

Date : January 28, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 22A14-PTH07

**Customer identification :** Vetiver Organic - Madagascar - V80106212R

**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 :** Sylvain Mercier, M. Sc., Chimiste 2014-005

**Analysis date :** January 26, 2022

Checked and approved by :

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

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#### *P*HYSICO*C*HEMICAL *D*ATA

**Physical aspect:** Brown viscous liquid

**Refractive index:**  $1.5267 \pm 0.0003$  (20 °C; method PC-MAT-016)

#### *C*ONCLUSION

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	0.03	Furan
4-Vinylguaiacol	0.05	Simple phenolic
Unknown	0.05	Sesquiterpene
2-Norprenzene	0.05	Sesquiterpene
Unknown	0.10	Unknown
Unknown	0.27	Norsesquiterpene
Cyclosativene II	0.01	Sesquiterpene
12-Norisoziza-5-ene	0.61	Norsesquiterpene
Unknown	0.14	Norsesquiterpene
$\alpha$ -Ylangene	0.04	Sesquiterpene
6-epi-Nigritene	1.04	Norsesquiterpene
Nigritene	2.22	Norsesquiterpene
Unknown	0.15	Unknown
Acora-3,7(14)-diene	0.12	Sesquiterpene
$\beta$ -Funebrene	0.14	Sesquiterpene
$\beta$ -Cedrene	0.10	Sesquiterpene
Prezizaene	0.42	Sesquiterpene
Unknown	0.89	Norsesquiterpene
Khusimene	0.43	Sesquiterpene
(E)-Isoeugenol	0.42	Phenylpropanoid
Unknown	0.40	Sesquiterpene
Unknown	0.19	Sesquiterpene
Unknown	0.51	Sesquiterpene
$\alpha$ -Amorphene	1.18	Sesquiterpene
$\alpha$ -Vetispirene	0.96	Sesquiterpene
$\beta$ -Vetispirene	0.86	Sesquiterpene
$\gamma$ -Amorphene	0.16	Sesquiterpene
$\delta$ -Selinene	0.78	Sesquiterpene
Eudesma-2,4(15),11-triene	0.43	Sesquiterpene
$\delta$ -Amorphene	0.71	Sesquiterpene
Nootkatene	0.32	Sesquiterpene
Spirovetiva-1(10),7(11)-diene	0.61	Sesquiterpene
trans-Calamenene	0.10	Sesquiterpene
$\delta$ -Cadinene	0.28	Sesquiterpene
$\gamma$ -Vetivenene	2.24	Sesquiterpene
$\alpha$ -Calacorene	0.61	Sesquiterpene
$\beta$ -Vetivenene	2.89	Sesquiterpene
$\alpha$ -Elemol	0.19	Sesquiterpenic alcohol
Eremophila-1(10),11-dien-9 $\beta$ -ol	1.70	Sesquiterpenic alcohol
Unknown	0.20	Oxygenated sesquiterpene
Gynuradienol?	0.10	Sesquiterpenic alcohol
Unknown	0.99	Sesquiterpene
Khusimone	0.84	Norsesquiterpenic ketone
Unknown	0.95	Sesquiterpene
10-epi- $\gamma$ -Eudesmol	0.50	Sesquiterpenic alcohol

