

Date : November 11, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22K04-PTH02

Customer identification : Lemongrass - India - L80114R

Type : Essential oil

Source : *Cymbopogon flexuosus*

Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-014  - 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 : November 09, 2022

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow liquid

Refractive index: 1.4853 ± 0.0003 (20 °C; method PC-MAT-016)

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	%	Class
2-Methyl-3-buten-2-ol	0.02	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
Hexanal	tr	Aliphatic aldehyde
Unknown	tr	Unknown
(3Z)-Hexenol	0.01	Aliphatic alcohol
4-Heptanone	0.01	Aliphatic ketone
Hexanol	tr	Aliphatic alcohol
Unknown	tr	Unknown
Tricyclene	0.12	Monoterpene
α -Pinene	0.13	Monoterpene
Camphene	0.90	Monoterpene
α -Fenchene	0.01	Monoterpene
Benzaldehyde	0.01	Simple phenolic
β -Pinene	0.01	Monoterpene
Sabinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Dehydro-1,8-cineole	0.03	Monoterpenic ether
Myrcene	0.07	Monoterpene
6-Methyl-5-hepten-2-ol	0.06	Aliphatic alcohol
α -Phellandrene	0.01	Monoterpene
Octanal	0.07	Aliphatic aldehyde
α -Terpinene	tr	Monoterpene
para-Cymene	0.01	Monoterpene
Limonene	0.71	Monoterpene
β -Phellandrene	0.03	Monoterpene
Benzeneacetaldehyde	0.01	Simple phenolic
(Z)- β -Ocimene	0.29	Monoterpene
(E)- β -Ocimene	0.18	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
γ -Terpinene	0.01	Monoterpene
cis-Sabinene hydrate	tr	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
4-Nonanone	0.99	Aliphatic ketone
Camphenilone	0.01	Normonoterpenic ketone
trans-Linalool oxide (fur.)	tr	Monoterpenic alcohol
Terpinolene	0.04	Monoterpene
para-Cymenene	0.01	Monoterpene
4-Nonanol	0.03	Aliphatic alcohol
Rosefuran	0.20	Monoterpenic ether
Linalool	1.11	Monoterpenic alcohol
cis-Chrysanthemal?	0.01	Monoterpenic aldehyde
(Z)-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone

α -Cyclocitral	0.01	Monoterpenic aldehyde
<i>trans</i> -para-Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
Unknown	0.13	Unknown
Unknown	0.01	Unknown
<i>trans</i> -Chrysanthemal	0.26	Monoterpenic aldehyde
exo-Isocitral	0.04	Monoterpenic aldehyde
Citronellal	0.29	Monoterpenic aldehyde
Borneol	0.16	Monoterpenic alcohol
α -Phellandren-8-ol	0.02	Monoterpenic alcohol
Isoneral	0.48	Monoterpenic aldehyde
Rosefuran oxide	0.23*	Monoterpenic ether
Terpinen-4-ol	0.23*	Monoterpenic alcohol
Unknown	0.09	Oxygenated monoterpene
Unknown	0.06	Unknown
Isogeranial	0.84	Monoterpenic aldehyde
Myrtenal	0.02	Monoterpenic aldehyde
α -Terpineol	0.12	Monoterpenic alcohol
Unknown	0.07	Unknown
<i>trans</i> -Isopiperitenol	0.04	Monoterpenic alcohol
Unknown	0.05	Oxygenated monoterpene
Decanal	0.16	Aliphatic aldehyde
<i>cis</i> -Isopiperitenol	0.04	Monoterpenic alcohol
2,3-Epoxyneral?	0.05	Monoterpenic aldehyde
Nerol	0.03	Monoterpenic alcohol
Citronellol	0.21	Monoterpenic alcohol
(<i>Z</i>)-Isogeraniol	0.02	Monoterpenic alcohol
Neral	31.07	Monoterpenic aldehyde
Piperitone	0.05	Monoterpenic ketone
Geraniol	7.06	Monoterpenic alcohol
Geranial	41.08	Monoterpenic aldehyde
Unknown	0.18	Oxygenated monoterpene
2-Undecanone	tr	Aliphatic ketone
Geranyl formate	tr	Monoterpenic ester
Methyl geranate	0.03	Monoterpenic ester
Neric acid	0.03	Monoterpenic acid
Unknown	0.04	Unknown
α -Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.03	Monoterpenic ester
Unknown	0.02	Unknown
Cyclosativene I	0.07	Sesquiterpene
Cyclosativene II	0.08	Sesquiterpene
Neryl acetate	0.02	Monoterpenic ester
α -Ylangene	0.04	Sesquiterpene
Geranic acid	0.16	Aliphatic acid
α -Copaene	0.03	Sesquiterpene
Unknown	0.05	Unknown
β -Bourbonene	0.03	Sesquiterpene
β -Cubebene	0.07	Sesquiterpene
Geranyl acetate	3.35	Monoterpenic ester
β -Elemene	0.08	Sesquiterpene
Longifolene	0.02	Sesquiterpene
β -Caryophyllene	1.35	Sesquiterpene

