

Introducing “DoPP”: A Graphical User-friendly Application for the Rapid Species Identification of Psychoactive Plant Materials and Quantification of Psychoactive Small Molecules Using DART-MS Data

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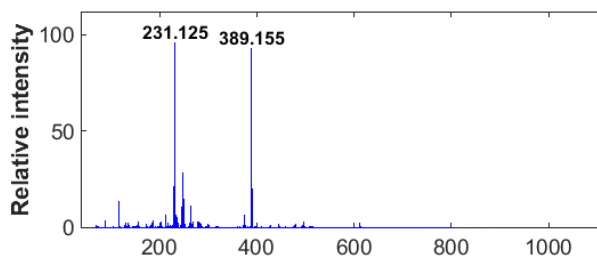
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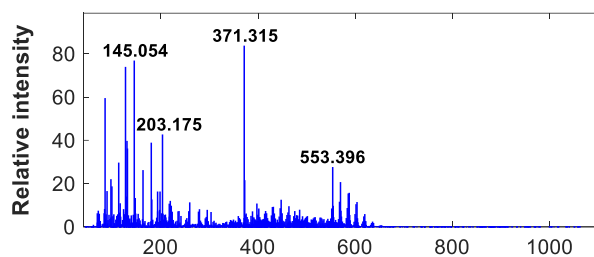
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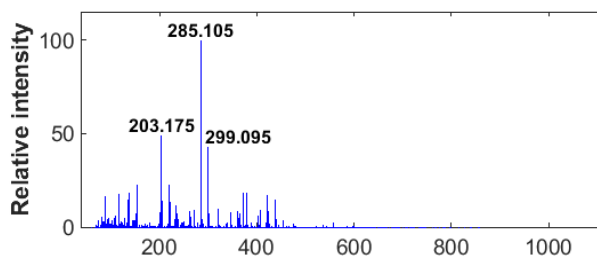
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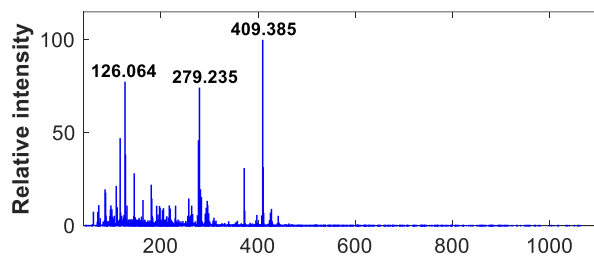
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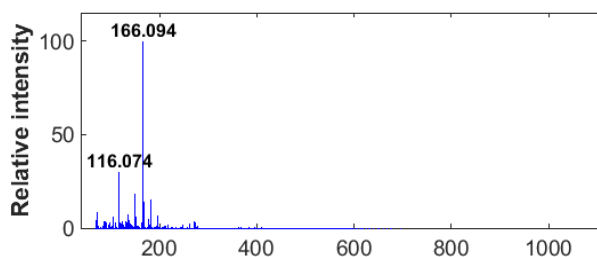
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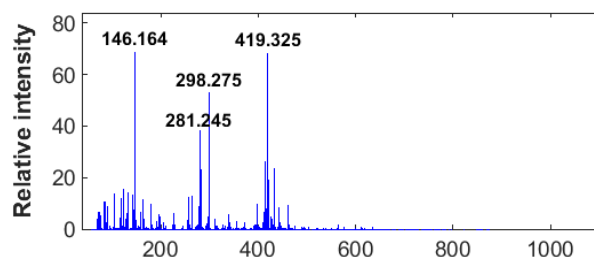
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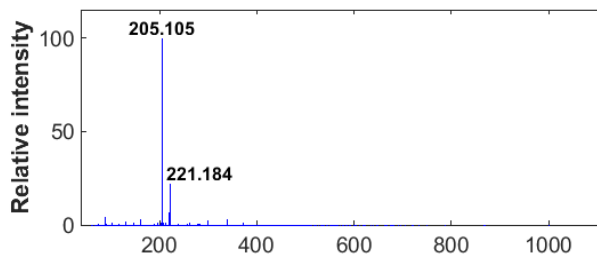
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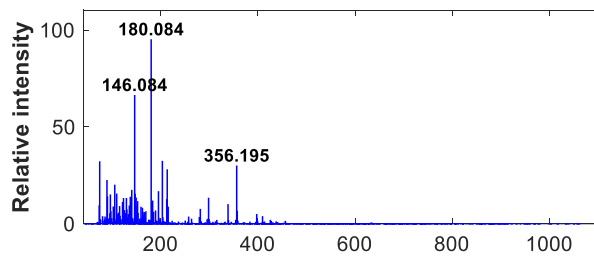
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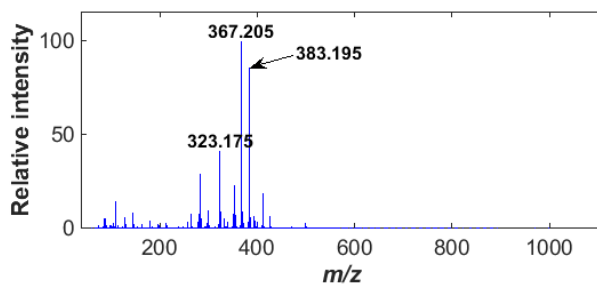
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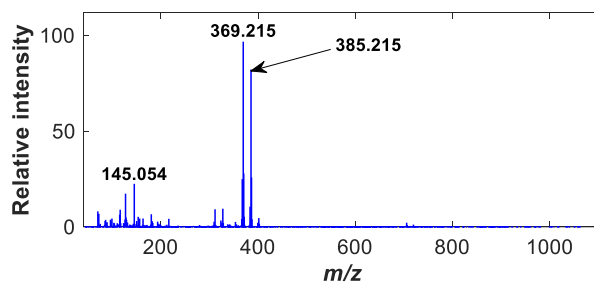
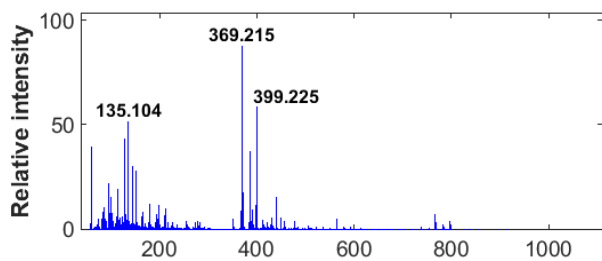
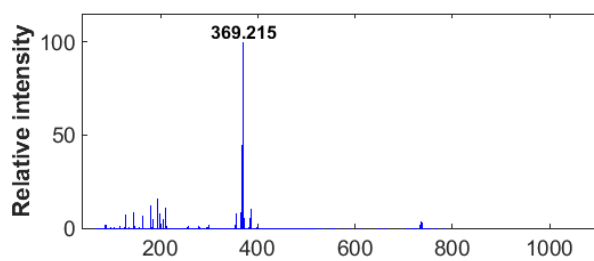


Figure S1. Representative DART high-resolution mass spectra of *A. absinthium*; *A. vulgaris*; *C. zacatechichi*; *L. virosa*; *S. tortuosum*; *E. lobata*; *A. peregrina*; *M. hostilis*, *P. nitida*; and *V. africana*.

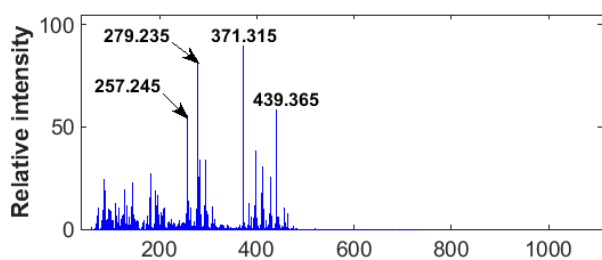
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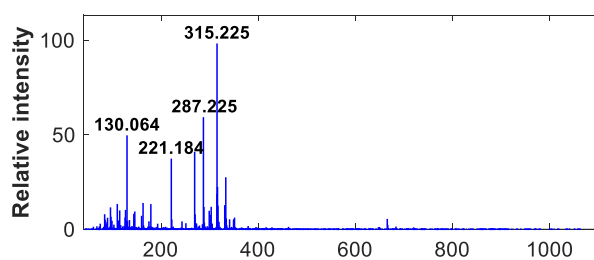
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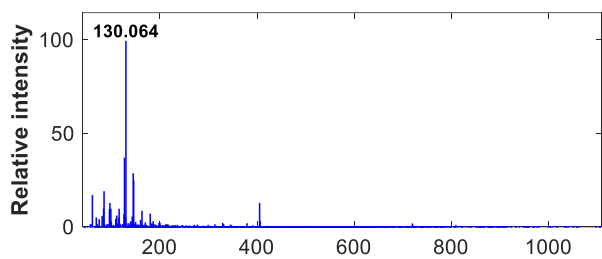
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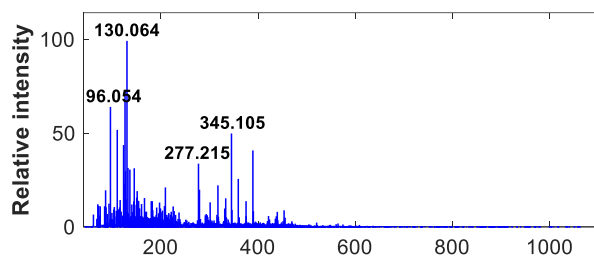
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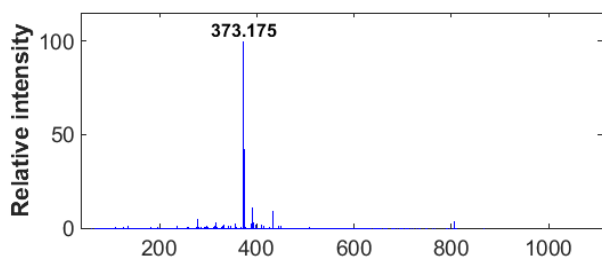
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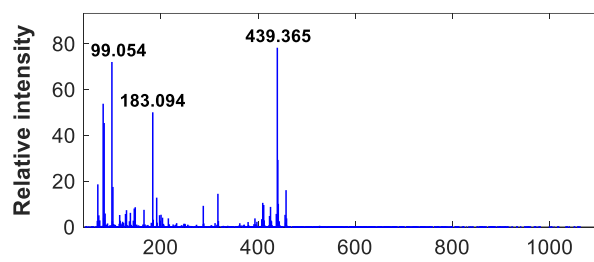
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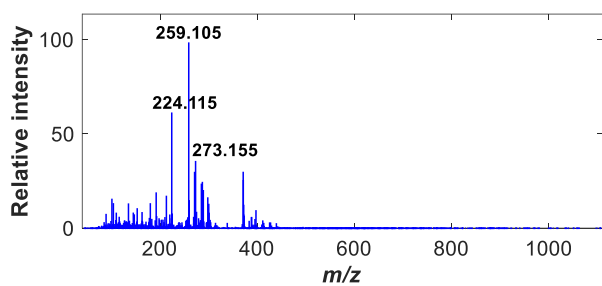
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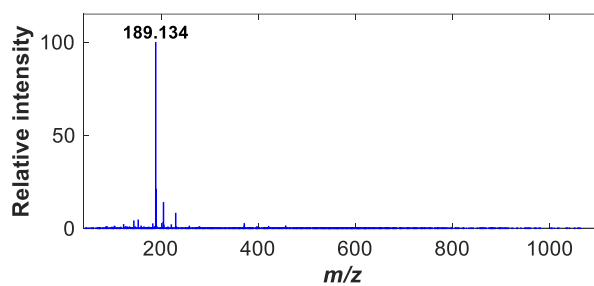
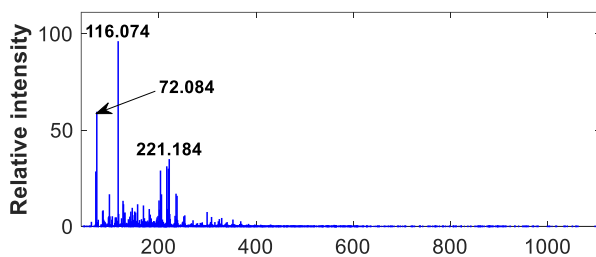
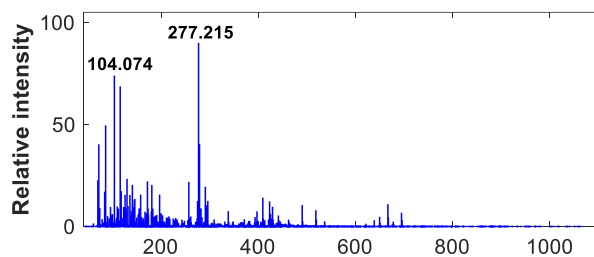


Figure S1 (continued). Representative DART high-resolution mass spectra of *M. speciosa*, *C. johimbe*; *P. viridis*; *L. leonurus*; *L. nepetifolia*; *L. sibiricus*; *S. divinorum*; *S. vulgaris*; *B. caapi* and *D. cabrerana*.

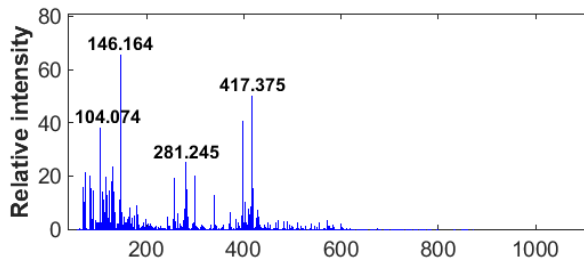
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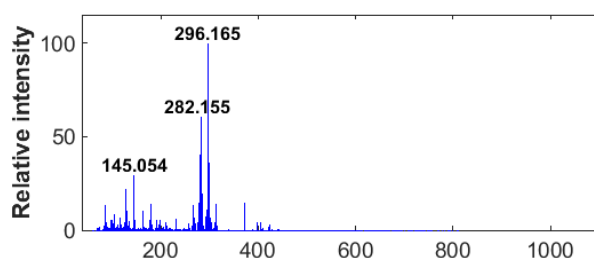
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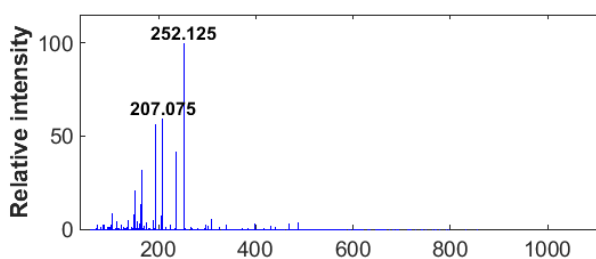
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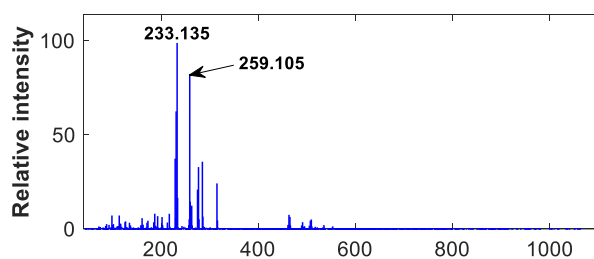
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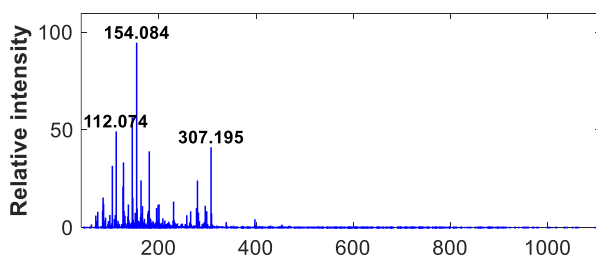
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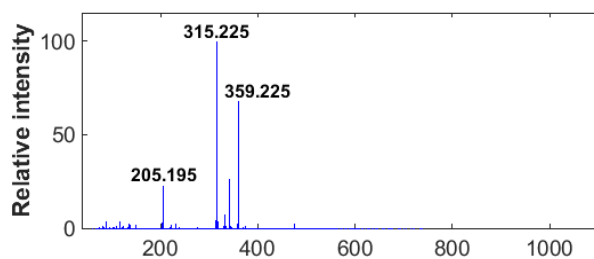
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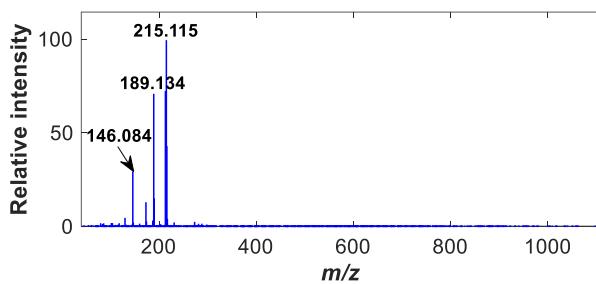
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C. sativa



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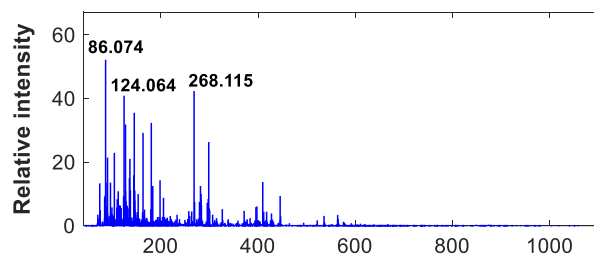
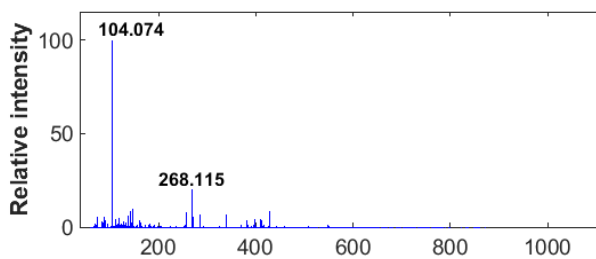
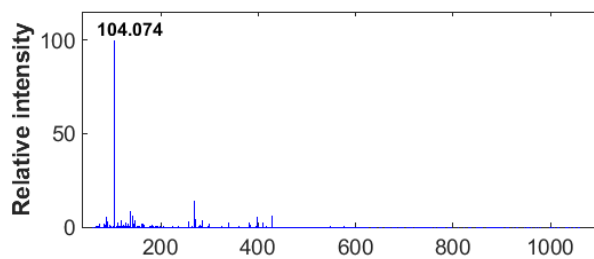


Figure S1 (continued). Representative DART high-resolution mass spectra of *T. diffusa*; *A. officinalis*; *T. populnea*; *N. caerulea*; *P. betel*; *P. methysticum*; *A. racemosa*; *C. sativa*; *P. harmala* and *A. nervosa*.

