Table 2. Area under the ROC curve (AUROC) for binary classification of nC8 using three different spectral measures for 20 fragment ion predictions. CNS = consensus approach, which measures each query spectrum to the mean of the training set. EASI = expert algorithm for substance identification.

Spectral measure	CNS	EASI
MAR	0.990	1.0000
Euclid	0.991	1.0000
PPMC	0.994	1.0000

Discriminating between the larger n-alkanes is more challenging because the spectral differences are smaller, and the molecular ions are less abundant or absent. As shown in Table 3, the consensus approach had AUROC values of 0.78-0.8, depending on the spectral measure. One can therefore expect a combined false positive and false negative error rate of about 20%, depending on the selected threshold. In contrast, The AUROCs for EASI were about 0.9, so the total error rate is expected to be about 10%, depending on the threshold.

Table 3. Area under the ROC curve (AUROC) for binary classification of nC20 using three different spectral measures for 20 fragment ion predictions. CNS = consensus approach, which measures each query spectrum to the mean of the training set. EASI = expert algorithm for substance identification.

Spectral measure	CNS	EASI
MAR	0.786	0.914
Euclid	0.780	0.899
PPMC	0.800	0.899

Databases #5 and 6. We are still finalizing work on these models. We have presented preliminary results (see list of presentations), and we will continue to disseminate the findings through peer reviewed publications in due course.

5) Applicability to the criminal justice system.

The goals were designed to address specific needs of the TWG for seized drugs, which are consensus requests for proposals germane to practitioners. As described in the products section, we have presented our findings in several outlets, including on-line workshops, in-person and on-line conferences, and peer-reviewed publications. Two of these presentations have led to the development of collaborations with practitioners in practicing crime laboratories, as they see value in the algorithm and would like to implement its capabilities on casework.

In one example, we were contact by Stephen Hokanson of the Virginia Department of Forensic Science (VDFS). They had a casework sample that contained a suspected synthetic cathinone that was similar to N-ethylpentylone (NEP), which they had seen for years in previous casework samples. The new substance was suspected to be N-propylbutylone (NPB) or N-isopropylbutylone (NIPB), which are both constitutional isomers of NEP and have seemingly indistinguishable GC-EI mass spectra. At the time, NPB and NIPB were on back-order at Cayman Chemical, so the lab was unable to acquire a contemporaneous spectrum of a reference material under the same conditions as the query sample, as is required in ASTM-2327 Standard Practice for Quality Assurance of Laboratories Performing Seized-Drug Analysis. This standard requires "Comparison to data obtained from a suitable drug reference material analyzed under the same analytical conditions as the test/case sample. The reference material may be analyzed: 1) contemporaneously with test/case sample; 2) as part of routine quality control (for example, daily check solutions); or 3) at a previous date (for example, method validation, in-house library)." We therefore worked with the laboratory to identify a suitable approach to establishing the applicability of our algorithm for identifying the substance on a GC-MS instrument on which a reference sample or training set had not been acquired. We have presented our results on three occasions at scientific conferences and are in the final stages of completing a manuscript to describe the results.

In the second example, we have recently been collaborating with Dr. Sandra Rodriguez-Cruz of the DEA Special Testing program to see if our algorithm would be applicable to distinguishing between spectrally similar compounds collected on their DART-MS/MS instruments. We are currently developing a research plan and plan to submit a new NIJ proposal in spring 2024 to address that question.

In addition to these collaborations with practitioners in the criminal justice system, we have signed a non-disclosure agreement with a major publisher of mass spectral libraries to help commercialize the algorithm. The goal of the software is to enable end-users in crime laboratories to have functional access to the algorithm so that they can compare the algorithm's output along with any existing analytical scheme for casework samples.

By understanding the variance that occurs in mass spectral fragmentation, and by explaining how to model and explain this variance, we have provided practitioners with a

way to make more reliable and more accurate identifications of seized drugs, even in the absence of reference spectra on the same instrument with the same conditions. Practitioners will need help implementing these profound capabilities, so we are currently working with a commercial vendor, which has expertise in this area, to help automate the data analysis and validation and ease its deployment in the criminal justice system. In addition to meeting several defined needs of the TWG for seized drugs, we are working hard to move the technology to practitioners.

Products

1) Peer-reviewed publications

1) G. P. Jackson, S.A. Mehnert, J. T. Davidson, B. D. Lowe, E. A. Ruiz, J. R. King, "Expert Algorithm for Substance Identification (EASI) using Mass Spectrometry: Part I. Statistical Foundations in Unimolecular Reaction Rate Theory," *J. Am. Soc. Mass Spectrom.* **2023**, 34(7), 1235-1247. https://doi.org/10.1021/jasms.3c00089

2) S.A. Mehnert, J. T. Davidson, A. Adeoye, B. D. Lowe, E. A. Ruiz, J.R. King, G. P. Jackson, "Expert Algorithm for Substance Identification (EASI) using Mass Spectrometry: Part II. Application to the Identification of Cocaine on Different Instruments using Binary Classification Models," *J. Am. Soc. Mass Spectrom.* **2023**, 34(7), 1248-1262. https://doi.org/10.1021/jasms.3c00090

