

Date : February 14, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23B08-PTH03

Customer identification : Vetiver ORGANIC - Madagascar - V80108R

Type : Essential oil

Source : *Vetiveria zizanioides*

Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-014  - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Amélie Simard, Analyste

Analysis date : February 13, 2023

Checked and approved by :

Alexis St-Gelais, Ph. D., Chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Orange brownish viscous liquid

Refractive index: 1.5263 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Furfural	0.05	Furan
Unknown	0.07	Sesquiterpene
2-Norprezizene	0.06	Sesquiterpene
Unknown	0.14	Unknown
12-Norisoziza-5-ene	0.85	Norsesquiterpene
Unknown	0.28	Norsesquiterpene
Cyclosativene II	0.01	Sesquiterpene
Unknown	0.20	Norsesquiterpene
α -Ylangene	0.05	Sesquiterpene
6-epi-Nigritene	1.43	Norsesquiterpene
Nigritene	2.84	Norsesquiterpene
Unknown	0.19	Unknown
Acora-3,7(14)-diene	0.13	Sesquiterpene
β -Funebrene	0.13	Sesquiterpene
β -Cedrene	0.14	Sesquiterpene
Prezizaene	0.43	Sesquiterpene
Unknown	0.79	Norsesquiterpene
Khusimene	0.48	Sesquiterpene
(E)-Isoeugenol	0.34	Phenylpropanoid
Unknown	0.39	Sesquiterpene
Unknown	0.20	Sesquiterpene
Unknown	0.38	Sesquiterpene
α -Amorphene	0.91	Sesquiterpene
α -Vetispirene	1.86	Sesquiterpene
β -Vetispirene	0.77	Sesquiterpene
δ -Selinene	0.66	Sesquiterpene
γ -Amorphene	0.07	Sesquiterpene
Eudesma-2,4(15),11-triene	0.14	Sesquiterpene
δ -Amorphene	0.41	Sesquiterpene
Nootkatene	0.32	Sesquiterpene
Spirovetiva-1(10),7(11)-diene	0.49	Sesquiterpene
<i>trans</i> -Calamenene	0.10	Sesquiterpene
δ -Cadinene	0.29	Sesquiterpene
γ -Vetivenene	1.89	Sesquiterpene
α -Calacorene	0.59	Sesquiterpene
α -Elemol	0.06	Sesquiterpenic alcohol
β -Vetivenene	2.40	Sesquiterpene
Eremophila-1(10),11-dien-9 β -ol	1.37	Sesquiterpenic alcohol
Unknown	0.32	Oxygenated sesquiterpene
Gynuradienol?	0.21	Sesquiterpenic alcohol
Unknown	0.64	Sesquiterpene
Khusimone	1.05	Norsesquiterpenic ketone
Junenol	0.48	Sesquiterpenic alcohol
10-epi- γ -Eudesmol	0.45	Sesquiterpenic alcohol
Unknown	0.52	Sesquiterpene