β-Ylangene	0.02	Sesquiterpene
β-Copaene	0.02	Sesquiterpene
<i>trans</i> -α-Bergamotene	0.01	Sesquiterpene
6,9-Guaiadiene	0.02	Sesquiterpene
(<i>E</i>)-Isoeugenol	0.44	Phenylpropanoid
α-Humulene	0.16	Sesquiterpene
<i>cis</i> -Muurolo-4(15),5-diene	0.03	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.03	Sesquiterpene
γ-Muurolole	0.01	Sesquiterpene
Germacrene D	0.19	Sesquiterpene
γ-Amorphene	0.02	Sesquiterpene
epi-Cubebol	0.09	Sesquiterpenic alcohol
α-Selinene	0.02	Sesquiterpene
α-Muurolole	0.02	Sesquiterpene
Methyl (<i>E</i>)-isoeugenol	0.03	Phenylpropanoid
γ-Cadinene	0.91	Sesquiterpene
Cubebol	0.26	Sesquiterpenic alcohol
δ-Cadinene	0.25	Sesquiterpene
10-epi-Cubebol?	0.04	Sesquiterpenic alcohol
(<i>E</i>)-γ-Bisabolene	0.13	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.02	Sesquiterpene
α-Cadinene	0.03	Sesquiterpene
Neryl butyrate	0.02	Monoterpenic ester
α-Elemol	0.05	Sesquiterpenic alcohol
Germacrene B	0.04	Sesquiterpene
Geranyl butyrate	0.08	Monoterpenic ester
Caryophyllene oxide	0.41	Sesquiterpenic ether
Caryophyllene oxide isomer	0.04	Sesquiterpenic ether
Humulene epoxide II	0.04	Sesquiterpenic ether
10-epi-Cubebol	0.02	Sesquiterpenic alcohol
Selin-6-en-4α-ol isomer	0.01	Sesquiterpenic alcohol
1-epi-Cubebol	0.03	Sesquiterpenic alcohol
τ-Muurolol	tr	Sesquiterpenic alcohol
τ-Cadinol	0.01	Sesquiterpenic alcohol
Cubebol	0.01	Sesquiterpenic alcohol
β-Eudesmol	0.01	Sesquiterpenic alcohol
α-Eudesmol	0.01	Sesquiterpenic alcohol
α-Cadinol	0.01	Sesquiterpenic alcohol
(2 <i>Z</i> ,6 <i>Z</i>)-Farnesol	0.01	Sesquiterpenic alcohol
Farnesal isomer	0.01	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	0.01	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	0.01	Sesquiterpenic aldehyde
Neophytadiene	0.03	Diterpene
Phytone	0.01	Terpenic ketone
Unknown	0.01	Unknown
Octadecanal	0.03	Aliphatic aldehyde
Unknown	0.02	Unknown
Unknown	0.05	Unknown
Unknown	0.02	Unknown
Dicitral	0.08	Diterpenic aldehyde
Unknown	0.02	Unknown
Unknown	0.01	Unknown

