Date : June 06, 2023

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 23E30-PTH01
Customer identification : Himalayan Cedarwood, Bulk - India - C50110R
Type : Essential oil
Source : *Cedrus deodara*
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 : Amélie Simard, Analyste
Analysis date : June 05, 2023

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow liquid
Refractive index: 1.5146 ± 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
Mesityl oxide	0.02	Aliphatic ketone
α-Pinene	0.06	Monoterpene
Camphene	0.01	Monoterpene
β-Pinene	0.03	Monoterpene
3-Methylpentyl acetate	0.01	Aliphatic ester
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Limonene	0.02	Monoterpene
Terpinolene	0.01	Monoterpene
para-Cymenene	0.01	Monoterpene
Unknown	0.01	Oxygenated monoterpene
Phenylethyl alcohol	0.01	Simple phenolic
Limona ketone	0.56	Normonoterpenic ketone
α,4-Dimethyl-3-cyclohexene-1-methanol	0.04	Normonoterpenic alcohol
α,4-Dimethyl-3-cyclohexene-1-methanol epimer	0.04	Normonoterpenic alcohol
Borneol	0.01	Monoterpenic alcohol
4-Methylacetophenone	0.08	Simple phenolic
α-Terpineol	0.03	Monoterpenic alcohol
α-Longipinene	0.08	Sesquiterpene
Longicyclene	0.01	Sesquiterpene
α-Ylangene	0.06	Sesquiterpene
Unknown	0.02	Terpene derivative
Unknown	0.01	Terpene derivative
Unknown	0.04	Sesquiterpene
(3*Z*)-Hexenyl (3*Z*)-hexenoate	0.05	Aliphatic ester
Unknown	0.08	Sesquiterpene
Sativene	0.11	Sesquiterpene
β-Elemene	0.01	Sesquiterpene
β-Longipinene	0.04	Sesquiterpene
Longifolene	0.52	Sesquiterpene
Sibirene	0.11	Sesquiterpene
(*Z*?)-Vestitenone, or analog	0.09	Terpenic ketone
Unknown	0.04	Unknown
Himachala-2,4-diene	0.49	Sesquiterpene
Unknown	0.02	Sesquiterpene
Unknown	0.16	Sesquiterpene
trans-α-Bergamotene	0.10	Sesquiterpene
Himachala-2,4-diene isomer	0.23	Sesquiterpene
α-Himachalene	13.75	Sesquiterpene
(*E*)-Vestitenone	0.47	Terpenic ketone
Unknown	0.17	Sesquiterpene
(*E*)-β-Farnesene	0.30	Sesquiterpene
Unknown	0.38	Sesquiterpene
Unknown	0.41	Sesquiterpene
γ-Himachalene	8.70	Sesquiterpene

11-αH-Himachala-1,4-diene	2.02	Sesquiterpene
Unknown	0.19	Sesquiterpenic ether
β-Himachalene	36.69	Sesquiterpene
α-Muurolene	0.09	Sesquiterpene
(*Z*)-α-Bisabolene	0.13	Sesquiterpene
Unknown	0.14	Sesquiterpene
Cycloisolongifol-5-ol	0.16	Sesquiterpenic alcohol
α-Dehydro-ar-himachalene	0.33	Sesquiterpene
trans-Calamenene	0.02	Sesquiterpene
γ-Dehydro-ar-himachalene	0.33	Sesquiterpene
Unknown	0.33	Sesquiterpene
Unknown	0.03	Sesquiterpene
ar-Himachalene	0.18	Sesquiterpene
α-Calacorene	0.14	Sesquiterpene
(*E*)-α-Bisabolene	1.13	Sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
(*E*)-Nerolidol	0.11	Sesquiterpenic alcohol
Unknown	0.19	Unknown
Himachalene epoxide	0.23	Sesquiterpenic ether
Unknown	0.03	Oxygenated sesquiterpene
Longiborneol	0.39	Sesquiterpenic alcohol
ar-Dihydroturmerone	0.05	Sesquiterpenic ketone
β-Himachalene oxide	0.35	Sesquiterpenic ether
Unknown	0.33	Oxygenated sesquiterpene
Unknown	0.19	Oxygenated sesquiterpene
1-epi-Cubenol	0.11	Sesquiterpenic alcohol
6-Methyl-6-meta-tolyl-heptan-2-one	0.17	Miscellaneous
Unknown	0.26	Oxygenated sesquiterpene
Unknown	0.18	Oxygenated sesquiterpene
Himachalol	1.51	Sesquiterpenic alcohol
Allohimachalol	1.07	Sesquiterpenic alcohol
β-Atlantone	0.57	Sesquiterpenic ketone
(*E*)-10,11-Dihydroatlantone	0.63	Sesquiterpenic ketone
Unknown	0.10	Oxygenated sesquiterpene
Deodarone epimer I	0.16	Sesquiterpenic ketone
(*Z*)-γ-Atlantone	3.07	Sesquiterpenic ketone
Deodarone epimer II	0.22	Sesquiterpenic ketone
(*E*)-γ-Atlantone	3.18	Sesquiterpenic ketone
(*Z*)-α-Atlantone	2.41	Sesquiterpenic ketone
Unknown	0.22	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.09	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.16	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
(*E*)-α-Atlantone	11.23	Sesquiterpenic ketone
Unknown	0.19	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Consolidated total	**97.00%**	

