CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23D12-PTH01
Customer identification : Palmarosa - India - P10111R
Type : Essential oil
Source : *Cymbopogon martini*
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 : April 18, 2023

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

✳ISO 17025:2017
MÉTHODE CERTIFIÉE
CERTIFIED METHOD

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid
Refractive index: 1.4733 ± 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
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.02	Aliphatic alcohol
Camphene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.06	Aliphatic ketone
trans-Dehydroxylinalool oxide	0.02	Monoterpenic ether
Myrcene	0.16	Monoterpene
cis-Dehydroxylinalool oxide	0.02	Monoterpenic ether
para-Cymene	0.02	Monoterpene
Limonene	0.16	Monoterpene
(*Z*)-β-Ocimene	0.38	Monoterpene
(*E*)-β-Ocimene	1.42	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
trans-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Terpinolene	0.02	Monoterpene
Rosefuran	0.01	Monoterpenic ether
Linalool	2.30	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
Unknown	0.01	Unknown
Citronellal	0.02	Monoterpenic aldehyde
Terpinen-4-ol	0.01	Monoterpenic alcohol
Menthol	0.01	Monoterpenic alcohol
α-Terpineol	0.02	Monoterpenic alcohol
Decanal	0.01	Aliphatic aldehyde
Nerol	0.19	Monoterpenic alcohol
Citronellol	0.01	Monoterpenic alcohol
Neral	0.19	Monoterpenic aldehyde
Geraniol	79.68	Monoterpenic alcohol
Geranial	0.40	Monoterpenic aldehyde
Geranyl formate	0.11	Monoterpenic ester
2,3-Epoxygeraniol?	0.03	Oxygenated monoterpene
Neryl acetate	0.02	Monoterpenic ester
Geranyl acetate	8.59	Monoterpenic ester
β-Elemene	0.08	Sesquiterpene
β-Caryophyllene	1.73	Sesquiterpene
α-Humulene	0.12	Sesquiterpene
Germacrene D	0.01	Sesquiterpene
Unknown	0.07	Sesquiterpene
β-Selinene	0.03	Sesquiterpene
Valencene	0.05	Sesquiterpene
α-Muurolene	0.02	Sesquiterpene
γ-Cadinene	0.04	Sesquiterpene