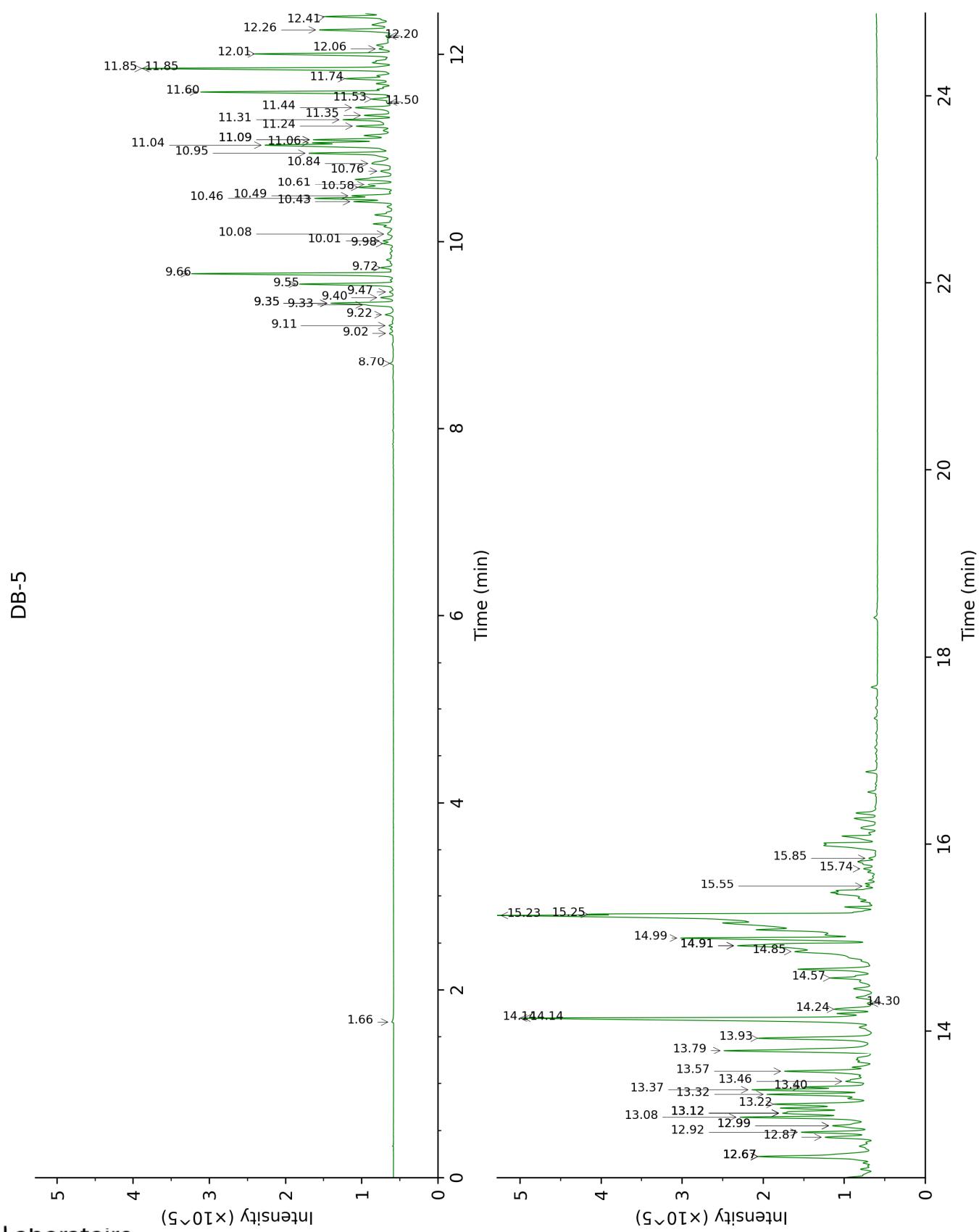
Selin-6-en-4a-ol isomer	0.61	Sesquiterpenic alcohol
Junenol	0.48	Sesquiterpenic alcohol
$\gamma$ -Eudesmol	0.79	Sesquiterpenic alcohol
Unknown	1.03	Unknown
Unknown	0.65	Unknown
Unknown	0.38	Oxygenated sesquiterpene
Unknown	1.93	Oxygenated sesquiterpene
Unknown	2.06	Unknown
Cyclocopacamphan-12-ol, epimer A	0.98	Sesquiterpenic alcohol
Unknown	0.29	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer B	1.62	Sesquiterpenic alcohol
Zizanol	1.40	Sesquiterpenic alcohol
Khusiol	1.62	Sesquiterpenic alcohol
epi-Zizanone	0.89	Sesquiterpenic ketone
Zizanal	0.44	Sesquiterpenic aldehyde
Unknown	1.49	Oxygenated sesquiterpene
Unknown	2.79	Oxygenated sesquiterpene
Vetiselinol	2.01	Sesquiterpenic alcohol
Khusimol	4.64	Sesquiterpenic alcohol
Unknown	1.38	Oxygenated sesquiterpene
10-epi-Acora-3,11-dien-15-al?	0.71	Sesquiterpenic aldehyde
Unknown	0.15	Oxygenated sesquiterpene
Unknown	0.58	Unknown
Nootkatone	1.13	Sesquiterpenic ketone
Isozizanoic acid	4.72	Sesquiterpenic acid
(Z)-Isovalencenal	0.34	Sesquiterpenic aldehyde
$\beta$ -Vetivone	2.71	Sesquiterpenic ketone
$\alpha$ -Vetivone	4.79	Sesquiterpenic ketone
Zizanoic acid	9.81	Sesquiterpenic acid
(E)-Isovalencenyl acetate?	0.10	Sesquiterpenic ester
Isovalencenal isomer II?	0.17	Sesquiterpenic aldehyde
Isovalencenal isomer I?	0.08	Sesquiterpenic aldehyde
<b>Consolidated total</b>	<b>78.74%</b>	