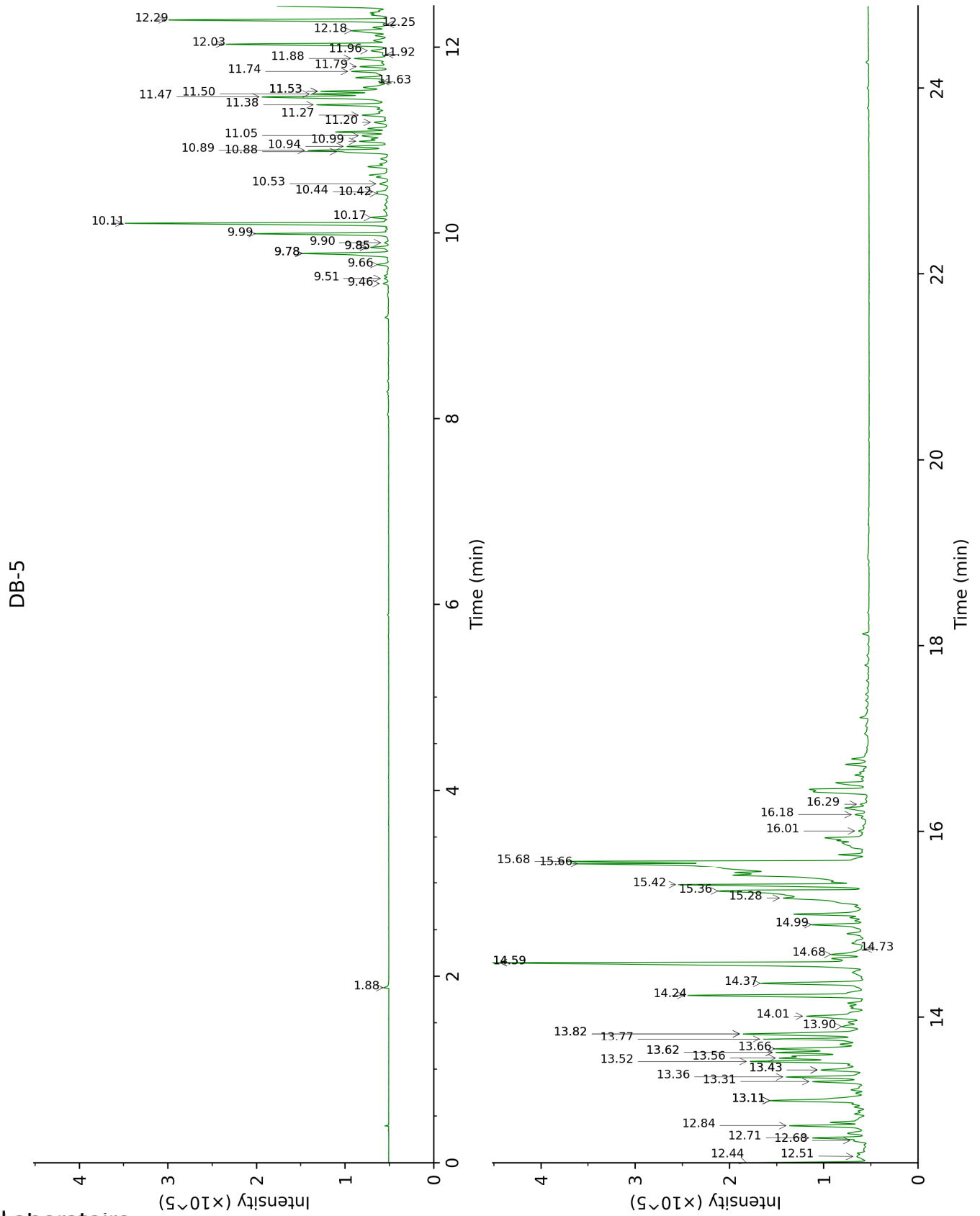
Selin-6-en-4 α -ol isomer	0.25	Sesquiterpenic alcohol
γ -Eudesmol	0.80	Sesquiterpenic alcohol
Unknown	1.19	Unknown
Unknown	0.51	Unknown
Unknown	0.38	Oxygenated sesquiterpene
Unknown	1.49	Oxygenated sesquiterpene
Cyclocopacamphan-12-ol, epimer A	1.95	Sesquiterpenic alcohol
Unknown	0.78	Unknown
Unknown	0.37	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer B	1.50	Sesquiterpenic alcohol
Zizanol	1.52	Sesquiterpenic alcohol
Khusiol	1.31	Sesquiterpenic alcohol
epi-Zizanone	0.46	Sesquiterpenic ketone
Zizanal	0.52	Sesquiterpenic aldehyde
Unknown	1.25	Oxygenated sesquiterpene
Unknown	2.34	Oxygenated sesquiterpene
Vetiselinenol	1.58	Sesquiterpenic alcohol
Unknown	0.44	Oxygenated sesquiterpene
Khusimol	5.51	Sesquiterpenic alcohol
10-epi-Acora-3,11-dien-15-al?	0.80	Sesquiterpenic aldehyde
Unknown	0.14	Oxygenated sesquiterpene
Unknown	0.98	Unknown
Isozizanoic acid	4.80	Sesquiterpenic acid
(Z)-Isovalencenal	0.48	Sesquiterpenic aldehyde
β -Vetivone	2.44	Sesquiterpenic ketone
Zizanoic acid	12.62	Sesquiterpenic acid
α -Vetivone	3.56	Sesquiterpenic ketone
(E)-Isovalencenyl acetate?	0.21	Sesquiterpenic ester
Isovalencenal isomer II?	0.19	Sesquiterpenic aldehyde
Isovalencenal isomer I?	0.13	Sesquiterpenic aldehyde
Consolidated total	76.08%	

