

Date : 2024-07-11

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24F26-PTH03

Customer Identification : Rose Absolute - Morocco - R30115R

Type : Absolute

Source : *Rosa x damascena*

Customer : Plant Therapy

Checked and approved by:

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

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GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-004 - Terpenes and volatiles profiling by response factor

Results : See analysis summary (next page)

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

Date : 2024-07-09

PHYSICOCHEMICAL DATA

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY

Identification	mg/g	% m/m	Class
Hexanol	0.18	0.02	Aliphatic alcohol
Heptanal	0.03	0.0	Aliphatic aldehyde
α -Pinene	0.09	0.01	Monoterpene
Benzaldehyde	0.05	0.01	Simple phenolic
β -Pinene	0.08	0.01	Monoterpene
Myrcene	0.21	0.02	Monoterpene
Valeral diethyl acetal?	0.28	0.03	Aliphatic acetal
<i>para</i> -Cymene	0.05	0.01	Monoterpene
Limonene	0.19	0.02	Monoterpene
Benzyl alcohol	1.17	0.12	Simple phenolic
Benzeneacetaldehyde	0.07	0.01	Simple phenolic
(<i>E</i>)- β -Ocimene	0.04	0.0	Monoterpene
γ -Terpinene	0.08	0.01	Monoterpene
<i>trans</i> -Sabinene hydrate	0.15	0.01	Monoterpenic alcohol
Linalool	0.20	0.02	Monoterpenic alcohol
Nonanal	0.14	0.01	Aliphatic aldehyde
Phenylethyl alcohol	337.11	33.71	Simple phenolic
Phenylethyl formate	0.24	0.02	Phenolic ester
Terpinen-4-ol	0.11	0.01	Monoterpenic alcohol
α -Terpineol	0.13	0.01	Monoterpenic alcohol
Nerol	1.93	0.19	Monoterpenic alcohol
Citronellol	92.37	9.24	Monoterpenic alcohol
Neral	0.19	0.02	Monoterpenic aldehyde
(<i>Z</i>)-Isogeraniol	0.05	0.01	Monoterpenic alcohol
Phenylethyl acetate	0.31	0.03	Phenolic ester
Geraniol	52.14	5.21	Monoterpenic alcohol
Geranial	0.50	0.05	Monoterpenic aldehyde
Citronellyl formate	0.18	0.02	Monoterpenic ester
Geranyl formate	0.15	0.01	Monoterpenic ester
<i>cis</i> -Rose oxide	0.34	0.03	Monoterpenic ether
Unknown	0.19	0.02	Unknown
Unknown	0.22	0.02	Unknown
Citronellyl acetate	0.24	0.02	Monoterpenic ester
Eugenol	4.86	0.49	Phenylpropanoid
Geranic acid	0.58	0.06	Aliphatic acid
Geranyl acetate	0.42	0.04	Monoterpenic ester
Ethyl decanoate	0.40	0.04	Aliphatic ester
Methyleugenol	1.22	0.12	Phenylpropanoid
β -Caryophyllene	1.24	0.12	Sesquiterpene
α -Guaiene	0.26	0.03	Sesquiterpene
α -Humulene	0.31	0.03	Sesquiterpene