Note: no correction factor was applied

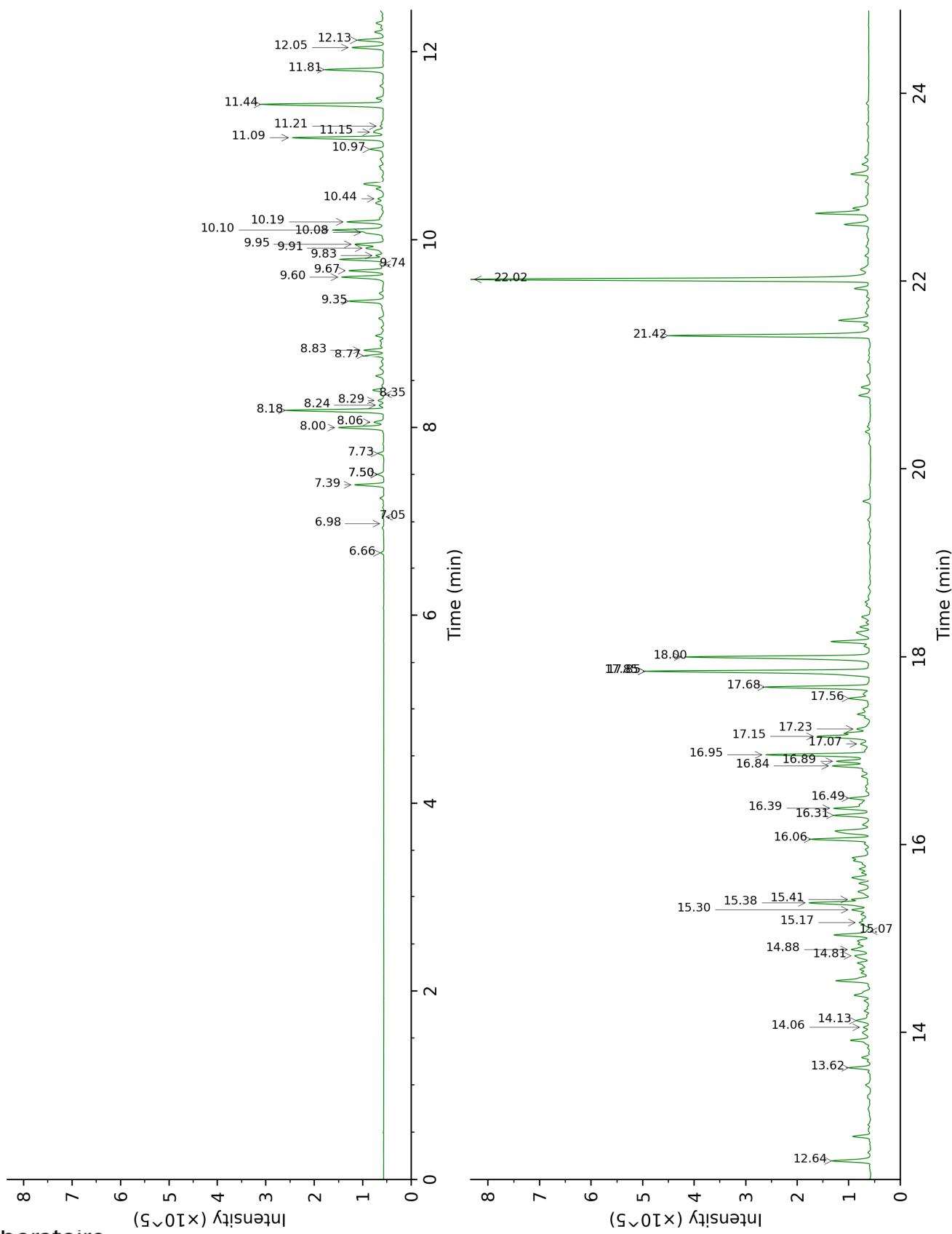
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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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DB-WAX



