

Date : May 20, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 22E18-PTH02

**Customer identification :** Ylang Ylang Complete ORGANIC - Madagascar - Y80107R

**Type :** Essential oil

**Source :** *Cananga odorata* var. *genuina* (Ylang-ylang)

**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. Carrier oil determination by PC-MAT-010 – GC-FID quantitation of fatty acid methyl esters after derivatization, against an internal standard of tridecanoic acid.

**Analyst :** Sylvain Mercier, M. Sc., Chimiste 2014-005

**Analysis date :** May 19, 2022

Checked and approved by :

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

#### *P*HYSICO*C*HEMICAL *D*ATA

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.5019 \pm 0.0003$  (20 °C; method PC-MAT-016)

#### *C*ARRIER *O*IL *D*ETERMINATION

After derivatization, 0.2% of fatty acids were observed.

#### *C*ONCLUSION

No adulterant, contaminant or diluent has been detected using this method. This sample is not diluted with a carrier oil.

## 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	0.01	Aliphatic alcohol
Ethyl acetate	0.02	Aliphatic ester
Octane	tr	Alkane
Butyl acetate	0.01	Aliphatic ester
Isoamyl acetate	0.01	Aliphatic ester
2-Methylbutyl acetate	0.01	Aliphatic ester
3-Methyl-3-butynyl acetate	0.03	Aliphatic ester
Prenyl acetate	0.10	Aliphatic ester
α-Pinene	0.19	Monoterpene
Camphepane	tr	Monoterpene
Benzaldehyde	0.03	Simple phenolic
Sabinene	0.01	Monoterpene
β-Pinene	0.06	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.10	Monoterpene
(3Z)-Hexenyl acetate	0.04	Aliphatic ester
para-Methylanisole	2.42	Simple phenolic
Hexyl acetate	0.03	Aliphatic ester
1,8-Cineole	0.17	Monoterpenic ether
Limonene	0.04	Monoterpene
Benzyl alcohol	0.05	Simple phenolic
(Z)-β-Ocimene	0.01	Monoterpene
(E)-β-Ocimene	0.02	Monoterpene
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.01	Monoterpene
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Methyl benzoate	1.23	Phenolic ester
para-Cresol	0.06	Simple phenolic
Linalool	6.20	Monoterpenic alcohol
ortho-Dimethoxybenzene	0.02	Simple phenolic
Benzyl acetate	1.20	Phenolic ester
Ethyl benzoate	0.05	Phenolic ester
α-Terpineol	0.18	Monoterpenic alcohol
Methylchavicol	0.12	Phenylpropanoid
Nerol	0.04	Monoterpenic alcohol
Neral	0.04	Monoterpenic aldehyde
Phenylethyl acetate	0.03	Phenolic ester
Geraniol	1.40	Monoterpenic alcohol
Geranal	0.08	Monoterpenic aldehyde
(E)-Anethole	0.06	Phenylpropanoid
1-Nitro-2-phenylethane	0.07	Simple phenolic
4-Vinylguaiacol	0.03	Simple phenolic
Bicycloelemene	0.03	Sesquiterpene
Methyl ortho-anisate	0.12	Phenolic ester
Benzyl butyrate	0.03	Phenolic ester