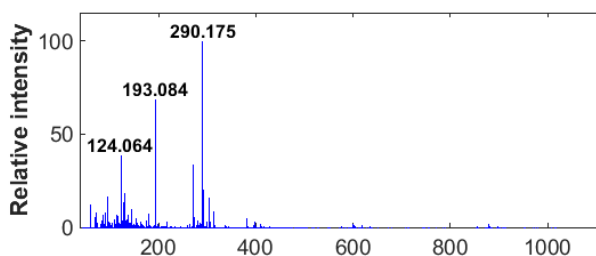
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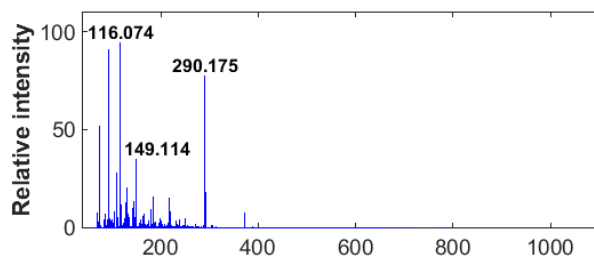
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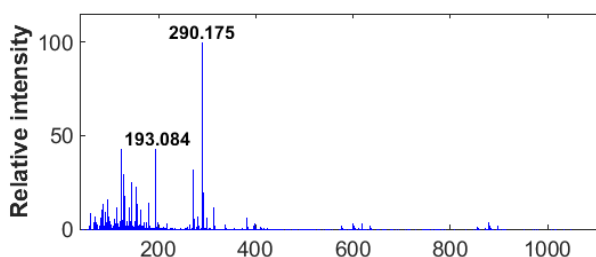
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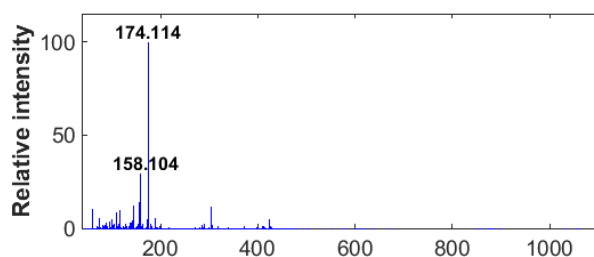
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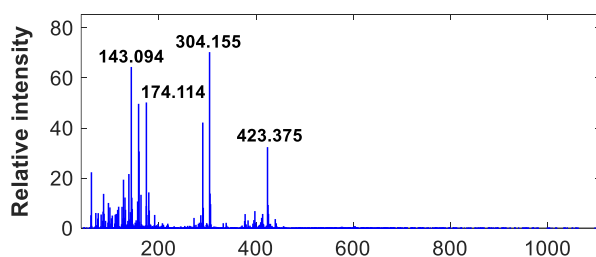
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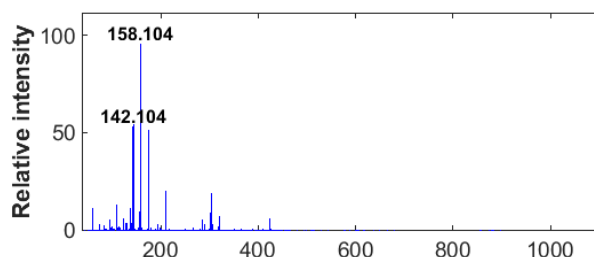
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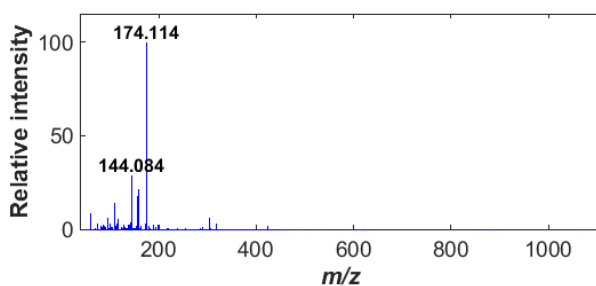
B. aurea



B. sanguinea



B. suaveolens



B. versicolor

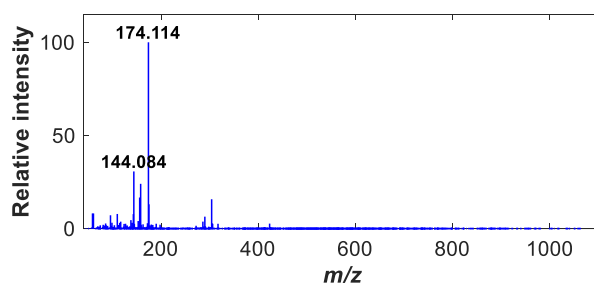
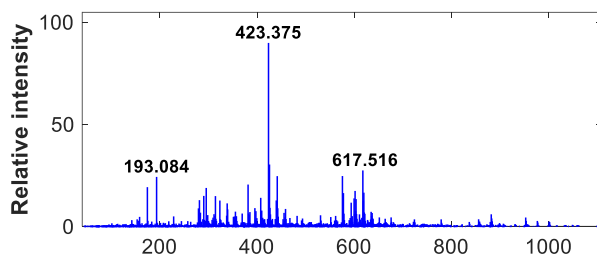
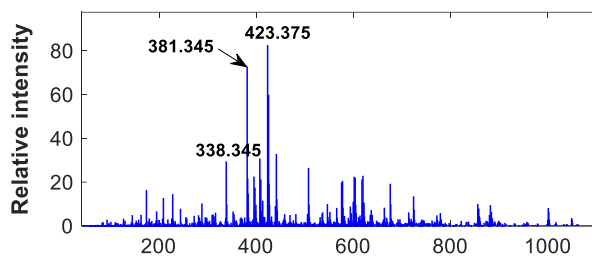


Figure S1 (continued). Representative DART high-resolution mass spectra of *C. tricolor*; *I. tricolor*; *A. baetica*; *A. belladonna*; *A. Komarovii*; *B. arborea*; *B. aurea*; *B. sanguinea*; *B. suaveolens* and *B. versicolor*.

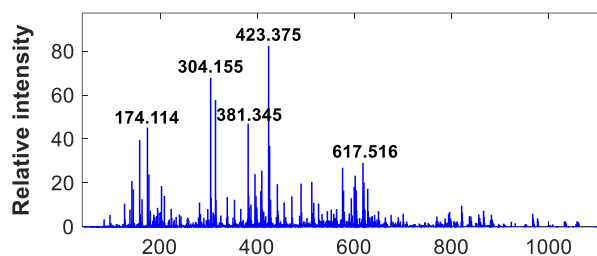
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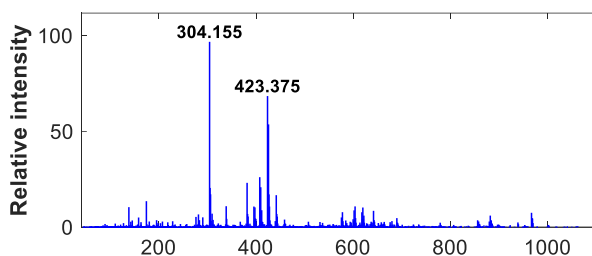
D. discolor



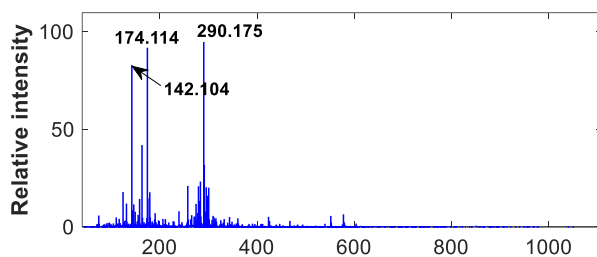
D. ferox



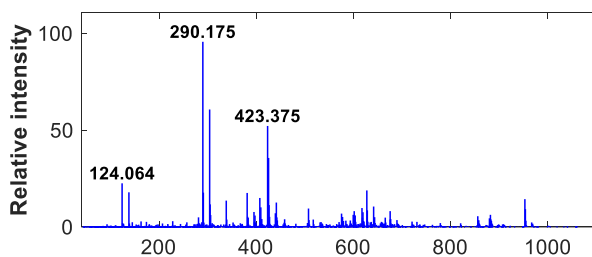
D. innoxia



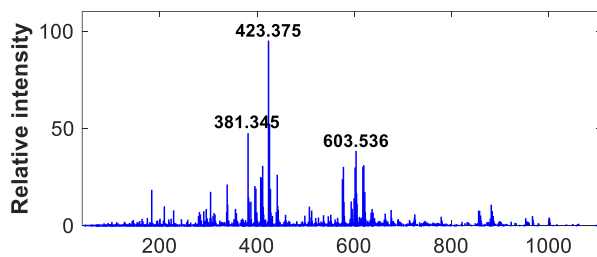
D. leichhardtii



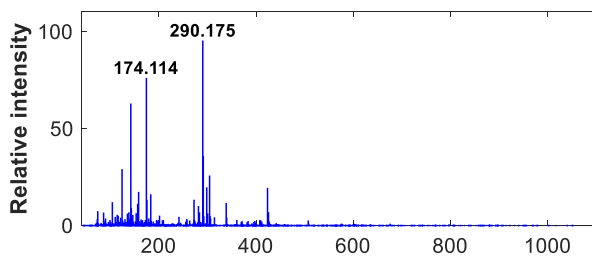
D. metel



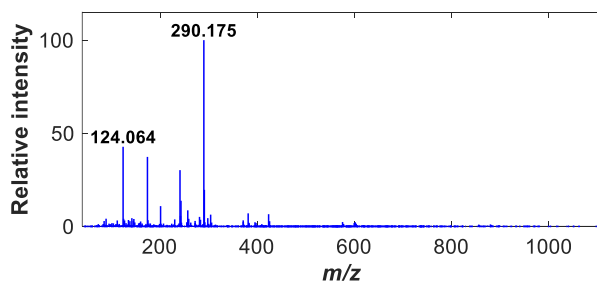
D. parajuli



D. quercifolia



D. stramonium



D. wrightii

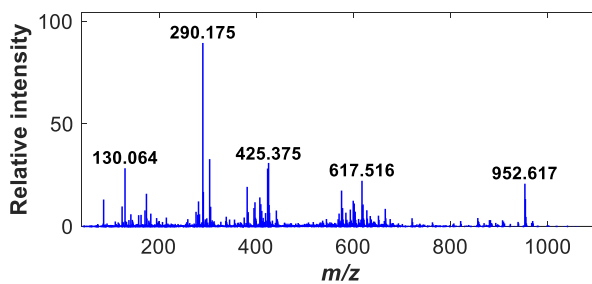
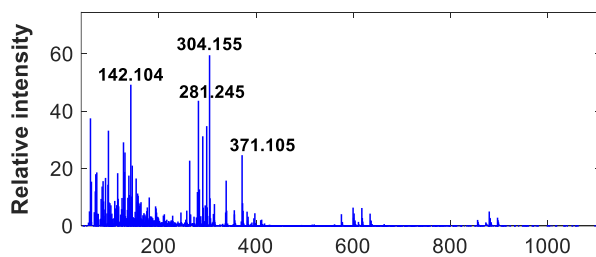
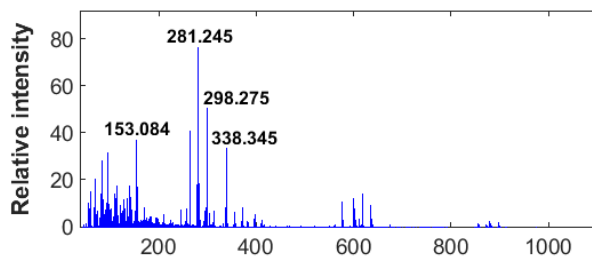


Figure S1 (continued). Representative DART high-resolution mass spectra of *D. ceratocaula*; *D. discolor*; *D. ferox*; *D. innoxia*; *D. leichhardtii*; *D. metel*; *D. parajuli*; *D. quercifolia*; *D. stramonium* and *D. wrightii*.

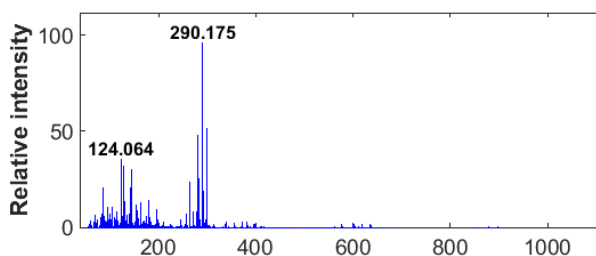
H. albus



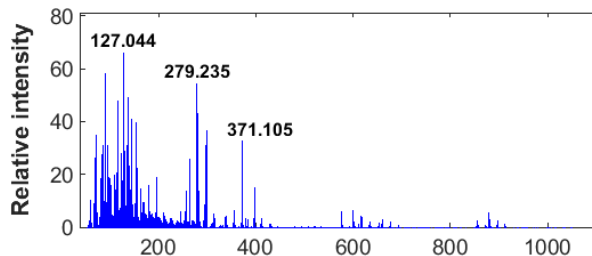
H. aureus



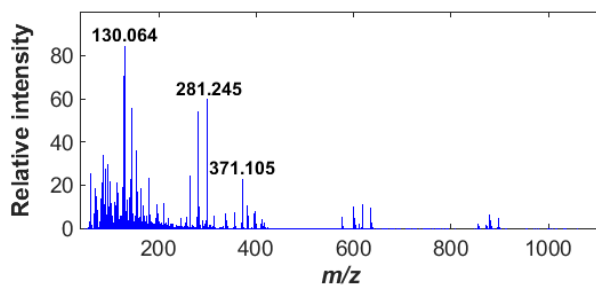
H. muticus



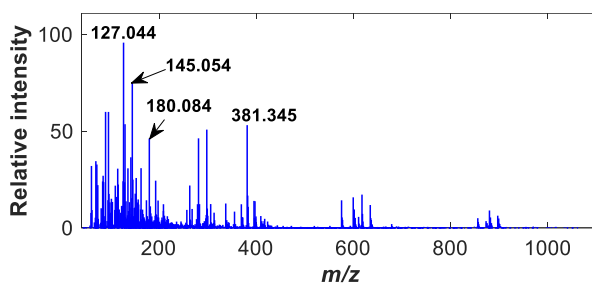
H. niger



H. pusillus



M. autumnalis



M. officinarum

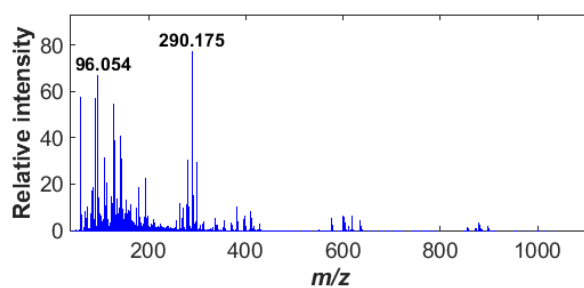


Figure S1 (continued). Representative DART high-resolution mass spectra of *H. albus*; *H. aureus*; *H. muticus*; *H. niger*; *H. pusillus*; *M. autumnalis*; and *M. officinarum*.

