

# Random Forest Processing of Direct Analysis in Real Time-Mass Spectrometric Data Enables Species Identification of Psychoactive Plants from Their Headspace Chemical Signatures

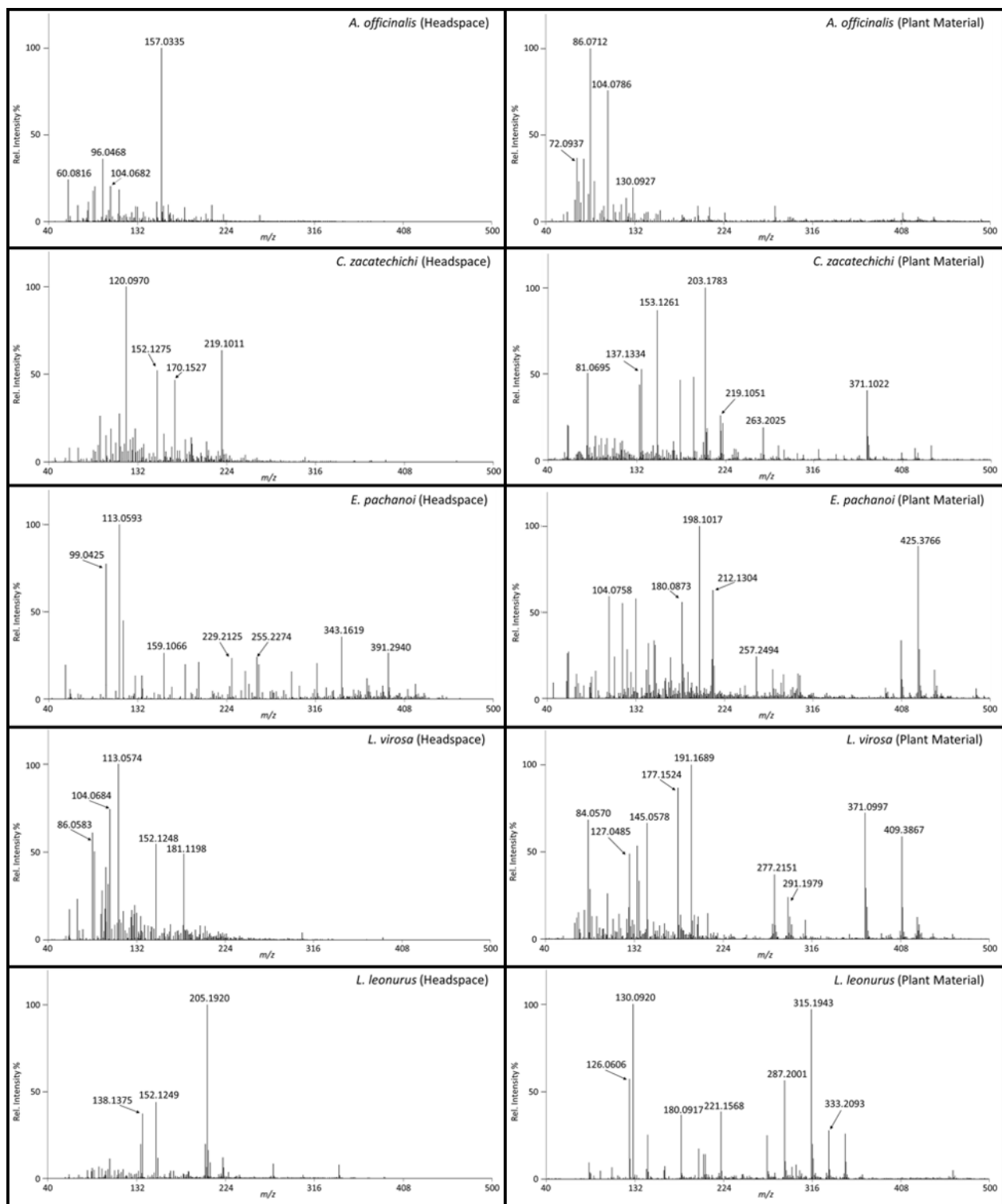
Meghan G. Appley<sup>1</sup>, Samira Beyramysoltan<sup>1</sup> and Rabi A. Musah<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, University at Albany, State University of New York, 1400 Washington Avenue, Albany, NY 12222, USA

\*Correspondence should be addressed to R.A.M. ([rmusah@albany.edu](mailto:rmusah@albany.edu))

## Supporting Information

This document contains: (1) representative mass spectra of the headspace and direct analysis of plant material; (2) the estimated error rate of the out-of-bag classifier on the training set for grown trees in the random forest modeling; (3) a 2-D plot of coordinate components of the multidimensional scaling of the proximity matrix resulting from RF modeling; (4) performance results for species discrimination using the RF model for the out-of-bag samples; (5) *p*-values from the RF conformal predictor for the unknowns representative of each species; (6) average relative intensities for *m/z* values ranked most highly significant; and (7) species-specific variables important for species discrimination.



**Figure S1.** Representative mass spectra of the headspace (left column) and plant material (right column) for each plant species analyzed by DART-HRMS.