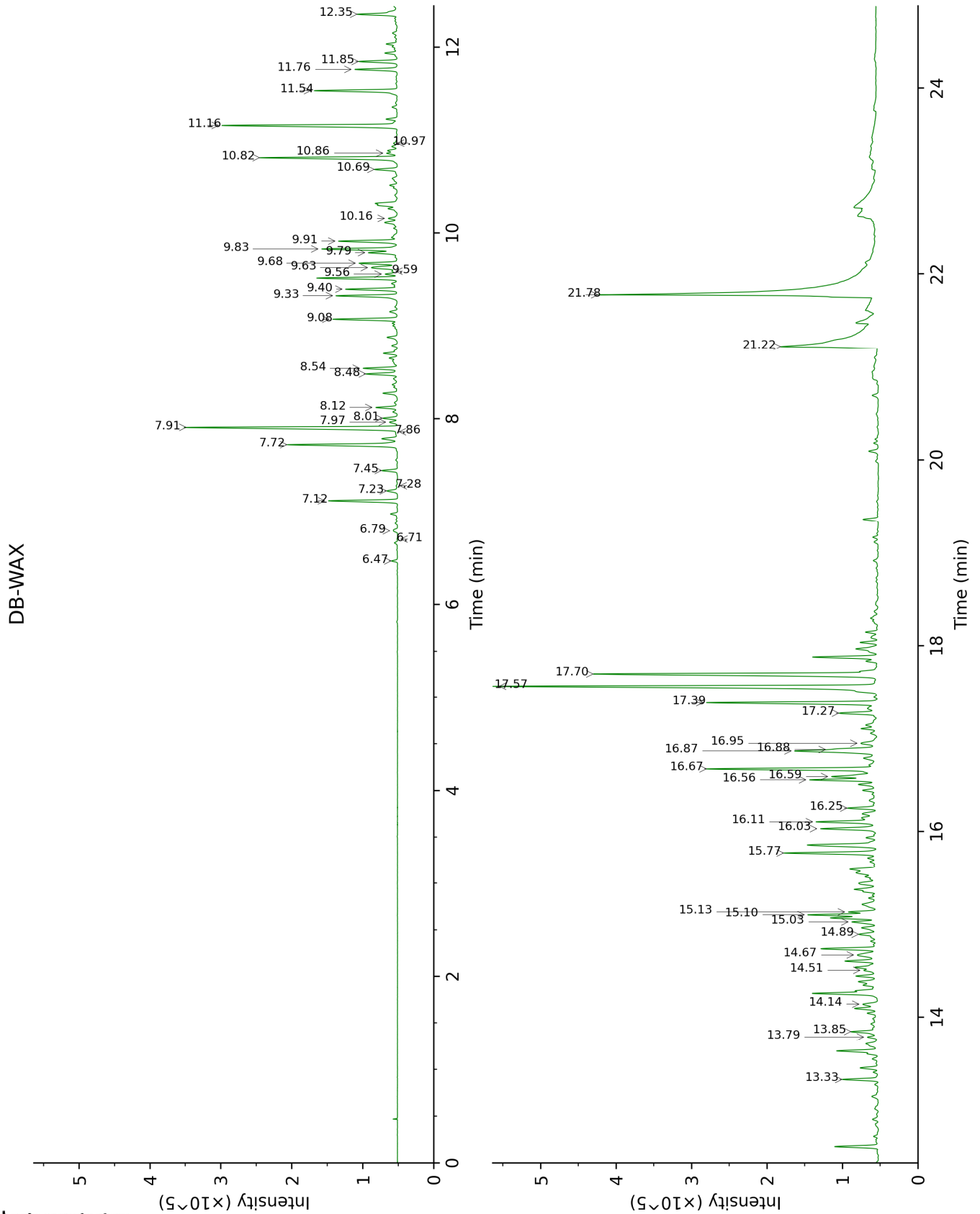
Note: no correction factor was applied

About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm is set to prioritize data from the most standard DB-5 column, and smallest values so as to avoid overestimating individual content. This process is semi-automatic. Advanced users are invited to consult the "Full analysis data" table after the chromatograms in this report to access the full untreated data and perform their own calculations if needed.