$\alpha$ -Cubebene	0.19	Sesquiterpene
Eugenol	0.58	Phenylpropanoid
Neryl acetate	0.03	Monoterpenic ester
$\alpha$ -Ylangene	0.23	Sesquiterpene
$\alpha$ -Copaene	1.10	Sesquiterpene
$\beta$ -Bourbonene	0.01	Sesquiterpene
$\beta$ -Cubebene	0.13	Sesquiterpene
Geranyl acetate	7.20	Monoterpenic ester
$\beta$ -Elemene	0.43	Sesquiterpene
Cyperene	0.06	Sesquiterpene
Isocaryophyllene	0.01	Sesquiterpene
$\alpha$ -Gurjunene	0.04	Sesquiterpene
Methyleugenol	0.01	Phenylpropanoid
$\beta$ -Caryophyllene	14.04	Sesquiterpene
Caryophylla-4(12),8(13)-diene	0.10	Sesquiterpene
$\beta$ -Copaene	0.58	Sesquiterpene
Aromadendrene	0.01	Sesquiterpene
$\alpha$ -Guaiene	0.07	Sesquiterpene
Isogermacrene D	0.02	Sesquiterpene
(E)-Cinnamyl acetate	0.56	Phenylpropanoid ester
trans-Muurola-3,5-diene	0.05	Sesquiterpene
Cadina-3,5-diene?	0.13	Sesquiterpene
(E)-Isoeugenol	0.14	Phenylpropanoid
$\alpha$ -Humulene	3.58	Sesquiterpene
$\epsilon$ -Muurolene?	0.35	Sesquiterpene
allo-Aromadendrene	0.05	Sesquiterpene
cis-Cadina-1(6),4-diene	0.10	Sesquiterpene
cis-Muurola-4(15),5-diene	0.07	Sesquiterpene
trans-Cadina-1(6),4-diene	0.29	Sesquiterpene
$\gamma$ -Muurolene	2.49	Sesquiterpene
Germacrene D	13.27	Sesquiterpene
trans-Muurola-4(15),5-diene	0.24	Sesquiterpene
Prenyl benzoate	0.17	Phenolic ester
epi-Cubebol	0.06	Sesquiterpenic alcohol
Viridiflorene	0.10	Sesquiterpene
Bicyclogermacrene	1.31	Sesquiterpene
$\alpha$ -Muurolene	0.09	Sesquiterpene
(3Z,6E)- $\alpha$ -Farnesene	0.05	Sesquiterpene
Methyl (E)-isoeugenol	0.98	Phenylpropanoid
$\delta$ -Amorphene	0.55	Sesquiterpene
Unknown	1.80	Sesquiterpene
Cubebol	0.05	Sesquiterpenic alcohol
(Z)- $\gamma$ -Bisabolene	0.31	Sesquiterpene
$\gamma$ -Cadinene	1.01	Sesquiterpene
(3E,6E)- $\alpha$ -Farnesene	7.59	Sesquiterpene
trans-Calamenene	0.07	Sesquiterpene
$\delta$ -Cadinene	4.03	Sesquiterpene
trans-Cadina-1,4-diene	0.23	Sesquiterpene
$\alpha$ -Cadinene	0.32	Sesquiterpene
$\alpha$ -Calacorene	0.04	Sesquiterpene
cis-Dracunculifoliol	0.02	Sesquiterpenic alcohol
$\alpha$ -Elemol	0.10	Sesquiterpenic alcohol

Laboratoire  
**PhytoChemia**

Plus que des analyses... des conseils

Germacrene B	0.03	Sesquiterpene
$\beta$ -Calacorene	0.02	Sesquiterpene
(E)-Nerolidol	0.16	Sesquiterpenic alcohol
(3Z)-Hexenyl benzoate	0.02	Phenolic ester
Spathulenol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide	0.16	Sesquiterpenic ether
Globulol	0.10	Sesquiterpenic alcohol
Unknown	0.11	Sesquiterpenic alcohol
Unknown	0.05	Oxygenated sesquiterpene
Guaiol	0.07	Sesquiterpenic alcohol
Copaborneol	0.09	Sesquiterpenic alcohol
Humulene epoxide II	0.06	Sesquiterpenic ether
10-epi-Cubenol	0.05	Sesquiterpenic alcohol
Junenol	0.35	Sesquiterpenic alcohol
(E)-Isoeugenyl acetate	0.01	Phenylpropanoid ester
1-epi-Cubenol	0.30	Sesquiterpenic alcohol
$\gamma$ -Eudesmol	0.17	Sesquiterpenic alcohol
$\tau$ -Cadinol	0.48	Sesquiterpenic alcohol
Cubenol	0.07	Sesquiterpenic alcohol
$\tau$ -Muurolol	tr	Sesquiterpenic alcohol
$\alpha$ -Muurolol	0.46	Sesquiterpenic alcohol
Unknown	0.29	Sesquiterpenic alcohol
cis-Calamenen-10-ol	0.04	Sesquiterpenic alcohol
$\alpha$ -Cadinol	1.77	Sesquiterpenic alcohol
trans-Calamenen-10-ol	0.04	Sesquiterpenic alcohol
Bulnesol	0.05	Sesquiterpenic alcohol
Unknown	0.20	Oxygenated sesquiterpene
Eudesma-4(15),7-dien-1 $\beta$ -ol	0.04	Sesquiterpenic alcohol
(2E,6Z)-Farnesol	0.01	Sesquiterpenic alcohol
(2Z,6E)-Farnesol	0.02	Sesquiterpenic alcohol
(2E,6E)-Farnesol	1.83	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.04	Sesquiterpenic aldehyde
Benzyl benzoate	6.59	Phenolic ester
Unknown	0.02	Unknown
(2E,6E)-Farnesyl acetate	1.70	Sesquiterpenic ester
Benzyl salicylate	1.69	Phenolic ester
Unknown	0.02	Unknown
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Geranyl benzoate	0.17	Phenolic ester
Unknown	0.07	Unknown
Unknown	0.03	Unknown
Unknown	0.07	Unknown
<b>Consolidated total</b>	<b>97.00%</b>	