Unknown	0.02	Unknown
Unknown	0.01	Unknown
Consolidated total	97.55%	

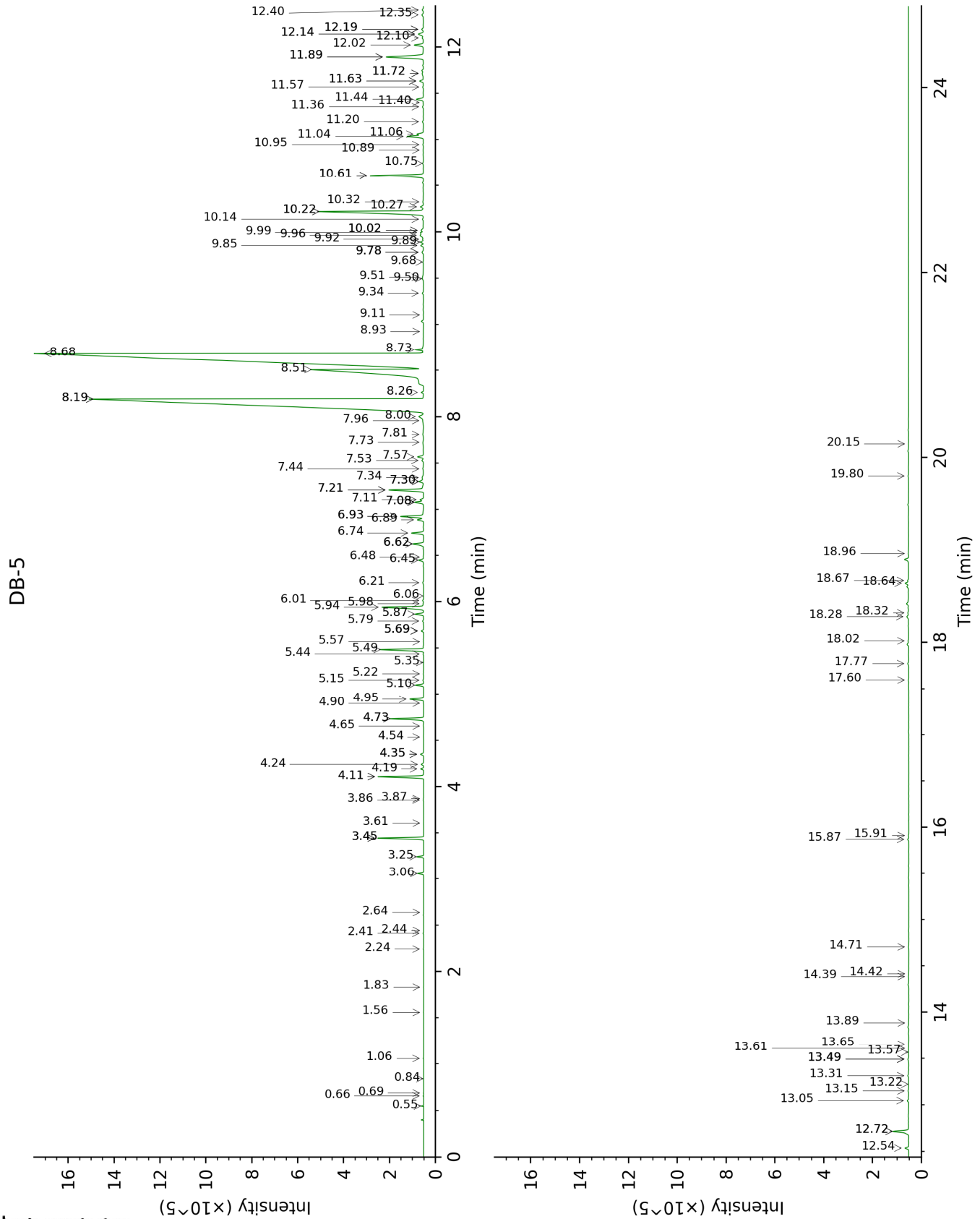
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered [xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