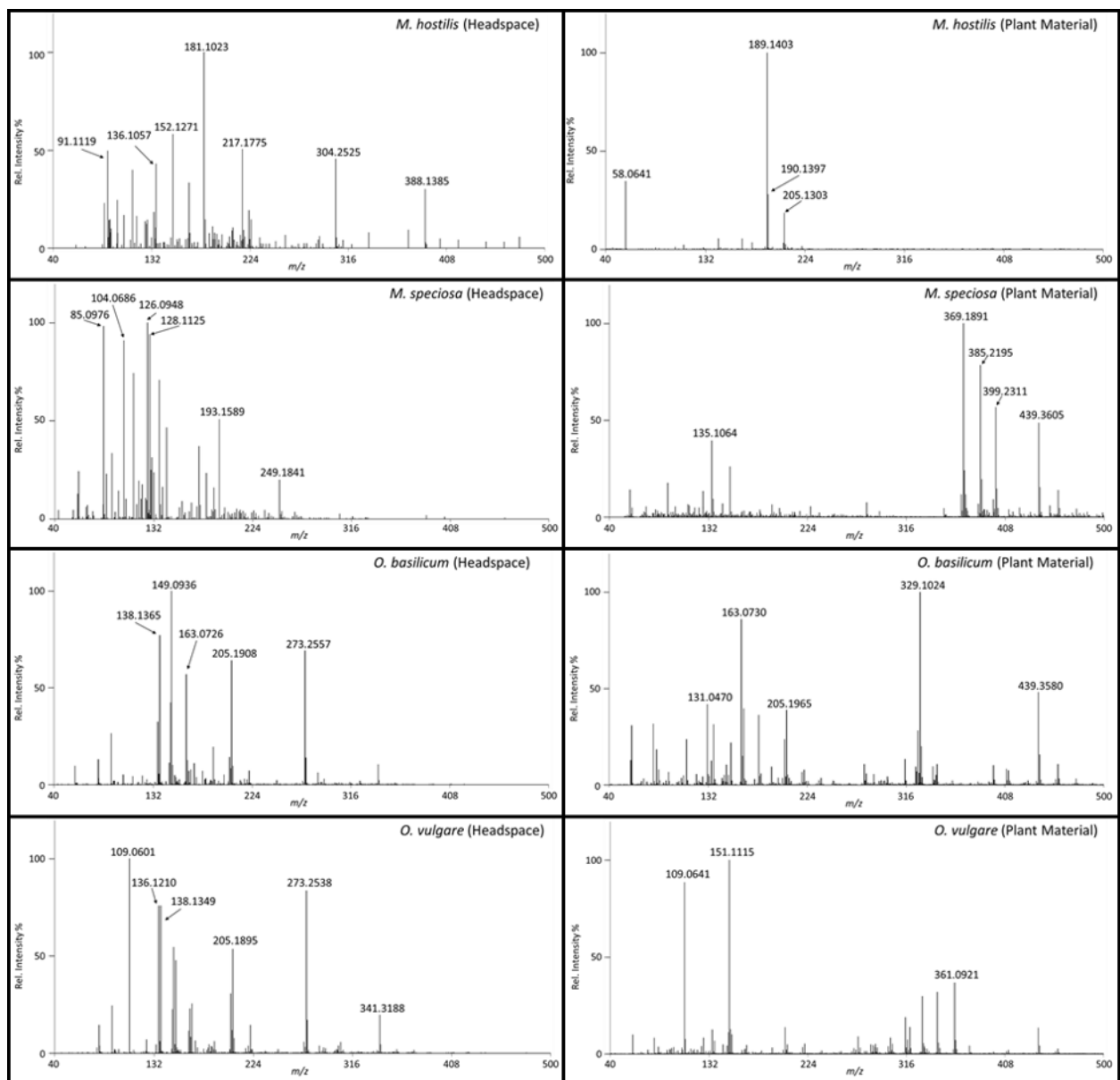
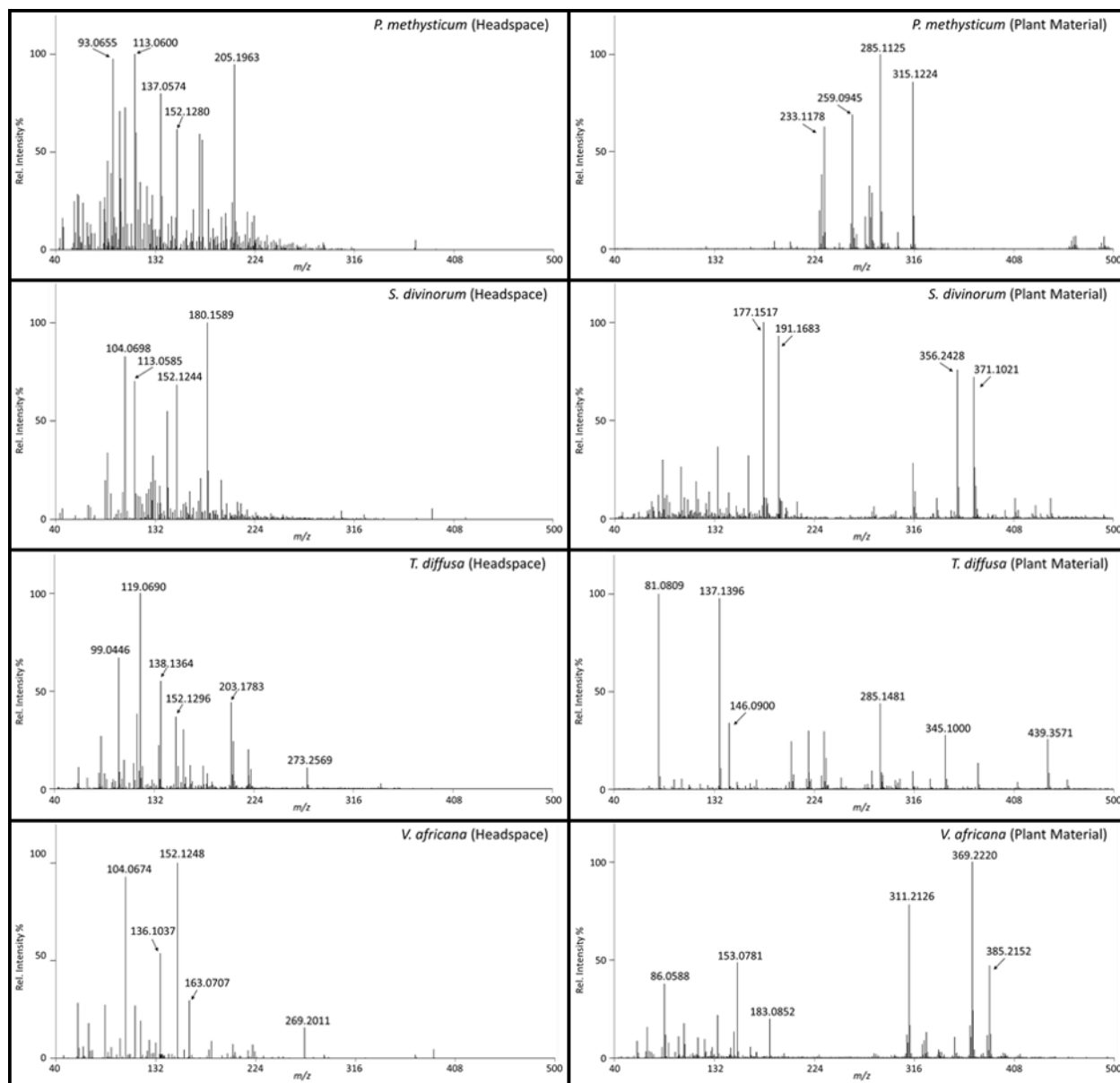