Laboratoire  
**PhytoChemia**

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Furfural	1.66	831	0.03	6.66	1410	0.07
4-Vinylguaiacol	8.70	1312	0.05	15.08	2126	0.07
Unknown [m/z 120, 91 (31), 92 (23), 121 (10), 105 (9), 119 (6)...202 (1)]	9.02	1335	0.05			
2-Norprezizene	9.11	1341	0.05	7.50*	1472	0.16
Unknown [m/z 119, 91 (23), 120 (17), 118 (11), 92 (7), 105 (6)...]	9.22	1349	0.10	7.50*	1472	[0.16]
Unknown [m/z 145, 188 (95), 117 (91), 173 (80), 91 (65), 131 (64)]	9.33†	1356	0.89			
Cyclosativene II	9.34*†	1358	[0.89]	6.98	1433	0.01
12-Norisoziza-5-ene	9.34*†	1358	[0.89]	7.39	1464	0.61
Unknown [m/z 119, 147 (85), 161 (75), 91 (69), 105 (62), 134 (60), 190 (43)]	9.40	1362	0.14	7.73	1489	0.14
α-Ylangene	9.47	1366	0.04	7.05	1439	0.04
6-epi-Nigritene	9.55	1372	1.04	8.00	1510	1.13
Nigritene	9.66	1380	2.22	8.18	1524	2.25
Unknown [m/z 119, 91 (24), 120 (17), 118 (10), 92 (8), 41 (7), 105 (6)...]	9.72	1384	0.15	8.29	1532	0.14
Acora-3,7(14)-diene	9.98	1403	0.12	8.24	1528	0.11
β-Funebrene	10.01	1405	0.14	8.06	1514	0.24
β-Cedrene	10.08	1410	0.10	8.35	1537	0.07
Prezizaene	10.43	1436	0.42	8.77	1569	0.45
Unknown [m/z 175, 190 (73), 161 (65), 119 (40), 105 (35), 91 (28), 133 (23)]	10.46	1439	0.89	9.35	1615	0.79
Khusimene	10.49	1441	0.43	8.83	1574	0.44
(E)-Isoeugenol	10.58	1447	0.42	16.49	2271	0.52
Unknown [m/z 119, 190 (99), 175 (95), 105 (71), 91 (59), 120 (57)... 204 (2)]	10.61	1450	0.40			
Unknown [m/z 119, 120 (31), 83 (23), 105 (22), 91 (21), 81 (18)... 202 (9)]	10.76	1461	0.19	9.74	1647	0.13
Unknown [m/z 145, 202 (85), 159 (64),	10.84	1467	0.51	9.91	1661	0.56

187 (39), 131 (35), 117 (34)]						
α-Amorphene	10.95	1475	1.18	9.60	1636	1.01
α-Vetispirene	11.04†	1482	2.82	10.10†	1676	[1.57]
β-Vetispirene	11.06†	1483	[2.82]	10.19	1683	0.86
γ-Amorphene	11.09*	1486	0.92	9.83	1654	0.16
δ-Selinene	11.09*	1486	[0.92]	9.67	1641	0.78
Eudesma-2,4(15),11-triene	11.24	1497	0.43	11.15	1764	0.37
δ-Amorphene	11.31	1502	0.71	9.95	1664	0.70
Nootkatene	11.35	1505	0.32	10.97	1749	0.35
Spirovetiva-1(10),7(11)-diene	11.44	1512	0.61	10.08†	1674	1.57
trans-Calamenene	11.50	1516	0.10	11.21	1770	0.08
δ-Cadinene	11.53	1519	0.28	10.44	1704	0.14
γ-Vetivenene	11.60	1525	2.24	11.09	1759	2.15
α-Calacorene	11.74	1536	0.61	12.13	1849	0.59
β-Vetivenene	11.85*	1545	3.00	11.44	1789	2.89
α-Elemol	11.85*	1545	[3.00]	14.06	2027	0.19
Eremophila-1(10),11-dien-9β-ol	12.01	1557	1.70	11.81	1822	1.36
Unknown [m/z 81, 200 (55), 143 (36), 93 (33), 91 (32), 185 (31), 129 (27), 128 (21)...]	12.06	1561	0.20			
Gynuradienol?	12.20	1572	0.10			
Unknown [m/z 202, 187 (63), 145 (43), 159 (34), 131 (29), 91 (22), 117 (20)]	12.26	1577	0.99	12.05	1842	0.71
Khusimone	12.41	1588	0.84			
Unknown [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	12.67*	1609	2.41	12.64	1895	0.95
10-epi-γ-Eudesmol	12.67*	1609	[2.41]	14.13	2034	0.50
Selin-6-en-4α-ol isomer	12.67*	1609	[2.41]	14.81	2100	0.61
Junenol	12.67*	1609	[2.41]	13.62	1985	0.48
γ-Eudesmol	12.87	1626	0.79	14.88	2107	0.69
Unknown [m/z 145, 59 (97), 161 (87), 218 (76), 43 (76), 179 (63)...]	12.92	1630	1.03			
Unknown [m/z 43, 91 (87), 71 (83), 93 (77), 95 (75), 135 (74)...]	12.99*	1636	1.02			
Unknown [m/z 187, 93 (35), 81 (34), 79]	12.99*	1636	[1.02]	15.41	2160	0.38

