Date : April 08, 2022

Certificate of Analysis – GC Profiling

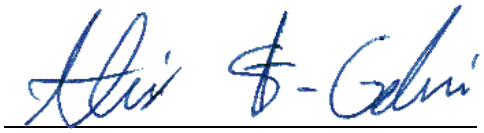
Sample identification

Internal code : 22D07-PTH04
Customer identification : Celery Seed - India - CH4101R
Type : Essential oil
Source : *Apium graveolens*
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 : April 08, 2022

Checked and approved by :



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

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Méthode certifiée ISO 17025:2017 Certified method

Laboratoire PhytoChemia

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow liquid
Refractive index: 1.4824 ± 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
Isobutyral	tr	Aliphatic aldehyde
Isovaleral	0.02	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Valeral	0.01	Aliphatic aldehyde
Hexanal	tr	Aliphatic aldehyde
2-Methyloctane	0.01	Alkane
Nonane	0.01	Alkane
α-Thujene	0.01	Monoterpene
α-Pinene	0.20	Monoterpene
Camphene	0.01	Monoterpene
Propylbenzene	0.01	Simple phenolic
β-Pinene	0.68	Monoterpene
Sabinene	0.10	Monoterpene
Myrcene	1.07	Monoterpene
α-Phellandrene	0.01	Monoterpene
Menthatriene isomer I	0.02	Monoterpene
Octanal	0.02	Aliphatic aldehyde
Δ3-Carene	0.04	Monoterpene
α-Terpinene	0.01	Monoterpene
para-Cymene	0.04	Monoterpene
Limonene	69.98	Monoterpene
β-Phellandrene	0.08	Monoterpene
(*Z*)-β-Ocimene	0.03	Monoterpene
(*E*)-β-Ocimene	0.01	Monoterpene
γ-Terpinene	0.12	Monoterpene
Octanol	0.04	Aliphatic alcohol
Terpinolene	0.02	Monoterpene
para-Cymenene	0.01	Monoterpene
Methyl benzoate	0.01	Phenolic ester
Perillene	0.01	Monoterpenic ether
Linalool	0.20	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
Hotrienol	0.01	Monoterpenic alcohol
Octen-3-yl acetate	0.02	Aliphatic ester
trans-para-Mentha-2,8-dien-1-ol	0.05	Monoterpenic alcohol
Limona ketone	0.02	Normonoterpenic ketone
Octan-3-yl acetate	0.01	Aliphatic ester
cis-Limonene oxide	0.04	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	0.09	Monoterpenic alcohol
Pentylbenzene	0.55	Simple phenolic
5-Pentylcyclohexa-1,3-diene	1.78	Alkene
2-Methylbutyl angelate	0.02	Aliphatic ester
Terpinen-4-ol	0.03	Monoterpenic alcohol
trans-Isocarveol	0.03	Monoterpenic alcohol
α-Terpineol	0.07	Monoterpenic alcohol

