Date : 2024-06-27

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 24F12-PTH04
Customer Identification : Vetiver - India - V30112R
Type : Essential Oil
Source : *Chrysopogon zizanioides ct. India*
Customer : Plant Therapy

Checked an 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

Laboratoire PhytoChemia

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Gas Chromatographic Analysis

Method : PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID
ISO
Results : See analysis summary (next page)
Analyst : Sylvain Mercier, M. Sc., Chimiste 2014-005
Date : 2024-06-18

Physicochemical data

Refractive index : 1.5265 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2024-06-14

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
Isovaleral	tr	Aliphatic aldehyde
Furfural	0.01	Furan
Limonene	0.01	Monoterpene
Menthol	0.01	Monoterpenic alcohol
4-Vinylguaiacol	0.03	Simple phenolic
α-Cubebene	0.01	Sesquiterpene
Unknown	0.02	Norsesquiterpene
Cyclosativene I	0.06	Sesquiterpene
12-Norisoziza-5-ene	0.05	Norsesquiterpene
α-Ylangene	0.09	Sesquiterpene
2-Norzizaene?	0.09	Norsesquiterpene
6-epi-Nigritene	0.11	Norsesquiterpene
Nigritene	0.30	Norsesquiterpene
β-Elemene	0.04	Sesquiterpene
Cyperene	0.03	Sesquiterpene
Acora-3,7(14)-diene	0.14	Sesquiterpene
α-Cedrene	0.09	Sesquiterpene
Cascarilladiene	0.03	Sesquiterpene
β-Caryophyllene	0.14	Sesquiterpene
β-Cedrene	0.08	Sesquiterpene
Unknown	0.19	Sesquiterpene
Prezizaene	0.44	Sesquiterpene
6,9-Guaiadiene	0.16	Sesquiterpene
Khusimene	0.59	Sesquiterpene
Selina-4(15),7-diene	0.17	Sesquiterpene
Unknown	0.34	Sesquiterpene
Unknown	0.29	Sesquiterpene
Unknown	0.33	Sesquiterpene
α-Amorphene	1.50	Sesquiterpene
α-Vetispirene	0.99	Sesquiterpene
Unknown	0.24	Unknown
β-Vetispirene	1.67	Sesquiterpene
Bicyclosesquiphellandrene?	0.55	Sesquiterpene
Eudesma-2,4(15),11-triene	0.57	Sesquiterpene
δ-Amorphene	1.00	Sesquiterpene
Nootkatene	0.45	Sesquiterpene
γ-Cadinene	0.11	Sesquiterpene
Spirovetiva-1(10),7(11)-diene	0.71	Sesquiterpene
δ-Cadinene	0.12	Sesquiterpene
trans-Calamenene	0.09	Sesquiterpene

