

Table S1. GC-qMS peak areas of the volatile metabolites identified in LC patients and healthy subjects (CTRL) organized by chemical family

label	Chemical Classes / Metabolites	CTRL				LC				Fold change	
		AVG	Max	Min	Freq (%)	AVG	Max	Min	Freq (%)		
Alcohols										LC-CTRL	% variation
40	Isopentanol	1.7E+05	6.0E+05	2.7E+04	100	2.9E+05 5	3.2E+06	0.0E+00 0	89	1.2E+05	42.1
62	1-Hexanol	1.0E+05	2.5E+05	0.0E+00	93	1.2E+05 5	9.1E+05	0.0E+00 0	82	1.8E+04	15.2
76	3,7-Dimethyl-3-octanol	2.3E+05	5.1E+05	1.3E+05	100	1.8E+05 5	6.2E+05	1.8E+04 4	100	- 5.5E+04	-31.0
77	2-Ethyl-1-hexanol	3.0E+05	5.4E+05	1.1E+05	100	2.2E+05 5	5.9E+05	0.0E+00 0	93	- 8.2E+04	-36.8
83	6,10-Dihydromyrcenol	1.2E+07	1.1E+08	2.6E+05	100	5.4E+05 5	2.4E+06	0.0E+00 0	96	- 1.2E+07	-2155.9
101	3,7-Dimethyl-1,6-octadien-3-ol	1.1E+05	7.0E+05	0.0E+00	93	4.1E+04 4	2.5E+05	0.0E+00 0	64	- 6.6E+04	-160.6
136	2-Furanmethanol	2.0E+05	6.9E+05	2.4E+04	100	1.6E+05 5	9.7E+05	0.0E+00 0	86	- 4.9E+04	-31.7
152	1-(3,5-Bis-trifluoromethylphenyl)ethanol	7.5E+04	5.8E+05	0.0E+00	44	1.7E+07 7	3.4E+08	0.0E+00 0	79	1.7E+07	99.6
165	2,4,6-Trimethylbenzyl alcohol	2.4E+06	1.3E+07	6.7E+03	100	2.8E+05 5	2.1E+06	0.0E+00 0	86	- 2.2E+06	-764.9
189	1,2-Decanediol	2.5E+08	4.0E+08	4.5E+07	100	1.7E+08 8	4.4E+08	8.8E+06 6	100	- 7.6E+07	-43.2
TOTAL AREA		2.7E+08				1.9E+08 8					
Aldehydes											
41	2-Hexenal	6.6E+05	4.4E+06	7.2E+04	100	4.9E+05 5	1.8E+06	9.5E+03 3	100	- 1.7E+05	-35

79	Furfural	3.1E+06	6.1E+06	1.2E+06	100	5.5E+06 6	1.4E+07	9.3E+05	100	2.3E+06	42.6
87	Decanal	2.3E+07	9.3E+07	1.5E+06	100	2.3E+07 7	5.4E+07	2.4E+05	100	- 6.2E+05	-2.7
164	Cuminaldehyde	5.7E+06	3.3E+07	1.1E+06	100	1.9E+06 6	7.1E+06	2.5E+05	100	- 3.8E+06	-205.2
TOTAL AREA		3.3E+07				3.1E+08					
						8					