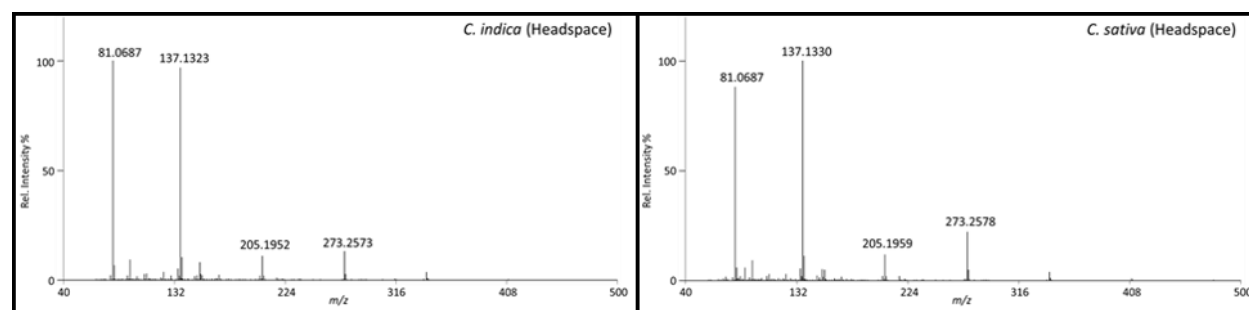