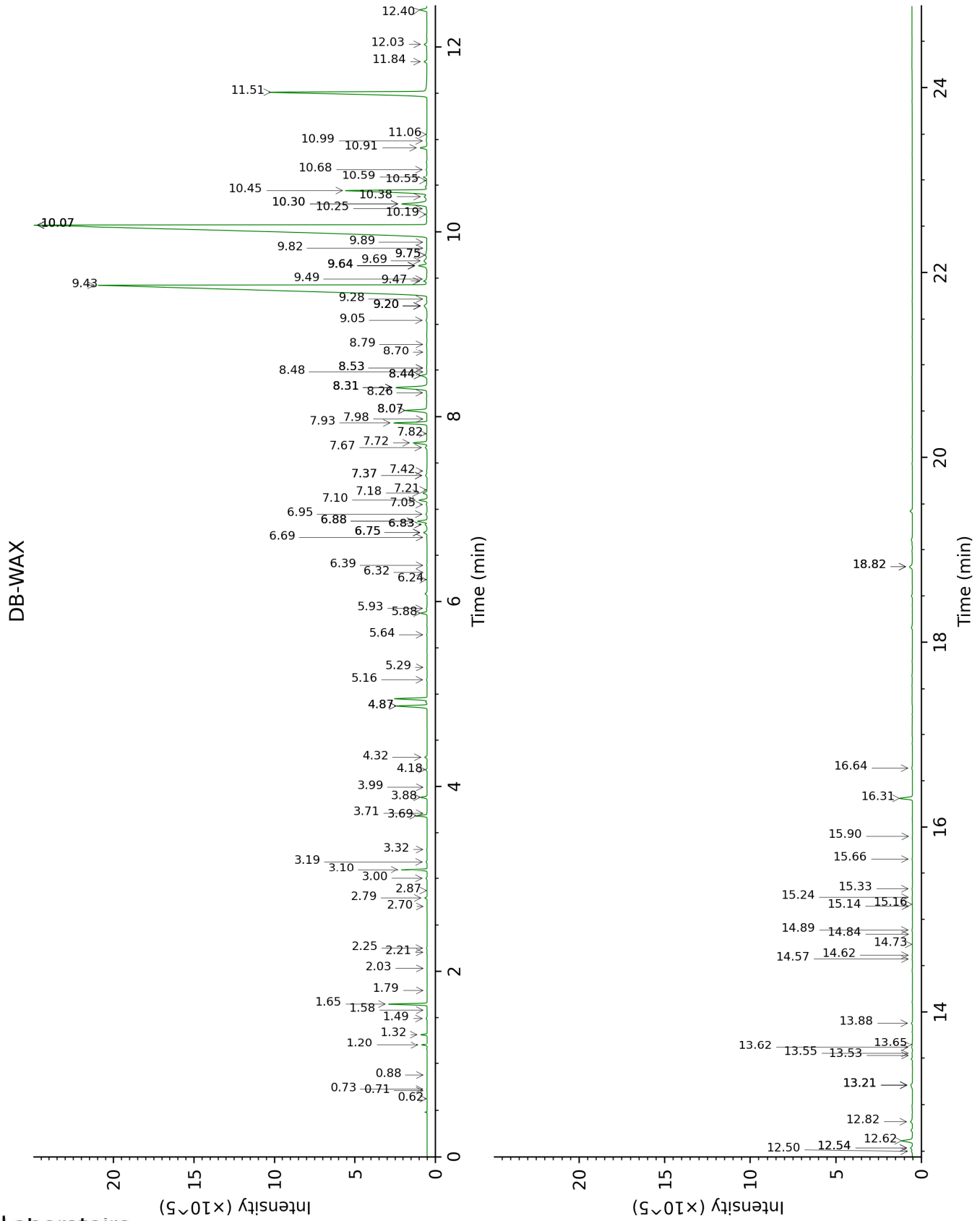
Note: no correction factor was applied

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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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
2-Methyl-3-buten-2-ol	0.55	608	0.02	1.49	1012	0.03
Isovaleral	0.66	642	0.01	0.73	887	0.01
2-Methylbutyral	0.69	652	tr	0.71	881	tr
2-Ethylfuran	0.84	699	tr	0.88	919	tr
Isoamyl alcohol	1.06	730	0.01	3.32	1177	0.01
Hexanal	1.56	798	tr	1.80	1042	0.01
Unknown [m/z 81, 69 (80), 41 (65), 83 (52), 109 (48), 55 (47)...]	1.83	822	tr	0.62	848	tr
(3Z)-Hexenol	2.24	856	0.01	5.64	1345	0.01
4-Heptanone	2.41	870	0.01	2.25	1089	0.02
Hexanol	2.44	872	tr	5.29	1320	0.01
Unknown [m/z 69, 41 (57), 81 (57), 80 (18), 79 (18), 67 (17)...]	2.64	888	tr			
Tricyclene	3.06	918	0.12	1.20	973	0.11
α-Pinene	3.24	931	0.13	1.32	993	0.13
Camphene	3.45*	944	0.91	1.65	1027	0.90
α-Fenchene	3.45*	944	[0.91]	1.58	1021	0.01
Benzaldehyde	3.61	954	0.01	7.21	1461	0.01
β-Pinene	3.86†	971	0.01	2.03	1066	0.01
Sabinene	3.87†	972	[0.01]	2.21	1084	0.01
6-Methyl-5-hepten-2-one	4.11*	987	0.99	4.87*	1296	1.00
Dehydro-1,8-cineole	4.11*	987	[0.99]	3.00	1151	0.03
Myrcene	4.19	993	0.07	2.79	1134	0.06
6-Methyl-5-hepten-2-ol	4.24	996	0.06	6.83*	1433	0.08
α-Phellandrene	4.35*	1003	0.08	2.70	1126	0.01
Octanal	4.35*	1003	[0.08]	4.32	1254	0.07
α-Terpinene	4.54	1015	tr	2.87	1140	0.01
para-Cymene	4.65	1022	0.01	3.99	1229	0.01
Limonene	4.73*	1027	0.73	3.10	1159	0.71
β-Phellandrene	4.73*	1027	[0.73]	3.19	1166	0.03
Benzeneacetaldehyde	4.90	1038	0.01	8.70	1575	0.02
(Z)-β-Ocimene	4.94	1040	0.29	3.69	1206	0.29
(E)-β-Ocimene	5.10	1050	0.18	3.88	1221	0.18
2,6-Dimethyl-5-heptenal (melonal)	5.15	1053	0.02	5.16	1310	0.02
γ-Terpinene	5.22	1058	0.01	3.71	1208	0.01
cis-Sabinene hydrate	5.35	1065	tr	6.74*	1426	0.13
cis-Linalool oxide (fur.)	5.44	1071	0.01	6.39	1400	0.01