Benzene Derivatives

46	<i>o</i> -Cymene	1.2E+08	5.0E+08	3.0E+04	100	3.6E+07 7	2.1E+08	0.0E+00	75	- 8.0E+07	-225.1
52	1-Isopropyl-3-methylbenzene	1.4E+07	1.6E+08	0.0E+00	85	3.8E+06 6	9.0E+07	0.0E+00	86	- 1.0E+07	-268.5
57	Hemimellitene	5.3E+06	1.7E+07	0.0E+00	96	3.3E+06 6	2.0E+07	0.0E+00	93	- 2.0E+06	-60.2
64	<i>p</i> -Cymenene	5.1E+07	1.6E+08	3.8E+04	100	1.1E+07 7	3.4E+07	0.0E+00	93	- 4.0E+07	-368.6
68	Toluene	5.5E+05	7.5E+06	1.3E+03	100	2.1E+05 5	1.7E+06	0.0E+00	89	- 3.4E+05	-161.4
71	(1,4-Dimethylpent-2-enyl)benzene	2.0E+06	9.5E+06	0.0E+00	74	1.4E+06 6	1.2E+07	0.0E+00	93	- 6.7E+05	-49.3
72	Benzene, 1-butenyl-, (Isomer)-	3.2E+07	1.8E+08	0.0E+00	93	1.4E+07 7	6.3E+07	0.0E+00	86	- 1.7E+07	-121
84	1,2,4,5-Tetramethylbenzene	8.4E+06	2.6E+07	3.5E+05	100	5.0E+06 6	1.4E+07	0.0E+00	96	-34E+06	-68.4
98	1H-Trindene, 2,3,4,5,6,7,8,9-octahydro-1,1,4,4,9,9-hexamethyl-	1.6E+06	6.3E+06	2.5E+05	100	2.9E+06 6	1.3E+07	1.3E+05	100	1.3E+06	43.8
153	Benzoyl isocyanate	1.4E+06	4.2E+06	1.3E+05	100	6.4E+05 5	3.2E+06	1.3E+05	100	-72E+05	-112.9
162	Oxime-,methoxy-phenyl-	1.9E+06	8.8E+06	4.5E+05	100	1.1E+06 6	7.1E+06	1.9E+03	100	- 7.4E+05	-65.8
176	α -Bromomesitylene	9.5E+06	7.5E+07	1.9E+05	100	6.2E+06 6	4.4E+07	0.0E+00	93	- 3.3E+06	-53.9

190	Tricyclazole	8.3E+06	4.1E+07	7.4E+05	100	8.5E+05	4.5E+06	5.4E+04	100	-	-871.7
198	4,4,5,8-tetramethylchromene	4.3E+07	1.9E+08	8.2E+06	100	1.8E+07	1.2E+08	7.8E+05	100	-	-135.9
202	Eugenol	1.7E+07	1.2E+08	1.0E+05	100	1.6E+06	1.2E+07	3.6E+04	100	-	-941.6
212	1H-Inden-1-one, 2,3-dihydro-3,3,4,5-pentamethyl-	1.4E+05	3.2E+05	3.5E+04	100	7.2E+04	2.9E+05	0.0E+00	82	-	-94.2
218	Indole	2.7E+06	2.5E+07	8.9E+04	100	2.0E+05	5.6E+05	0.0E+00	82	-	46.6
TOTAL AREA		3.2E+08				1.2E+08					

Esters

125	Methyl benzoate	1.3E+06	8.0E+06	7.3E+04	100	1.2E+06	5.4E+06	1.7E+05	100	-	-10.4
177	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	2.2E+07	5.4E+07	2.7E+06	100	8.9E+06	2.3E+07	1.6E+05	100	-	-142.2
220	Diisobutyl phthalate	2.7E+05	1.5E+06	0.0E+00	48	2.0E+06	1.5E+07	0.0E+00	86	-	86.4
TOTAL AREA		2.3E+07				1.2E+07					

Furans

3	Furan	1.6E+06	5.1E+06	0.0E+00	96	2.4E+05	1.7E+06	0.0E+00	46	-	-551.4
13	2,5-Dimethylfuran	7.2E+05	2.3E+06	0.0E+00	89	7.0E+05	2.3E+06	3.3E+04	100	-	-2.3
15	2-Ethyl-5-methylfuran	4.5E+06	3.7E+07	3.0E+05	100	1.9E+06	1.2E+07	8.3E+04	100	-	-131.8
44	2,2-Dimethyl-5-(1-methyl-1-propenyl)-tetrahydrofuran	2.0E+06	8.2E+06	1.5E+05	100	8.0E+05	3.6E+06	0.0E+00	96	-	-149.2

61	2-Methyl-3-(methylthio)furan	6.4E+05	1.5E+06	3.6E+04	100	8.0E+05	3.2E+06	0.0E+00	93	1.6E+05	20.2
75	5-Ethenyltetrahydro-5-trimethyl-trans-2-furanmethanol	9.0E+05	3.9E+06	7.1E+04	100	8.6E+05	6.0E+06	1.6E+04	100	-	-3.8
81	Linalool oxide	8.2E+06	5.1E+07	2.6E+05	100	4.2E+05	2.3E+06	0.0E+00	96	-	-1853.2
105	5-Methyl-2-furancarboxaldehyde	3.7E+06	9.7E+06	9.9E+05	100	5.1E+06	3.6E+07	6.3E+05	100	1.4E+06	28.3
122	Dihydro-5-methyl-2(3H)-furanone	3.4E+05	1.4E+06	4.8E+03	100	2.7E+05	1.5E+06	0.0E+00	79	-	-27.4
145	Benzofuran, 4,7-dimethyl-	2.3E+06	8.0E+06	3.0E+05	100	1.5E+06	7.9E+06	8.0E+04	100	-	-56.7
203	2-[(E)-(2-ethoxy-3,4-dimethylcyclohex-2-en-1-ylidene)methyl]furan	1.6E+06	1.2E+07	4.5E+04	100	9.8E+04	6.3E+05	1.1E+04	100	-	-1538.7
TOTAL AREA		2.6E+07				1.3E+07					

