Date : May 10, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22E04-PTH02
Customer identification : Vetiver ORGANIC - Madagascar - V80107R
Type : Essential oil
Source : *Vetiveria zizanioides*
Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-014 ✳ISO - 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 : May 06, 2022

Checked and approved by :

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

MÉTHODE CERTIFIÉE
✳ISO 17025:2017
CERTIFIED METHOD

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PHYSICOCHEMICAL DATA

Physical aspect: Light brown liquid
Refractive index: 1.5262 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

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

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ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

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

Identification	%	Class
Furfural	0.06	Furan
Unknown	0.06	Sesquiterpene
2-Norprezizene	0.06	Sesquiterpene
Unknown	0.14	Unknown
Unknown	0.21	Norsesquiterpene
Cyclosativene II	0.01	Sesquiterpene
12-Norisoziza-5-ene	0.95	Norsesquiterpene
Unknown	0.27	Norsesquiterpene
α-Ylangene	0.06	Sesquiterpene
6-epi-Nigritene	1.43	Norsesquiterpene
Nigritene	2.76	Norsesquiterpene
Unknown	0.23	Unknown
Acora-3,7(14)-diene	0.13	Sesquiterpene
β-Funebrene	0.14	Sesquiterpene
β-Cedrene	0.16	Sesquiterpene
Unknown	0.86	Norsesquiterpene
Prezizaene	0.47	Sesquiterpene
Khusimene	0.47	Sesquiterpene
(*E*)-Isoeugenol	0.22	Phenylpropanoid
Unknown	0.40	Sesquiterpene
Unknown	0.26	Sesquiterpene
Unknown	0.44	Sesquiterpene
α-Amorphene	1.12	Sesquiterpene
α-Vetispirene	1.18	Sesquiterpene
β-Vetispirene	0.91	Sesquiterpene
γ-Amorphene	0.10	Sesquiterpene
δ-Selinene	0.84	Sesquiterpene
Eudesma-2,4(15),11-triene	0.16	Sesquiterpene
δ-Amorphene	0.61	Sesquiterpene
Nootkatene	0.37	Sesquiterpene
Spirovetiva-1(10),7(11)-diene	0.57	Sesquiterpene
trans-Calamenene	0.10	Sesquiterpene
δ-Cadinene	0.34	Sesquiterpene
γ-Vetivenene	2.03	Sesquiterpene
α-Calacorene	0.45	Sesquiterpene
β-Vetivenene	2.98	Sesquiterpene
α-Elemol	0.20	Sesquiterpenic alcohol
Eremophila-1(10),11-dien-9β-ol	1.47	Sesquiterpenic alcohol
Unknown	0.27	Oxygenated sesquiterpene
Gynuradienol?	0.33	Sesquiterpenic alcohol
Unknown	0.86	Sesquiterpene
Khusimone	0.90	Norsesquiterpenic ketone
Selin-6-en-4α-ol isomer	0.38	Sesquiterpenic alcohol
Junenol	0.46	Sesquiterpenic alcohol
Unknown	1.06	Sesquiterpene