Germacrene D	0.51	0.05	Sesquiterpene
Aciphyllene	0.07	0.01	Sesquiterpene
Pentadecane	0.17	0.02	Alkane
δ -Guaiene	0.25	0.03	Sesquiterpene
α -Elemol	0.36	0.04	Sesquiterpenic alcohol
Caryophyllene oxide	0.30	0.03	Sesquiterpenic ether
Ethyl laurate	0.21	0.02	Aliphatic ester
Hexadecane	0.08	0.01	Alkane
(8Z)-Heptadecene	0.14	0.01	Alkene
α -Bisabolol	0.17	0.02	Sesquiterpenic alcohol
(2E,6Z)-Farnesol	0.10	0.01	Sesquiterpenic alcohol
Heptadecane	0.50	0.05	Alkane
(2E,6E)-Farnesol	0.49	0.05	Sesquiterpenic alcohol
α -Bisabolol oxide A	0.26	0.03	Sesquiterpenic alcohol
Benzyl benzoate	0.15	0.01	Phenolic ester
Octadecane	0.13	0.01	Alkane
Phenylethyl benzoate	0.16	0.02	Phenolic ester
(9Z)-Nonadecene	1.56	0.16	Alkene
Phenylethyl phenylacetate	0.11	0.01	Phenolic ester
Nonadecane	1.79	0.18	Alkane
Palmitic acid	1.83	0.18	Aliphatic acid
(9Z)-Eicosene	0.18	0.02	Alkene
Ethyl palmitate	0.60	0.06	Aliphatic ester
Eicosane	0.16	0.02	Alkane
(10Z)-Heneicosene	0.19	0.02	Alkene
Heneicosane	0.30	0.03	Alkane
Citronellyl caprate	0.10	0.01	Monoterpenic ester
Linoleic acid	9.15	0.92	Aliphatic acid
Geranyl caprate	0.61	0.06	Monoterpenic ester
Oleic acid	2.33	0.23	Aliphatic acid
Ethyl linoleate	1.81	0.18	Aliphatic ester
Ethyl oleate	1.65	0.16	Aliphatic ester
Docosane	0.21	0.02	Alkane
Tricosane	0.10	0.01	Alkane
Citronellyl laurate	0.12	0.01	Monoterpenic ester
Geranyl laurate	0.11	0.01	Monoterpenic ester
Tetradecyl octanoate	0.29	0.03	Aliphatic ester
Tetradecyl nonanoate	0.43	0.04	Aliphatic ester
Pentadecyl octanoate	0.72	0.07	Aliphatic ester
Phenylethyl myristate	0.15	0.01	Phenolic ester
Pentacosane	2.15	0.21	Alkane
Citronellyl myristate	0.12	0.01	Monoterpenic ester
Geranyl myristate	0.14	0.01	Monoterpenic ester
Unknown	2.09	0.21	Phenolic ester
Phenylethyl palmitoleate?	0.76	0.08	Phenolic ester

Phenylethyl palmitate	0.10	0.01	Phenolic ester
Citronellyl palmitoleate?	0.10	0.01	Monoterpenic ester
Citronellyl palmitate	0.48	0.05	Monoterpenic ester
Geranyl palmitate	0.38	0.04	Monoterpenic ester
α -Tocopherol	0.14	0.01	Tocopherol
Consolidated total	533.71	53.37	

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

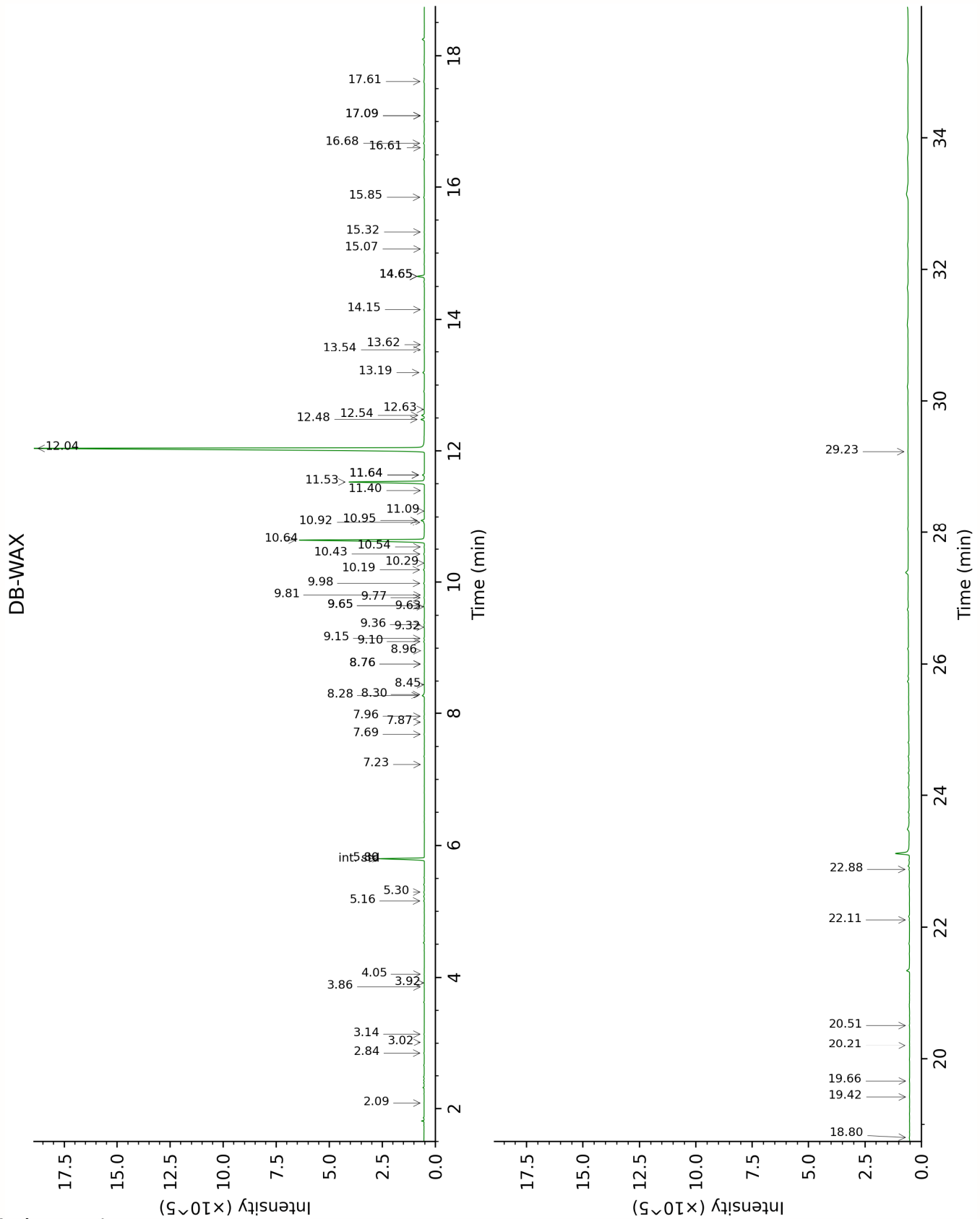
Note: Individual compounds contents were corrected following the method of Cachet et al., 2016 (Flavour and Fragrance Journal guidelines).