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.

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

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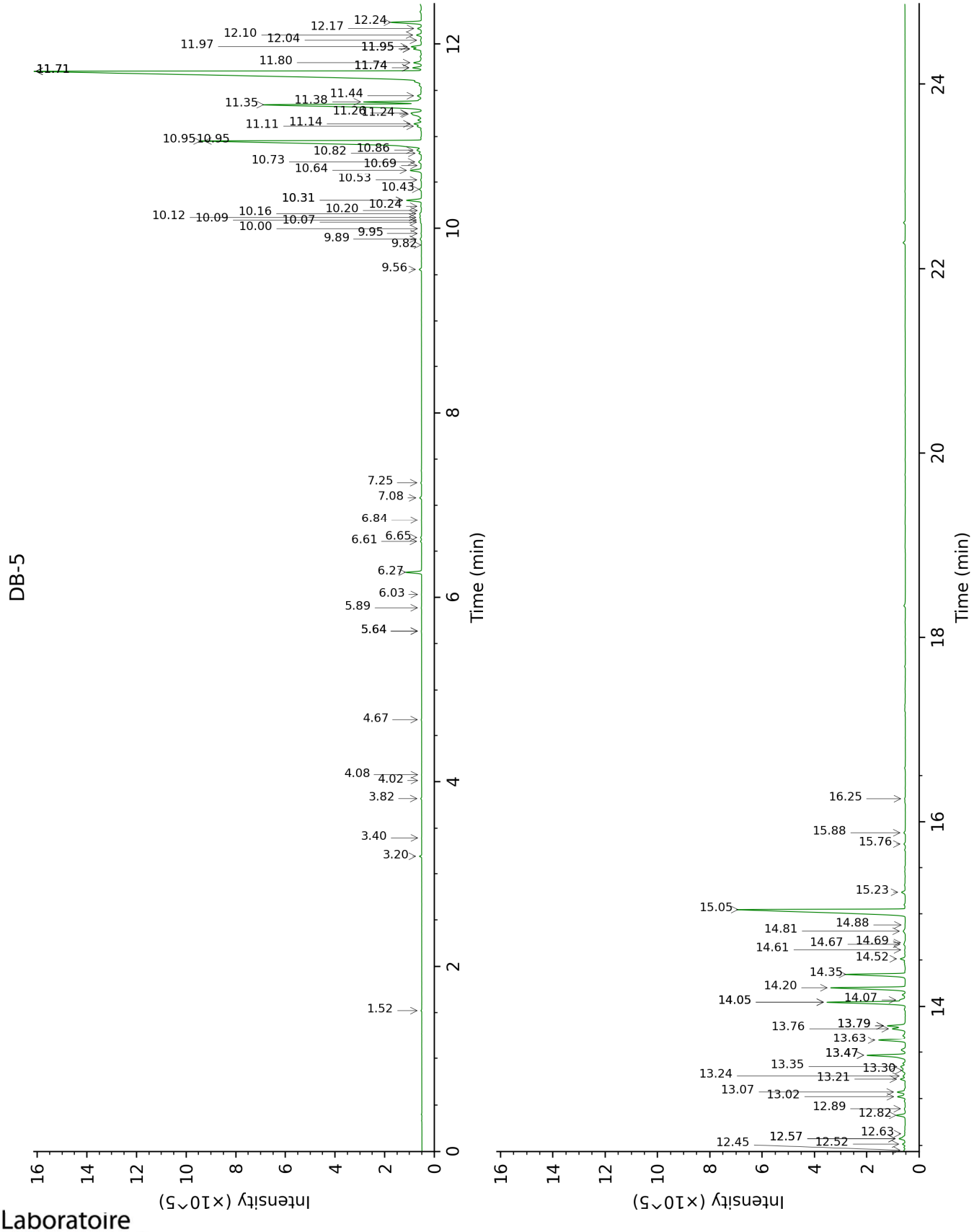
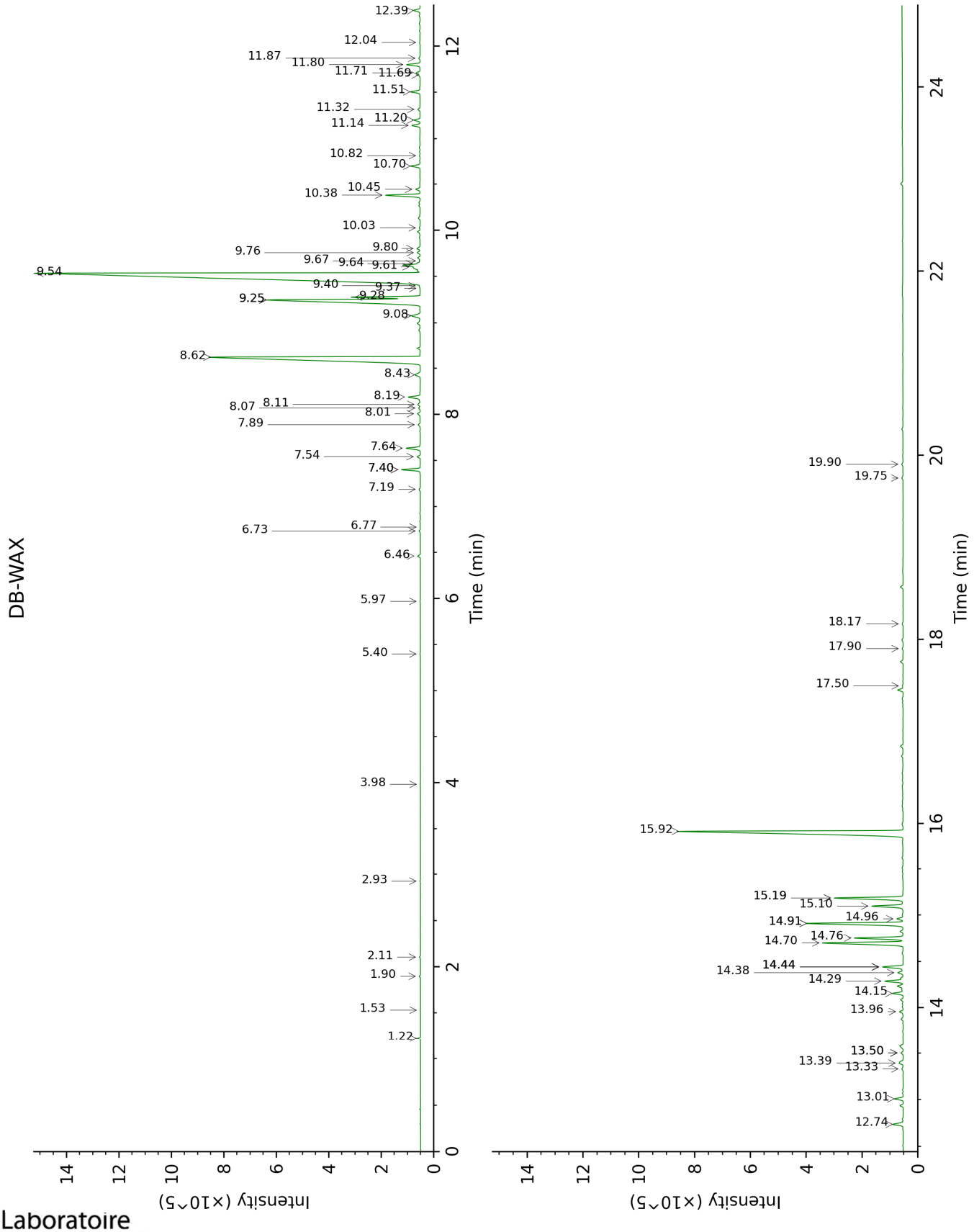