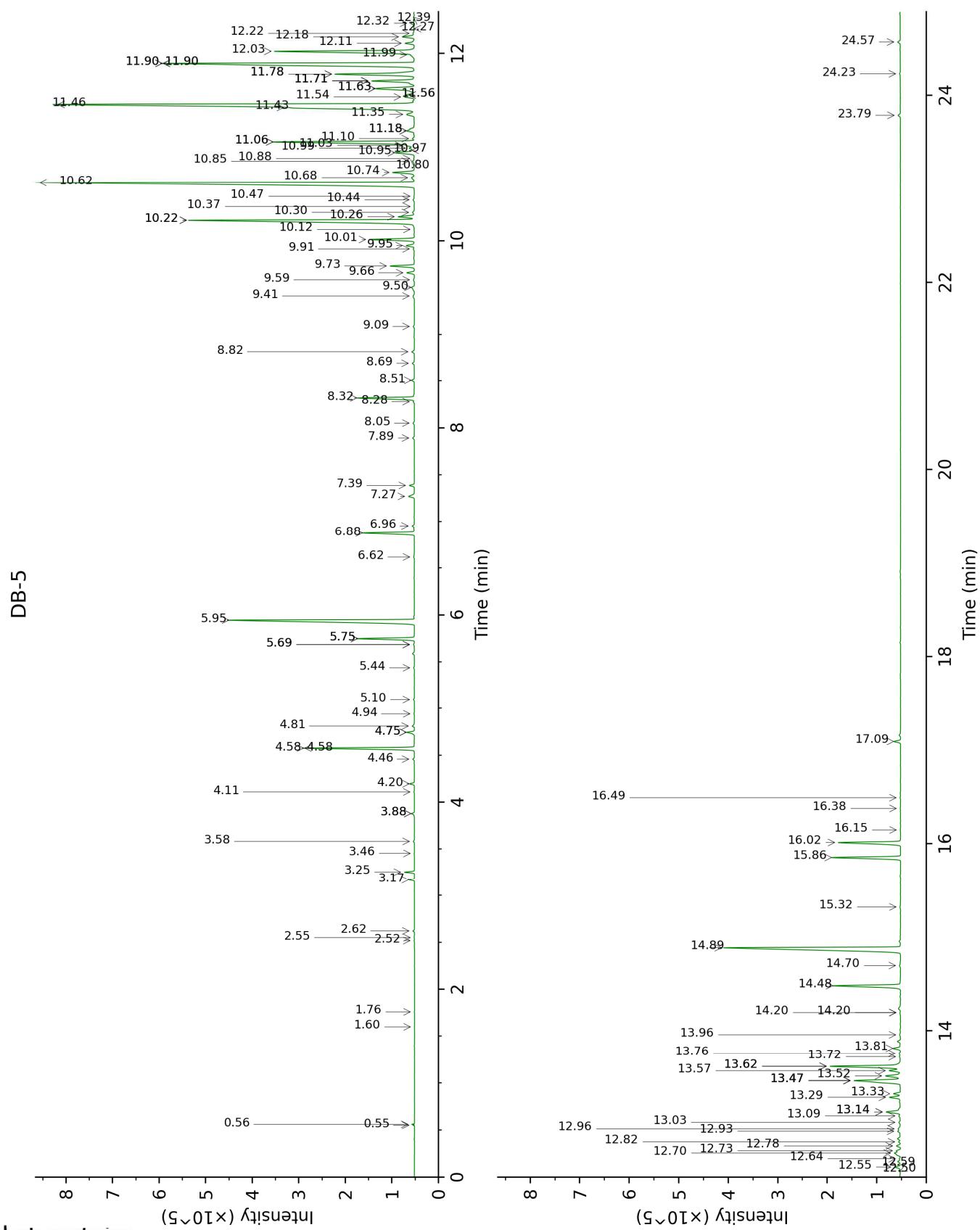
tr: The compound has been detected below 0.005% of total signal.