Unknown compounds are expressed in equivalents of internal standard without correction.

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: The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

Bracketed value ([xx]): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.



FULL ANALYSIS DATA

Hexanol	Column DB-WAX			Column DB-5		
	5.30	1320.8	0.06	2.33	876.0	0.02
Heptanal	3.02	1149.0	0.01	2.68	905.1	tr
α -Pinene				3.10	933.5	0.01
Benzaldehyde	7.23	1461.4	0.01	3.42	954.4	0.01
β -Pinene	2.09	1070.3	0.01	3.71	973.6	0.01
Myrcene	2.84	1135.5	0.04	4.02	994.4	0.03
Valeral diethyl acetal?				4.39	1018.5	0.04
<i>para</i> -Cymene	4.05	1226.2	0.02	4.50	1025.3	0.01
Limonene	3.14	1158.6	0.03	4.54	1028.0	0.03
Benzyl alcohol	11.64*	1816.2	[0.21]	4.63	1034.0	0.18
Benzeneacetaldehyde	8.76*	1578.2	[0.02]	4.71	1038.7	0.01
(<i>E</i>)- β -Ocimene	3.92	1216.8	0.01	4.90	1051.2	0.01
γ -Terpinene	3.86	1212.5	0.01	5.02	1058.8	0.01
<i>trans</i> -Sabinene hydrate	7.87	1509.5	0.01	5.67	1099.6	0.02
Linalool	7.96	1516.3	0.03	5.71	1102.7	0.03
Nonanal				5.75	1105.2	0.02
Phenylethyl alcohol	12.04	1851.9	54.88	5.95	1117.6	51.88
Phenylethyl formate	10.54	1722.1	0.04	6.81	1173.9	0.03
Terpinen-4-ol	8.45	1554.1	0.03	6.84	1175.8	0.02
α -Terpineol	9.63	1647.6	0.02	7.06	1190.0	0.02
Nerol	10.95	1756.8	0.35	7.68	1231.4	0.29
Citronellol	10.64	1730.8	14.84	7.76	1236.8	13.98
Neral	9.36	1625.6	0.04	7.83	1242.0	0.03
(<i>Z</i>)-Isogeraniol	11.09	1768.9	0.02	7.92	1247.9	0.01
Phenylethyl acetate	10.92	1754.5	0.06	8.06	1257.2	0.04
Geraniol	11.53	1806.8	8.26	8.12	1261.8	7.74
Geranial	9.98	1676.3	0.09	8.29	1272.8	0.07
Citronellyl formate	8.76*	1578.2	[0.02]	8.41	1281.2	0.02
Geranyl formate	9.81	1662.0	0.02	8.72	1302.7	0.02
<i>cis</i> -Rose oxide	5.16	1311.1	0.05			
Unknown FRAG CDLXV [m/z 41, 43 (88), 69 (85), 67 (73), 109 (72), 82 (57)...]	14.15	2047.6	0.03	9.24	1335.9	0.02
Unknown MISC LVII [m/z 43, 59 (52), 139 (51), 69 (43), 41 (42), 55 (37)...]	15.07	2137.6	0.02	9.29	1339.1	0.03
Citronellyl acetate	9.32	1622.6	0.03	9.50*	1354.2	[0.69]
Eugenol	14.65*	2096.3	[0.76]	9.50*	1354.2	[0.69]
Geranic acid				9.60	1361.3	0.07
Geranyl acetate	10.43	1712.9	0.08	9.95	1386.0	0.06