Unknowns: Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Furfural	1.88	829	0.05	6.47	1414	0.07
Unknown [m/z 120, 91 (31), 92 (23), 121 (10), 105 (9), 119 (6)...202 (1)]	9.46	1336	0.07			
2-Norprezizene	9.51	1340	0.06	7.28	1474	0.02
Unknown [m/z 119, 91 (23), 120 (17), 118 (11), 92 (7), 105 (6)...]	9.66	1350	0.14	7.23	1470	0.17
12-Norisoziza-5-ene	9.78*	1359	1.13	7.12	1462	0.85
Unknown [m/z 145, 188 (95), 117 (91), 173 (80), 91 (65), 131 (64)]	9.78*	1359	[1.13]			
Cyclosativene II	9.85*	1364	0.21	6.70	1431	0.01
Unknown [m/z 119, 147 (85), 161 (75), 91 (69), 105 (62), 134 (60), 190 (43)]	9.85*	1364	[0.21]	7.45	1486	0.20
α-Ylangene	9.90	1367	0.05	6.79	1438	0.04
6-epi-Nigritene	9.99	1374	1.43	7.72	1507	1.53
Nigritene	10.10	1382	2.84	7.91	1522	2.98
Unknown [m/z 119, 91 (24), 120 (17), 118 (10), 92 (8), 41 (7), 105 (6)...]	10.17	1386	0.19	8.01	1529	0.19
Acora-3,7(14)-diene	10.42	1404	0.13	7.97	1526	0.12
β-Funebrene	10.44	1405	0.13	7.86	1518	0.04
β-Cedrene	10.53	1412	0.14	8.12	1538	0.28
Prezizaene	10.88†	1438	1.25	8.48	1566	0.43
Unknown [m/z 175, 190 (73), 161 (65), 119 (40), 105 (35), 91 (28), 133 (23)]	10.89†	1439	[1.25]	9.08	1613	0.79
Khusimene	10.94	1442	0.48	8.54	1571	0.45
(E)-Isoeugenol	10.99	1446	0.34	16.25	2273	0.45
Unknown [m/z 119, 190 (99), 175 (95), 105 (71), 91 (59), 120 (57)... 204 (2)]	11.05	1451	0.39			
Unknown [m/z 119, 120 (31), 83 (23), 105 (22), 91 (21), 81 (18)... 202 (9)]	11.20	1462	0.20	9.56	1652	0.15
Unknown [m/z 145, 202 (85), 159 (64), 187 (39), 131 (35), 117 (34)]	11.27	1467	0.38	9.63	1658	0.47