Hydrocarbons

104	2-Methyl-1-butene	1.7E+05	5.9E+05	0.0E+00	81	1.1E+05	3.6E+05	0.0E+00	82	-	-53.6
159	4,5-Dehydro-Isolongifolene	2.2E+06	1.4E+07	2.3E+05	100	1.4E+06	6.0E+06	3.9E+04	100	-	-57.6
183	4,5,9,10-Dehydroisolongifolene	2.9E+06	3.2E+07	7.9E+04	100	2.0E+06	1.2E+07	0.0E+00	89	-	-43.0
TOTAL AREA		5.3E+06				3.6E+06					

Ketones

4	Acetone	1.2E+07	2.3E+07	1.5E+06	100	1.8E+07	9.5E+07	1.2E+06	100	6.2E+06	34.8
8	Butanone	4.1E+06	1.4E+07	5.4E+05	100	7.7E+06	3.6E+07	2.7E+05	100	3.6E+06	46.8
14	2-Pentanone	2.1E+07	9.4E+07	1.7E+06	100	5.0E+07	2.4E+08	1.2E+06	100	2.9E+07	58.2

22	3-Hexanone	2.1E+06	6.0E+06	1.3E+05	100	3.6E+06	1.4E+07	2.0E+05	100	1.5E+06	40.9
27	4-Heptanone	6.1E+07	1.8E+08	5.6E+06	100	7.0E+07	3.2E+08	0.0E+00	96	9.0E+06	12.8
32	2-Heptanone	2.6E+06	5.8E+06	1.1E+05	100	6.3E+06	7.4E+07	1.8E+05	100	3.7E+06	58.8
60	3-Ethylcyclopentanone	2.0E+05	1.2E+06	0.0E+00	93	3.3E+05	4.5E+06	0.0E+00	89	1.3E+05	38.9
69	3,5,5-Trimethyl-2-cyclohexen-1-one	7.2E+05	2.1E+06	1.3E+05	100	1.4E+06	5.4E+06	3.3E+04	100	6.6E+05	48.0
82	6-Camphenone	2.8E+05	1.1E+06	3.2E+04	100	2.2E+05	1.1E+06	0.0E+00	96	-	-29.4
86	2-Decanone	2.3E+07	9.3E+07	1.4E+06	100	1.9E+07	5.4E+07	0.0E+00	93	-	-25.7
91	2-Acetylfuran	9.6E+06	3.9E+07	1.3E+06	100	1.1E+07	3.0E+07	1.0E+06	100	1.1E+06	10
94	1-(4-Methoxyphenyl)-1,3-butanedi-one	2.8E+05	1.2E+06	0.0E+00	93	4.5E+05	2.6E+06	0.0E+00	93	1.8E+05	38.7
115	4-Cyclopentene-1,3-dione	4.2E+05	8.0E+05	1.8E+05	100	6.4E+05	5.4E+06	1.2E+05	100	2.2E+05	34.8
134	Acetophenone	2.3E+06	2.6E+07	2.5E+05	100	1.2E+06	3.6E+06	1.6E+05	100	-	-90.7
139	4-Hydroxy-4-methyl-5-hexenoic acid γ -lactone	8.3E+05	3.5E+06	0.0E+00	81	7.9E+05	4.8E+06	0.0E+00	79	-	-4.1
154	1-H-Inden-1-one,2,3-dihydro-3,3,5,6-tetramethyl	2.5E+07	8.1E+07	3.6E+06	100	1.3E+07	7.5E+07	6.8E+05	100	-	-90.5
158	Cyclopenten-4-one, 1,2,3,3-tetramethyl-	6.4E+05	1.8E+06	1.6E+05	100	3.2E+05	1.5E+06	0.0E+00	89	-	-97.9
163	m-Methylacetophenone	5.5E+06	2.6E+07	5.9E+05	100	4.7E+06	4.8E+07	3.4E+05	100	-	-16.7
166	γ -Caprolactone	2.8E+05	2.0E+06	0.0E+00	96	2.7E+05	1.6E+06	0.0E+00	89	-	-0.8
168	β -Damascenone	7.9E+06	2.2E+07	1.5E+06	100	5.8E+06	4.3E+07	1.1E+05	100	-	-37.3