γ-Vetivenene	0.90	Sesquiterpene
α-Calacorene	0.43	Sesquiterpene
α-Elemol	0.41	Sesquiterpenic alcohol
β-Vetivenene	5.08	Sesquiterpene
Unknown	0.32	Sesquiterpene
Eremophila-1(10),11-dien-9β-ol	0.69	Sesquiterpenic alcohol
cis-Eudes*m*-6-en-11-ol	0.76	Sesquiterpenic alcohol
Unknown	0.37	Oxygenated sesquiterpene
Gynuradienol?	0.36	Sesquiterpenic alcohol
Unknown	0.67	Sesquiterpene
Unknown	0.29	Oxygenated sesquiterpene
Unknown	0.40	Sesquiterpene
Khusimone	0.42	Norsesquiterpenic ketone
Eudes*m*-4-en-7α-ol	0.21	Sesquiterpenic alcohol
Unknown	0.75	Sesquiterpene
10-epi-γ-Eudesmol	0.55	Sesquiterpenic alcohol
Selin-6-en-4α-ol isomer	1.12	Sesquiterpenic alcohol
Selin-6-en-4α-ol	0.48	Sesquiterpenic alcohol
Unknown	0.52	Oxygenated sesquiterpene
Unknown	1.04	Unknown
Unknown	1.11	Oxygenated sesquiterpene
Unknown	1.59	Oxygenated sesquiterpene
Cyclocopacamphan-12-ol, epimer A	1.02	Sesquiterpenic alcohol
Unknown	1.43	Sesquiterpenic alcohol
Unknown	1.02	Oxygenated sesquiterpene
Cyclocopacamphan-12-ol, epimer B	0.86	Sesquiterpenic alcohol
Unknown	1.36	Oxygenated sesquiterpene
Khusinol	0.34	Sesquiterpenic alcohol
Zizanol	1.48	Sesquiterpenic alcohol
Zizanone analog	0.30	Sesquiterpenic ketone
epi-Zizanone	0.18	Sesquiterpenic ketone
Khusiol	1.53	Sesquiterpenic alcohol
Zizanal	0.88	Sesquiterpenic aldehyde
Unknown	1.53	Oxygenated sesquiterpene
Juniper camphor	0.68	Sesquiterpenic alcohol
Unknown	1.41	Oxygenated sesquiterpene
Unknown	0.21	Oxygenated sesquiterpene
Vetiselinenol	2.53	Sesquiterpenic alcohol
α-Vetivol?	0.30	Sesquiterpenic alcohol
Unknown	0.19	Oxygenated sesquiterpene
Unknown	0.74	Oxygenated sesquiterpene
Khusimol	9.12	Sesquiterpenic alcohol
10-epi-Acora-3,11-dien-15-al?	1.09	Sesquiterpenic aldehyde
Unknown	0.31	Unknown
(*E*)-Isovalencenol	5.87	Sesquiterpenic alcohol

Unknown	1.99	Oxygenated sesquiterpene
Unknown	0.32	Oxygenated sesquiterpene
Nootkatone	0.43	Sesquiterpenic ketone
(*Z*)-Isovalencenal	1.02	Sesquiterpenic aldehyde
β-Vetivone	3.61	Sesquiterpenic ketone
Zizanoic acid	5.80	Sesquiterpenic acid
(*E*)-Isovalencenal	0.64	Sesquiterpenic aldehyde
α-Vetivone	2.89	Sesquiterpenic ketone
Unknown	0.57	Oxygenated sesquiterpene
Isovalencenal isomer II?	0.42	Sesquiterpenic aldehyde
Isovalencenal isomer I?	0.21	Sesquiterpenic aldehyde
β-Cyclodihydrocostunolide?	0.18	Sesquiterpenic lactone
Consolidated total	**82.80**	