cis-Dihydrocarvone	0.01	Monoterpenic ketone
Unknown	0.04	Unknown
Unknown	0.02	Unknown
trans-Isopiperitenol	0.04	Monoterpenic alcohol
Decanal	0.03	Aliphatic aldehyde
cis-Isopiperitenol	0.02	Monoterpenic alcohol
trans-Carveol	0.06	Monoterpenic alcohol
Unknown	0.02	Unknown
cis-Isocarveol	0.03	Monoterpenic alcohol
Coumaran	0.02	Simple phenolic
cis-Carveol	0.04	Monoterpenic alcohol
Carvone	0.03	Monoterpenic ketone
Neral	0.01	Monoterpenic aldehyde
Linalyl acetate	0.01	Monoterpenic ester
Perillaldehyde	0.03	Monoterpenic aldehyde
Geranial	0.02	Monoterpenic aldehyde
Limonen-10-ol	0.01	Monoterpenic alcohol
Perilla alcohol	0.07	Monoterpenic alcohol
trans-Pinocarvyl acetate	0.01	Monoterpenic ester
4-Vinylguaiacol	0.07	Simple phenolic
trans-Carvyl acetate	0.03	Monoterpenic ester
Fenipentol	0.02	Simple phenolic
Valerophenone	0.49	Simple phenolic
cis-Carvyl acetate	0.01	Monoterpenic ester
Unknown	0.01	Unknown
β-Elemene	0.08	Sesquiterpene
Unknown	0.05	Unknown
α-Cedrene	0.01	Sesquiterpene
Unknown	0.01	Unknown
2-Pentylphenol	0.02	Simple phenolic
β-Caryophyllene	0.78	Sesquiterpene
α-Humulene	0.09	Sesquiterpene
(*E*)-β-Farnesene	0.02	Sesquiterpene
4-Pentylphenol	0.02	Simple phenolic
Selina-4,11-diene	0.02	Sesquiterpene
β-Selinene	10.30	Sesquiterpene
α-Selinene	1.71	Sesquiterpene
Selina-4(15),7(11)-diene	0.06	Sesquiterpene
Selina-3,7(11)-diene	0.03	Sesquiterpene
Unknown	0.03	Unknown
α-Elemol	0.03	Sesquiterpenic alcohol
(*E*)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.13	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Unknown	0.03	Unknown
Humulene epoxide II	0.02	Sesquiterpenic ether
Unknown	0.12	Unknown
Dill apiole	0.01	Phenylpropanoid
β-Eudesmol	0.28	Sesquiterpenic alcohol
3-Butylphthalide	1.29	Phthalide
α-Eudesmol	0.01	Sesquiterpenic alcohol
(3*Z*)-Butylidenephthalide	0.46	Phthalide

Sedanenolide	5.15	Phthalide
Sedanolide?	0.35	Phthalide
(*Z*)-Ligustilide	0.09	Phthalide
Neophytadiene	0.05	Diterpene
Senkyunolide N?	0.01	Phthalide
Unknown	0.07	Unknown
Unknown	0.14	Unknown
Menthatriene isomer II	tr	Monoterpene
3-Methylpentylbenzene	0.01	Simple phenolic
(1*E*)-Pentenylbenzene	0.01	Simple phenolic
Consolidated total	**98.14%**	