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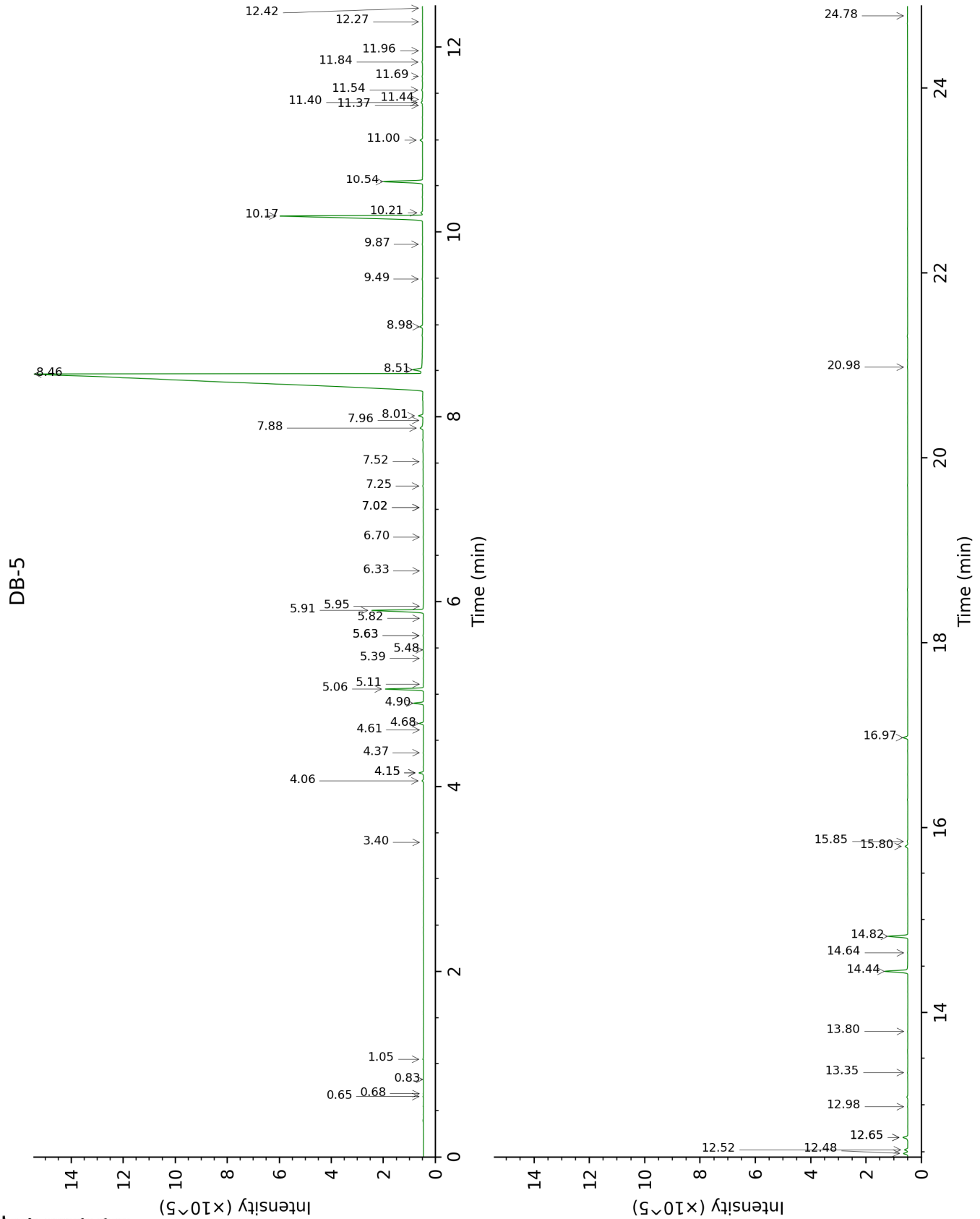|		
δ-Cadinene	0.01	Sesquiterpene
α-Elemol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Unknown
Geranyl butyrate	0.18	Monoterpenic ester
(*E*)-Nerolidol	0.13	Sesquiterpenic alcohol
Caryophyllene oxide	0.20	Sesquiterpenic ether
Caryophyllene oxide isomer	0.03	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
Caryophylladienol II	0.02	Sesquiterpenic alcohol
(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	0.01	Sesquiterpenic alcohol
(2*E*,6*E*)-Farnesol	1.05	Sesquiterpenic alcohol
(2*E*,6*E*)-Farnesal	0.02	Sesquiterpenic aldehyde
Geranyl caproate	0.83	Monoterpenic ester
(2*E*,6*E*)-Farnesyl acetate	0.12	Sesquiterpenic ester
Phytone	0.03	Terpenic ketone
Geranyl caprylate	0.20	Monoterpenic ester
Unknown	0.02	Unknown
Unknown	0.01	Unknown
Consolidated total	**99.04%**	