Ethyl decanoate	9.10	1605.0	0.06	10.14	1399.8	0.06
Methyleugenol	13.19	1956.4	0.18	10.20	1403.8	0.17
β -Caryophyllene	8.28	1541.3	0.23	10.34	1414.2	0.21
α -Guaiene	8.30	1542.6	0.05	10.64	1436.6	0.04
α -Humulene	9.15	1608.9	0.05	10.80	1448.4	0.05
Germacrene D	9.65*	1648.9	[0.07]	11.17	1476.6	0.09
Aciphyllene	9.65*	1648.9	[0.07]	11.43	1496.0	0.01
Pentadecane	7.69	1495.3	0.03	11.51*	1501.8	[0.06]
δ -Guaiene	9.77	1658.7	0.05	11.51*	1501.8	[0.06]
α -Elemol				12.08	1547.2	0.06
Caryophyllene oxide	12.63	1904.7	0.04	12.44	1575.5	0.05
Ethyl laurate	11.64*	1816.2	[0.21]	12.75*	1599.5	[0.05]
Hexadecane	8.96	1593.8	0.02	12.75*	1599.5	[0.05]
(8Z)-Heptadecene	10.29	1701.4	0.03	13.73*	1680.9	[0.04]
α -Bisabolol	15.32	2163.4	0.03	13.73*	1680.9	[0.04]
(2E,6Z)-Farnesol				13.95	1699.2	0.02
Heptadecane	10.19	1692.8	0.09	14.04	1706.2	0.09
(2E,6E)-Farnesol	16.68	2304.0	0.10	14.22	1722.5	0.08
α -Bisabolol oxide A	17.09*	2349.4	[0.02]	14.41	1738.7	0.04
Benzyl benzoate				14.59	1754.6	0.02
Octadecane	11.40	1795.4	0.01	15.19	1806.4	0.02
Phenylethyl benzoate	19.42	2615.1	0.03	15.60	1843.7	0.02
(9Z)-Nonadecene	12.54	1896.4	0.29	15.98	1878.6	0.28
Phenylethyl phenylacetate	20.21	2710.8	0.02	16.24	1902.1	0.02
Nonadecane	12.48	1890.7	0.34	16.29	1906.5	0.32
Palmitic acid				16.93	1967.8	0.27
(9Z)-Eicosene	13.62	1996.7	0.04	17.03	1977.3	0.03
Ethyl palmitate	15.85	2217.1	0.08	17.26	1999.2	0.09
Eicosane	13.54	1989.2	0.03	17.33	2006.1	0.03
(10Z)-Heneicosene	14.65*	2096.3	[0.76]	18.04	2076.7	0.03
Heneicosane	14.65*	2096.3	[0.76]	18.34	2106.1	0.05
Citronellyl caprate	17.09*	2349.4	[0.02]	18.42	2115.0	0.02
Linoleic acid				18.70*	2143.0	[1.46]
Geranyl caprate	17.61	2406.3	0.10	18.70*	2143.0	[1.46]
Oleic acid				18.74	2147.6	0.35
Ethyl linoleate				18.88	2162.6	0.28
Ethyl oleate				18.94	2168.3	0.25
Docosane				19.23	2198.0	0.04
Tricosane	16.61	2296.8	0.02	20.23	2305.4	0.02
Citronellyl laurate	18.80	2542.1	0.06	20.30	2313.2	0.02
Geranyl laurate	19.66	2644.2	0.02	20.61	2347.8	0.02
Tetradecyl octanoate				20.78	2367.8	0.05
Tetradecyl nonanoate				21.62	2463.7	0.07
Pentadecyl octanoate				21.72	2474.8	0.11

Phenylethyl myristate	22.12	2956.6	0.03	21.86	2491.3	0.02
Pentacosane				22.01	2509.0	0.39
Citronellyl myristate	20.51	2749.2	0.04	22.07	2515.6	0.02
Geranyl myristate				22.34	2548.1	0.02
Unknown ROAB II [m/z 105, 79 (23), 104 (16), 67 (12), 95 (12), 106 (9)... 382 (1)]				22.55	2574.0	0.27
Phenylethyl palmitoleate?				23.33	2669.8	0.12
Phenylethyl palmitate				23.53	2694.6	0.02
Citronellyl palmitoleate?				23.60	2702.5	0.02
Citronellyl palmitate				23.67	2712.6	0.08
Geranyl palmitate	22.88	3060.8	0.05	23.95	2747.8	0.06
α -Tocopherol	29.23	3873.3	0.05	26.82	3122.2	0.02
Total reported		86.72%			85.62%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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