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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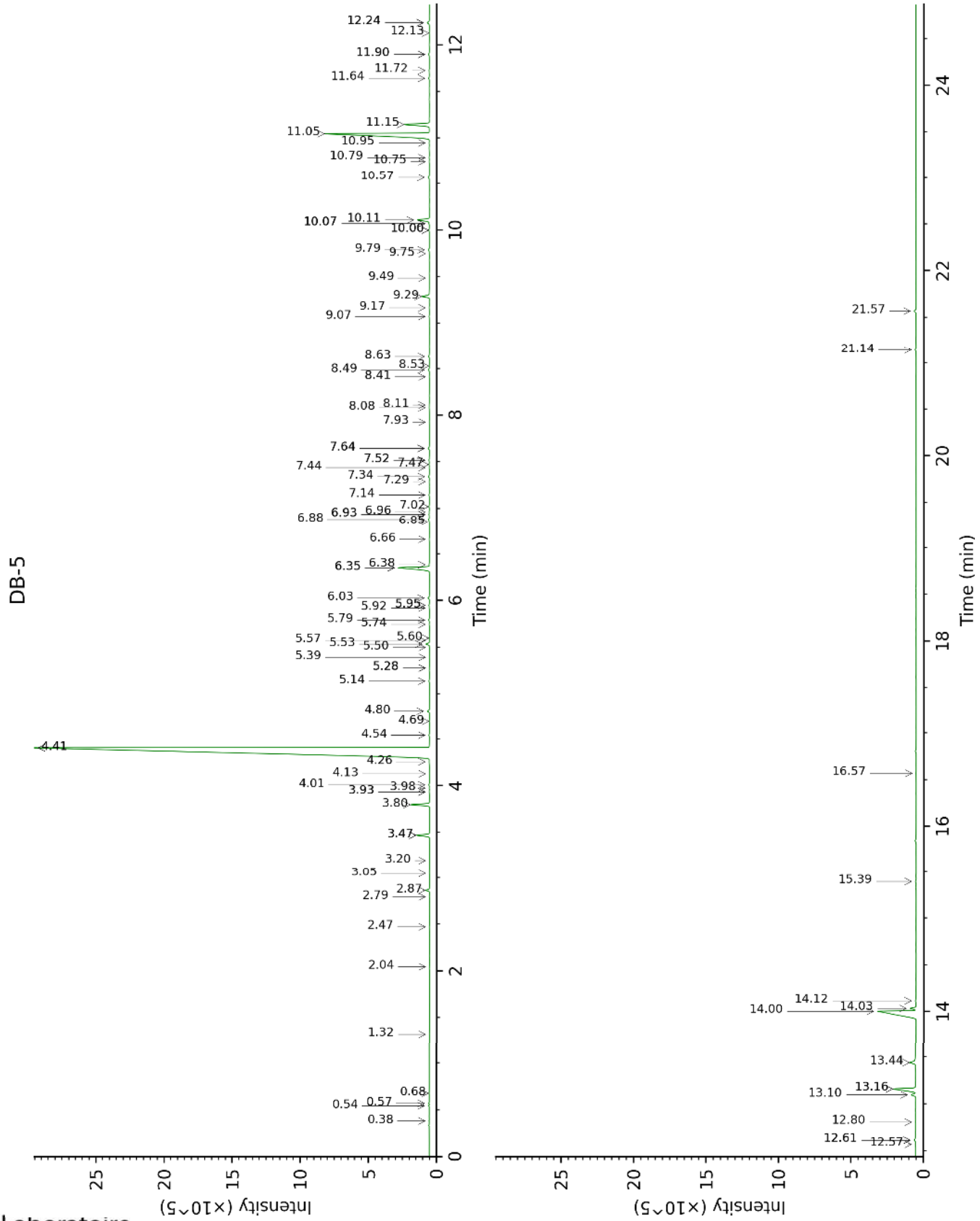
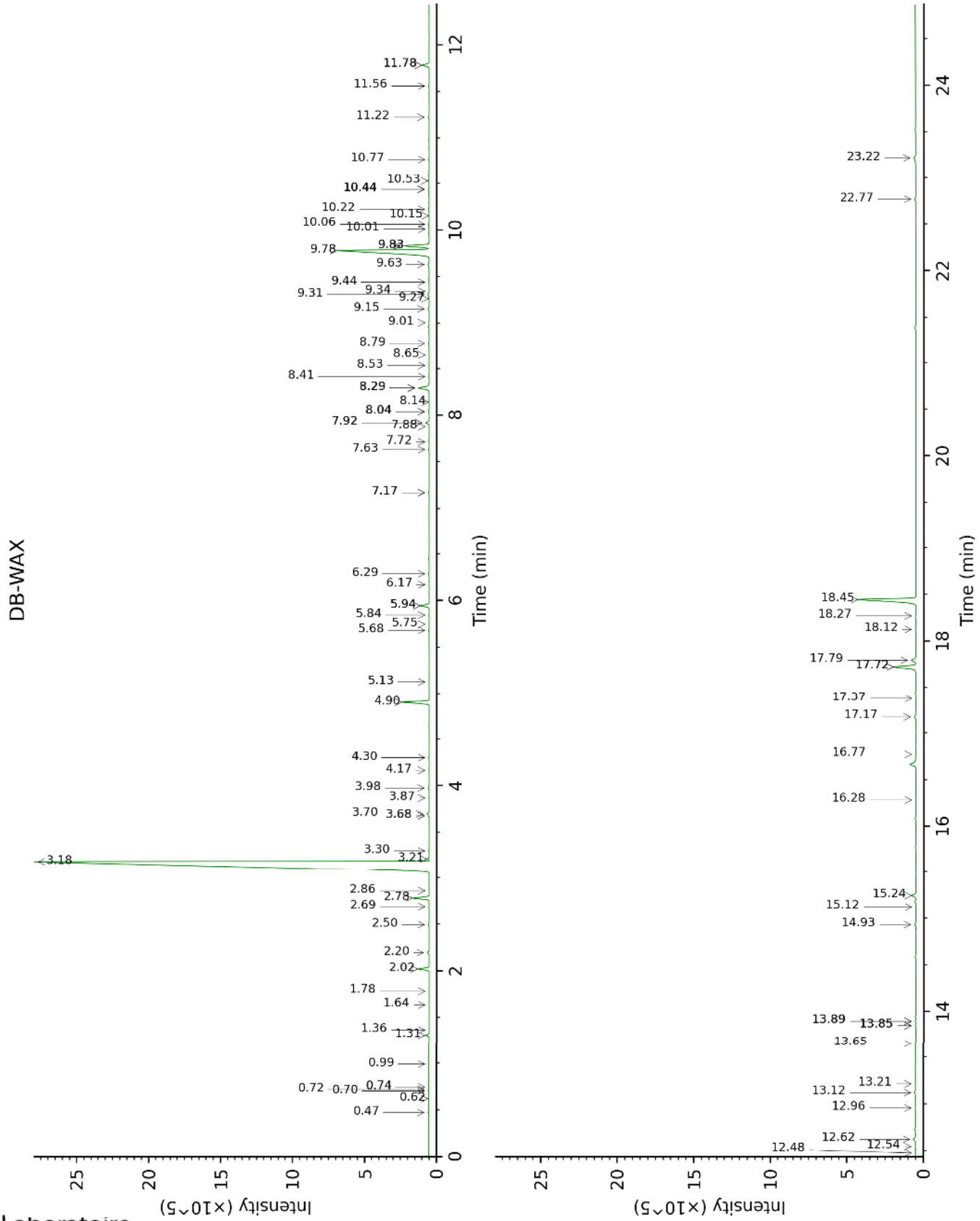