(31), 41 (30), 91 (30), 107 (29)... 220 (4)]						
Unknown [m/z 121, 107 (69), 93 (64), 79 (60), 177 (59), 136 (58), 91 (57), 41 (56)... 220 (21)]	13.08	1643	1.93	15.38	2156	1.78
Unknown [m/z 159, 91 (58), 105 (54), 93 (51), 81 (50), 177 (44)...]	13.12*†	1647	3.32			
Cyclocopacamphan- 12-ol, epimer A	13.12*†	1647	[3.32]	16.31	2252	0.98
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.12*†	1647	[3.32]	15.17	2135	0.29
Cyclocopacamphan- 12-ol, epimer B	13.22	1655	1.62	16.39	2260	0.92
Zizanol	13.32	1663	1.40	16.84	2307	1.01
Khusiol	13.37	1667	1.62	16.06	2226	1.40
epi-Zizanone	13.40	1670	0.89	15.30	2149	0.51
Zizanal	13.46	1675	0.44	17.23	2349	0.49
Unknown [m/z 145, 147 (98), 105 (93), 159 (91), 91 (90), 119 (76)...220 (30)]	13.57	1684	1.49			
Unknown [m/z 189, 159 (82), 133 (44), 91 (29), 105 (29), 205 (25)... 220 (13)]	13.79	1702	2.79	16.95	2320	2.51
Vetiselinol	13.93	1714	2.01	17.15	2341	1.55
Khusimol	14.14*†	1732	6.01	17.85*†	2417	5.76
Unknown [m/z 189, 187 (29), 159 (23), 43 (20), 133 (16)...]	14.14*†	1732	[6.01]			
10-epi-Acora-3,11- dien-15-al?	14.24	1740	0.71			
Unknown [m/z 91, 105 (89), 79 (84), 93 (77), 107 (67), 189 (64), 145 (62), 119 (61)... 220 (16)...]	14.30	1746	0.15			
Unknown [m/z 174, 131 (37), 159 (25), 91 (20), 175 (14)....]	14.57	1769	0.58	17.56	2385	0.54
Nootkatone	14.85†	1794	6.19	17.85*†	2417	[5.76]
Isozizanoic acid	14.91*†	1799	[6.19]	21.42	2842	4.72
(Z)-Isovalencenal	14.91*†	1799	[6.19]	17.07	2332	0.34
β-Vetivone	14.99	1806	2.71	17.68	2398	2.54

α-Vetivone	15.23†	1828	16.70	18.00	2434	4.79
Zizanoic acid	15.25†	1830	[16.70]	22.02	2919	9.81
(E)-Isovalencenyl acetate?	15.55	1857	0.10	16.88	2312	0.88
Isovalencenal isomer II?	15.74	1874	0.17			
Isovalencenal isomer I?	15.85	1885	0.08			
<b>Total identified</b>		<b>69.10%</b>			<b>57.40%</b>	
<b>Total reported</b>		<b>81.59%</b>			<b>66.31%</b>	

\*: 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