182	(E)-(2,4,4-Trimethylcyclohex-1,5-dien-1-yl]but-3-en-2-one	9.3E+05	3.8E+06	0.0E+00	96	3.9E+05	2.5E+06	0.0E+00	96	-	-140.4
200	2,3,3-Trimethyl-2H-inden-1-one	6.3E+05	1.9E+06	7.2E+04	100	2.0E+05	7.5E+05	0.0E+00	96	-	-215.8
210	4-(2,3,6-Trimethylphenyl)-2-butanone	1.4E+06	6.7E+06	2.6E+05	100	8.8E+05	3.3E+06	4.3E+04	100	-	-55.8
216	1-(4-Hydroxy-3,5-di-tert-butylphenyl)-2-methyl-3-morpholinopropan-1-one	1.5E+07	8.6E+07	0.0E+00	96	3.8E+05	1.4E+06	0.0E+00	46	-	-3706.2
TOTAL AREA		3.8E+08					5.3E+08				

Naphthalene derivatives

73	α -Ionene	1.2E+07	3.6E+07	0.0E+00	93	6.2E+06	4.0E+07	0.0E+00	86	-	-97.6
93	2(1H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-1,1,4a-trimethyl-	6.4E+06	3.6E+07	4.4E+05	100	1.1E+07	8.0E+07	0.0E+00	96	4.6E+06	41.6
156	1,2-Dihydro-1,1,6-trimethylnaphthalene	8.2E+07	1.7E+08	1.2E+07	100	6.0E+07	1.8E+08	4.8E+06	100	-	-37.4
186	1,7-Dimethylnaphthalene	3.7E+06	2.2E+07	4.0E+05	100	9.5E+05	4.4E+06	4.4E+04	100	-	-294.4
191	6-Hydroxy-3,8-dimethyl-5-propan-2-yl-naphthalene-1,2-dione	7.2E+06	3.2E+07	4.0E+05	100	1.9E+06	8.4E+06	9.8E+04	100	-	-272.8
208	Cadalene	5.2E+07	1.9E+08	5.8E+06	100	2.0E+07	5.9E+07	1.1E+06	100	-	-160.9
TOTAL		3.8E+08					5.3E+08				

Fatty Acids

78	Acetic acid	6.7E+06	1.8E+07	7.5E+04	100	1.7E+07	1.3E+08	0.0E+00	96	1.0E+07	60.5
114	Isobutyric acid	4.3E+05	1.5E+06	1.4E+05	100	4.4E+05	3.2E+06	0.0E+00	93	1.0E+04	2.3

116	3-Pentenoic acid, 4-methyl-	3.6E+05	1.2E+06	5.9E+04	100	4.4E+05	1.3E+06	2.9E+04	100	8.3E+04	18.7
141	Ethylmethylacetic acid	6.4E+05	2.0E+06	0.0E+00	93	1.2E+06	9.2E+06	0.0E+00	68	5.6E+05	46.8
192	Caprylic acid	7.6E+06	2.8E+07	1.3E+06	100	6.0E+06	2.5E+07	1.0E+06	100	-	-25.7
201	Pelargonic acid	1.8E+06	2.7E+06	6.2E+05	100	1.1E+06	3.3E+06	1.0E+05	100	-	-54.1
213	Capric acid	4.0E+06	9.4E+06	5.8E+05	100	2.4E+06	1.5E+07	9.0E+04	100	-	-65.4
219	Dodecanoic acid	1.3E+06	3.2E+06	2.8E+05	100	1.5E+06	8.8E+06	0.0E+00	89	1.6E+05	11.1
	TOTAL	2.3E+07				3.0E+07					