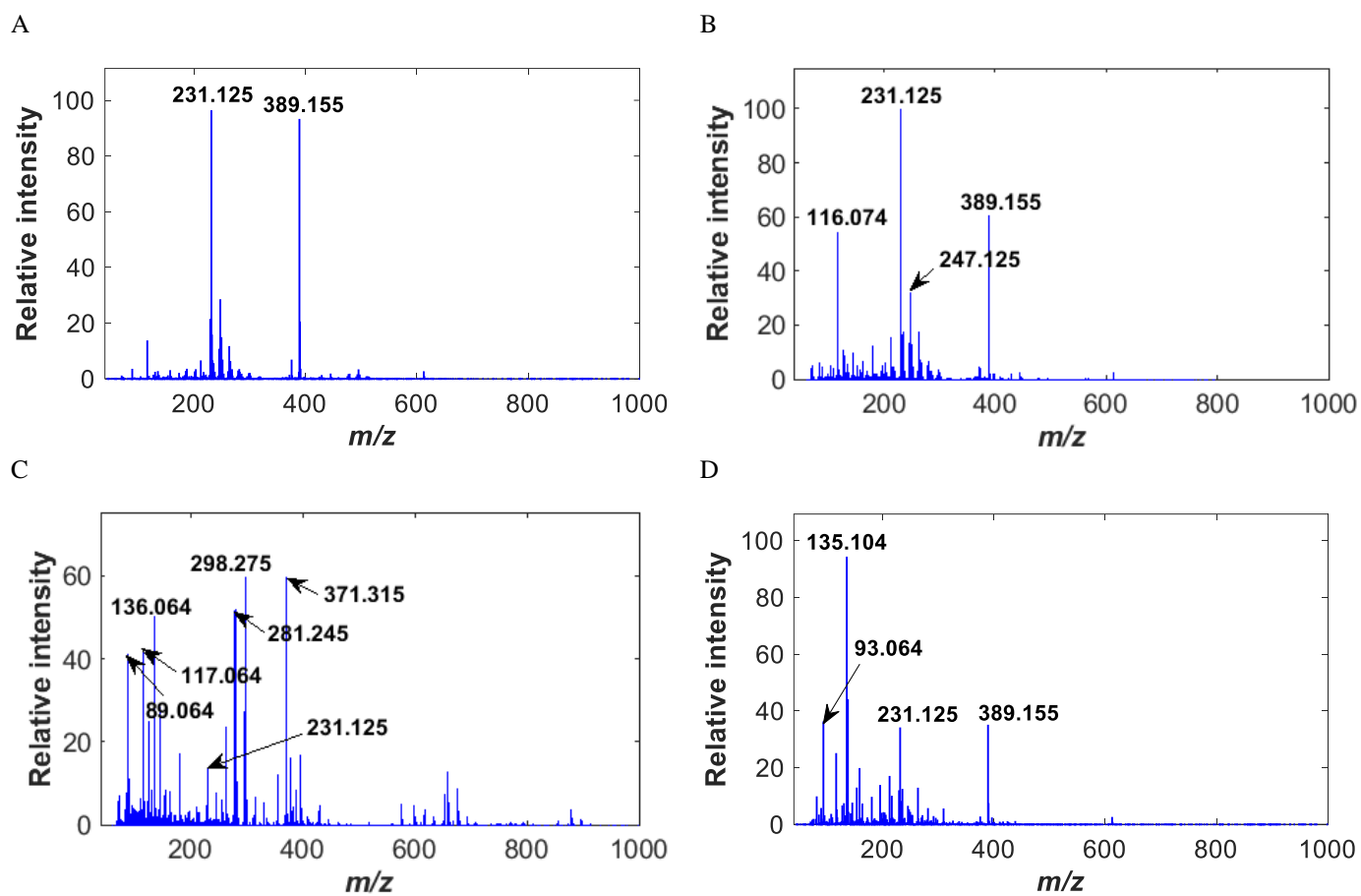


Figure S2. Representative 20 V soft ionization DART mass spectra of: (A) dried herb; (B) powder; (C) seed; and (D) tincture of *A. absinthium*.

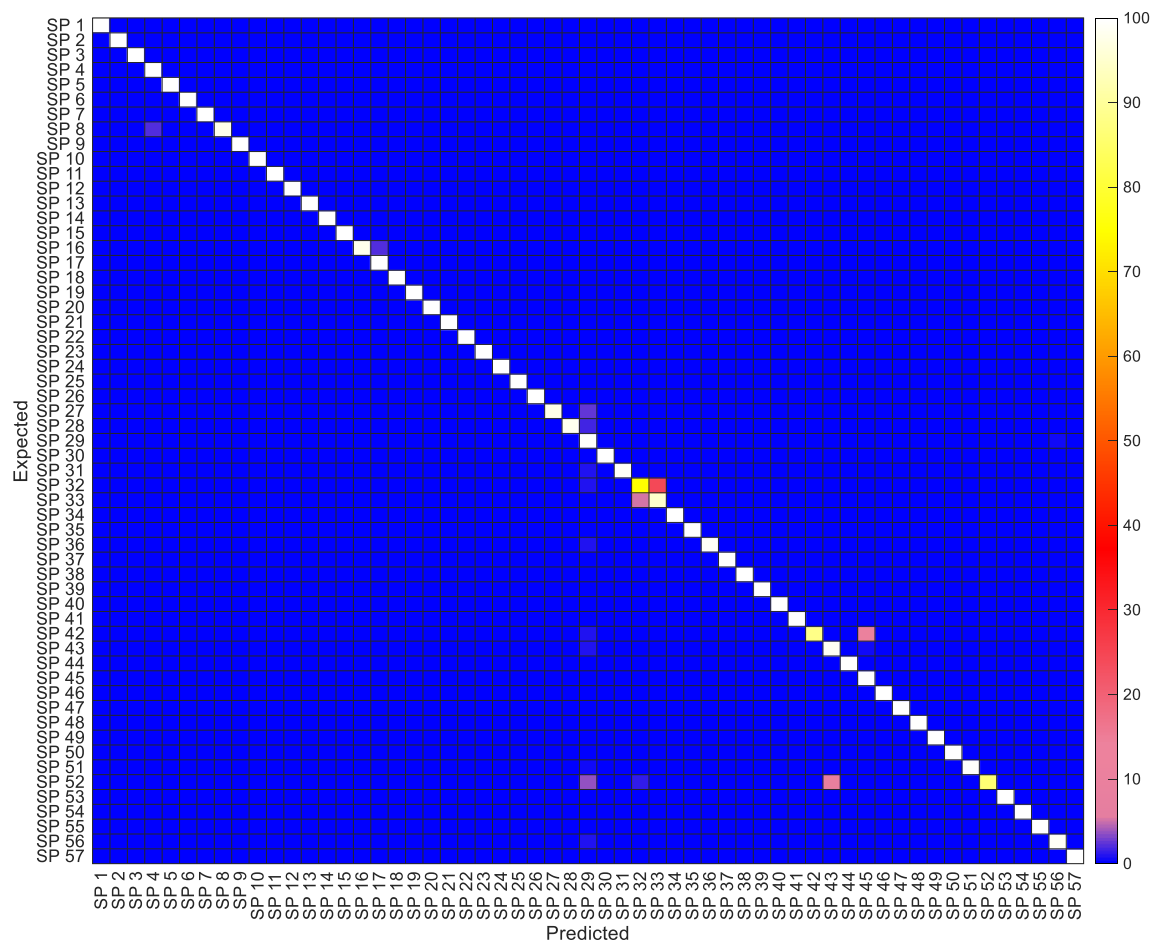


Figure S3. Normalized confusion matrix presenting the external validation results of the hierarchical classification tree. The color gradient extends from blue to white, where blue represents 0% and white presents 100% prediction rates. The x- and y-axes display the prediction and true values, respectively. Diagonal elements in the confusion matrix correspond to true positive rates and non-diagonal elements are indicative of false positive and false negative rates. Sp 1: *A. baetica*; Sp 2: *A. belladonna*; Sp 3: *A. komarovii*; Sp 4: *B. arborea*; Sp 5: *B. aurea*; Sp 6: *B. sanguinea*; Sp 7: *B. suaveolens*; Sp 8: *B. versicolor*; Sp 9: *D. ceratocaula*; Sp 10: *D. discolor*; Sp 11: *D. ferox*; Sp 12: *D. innoxia*; Sp 13: *D. leichhardtii*; Sp 14: *D. metel*; Sp 15: *D. parajuli*; Sp 16: *D. quercifolia*; Sp 17: *D. stramonium*; Sp 18: *D. wrightii*; Sp 19: *H. albus*; Sp 20: *H. aureus*; Sp 21: *H. muticus*; Sp 22: *H. niger*; Sp 23: *H. pusillus*; Sp 24: *M. autumnalis*; Sp 25: *M. officinarum*; Sp 26: *A. absinthium*; Sp 27: *A. vulgaris*; Sp 28: *C. zacatechichi*; Sp 29: *L. virosa*; Sp 30: *P. nitida*; Sp 31: *V. africana*; Sp 32: *A. nervosa*; Sp 33: *C. tricolor*; Sp 34: *I. tricolor*; Sp 35: *A. peregrina*; Sp 36: *M. hostilis*; Sp 37: *B. caapi*; Sp 38: *D. cabrerana*; Sp 39: *L. leonurus*; Sp 40: *L. sibiricus*; Sp 41: *L. nepetifolia*; Sp 42: *S. divinorum*; Sp 43: *M. speciosa*; Sp 44: *C. johimbe*; Sp 45: *P. viridis*; Sp 46: *A. officinalis*; Sp 47: *T. populnea*; Sp 48: *P. betel*; Sp 49: *P. methysticum*; Sp 50: *E. lobata*; Sp 51: *C. sativa*; Sp 52: *S. tortuosum*; Sp 53: *P. harmala*; Sp 54: *A. racemosa*; Sp 55: *S. vulgaris*; Sp 56: *N. caerulea*; Sp 57: *T. diffusa*. The confusion matrix reveals a prediction accuracy of 74.75%, 86.2% and 87.91% for Sp32, Sp42 and Sp52, respectively. These accuracies show that the model can still be considered to be well-fitted for Sp42 (dried herb, extract, powder and root) and Sp52 (leaf and extracts with different concentrations). However, it remains uncertain why the results are not as accurate for Sp32 (only in seed form).

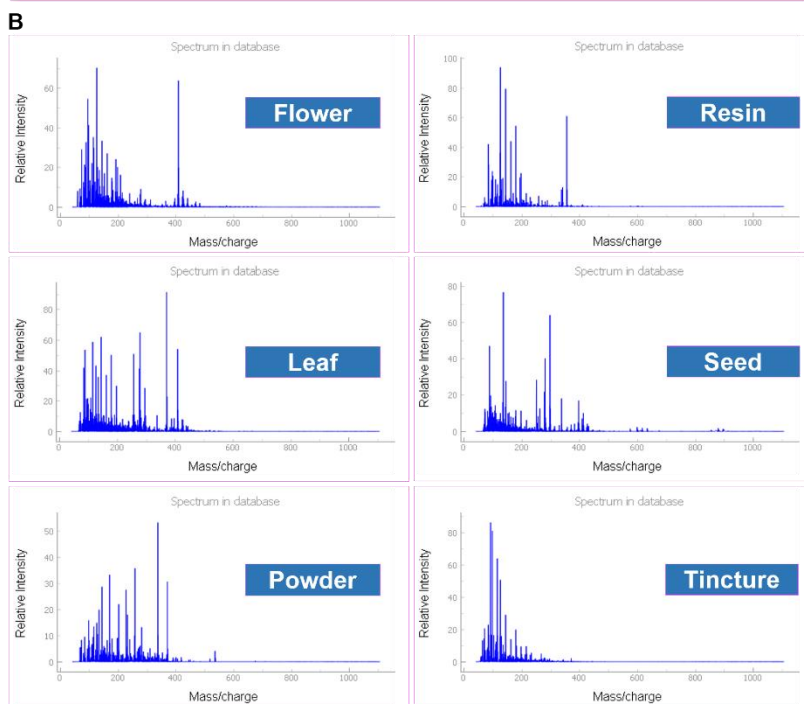
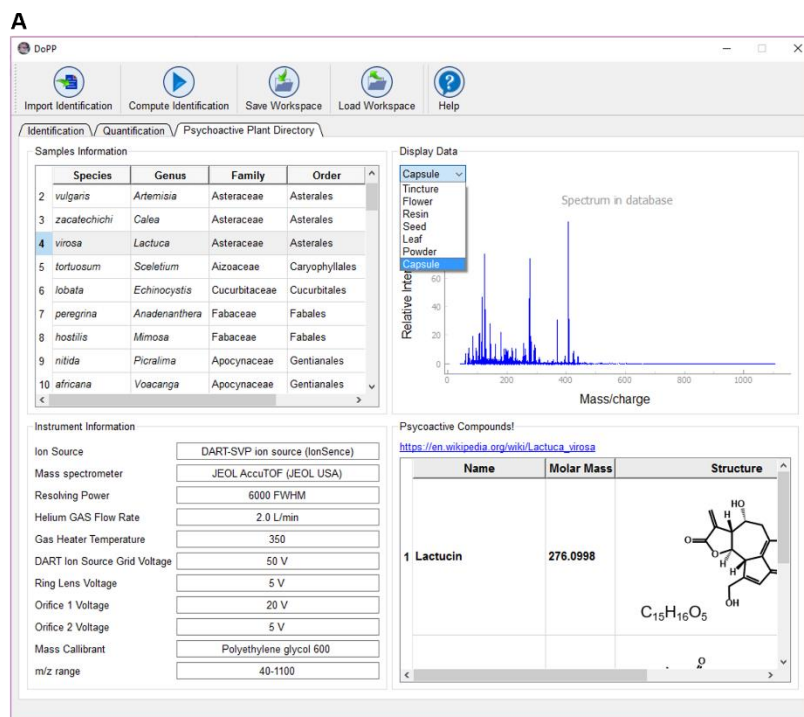


Figure S4. Illustration of the “Psychoactive plant directory” tab of DoPP. (A) Information about the *Lactuca virosa* species that is observed after right clicking on the species tab in the “Sample Information” section. The information includes: a link to the Wikipedia page describing the species and a table containing its known psychoactive components (names and structures) under “Psychoactive Compound” section; and the mass spectra of the various products derived from the species under “Display Data” section; (B) Retrieved mass spectra for *L. virosa* representing flower, resin, leaf, seed, powder and tincture forms.

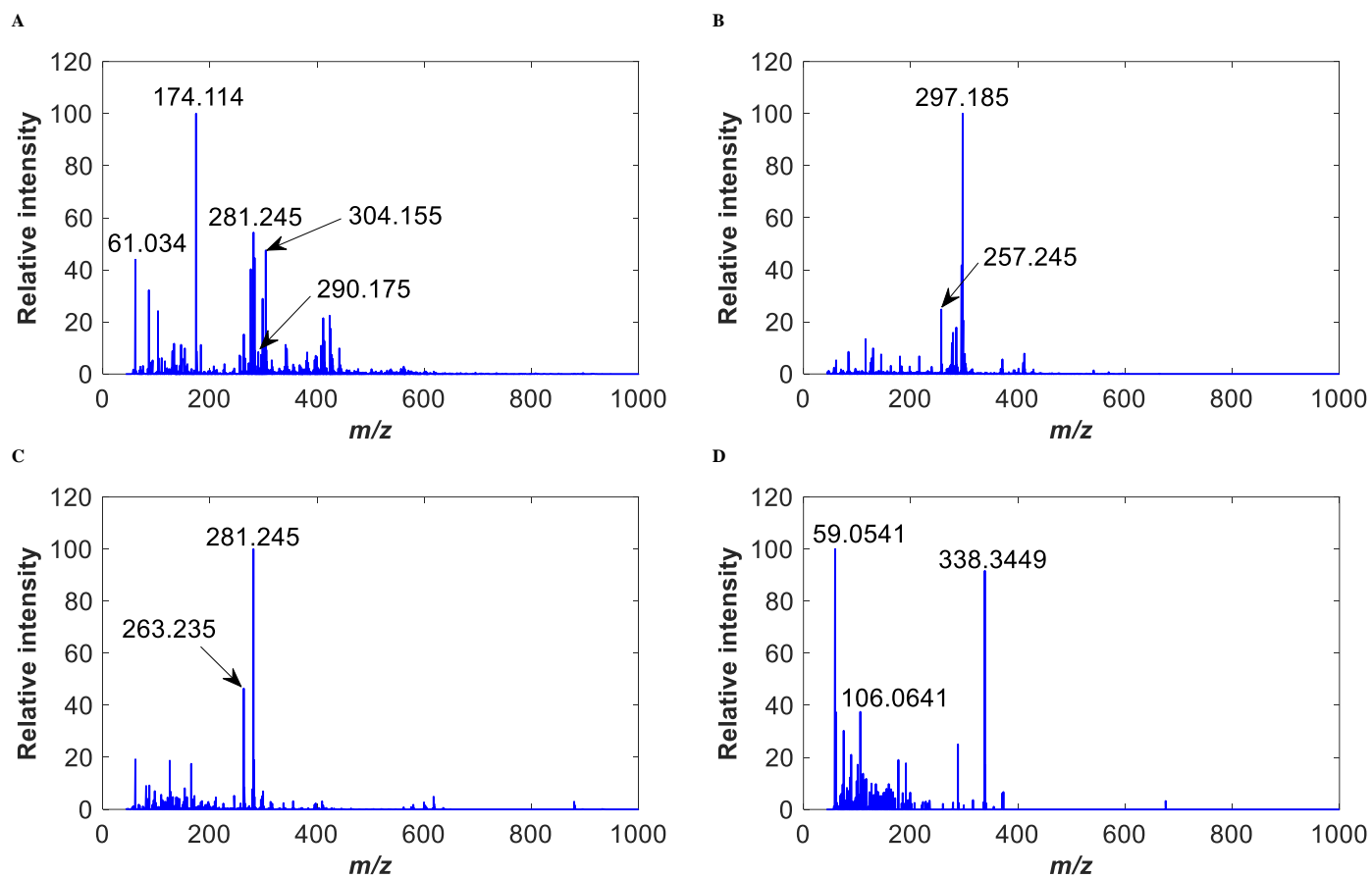


Figure S5. Representative 20 V soft ionization DART mass spectra of (A) *D. wrightii*; (B) *S. miltiorrhiza*; (C) *R. communis*; and (D) plastic bag.