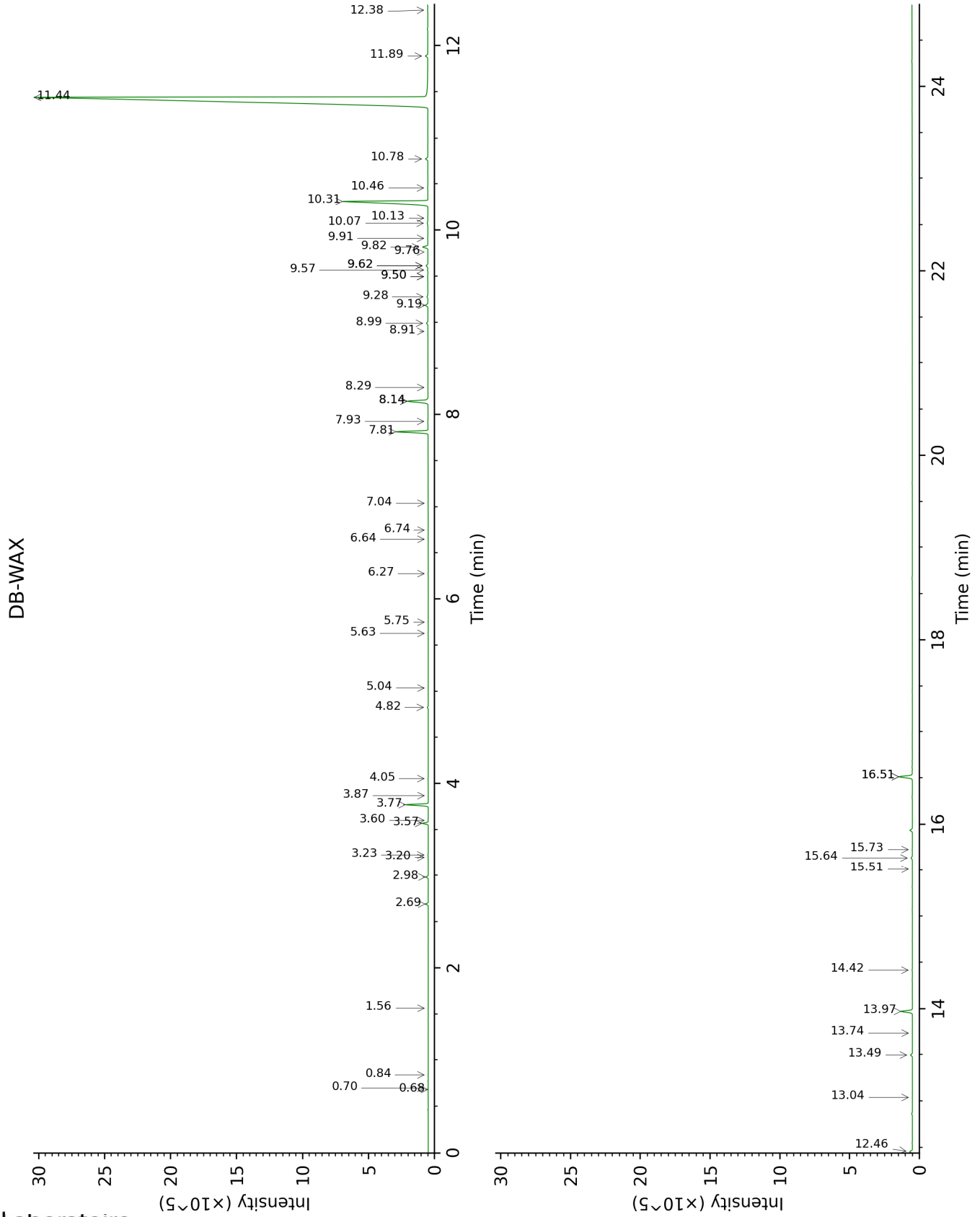tr: The compound has been detected below 0.005% of total signal.

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)

Time (min)

Intensity (×10^5)

DB-WAX

Top chromatogram (0–12 min):

12.38
11.89
11.44
10.78
10.46
10.31
10.13
10.07
9.91
9.82
9.76
9.62
9.57
9.50
9.28
9.19
8.99
8.91
8.29
8.14
7.93
7.81
7.04
6.74
6.64
6.27
5.75
5.63
5.04
4.82
4.05
3.87
3.77
3.60
3.57
3.23
3.20
2.98
2.69
1.56
0.84
0.70
0.68

Intensity (×10^5)

30 25 20 15 10 5 0

Time (min)

Bottom chromatogram (12–25 min):

16.51
15.73
15.64
15.51
14.42
13.97
13.74
13.49
13.04
12.46

Intensity (×10^5)

30 25 20 15 10 5 0

Time (min)