4-Nonanone	5.48	1074	0.99	4.87*	1296	[1.00]
Camphenilone	5.57	1079	0.01	6.32	1394	0.01
trans-Linalool oxide (fur.)	5.69*	1086	0.06	6.74*	1426	[0.13]

Terpinolene	5.69*	1086	[0.06]	4.18	1244	0.04
para-Cymenene	5.69*	1086	[0.06]	6.24	1388	0.01
4-Nonanol	5.79	1093	0.03			
Rosefuran	5.87	1098	0.20	5.88	1362	0.21
Linalool	5.94	1102	1.11	7.93	1516	1.06
cis-Chrysanthemal?	5.98	1105	0.01	5.93	1366	0.03
(Z)-6-Methyl-3,5-heptadien-2-one	6.01	1107	0.03	8.07*	1526	0.87
α-Cyclocitral	6.06	1110	0.01			
trans-para-Mentha-2,8-dien-1-ol	6.20	1119	0.03	8.79	1582	0.03
Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.45	1135	0.13	6.74*	1426	[0.13]
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	6.48	1137	0.01	7.42	1476	0.02
trans-Chrysanthemal	6.62*	1146	0.30	7.10	1453	0.26
exo-Isocitral	6.62*	1146	[0.30]	7.37*	1473	0.07
Citronellal	6.74	1153	0.29	6.88*	1436	0.34
Borneol	6.89	1163	0.16	9.64*	1651	0.34
α-Phellandren-8-ol	6.93*	1165	0.57	10.07*	1686	41.17
Isoneral	6.93*	1165	[0.57]	7.72	1499	0.48
Rosefuran oxide	7.08*	1175	0.23	8.44*	1556	0.24
Terpinen-4-ol	7.08*	1175	[0.23]	8.44*	1556	[0.24]
Unknown [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	7.11	1177	0.09	9.47	1637	0.11
Unknown [m/z 69, 41 (65), 109 (36), 67 (16), 84 (11), 43 (10), 55 (9)...]	7.21*	1184	0.90			
Isogeranial	7.21*	1184	[0.90]	8.07*	1526	[0.87]
Myrtenal	7.30*	1189	0.14	8.53*	1562	0.04
α-Terpineol	7.30*	1189	[0.14]	9.64*	1651	[0.34]
Unknown [m/z 43, 81 (47), 67 (45), 69 (944), 41 (42), 59 (40), 55 (39)...]	7.34	1192	0.07	9.05	1603	0.04
trans-Isopiperitenol	7.44	1198	0.04	10.25	1701	0.03
Unknown [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	7.53	1204	0.05	10.07*	1686	[41.17]
Decanal	7.57	1206	0.16	7.18	1458	0.13
cis-Isopiperitenol	7.73	1217	0.04	10.19	1696	0.02
2,3-Epoxyneral?	7.81	1222	0.05			
Nerol	7.96	1232	0.03	10.91	1758	0.23
Citronellol	8.00	1235	0.21	10.59	1730	0.13