DB-5
Time (min)
Intensity (×10^5)
12.24
12.13
11.90
11.72
11.64
11.15
11.05
10.95
10.79
10.75
10.57
10.07
10.11
10.00
9.79
9.75
9.49
9.29
9.17
9.07
8.63
8.49
8.53
8.41
8.08
8.11
7.93
7.64
7.52
7.47
7.44
7.34
7.29
7.14
7.02
6.96
6.93
6.88
6.85
6.66
6.38
6.35
6.03
5.92
5.95
5.79
5.74
5.60
5.57
5.53
5.50
5.39
5.28
5.14
4.80
4.69
4.54
4.41
4.26
4.13
4.01
3.98
3.93
3.80
3.47
3.20
3.05
2.87
2.79
2.47
2.04
1.32
0.68
0.57
0.54
0.38
21.57
21.14
16.57
15.39
14.12
14.03
14.00
13.44
13.16
13.10
12.80
12.61
12.57


DB-WAX
Time (min)
Intensity (×10^5)
11.78
11.56
11.22
10.77
10.53
10.44
10.22
10.15
10.06
10.01
9.83
9.78
9.63
9.44
9.34
9.31
9.27
9.15
9.01
8.79
8.65
8.53
8.41
8.29
8.14
8.04
7.92
7.88
7.72
7.63
7.17
6.29
6.17
5.94
5.84
5.75
5.68
5.13
4.90
4.30
4.17
3.98
3.87
3.70
3.68
3.30
3.21
3.18
2.86
2.78
2.69
2.50
2.20
2.02
1.78
1.64
1.36
1.31
0.99
0.74
0.72
0.70
0.62
0.47
23.22
22.77
18.45
18.27
18.12
17.79
17.72
17.37
17.17
16.77
16.28
15.24
15.12
14.93
13.89
13.85
13.65
13.21
13.12
12.96
12.62
12.54
12.48