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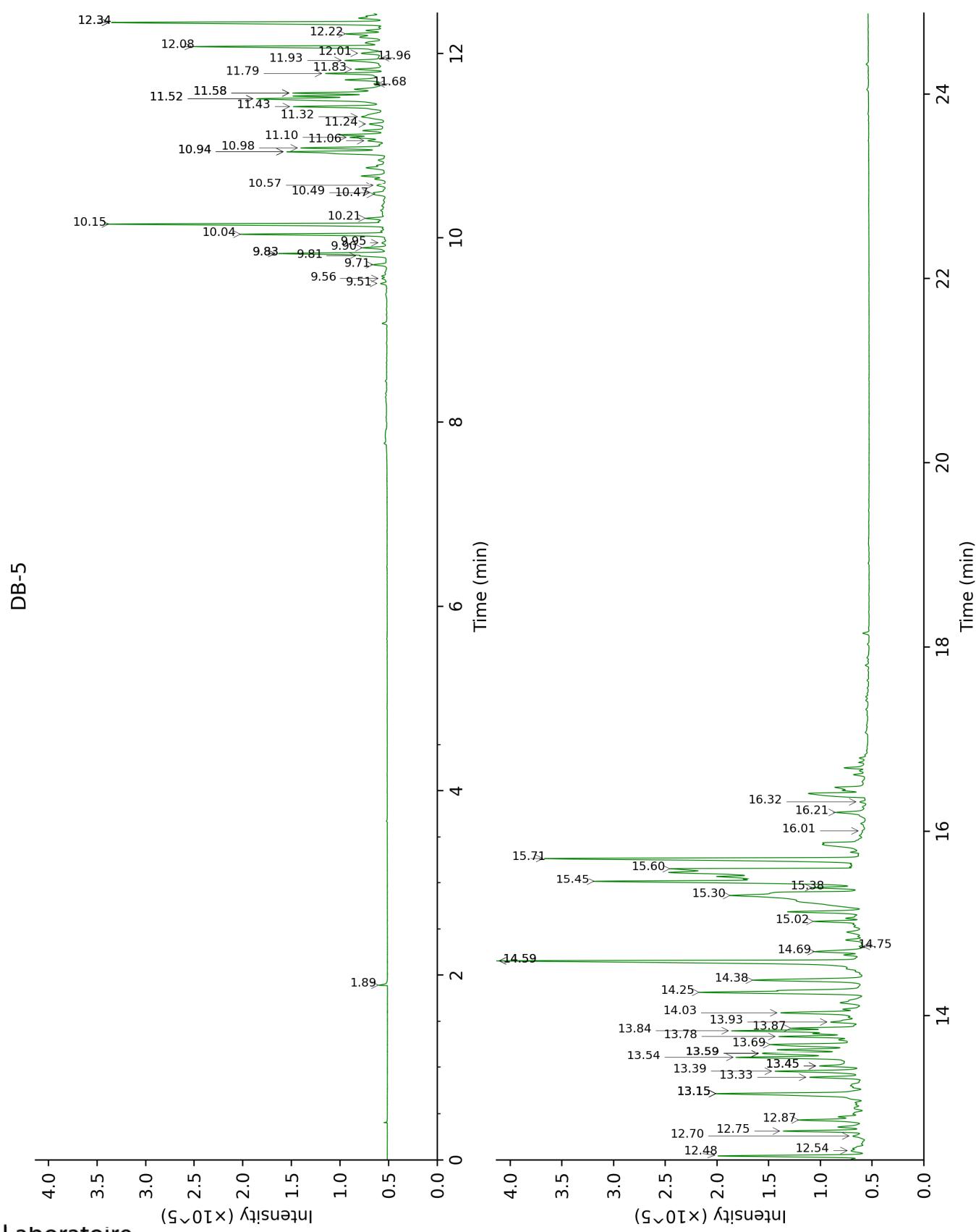
|		
10-epi-γ-Eudesmol	0.49	Sesquiterpenic alcohol
γ-Eudesmol	0.71	Sesquiterpenic alcohol
Unknown	1.24	Unknown
Unknown	0.38	Oxygenated sesquiterpene
Unknown	0.36	Unknown
Unknown	1.79	Oxygenated sesquiterpene
Unknown	1.65	Unknown
Unknown	0.36	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer A	0.87	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer B	1.64	Sesquiterpenic alcohol
Zizanol	0.97	Sesquiterpenic alcohol
Khusiol	1.46	Sesquiterpenic alcohol
epi-Zizanone	0.77	Sesquiterpenic ketone
Zizanal	0.46	Sesquiterpenic aldehyde
Unknown	1.30	Oxygenated sesquiterpene
Unknown	2.14	Oxygenated sesquiterpene
Vetiselinenol	1.77	Sesquiterpenic alcohol
Khusimol	4.91	Sesquiterpenic alcohol
Unknown	0.68	Oxygenated sesquiterpene
10-epi-Acora-3,11-dien-15-al?	0.78	Sesquiterpenic aldehyde
Unknown	0.11	Oxygenated sesquiterpene
Unknown	0.58	Unknown
Isozizanoic acid	6.05	Sesquiterpenic acid
(Z)-Isovalencenal	0.63	Sesquiterpenic aldehyde
β-Vetivone	2.21	Sesquiterpenic ketone
Zizanoic acid	9.01	Sesquiterpenic acid
α-Vetivone	4.31	Sesquiterpenic ketone
(E)-Isovalencenyl acetate?	0.08	Sesquiterpenic ester
Isovalencenal isomer II?	0.58	Sesquiterpenic aldehyde
Isovalencenal isomer I?	0.10	Sesquiterpenic aldehyde
Consolidated total	**75.82%**	

