

Date : 2024-01-22

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 24A15-PTH03

**Customer Identification :** Patchouli - Indonesia - P20112R

**Type :** Essential Oil

**Source :** *Pogostemon cablin*

**Customer :** Plant Therapy

Checked and approved by:

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

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## GAS CHROMATOGRAPHIC ANALYSIS

**Method :** PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

**\*ISO**

**Results :** See analysis summary (next page)

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

**Date :** 2024-01-18

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.5081 \pm 0.0003$  (20 °C)

**Method :** PC-MAT-016 - Measure of the refractive index of a liquid.

**Analyst :** Cindy Caron B. Sc.

**Date :** 2024-01-16

## 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
5-Methyl-2-hexanone	0.01	Aliphatic ketone
$\alpha$ -Pinene	0.09	Monoterpene
Camphene	tr	Monoterpene
$\beta$ -Pinene	0.21	Monoterpene
Sabinene	tr	Monoterpene
Octen-3-ol	0.01	Aliphatic alcohol
Octan-3-one	0.01	Aliphatic ketone
Myrcene	0.01	Monoterpene
Octan-3-ol	0.01	Aliphatic alcohol
Limonene	0.02	Monoterpene
Terpinolene	0.01	Monoterpene
Linalool	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
$\delta$ -Elemene	0.17	Sesquiterpene
$\alpha$ -Copaene	tr	Sesquiterpene
$\beta$ -Patchoulene	2.58	Sesquiterpene
$\beta$ -Bourbonene	0.01	Sesquiterpene
<i>cis</i> - $\beta$ -Elemene	0.06	Sesquiterpene
$\beta$ -Elemene	1.06	Sesquiterpene
Cycloseychellene	0.58	Sesquiterpene
Isocaryophyllene	0.02	Sesquiterpene
$\beta$ -Caryophyllene	3.28	Sesquiterpene
Seychellene	6.77	Sesquiterpene
Selina-5,11-diene	0.05	Sesquiterpene
$\alpha$ -Guaiene	13.73	Sesquiterpene
Unknown	0.05	Sesquiterpene
$\alpha$ -Humulene	0.59	Sesquiterpene
$\alpha$ -Patchoulene	4.72	Sesquiterpene
$\gamma$ -Patchoulene	0.97	Sesquiterpene
Patchoulene analog I	1.55	Sesquiterpene
9- <i>epi</i> - $\beta$ -Caryophyllene	0.02	Sesquiterpene
Unknown	0.44	Sesquiterpene
Unknown	0.51	Sesquiterpene
Selina-4,11-diene	0.07	Sesquiterpene
Patchoulene analog II	0.01	Sesquiterpene
$\beta$ -Selinene	0.07	Sesquiterpene
Unknown	0.54	Sesquiterpene
$\delta$ -Selinene	0.17	Sesquiterpene
Unknown	0.09	Sesquiterpene
$\alpha$ -Selinene	0.10	Sesquiterpene

Aciphyllene	3.06	Sesquiterpene
Eudesma-2,4(15),11-triene	0.12	Sesquiterpene
δ-Guaiene	18.36	Sesquiterpene
Pentadecane	0.05	Alkane
Nootkatene	0.01	Sesquiterpene
γ-Cadinene	0.49	Sesquiterpene
7-epi-α-Selinene	0.21	Sesquiterpene
Unknown	0.08	Sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.13	Oxygenated sesquiterpene
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.01	Sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Norpatchoulenol	0.58	Norsesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.17	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Caryophyllene oxide isomer	0.07	Sesquiterpenic ether
Caryophyllene oxide	0.26	Sesquiterpenic ether
Unknown	0.52	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Hexadecane	0.04	Alkane
Humulene epoxide II	0.08	Sesquiterpenic ether
Unknown	0.09	Oxygenated sesquiterpene
Unknown	0.24	Oxygenated sesquiterpene
Unknown	0.23	Oxygenated sesquiterpene
Unknown	0.59	Oxygenated sesquiterpene
Caryophylladienol II	0.19	Sesquiterpenic alcohol
Hinesol	0.29	Sesquiterpenic alcohol
Patchoulol	28.45	Sesquiterpenic alcohol
Pogostol	2.03	Sesquiterpenic alcohol
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.16	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Rotundone	0.12	Sesquiterpenic ketone
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Pogostone	1.20	Terpenic lactone
Unknown	0.18	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene

Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Phytol	0.03	Diterpenic alcohol
<b>Consolidated total</b>	<b>97.76</b>	