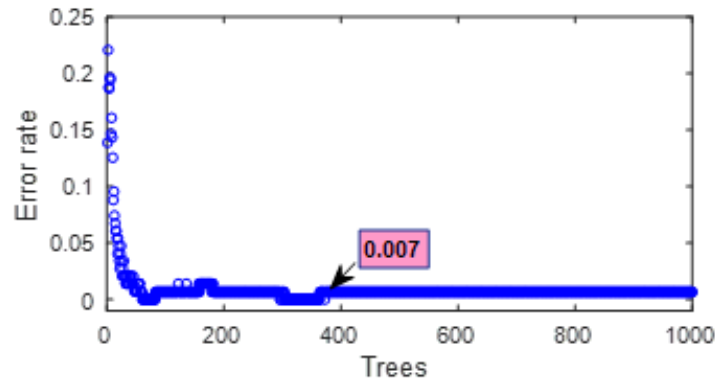
Figure S1. (continued)



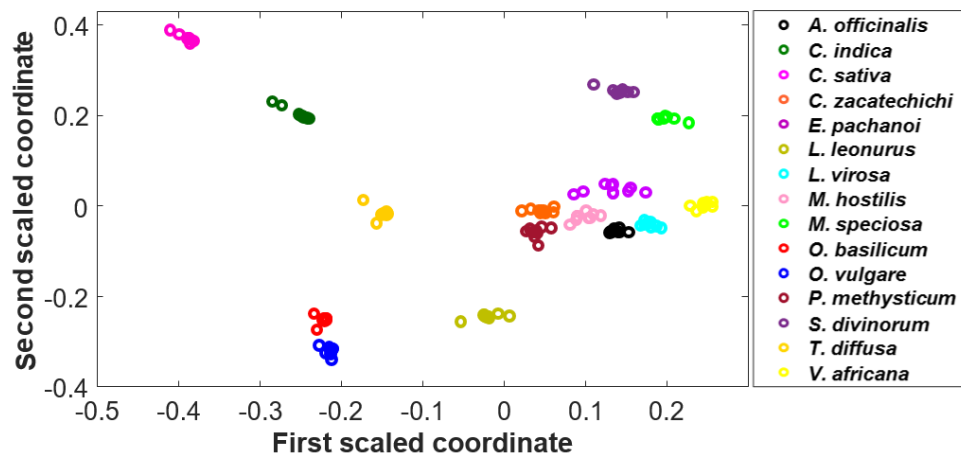
**Figure S1.** (continued)



**Figure S2.** Representative mass spectra of the headspace of *C. indica* (left panel) and *C. sativa* (right panel) analyzed by DART-HRMS.



**Figure S3.** The estimated error rate of the out-of-bag classifier on the training set is illustrated for grown trees in the random forest (RF) modeling. The error plot displays an error level of 0.007 for 1000 grown trees.



**Figure S4.** 2-D plot of the coordinate components of the multidimensional scaling of the proximity matrix resulting from RF modeling. The plot shows 15 clear clusters, which correspond to the 15 plant species studied. The species inter-relationships that were revealed by this method were consistent with those observed by PCA and *g*-SNE. The results indicate close similarity between *O. vulgare*, *O. basilicum*, *L. leonurus*, *T. diffusa*, and *P. methysticum*; and between *E. pachanoi*, *V. africana*, *L. virosa*, *A. officinalis*, and *M. hostilis*.

**Table S1.** Performance results for species discrimination using the RF model (accuracy of 99%) for the out-of-bag samples based on the maximum scores given to each sample.

Species	Classification model performance		
	Sensitivity*	Specificity**	Precision
<i>A. officinalis</i>	1	1	1
<i>C. indica</i>	0.9	1	1
<i>C. sativa</i>	1	1	1
<i>C. zacatechichi</i>	1	1	1
<i>E. pachanoi</i>	1	0.99	0.91
<i>L. leonurus</i>	1	1	1
<i>L. virosa</i>	1	1	1
<i>M. hostilis</i>	1	1	1
<i>M. speciosa</i>	1	1	1
<i>O. basilicum</i>	1	1	1
<i>O. vulgare</i>	1	1	1
<i>P. methysticum</i>	1	1	1
<i>S. divinorum</i>	1	1	1
<i>T. diffusa</i>	1	1	1
<i>V. africana</i>	1	1	1

\*Sensitivity refers to the true positive rate.

\*\*Specificity refers to the true negative rate

**Table S2.** The resulting  $p$ -values from the RF conformal predictor for the unknowns representative of each species. The first column displays 14 sample unknowns, and the first row shows the species classes of the training samples. According to the  $p$ -values of the sample unknowns, *M. hostilis*, *O. vulgare*, *E. pachanoi*, and *C. sativa* received dual class assignments at the 8% significance level. All other unknowns were assigned a single label.

Class Test sample	<i>A. officinalis</i>	<i>C. indica</i>	<i>C. sativa</i>	<i>C. zacatechichi</i>	<i>E. pachanoi</i>	<i>L. leonurus</i>	<i>L. virosa</i>	<i>M. hostilis</i>	<i>M. speciosa</i>	<i>O. vulgare</i>	<i>O. basilicum</i>	<i>P. methysticum</i>	<i>S. divinorum</i>	<i>T. diffusa</i>	<i>V. africana</i>
<i>A. officinalis</i>	<b>0.09</b>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>C. indica</i>	0.00	<b>0.27</b>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>C. sativa</i>	0.00	0.00	<b>0.09</b>	0.00	0.00	<b>0.09</b>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>C. zacatechichi</i>	0.00	0.00	0.00	<b>0.90</b>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>E. pachanoi</i>	0.00	0.00	0.00	0.00	<b>0.09</b>	<b>0.09</b>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>L. leonurus</i>	0.00	0.00	0.00	0.00	0.00	<b>0.09</b>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>L. virosa</i>	0.00	0.00	0.00	0.00	0.00	0.00	<b>1.00</b>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>M. hostilis</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	<b>0.09</b>	0.00	0.00	<b>0.09</b>	0.00	0.00	0.00	0.00
<i>M. speciosa</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	<b>0.45</b>	0.00	0.00	0.00	0.00	0.00	0.00
<i>O. basilicum</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	<b>0.09</b>	0.00	0.00	0.00	0.00	0.00
<i>O. vulgare</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	<b>0.09</b>	0.00	0.00	<b>0.18</b>	0.00	0.00	0.00	0.00
<i>P. methysticum</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	<b>0.45</b>	0.00	0.00	0.00
<i>S. divinorum</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	<b>0.36</b>	0.00	0.00
<i>T. diffusa</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	<b>0.55</b>	0.00

**Table S3-a.** The average of the relative intensities for the  $m/z$  values ranked most highly significant by PCA-VIP and RF modeling (in the range  $m/z$  60-101).