Organosulphurs

2	Methanethiol	1.2E+07	3.2E+07	3.3E+06	100	1.1E+07	4.4E+07	1.1E+06	100	-	-1.4
5	1-Propanethiol	1.8E+05	1.0E+06	0.0E+00	85	7.4E+04	7.8E+05	0.0E+00	39	-	-138.6
24	Dimethyldisulfide	1.8E+08	4.3E+08	3.7E+07	100	3.2E+08	1.3E+09	4.1E+07	100	1.4E+08	43.0
42	Methyl propyl disulfide	5.8E+05	2.0E+06	1.0E+04	100	4.9E+05	3.8E+06	0.0E+00	89	-	-19.9
45	2,4-Dimethylthiophene	3.2E+06	1.5E+07	0.0E+00	85	1.5E+06	9.3E+06	0.0E+00	75	-	-108.2
51	Methyl 2-propenyl disulfide	5.6E+06	3.3E+07	7.2E+04	100	2.7E+06	1.6E+07	1.8E+01	100	-	-103.4
97	3-(Methylthio)thiophene	4.9E+05	1.8E+06	1.0E+05	100	3.8E+05	2.2E+06	2.6E+04	100	-	-30.5
143	2,5-Dimethylthiophene	1.5E+06	3.7E+06	3.5E+05	100	1.4E+06	3.6E+06	3.1E+05	100	-	-5.3
178	Dimethyl sulfone	9.2E+05	2.1E+06	1.8E+05	100	7.5E+05	2.9E+06	0.0E+00	96	-	-22.6

TOTAL		2.1E+08				3.4E+08					
						8					
Phenols											
171	2-Chlorophenol	3.1E+05	1.2E+06	4.7E+03	100	2.9E+05	1.7E+06	0.0E+00	96	-	-5.2
173	Guaiacol	3.5E+06	2.1E+07	9.2E+03	100	3.0E+06	1.8E+07	2.7E+04	100	-	-16.3
184	2-Bromophenol	1.4E+05	2.6E+05	0.0E+00	96	2.9E+04	1.7E+05	0.0E+00	64	-	-389.4
188	Phenol	2.9E+07	9.1E+07	3.7E+02	100	5.6E+07	6.9E+08	0.0E+00	68	2.6E+07	47.6
195	p-Cresol	7.0E+07	3.6E+08	7.7E+05	100	2.5E+08	1.8E+09	7.5E+06	100	1.8E+08	72.6
196	2,4,6-Triisopropylphenol	1.5E+05	5.6E+05	0.0E+00	93	6.0E+04	4.7E+05	0.0E+00	71	-	-152
197	4-tert-Butyl-2-chlorophenol	1.9E+05	5.4E+05	0.0E+00	96	1.5E+05	4.0E+05	4.5E+04	100	-	-23.2
204	3-Hydroxybenzotrifluoride	1.1E+06	8.1E+06	8.9E+04	100	1.9E+05	8.2E+05	0.0E+00	96	-	-451.2
205	5-Isopropyl-2-methylphenol	8.9E+06	9.5E+07	4.9E+05	100	3.2E+06	1.7E+07	2.5E+05	100	-	-177.8
206	Thymol	1.4E+07	9.5E+07	1.3E+06	100	3.9E+06	2.5E+07	1.2E+05	100	-	-272.2
207	4-tert-Butyl-2-Bromophenol	3.1E+05	7.1E+05	8.0E+04	100	1.2E+05	6.2E+05	1.1E+04	100	-	-155.3
214	4-tert-Butylphenol	4.0E+05	9.4E+05	1.2E+05	100	3.9E+05	1.1E+06	1.2E+05	100	-	-2.3
215	2,4-Di-tert-butylphenol	8.9E+07	1.9E+08	1.8E+07	100	6.1E+07	1.5E+08	6.7E+06	100	-	-45.6
TOTAL		2.2E+08				3.8E+08					
						8					
Terpene Derivatives											