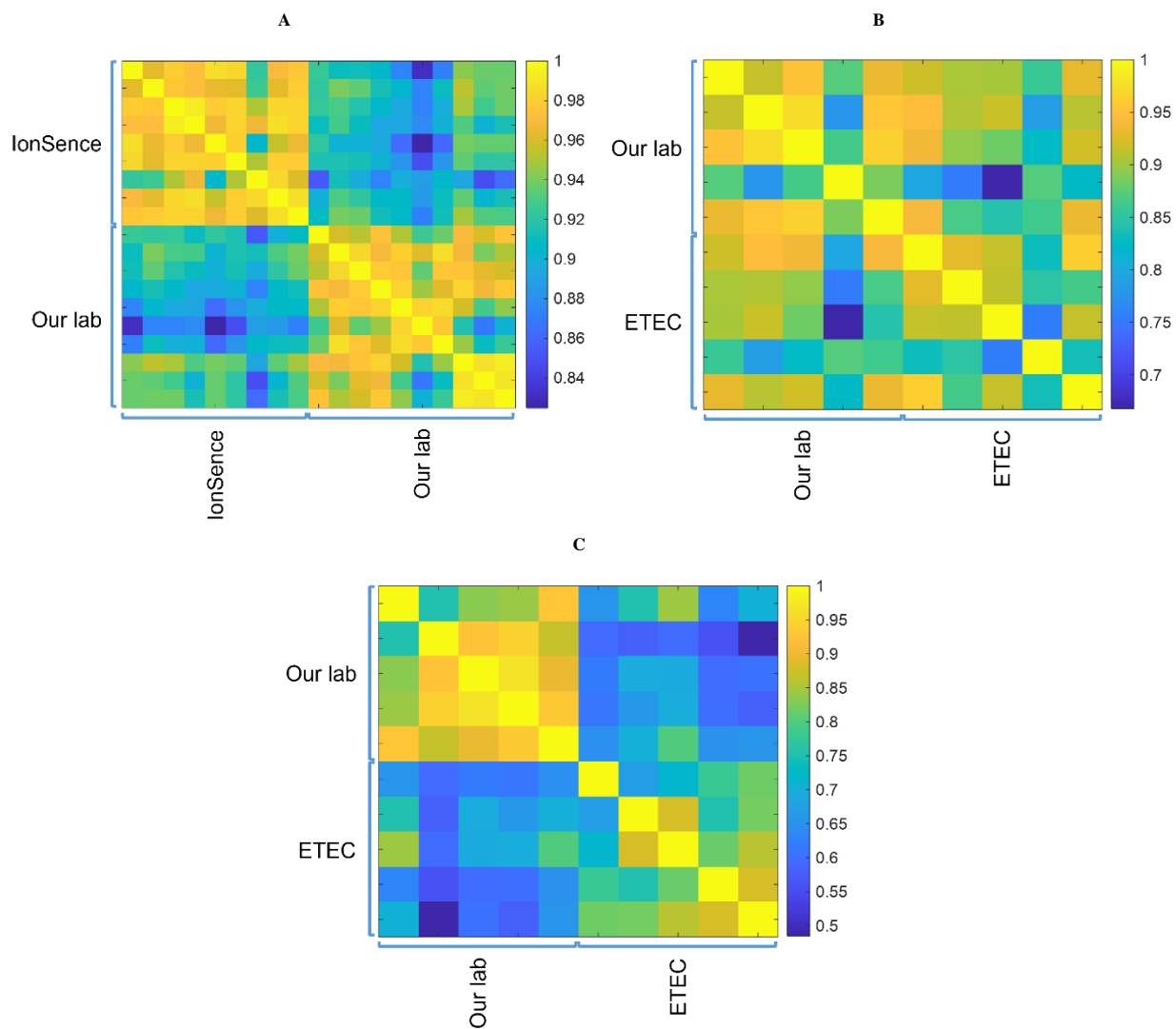


Figure S6. Pairwise inter-spectral similarities estimated using correlation coefficients. The plot illustrates the similarities between the DART-HR mass spectra of kratom (A), *D. innoxia* (B) and *D. wrightii* (C) analyzed in two different laboratories, with the brightest shade of yellow representing the highest correlation (i.e., 1) and the darkest shade of blue representing the lowest (i.e., 0.82).

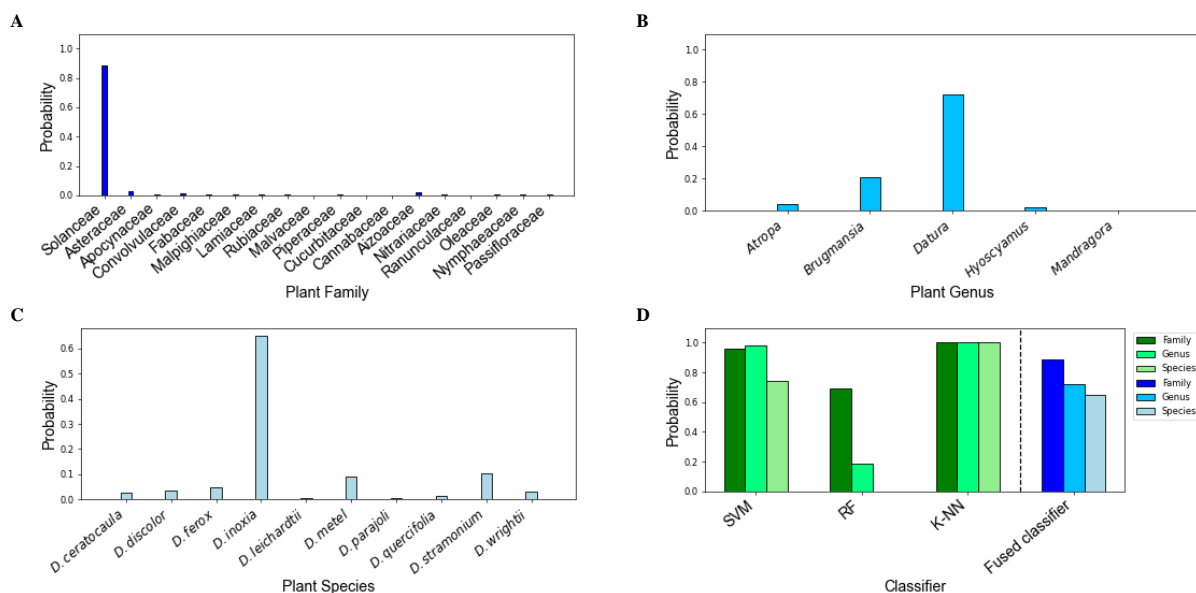


Figure S7. Identification result for *D. innoxia* seed analyzed by DART-HRMS in our laboratory. Panels A-C present three bar plots displaying the probabilities for identification of the family, genus and species levels acquired using the fused classifier; (D) Bar plot showing the probabilities associated with the identification of the family, genus, and species by the embedded classifiers (i.e., SVM, RF, K-NN and the fused classifier) in the hierarchical classification tree. DoPP identified the material as Solanaceae, *Datura*, and *innoxia* with probabilities of 0.88, 0.72, and 0.65 for the averaged spectra of three DART-HRMS replicates.

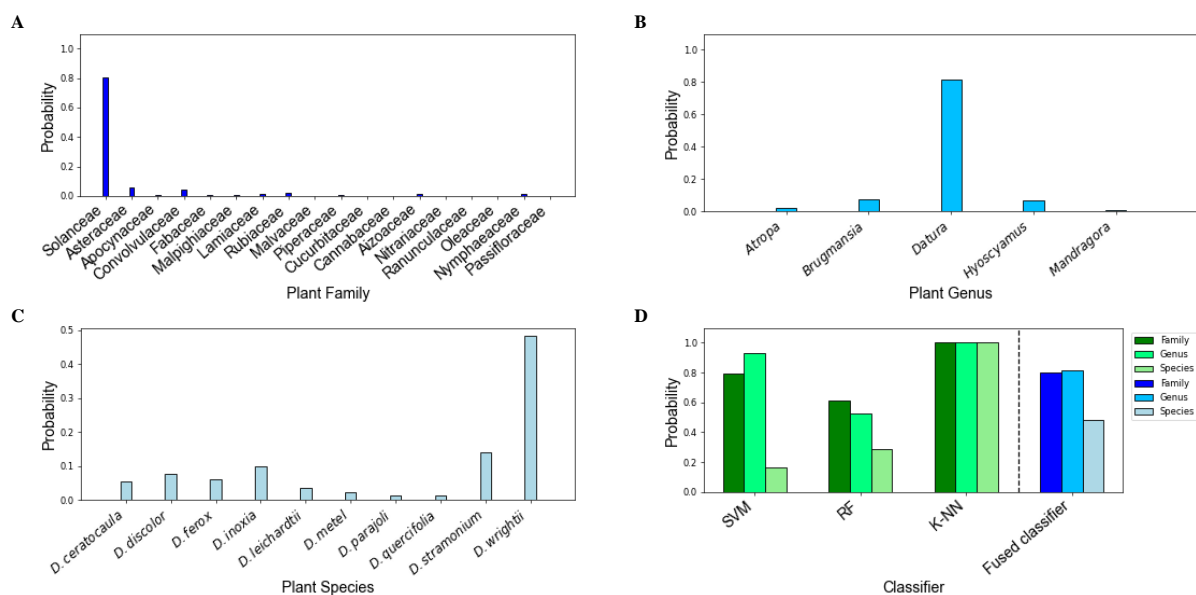


Figure S8. Identification result for *D. wrightii* seed analyzed by DART-HRMS in our laboratory. Panels A-C present three bar plots displaying the probabilities for identification of the family, genus and species levels respectively, acquired using the fused classifier; (D) Bar plot showing the probabilities associated with the identification of the family, genus, and species by the embedded classifiers (i.e., SVM, RF, K-NN and the fused classifier) in the hierarchical classification tree. DoPP identified the material as Solanaceae, *Datura*, and *wrightii* with probabilities of 0.80, 0.82, and 0.48 for the averaged spectra of three DART-HRMS replicates.

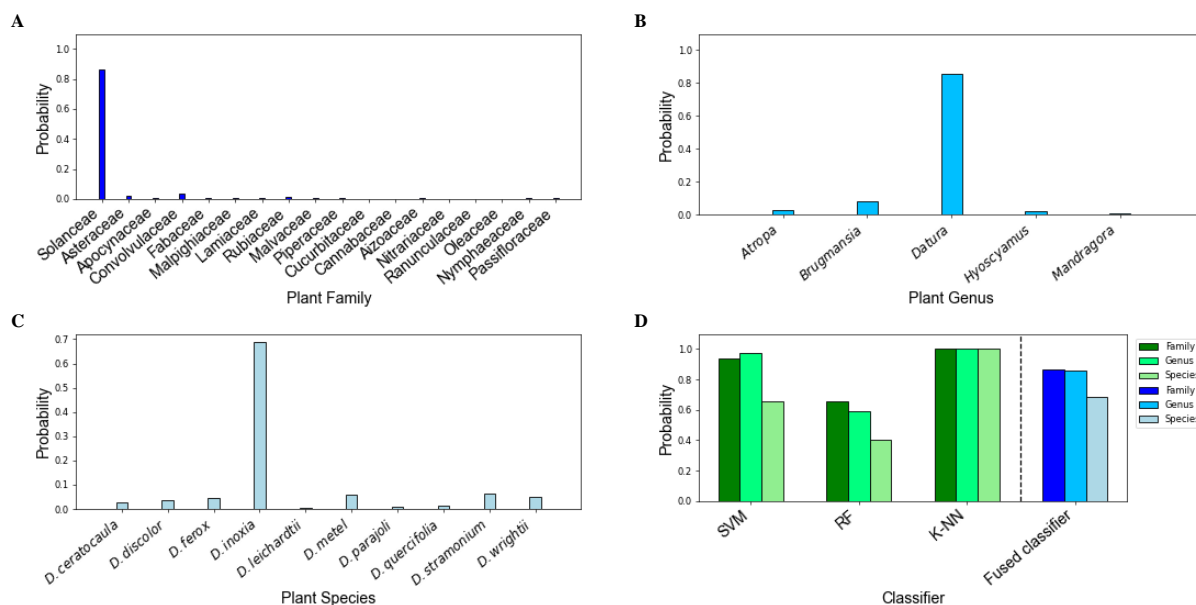


Figure S9. Identification result for *D. innoxia* seed analyzed by DART-HRMS in the ETEC laboratory. Panels A-C present three bar plots displaying the probabilities for identification of the family, genus and species levels acquired using the fused classifier; (D) Bar plot showing the probabilities associated with the identification of the family, genus, and species by the embedded classifiers (i.e., SVM, RF, K-NN and fused classifier) in the hierarchical classification tree. DoPP identified the material as Solanaceae, *Datura*, and *innoxia* with probabilities of 0.86, 0.86, and 0.69 for the averaged spectra of three replicates.

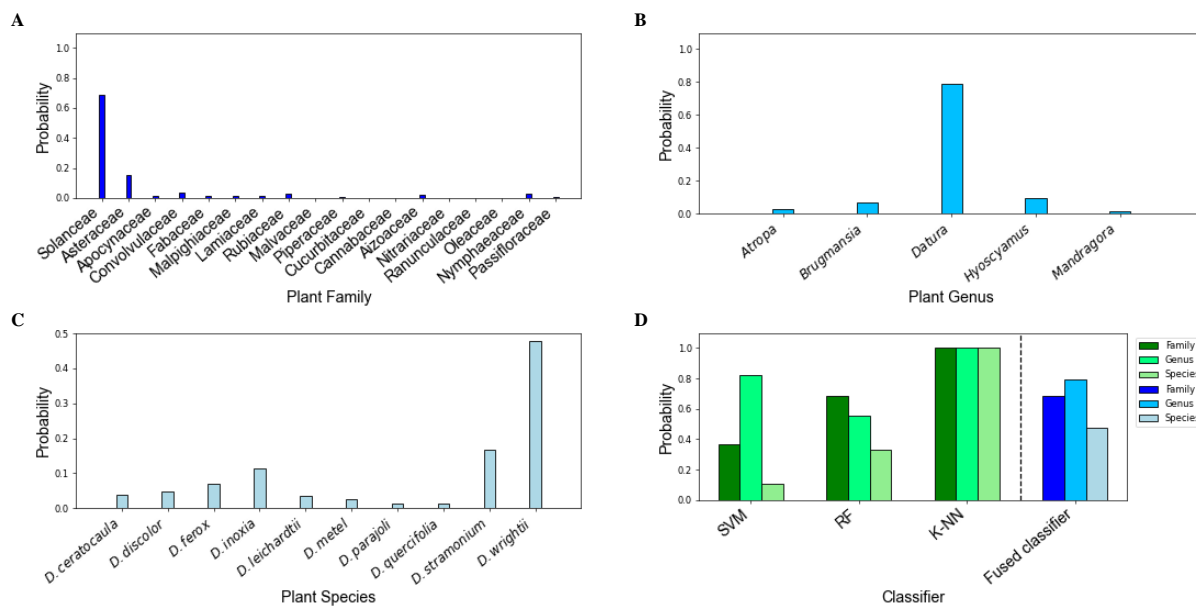


Figure S10. Identification result for *D. wrightii* seed analyzed by DART-HRMS in the ETEC laboratory. Panels A-C present three bar plots displaying the probabilities for identification of the family, genus and species levels acquired using the fused classifier; (D) Bar plot showing the probabilities associated with the identification of the family, genus, and species by the embedded classifiers (i.e., SVM, RF, K-NN and fused classifier) in the hierarchical classification tree. DoPP identified the material as Solanaceae, *Datura*, and *wrightii* with probabilities of 0.68, 0.79, and 0.48 for the averaged spectra of three replicates.

