

**Date :** March 24, 2020

**CERTIFICATE OF ANALYSIS – GC PROFILING**

**SAMPLE IDENTIFICATION**

**Internal code :** 20C11-PSC12

**Customer identification :** Vetiver - India - 200819

**Type :** Essential oil

**Source :** *Vetiveria zizanioides* ct. India

**Customer :** Pacha Soap Co.

**ANALYSIS**

**Method:** PC-MAT-007 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Sylvain Mercier, M. Sc., Chimiste

**Analysis date :** March 23, 2020

Checked and approved by :

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Alexis St-Gelais, M. Sc., chimiste 2013-174

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Bright yellow viscous liquid

**Refractive index:**  $1.5248 \pm 0.0003$  (20 °C)

*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	%	Classe
Limonene	0.01	Monoterpene
4-Vinylguaiaicol	0.01	Simple phenolic
$\alpha$ -Cubebene	0.01	Sesquiterpene
Cyclosativene I	0.07	Sesquiterpene
Unknown	0.03	Norsesquiterpene
$\alpha$ -Ylangene	0.11	Sesquiterpene
2-Norzizaene?	0.14	Norsesquiterpene
$\alpha$ -Copaene	0.01	Sesquiterpene
6-epi-Nigritene	0.08	Norsesquiterpene
Nigritene	0.06	Norsesquiterpene
Unknown	0.05	Norsesquiterpene
$\alpha$ -Funebrene	0.06	Sesquiterpene
Cyperene	0.07	Sesquiterpene
Acora-3,7(14)-diene	0.19	Sesquiterpene
$\alpha$ -Cedrene	0.11	Sesquiterpene
$\beta$ -Cedrene	0.11	Sesquiterpene
Cascarilladiene	0.11	Sesquiterpene
$\beta$ -Copaene	0.13	Sesquiterpene
Prezizaene	0.59	Sesquiterpene
6,9-Guaiadiene	0.16	Sesquiterpene
Khusimene	0.88	Sesquiterpene
Unknown	0.32	Sesquiterpene
Unknown	0.17	Sesquiterpene
Unknown	0.34	Sesquiterpene
Unknown	0.36	Sesquiterpene
$\alpha$ -Amorphene	1.59	Sesquiterpene
$\alpha$ -Vetispirene	0.82	Sesquiterpene
$\beta$ -Vetispirene	1.78	Sesquiterpene
$\gamma$ -Amorphene	0.19	Sesquiterpene
$\delta$ -Selinene	0.54	Sesquiterpene
Eudesma-2,4(15),11-triene	0.53	Sesquiterpene
$\delta$ -Amorphene	0.87	Sesquiterpene
Nootkatene	0.29	Sesquiterpene
Spirovetiva-1(10),7(11)-diene	0.93	Sesquiterpene
$\delta$ -Cadinene	0.34	Sesquiterpene
$\gamma$ -Vetivenene	0.51	Sesquiterpene
11,12,13-trinor- <i>trans</i> -Eudesm-5-en-7-one	0.37	Terpenic ketone
$\alpha$ -Calacorene	0.32	Sesquiterpene
Selina-3,7(11)-diene	0.31	Sesquiterpene
$\beta$ -Vetivenene	4.13	Sesquiterpene
$\alpha$ -Elemol	0.28	Sesquiterpenic alcohol
<i>cis</i> -Eudesm-6-en-11-ol	1.48	Sesquiterpenic alcohol
Unknown	0.49	Oxygenated sesquiterpene
Unknown	0.48	Sesquiterpene
Unknown	0.26	Oxygenated sesquiterpene
Khusimone	0.56	Norsesquiterpenic ketone
Unknown	0.29	Oxygenated sesquiterpene