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

Bracketed value ([xx]): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

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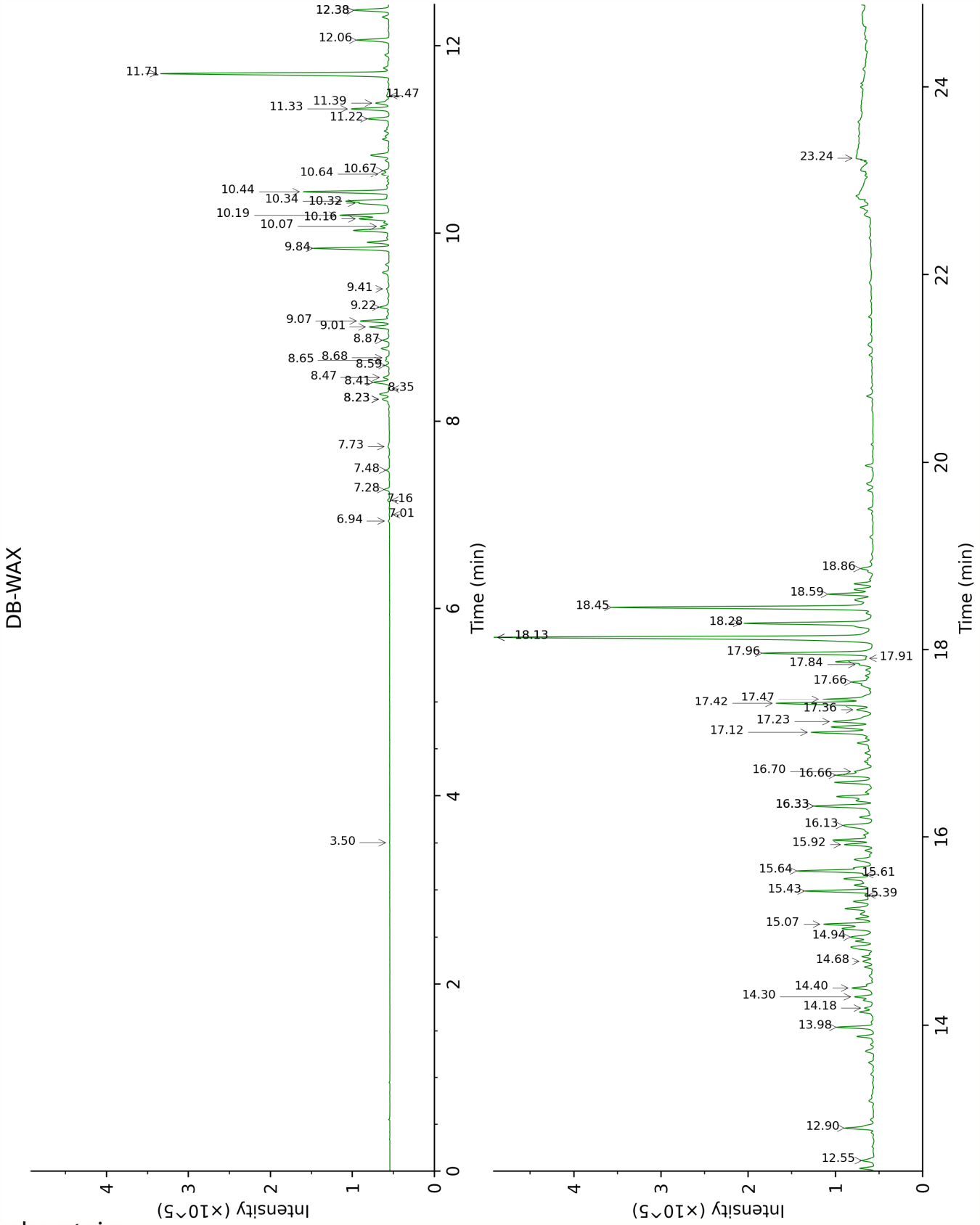
DB-WAX
Intensity (×10^5)
Time (min)
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12.06
11.71
11.47
11.39
11.33
11.22
10.67
10.64
10.44
10.34