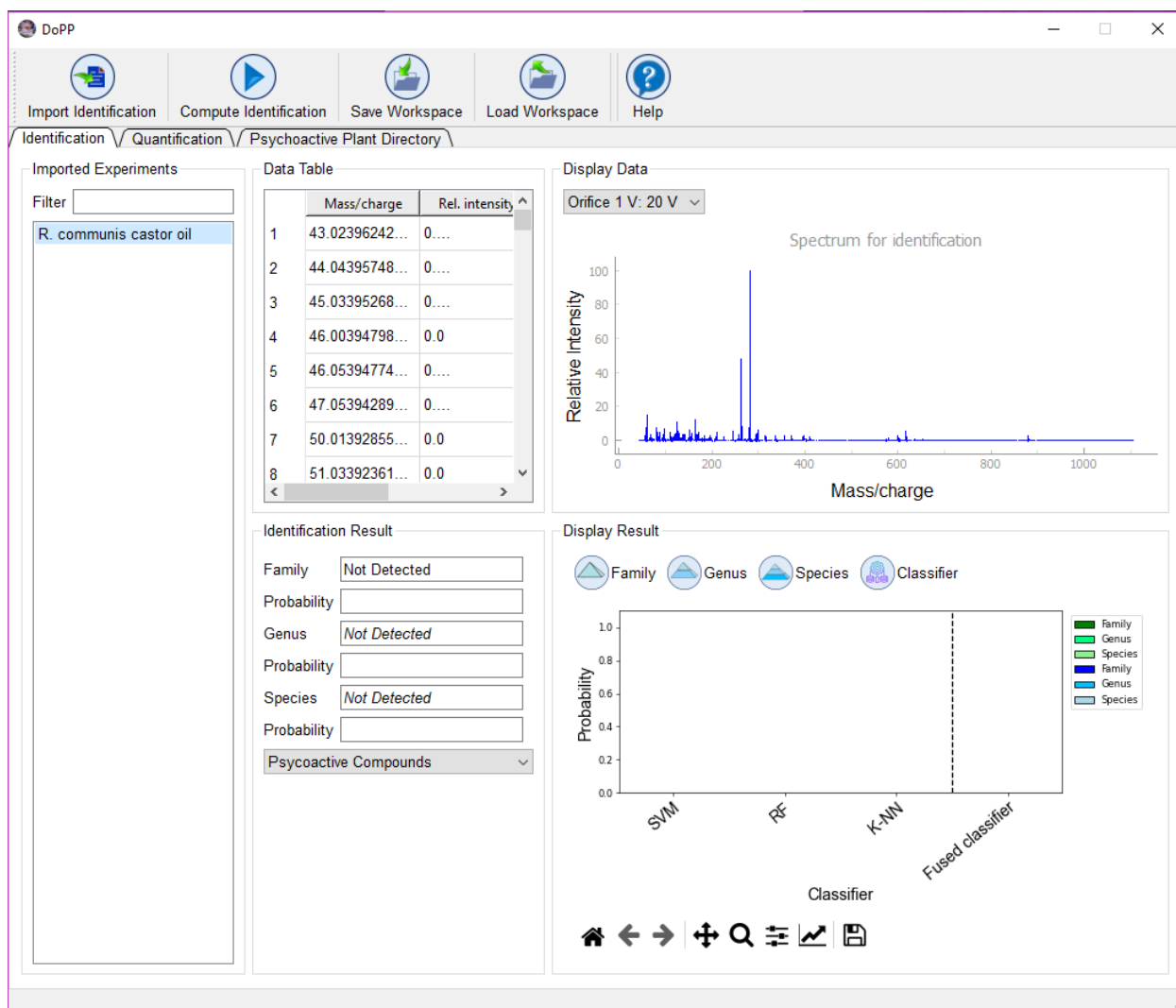


Figure S11. Identification result for *R. communis* castor oil (a species that is not represented in the database) analyzed by DART-HRMS. DoPP detected the material as an outlier and the sample is classified as “Not Detected”.

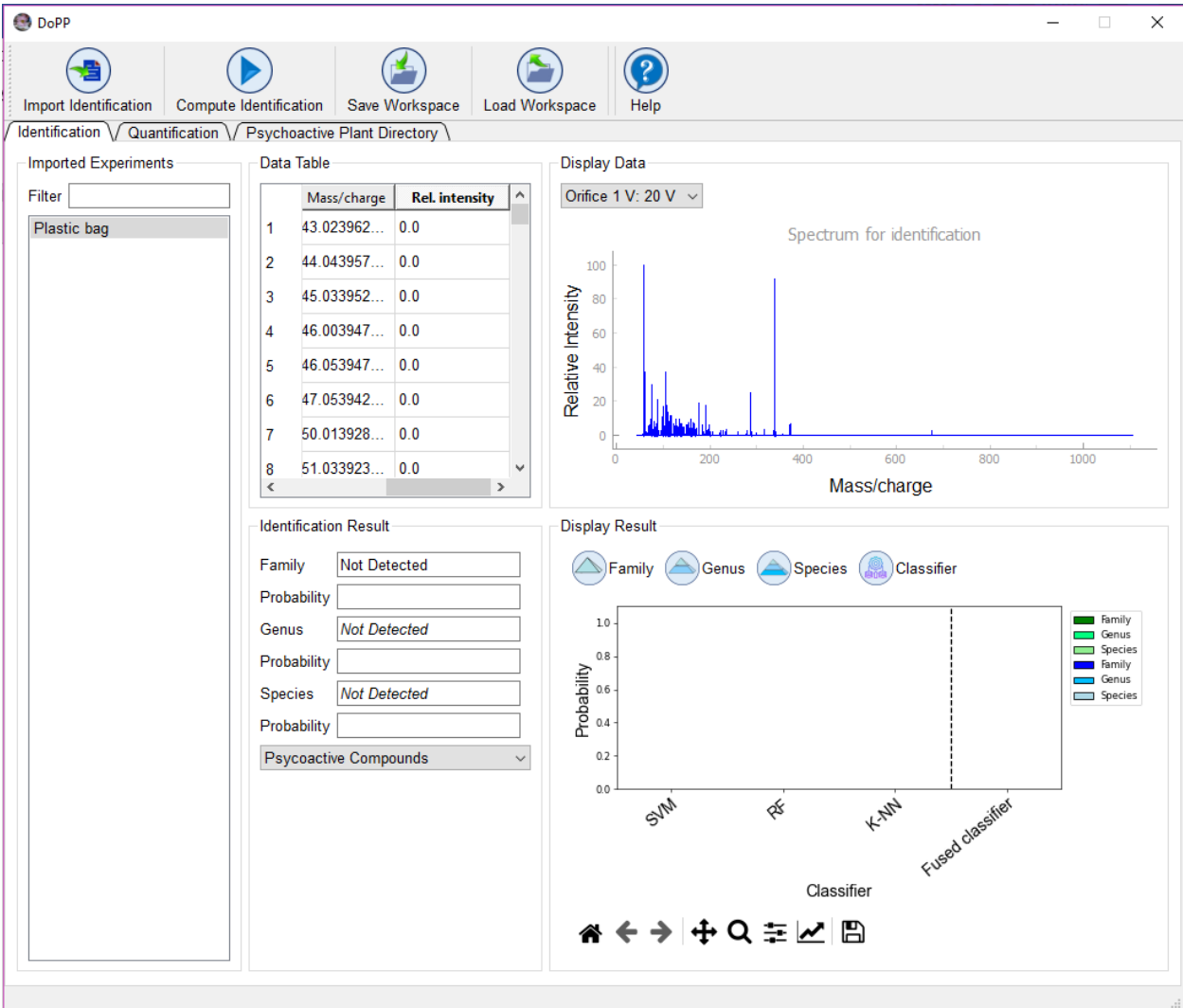
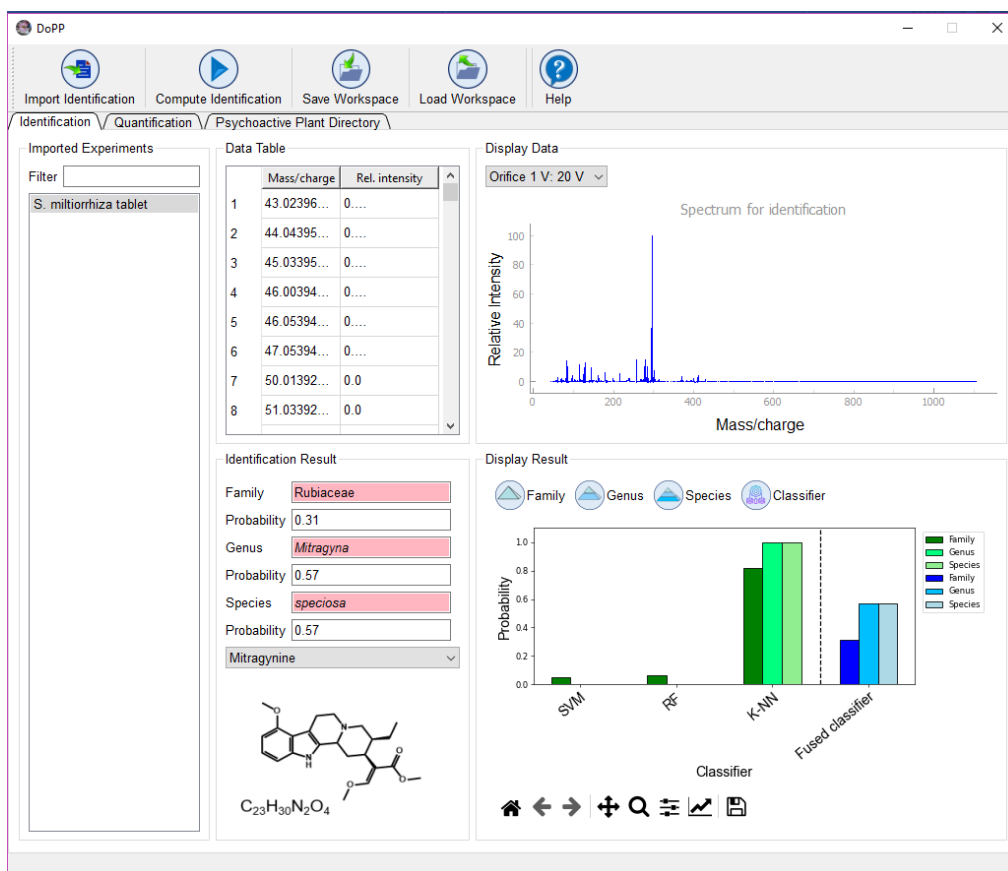
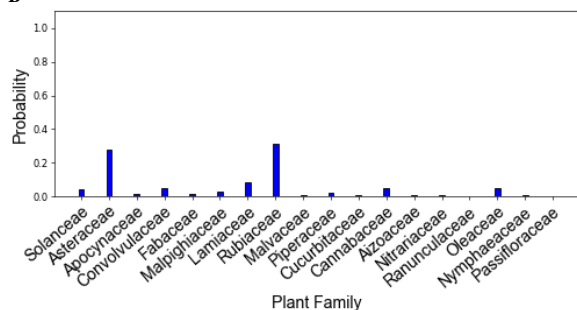


Figure S12. Identification result for plastic bag sample analyzed by DART-HRMS. DoPP detected the material as an outlier and presented the result as “Not Detected”.

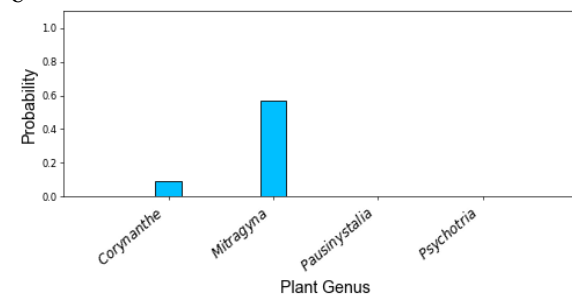
A



B



C



D

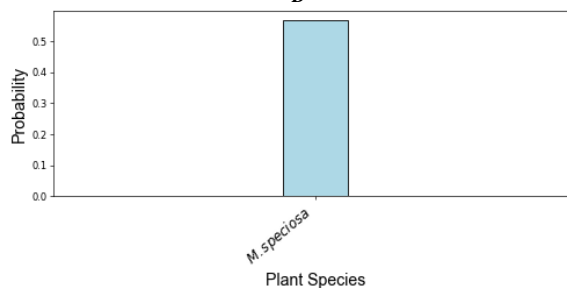
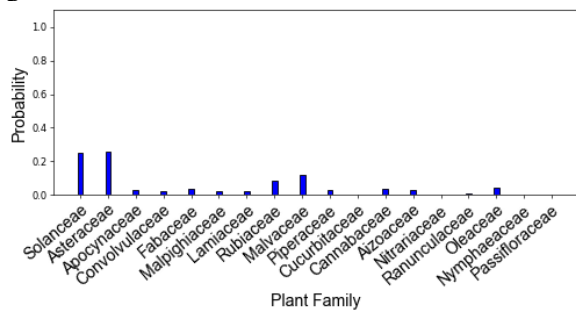


Figure S13. (A) Identification result for a *Salvia miltiorrhiza* tablet (a species that is not represented in the database) analyzed by DART-HRMS. Panels B-D present three bar plots displaying the probabilities for identification of the family, genus and species levels acquired using the fused classifier. While DoPP shows a computed result in each level, the material is suggested to be non-assigned based on the appearance of the pink background color, since the family probability is 0.31, which is lower than the computed threshold (0.45) for Rubiaceae class.

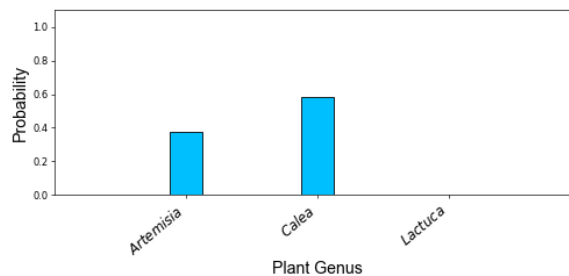
A



B



C



D

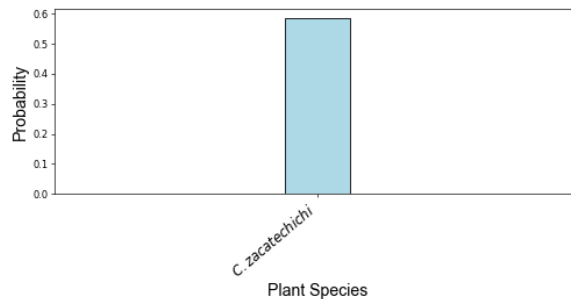


Figure 14. (A) Identification result for a *D. wrightii* spectrum that was not corrected for background following analysis by DART-HRMS. Panels B-D present three bar plots displaying the probabilities for identification of the family, genus and species levels acquired using the fused classifier. While DoPP shows a computed result at each level, it nevertheless suggests that the sample is unclassified, which is indicated by the appearance of the pink background color. This is because the probability for the family classification is lower than the threshold of 0.45 for the Rubiaceae class (with a value of 0.26).

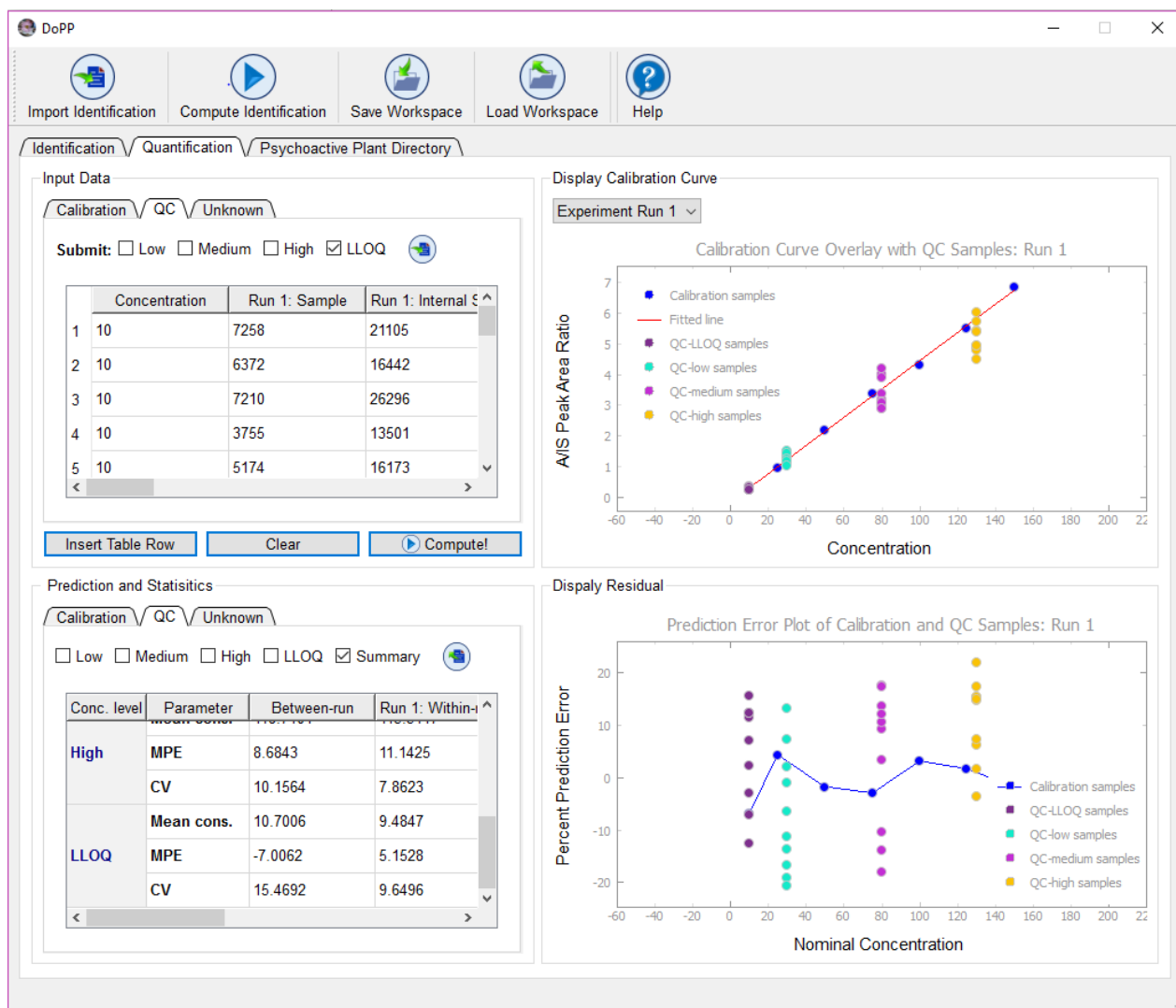
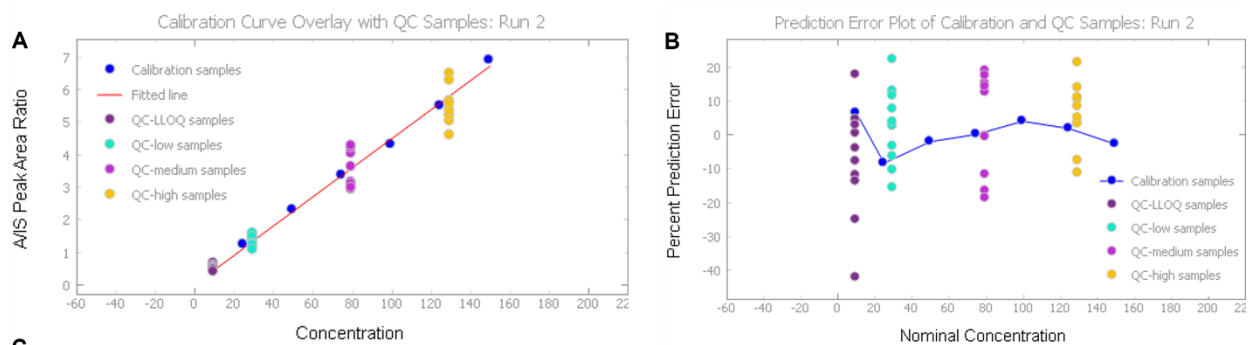