Selin-6-en-4 $\alpha$ -ol isomer	1.08	Sesquiterpenic alcohol
Unknown	0.41	Sesquiterpene
Selin-6-en-4 $\alpha$ -ol	0.69	Sesquiterpenic alcohol
Unknown	0.65	Oxygenated sesquiterpene
Unknown	1.24	Unknown
Unknown	1.23	Unknown
Unknown	0.32	Oxygenated sesquiterpene
Unknown	1.80	Oxygenated sesquiterpene
Unknown	0.73	Oxygenated sesquiterpene
Unknown	1.46	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer A	1.57	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer B	1.56	Sesquiterpenic alcohol
Zizanone analog	2.27	Sesquiterpenic ketone
Zizanol	1.24	Sesquiterpenic alcohol
epi-Zizanone	0.39	Sesquiterpenic ketone
Khusiol	1.61	Sesquiterpenic alcohol
Zizanal	0.42	Sesquiterpenic aldehyde
Unknown	1.28	Oxygenated sesquiterpene
Unknown	0.21	Oxygenated sesquiterpene
Vetiselinenol	2.63	Sesquiterpenic alcohol
$\alpha$ -Vetivol?	0.43	Sesquiterpenic alcohol
Unknown	0.44	Oxygenated sesquiterpene
Khusimol	12.51	Sesquiterpenic alcohol
Unknown	1.26	Oxygenated sesquiterpene
10-epi-Acora-3,11-dien-15-al?	1.10	Sesquiterpenic aldehyde
Unknown	0.19	Oxygenated sesquiterpene
Unknown	0.43	Oxygenated sesquiterpene
Unknown	0.22	Unknown
( <i>E</i> )-Isovalencenol	6.74	Sesquiterpenic alcohol
Unknown	0.99	Oxygenated sesquiterpene
Unknown	0.57	Oxygenated sesquiterpene
Nootkatone	0.14	Sesquiterpenic ketone
( <i>Z</i> )-Isovalencenal	0.46	Sesquiterpenic aldehyde
$\beta$ -Vetivone	1.97	Sesquiterpenic ketone
Zizanoic acid	3.02	Sesquiterpenic acid
( <i>E</i> )-Isovalencenal	1.22	Sesquiterpenic aldehyde
$\alpha$ -Vetivone	1.97	Sesquiterpenic ketone
Unknown	0.21	Oxygenated sesquiterpene
Unknown	0.21	Sesquiterpenic ester
$\beta$ -Cyclodihydrocostunolide?	0.14	Sesquiterpenic lactone
<b>Consolidated total</b>	<b>78.54%</b>	