	<b>60.0802</b>	<b>81.0500</b>	<b>85.0999</b>	<b>88.0800</b>	<b>93.0699</b>	<b>96.0500</b>	<b>99.0399</b>	<b>100.0899</b>
<i>A. officinalis</i>	38.58	0.00	0.00	11.66	0.00	42.97	1.09	2.95
<i>C. indica</i>	0.00	94.48	4.79	4.47	3.20	0.70	6.24	1.41
<i>C. sativa</i>	0.00	88.58	2.65	0.00	1.80	0.00	0.00	0.00
<i>C. zacatechichi</i>	0.15	0.00	0.00	17.41	18.57	2.10	21.60	12.65
<i>E. pachanoi</i>	0.46	0.00	2.03	6.09	5.40	0.33	9.06	0.81
<i>L. leonurus</i>	2.25	0.00	0.40	4.80	3.62	9.73	1.19	4.89
<i>L. virosa</i>	0.81	0.74	0.00	13.81	2.31	28.13	9.12	34.94
<i>M. hostilis</i>	0.21	0.00	0.45	16.32	24.51	1.03	1.14	2.67
<i>M. speciosa</i>	0.00	0.00	39.37	9.30	9.08	4.05	7.45	4.02
<i>O. basilicum</i>	0.00	0.00	0.00	0.18	18.09	0.17	0.65	0.00
<i>O. vulgare</i>	0.00	0.00	0.00	0.20	19.31	0.00	1.13	0.00
<i>P. methysticum</i>	13.08	20.14	14.58	22.71	91.67	10.91	59.93	27.65
<i>S. divinorum</i>	3.45	0.00	5.59	36.19	4.34	2.45	0.15	2.57
<i>T. diffusa</i>	0.00	0.51	0.00	1.38	1.17	2.28	54.98	4.66
<i>V. africana</i>	27.02	0.00	4.12	15.39	0.00	1.00	1.60	1.60

**Table S3-b.** The average of the relative intensities for the  $m/z$  values ranked most highly significant by PCA-VIP and RF modeling (in the range  $m/z$  104-121).

	<b>104.0698</b>	<b>109.0698</b>	<b>112.0397</b>	<b>113.0597</b>	<b>114.0897</b>	<b>118.0898</b>	<b>119.0697</b>	<b>120.0997</b>
<i>A. officinalis</i>	11.58	0.23	5.30	16.41	2.74	3.64	0.00	3.66
<i>C. indica</i>	0.94	10.07	0.00	5.25	5.93	0.54	4.17	0.00
<i>C. sativa</i>	0.00	4.32	0.00	0.00	0.00	0.00	0.00	0.00
<i>C. zacatechichi</i>	18.84	9.74	0.00	32.42	24.67	9.27	0.00	79.64
<i>E. pachanoi</i>	2.49	0.58	0.00	24.08	8.61	1.96	0.00	1.93
<i>L. leonurus</i>	18.57	2.22	3.26	4.72	2.44	7.41	0.00	1.42
<i>L. virosa</i>	62.30	1.51	12.11	57.58	10.51	13.68	0.00	4.53
<i>M. hostilis</i>	13.90	0.00	0.27	1.51	25.14	9.52	0.00	1.98
<i>M. speciosa</i>	99.10	6.73	0.00	51.10	6.85	20.42	0.00	10.62
<i>O. basilicum</i>	4.77	0.00	0.00	2.89	0.00	0.14	0.00	0.00
<i>O. vulgare</i>	0.36	75.77	0.00	1.86	0.00	0.10	0.00	0.00
<i>P. methysticum</i>	67.20	3.77	0.00	90.15	30.95	25.45	0.00	2.47
<i>S. divinorum</i>	66.84	0.00	0.00	51.49	9.06	9.07	0.00	5.70
<i>T. diffusa</i>	8.26	1.68	0.00	7.61	1.23	6.45	100.00	0.00
<i>V. africana</i>	83.58	1.69	0.46	12.84	8.34	16.84	0.00	3.40



**Table S3-c.** The average of the relative intensities for the  $m/z$  values ranked most highly significant by PCA-VIP and RF modeling (in the range  $m/z$  136-151).