DB-5
Time (min)
Intensity (×10^5)
12.24
12.17
12.10
12.04
11.97
11.95
11.80
11.74
11.71
11.44
11.38
11.35
11.26
11.24
11.14
11.11
10.95
10.95
10.86
10.82
10.73
10.69
10.64
10.53
10.43
10.31
10.24
10.20
10.16
10.12
10.09
10.07
10.00
9.95
9.89
9.82
9.56
7.25
7.08
6.84
6.65
6.61
6.27
6.03
5.89
5.64
4.67
4.08
4.02
3.82
3.40
3.20
1.52
16.25
15.88
15.76
15.23
15.05
14.88
14.81
14.69
14.67
14.61
14.52
14.35
14.20
14.07
14.05
13.79
13.76
13.63
13.47
13.35
13.30
13.24
13.21
13.07
13.02
12.89
12.82
12.63
12.57
12.52
12.45


DB-WAX
Time (min)
Intensity (×10^5)
12.39
12.04
11.87
11.80
11.71
11.69
11.51
11.32
11.20
11.14
10.82
10.70
10.45
10.38
10.03
9.80
9.76
9.67
9.64
9.61
9.54
9.40
9.37
9.28
9.25
9.08
8.62
8.43
8.19
8.11
8.07
8.01
7.89
7.64
7.54
7.40
7.19
6.77
6.73
6.46
5.97
5.40
3.98
2.93
2.11
1.90
1.53
1.22
19.90
19.75
18.17
17.90
17.50
15.92
15.19
15.10
14.96
14.91
14.76
14.70
14.44
14.38
14.29
14.15
13.96
13.50
13.39
13.33
13.01
12.74

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Mesityl oxide	1.52	797	0.02	2.11	1088	0.02
α-Pinene	3.20	930	0.06	1.22	993	0.06
Camphene	3.40	943	0.01	1.53	1029	tr
β-Pinene	3.82	971	0.03	1.90	1067	0.03
3-Methylpentyl acetate	4.02	984	0.01			
6-Methyl-5-hepten-2-one	4.08	988	0.01			
Limonene	4.67	1026	0.02	2.93	1159	0.01
Terpinolene	5.64*	1086	0.02	3.98	1244	0.01
para-Cymenene	5.64*	1086	[0.02]	5.97	1386	0.01
Unknown [m/z 95, 150 (45), 110 (35), 107 (23), 109 (21)]	5.89	1102	0.01	5.40	1344	0.01
Phenylethyl alcohol	6.03	1111	0.01	11.69	1849	0.04
Limona ketone	6.27	1126	0.56	7.40*	1494	0.59
α,4-Dimethyl-3-cyclohexene-1-methanol	6.61	1148	0.04			
α,4-Dimethyl-3-cyclohexene-1-methanol epimer	6.65	1150	0.04			
Borneol	6.84	1163	0.01	9.37	1650	0.01
4-Methylacetophenone	7.08	1178	0.08	10.03	1704	0.03
α-Terpineol	7.25	1188	0.03	9.40	1653	0.03
α-Longipinene	9.56	1344	0.08	6.46	1422	0.09
Longicyclene	9.82	1363	0.01	6.77	1446	0.01
α-Ylangene	9.89	1367	0.06	6.73	1443	0.04
Unknown [m/z 105, 120 (38), 145 (37), 121 (34), 93 (28), 91 (26)...]	9.95	1371	0.02			
Unknown [m/z 119, 161 (36), 43 (33), 176 (26), 91 (24), 105 (22)]	10.00	1375	0.01	12.04	1881	0.02
Unknown epimer I [m/z 131, 146 (36), 91 (22), 145 (19), 202 (18)]	10.07	1380	0.04	7.89	1531	0.09
(3*Z*)-Hexenyl (3*Z*)-hexenoate	10.09	1382	0.05	9.67	1675	0.02
Unknown epimer II [m/z 131, 146 (33), 91 (20), 202 (18)]	10.12	1384	0.08	8.01	1541	0.12
Sativene	10.16	1386	0.11	7.19	1478	0.04
β-Elemene	10.20	1389	0.01	8.07	1546	0.06
β-Longipinene	10.24	1392	0.04	7.40*	1494	[0.59]