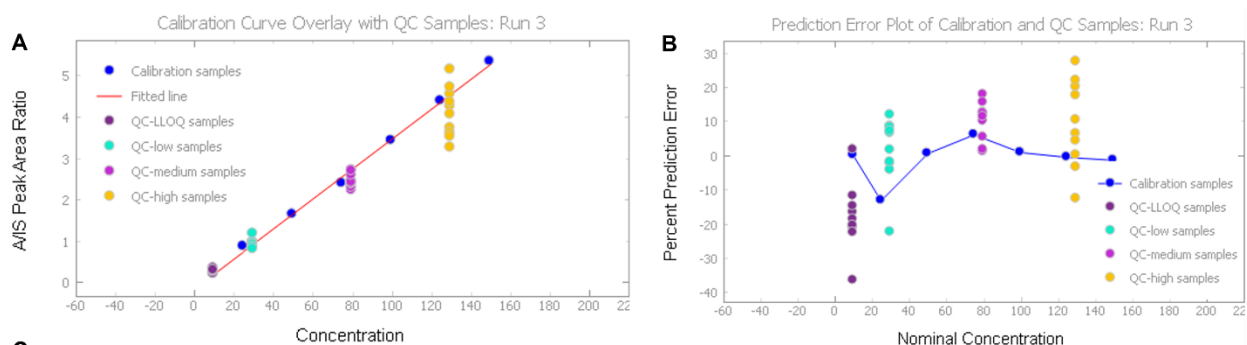
Figure S15. Illustration of DoPP for the quantification of the psychoactive component DMT. The calibrators and QC samples were imported into the application and the calculated results for the calibration curve and validation of QC samples appear in the quantification tab. Also shown is the prediction error plot with an overlay on the calibration curve of the QC samples for Run 1 of the experiment.



Regression Statistics: Run 2						
No. of calibration stds.	R-squared	Adjusted R-squared	Std. error	F-statistic	Probability	Confidence level
7	0.997	0.997	0.089	1798	0	95
Summary						
Index	Coefficient	Std. error	t-statistic	P > t	Lower limit of 95% CI*	Lower limit of 95% CI*
Intercept	0.0227	0.095	0.239	0.82	-0.221	0.267
Slope	0.0446	0.001	42.403	0	0.042	0.047
Analysis of Variance (ANOVA)						
Index	DoF**	Sum of square	Mean square	F-statistic	P > F	
Model	1	31.9959	31.9959	1797.999	0	
Residual	5	0.089	0.0178			

*CI refers to Confidence Interval; **DoF refers to Degree of Freedom.

Figure S16. Results of calibration curve analysis for Run 2 using DoPP. (A) Calibration curve; (B) prediction error plot with overlay of QC samples in Run 2; (C) Report of the goodness of fit. These are further described in the “Regression Statistics” section. The parameters for interpretation of the regression coefficients are described in the “Summary Table” section, and the ANOVA table is shown in the “Analysis of Variance (ANOVA)” section of the manuscript.



Regression Statistics: Run 3						
No. of calibration stds.	R-squared	Adjusted R-squared	Std. error	F-statistic	Probability	Confidence level
8	0.997	0.997	0.0736	2190	0	95
Summary						
Index	Coefficient	Std. error	t-statistic	P > t	Lower limit of 95% CI*	Lower limit of 95% CI*
Intercept	-0.0954	0.064	-1.486	0.188	-0.252	0.062
Slope	0.0356	0.001	46.792	0	0.034	0.037
Analysis of Variance (ANOVA)						
Index	DoF**	Sum of square	Mean square	F-statistic	P > F	
Model	1	26.8483	26.8483	2189.523	0	
Residual	6	0.0736	0.0123			

*CI refers to Confidence Interval; **DoF refers to Degree of Freedom.

Figure S17. Results of calibration curve analysis for Run 3 using DoPP. (A) Calibration curve; (B) prediction error plot with overlay of QC samples in Run 3; (C) Report of the goodness of fit. These are further described in the “Regression Statistics” section. The parameters for interpretation of the regression coefficients are described in the “Summary Table” section, and the ANOVA table is shown in the “Analysis of Variance (ANOVA)” section of the manuscript.

Supporting Tables.

Table S1. Plant materials analyzed and related taxonomical information including order, family, genus, and species, and the matrix of each.

Index	Order	Family	Genus	Species	Matrix	Vendor					
1	Asterales	Asteraceae	<i>Artemisia</i>	<i>absinthium</i>	Dried herb	Brewer's Best Salem					
					Powder	Penn Herb Co. Ltd.					
					Seed	Strictly Medicinal Seeds					
					Tincture	Herb Pharm Starwest Botanicals					
2	Asterales	Asteraceae	<i>Artemisia</i>	<i>vulgaris</i>	Seed	World Seed Supply					
3	Asterales	Asteraceae	<i>Calea</i>	<i>zacatechichi</i>	Leaf	World Seed Supply					
					Seed pod	World Seed Supply					
					Seed	World Seed Supply					
					Syrup	Hawaii Pharm					
					Tincture	Hawaii Pharm					
4	Asterales	Asteraceae	<i>Lactuca</i>	<i>virosa</i>	Capsule	Swanson					
					Leaf	Mr. Botanicals Schmerbals Herbals World Seed Supply					
						Powder	Mr. Botanicals Schmerbals Herbal World Seed Supply				
							Resin	World Seed Supply			
					Seed	Schmerbals Herbal World Seed Supply					
					Tincture	Schmerbals Herbal					
					5	Caryophyllales	Aizoaceae	<i>Sceletium</i>	<i>tortuosum</i>	Dried herb	eBay Herb Stomp Schmerbals Herbal World Seed Supply
											Extract
Powder	Herb Stomp World Seed Supply										
	Root	eBay									
6	Cucurbitales	Cucurbitaceae	<i>Echinocystis</i>	<i>lobata</i>						Seed	Prairie Moon Nursery
7	Fabales	Fabaceae	<i>Anadenanthera</i>	<i>peregrina</i>	Seed	Herbal Flame World Seed Supply					
						8	Fabales	Fabaceae	<i>Mimosa</i>	<i>hostilis</i>	Bark
Powder	Heavenly Products										
Root	Unknown										
Seed	Heavenly Products										

Table S1 (continued). Plant materials analyzed and related taxonomical information including order, family, genus, and species, and the matrix of each.

Index	Order	Family	Genus	Species	Matrix	Vendor
9	Gentianales	Apocynaceae	<i>Picralima</i>	<i>nitida</i>	Powder	World Seed Supply
					Seed	World Seed Supply
10	Gentianales	Apocynaceae	<i>Voacanga</i>	<i>africana</i>	Bark	World Seed Supply
					Powder	Amazon
						Om-Chi
Seed	World Seed Supply					
11	Gentianales	Rubiaceae	<i>Mitragyna</i>	<i>speciosa</i>	Capsule	Kratom Crazy
					Leaf	Kratom King
					Powder	Authentic Kratom
Herbal Flame						
					Kratom Underground	
12	Gentianales	Rubiaceae	<i>Corynanthe</i>	<i>johimbe</i>	Bark	Bouncing Bear Botanicals
13	Gentianales	Rubiaceae	<i>Psychotria</i>	<i>viridis</i>	Leaf	Mr. Botanicals
					Powder	USA Botanicals
					Seed	World Seed Supply
14	Lamiales	Lamiaceae	<i>Leonotis</i>	<i>leonurus</i>	Extract	Schmerbals Herbs
					Flower	World Seed Supply
					Leaf	Herbal Fire Botanicals
					Powder	Herbal Fire Botanicals
15	Lamiales	Lamiaceae	<i>Leonotis</i>	<i>nepetifolia</i>	Flower	Schmerbals Herbs
16	Lamiales	Lamiaceae	<i>Leonurus</i>	<i>sibiricus</i>	Extract	Mr. Botanicals
17	Lamiales	Lamiaceae	<i>Salvia</i>	<i>divinorum</i>	Leaf	Arena Ethnobotanicals
						Salvia Dragon
18	Lamiales	Oleaceae	<i>Syringa</i>	<i>vulgaris</i>	Leaf	Unknown
19	Malpighiales	Malpighiaceae	<i>Banisteriopsis</i>	<i>caapi</i>	Leaf	World Seed Supply
					Powder	World Seed Supply
					Rootbark	World Seed Supply
					Seed	World Seed Supply
20	Malpighiales	Malpighiaceae	<i>Diplopterys</i>	<i>cabrerana</i>	Leaf	Herbal Flame
					Powder	USA Botanicals
21	Malpighiales	Passifloraceae	<i>Turnera</i>	<i>diffusa</i>	Capsule	Penn Herb Co. Ltd.
					Extract	Strictly Medicinal Seeds
					Leaf	Bouncing Bear Botanicals
						Monterey Bay Spice Co.
Powder	Monterey Bay Spice Co.					

Table S1 (continued). Plant materials analyzed and related taxonomical information including order, family, genus, and species, and the matrix of each.

Index	Order	Family	Genus	Species	Matrix	Vendor
22	Malvales	Malvaceae	<i>Althaea</i>	<i>officinalis</i>	Leaf	Bouncing Bear Botanicals
						World Seed Supply
23	Malvales	Malvaceae	<i>Thespesia</i>	<i>populnea</i>	Seeds	Amazon
24	Nymphaeales	Nymphaeaceae	<i>Nymphaea</i>	<i>caerulea</i>	Extract	Unknown
					Flower	Schmerbals Herbals
					Leaves	World Seed Supply
					Powder	Herb Stomp
						Lotus Extracts
					Resin	Etsy (Schmerbals Herbals)
					Seed	World Seed Supply
Tincture	World Seed Supply					
25	Piperales	Piperaceae	<i>Piper</i>	<i>betel</i>	Leaf	Live Plant
					Essential Oil	Healing Solutions
26	Piperales	Piperaceae	<i>Piper</i>	<i>methysticum</i>	Capsule	Starwest Botanicals
					Powder	Bouncing Bear Botanicals
						World Seed Supply
					Root	Bouncing Bear Botanicals
					Tincture	Herbal Island
Root of Happiness						
	Happy Kava Brand					
27	Ranunculales	Ranunculaceae	<i>Actaea</i>	<i>racemosa</i>	Root	Bouncing Bear Botanicals
28	Rosales	Cannabaceae	<i>Cannabis</i>	<i>sativa</i>	Flower	Berkshire CBD
						Plain Jane
						Stewart Rose Farms
29	Sapindales	Nitrariaceae	<i>Peganum</i>	<i>harmala</i>	Capsule	Herb Stomp
					Seed	World Seed Supply
					Powder	Waking Herbs
30	Solanales	Convolvulaceae	<i>Argyreia</i>	<i>nervosa</i>	Seed	World Seed Supply
31	Solanales	Convolvulaceae	<i>Convolvulus</i>	<i>tricolor</i>	Seed	World Seed Supply
32	Solanales	Convolvulaceae	<i>Ipomoea</i>	<i>tricolor</i>	Seed	World Seed Supply
33	Solanales	Solanaceae	<i>Atropa</i>	<i>baetica</i>	Seed	eBay
34	Solanales	Solanaceae	<i>Atropa</i>	<i>belladonna</i>	Seed	World Seed Supply
					Extract	Hawaii Pharm
35	Solanales	Solanaceae	<i>Atropa</i>	<i>komarovii</i>	Seed	Strictly Medicinal Seeds

Table S1 (continued). Plant materials analyzed and related taxonomical information including order, family, genus, and species, and the matrix of each.

Index	Order	Family	Genus	Species	Matrix	Vendor
36	Solanales	Solanaceae	<i>Brugmansia</i>	<i>arborea</i>	Seed	Georgia Vines
37	Solanales	Solanaceae	<i>Brugmansia</i>	<i>aurea</i>	Seed	Seedman's
38	Solanales	Solanaceae	<i>Brugmansia</i>	<i>sanguinea</i>	Seed	Seedman's
39	Solanales	Solanaceae	<i>Brugmansia</i>	<i>suaveolens</i>	Seed	Seedman's
40	Solanales	Solanaceae	<i>Brugmansia</i>	<i>versicolor</i>	Seed	Seedman's
41	Solanales	Solanaceae	<i>Datura</i>	<i>ceratocaula</i>	Seed	World Seed Supply
						Georgia Vines
						Hudson
42	Solanales	Solanaceae	<i>Datura</i>	<i>discolor</i>	Seed	World Seed Supply
						Hudson
43	Solanales	Solanaceae	<i>Datura</i>	<i>ferox</i>	Seed	World Seed Supply
						Georgia Vines
44	Solanales	Solanaceae	<i>Datura</i>	<i>innoxia</i>	Seed	World Seed Supply
						Georgia Vines
						Horizon Herbs
45	Solanales	Solanaceae	<i>Datura</i>	<i>leichhardtii</i>	Seed	Hudson
46	Solanales	Solanaceae	<i>Datura</i>	<i>metel</i>	Seed	Georgia Vines
47	Solanales	Solanaceae	<i>Datura</i>	<i>parajuli</i>	Seed	Georgia Vines
48	Solanales	Solanaceae	<i>Datura</i>	<i>quercifolia</i>	Seed	Hirts Gardens
49	Solanales	Solanaceae	<i>Datura</i>	<i>stramonium</i>	Seed	World Seed Supply
						Hudson
						Horizon Herbs
					Georgia Vines	
					Powder	Amazon Shopping Universe
50	Solanales	Solanaceae	<i>Datura</i>	<i>wrightii</i>	Seed	Georgia Vines
						Hudson
51	Solanales	Solanaceae	<i>Hyocyamus</i>	<i>albus</i>	Seed	eBay
52	Solanales	Solanaceae	<i>Hyocyamus</i>	<i>aureus</i>	Seed	eBay
53	Solanales	Solanaceae	<i>Hyocyamus</i>	<i>muticus</i>	Seed	eBay
54	Solanales	Solanaceae	<i>Hyocyamus</i>	<i>niger</i>	Seed	Horizon Herbs
						Amazon
55	Solanales	Solanaceae	<i>Hyocyamus</i>	<i>pusillus</i>	Seed	eBay
56	Solanales	Solanaceae	<i>Mandragora</i>	<i>autumnalis</i>	Seed	Amazon
57	Solanales	Solanaceae	<i>Mandragora</i>	<i>officinarum</i>	Seed	eBay

Table S2. Known molecules of interest in the indicated species.

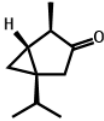
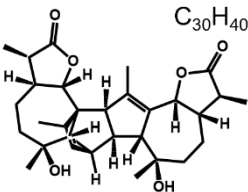
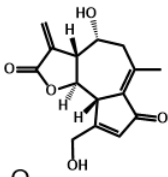
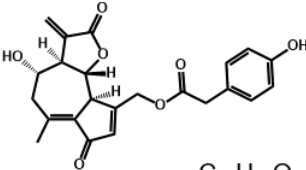
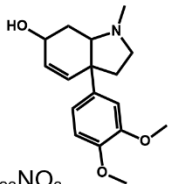
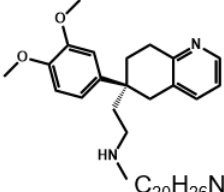
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
1	<i>A. absinthium</i>	(-)-thujone	152.1201	 $C_{10}H_{16}O$
		Absinthin	496.2824	 $C_{30}H_{40}O_6$
2	<i>A. vulgaris</i>	None	None	None
3	<i>C. zacatechichi</i>	Sesquiterpene alkaloids	-----	-----
		Caleicines	-----	-----
		Caleochromenes	-----	-----
4	<i>L. virosa</i>	Lactucin	276.0998	 $C_{15}H_{16}O_5$
		Lactucopicrin	410.1366	 $C_{23}H_{22}O_7$
5	<i>S. tortuosum</i>	Mesembrenol	289.1678	 $C_{17}H_{23}NO_3$
		Tortuosamine	326.1994	 $C_{20}H_{26}N_2O_2$

Table S2 (continued). Known molecules of interest in the indicated species.