	<b>136.1096</b>	<b>137.1096</b>	<b>138.1296</b>	<b>143.1394</b>	<b>147.0795</b>	<b>148.0895</b>	<b>149.0895</b>	<b>150.0994</b>
<i>A. officinalis</i>	0.70	0.53	6.01	0.00	0.00	1.38	0.30	0.98
<i>C. indica</i>	1.76	51.53	9.37	2.89	0.63	0.00	2.68	0.00
<i>C. sativa</i>	2.02	2.60	10.77	0.00	0.00	0.00	3.21	0.00
<i>C. zacatechichi</i>	21.13	0.00	5.09	1.73	1.62	2.77	0.74	2.99
<i>E. pachanoi</i>	18.42	0.15	1.90	0.00	0.23	0.45	0.53	3.23
<i>L. leonurus</i>	6.78	0.25	8.44	0.00	0.00	2.80	0.00	2.26
<i>L. virosa</i>	9.12	1.03	3.32	0.00	4.03	5.64	2.61	4.45
<i>M. hostilis</i>	13.01	0.22	2.83	0.65	3.15	4.10	0.00	6.68
<i>M. speciosa</i>	4.12	33.15	4.60	0.00	0.20	3.51	0.48	2.50
<i>O. basilicum</i>	21.76	0.00	61.27	0.00	9.42	34.87	98.95	10.24
<i>O. vulgare</i>	84.24	0.00	91.48	0.00	0.00	2.14	21.95	64.41
<i>P. methysticum</i>	3.02	66.98	27.07	1.06	17.21	5.29	0.00	2.11
<i>S. divinorum</i>	13.85	9.16	2.72	44.12	0.00	2.63	0.26	3.20
<i>T. diffusa</i>	11.92	10.96	21.17	0.00	0.13	0.66	0.00	0.94
<i>V. africana</i>	12.27	0.15	2.25	0.18	3.11	3.89	0.00	4.84

**Table S3-d.** The average of the relative intensities for the  $m/z$  values ranked most highly significant by PCA-VIP and RF modeling (in the range  $m/z$  152-174).

	<b>152.1294</b>	<b>153.1294</b>	<b>157.0392</b>	<b>160.1394</b>	<b>163.0693</b>	<b>165.1092</b>	<b>167.1094</b>	<b>173.0992</b>
<i>A. officinalis</i>	12.04	0.00	86.38	0.99	0.00	0.35	1.11	0.49
<i>C. indica</i>	0.75	9.06	0.99	0.51	3.30	0.82	1.60	0.98
<i>C. sativa</i>	0.00	5.82	0.00	0.00	0.00	0.00	0.28	0.00
<i>C. zacatechichi</i>	54.89	0.00	0.00	2.38	0.00	2.39	12.87	3.37
<i>E. pachanoi</i>	62.93	0.00	0.00	2.30	0.00	0.69	5.37	0.00
<i>L. leonurus</i>	32.43	0.00	0.00	0.72	0.00	0.00	3.05	0.26
<i>L. virosa</i>	58.36	0.00	5.20	3.30	0.00	1.90	5.92	3.76
<i>M. hostilis</i>	93.80	0.00	0.00	3.62	0.00	1.68	8.14	0.21
<i>M. speciosa</i>	36.33	0.00	0.00	4.07	0.00	1.69	7.64	0.71
<i>O. basilicum</i>	0.54	0.00	0.00	0.00	79.15	7.28	8.21	0.00
<i>O. vulgare</i>	2.05	0.00	0.00	0.00	0.00	28.89	29.98	0.12
<i>P. methysticum</i>	30.75	0.00	0.00	2.09	0.00	4.90	9.35	46.36
<i>S. divinorum</i>	55.76	0.00	0.00	7.46	0.00	1.10	5.05	0.29
<i>T. diffusa</i>	11.56	2.85	2.77	1.75	0.00	4.25	3.11	1.77
<i>V. africana</i>	88.28	0.00	0.00	2.82	4.34	0.84	6.43	0.50

**Table S3-e.** The average of the relative intensities for the  $m/z$  values ranked most highly significant by PCA-VIP and RF modeling (in the range  $m/z$  174-204).

	<b>174.1492</b>	<b>175.1191</b>	<b>177.1093</b>	<b>180.1592</b>	<b>181.1192</b>	<b>187.1292</b>	<b>193.1590</b>	<b>203.1789</b>
<i>A. officinalis</i>	1.52	0.43	0.10	2.00	5.82	0.00	0.76	2.72
<i>C. indica</i>	0.38	0.57	4.21	0.70	1.21	1.06	0.51	1.83
<i>C. sativa</i>	0.00	0.00	0.09	0.00	0.00	0.00	0.00	3.23
<i>C. zacatechichi</i>	1.56	9.52	0.00	2.96	20.31	36.76	4.38	16.95
<i>E. pachanoi</i>	3.84	1.05	0.00	3.18	6.20	0.98	4.67	0.10
<i>L. leonurus</i>	0.79	0.13	0.00	2.87	2.88	0.23	0.26	22.71
<i>L. virosa</i>	4.16	3.63	0.26	12.34	38.53	2.53	4.30	5.55
<i>M. hostilis</i>	5.36	5.70	0.75	13.03	39.06	4.04	7.80	5.29
<i>M. speciosa</i>	22.52	5.24	0.00	5.23	26.30	4.07	33.26	2.09
<i>O. basilicum</i>	0.11	0.00	0.00	0.00	3.46	1.30	1.77	11.99
<i>O. vulgare</i>	0.00	0.00	0.00	0.27	1.64	2.34	0.10	45.44
<i>P. methysticum</i>	2.24	46.55	0.00	1.07	14.70	2.63	8.26	17.82
<i>T. diffusa</i>	17.97	3.43	0.00	100.00	28.40	2.31	21.83	1.51
<i>S. divinorum</i>	0.00	3.08	24.58	1.01	3.45	0.00	0.13	26.88
<i>V. africana</i>	2.51	1.74	0.00	5.58	3.35	1.51	1.65	4.42

**Table S3-f.** The average of the relative intensities for the  $m/z$  values ranked most highly significant by PCA-VIP and RF modeling (in the range  $m/z$  205-275).