Note: no correction factor was applied
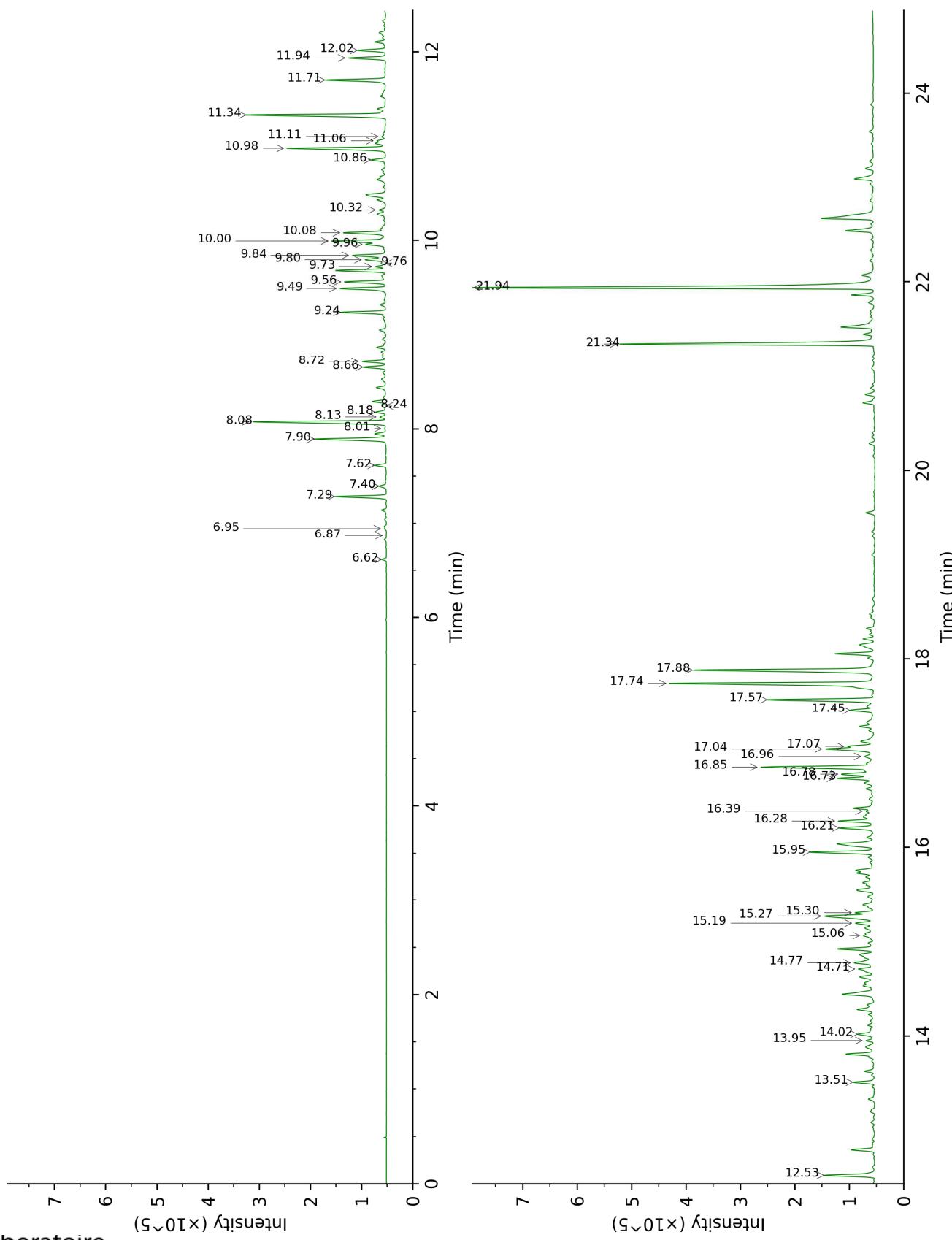
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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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This page was intentionally left blank. The following pages present the complete data of the analysis.