α-Amorphene	11.38	1476	0.91	9.33	1633	0.84
α-Vetispirene	11.47	1482	1.86	9.83	1674	1.02
β-Vetispirene	11.50	1484	0.77	9.91	1681	0.80
δ-Selinene	11.53*	1486	0.75	9.40	1639	0.66
γ-Amorphene	11.53*	1486	[0.75]	9.59	1655	0.07
Eudesma-2,4(15),11-triene	11.63	1494	0.14	10.86	1761	0.15
δ-Amorphene	11.74	1502	0.41	9.68	1662	0.50
Nootkatene	11.79	1506	0.32	10.69	1746	0.30
Spirovetiva-1(10),7(11)-diene	11.88	1513	0.49	9.79	1671	0.39
trans-Calamenene	11.92	1516	0.10	10.97	1770	0.05
δ-Cadinene	11.96	1519	0.29	10.16	1701	0.13
γ-Vetivenene	12.03	1525	1.89	10.82	1756	1.84
α-Calacorene	12.18	1536	0.59	11.85	1846	0.50
α-Elemol	12.25	1542	0.06	13.79	2025	0.18
β-Vetivenene	12.29	1545	2.40	11.16	1786	2.38
Eremophila-1(10),11-dien-9β-ol	12.44	1557	1.37	11.54	1819	1.09
Unknown [m/z 81, 200 (55), 143 (36), 93 (33), 91 (32), 185 (31), 129 (27), 128 (21)...]	12.51	1562	0.32			
Gynuradienol?	12.68	1576	0.21	14.14	2059	0.31
Unknown [m/z 202, 187 (63), 145 (43), 159 (34), 131 (29), 91 (22), 117 (20)]	12.71	1578	0.64	11.76	1839	0.54
Khusimone	12.84	1588	1.05			
Junenol	13.11*	1609	1.83	13.33	1982	0.48
10-epi-γ-Eudesmol	13.11*	1609	[1.83]	13.85	2031	0.45
Unknown [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	13.11*	1609	[1.83]	12.35	1891	0.52
Selin-6-en-4α-ol isomer	13.11*	1609	[1.83]	14.51	2094	0.25
γ-Eudesmol	13.31	1626	0.80	14.67	2111	0.57
Unknown [m/z 145, 59 (97), 161 (87), 218 (76), 43 (76), 179 (63)...]	13.36	1630	1.19			
Unknown [m/z 43, 91 (87), 71 (83), 93 (77), 95 (75), 135 (74)...]	13.43*	1636	0.89			
Unknown [m/z 187, 93 (35), 81 (34), 79 (31), 41 (30), 91 (30), 107 (29)... 220 (4)]	13.43*	1636	[0.89]	15.13	2157	0.38

Unknown [m/z 121, 107 (69), 93 (64), 79 (60), 177 (59), 136 (58), 91 (57), 41 (56)... 220 (21)]	13.52	1644	1.49	15.10	2154	0.87
Cyclocopacamphan-12-ol, epimer A	13.56	1646	1.95	16.03	2250	0.93
Unknown [m/z 159, 91 (58), 105 (54), 93 (51), 81 (50), 177 (44)...]	13.62*	1652	1.15			
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.62*	1652	[1.15]	14.89	2133	0.37
Cyclocopacamphan-12-ol, epimer B	13.66	1655	1.50	16.11	2257	0.94
Zizanol	13.77	1664	1.52	16.56	2305	0.91
Khusiol	13.82*	1668	2.29	15.77	2222	1.31
epi-Zizanone	13.82*	1668	[2.29]	15.03	2146	0.46
Zizanal	13.90	1675	0.52	16.95	2347	0.45
Unknown [m/z 145, 147 (98), 105 (93), 159 (91), 91 (90), 119 (76)...220 (30)]	14.01	1684	1.25			
Unknown [m/z 189, 159 (82), 133 (44), 91 (29), 105 (29), 205 (25)... 220 (13)]	14.24	1702	2.34	16.67	2318	2.40
Vetiselinenol	14.37	1714	1.58	16.87	2338	1.37
Unknown [m/z 189, 187 (29), 159 (23), 43 (20), 133 (16)...]	14.59*	1733	5.96			
Khusimol	14.59*	1733	[5.96]	17.57	2415	5.51
10-epi-Acora-3,11-dien-15-al?	14.68	1740	0.80			
Unknown [m/z 91, 105 (89), 79 (84), 93 (77), 107 (67), 189 (64), 145 (62), 119 (61)... 220 (16)...]	14.73	1745	0.14			
Unknown [m/z 174, 131 (37), 159 (25), 91 (20), 175 (14)...]	15.00	1768	0.98	17.27	2382	0.60
Isozizanoic acid	15.28†	1793	5.97	21.22	2854	4.80
(Z)-Isovalencenal	15.36†	1799	[5.97]	16.88	2340	0.48
β-Vetivone	15.42	1805	2.44	17.38	2395	2.24
Zizanoic acid	15.66	1826	12.62	21.78	2927	10.52
α-Vetivone	15.68	1828	3.56	17.70	2430	4.34

(E)-Isovalencenyl acetate?	16.01	1858	0.21	16.59	2309	0.82
Isovalencenal isomer II?	16.18	1874	0.19			
Isovalencenal isomer I?	16.29	1884	0.13			
Total identified		67.77%			55.31%	
Total reported		77.48%			62.95%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

†: Peaks apexes were resolved, but peaks overlapped and were summed for analysis

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index