	<b>205.1888</b>	<b>219.0989</b>	<b>220.1086</b>	<b>222.1088</b>	<b>257.1084</b>	<b>273.2583</b>	<b>274.2583</b>
<i>A. officinalis</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>C. indica</i>	11.26	0.00	0.63	0.00	0.00	11.76	2.35
<i>C. sativa</i>	20.51	0.00	0.00	0.00	0.00	17.63	3.74
<i>C. zacatechichi</i>	8.09	83.10	8.53	0.15	0.00	0.22	0.16
<i>E. pachanoi</i>	0.10	0.18	0.27	0.55	0.00	0.48	0.12
<i>L. leonurus</i>	100.00	1.21	0.00	6.13	0.00	0.84	0.15
<i>L. virosa</i>	2.20	3.09	0.52	1.41	0.00	0.13	0.00
<i>M. hostilis</i>	2.72	0.23	1.83	1.98	11.78	0.62	1.49
<i>M. speciosa</i>	0.86	0.00	0.00	0.97	0.00	0.00	0.00
<i>O. basilicum</i>	55.01	0.00	0.00	0.12	0.00	50.54	0.00
<i>O. vulgare</i>	66.80	0.00	0.00	1.99	0.00	90.14	0.00
<i>P. methysticum</i>	72.38	0.00	0.19	1.06	0.64	0.26	0.15
<i>T. diffusa</i>	11.32	13.44	1.41	0.13	0.00	1.76	0.20
<i>S. divinorum</i>	0.00	0.00	0.00	1.47	0.00	0.00	0.00
<i>V. africana</i>	1.01	0.00	0.00	0.86	0.00	0.00	0.22

**Table S4-a.** The twenty species-specific variables (i.e.  $m/z$  values) found to be most important for species discrimination, based on their variable importance scores computed by RF analysis. The  $m/z$  values are listed in order of decreasing magnitude of the importance score.

#	Plant species									
	<i>A. officinalis</i>		<i>C. indica</i>		<i>C. sativa</i>		<i>C. zacatechichi</i>		<i>E. pachanoi</i>	
	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance
1	157.0392	29.20	81.0500	18.70	274.2583	20.91	120.0997	15.68	203.1789	36.39
2	60.0802	9.80	153.1294	12.60	203.1789	10.20	219.0989	14.70	96.0500	7.67
3	96.0500	9.21	203.1789	10.53	135.0995	9.51	187.1292	14.46	205.1889	7.53
4	100.0899	7.99	60.0802	8.71	155.0893	9.18	220.1086	11.51	157.0392	7.48
5	203.1789	7.66	205.1889	8.56	89.1000	8.27	203.1789	8.38	104.0698	7.07
6	112.0397	7.21	151.1494	7.47	60.0802	8.09	60.0802	7.85	100.0899	6.69
7	205.1889	7.01	100.0899	7.34	205.1889	7.88	205.1889	7.40	112.0397	6.55
8	136.1096	6.94	157.0392	6.94	81.0500	7.09	112.0397	6.34	120.0997	6.09
9	165.0194	6.36	120.0997	6.56	120.0997	6.70	157.0392	6.21	274.2583	5.85
10	274.2583	5.97	112.0397	6.51	157.0392	6.63	96.0500	5.40	222.1088	5.79
11	120.0997	5.96	222.1088	6.16	100.0899	6.37	222.1088	5.32	257.1084	5.70
12	222.1088	5.90	219.0989	6.04	112.0397	6.22	274.2583	5.26	219.0989	5.33
13	147.0795	5.84	101.0798	6.01	273.2583	6.22	170.1493	5.24	81.0500	5.09
14	164.0992	5.46	104.0698	5.91	222.1088	6.16	257.1084	5.06	136.1096	4.98
15	257.1084	5.46	96.0500	5.87	219.0989	5.90	84.0501	5.00	177.1093	4.89
16	219.0989	5.27	257.1084	5.85	257.1084	5.84	81.0500	4.79	118.0898	4.78
17	81.0500	4.90	147.0795	5.52	73.0500	5.69	177.1093	4.58	193.1590	4.75
18	78.0368	4.87	135.0995	5.51	153.1294	5.53	119.0697	4.56	119.0697	4.63
19	388.1372	4.86	138.1296	5.44	147.0795	5.39	193.1590	4.46	147.0795	4.52
20										

**Table S4-b.** The twenty species-specific variables (i.e.  $m/z$  values) found to be most important for species discrimination, based on their variable importance scores computed by RF analysis. The  $m/z$  values are listed in order of decreasing magnitude of the importance score.