10.32
10.19
10.16
10.07
9.84
9.41
9.22
9.07
9.01
8.87
8.68
8.65
8.59
8.47
8.41
8.35
8.23
7.73
7.48
7.28
7.16
7.01
6.94
3.50
23.24
18.86
18.59
18.45
18.28
18.13
17.96
17.91
17.84
17.66
17.47
17.42
17.36
17.23
17.12
16.70
16.66
16.33
16.13
15.92
15.64
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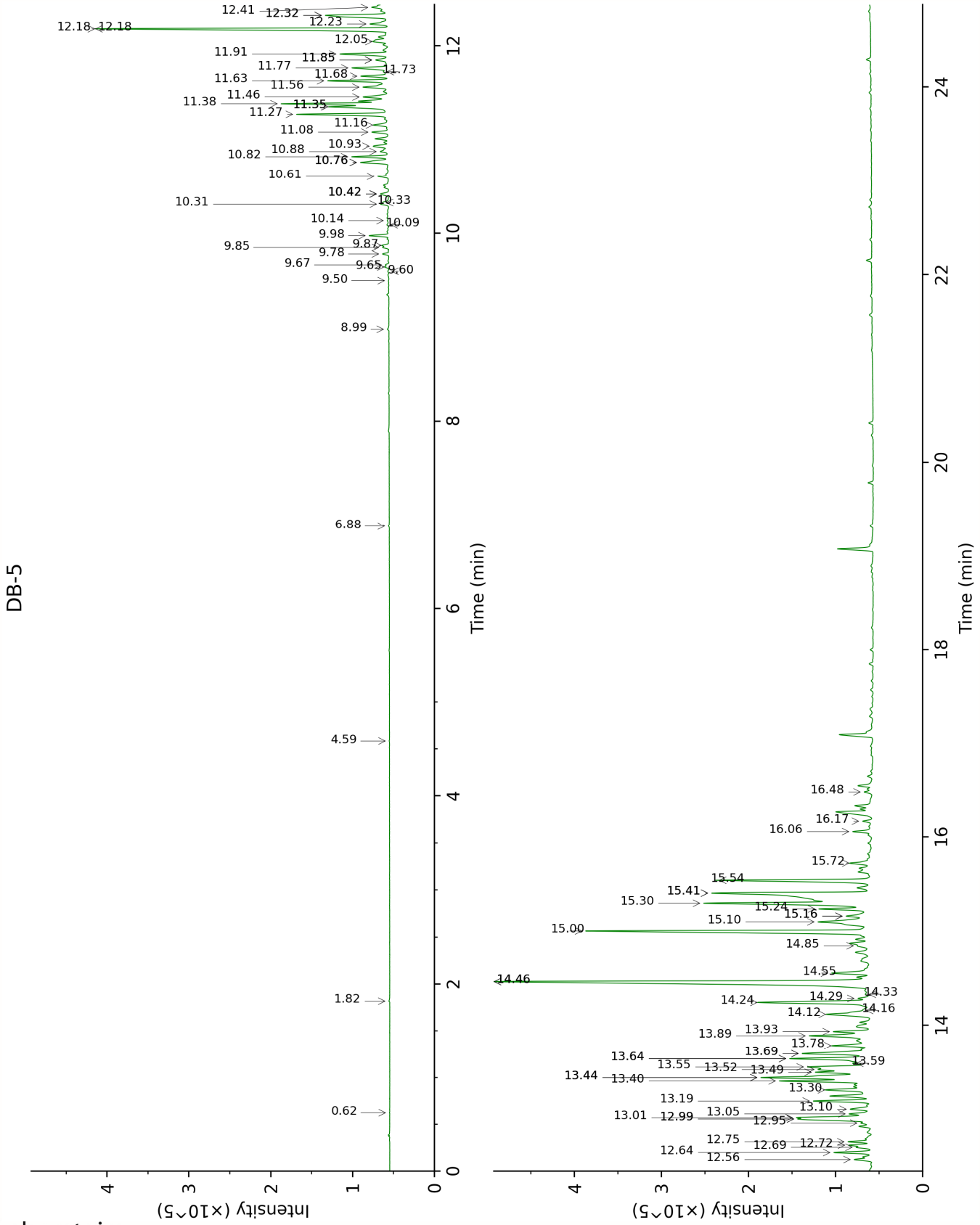
14.40
14.30
14.18
13.98
12.90
12.55