34	Limonene (isomer)	3.3E+05	1.9E+06	4.5E+04	100	3.3E+0 5	1.6E+06	0.0E+0 0	89	-	-1.4
90	α -Carene	1.1E+06	8.7E+06	0.0E+00	93	7.7E+0 5	3.0E+06	0.0E+0 0	89	-	-44.3
92	α -Ionone	3.6E+06	1.3E+07	4.0E+05	100	4.5E+0 6	3.0E+07	4.9E+0 4	100	8.8E+05	19.8
95	β -Ionone	1.9E+06	8.3E+06	0.0E+00	96	2.2E+0 6	1.7E+07	0.0E+0 0	89	3.2E+05	14.1
100	α -Cedrene	2.2E+06	1.6E+07	1.6E+05	100	9.8E+0 5	6.7E+06	0.0E+0 0	96	-	-123.5
107	Terpinenol	5.8E+05	1.6E+06	9.4E+04	100	6.9E+0 5	4.8E+06	7.5E+0 4	100	1.1E+05	16.4
118	(-)-Neoisomenthol	3.7E+06	3.1E+07	0.0E+00	96	3.4E+0 6	4.4E+07	1.6E+0 4	100	-	-8.5
119	<i>p</i> -Menth-1-en-4-ol	4.2E+06	3.1E+07	0.0E+00	96	3.6E+0 6	4.8E+07	0.0E+0 0	89	-	-16.1
123	Ylangene	2.1E+06	1.6E+07	4.0E+05	100	1.0E+0 6	2.6E+06	2.4E+0 3	100	-	-106.1
124	α -Caryophyllene	1.9E+06	4.2E+06	1.9E+05	100	1.4E+0 6	9.8E+06	7.3E+0 4	100	-	-37.2
126	Myrtenal	5.6E+05	3.6E+06	1.5E+04	100	4.0E+0 5	2.6E+06	0.0E+0 0	96	-	-42.4
129	Isolatedene	4.0E+06	3.1E+07	1.6E+04	100	1.2E+0 6	6.8E+06	0.0E+0 0	89	-	-235.1
130	Menthol	2.1E+07	7.7E+07	0.0E+00	96	6.1E+0 6	4.8E+07	0.0E+0 0	96	-	-246.9
131	β -Chamigrene	4.9E+06	1.6E+07	8.6E+05	100	2.9E+0 6	1.1E+07	0.0E+0 0	96	-	-71.0
132	Viridiflorene	2.3E+06	5.4E+06	4.2E+05	100	1.1E+0 6	5.6E+06	1.8E+0 5	100	-	-104.6
133	β -Guaiene	6.1E+06	1.5E+07	1.4E+06	100	3.2E+0 6	1.4E+07	2.1E+0 5	100	-	-90.1
135	α -Amorphene	6.2E+06	5.1E+07	0.0E+00	93	1.9E+0 6	1.1E+07	0.0E+0 0	89	-	-231.6

140	(S)-Carvone	1.1E+07	3.1E+07	1.4E+06	100	6.1E+0 6	3.6E+07	1.4E+0 5	100	-	-85.3
142	4,4-Dimethyl-3-(3-methylbut-3-enylidene)-2-methylenebicyclo[4.1.0]heptane	2.2E+06	1.6E+07	2.0E+05	100	9.9E+0 5	4.3E+06	8.5E+0 4	100	-	-124.2
144	α -Terpineol	9.2E+04	3.0E+05	0.0E+00	89	1.5E+0 5	6.9E+05	0.0E+0 0	61	5.7E+04	38.1
146	α -Muurokene	1.4E+06	9.3E+06	6.6E+04	100	1.0E+0 6	6.6E+06	2.2E+0 4	100	-	-43.5
147	β -Vatirene	1.9E+06	8.1E+06	1.7E+05	100	1.1E+0 6	4.7E+06	1.9E+0 4	100	-	-77.3
148	α -Chamigrene	6.1E+06	4.9E+07	0.0E+00	96	2.2E+0 6	9.7E+06	0.0E+0 0	96	-	-183.2
150	Spathulenol	2.1E+07	1.0E+08	1.9E+06	100	1.5E+0 7	8.5E+07	1.3E+0 5	100	-	-34.6
151	Phellandral	2.1E+06	1.4E+07	1.9E+05	100	9.4E+0 5	3.3E+06	1.5E+0 4	100	-	-119.6
161	α -Curcumene	1.4E+07	7.3E+07	9.2E+05	100	5.7E+0 6	4.0E+07	1.8E+0 4	100	-	-140.1
167	9-Isopropyl-1-methyl-2-methylene-5-oxatricyclo[5.4.0.0(3,8)]undecane	3.8E+06	1.4E+07	1.7E+05	100	3.0E+0 6	3.4E+07	1.7E+0 4	100	-	-26.6
169	Calamenene	2.4E+07	1.3E+08	9.4E+05	100	1.4E+0 7	5.9E+07	3.5E+0 5	100	-	-73.7
179	α -Calacorene	1.3E+07	7.1E+07	4.8E+05	100	3.9E+0 6	2.2E+07	6.0E+0 4	100	-	-236.0
187	Dehydro- β -Ionone	6.9E+06	1.9E+07	4.4E+05	100	1.7E+0 6	5.9E+06	0.0E+0 0	89	-	-314.0
193	γ -Muurokene	5.8E+06	1.6E+07	5.1E+05	100	9.2E+0 6	7.1E+07	1.8E+0 5	100	3.4E+06	37.1
199	(8 <i>S</i> ,8 <i>aS</i>)-3,8-dimethyl-4-propan-2-ylidene-1,2,6,7,8,8 <i>a</i> -hexahydroazulen-5-one	8.8E+05	4.7E+06	4.7E+04	100	3.6E+0 5	1.7E+06	2.9E+0 4	100	-	-146.1