(Z)-Isogeraniol	8.19*	1248	31.16	11.06	1770	0.02
Neral	8.19*	1248	[31.16]	9.42	1634	31.07
Piperitone	8.26	1253	0.05	9.75*	1660	0.12
Geraniol	8.51	1269	7.06	11.51	1809	7.27
Geranial	8.68	1281	41.08	10.07*	1686	[41.17]
Unknown [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	8.73	1284	0.18	12.82	1927	0.10
2-Undecanone	8.93	1297	tr	8.48	1559	0.01
Geranyl formate	9.11	1307	tr	9.75*	1660	[0.12]
Methyl geranate	9.34	1324	0.03	9.64*	1651	[0.34]
Neric acid	9.50	1334	0.03			
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	9.51	1336	0.04	12.54*	1901	0.08
α-Cubebene	9.68	1347	0.02	6.69	1422	0.01
Citronellyl acetate	9.78*	1355	0.05	9.28	1622	0.03
Unknown [m/z 110, 95 (98), 109 (40), 43 (35), 111 (32)... 153 (13)...]	9.78*	1355	[0.05]	13.21*	1963	0.11
Cyclosativene I	9.85	1360	0.07	6.83*	1433	[0.08]
Cyclosativene II	9.89	1362	0.08	6.88*	1436	[0.34]
Neryl acetate	9.92	1364	0.02	10.07*	1686	[41.17]
α-Ylangene	9.96†	1367	0.20	6.95	1442	0.04
Geranic acid	9.99†	1370	[0.20]			
α-Copaene	10.02*	1371	0.08	7.05	1449	0.03
Unknown [m/z 81, 59 (94), 41 (74), 85 (40), 43 (55)...]	10.02*	1371	[0.08]	13.21*	1963	[0.11]
β-Bourbonene	10.14	1380	0.03	7.37*	1473	[0.07]
β-Cubebene	10.22*	1386	3.36	7.67	1495	0.07
Geranyl acetate	10.22*	1386	[3.36]	10.45	1718	3.35
β-Elementene	10.27	1389	0.08	8.32*	1546	1.44
Longifolene	10.32	1393	0.02	7.82	1507	0.03
β-Caryophyllene	10.61*	1414	1.42	8.32*	1546	[1.44]
β-Ylangene	10.61*	1414	[1.42]	7.98	1519	0.02
β-Copaene	10.75	1424	0.02	8.26	1541	0.03
trans-α-Bergamotene	10.89	1434	0.01	8.32*	1546	[1.44]
6,9-Guaiadiene	10.95	1439	0.02	8.53*	1562	[0.04]
(E)-Isoeugenol	11.04	1446	0.44	16.31	2271	0.43
α-Humulene	11.06	1447	0.16	9.20*	1616	0.18
cis-Muurolo-4(15),5-diene	11.20	1457	0.03	9.20*	1616	[0.18]
trans-Cadina-1(6),4-diene	11.36	1469	0.03	9.20*	1616	[0.18]
γ-Muurolole	11.40	1473	0.01	9.49	1639	0.03
Germacrene D	11.44	1475	0.19	9.64*	1651	[0.34]
γ-Amorphene	11.57	1485	0.02	9.69	1655	0.19
epi-Cubebol	11.63*	1490	0.10	11.84	1839	0.09
α-Selinene	11.63*	1490	[0.10]	9.82	1666	0.02
α-Muurolole	11.72*	1496	0.06	9.89	1672	0.02