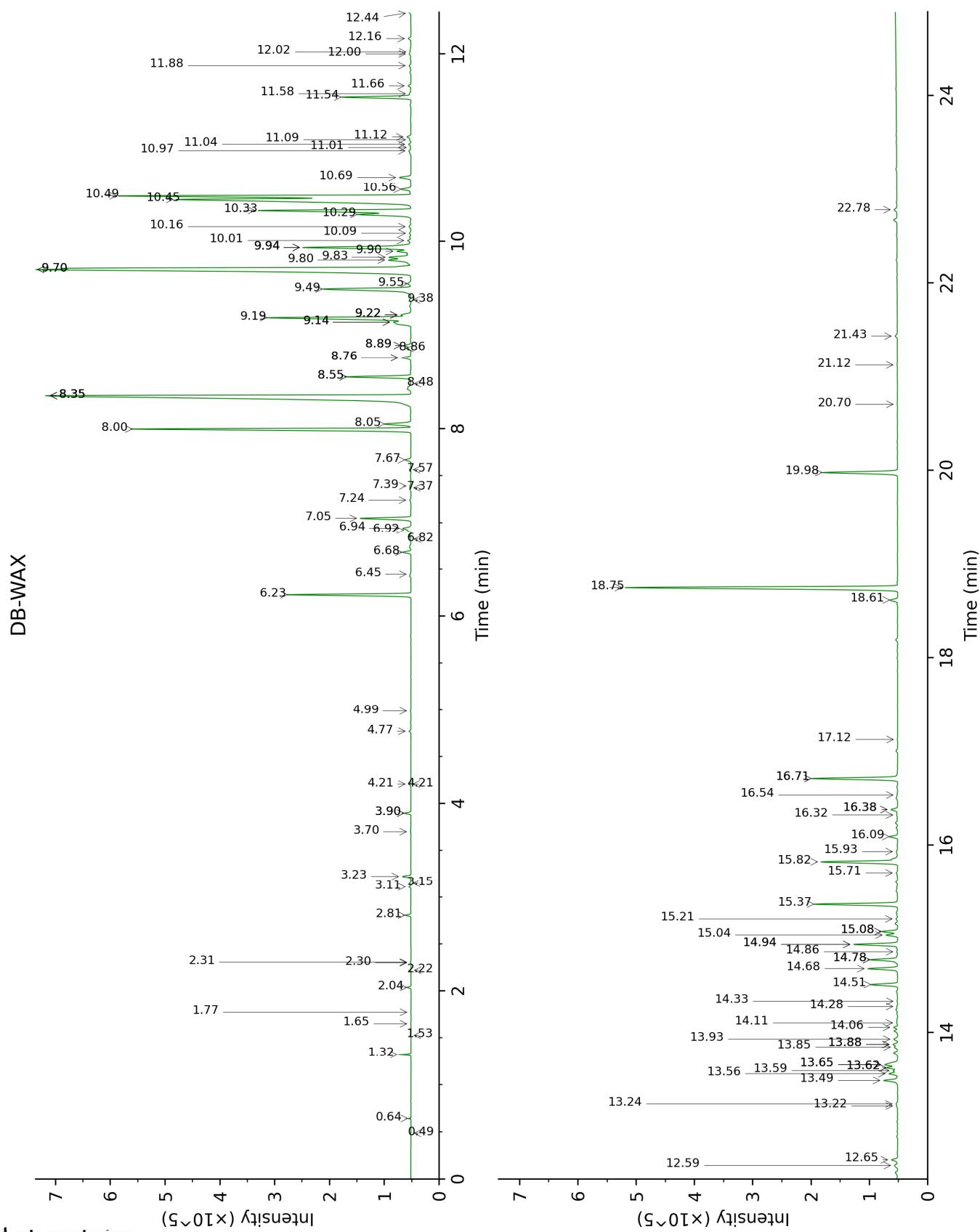
Note: no correction factor was applied

**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.

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





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	0.01	1.53	1013	0.01
Ethyl acetate	0.56	611	0.02	0.64	849	0.02
Octane	1.60	803	tr	0.49	784	0.01
Butyl acetate	1.76	816	0.01	1.78	1038	tr
Isoamyl acetate	2.52	877	0.01	2.31	1091	0.01
2-Methylbutyl acetate	2.55	879	0.01	2.30	1090	0.01
3-Methyl-3-butenyl acetate	2.62	885	0.03	3.15	1159	0.03
Prenyl acetate	3.17	924	0.10	3.90*	1217	0.12
$\alpha$ -Pinene	3.26	930	0.19	1.32	989	0.18
Camphene	3.46	943	tr	1.65	1025	0.01
Benzaldehyde	3.58	951	0.03	7.24	1460	0.03
Sabinene	3.88*	971	0.08	2.22	1082	0.01
$\beta$ -Pinene	3.88*	971	[0.08]	2.04	1064	0.06
6-Methyl-5-hepten-2-one	4.11	986	0.01	4.99	1297	0.01
Myrcene	4.20	992	0.10	2.81	1132	0.10
(3Z)-Hexenyl acetate	4.46	1009	0.04	4.77	1281	0.04
para-Methylanisole	4.58*	1016	2.46	6.23	1385	2.42
Hexyl acetate	4.58*	1016	[2.46]	4.21*	1240	0.04
1,8-Cineole	4.74*	1027	0.19	3.22	1165	0.17
Limonene	4.74*	1027	[0.19]	3.11	1156	0.04
Benzyl alcohol	4.81	1031	0.05	11.66	1816	0.06
(Z)- $\beta$ -Ocimene	4.94	1039	0.01	3.70	1203	0.01
(E)- $\beta$ -Ocimene	5.10	1049	0.02	3.90*	1217	[0.12]
cis-Linalool oxide (fur.)	5.44	1071	0.02	6.45	1401	0.02
Terpinolene	5.69*	1086	0.03	4.21*	1240	[0.04]
trans-Linalool oxide (fur.)	5.69*	1086	[0.03]	6.82	1429	0.02
Methyl benzoate	5.75*	1090	1.30	8.55*	1560	1.33
para-Cresol	5.75*	1090	[1.30]	13.88*	2018	0.11
Linalool	5.95	1103	6.20	8.00	1517	6.15
ortho-Dimethoxybenzene	6.62	1146	0.02			
Benzyl acetate	6.88	1163	1.20	9.94*	1670	2.61
Ethyl benzoate	6.96	1168	0.05	9.22*	1612	0.24
$\alpha$ -Terpineol	7.27	1189	0.18	9.70*	1651	15.42
Methylchavicol	7.39	1196	0.12	9.22*	1612	[0.24]
Nerol	7.89	1230	0.04	10.97	1756	0.04
Neral	8.05	1241	0.04	9.38	1625	0.05
Phenylethyl acetate	8.28	1257	0.03	11.01	1759	0.02
Geraniol	8.32	1260	1.40	11.54	1805	1.43
Geranal	8.51	1272	0.08	10.01	1676	0.07