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isobutyral	0.38	538	tr	0.47	785	0.02
Isovaleral	0.54	642	0.02	0.72	887	0.02
2-Methylbutyral	0.57	652	0.01	0.70	882	0.02
Valeral	0.68	695	0.01	0.99	940	tr
Hexanal	1.32	801	tr	1.78	1043	tr
2-Methyloctane	2.04	865	0.01	0.62	851	0.01
Nonane	2.47	902	0.01	0.74	897	0.01
α-Thujene	2.80	924	0.01	1.36	1002	0.01
α-Pinene	2.86	929	0.20	1.31	993	0.20
Camphene	3.05	942	0.01	1.64	1029	tr
Propylbenzene	3.20	952	0.01			
β-Pinene	3.47*	970	0.78	2.02	1067	0.68
Sabinene	3.47*	970	[0.78]	2.20	1085	0.10
Myrcene	3.80	992	1.07	2.78	1135	1.07
α-Phellandrene	3.93*	1001	0.03	2.69	1127	0.01
Menthatriene isomer I	3.93*	1001	[0.03]	3.30	1176	0.02
Octanal	3.98	1004	0.02	4.30	1253	0.03
Δ3-Carene	4.01	1006	0.04	2.50	1112	0.04
α-Terpinene	4.13	1014	0.01	2.86	1141	0.01
para-Cymene	4.26	1022	0.04	3.98	1228	0.06
Limonene	4.41*	1031	70.20	3.18	1167	69.98
β-Phellandrene	4.41*	1031	[70.20]	3.22	1169	0.08
(*Z*)-β-Ocimene	4.54	1040	0.03	3.68*	1206	0.03
(*E*)-β-Ocimene	4.69	1049	0.01	3.87	1220	0.01
γ-Terpinene	4.80	1056	0.12	3.70	1208	0.14
Octanol	5.14	1077	0.04	8.04*	1524	0.04
Terpinolene	5.28*†	1086	0.02	4.16	1243	0.02
para-Cymenene	5.28*†	1086	[0.02]	6.17	1386	0.01
Methyl benzoate	5.39	1094	0.01	8.53	1563	0.01
Perillene	5.50	1100	0.01	5.94*	1370	0.56
Linalool	5.53	1102	0.20	7.92*	1515	0.21
Nonanal	5.57	1105	0.01	5.74	1356	0.01
Hotrienol	5.60	1106	0.01	8.65	1572	0.01
Octen-3-yl acetate	5.74	1116	0.02	5.68	1351	0.04
trans-para-Mentha-2,8-dien-1-ol	5.79	1119	0.05	8.78	1582	0.05
Limona ketone	5.92	1127	0.02	7.72	1500	0.03
Octan-3-yl acetate	5.95*	1129	0.04	5.13	1312	0.01
cis-Limonene oxide	5.95*	1129	[0.04]	6.29	1394	0.04
cis-para-Mentha-2,8-dien-1-ol	6.03	1134	0.09	9.31	1624	0.11
Pentylbenzene	6.35*	1155	2.34	5.94*	1370	[0.56]
5-Pentylcyclohexa-1,3-diene	6.35*	1155	[2.34]	4.90	1298	1.78
2-Methylbutyl angelate	6.38	1157	0.02	5.84	1363	0.02
Terpinen-4-ol	6.66	1174	0.03	8.42	1554	0.02

trans-Isocarveol	6.85	1187	0.03	10.77	1745	0.03
α-Terpineol	6.88	1189	0.07	9.63	1650	0.11
cis-Dihydrocarvone	6.94*†	1192	0.05	8.29*	1544	0.85
Unknown [m/z 121, 79 (98), 93 (87), 94 (73), 91 (63), 105 (45)...]	6.94*†	1192	[0.05]	7.63	1494	0.04
Unknown [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...]	6.96	1194	0.02	7.92*	1515	[0.21]
trans-Isopiperitenol	7.02	1198	0.04	10.22	1698	0.05
Decanal	7.14	1206	0.03	7.17*	1459	0.04
cis-Isopiperitenol	7.29	1215	0.02	10.15	1693	0.01
trans-Carveol	7.34	1219	0.06	11.22	1784	0.06
Unknown [m/z 92, 91 (76), 41 (47), 69 (45), 109 (42)... 162 (15)]	7.44	1225	0.02			
cis-Isocarveol	7.47	1228	0.03	11.78*	1833	0.50
Coumaran	7.52*	1231	0.04	16.77	2323	0.02
cis-Carveol	7.52*	1231	[0.04]	11.56	1813	0.04
Carvone	7.64*	1239	0.08	9.83*	1667	1.74
Neral	7.64*	1239	[0.08]	9.34	1627	0.01
Linalyl acetate	7.93	1258	0.01	8.04*	1524	[0.04]
Perillaldehyde	8.08	1268	0.03	10.53	1724	0.06
Geranial	8.11	1270	0.02	10.01	1681	0.01
Limonen-10-ol	8.41	1290	0.01	12.96	1939	0.02
Perilla alcohol	8.49	1295	0.07	13.12	1954	0.07
trans-Pinocarvyl acetate	8.53	1298	0.01	9.01	1600	0.01
4-Vinylguaiacol	8.63	1305	0.07	14.93	2130	0.08
trans-Carvyl acetate	9.07	1336	0.03	10.06	1686	0.05
Fenipentol	9.17	1343	0.02	13.85*	2023	0.03
Valerophenone	9.29	1351	0.49	11.78*	1833	[0.50]
cis-Carvyl acetate	9.49	1365	0.01	10.44*	1716	0.07
Unknown [m/z 109, 95 (24), 79 (19), 91 (19), 166 (18)]	9.75	1384	0.01	13.90*	2028	0.03
β-Elemene	9.79	1387	0.08	8.29*	1544	[0.85]
Unknown [m/z 109, 95 (28), 166 (22), 79 (21), 81 (19), 91 (19)]	10.00*	1401	0.05			
α-Cedrene	10.00*	1401	[0.05]	7.88	1512	0.01
Unknown [m/z 109, 95 (22), 166 (20), 79 (16)... 180? (t)]	10.07*	1407	0.03	13.85*	2023	[0.03]
2-Pentylphenol	10.07*	1407	[0.03]			
β-Caryophyllene	10.11	1410	0.78	8.29*	1544	[0.85]
α-Humulene	10.57	1444	0.09	9.15	1611	0.08
(*E*)-β-Farnesene	10.75	1457	0.02	9.44	1635	0.03
4-Pentylphenol	10.79	1460	0.02	17.37	2389	0.01
Selina-4,11-diene	10.95	1472	0.02	9.26	1620	0.02
β-Selinene	11.05	1479	10.30	9.78	1662	10.13