3) G. P. Jackson, Mark A. Barkett, "Forensic Mass Spectrometry: Scientific and Legal Precedents, *J. Am. Soc. Mass Spectrom.,* **2023**, 34(7), 1210-1224. https://doi.org/10.1021/jasms.3c00124

2) Book chapters and theses

1) Isabel Cristina Gálvez Valencia, The Influence of Instrumental Sources of Variance on Mass spectral Comparison Algorithms, 2023. Graduate Thesis, 12104. https://doi.org/10.33915/etd.12104
2) Alexandra Adeoye, "Development of an Expert Algorithm for Substance Identification (EASI) to Discriminate between Spectrally Similar Fentanyl Analogs in Mass Spectrometry" (2022). *Graduate Theses*. 11164. https://doi.org/10.33915/etd.11164

3) Archived research data.

The cocaine dataset that was used in the first two publications has been submitted for data archiving a public access through Mendeley. The link to the open-access datafile is here:
Jackson, Glen P. (2024), "Data for: Expert Algorithm for Substance Identification (EASI) using Mass Spectrometry: Parts I and II. J. Am. Soc. Mass Spectrom., 2023, Vol 34(7), 1428-1447. ", Mendeley Data, V1, doi: 10.17632/4b4fry23r3.1

Other databases will be made available as they are published. This funding source from NIJ will continue to be cited in future publications and data archives.

4) Conference presentations

The following presentations were invited (asterisks) or accepted as oral or poster presentations in traditional conference vanues.

1) A. Pfeffer, G. P. Jackson, "Application of the Expert Algorithm for Substance Identification (EASI) to n-Alkanes" at the 21st Undergraduate Research Day at the Capitol, Charleston, WV, 2024. (Poster)

2) A. Adeoye, J. King, G. P. Jackson, "Application of the Expert Algorithm for Substance Identification (EASI) to Resolve THC and CBD ESI-Mass Spectra" at the 76th American Academy of Forensic Sciences Meeting, Denver, CO, 2024. (Oral)

3) G. P. Jackson, A. Pfeffer, A. Adeoye, C. McQuain, J. Orris, S Hokanson, "Application of the Expert Algorithm for Substance Identification (EASI) to the Mass Spectral Identification of Bath Salts (Synthetic Cathinones)" at the 76th American Academy of Forensic Sciences Meeting, Denver, CO, 2024. (Poster)

4) G. P. Jackson, A. Adeoye, E. A. Ruiz, J. T. Davidson, "Expert Algorithm for Substance Identification (EASI) Applied to the Tandem Mass Spectra of Seized Drugs" at the NIJ Forensic Science Research and Development Symposium, Denver, CO, 2024. (Oral)

5) A. Adeoye, G. P. Jackson, "Expert Algorithm for Substance Identification (EASI) Applied to Cathinones," at NIJ's Graduate Research Symposium at the Forensic Technology Center of Excellence, 2023. (Oral, via Zoom)

6) G. P. Jackson, A. Adeoye, "Expert Algorithm for Substance Identification (EASI) Applied to the Mass Spectra of Seized Drugs," at SciX Conference, Reno, NV, 2023. (Oral)

7) J. Orris, A. Adeoye, S. Hokanson, G. P. Jackson, "Application of the Expert Algorithm for Substance Identification (EASI) to Mass Spectra of Synthetic Cathinones" at the Spring ACS Meeting, Indianapolis, IN, 2023. (Poster)

8) *G. P. Jackson, J. T. Davidson, A. Adeoye, E. Ruiz, B. Lowe, J. King "Expert Algorithm for Substance Identification (EASI) Applied to the Mass Spectra of Structurally Similar Fentanyl Analogs," at the Pittsburgh Conference, Philadelphia, PA, 2023. (Oral)

9) *G. P. Jackson, A. Adeoye, J. Orris, S. Hokanson, "Application of the Expert Algorithm for Substance Identification (EASI) to Mass Spectra of Synthetic Cathinones," at the Pittsburgh Conference, Philadelphia, PA, 2023. (Oral)

10) G. P. Jackson, A. Adeoye, J. Orris, S. Hokanson, "B83 The Application of the Expert Algorithm for Substance Identification (EASI) on Synthetic Cathinones Using Mass Spectrometry (MS)," at the 75th American Academy of Forensic Sciences Meeting, Orlando, FL, 2023. (Oral)

11) A. Adeoye, G. P. Jackson, "B84 The Application of the Expert Algorithm for Substance Identification (EASI) to the Mass Spectral Identification of Fentanyl Analogs," at the 75th American Academy of Forensic Sciences Meeting, Orlando, FL, 2023. (Oral)

12) C. S. Poulos and G. P. Jackson, "B115 A Mass Spectral Interpretation of PINACA-Type Novel Psychoactive Substances (NPS)," at the 75th American Academy of Forensic Sciences Meeting, Orlando, FL, 2023. (Poster)