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isovaleral	0.65	641	0.01	0.70	886	0.01
2-Methylbutyral	0.68	651	tr	0.68	880	tr
2-Ethylfuran	0.83	702	tr	0.84	918	tr
Isoamyl alcohol	1.05	732	0.02	3.23	1177	0.02
Camphene	3.40	944	0.01	1.56	1026	tr
6-Methyl-5-hepten-2-one	4.06	987	0.06	4.82	1302	0.06
trans-Dehydroxylinalool oxide	4.15*	993	0.18	3.20	1175	0.02
Myrcene	4.15*	993	[0.18]	2.69	1133	0.16
cis-Dehydroxylinalool oxide	4.37	1007	0.02	3.60	1208	0.02
para-Cymene	4.61	1022	0.02	3.87	1228	0.01
Limonene	4.68	1027	0.16	2.98	1157	0.16
(*Z*)-β-Ocimene	4.90	1040	0.38	3.57	1205	0.37
(*E*)-β-Ocimene	5.06	1050	1.42	3.77	1221	1.43
2,6-Dimethyl-5-heptenal (melonal)	5.11	1054	0.02	5.04	1310	0.01
cis-Linalool oxide (fur.)	5.39	1071	0.02	6.27	1400	0.02
Octanol	5.48	1077	0.02	7.93	1525	0.02
trans-Linalool oxide (fur.)	5.64*	1086	0.03	6.64	1428	0.01
Terpinolene	5.64*	1086	[0.03]	4.05	1242	0.02
Rosefuran	5.82	1098	0.01	5.75	1362	0.01
Linalool	5.91	1103	2.30	7.81	1517	2.25
Nonanal	5.95	1106	0.01	5.63	1353	0.01
Unknown [m/z 95, 123 (73), 67 (64), 82 (54), 41 (47), 55 (27)...]	6.33	1130	0.01			
Citronellal	6.70	1153	0.02	6.74	1436	tr
Terpinen-4-ol	7.02*	1174	0.01	8.29	1554	0.01
Menthol	7.02*	1174	[0.01]	8.91	1602	0.01
α-Terpineol	7.26	1189	0.02	9.50*	1650	0.03
Decanal	7.52	1206	0.01	7.04	1458	0.01
Nerol	7.88	1230	0.19	10.78	1757	0.18
Citronellol	7.96	1235	0.01	10.46	1730	0.02
Neral	8.01	1239	0.19	9.19	1625	0.21
Geraniol	8.46†	1269	80.05	11.44	1815	79.68
Geranial	8.51†	1272	[80.05]	9.82	1677	0.40
Geranyl formate	8.98	1303	0.11	9.62*	1660	0.14
2,3-Epoxygeraniol?	9.49	1339	0.03			
Neryl acetate	9.87	1366	0.02	9.91	1684	0.02

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Compound	RT	RI	%	RT	RI	%
Geranyl acetate	10.17	1387	8.59	10.31	1718	8.50
β-Elemene	10.21	1390	0.08	8.14*	1542	1.79
β-Caryophyllene	10.54	1414	1.73	8.14*	1542	[1.79]
α-Humulene	11.00	1448	0.12	8.99	1609	0.12
Germacrene D	11.37	1476	0.01	9.50*	1650	[0.03]
Unknown [m/z 189, 133 (75), 91 (71), 105 (69), 93 (44)... 204 (33)]	11.40	1478	0.07	9.28	1633	0.09
β-Selinene	11.44	1480	0.03	9.57	1656	0.03
Valencene	11.54	1488	0.05	9.62*	1660	[0.14]
α-Muurolene	11.69	1499	0.02	9.76	1672	0.02
γ-Cadinene	11.84	1510	0.04	10.07	1698	0.06
δ-Cadinene	11.96	1520	0.01	10.13	1702	0.01
α-Elemol	12.27	1544	0.01	13.74	2026	0.01
Unknown [m/z 59, 68 (63), 43 (31), 67 (27), 81 (27), 94 (25), 69 (23), 41 (22), 84 (20)...]	12.42	1556	0.02			
Geranyl butyrate	12.48	1561	0.18	11.89	1855	0.18
(*E*)-Nerolidol	12.52	1564	0.13	13.49	2002	0.13
Caryophyllene oxide	12.65*	1574	0.23	12.46	1906	0.20
Caryophyllene oxide isomer	12.65*	1574	[0.23]	12.38	1899	0.03
Humulene epoxide II	12.98	1600	0.01	13.04	1960	0.01
Caryophylladienol II	13.35	1630	0.02	15.73	2224	0.02
(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	13.80	1667	0.01	16.51*	2306	1.08
(2*E*,6*E*)-Farnesol	14.44	1721	1.05	16.51*	2306	[1.08]
(2*E*,6*E*)-Farnesal	14.64	1738	0.02	15.51	2201	0.01
Geranyl caproate	14.82	1754	0.83	13.97	2048	0.85
(2*E*,6*E*)-Farnesyl acetate	15.80	1840	0.12	15.64	2214	0.11
Phytone	15.85	1845	0.03	14.42	2091	0.02
Geranyl caprylate	16.97	1949	0.20			
Unknown [m/z 69, 81 (70), 93 (37), 95 (31), 41 (24)...]	20.98	2362	0.02			
Unknown [m/z 69, 81 (64), 95 (29), 137 (19), 41 (19)...]	24.78	2826	0.01			
Total identified		98.87%			98.52%	
Total reported		99.00%			98.60%	

*: 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

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Essential oil, *Cymbopogon martini*
Internal code: 23D12-PTH01

Palmarosa - India - P10111R

Report prepared for
Plant Therapy

R.T.: Retention time (minutes)
R.I.: Retention index

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