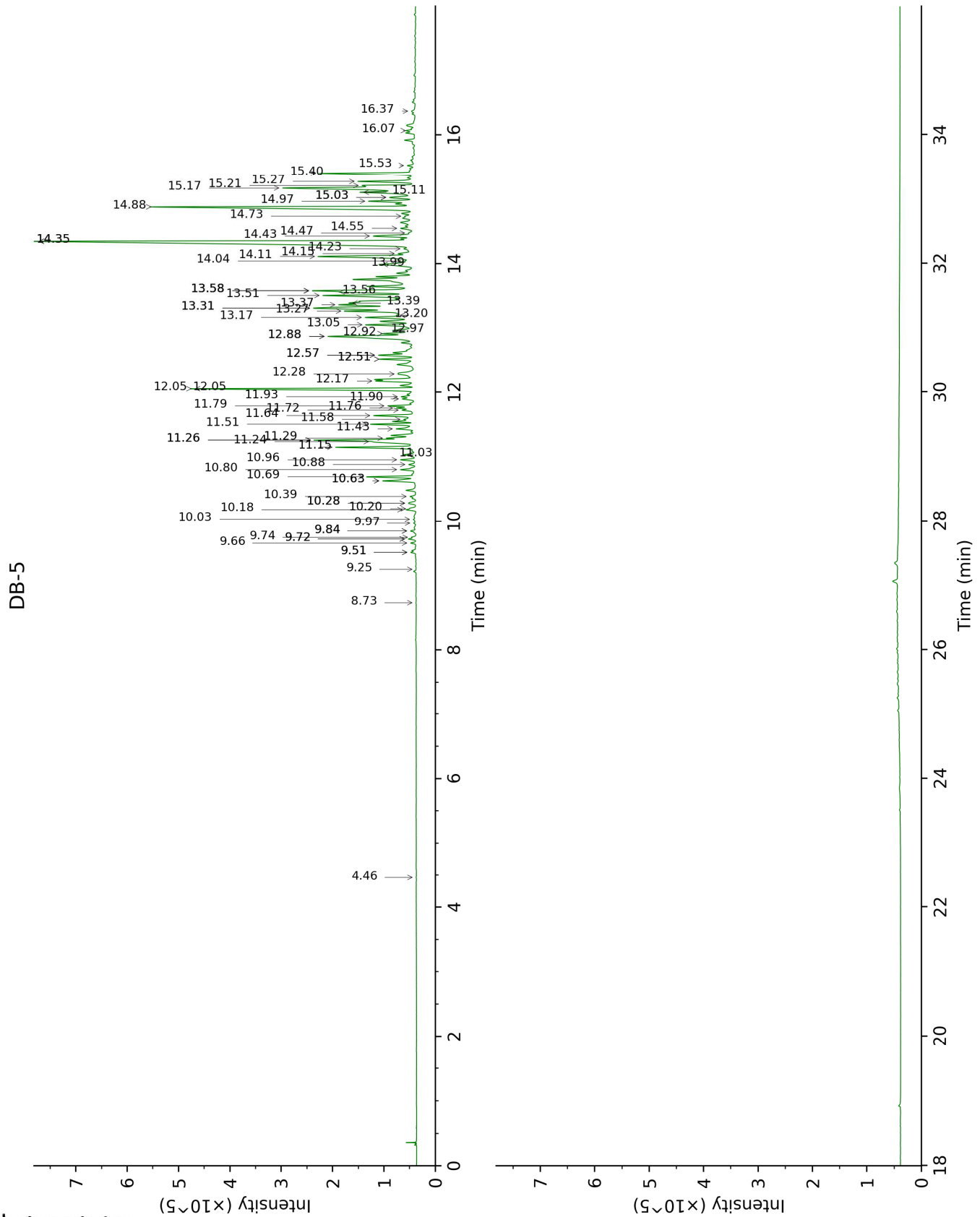
tr: The compound has been detected below 0.005% of total signal.