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DB-5

Top chromatogram (Time 0–12 min):
12.34, 12.22, 12.08, 12.01, 11.96, 11.93, 11.83, 11.79, 11.68, 11.58, 11.52, 11.43, 11.32, 11.24, 11.10, 11.06, 10.94, 10.98, 10.57, 10.49, 10.47, 10.15, 10.21, 10.04, 9.95, 9.90, 9.83, 9.81, 9.71, 9.56, 9.51, 1.89

Bottom chromatogram (Time 14–24 min):
16.32, 16.21, 16.01, 15.71, 15.60, 15.45, 15.38, 15.30, 15.02, 14.75, 14.69, 14.59, 14.38, 14.25, 14.03, 13.93, 13.87, 13.84, 13.78, 13.69, 13.59, 13.54, 13.45, 13.39, 13.33, 13.15, 12.87, 12.75, 12.70, 12.54, 12.48

DB-WAX

Time (min)

Intensity (×10^5)

Time (min)

Intensity (×10^5)

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Furfural	1.89	826	0.06	6.62	1414	0.08
Unknown [m/z 120, 91 (31), 92 (23), 121 (10), 105 (9), 119 (6)...202 (1)]	9.51	1337	0.06			
2-Norprezizene	9.56	1341	0.06	7.40*	1471	0.17
Unknown [m/z 119, 91 (23), 120 (17), 118 (11), 92 (7), 105 (6)...]	9.71	1352	0.14	7.40*	1471	[0.17]
Unknown [m/z 145, 188 (95), 117 (91), 173 (80), 91 (65), 131 (64)]	9.81	1358	0.21			
Cyclosativene II	9.83*	1360	1.05	6.87	1432	0.01
12-Norisoziza-5-ene	9.83*	1360	[1.05]	7.29	1463	0.95
Unknown [m/z 119, 147 (85), 161 (75), 91 (69), 105 (62), 134 (60), 190 (43)]	9.90	1365	0.27	7.62	1488	0.22
α-Ylangene	9.95	1368	0.06	6.95	1438	0.04
6-epi-Nigritene	10.04	1375	1.43	7.90	1509	1.51
Nigritene	10.15	1383	2.76	8.08	1523	2.77
Unknown [m/z 119, 91 (24), 120 (17), 118 (10), 92 (8), 41 (7), 105 (6)...]	10.22	1387	0.23	8.18	1531	0.24
Acora-3,7(14)-diene	10.47	1406	0.13	8.13	1527	0.14
β-Funebrene	10.49	1407	0.14	8.01	1517	0.04
β-Cedrene	10.57	1413	0.16	8.24	1536	0.10
Unknown [m/z 175, 190 (73), 161 (65), 119 (40), 105 (35), 91 (28), 133 (23)]	10.94*†	1440	2.28	9.24	1614	0.86
Prezizaene	10.94*†	1440	[2.28]	8.66	1568	0.47
Khusimene	10.98†	1444	[2.28]	8.72	1572	0.47
(*E*)-Isoeugenol	11.06	1449	0.22	16.38	2270	0.16
Unknown [m/z 119, 190 (99), 175 (95), 105 (71), 91 (59), 120 (57)... 204 (2)]	11.10	1452	0.40			
Unknown [m/z 119, 120 (31), 83 (23), 105 (22), 91 (21), 81 (18)... 202 (9)]	11.24	1463	0.26	9.73	1653	0.20
Unknown [m/z 145, 202 (85), 159 (64), 187 (39), 131 (35), 117 (34)]	11.32	1469	0.44	9.80	1659	0.49