α-Selinene	11.15	1487	1.71	9.83*	1667	[1.74]
Selina-4(15),7(11)-diene	11.64	1525	0.06	10.44*	1716	[0.07]
Selina-3,7(11)-diene	11.72	1531	0.03	10.44*	1716	[0.07]
Unknown [m/z 84, 83 (15), 95 (15), 41 (14), 113 (12), 67 (12), 55 (10), 125 (9)...]	11.90*	1545	0.06	18.27	2491	0.03
α-Elemol	11.90*	1545	[0.06]	13.90*	2028	[0.03]
(*E*)-Nerolidol	12.13	1562	0.02	13.65	2004	0.01
Caryophyllene oxide	12.24*	1571	0.15	12.62	1908	0.13
Caryophyllene oxide isomer	12.24*	1571	[0.15]	12.54	1901	0.02
Unknown [m/z 123, 138 (99), 95 (97), 67 (64), 180 (45), 96 (40)...]	12.57	1597	0.03			
Humulene epoxide II	12.61*	1601	0.12	13.21	1963	0.02
Unknown [m/z 95, 123 (98), 133 (83), 138 (82), 67 (65), 41 (47), 180 (40)]	12.61*	1601	[0.12]	17.17	2367	0.12
Dill apiole	12.80	1616	0.01	16.28	2270	0.01
β-Eudesmol	13.10	1640	0.28	15.24	2162	0.28
3-Butylphthalide	13.16*	1646	1.76	17.72*	2428	1.76
α-Eudesmol	13.16*	1646	[1.76]	15.12	2149	0.01
(3*Z*)-Butylidenephthalide	13.44	1669	0.46	17.72*	2428	[1.76]
Sedanenolide	14.00	1716	5.15	18.45	2511	5.06
Sedanolide?	14.03	1719	0.35	17.79	2436	0.35
(*Z*)-Ligustilide	14.12	1726	0.09	18.12	2474	0.03
Neophytadiene	15.40	1838	0.05	12.48	1895	0.01
Senkyunolide N?	16.57	1947	0.01			
Unknown [m/z 192, 193 (19), 136 (19), 108 (18), 41 (13)...]	21.14	2426	0.07	22.77	3065	0.07
Unknown [m/z 192, 193 (15), 136 (14), 108 (12), 150 (9), 41 (7)...]	21.57	2475	0.14	23.22	3129	0.19
Menthatriene isomer II				3.68*	1206	[0.03]
3-Methylpentylbenzene				7.17*	1459	[0.04]
(1*E*)-Pentenylbenzene				8.14	1532	0.01
Total identified		**98.46%**			**97.38%**	
Total reported		**98.74%**			**97.82%**	

*: 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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