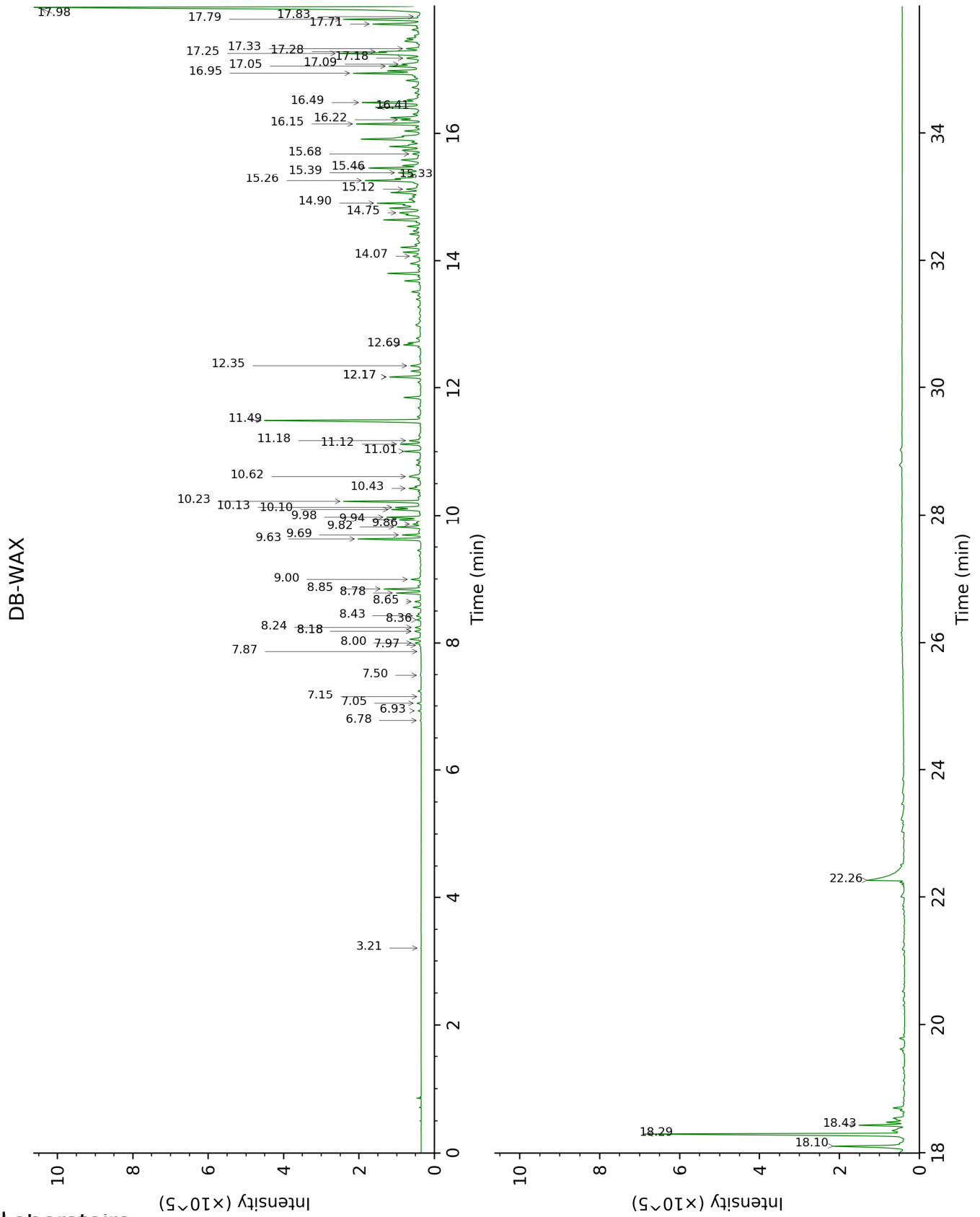
Note: no correction factor was applied

**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.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Limonene	4.46	1025	0.01	3.21	1158	tr
4-Vinylguaiacol	8.73	1308	0.01	15.12	2125	0.48
$\alpha$ -Cubebene	9.25	1346	0.01	6.78	1416	0.02
Cyclosativene I	9.51*	1357	0.10	6.93	1428	0.07
Unknown [m/z 145, 188 (95), 117 (91), 173 (80), 91 (65), 131 (64)]	9.51*	1357	[0.10]			
$\alpha$ -Ylangene	9.66	1368	0.11	7.05	1436	0.09
2-Norzizaene?	9.72*	1372	0.15			
$\alpha$ -Copaene	9.72*	1372	[0.15]	7.15	1444	0.01
6-epi-Nigritene	9.74	1374	0.08	7.97	1505	0.05
Nigritene	9.84*	1381	0.11	8.18*	1522	0.17
Unknown [m/z 145, 146 (35), 131 (42), 117 (22), 173 (22), 91 (20)... 188 (6)]	9.84*	1381	[0.11]			
$\alpha$ -Funebrene	9.97	1389	0.06	7.87	1497	0.01
Cyperene	10.03	1394	0.07	7.50	1470	0.03
Acora-3,7(14)-diene	10.18	1405	0.19	8.24	1526	0.17
$\alpha$ -Cedrene	10.20	1406	0.11	8.00	1508	0.16
$\beta$ -Cedrene	10.28*	1412	0.22	8.36	1535	0.11
Cascarilladiene	10.28*	1412	[0.22]	8.18*	1522	[0.17]
$\beta$ -Copaene	10.39	1420	0.13	8.42	1540	0.12
Prezizaene	10.63*	1438	0.78	8.78	1568	0.59
6,9-Guaiadiene	10.63*	1438	[0.78]	8.65	1557	0.16
Khusimene	10.69	1443	0.88	8.85	1572	0.85
Unknown [m/z 105, 161 (78), 93 (70), 133 (67), 91 (66), 204 (63), 119 (41)]	10.80	1451	0.32	9.00	1584	0.24
Unknown [m/z 119, 190 (99), 175 (95), 105 (71), 91 (59), 120 (57)... 204 (2)]	10.88	1457	0.17			
Unknown [m/z 119, 120 (31), 83 (23), 105 (22), 91 (21), 81 (18)... 202 (9)]	10.96	1462	0.34	9.82	1650	0.62
Unknown [m/z 145, 202 (85), 159 (64), 187 (39), 131 (35), 117 (34)]	11.03	1468	0.36	9.94	1660	0.54
$\alpha$ -Amorphene	11.15	1477	1.59	9.63	1635	1.48
$\alpha$ -Vetispirene	11.24	1483	0.82	10.10†	1673	1.38
$\beta$ -Vetispirene	11.26*	1485	1.94	10.23	1683	1.78
$\gamma$ -Amorphene	11.26*	1485	[1.94]	9.86	1653	0.19
$\delta$ -Selinene	11.29	1487	0.54	9.69	1640	0.44
Eudesma-2,4(15),11-triene	11.43	1498	0.53	11.18	1762	0.31
$\delta$ -Amorphene	11.51	1503	0.87	9.98	1663	0.82
Nootkatene	11.58	1509	0.29	11.01	1748	0.39
Spirovetiva-1(10),7(11)-diene	11.64	1514	0.93	10.13†	1675	[1.38]