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Compound						
α-Amorphene	11.43	1477	1.12	9.49	1634	0.96
α-Vetispirene	11.52*	1483	2.03	10.00	1675	1.18
β-Vetispirene	11.52*	1483	[2.03]	10.08	1682	0.91
γ-Amorphene	11.58*	1488	1.00	9.76	1656	0.10
δ-Selinene	11.58*	1488	[1.00]	9.56	1640	0.84
Eudesma-2,4(15),11-triene	11.68	1495	0.16	11.06	1764	0.18
δ-Amorphene	11.79	1504	0.61	9.84	1662	0.74
Nootkatene	11.83	1507	0.37	10.86	1747	0.32
Spirovetiva-1(10),7(11)-diene	11.93	1515	0.57	9.96	1672	0.41
trans-Calamenene	11.96	1517	0.10	11.11	1768	0.10
δ-Cadinene	12.01	1521	0.34	10.32	1702	0.16
γ-Vetivenene	12.08	1526	2.03	10.98	1758	2.03
α-Calacorene	12.22	1537	0.45	12.02	1848	0.58
β-Vetivenene	12.34*	1547	3.04	11.34	1787	2.98
α-Elemol	12.34*	1547	[3.04]	13.95	2026	0.20
Eremophila-1(10),11-dien-9β-ol	12.48	1558	1.47	11.70	1820	1.26
Unknown [m/z 81, 200 (55), 143 (36), 93 (33), 91 (32), 185 (31), 129 (27), 128 (21)...]	12.54	1563	0.27			
Gynuradienol?	12.70	1575	0.33			
Unknown [m/z 202, 187 (63), 145 (43), 159 (34), 131 (29), 91 (22), 117 (20)]	12.75	1579	0.86	11.94	1840	0.76
Khusimone	12.87	1589	0.90			
Selin-6-en-4α-ol isomer	13.15*	1611	2.36	14.71	2098	0.38
Junenol	13.15*	1611	[2.36]	13.51	1983	0.46
Unknown [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	13.15*	1611	[2.36]	12.53	1893	1.06
10-epi-γ-Eudesmol	13.15*	1611	[2.36]	14.02	2032	0.49
γ-Eudesmol	13.33	1626	0.71	14.77	2105	0.64
Unknown [m/z 145, 59 (97), 161 (87), 218 (76), 43 (76), 179 (63)...]	13.39	1631	1.24			
Unknown [m/z 187, 93 (35), 81 (34), 79 (31), 41 (30), 91 (30), 107 (29)... 220 (4)]	13.45*	1636	0.74	15.30	2158	0.38
Unknown [m/z 43, 91 (87), 71 (83), 93 (77), 95 (75), 135 (74)...]	13.45*	1636	[0.74]			

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Compound	RT	RI	%	RT	RI	%
Unknown [m/z 121, 107 (69), 93 (64), 79 (60), 177 (59), 136 (58), 91 (57), 41 (56)... 220 (21)]	13.54	1644	1.79	15.27	2155	1.54
Unknown [m/z 159, 91 (58), 105 (54), 93 (51), 81 (50), 177 (44)...]	13.59*†	1647	2.88			
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.59*†	1647	[2.88]	15.06	2134	0.36
Cyclocopacamphan-12-ol, epimer A	13.59*†	1647	[2.88]	16.21	2251	0.87
Cyclocopacamphan-12-ol, epimer B	13.69	1656	1.64	16.28	2259	0.79
Zizanol	13.78	1663	0.97	16.73	2307	0.79
Khusiol	13.84	1668	1.46	15.95	2225	1.32
epi-Zizanone	13.86	1670	0.77	15.19	2147	0.47
Zizanal	13.93	1676	0.46	17.07	2343	0.48
Unknown [m/z 145, 147 (98), 105 (93), 159 (91), 91 (90), 119 (76)...220 (30)]	14.03	1684	1.30			
Unknown [m/z 189, 159 (82), 133 (44), 91 (29), 105 (29), 205 (25)... 220 (13)]	14.25	1702	2.14	16.85	2319	2.40
Vetiselinenol	14.38	1714	1.77	17.04	2340	1.29
Khusimol	14.59*†	1732	5.58	17.74	2417	4.91
Unknown [m/z 189, 187 (29), 159 (23), 43 (20), 133 (16)...]	14.59*†	1732	[5.58]			
10-epi-Acora-3,11-dien-15-al?	14.69	1740	0.78			
Unknown [m/z 91, 105 (89), 79 (84), 93 (77), 107 (67), 189 (64), 145 (62), 119 (61)... 220 (16)...]	14.75	1745	0.11			
Unknown [m/z 174, 131 (37), 159 (25), 91 (20), 175 (14)....]	15.02	1769	0.58	17.45	2384	0.54
Isozizanoic acid	15.30	1793	6.05	21.34	2848	5.26
(*Z*)-Isovalencenal	15.38	1800	0.63	16.96	2332	0.34
β-Vetivone	15.45†	1806	13.02	17.57	2397	2.21
Zizanoic acid	15.60†	1819	[13.02]	21.94	2926	9.01
α-Vetivone	15.71	1829	4.31	17.88	2432	4.16

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	R.T.	R.I.	%	R.T.	R.I.	%
(*E*)-Isovalencenyl acetate?	16.01	1856	0.08	16.78	2311	0.79
Isovalencenal isomer II?	16.21	1875	0.58			
Isovalencenal isomer I?	16.32	1885	0.10			
Total identified	**67.73%**			**54.49%**		
Total reported	**78.02%**			**63.52%**		

*: 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

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