DB-5
Intensity (×10^5)
Time (min)
12.41
12.32
12.23
12.18
12.18
12.05
11.91
11.85
11.77
11.73
11.68
11.63
11.56
11.46
11.38
11.35
11.27
11.16
11.08
10.93
10.88
10.82
10.76
10.61
10.42
10.33
10.31
10.14
10.09
9.98
9.87
9.85
9.78
9.67
9.65
9.60
9.50
8.99
6.88
4.59
1.82
0.62
16.48
16.17
16.06
15.72
15.54
15.41
15.30
15.24
15.16
15.10
15.00
14.85
14.55
14.46
14.33
14.29
14.24
14.16
14.12
13.93
13.89
13.78
13.69
13.64
13.59
13.55
13.52
13.49
13.44
13.40
13.30
13.19
13.10
13.05
13.01
12.99
12.95
12.75
12.72
12.69
12.64
12.56

FULL ANALYSIS DATA

Isovaleral	Column DB-WAX			Column DB-5		
				0.62	639.2	tr
Furfural	6.94	1412.5	0.03	1.82	829.0	0.01
Limonene	3.50	1164.2	0.01	4.59	1026.2	0.01
Menthol	9.41	1599.9	0.07	6.88	1171.5	0.01
4-Vinylguaiacol	15.39	2126.6	0.29	8.99	1311.3	0.03
α-Cubebene	7.01	1417.4	0.01	9.50	1347.6	0.01
Unknown CHZI VIII [m/z 145, 188 (95), 117 (91), 173 (80), 91 (65), 131 (64)]				9.60	1354.6	0.02
Cyclosativene I	7.16	1428.8	0.04	9.65	1357.9	0.06
12-Norisoziza-5-ene	7.48	1452.4	0.07	9.67	1359.4	0.05
α-Ylangene	7.28	1437.2	0.11	9.78	1367.6	0.09
2-Norzizaene?				9.85	1372.5	0.09
6-epi-Nigritene	8.24*	1508.8	[0.19]	9.87	1374.0	0.11
Nigritene	8.42	1522.7	0.38	9.98	1381.3	0.30
β-Elemene	8.68*†	1542.8	[0.08]	10.09	1389.4	0.04
Cyperene	7.73	1471.0	0.06	10.14	1392.5	0.03
Acora-3,7(14)-diene	8.47	1526.7	0.15	10.31	1404.9	0.14
α-Cedrene	8.24*	1508.8	[0.19]	10.33	1406.2	0.09
Cascarilladiene	8.34	1517.3	0.03	10.42*	1412.9	[0.18]
β-Caryophyllene	8.65*†	1540.6	[0.10]	10.42*	1412.9	[0.18]
β-Cedrene	8.59	1536.5	0.08	10.42*	1412.9	[0.18]
Unknown POBA XXIV [m/z 161, 105 (35), 119 (23), 93 (16), 91 (16), 81 (15)... 204 (3)]				10.61	1427.0	0.19
Prezizaene	9.01	1568.5	0.44	10.76*	1438.3	[0.65]
6,9-Guaiadiene	8.87	1557.6	0.16	10.76*	1438.3	[0.65]
Khusimene	9.07	1573.3	0.61	10.82	1442.9	0.59
Selina-4(15),7-diene	9.22	1584.6	0.26	10.88	1447.0	0.17
Unknown CHZI X [m/z 119, 190 (99), 175 (95), 105 (71), 91 (59), 120 (57)... 204 (2)]				10.93	1451.2	0.34
Unknown CHZI XI [m/z 119, 120 (31), 83 (23), 105 (22), 91 (21), 81 (18)... 202 (9)]	10.08	1653.1	0.17	11.08	1462.4	0.29
Unknown CHZI XII [m/z 145, 202 (85), 159 (64), 187 (39), 131 (35), 117 (34)]	10.16	1659.5	0.68	11.16	1468.0	0.33
α-Amorphene	9.84	1634.4	1.56	11.27	1476.5	1.50
α-Vetispirene	10.34	1674.5	0.99	11.35*	1482.5	[1.23]
Unknown MISC CLXXI [m/z 160, 145 (78), 91 (37), 108				11.35*	1482.5	[1.23]