δ-Cadinene	11.72	1520	0.34	10.43	1700	0.33
γ-Vetivenene	11.76†	1523	0.88	11.12	1758	0.51
11,12,13-trinor- <i>trans</i> -Eudesm-5-en-7-one	11.79†	1525	[0.88]			
α-Calacorene	11.90	1534	0.32	12.17*	1849	0.80
Selina-3,7(11)-diene	11.93	1537	0.31	10.62	1715	0.47
β-Vetivenene	12.05*	1546	4.43	11.49	1789	4.13
α-Elemol	12.05*	1546	[4.43]	14.07	2023	0.28
<i>cis</i> -Eudesm-6-en-11-ol	12.17	1556	1.48			
Unknown [m/z 81, 200 (55), 143 (36), 93 (33), 91 (32), 185 (31), 129 (27), 128 (21)...]	12.28	1564	0.49			
Unknown [m/z 202, 187 (63), 145 (43), 159 (34), 131 (29), 91 (22), 117 (20)]	12.51*	1582	0.74	12.17*	1849	[0.80]
Unknown [m/z 59, 43 (56), 205 (47), 91 (41), 220 (32), 105 (30), 147 (21)]	12.51*	1582	[0.74]			
Khusimone	12.57*	1587	0.85			
Unknown [m/z 161, 119 (78), 105 (75), 120 (72), 43 (64)... 218 (4)]	12.57*	1587	[0.85]	12.35	1864	0.29
Selin-6-en-4α-ol isomer	12.88*	1611	2.90	14.90	2103	1.08
Unknown [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	12.88*	1611	[2.90]	12.69	1894	0.41
Selin-6-en-4α-ol	12.92	1615	0.69	15.68	2181	0.22
Unknown [m/z 59, 149 (94), 43 (82), 205 (65)... 220 (6)]	12.97	1619	0.65			
Unknown [m/z 145, 59 (97), 161 (87), 218 (76), 43 (76), 179 (63)...]	13.06	1626	1.24			
Unknown [m/z 43, 91 (87), 71 (83), 93 (77), 95 (75), 135 (74)...]	13.17	1635	1.23			
Unknown [m/z 187, 93 (35), 81 (34), 79 (31), 41 (30), 91 (30), 107 (29)... 220 (4)]	13.20	1638	0.32	15.39	2152	0.76
Unknown [m/z 121, 107 (69), 93 (64), 79 (60), 177 (59), 136 (58), 91 (57), 41 (56)... 220 (21)]	13.27	1643	1.80	15.46	2159	1.34
Unknown [m/z 161, 59 (67), 95 (45), 93 (40), 105 (40), 149 (39), 81 (39), 43 (38), 204 (37)... 220 (5)]	13.31*	1647	3.15	14.75	2088	0.73
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109	13.31*	1647	[3.15]	15.26	2138	1.46