209	2,4a-Methanonaphthalen-7(4aH)-one, 1,2,3,4,5,6-hexahydro-1,1,5,5-tetramethyl-, (2s-cis)-	8.2E+06	7.5E+07	3.4E+05	100	1.1E+07	6.6E+07	4.6E+04	100	2.6E+06	24.0
211	ar-Turmerone	4.2E+06	2.7E+07	4.8E+05	100	4.0E+06	2.2E+07	8.4E+04	100	- 2.7E+05	-6.8
	TOTAL	1.9E+08				1.2E+08					
Other Compounds											
1	1,2-Diaminopropane	8.5E+07	2.6E+08	5.7E+07	100	8.6E+07	2.4E+08	2.2E+07	100	8.6E+05	1.0
23	3,4,5-Trimethylpyrazole	4.5E+05	1.7E+06	2.6E+04	100	4.5E+05	1.7E+06	0.0E+00	93	- 2,1E+03	-0.5
26	Linaloyl oxide	1.6E+05	5.4E+05	0.0E+00	93	5.2E+05	4.0E+06	0.0E+00	86	3,6E+05	69.3
149	3,6-dimethyl-2H-indazole	1.6E+06	6.3E+06	3.3E+05	100	7.2E+05	2.7E+06	0.0E+00	96	- 9.3E+05	-129.3
217	Benzoic acid	4.8E+06	2.5E+07	8.7E+03	100	9.0E+06	9.8E+07	2.1E+05	100	8.6E+05	1.0
	TOTAL	8.7E+07				8.7E+07					

Table S2. Results of the target groups discrimination following the use of different classification algorithms. The variables (uVOMs) used in each assay are described in Table 4.

All data processing				
<i>Algorithm</i>	<i>Accuracy</i>	<i>Sensitivity (CTL)</i>	<i>Specificity (LC)</i>	<i>AUC</i>
<i>SVM</i>	96.33	92.59	100	0.975
<i>RF</i>	94.66	88.88	100	0.984
<i>PLS-DA</i>	96.33	96.29	96.42	0.989
<i>MLP</i>	98	96.29	100	0.999
Upon CFS variable selection				
<i>Algorithm</i>	<i>Accuracy</i>	<i>Sensitivity (CTL)</i>	<i>Specificity (LC)</i>	<i>AUC</i>
<i>SVM</i>	96.31	92.59	100	0.996
<i>RF</i>	96.46	96.29	96.42	0.997
<i>PLS-DA</i>	96.31	92.59	100	0.998
<i>MLP</i>	97.83	97.40	98.21	0.999
Upon CFS + F-score variable selection				
<i>Algorithm</i>	<i>Accuracy</i>	<i>Sensitivity (CTL)</i>	<i>Specificity (LC)</i>	<i>AUC</i>
<i>SVM</i>	100	100	100	1
<i>RF</i>	98.33	96.29	100	0.999
<i>PLS-DA</i>	96	92.59	100	0.997
<i>MLP</i>	100	97.40	98.21	0.999

Table S3. Pathway analysis results

<i>Pathway name</i>	<i>Total com-pounds</i>	<i>Match status</i>	<i>p</i>	<i>-log(p)</i>	<i>Holm p</i>	<i>FDR</i>	<i>Impact</i>
Pyruvate metabolism	22	1	0.057608	1.2395	0.28804	0.096014	0.06065
Glycolysis / Gluconeogenesis	26	1	0.057608	1.2395	0.28804	0.096014	0.02906
Glyoxylate and dicarboxylate metabolism	32	1	0.057608	1.2395	0.28804	0.096014	0
Fatty acid biosynthesis	47	3	0.23999	0.6198	0.47998	0.29999	0
Sulfur metabolism	8	1	0.95175	0.021475	0.95175	0.95175	0