#	Plant species type									
	<i>L. leonurus</i>		<i>L. virosa</i>		<i>M. hostilis</i>		<i>M. speciosa</i>		<i>O. basilicum</i>	
	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance
1										
2	205.1889	20.76	100.0899	15.88	257.1084	19.32	120.0997	12.82	148.0895	12.55
3	222.1088	20.75	112.0397	14.78	225.1600	9.05	249.1884	10.41	149.0895	12.12
4	203.1789	9.84	95.0198	10.50	203.1789	9.03	132.0996	10.02	163.0693	11.74
5	221.1888	7.94	96.0500	9.61	60.0802	8.17	174.1492	9.83	203.1789	10.00
6	100.0899	7.31	203.1789	9.22	225.0587	7.13	60.0802	8.51	180.0892	8.64
7	238.1611	7.31	86.0601	7.69	157.0392	6.39	193.1590	8.06	60.0802	8.13
8	157.0392	6.89	205.1889	7.41	120.0997	6.24	100.0899	6.81	178.0990	7.54
9	120.0997	6.15	157.0392	7.17	186.1490	6.17	212.1989	6.77	205.1889	7.41
10	96.0500	6.05	222.1088	6.36	205.1889	6.15	157.0392	6.74	157.0392	6.93
11	274.2583	5.97	120.0997	6.27	104.0698	6.12	205.1889	6.67	285.2282	6.80
12	147.0795	5.59	219.0989	5.90	258.1683	5.78	125.2495	6.61	100.0899	6.75
13	257.1084	5.43	181.1192	5.64	222.1088	5.74	96.0500	6.20	112.0397	6.49
14	219.0989	5.30	274.2583	5.60	274.2583	5.39	112.0397	6.11	274.2583	6.36
15	81.0500	5.18	257.1084	5.34	96.0500	5.20	222.1088	5.81	222.1088	6.27
16	119.0697	4.99	81.0500	5.14	219.0989	4.79	274.2583	5.76	120.0997	6.18
17	177.1093	4.79	174.1492	4.89	81.0500	4.79	219.0989	5.70	257.1084	5.91
18	174.1492	4.67	147.0795	4.71	208.1888	4.64	257.1084	5.66	81.0500	5.75
19	193.1590	4.52	193.1590	4.68	177.1093	4.57	85.0299	5.57	219.0989	5.68
20	70.0701	4.51	119.0697	4.62	233.1187	4.57	137.1096	5.39	147.0795	5.52

**Table S4-c.** The twenty species-specific variables (i.e.  $m/z$  values) found to be most important for species discrimination, based on their variable importance scores computed by RF analysis. The  $m/z$  values are listed in order of decreasing magnitude of the importance score.

#	Plant species type									
	<i>O. vulgare</i>		<i>P. methysticum</i>		<i>S. divinorum</i>		<i>T. diffusa</i>		<i>V. africana</i>	
1	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance	$m/z$	Importance
2	203.1789	9.40	175.1191	11.29	143.1394	13.69	177.1093	17.44	60.0802	16.67
3	60.0802	8.02	173.0992	11.22	180.1592	13.50	119.0697	17.20	104.0698	9.28
4	205.1889	7.43	147.0795	11.19	160.1394	13.50	159.0994	11.07	203.1789	8.83
5	136.1096	7.29	93.0699	11.09	174.1492	7.35	203.1789	9.33	205.1889	8.38
6	165.1092	7.19	122.0796	8.74	193.0890	7.18	219.0989	9.29	100.0899	8.26
7	341.3176	6.99	203.1789	8.10	325.2578	6.96	60.0802	8.06	147.0795	8.16
8	157.0392	6.94	100.0899	7.83	211.1389	6.71	205.1889	7.68	388.1372	7.43
9	305.2480	6.89	157.0392	6.27	157.0392	6.51	94.1200	7.39	152.1294	7.36
10	100.0899	6.83	112.0397	6.20	100.0899	6.39	157.0392	6.89	157.0392	7.09
11	339.4282	6.83	193.0890	6.00	205.1889	6.23	100.0899	6.58	96.0500	6.96
12	150.0994	6.76	120.0997	5.86	120.0997	6.19	112.0397	6.27	120.0997	6.61
13	303.2281	6.76	197.0989	5.21	222.1088	6.07	120.0997	6.27	222.1088	6.55
14	273.2583	6.75	274.2583	5.18	147.0795	5.87	116.0798	6.02	81.0500	5.90
15	342.3275	6.66	222.1088	5.08	274.2583	5.84	222.1088	5.84	274.2583	5.89
16	151.2894	6.66	219.0989	5.05	96.0500	5.82	274.2583	5.82	219.0989	5.76
17	109.0698	6.59	96.0500	4.97	112.0397	5.81	257.1084	5.77	138.1296	5.61
18	137.2996	6.52	138.1296	4.96	193.1590	5.69	99.0399	5.74	257.1084	5.59
19	112.0397	6.18	81.0500	4.86	219.0989	5.25	81.0500	5.59	108.1698	5.54
20	120.0997	6.15	137.1096	4.54	81.0500	5.20	96.0500	5.22	193.1590	5.40