)40)... 204 (35), 222 (2)]						
Cyclocopacamphan-12-ol, epimer A	13.36	1652	1.57	16.41	2256	1.32
Cyclocopacamphan-12-ol, epimer B	13.39	1654	1.56	16.49	2264	1.51
Zizanone analog	13.51	1663	2.27			
Zizanol	13.56	1668	1.24	16.94	2312	1.62
epi-Zizanone	13.58*	1670	2.16	15.33	2146	0.39
Khusiol	13.58*	1670	[2.16]	16.15	2229	1.61
Zizanal	13.58*	1670	[2.16]	17.33	2354	0.42
Unknown [m/z 189, 159 (82), 133 (44), 91 (29), 105 (29), 205 (25)... 220 (13)]	13.99	1703	1.28	17.06	2324	0.89
Unknown [m/z 204, 189 (99), 43 (83), 161 (75), 105 (55), 91 (44), 119 (33)... 220 (13)]	14.04	1708	0.21			
Vetiselinenol	14.11	1714	2.63	17.26	2346	2.39
α-Vetivol?	14.16	1718	0.43	17.71	2396	1.34
Unknown [m/z 136, 121 (98), 137 (90), 119 (68), 107 (55), 135 (55)... 202 (30), 220 (27)]	14.23	1724	0.44			
Khusimol	14.35*	1734	13.77	17.98	2425	12.51
Unknown [m/z 189, 187 (29), 159 (23), 43 (20), 133 (16)...]	14.35*	1734	[13.77]			
10-epi-Acora-3,11-dien-15-al?	14.43	1741	1.10			
Unknown [m/z 91, 105 (89), 79 (84), 93 (77), 107 (67), 189 (64), 145 (62), 119 (61)... 220 (16)...]	14.47	1745	0.19			
Unknown [m/z 91, 175 (51), 105 (47), 133 (50)... 218 (20), 232? (1)]	14.55	1752	0.43	16.22	2236	0.47
Unknown [m/z 174, 131 (37), 159 (25), 91 (20), 175 (14)...]	14.73	1768	0.22			
(E)-Isovalencenol	14.88	1780	6.74	18.29	2460	6.53
Unknown [m/z 120, 121 (93), 93 (85), 105 (74), 119 (68), 91 (58), 123 (49)... 220 (8)]	14.97	1788	0.99	18.43	2475	1.06
Unknown [m/z 202, 187 (91), 93 (70), 91 (69), 105 (67)...]	15.02*	1793	0.71			
Nootkatone	15.02*	1793	[0.71]	17.83	2408	0.14
(Z)-Isovalencenal	15.10†	1800	6.15	17.18	2338	0.46
β-Vetivone	15.17†	1806	[6.15]	17.79	2404	1.97
Zizanoic acid	15.21†	1810	[6.15]	22.26	2944	3.02
(E)-Isovalencenal	15.27	1815	1.22	17.28	2348	0.93

α-Vetivone	15.40	1827	1.97	18.10	2439	2.19
Unknown [m/z 105, 179 (87), 91 (67), 161 (61), 121 (57), 119 (56), 163 (50), 43 (50)...]	15.53	1838	0.21			
Unknown [m/z 202, 187 (72), 160 (48), 43 (44), 159 (43), 145 (37)...]	16.07	1888	0.21	17.09	2328	0.59
β-Cyclodihydrocostunolide?	16.37	1916	0.14			
<b>Total identified</b>		<b>70.27%</b>			<b>56.07%</b>	
<b>Total reported</b>		<b>81.36%</b>			<b>65.46%</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

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied  
R.T.: Retention time (minutes)  
R.I.: Retention index