Longifolene	10.31*	1397	0.59	7.64	1511	0.52
Sibirene	10.31*	1397	[0.59]	7.54	1504	0.11
(*Z*?)-Vestitenone, or analog	10.42	1405	0.09	11.32	1816	0.08
Unknown [m/z 105, 93 (61), 120 (55), 145 (54), 91 (52)...]	10.53	1413	0.04	11.87	1865	0.05
Himachala-2,4-diene	10.64	1421	0.49	8.19	1555	0.47
Unknown [m/z 91, 93 (90), 105 (72), 202 (71), 131 (68), 77 (63), 107 (55), 187 (54)]	10.69	1425	0.02			
Unknown [m/z 105, 91 (70), 93 (65), 43 (61), 120 (57), 145 (50)... 204 (6)]	10.73	1428	0.16			
trans-α-Bergamotene	10.82	1435	0.10	8.11	1549	0.10
Himachala-2,4-diene isomer	10.86	1437	0.23	8.43	1574	0.26
α-Himachalene	10.95*	1444	14.29	8.62	1589	13.75
(*E*)-Vestitenone	10.95*	1444	[14.29]	11.80	1859	0.47
Unknown [m/z 187, 131 (78), 202 (76), 105 (74), 91 (74), 117 (53), 145 (52)]	11.11	1456	0.17	9.61†	1670	0.95
(*E*)-β-Farnesene	11.14	1458	0.30	9.25*	1640	8.76
Unknown [m/z 119, 91 (85), 93 (77), 105 (76), 79 (61), 134 (60), 94 (49), 204 (46)]	11.24	1466	0.38	9.08	1626	0.40
Unknown [m/z 131, 202 (78), 91 (74), 105 (68), 187 (68), 119 (53), 145 (52)]	11.26	1467	0.41			
γ-Himachalene	11.35	1474	8.70	9.25*	1640	[8.76]
11-αH-Himachala-1,4-diene	11.38	1476	2.02	9.28	1642	2.00
Unknown [m/z 137, 43 (84), 138 (63), 109 (53), 95 (51), 93 (50), 207 (46)... 222 (21)]	11.44	1481	0.19	9.76	1682	0.11
β-Himachalene	11.71*†	1500	36.91	9.54	1664	36.69
α-Muurolene	11.71*†	1500	[36.91]	9.64†	1672	[0.95]
(*Z*)-α-Bisabolene	11.71*†	1500	[36.91]	9.80	1686	0.13
Unknown [m/z 105, 119 (89), 91 (69), 159 (62), 131 (42), 93 (41), 202 (38)]	11.74*	1503	0.30			
Cycloisolongifol-5-ol	11.74*	1503	[0.30]	10.44	1740	0.16
α-Dehydro-ar-himachalene	11.80	1508	0.33	11.14	1800	0.28
trans-Calamenene	11.95*†	1519	0.67	10.82	1772	0.02