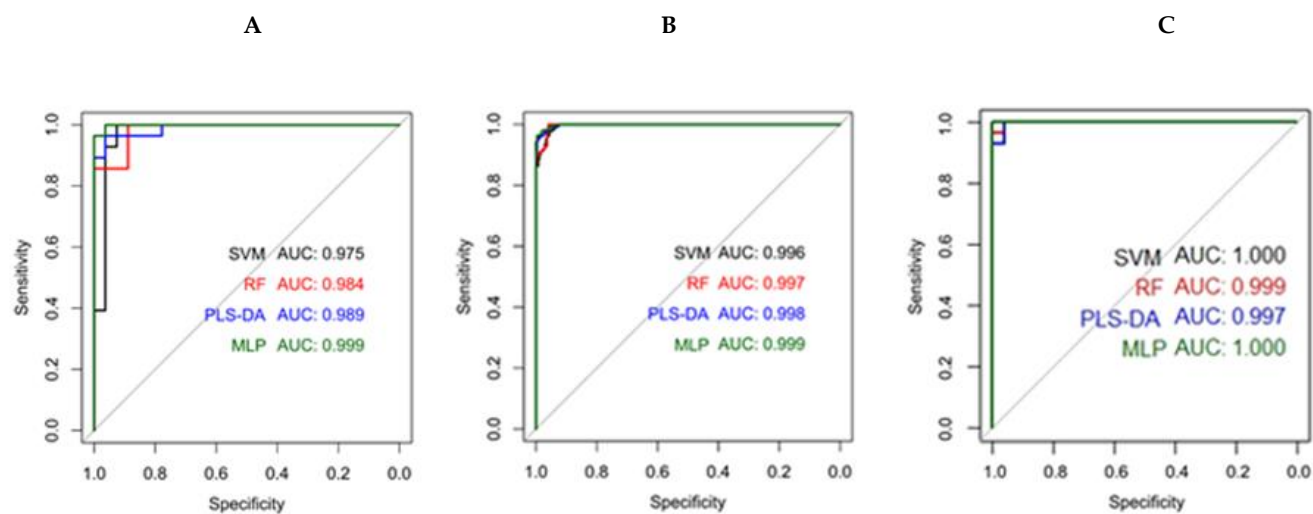


Figure S1. Performance of the variables identified with the different algorithms described in Table 2 and Table S3.

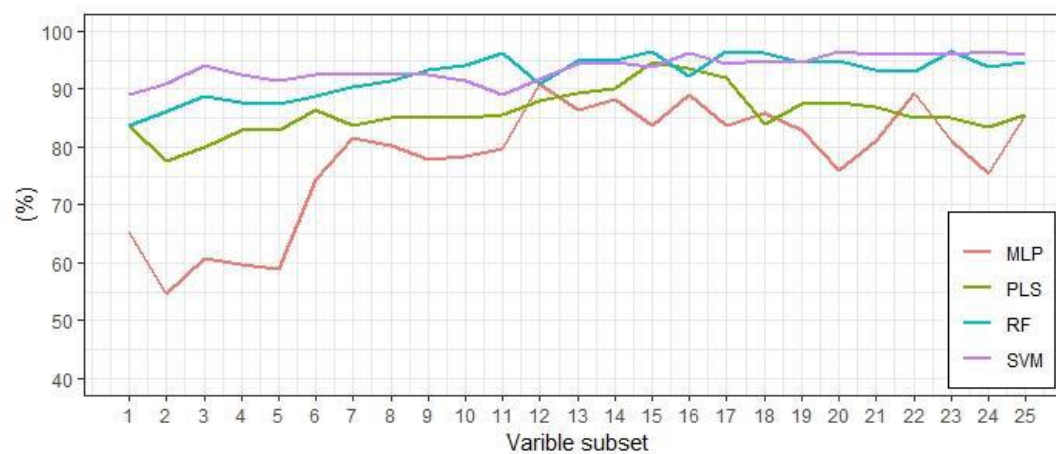


Figure S2. Results of the classification of the 25 groups generated from the F-score classification of the uVOMs identified in this work.