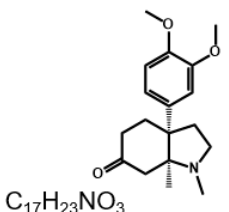
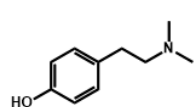
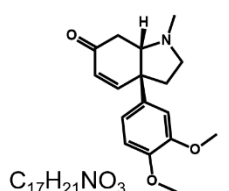
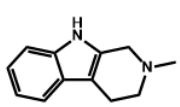
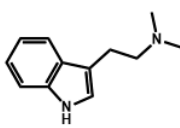
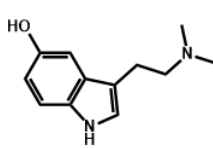
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
5	<i>S. tortuosum</i>	Mesembrine	289.1678	 <chem>C17H23NO3</chem>
		Hordenine	165.1154	 <chem>C10H15NO</chem>
		Mesembrenone	287.1521	 <chem>C17H21NO3</chem>
6	<i>E. lobata</i>	None	None	None
7	<i>A. peregrina</i>	2-Methyltryptoline	186.1157	 <chem>C12H14N2</chem>
		<i>N,N</i> -Dimethyltryptamine (DMT)	188.1313	 <chem>C12H16N2</chem>
		Bufotenin	204.1263	 <chem>C12H16N2O</chem>

Table S2 (continued). Known molecules of interest in the indicated species.

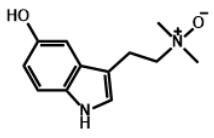
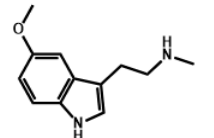
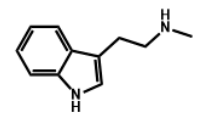
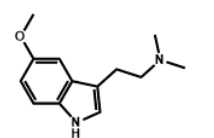
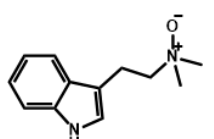
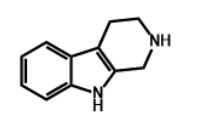
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
7	<i>A. peregrina</i>	Bufotenin-oxide	220.1212	 <chem>C12H16N2O2</chem>
		5-Methoxy- <i>N</i> -methyltryptamine	204.1263	 <chem>C12H16N2O</chem>
		<i>N</i> -Methyltryptamine	174.1157	 <chem>C11H14N2</chem>
		5-Methoxy DMT	218.1419	 <chem>C13H18N2O</chem>
		DMT-oxide	204.1263	 <chem>C12H16N2O</chem>
		Tryptoline	172.1000	 <chem>C11H12N2</chem>

Table S2 (continued). Known molecules of interest in the indicated species.

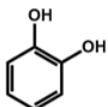
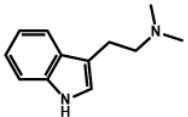
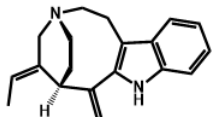
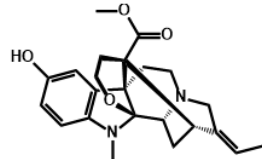
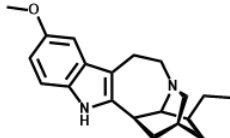
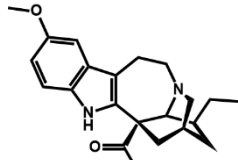
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
7	<i>A. peregrina</i>	Catechol	110.0368	 <chem>Oc1ccccc1O</chem> $C_6H_6O_2$
8	<i>M. hostilis</i>	<i>N,N</i> -Dimethyltryptamine (DMT)	188.1313	 <chem>CN(C)CCc1c[nH]c2ccccc12</chem> $C_{12}H_{16}N_2$
9	<i>P. nitida</i>	Pericine	278.1783	 <chem>CN1CC[C@H]2C[C@@H]3C[C@H]1C[C@@H]2C=C3</chem> $C_{19}H_{22}N_2$
		Akuammine	382.1893	 <chem>CN1CC[C@H]2C[C@@H]3C[C@H]1C[C@@H]2C=C3C(=O)O</chem> $C_{22}H_{26}N_2O_4$
10	<i>V. africana</i>	Ibogaine	310.2045	 <chem>CN1CC[C@H]2C[C@@H]3C[C@H]1C[C@@H]2C=C3OC</chem> $C_{20}H_{26}N_2O$
		Voacangine	368.2100	 <chem>CN1CC[C@H]2C[C@@H]3C[C@H]1C[C@@H]2C=C3OC(=O)OC</chem> $C_{22}H_{28}N_2O_3$

Table S2 (continued). Known molecules of interest in the indicated species.

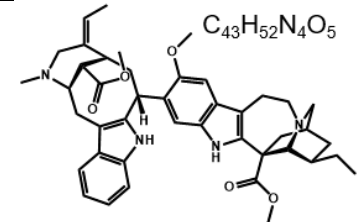
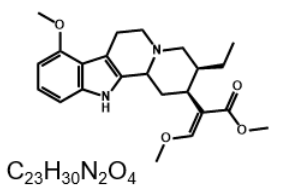
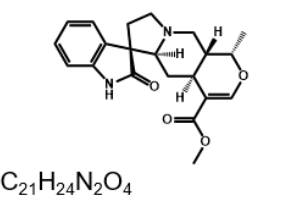
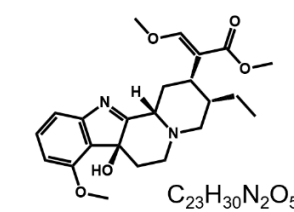
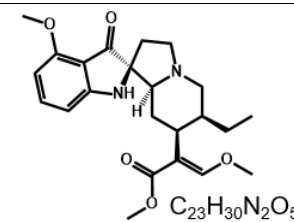
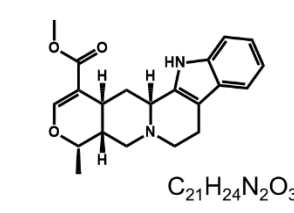
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
10	<i>V. africana</i>	Voacamine	704.3938	 C ₄₃ H ₅₂ N ₄ O ₅
11	<i>M. speciosa</i>	Mitragynine	398.2206	 C ₂₃ H ₃₀ N ₂ O ₄
		Mitraphylline	368.1736	 C ₂₁ H ₂₄ N ₂ O ₄
		7-Hydroxymitragynine	414.2155	 C ₂₃ H ₃₀ N ₂ O ₅
		Mitragynine pseudoindoxyl	414.2155	 C ₂₃ H ₃₀ N ₂ O ₅
		Ajmalicine	352.1787	 C ₂₁ H ₂₄ N ₂ O ₃

Table S2 (continued). Known molecules of interest in the indicated species.

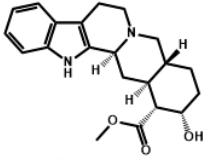
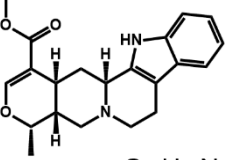
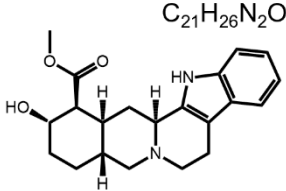
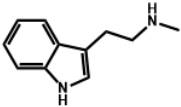
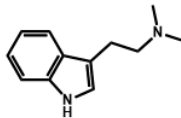
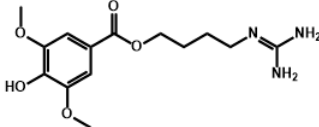
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
12	<i>C. johimbe</i>	Yohimbine	354.1943	 <chem>C21H26N2O3</chem>
		Ajmalicine	352.1787	 <chem>C21H24N2O3</chem>
		Corynanthine	354.1943	 <chem>C21H26N2O3</chem>
13	<i>P. viridis</i>	<i>N</i> -Methyltryptamine	174.1157	 <chem>C11H14N2</chem>
		<i>N,N</i> -Dimethyltryptamine (DMT)	188.1313	 <chem>C12H16N2</chem>
14	<i>L. leonurus</i>	Leonurine	311.1481	 <chem>C14H21N3O5</chem>

Table S2 (continued). Known molecules of interest in the indicated species.

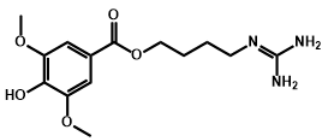
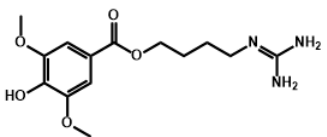
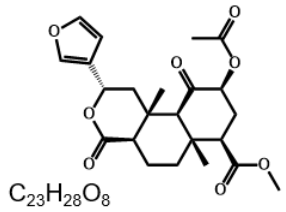
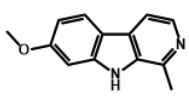
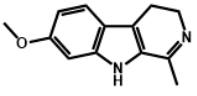
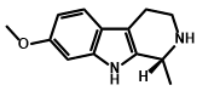
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
15	<i>L. nepetifolia</i>	Leonurine	311.1481	 $C_{14}H_{21}N_3O_5$
16	<i>L. sibiricus</i>	Leonurine	311.1481	 $C_{14}H_{21}N_3O_5$
17	<i>S. divinorum</i>	Salvinorin A	432.1784	 $C_{23}H_{28}O_8$
18	<i>S. vulgaris</i>	None	None	None
19	<i>B. caapi</i>	Harmine	212.0950	 $C_{13}H_{12}N_2O$
		Harmaline	214.1106	 $C_{13}H_{14}N_2O$
		Tetrahydroharmine	216.1263	 $C_{13}H_{16}N_2O$

Table S2 (continued). Known molecules of interest in the indicated species.

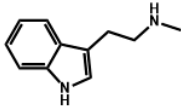
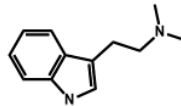
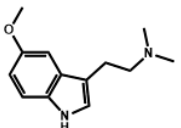
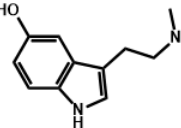
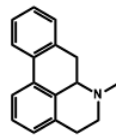
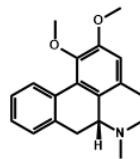
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
20	<i>D. cabrerana</i>	<i>N</i> -Methyltryptamine	174.1157	 <chem>CNCCc1c[nH]c2ccccc12</chem> $C_{11}H_{14}N_2$
		<i>N,N</i> -Dimethyltryptamine (DMT)	188.1313	 <chem>CN(C)CCc1c[nH]c2ccccc12</chem> $C_{12}H_{16}N_2$
		5-Methoxy DMT	218.1419	 <chem>CN(C)CCc1c[nH]c2cc(OC)ccc12</chem> $C_{13}H_{18}N_2O$
		Bufotenin	204.1263	 <chem>CN(C)CCc1c[nH]c2cc(O)ccc12</chem> $C_{12}H_{16}N_2O$
21	<i>T. diffusa</i>	Damianin	Unknown	Unknown
22	<i>A. officinalis</i>	None	None	None
23	<i>T. populnea</i>	None	None	None
24	<i>N. caerulea</i>	Aporphine	235.1361	 <chem>CN1CCc2c3ccccc3c4c2ccc5c4NCC5</chem> $C_{17}H_{17}N$
		Nuciferine	295.1572	 <chem>CN1CCc2c3cc(OC)c(OC)c3c4c2ccc5c4NCC5</chem> $C_{19}H_{21}NO_2$

Table S2 (continued). Known molecules of interest in the indicated species.

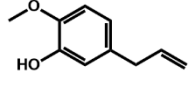
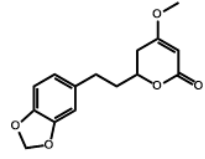
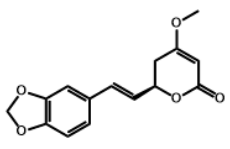
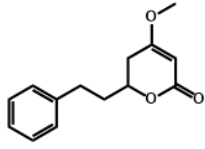
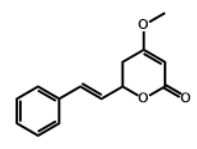
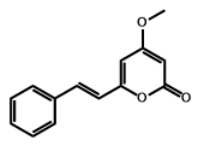
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
25	<i>P. betel</i>	Chavibetol	164.0837	$C_{10}H_{12}O_2$ 
26	<i>P. methysticum</i>	Dihydromethysticin	276.0998	$C_{15}H_{16}O_5$ 
		Methysticin	274.0841	$C_{15}H_{14}O_5$ 
		Dihydrokavain	232.1099	$C_{14}H_{16}O_3$ 
		Kavain	230.0943	$C_{14}H_{14}O_3$ 
		Desmethoxyyangonin	228.0786	$C_{14}H_{12}O_3$ 

Table S2 (continued). Known molecules of interest in the indicated species.

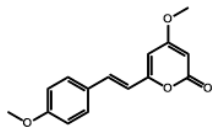
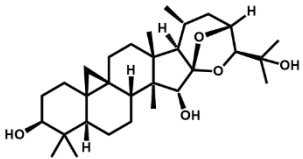
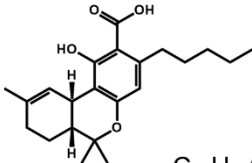
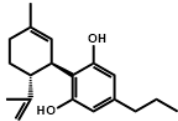
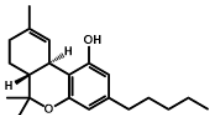
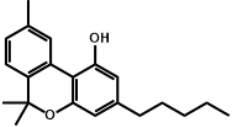
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
26	<i>P. methysticum</i>	Yangonin	258.0892	$C_{15}H_{14}O_4$ 
27	<i>A. racemosa</i>	Cimigenol	488.3502	 $C_{30}H_{48}O_5$
28	<i>C. sativa</i>	Tetrahydrocannabinolic acid (THCA)	358.2144	 $C_{22}H_{30}O_4$
		Cannabidivarin (CBDV)	286.1933	 $C_{19}H_{22}O_2$
		Tetrahydrocannabinol (THC)	314.2246	 $C_{21}H_{30}O_2$
		Cannabinol (CBN)	310.1933	 $C_{21}H_{26}O_2$

Table S2 (continued). Known molecules of interest in the indicated species.

Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
28	<i>C. sativa</i>	Cannabidiol (CBD)	314.2246	$C_{21}H_{30}O_2$
		Cannabidiolic acid (CBDA)	358.2144	$C_{22}H_{30}O_4$
		Tetrahydrocannabivarin (THCV)	286.1933	$C_{19}H_{26}O_2$
29	<i>P. harmala</i>	Vasicinone	202.0742	 $C_{11}H_{10}N_2O_2$
		Harmalol	200.0950	 $C_{12}H_{12}N_2O$
		Harmine	212.0950	 $C_{13}H_{12}N_2O$

Table S2 (continued). Known molecules of interest in the indicated species.

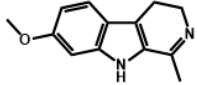
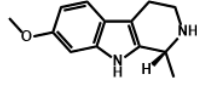
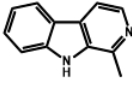
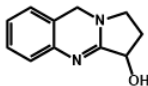
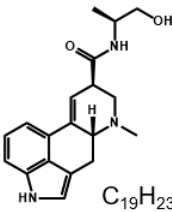
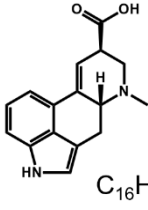
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
29	<i>P. harmala</i>	Harmaline	214.1106	 <chem>Cc1c2c(c3c1OCCN3)ccc(OC)c2</chem> $C_{13}H_{14}N_2O$
		Tetrahydroharmine	216.1263	 <chem>Cc1c2c(c3c1OCCN3)ccc(OC)c2</chem>
		Harmane	182.0844	 <chem>Cc1c2c(c3c1OCCN3)cccc2</chem> $C_{12}H_{10}N_2$
		Vasicine (peganine)	188.0950	 <chem>Oc1c2c(c3c1OCCN3)cccc2</chem> $C_{11}H_{12}N_2O$
30	<i>A. nervosa</i>	Ergometrine	325.1790	 <chem>CN1CC[C@H]2[C@@H]3C=C[C@H]4[C@@H]1Cc5c[nH]c6c5C[C@H]2C34</chem> $C_{19}H_{23}N_3O_2$
		Lysergic acid	268.1212	 <chem>CN1CC[C@H]2[C@@H]3C=C[C@H]4[C@@H]1Cc5c[nH]c6c5C[C@H]2C34C(=O)O</chem> $C_{16}H_{16}N_2O_2$

Table S2 (continued). Known molecules of interest in the indicated species.