γ-Dehydro-ar-himachalene	11.95*†	1519	[0.67]	11.51	1833	0.33
Unknown [m/z 131, 202 (28), 91 (22), 159 (16), 145 (16), 132 (15), 115 (14)]	11.97†	1521	[0.67]	10.70	1762	0.33
Unknown [m/z 93, 187 (70), 145 (59), 119 (42), 131 (39), 202 (33)]	12.04	1526	0.03			
ar-Himachalene	12.10	1531	0.18	11.20	1805	0.21
α-Calacorene	12.17	1536	0.14	11.71	1851	0.14
(*E*)-α-Bisabolene	12.24	1542	1.13	10.38	1735	1.15
Unknown [m/z 189, 91 (85), 43 (74), 105 (67), 133 (66), 107 (63), 135 (52)... 220 (20)]	12.45	1558	0.06	13.50*	2017	0.08
(*E*)-Nerolidol	12.52	1564	0.11	13.40	2007	0.21
Unknown [m/z 96, 95 (18), 83 (15), 125 (13), 119 (12), 55 (12), 41 (11)... 218? (tr)]	12.57*	1568	0.35	14.38	2103	0.19
Himachalene epoxide	12.57*	1568	[0.35]	12.39	1912	0.23
Unknown [m/z 177, 202 (79), 91 (76), 159 (75), 43 (65), 107 (59), 105 (57)...]	12.63	1572	0.03	13.96	2062	0.13
Longiborneol	12.82	1588	0.39	14.16	2081	0.36
ar-Dihydroturmerone	12.89	1593	0.05	13.50*	2017	[0.08]
β-Himachalene oxide	13.02	1604	0.35	12.74	1945	0.40
Unknown [m/z 138, 110 (77), 137 (75), 107 (62), 91 (61), 93 (60), 109 (57)... 220 (34)]	13.07	1608	0.33	13.01	1970	0.29
Unknown [m/z 137, 119 (69), 43 (51), 95 (50), 109)40)... 222 (1)]	13.21	1619	0.19	14.44*	2109	0.71
1-epi-Cubenol	13.24	1622	0.11	13.33	2001	0.07
6-Methyl-6-meta-tolyl-heptan-2-one	13.30	1627	0.17	15.19*	2185	2.40
Unknown [m/z 119, 163 (80), 107 (64), 95 (61), 93 (57), 91 (53)... 220 (11)]	13.35	1630	0.26			
Unknown [m/z 119, 91 (44), 94 (36), 107 (35), 93 (29)... 202 (19)...]	13.47*	1640	1.69			

Himachalol	13.47*	1640	[1.69]	14.76	2141	1.51
Allohimachalol	13.63	1654	1.07	15.10	2176	1.05
β-Atlantone	13.76	1664	0.57	14.44*	2109	[0.71]
(*E*)-10,11-Dihydroatlantone	13.79*	1667	0.73	14.29	2094	0.63
Unknown [m/z 83, 55 (19), 119 (14), 120 (10), 84 (6)... 218 (1)]	13.79*	1667	[0.73]	14.44*	2109	[0.71]
Deodarone epimer I	14.05*†	1688	3.52	14.91*	2157	3.34
(*Z*)-γ-Atlantone	14.05*†	1688	[3.52]	14.70	2135	3.07
Deodarone epimer II	14.07†	1690	[3.52]	14.96	2162	0.22
(*E*)-γ-Atlantone	14.20	1701	3.18	14.91*	2157	[3.34]
(*Z*)-α-Atlantone	14.35	1713	2.41	15.19*	2185	[2.40]
Unknown [m/z 105, 119 (89), 59 (68), 120 (65), 43 (65), 93 (62), 121 (61)...]	14.52	1728	0.22			
Unknown [m/z 91, 79 (83), 105 (68), 109 (63), 41 (590), 93 (58), 107 (57)...]	14.61	1736	0.05	17.50	2434	0.03
Unknown [m/z 83, 91 (28), 105 (25), 55 (21), 43 (17), 119 (17)...]	14.67	1741	0.09			
Unknown [m/z 43, 105 (99), 119 (90), 91 (87), 147 (76), 41 (69), 93 (63)...]	14.69	1743	0.03			
Unknown [m/z 83, 55 (17), 91 (14), 105 (9), 216 (6)...]	14.81	1753	0.16			
Unknown [m/z 91, 105 (74), 93 (67), 79 (59), 133 (54), 41 (47), 107 (46)...]	14.88	1759	0.02	17.90	2479	0.04
(*E*)-α-Atlantone	15.05	1774	11.23	15.92	2261	11.16
Unknown [m/z 95, 43 (59), 69, (57), 67 (43), 163 (42), 94 (37), 107 (37)... 178 (26), 218 (2)]	15.24	1790	0.19			
Unknown [m/z 83, 134 (28), 119 (19), 55 (18), 91 (14), 43 (11), 109 (10)... 216 (4), 249? (0)]	15.76	1837	0.06	19.76	2700	0.05
Unknown [m/z 83, 134 (30), 119 (19), 55 (18), 91 (12)... 216 (4)...]	15.88	1848	0.07	19.90	2718	0.05
Unknown [m/z 173, 83 (83), 91 (80), 201	16.25	1882	0.04	18.17	2510	0.04

(79), 115 (65)... 216 (31)]		
Total identified	**93.66%**	**92.15%**
Total reported	**97.03%**	**95.07%**

*: 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

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