Laboratoire  
**PhytoChemia**

Plus que des analyses... des conseils

(E)-Anethole	8.69	1285	0.06	11.09	1766	0.04
1-Nitro-2-phenylethane	8.82	1294	0.07	14.10	2040	0.03
4-Vinylguaiacol	9.09	1307	0.03	15.04†	2132	0.59
Bicycloelemene	9.41	1330	0.03	6.92	1436	0.05
Methyl ortho-anisate	9.50	1337	0.12	13.56	1988	0.21
Benzyl butyrate	9.58	1343	0.03	11.58	1808	0.04
α-Cubebene	9.66	1348	0.19	6.68	1418	0.18
Eugenol	9.73	1353	0.58	14.68	2096	0.64
Neryl acetate	9.91	1366	0.03	10.09	1682	0.04
α-Ylangene	9.95	1368	0.23	6.94	1438	0.22
α-Copaene	10.01	1373	1.10	7.05	1446	1.09
β-Bourbonene	10.12	1381	0.01	7.39	1471	0.03
β-Cubebene	10.22*	1388	7.33	7.67	1492	0.13
Geranyl acetate	10.22*	1388	[7.33]	10.49†	1715	[14.96]
β-Elemene	10.26	1390	0.43	8.35*	1544	14.28
Cyperene	10.30	1393	0.06	7.37	1470	0.03
Isocaryophyllene	10.36	1398	0.01	8.05	1521	0.66
α-Gurjunene	10.44	1403	0.04	7.57	1484	0.04
Methyleugenol	10.48	1406	0.01	13.24	1958	0.04
β-Caryophyllene	10.62	1417	14.04	8.35*	1544	[14.28]
Caryophylla-4(12),8(13)-diene	10.68	1421	0.10	8.55*	1560	[1.33]
β-Copaene	10.74	1425	0.58	8.35*	1544	[14.28]
Aromadendrene	10.80	1430	0.01	8.48	1554	0.01
α-Guaiene	10.85	1434	0.07	8.35*	1544	[14.28]
Isogermacrene D	10.88	1436	0.02	8.86	1584	0.11
(E)-Cinnamyl acetate	10.95	1441	0.56	14.51	2079	0.58
trans-Muurola-3,5-diene	10.97	1443	0.05	8.76*	1576	0.22
Cadina-3,5-diene?	10.99	1444	0.13	8.76*	1576	[0.22]
(E)-Isoeugenol	11.02	1447	0.14	16.38*	2269	0.17
α-Humulene	11.06*	1449	4.00	9.19	1610	3.58
ε-Muurolene?	11.06*	1449	[4.00]	9.14*	1606	0.65
allo-Aromadendrene	11.10	1452	0.05	8.89*	1586	0.15
cis-Cadina-1(6),4-diene	11.18*	1458	0.23	8.89*	1586	[0.15]
cis-Muurola-4(15),5-diene	11.18*	1458	[0.23]	9.22*	1612	[0.24]
trans-Cadina-1(6),4-diene	11.35	1471	0.29	9.14*	1606	[0.65]
γ-Muurolene	11.43†	1477	15.77	9.49	1634	2.49
Germacrene D	11.46†	1479	[15.77]	9.70*	1651	[15.42]
trans-Muurola-4(15),5-diene	11.54	1485	0.24	9.80	1659	0.58
Prenyl benzoate	11.56*	1487	0.23	13.62*	1994	0.24
epi-Cubebol	11.56*	1487	[0.23]	11.88	1835	0.06
Viridiflorene	11.63*	1492	1.41	9.55	1639	0.10
Bicyclogermacrene	11.63*	1492	[1.41]	9.94*	1670	[2.61]