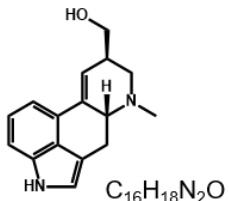
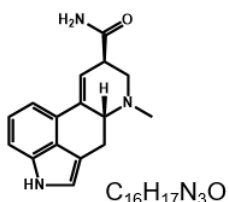
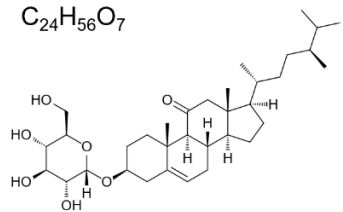
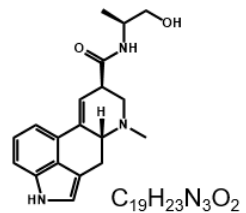
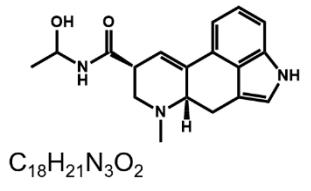
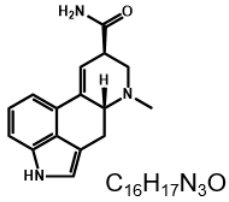
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
30	<i>A. nervosa</i>	Lysergol	254.1419	 <chem>C16H18N2O</chem>
		Ergine	267.1372	 <chem>C16H17N3O</chem>
		Argyroside	576.4026	 <chem>C24H56O7</chem>
31	<i>C. tricolor</i>	Unknown	-----	-----
32	<i>I. tricolor</i>	Ergometrine	325.1790	 <chem>C19H23N3O2</chem>
		Lysergic acid- α -hydroxyethylamide	311.1634	 <chem>C18H21N3O2</chem>
		Ergine	267.1372	 <chem>C16H17N3O</chem>

Table S2 (continued). Known molecules of interest in the indicated species.

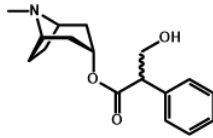
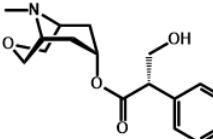
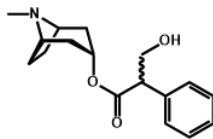
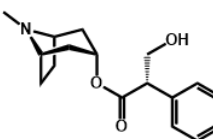
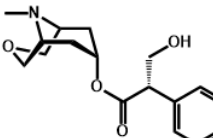
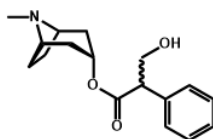
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
33	<i>A. baetica</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
34	<i>A. belladonna</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
34	<i>A. belladonna</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
35	<i>A. komarovii</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

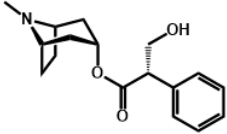
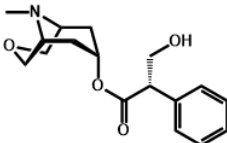
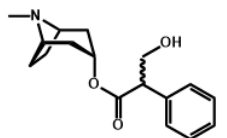
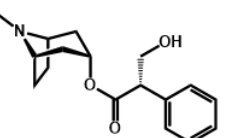
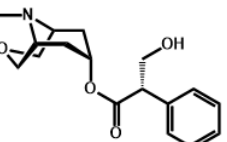
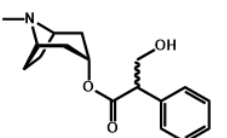
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
35	<i>A. komarovii</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
36	<i>B. arborea</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
37	<i>B. aurea</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

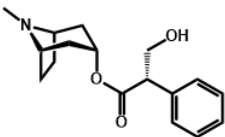
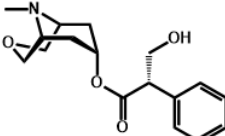
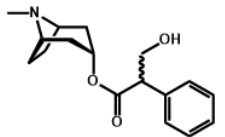
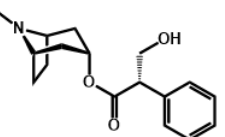
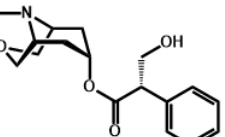
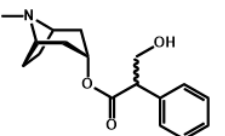
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
37	<i>B. aurea</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
38	<i>B. sanguinea</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
39	<i>B. suaveolens</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

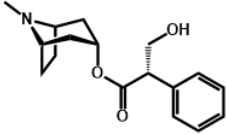
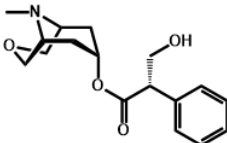
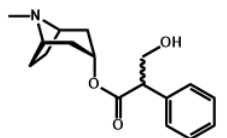
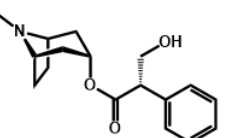
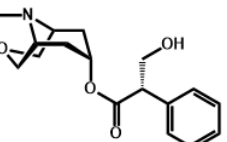
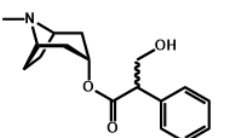
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
39	<i>B. suaveolens</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
40	<i>B. versicolor</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
41	<i>D. ceratocaula</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

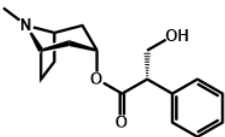
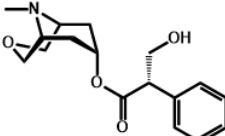
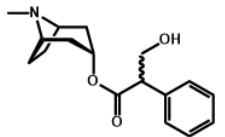
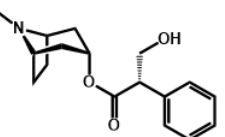
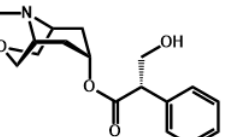
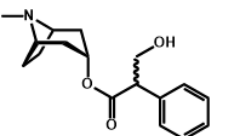
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
41	<i>D. ceratocaula</i>	Hyoscyamine	289.1678	 <chem>C17H23NO3</chem>
		Hyoscine (Scopolamine)	303.1471	 <chem>C17H21NO4</chem>
42	<i>D. discolor</i>	Atropine	289.1678	 <chem>C17H23NO3</chem>
		Hyoscyamine	289.1678	 <chem>C17H23NO3</chem>
		Hyoscine (Scopolamine)	303.1471	 <chem>C17H21NO4</chem>
43	<i>D. ferox</i>	Atropine	289.1678	 <chem>C17H23NO3</chem>

Table S2 (continued). Known molecules of interest in the indicated species.

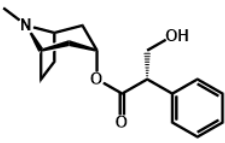
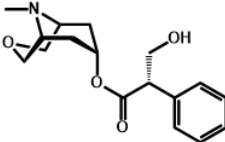
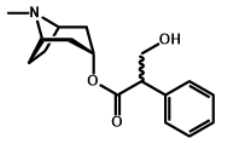
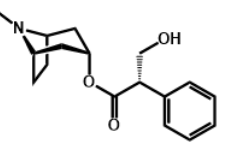
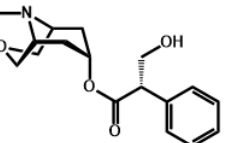
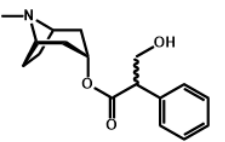
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
43	<i>D. ferox</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
44	<i>D. innoxia</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
45	<i>D. leichhardtii</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

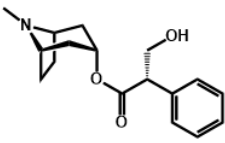
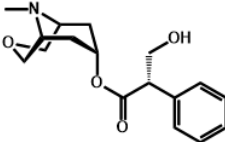
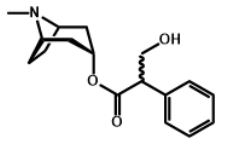
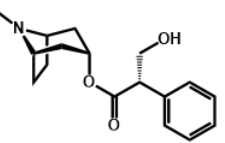
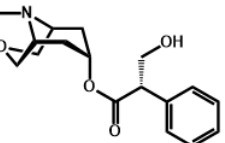
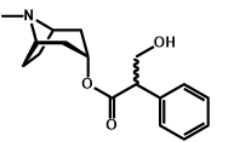
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
45	<i>D. leichhardtii</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
46	<i>D. metel</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
47	<i>D. parajuli</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

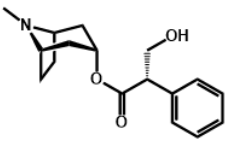
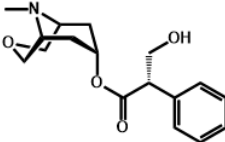
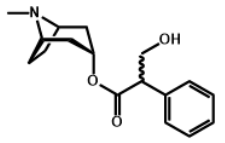
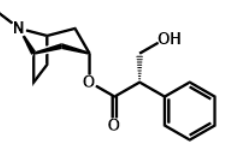
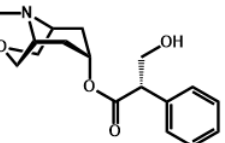
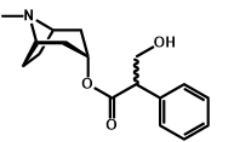
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
47	<i>D. parajuli</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
48	<i>D. quercifolia</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
49	<i>D. stramonium</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

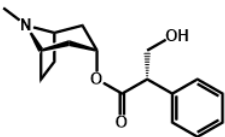
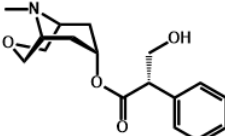
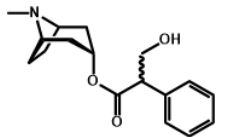
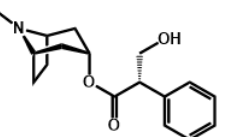
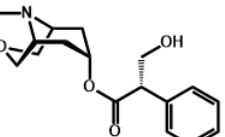
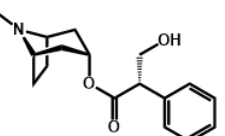
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
49	<i>D. stramonium</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
50	<i>D. wrightii</i>	Atropine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$
		Hyoscine (Scopolamine)	303.1471	 $C_{17}H_{21}NO_4$
51	<i>H. albus</i>	Hyoscyamine	289.1678	 $C_{17}H_{23}NO_3$

Table S2 (continued). Known molecules of interest in the indicated species.

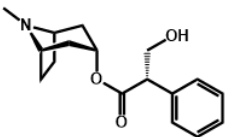
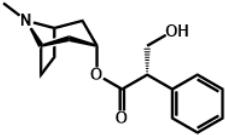
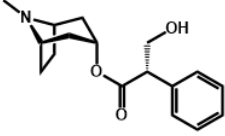
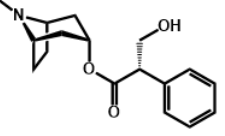
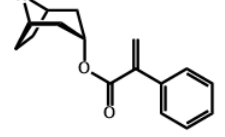
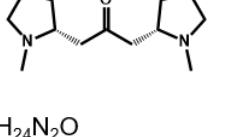
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
52	<i>H. aureus</i>	Hyoscyamine	289.1678	 <chem>CN1[C@H]2CC[C@@H]1[C@@H](C(=O)O[C@H](C2)c3ccccc3)O</chem> $C_{17}H_{23}NO_3$
53	<i>H. muticus</i>	Hyoscyamine	289.1678	 <chem>CN1[C@H]2CC[C@@H]1[C@@H](C(=O)O[C@H](C2)c3ccccc3)O</chem> $C_{17}H_{23}NO_3$
54	<i>H. niger</i>	Hyoscyamine	289.1678	 <chem>CN1[C@H]2CC[C@@H]1[C@@H](C(=O)O[C@H](C2)c3ccccc3)O</chem> $C_{17}H_{23}NO_3$
55	<i>H. pusillus</i>	Hyoscyamine	289.1678	 <chem>CN1[C@H]2CC[C@@H]1[C@@H](C(=O)O[C@H](C2)c3ccccc3)O</chem> $C_{17}H_{23}NO_3$
56	<i>M. autumnalis</i>	Apoatropine	271.1572	 <chem>CN1[C@H]2CC[C@@H]1[C@@H](C(=O)O[C@H](C2)C(=C)c3ccccc3)C</chem> $C_{17}H_{21}NO_2$
		Cuscohygrine	224.1889	 <chem>CN1CC[C@H]1C(=O)C2CCN2</chem> $C_{13}H_{24}N_2O$

Table S2 (continued). Known molecules of interest in the indicated species.

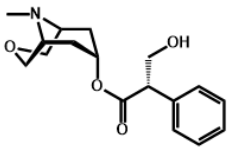
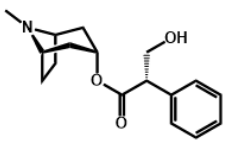
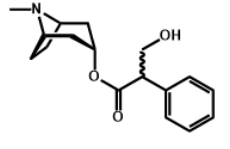
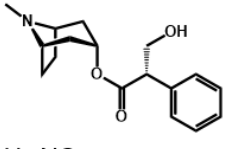
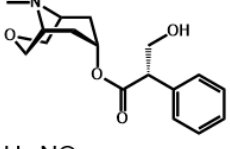
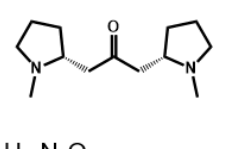
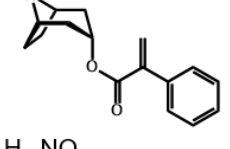
Index	Species	Molecules of Interest	Monoisotopic Mass	Structure
56	<i>M. autumnalis</i>	Hyoscine (Scopolamine)	303.1471	 <chem>C17H21NO4</chem>
		Hyoscyamine	289.1678	 <chem>C17H23NO3</chem>
57	<i>M. officinarum</i>	Atropine	289.1678	 <chem>C17H23NO3</chem>
58	<i>M. officinarum</i>	Hyoscyamine	289.1678	 <chem>C17H23NO3</chem>
		Hyoscine (Scopolamine)	303.1471	 <chem>C17H21NO4</chem>
		Cuscohygrine	224.1889	 <chem>C13H24N2O</chem>
		Apoatropine	271.1572	 <chem>C17H21NO2</chem>

Table S3. Validation results of the calibration curve using QC samples in (A) medium, (B) high and (C) LLOQ concentrations. The calculated concentrations and residuals for Runs 1-3 are shown. Cells highlighted in pink show percent error of values that deviate by greater than $\pm 15\%$ from the standard concentrations for the low, medium and high calibrators, and deviate by greater than $\pm 20\%$ from the LLOQ calibrator concentration.

A

Medium concentration level: Statistics						
Nominal conc. (mg/L)	Run 1		Run 2		Run 3	
	Calculated	Percent prediction error	Calculated	Percent prediction error	Calculated	Percent prediction error
80	72.4943	9.3822	80.3987	-0.4983	70.5257	11.8429
80	91.0445	-13.8056	89.482	-11.8525	65.7704	17.7870
80	88.2106	-10.2633	93.3318	-16.6648	67.5996	15.5006
80	94.3631	-17.9539	95.0658	-18.8323	69.9722	12.5347
80	77.2261	3.4674	80.5431	-0.6789	70.149	12.3137
80	69.1629	13.5464	67.8408	15.199	71.9711	10.0361
80	65.9606	17.5493	64.8473	18.9409	70.955	11.3063
80	71.493	10.6337	69.9804	12.5245	79.0988	1.1265
80	70.2135	12.2331	68.6396	14.2006	75.7306	5.3367
80	66.1406	17.3243	66.0471	17.4411	78.6544	1.6820

Cells highlighted in pink show the percent prediction error for concentrations that deviated from the nominal concentrations by greater than $\pm 15\%$

B

High concentration level: Statistics						
Nominal conc. (mg/L)	Run 1		Run 2		Run 3	
	Calculated	Percent prediction error	Calculated	Percent prediction error	Calculated	Percent prediction error
130	109.8795	15.4773	111.9699	13.8693	121.8128	6.2978
130	110.1051	15.3037	116.5366	10.3564	129.8995	0.0773
130	101.5727	21.8671	102.2869	21.3178	116.5247	10.3656
130	127.7046	1.7657	144.7874	-11.3749	134.4559	-3.4276
130	107.5195	17.2927	125.5875	3.3943	107.2454	17.5036
130	110.9048	14.6886	115.7273	10.979	103.9726	20.0211
130	121.7755	6.3265	125.8761	3.1722	101.5331	21.8976
130	110.6764	14.8643	119.1676	8.3326	124.4756	4.2496
130	120.4008	7.384	123.5716	4.945	146.4354	-12.6426
130	134.6083	-3.5448	139.9951	-7.6886	94.3027	27.4595

Cells highlighted in pink show the percent prediction error for concentrations that deviated from the nominal concentrations by greater than $\pm 15\%$

C

LLOQ concentration level: Statistics						
Nominal conc. (mg/L)	Run 1		Run 2		Run 3	
	Calculated	Percent prediction error	Calculated	Percent prediction error	Calculated	Percent prediction error
10	10.2858	-2.858	10.4084	-4.0837	12.0965	-20.9649
10	11.2403	-12.4035	9.5491	4.5089	11.6656	-16.6557
10	8.7611	12.389	14.2323	-42.3227	11.4855	-14.8548
10	8.8473	11.5269	12.5207	-25.207	13.6484	-36.4838
10	9.7613	2.3874	11.2025	-12.0251	11.8683	-18.6829
10	8.4348	15.6524	11.3871	-13.8711	9.8285	1.7153
10	8.765	12.3503	10.7898	-7.8979	11.1877	-11.877
10	9.2819	7.1811	9.9664	0.3364	12.0803	-20.8035
10	10.7001	-7.0006	9.7253	2.7467	12.0495	-20.4949
10	10.7001	-7.0006	9.7253	2.7467	12.0495	-20.4949

Cells highlighted in pink show the percent prediction error for concentrations that deviated from the nominal concentrations by greater than $\pm 20\%$