13) A. Pfeffer and G. P. Jackson, "B116 The Application of the Expert Algorithm for Substance Identification (EASI) on N-Alkanes," at the 75th American Academy of Forensic Sciences Meeting, Orlando, FL, 2023. (Poster)

14) I. Galvez and G. P. Jackson, "B117 The Influence of Instrument Parameters on Replicate Mass Spectra and Spectral Comparison Algorithms," at the 75th American Academy of Forensic Sciences Meeting, Orlando, FL, 2023. (Poster)

15) *G. P. Jackson, J. T. Davidson. A. Adeoye, S. Mehnert, E. Ruiz, J. King, "Expert Algorithm for Substance Identification (EASI): A New Paradigm for Mass Spectral Identifications," presented at SciX Conference, Providence, RI, Oct 2022. (Oral)

16) J. King, G. P. Jackson, "Expert Algorithm for Substance Identification (EASI) from Mass Spectra," presented at the 35th Annual ACS Regional Symposium, (virtual due to COVID) Apr 2022. (Poster)

17) *G. P. Jackson, S. Mehnert, J. T. Davidson, B. Lowe, A. Adeoye, E. Ruiz, "Expert Algorithm for Substance Identification (EASI) from Mass Spectra," presented at the NIJ Forensic Science Research and Development Symposium, (virtual due to COVID) Mar 2022. (Oral)

18) A. Adeoye, G. P. Jackson, "The Development of an Expert Algorithm for Substance Identification (EASI) of Fentanyl Analogs Using Mass Spectrometry," at the 74th Meeting of the American Academy of Forensic Sciences, Seattle, WA, Feb 2022. (Oral)

5) Webinars and workshops

Glen P. Jackson, How Did We Get Here? Cannabis Legalization, the Farm Bill, Cannabinoid Analogues, & Chemistry." At the 2023 Continuing Education Workshop for the American College of Medical Toxicology (ACMT) Seminar Series in Forensic Toxicology.

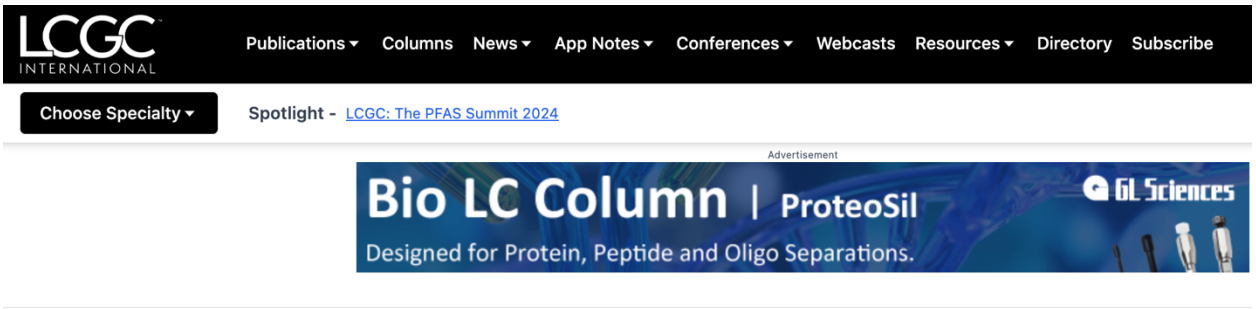
I was invited to provide the opening 30-minute presentation for the workshop, which was attended (remotely) by more than 220 attendees from around the world.

Alex Adeoye and Glen P. Jackson, Expert Algorithm for Substance Identification Applied to Cathinones." At the NIJ Graduate Research Symposium and Poster Session (Virtual), organized by the Forensic Technology Center for Research and Education (FTCOE), Sept 20, 2023

6) General press, podcasts etc.

In March 2022, LCGC published an interview with me regarding my receipt of the FACSS Innovation award at SciX Conference in Oct 2021. The award, for the most innovative research presented for the first time at SciX conference, was based on the EASI algorithm.
The link to the story is here:

https://www.chromatographyonline.com/view/a-new-paradigm-for-mass-spectral-identifications



A New Paradigm for Mass Spectral Identifications

March 2, 2022
John Chasse

Article

There is a growing school of thought among practitioners that what is considered to be the prevailing existing paradigm for mass spectral identification is lacking. Glen Jackson, Professor of Forensic and Investigative Science at West Virginia University, addressed this need with his presentation "Expert Algorithm for Substance Identification (EASI): A New Paradigm for Mass Spectral Identifications" at SciX 2021, where it earned the FACSS Innovations Award. These awards are given for the most innovative and outstanding *new* research advancements debuted orally at the SciX Conference. Jackson spoke to *Current Trends in Mass Spectrometry* about this presentation and filling the aforementioned need.

Your presentation won the FACSS Innovation Award at the 2021 SciX Conference this past fall. Why did you see a need for a new paradigm?

John Chasse, A New Paradigm for Mass Spectral Identifications, LCGC Magazine, March 2, 2022.

7) Other products.

The project did not result in any website(s) or other internet site(s), technologies or techniques, inventions, patent applications, and/or licenses.