Laboratoire  
**PhytoChemia**

Plus que des analyses... des conseils

$\alpha$ -Muurolene	11.71*	1498	1.13	9.94*	1670	[2.61]
(3Z,6E)- $\alpha$ -Farnesene	11.71*	1498	[1.13]	10.16	1688	0.05
Methyl ( <i>E</i> )-isoeugenol	11.71*	1498	[1.13]	14.94*	2121	0.96
$\delta$ -Amorphene	11.78*	1503	2.35	9.83	1662	0.55
Unknown [m/z 119, 41 (95), 123 (53), 80 (49), 161 (44), 105 (42)... 204 (2)]	11.78*	1503	[2.35]			
Cubebol	11.90*	1512	8.96	12.44	1885	0.05
( <i>Z</i> )- $\gamma$ -Bisabolene	11.90*	1512	[8.96]	9.90	1667	0.31
$\gamma$ -Cadinene	11.90*	1512	[8.96]	10.29†	1698	5.03
(3 <i>E</i> ,6 <i>E</i> )- $\alpha$ -Farnesene	11.90*	1512	[8.96]	10.45†	1712	14.96
<i>trans</i> -Calamenene	11.99	1519	0.07	11.12	1769	0.09
$\delta$ -Cadinene	12.02	1522	4.03	10.33†	1702	[5.03]
<i>trans</i> -Cadina-1,4-diene	12.11	1529	0.23	10.56	1721	0.24
$\alpha$ -Cadinene	12.18	1534	0.32	10.69	1732	0.29
$\alpha$ -Calacorene	12.22	1537	0.04	12.02	1848	0.03
<i>cis</i> -Dracunculifolol	12.27	1541	0.02	12.00	1846	0.06
$\alpha$ -Elemol	12.32	1546	0.10	13.93	2023	0.10
Germacrene B	12.39	1551	0.03	11.04	1762	0.05
$\beta$ -Calacorene	12.50	1560	0.02	12.59	1898	0.11
( <i>E</i> )-Nerolidol	12.55	1564	0.16	13.65*	1997	0.41
(3 <i>Z</i> )-Hexenyl benzoate	12.59	1567	0.02	14.28	2057	0.02
Spathulenol	12.64	1571	0.03	14.33	2062	0.01
Caryophyllene oxide	12.70	1575	0.16	12.65	1904	0.16
Globulol	12.73	1577	0.10	13.85	2015	0.08
Unknown cadinol or muurolol analog [m/z 161, 119 (77), 120 (76), 105 (73), 93 (57)... 204 (36)]	12.78	1581	0.11	12.16	1860	0.07
Unknown [m/z 161, 105 (84), 43 (80), 119 (72), 93 (62), 121 (54)... 204 (38), 222 (2)]	12.82	1585	0.05	13.88*	2018	[0.11]
Guaiol	12.93	1594	0.07	14.06	2035	0.08
Copaborneol	12.96	1596	0.09	14.86	2114	0.03
Humulene epoxide II	13.03	1601	0.06	13.22	1956	0.03
10-epi-Cubenol	13.09	1606	0.05	13.59	1991	0.09
Junenol	13.14*	1610	0.43	13.49	1981	0.35
( <i>E</i> )-Isoeugenyl acetate	13.14*	1610	[0.43]	17.12	2349	0.01
1-epi-Cubenol	13.29	1623	0.30	13.65*	1997	[0.41]
$\gamma$ -Eudesmol	13.33	1626	0.17	14.78*	2105	0.66
$\tau$ -Cadinol	13.47*	1637	1.64	14.78*	2105	[0.66]