(31), 105 (28)...]						
β-Vetispirene	10.44	1682.5	1.78	11.38	1484.9	1.67
Bicyclosesquiphellandrene?				11.46	1490.2	0.55
Eudesma-2,4(15),11-triene	11.39	1761.9	0.35	11.56	1498.1	0.57
δ-Amorphene	10.19	1662.6	1.03	11.63	1503.1	1.00
Nootkatene	11.22	1747.9	0.45	11.68	1506.9	0.45
γ-Cadinene	10.64	1698.5	0.19	11.73	1510.6	0.11
Spirovetiva-1(10),7(11)-diene	10.32	1672.9	0.52	11.77	1513.8	0.71
δ-Cadinene	10.67	1701.6	0.12	11.85*	1520.4	[0.31]
trans-Calamenene	11.47	1768.6	0.09	11.85*	1520.4	[0.31]
γ-Vetivenene	11.33	1756.7	0.79	11.91	1525.4	0.90
α-Calacorene	12.38*	1847.3	[0.76]	12.05	1535.8	0.43
α-Elemol	14.30	2022.4	0.41	12.18*	1546.4	[4.83]
β-Vetivenene	11.70	1788.2	5.08	12.18*	1546.4	[4.83]
Unknown CHZI XLIII [m/z 200, 185 (82), 143 (54), 157 (36), 123 (34), 128 (32)...]				12.23	1550.5	0.32
Eremophila-1(10),11-dien-9β-ol	12.06	1819.5	0.69	12.32*	1557.6	[1.52]
cis-Eudes*m*-6-en-11-ol	13.98	1991.6	0.76	12.32*	1557.6	[1.52]
Unknown CHZI XIII [m/z 81, 200 (55), 143 (36), 93 (33), 91 (32), 185 (31), 129 (27), 128 (21)...]				12.41	1564.4	0.37
Gynuradienol?	14.68	2058.1	0.28	12.56	1576.4	0.36
Unknown CHZI V [m/z 202, 187 (63), 145 (43), 159 (34), 131 (29), 91 (22), 117 (20)]	12.38*	1847.3	[0.76]	12.64	1582.3	0.67
Unknown POBA V [m/z 161, 119 (78), 105 (75), 120 (72), 43 (64)... 218 (4)]	12.55	1862.4	0.32	12.69	1586.7	0.29
Unknown CHZI XLIV [m/z 162, 119 (83), 43 (60), 147 (53), 91 (36), 204 (32)]				12.72	1588.5	0.40
Khusimone				12.75	1591.3	0.42
Eudes*m*-4-en-7α-ol	14.18	2011.0	0.23	12.95	1607.1	0.21
Unknown CHZI VI [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	12.90	1892.9	0.75	13.00*	1610.7	[1.39]
10-epi-γ-Eudesmol	14.40	2031.2	0.55	13.00*	1610.7	[1.39]
Selin-6-en-4α-ol isomer	15.08	2096.0	1.10	13.01	1611.8	1.12
Selin-6-en-4α-ol	15.92	2179.2	0.65	13.05	1615.2	0.48
Unknown CHZI XXVIII [m/z 59, 149 (94), 43 (82), 205				13.10	1619.3	0.52

