

Supplemental Material

TABLE S1. Retention times, retention indices, quantification ions of studied compounds.

	LRI ¹	Identification ²	Quantitation ion <i>m/z</i>	Qualifier ions <i>m/z</i>	LOD ($\mu\text{g/L}$)	LOQ ($\mu\text{g/L}$)	Recovery RSD % ($\mu\text{g/L}$)	R ²
Linalool	1547	RS	71	121, 93	0.08	0,25	91.2 (10.7)	0.9997
Geraniol	1860	RS	93	123, 121, 105	0.06	0,20	89.3 (12.1)	0.9978
β -Citronellol	1771	RS	69	82, 81, 67	0.07	0,21	95.7 (11.0)	0.9993
α -Terpineol	1701	RS	136	121, 93, 59	0.23	0,70	105.1 (22.3)	0.9927
3-Carene	1150	RS	93	91, 79	0.03	0,10	85.7 (9.87)	0.9965
α -Phellandrene	1180	RS	93	136, 91	0.11	0,34	87.9 (14.6)	0.9994
γ -Terpinene	1175	RS	121	136, 93	0.03	0,1	90.7 (12.4)	0.9955
α -Terpinene	1188	RS	121	93, 126	0.03	0,10	111.2 (10.5)	0.9998
Limonene	1198	RS	136	139, 125, 111	0.03	0,10	99.4 (10.5)	0.9975
1,4-Cineole	1186	RS	154	139, 125, 111	0.003	0,01	98.7 (9.5)	0.9998
1,8-Cineole	1217	RS	154	139, 111, 108	0.003	0,01	96.9 (7.2)	0.9999
p-Cymene	1271	RS	119	134, 91	0.04	0,10	101.3 (25.0)	0.9999
Terpinolene	1283	RS	121	136, 93	0.04	0,10	100.6 (17.4)	0.9993
Terpinen-1-ol	1581	LRI MS	136	121, 81	-	-	-	-
Terpinen-4-ol	1614	RS	71	111, 93, 86	0.02	0,05	87.9 (10.5)	0.9996
Nerol	1812	RS	93	121, 84, 69	0.04	0,12	90.7 (18.7)	0.9989
β -Damascenone	1825	RS	69	190, 121, 105	0.01	0,03	97.8 (8.50)	0.9982
α -Ionone	1853	RS	121	192, 136	0.003	0,01	89.5 (3.7)	0.9974
β -Ionone	1951	RS	177	192, 135	0.3	1,2	86.7 (10.1)	0.9943
TDN	1745	RS	157	172, 142	0.1	0,3	94.8 (7.8)	0.9996
TPB	1828	LRI MS	172	157, 142	-	-	-	-
Vitispirane	1524	LRI MS	192	177, 93	-	-	-	-

¹ Linear Retention Index (LRI) were determined on DB-WAX polar column, as described by van Den Dool and Kratz (1963).

² RS identified using reference standard; LRI MS tentatively identified by comparing the Linear Retention Index and mass spectra with those of literature.