Cubenol	13.47*	1637	[1.64]	13.62*	1994	[0.24]
τ-Muurolol	13.47*	1637	[1.64]	14.94*	2121	[0.96]
α-Muurolol	13.52	1642	0.46	15.08*†	2135	[0.59]
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.57	1646	0.29	15.08*†	2135	[0.59]
cis-Calamenen-10-ol	13.62*	1650	1.92	16.32	2263	0.04
α-Cadinol	13.62*	1650	[1.92]	15.37	2165	1.77
trans-Calamenen-10-ol	13.72	1658	0.04	16.71*	2304	1.89
Bulnesol	13.76	1661	0.05	15.21	2149	0.04
Unknown [m/z 123, 95 (31), 81 (29), 105 (27)... 222 (5)]	13.82	1666	0.20	16.09	2239	0.18
Eudesma-4(15),7-dien-1β-ol	13.96	1678	0.04	15.93	2223	0.05
(2E,6Z)-Farnesol	14.20*	1698	0.02	16.38*	2269	[0.17]
(2Z,6E)-Farnesol	14.20*	1698	[0.02]	16.54	2285	0.02
(2E,6E)-Farnesol	14.48	1722	1.83	16.71*	2304	[1.89]
(2E,6E)-Farnesal	14.70	1741	0.04	15.71	2199	0.05
Benzyl benzoate	14.89	1757	6.59	18.75	2531	6.59
Unknown [m/z 121, 107 (86), 81 (71), 93 (71), 59 (68), 43 (67)...]	15.32	1795	0.02			
(2E,6E)-Farnesyl acetate	15.86	1843	1.70	15.82	2211	1.75
Benzyl salicylate	16.02	1857	1.69	19.98	2677	1.68
Unknown [m/z 91, 93 (98), 81 (92), 41 (92), 105 (86), 107 (86)...]	16.15	1870	0.02	20.70	2767	0.01
Unknown [m/z 123, 81 (96), 41 (74), 43 (64), 91 (62), 95 (57)...]	16.38	1890	0.01			
Unknown [m/z 123, 81 (47), 43 (35), 91 (30), 41 (27), 79 (24)..]	16.49	1901	0.01	21.12	2820	0.02
Geranyl benzoate	17.09	1957	0.17	18.62	2516	0.19
Unknown [m/z 69, 83 (59), 81 (56), 137 (48), 41 (29), 139 (28)...]	23.79	2692	0.07	21.44	2860	0.06
Unknown [m/z 69, 81 (44), 147 (31), 41	24.23	2749	0.03			

(26), 119 (26), 93 (24)...					
Unknown [m/z 69, 81 (42), 147 (26), 119 (25), 93 (25), 41 (24)...	24.57	2792	0.07	22.78	3038
<b>Total identified</b>	<b>97.52%</b>				<b>97.03%</b>
<b>Total reported</b>	<b>98.40%</b>				<b>97.45%</b>

\*: 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