(65)... 220 (6)]						
Unknown CHZI XXV [m/z 145, 59 (97), 161 (87), 218 (76), 43 (76), 179 (63)...]				13.19	1626.5	1.04
Unknown CASA XXIX [m/z 187, 93 (35), 81 (34), 79 (31), 41 (30), 91 (30), 107 (29)... 220 (4)]				13.30	1636.3	1.11
Unknown CHZI II [m/z 121, 107 (69), 93 (64), 79 (60), 177 (59), 136 (58), 91 (57), 41 (56)... 220 (21)]	15.64	2151.7	1.67	13.40	1644.2	1.59
Cyclocopacamphan-12-ol, epimer A	16.66	2254.6	1.02	13.44*	1647.2	[2.71]
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	15.43	2130.7	1.43	13.44*	1647.2	[2.71]
Unknown CHZI XV [m/z 161, 59 (67), 95 (45), 93 (40), 105 (40), 149 (39), 81 (39), 43 (38), 204 (37)... 220 (5)]	14.94	2082.6	0.72	13.49	1651.9	1.02
Cyclocopacamphan-12-ol, epimer B	16.70	2258.5	0.55	13.52	1654.3	0.86
Unknown CHZI XXVII [m/z 84, 119 (77), 41 (72), 81 (68), 95 (68), 93 (68), 109 (63)... 222 (17)]				13.55	1656.5	1.36
Khusinol	16.13	2200.0	1.34	13.59	1659.8	0.34
Zizanol	17.12	2301.9	1.48	13.64*	1663.9	[1.78]
Zizanone analog				13.64*	1663.9	[1.78]
epi-Zizanone	15.60	2148.1	0.18	13.69*	1668.4	[1.71]
Khusiol	16.33*	2221.0	[1.58]	13.69*	1668.4	[1.71]
Zizanal	17.47	2339.6	1.44	13.78	1675.7	0.88
Unknown CHZI XXVI [m/z 189, 43 (91), 81 (89), 105 (81), 91 (74), 93 (74), 133 (67), 41 (67)... 222 (37)]				13.89	1684.5	1.53
Juniper camphor	16.33*	2221.0	[1.58]	13.93	1688.2	0.68
Unknown CHZI I [m/z 189, 159 (82), 133 (44), 91 (29), 105 (29), 205 (25)... 220 (13)]	17.23	2314.0	1.42	14.12	1703.4	1.41
Unknown CHZI XIX [m/z 204, 189 (99), 43 (83), 161				14.16	1707.0	0.21

(75), 105 (55), 91 (44), 119 (33)... 220 (13)]						
Vetiselinenol	17.42	2334.5	2.39	14.24	1714.4	2.53
α-Vetivol?	17.91	2386.3	0.14	14.29	1718.0	0.30
Unknown CHZI XX [m/z 136, 121 (98), 137 (90), 119 (68), 107 (55), 135 (55)... 202 (30), 220 (27)]	17.66	2359.2	0.53	14.33	1721.9	0.19
Unknown CHZI XXIII [m/z 189, 187 (29), 159 (23), 43 (20), 133 (16)...]				14.46*	1733.6	[9.86]
Khusimol	18.13*	2410.6	[9.55]	14.46*	1733.6	[9.86]
10-epi-Acora-3,11-dien-15-al?				14.56	1741.4	1.09
Unknown CHZI XXXVIII [m/z 174, 131 (37), 159 (25), 91 (20), 175 (14)....]	17.84	2379.0	0.27	14.85	1766.7	0.31
(*E*)-Isovalencenol	18.45	2445.5	5.89	15.00	1780.3	5.87
Unknown CHZI VII [m/z 120, 121 (93), 93 (85), 105 (74), 119 (68), 91 (58), 123 (49)... 220 (8)]	18.59	2460.8	0.97	15.10	1788.7	1.99
Unknown CHZI XXI [m/z 202, 187 (91), 93 (70), 91 (69), 105 (67)...]	18.86	2491.2	0.32	15.16*	1794.0	[0.75]
Nootkatone	18.13*	2410.6	[9.55]	15.16*	1794.0	[0.75]
(*Z*)-Isovalencenal	17.36	2327.3	0.48	15.24	1800.7	1.02
β-Vetivone	17.96	2392.2	2.46	15.30	1806.0	3.61
Zizanoic acid	23.24	3023.7	5.80	15.41*	1815.8	[6.44]
(*E*)-Isovalencenal				15.41*	1815.8	[6.44]
α-Vetivone	18.28	2426.9	3.06	15.54	1828.2	2.89
Unknown CHZI XXIX [m/z 105, 179 (87), 91 (67), 161 (61), 121 (57), 119 (56), 163 (50), 43 (50)...]				15.72	1844.8	0.57
Isovalencenal isomer II?				16.06	1875.3	0.42
Isovalencenal isomer I?				16.17	1885.4	0.21
β-Cyclodihydrocostunolide?				16.48	1914.1	0.18
Total reported		68.16%			82.63%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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

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