Methyl (E)-isoeugenol	11.72*	1496	[0.06]	14.89	2124	0.03
γ-Cadinene	11.89*	1510	1.25	10.30*	1706	1.17
Cubebol	11.89*	1510	[1.25]	12.40	1888	0.26
δ-Cadinene	12.02	1520	0.25	10.30*	1706	[1.17]
10-epi-Cubebol?	12.10	1526	0.04	13.62	2001	0.04
(E)-γ-Bisabolene	12.14*	1529	0.17	10.38	1712	0.13
trans-Cadina-1,4-diene	12.14*	1529	[0.17]	10.55	1727	0.02
α-Cadinene	12.19*	1533	0.05	10.68	1738	0.03
Neryl butyrate	12.19*	1533	[0.05]			
α-Elemol	12.35	1545	0.05	13.88	2026	0.03
Germacrene B	12.40	1549	0.04	10.99	1764	0.03
Geranyl butyrate	12.54	1560	0.08	12.03	1855	0.09
Caryophyllene oxide	12.72*	1574	0.46	12.62	1908	0.41
Caryophyllene oxide isomer	12.72*	1574	[0.46]	12.54*	1901	[0.08]
Humulene epoxide II	13.05	1600	0.04	13.21*	1963	[0.11]
10-epi-Cubenol	13.15	1608	0.02	13.55	1994	0.02
Selin-6-en-4α-ol isomer	13.22	1614	0.01	14.62	2097	0.02
1-epi-Cubenol	13.31	1622	0.03	13.65	2004	0.02
τ-Muurolol	13.49*	1636	0.03	14.84	2120	tr
τ-Cadinol	13.49*	1636	[0.03]	14.73	2109	0.01
Cubenol	13.49*	1636	[0.03]	13.53	1992	0.01
β-Eudesmol	13.57	1642	0.01	15.24	2160	0.02
α-Eudesmol	13.61	1646	0.01	15.16	2152	tr
α-Cadinol	13.65	1650	0.01	15.33	2169	0.03
(2Z,6Z)-Farnesol	13.89	1669	0.01	15.90	2228	tr
Farnesal isomer	14.39	1710	0.01			
(2E,6Z)-Farnesal	14.42	1713	0.01	15.14	2150	0.01
(2E,6E)-Farnesal	14.71	1738	0.01	15.66	2202	0.02
Neophytadiene	15.87	1840	0.03	12.50	1897	0.04
Phytone	15.91	1844	0.01	14.57	2093	0.02
Unknown [m/z 41, 69 (95), 109 (41), 95 (39), 55 (36), 121 (36)...]	17.60	2000	0.01			
Octadecanal	17.77	2017	0.03	16.64	2305	0.04
Unknown [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]	18.02	2042	0.02			
Unknown [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]	18.28	2067	0.05			
Unknown [m/z 57, 85 (55), 163 (47), 41 (44), 120 (35), 202 (30), 145 (25)... 219 (17), 304 (t)]	18.32	2071	0.02	18.82*	2548	0.14
Dicital	18.64	2103	0.08			
Unknown [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	18.67	2106	0.02	18.82*	2548	[0.14]

Unknown [m/z 69, 41 (38), 151 (36), 123 (34), 82 (24), 43 (23), 109 (21)...]	18.96	2135	0.01	
Unknown [m/z 94, 43 (56), 123 (55), 69 (53), 95 (42), 79 (39)...]	19.80	2223	0.02	
Unknown [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...]	20.15	2259	0.01	
Total identified		98.00%		96.99%
Total reported		98.75%		97.27%

*: 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