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

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

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





FULL ANALYSIS DATA

5-Methyl-2-hexanone	Column DB-WAX			Column DB-5		
	2.67	1105.3	0.01	2.18	855.5	0.01
$\alpha$ -Pinene	1.48	991.6	0.09	3.18	931.1	0.09
Camphene	1.84	1028.0	tr	3.37	943.6	tr
$\beta$ -Pinene	2.24	1066.4	0.21	3.80*	971.9	[0.22]
Sabinene	2.43	1083.9	tr	3.80*	971.9	[0.22]
Octen-3-ol	6.96	1418.6	0.01	3.98	983.9	0.01
Octan-3-one	4.13	1214.9	0.01	4.03	987.3	0.01
Myrcene	3.03	1132.4	tr	4.11	992.6	0.01
Octan-3-ol	6.23	1365.9	0.01	4.22	999.9	0.01
Limonene	3.34	1156.5	0.02	4.64	1026.6	0.02
Terpinolene	4.45	1238.0	tr	5.60	1086.0	0.01
Linalool	8.24	1514.1	0.01	5.85	1102.1	0.01
Unknown POCA I [m/z 159, 117 (68), 132 (55), 200 (35)]	7.34*	1447.3	[0.02]	9.12	1316.3	0.01
$\delta$ -Elemene	7.19*	1436.2	[2.76]	9.39	1335.3	0.17
$\alpha$ -Copaene	7.34*	1447.3	[0.02]	9.92	1372.4	tr
$\beta$ -Patchoulene	7.19*	1436.2	[2.76]	9.97	1375.7	2.58
$\beta$ -Bourbonene	7.68	1471.8	0.01	10.03	1379.9	0.01
<i>cis</i> - $\beta$ -Elemene	8.50	1534.3	0.04	10.06	1382.0	0.06
$\beta$ -Elemene	8.64*	1544.7	[4.67]	10.16	1389.7	1.06
Cycloseychellene	8.09	1502.5	0.58	10.32*	1400.7	[0.60]
Isocaryophyllene	8.38	1524.8	0.02	10.32*	1400.7	[0.60]
$\beta$ -Caryophyllene	8.64*	1544.7	[4.67]	10.50	1414.1	3.28
Seychellene	9.05*†	1576.4	[7.68]	10.78	1434.6	6.77
Selina-5,11-diene	8.94	1568.2	0.05	10.84*	1439.0	[13.69]
$\alpha$ -Guaiane	8.70	1549.4	13.73	10.84*	1439.0	[13.69]
Unknown POCA III [m/z 91, 93 (98), 79 (82), 81 (82), 105 (71), 107 (70)... 204 (38)]	9.41	1604.6	0.08	10.87	1441.3	0.05
$\alpha$ -Humulene	9.49	1611.3	0.59	10.98*	1449.3	[5.31]
$\alpha$ -Patchoulene	9.05*†	1576.4	[7.68]	10.98*	1449.3	[5.31]
$\gamma$ -Patchoulene	9.24	1591.4	0.97	11.02*	1452.5	[2.80]
Patchoulene analog I	9.09	1579.6	1.55	11.02*	1452.5	[2.80]
9-epi- $\beta$ - Caryophyllene	9.56*	1617.0	[0.90]	11.10	1458.1	0.02
Unknown POCA IV [m/z 159, 91 (88), 93 (72), 79	9.56*	1617.0	[0.90]	11.15	1462.0	0.44

(69), 105 (68), 41 (66), 81 (54), 202? (50)...						
Unknown POCA V [m/z 147, 93 (87), 107 (77), 105 (77), 91 (73), 79 (63)... 204 (21)]	9.56*	1617.0	[0.90]	11.30*	1473.0	[0.58]
Selina-4,11-diene	9.64	1622.8	0.07	11.30*	1473.0	[0.58]
Patchoulene analog II	9.98*	1650.3	[3.10]	11.39*	1480.0	[0.08]
β-Selinene	10.08	1658.4	0.07	11.39*	1480.0	[0.08]
Unknown POCA VI [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	9.89	1643.6	0.24	11.44	1483.5	0.54
δ-Selinene	9.86	1641.0	0.17	11.48*	1486.7	[0.26]
Unknown POCA VII [m/z 161, 189 (96), 91 (74), 204 (73), 105 (69), 41 (52)]	9.98*	1650.3	[3.10]	11.48*	1486.7	[0.26]
α-Selinene	10.18*	1666.4	[18.71]	11.52	1489.4	0.10
Aciphyllene	9.98*	1650.3	[3.10]	11.60*	1495.7	[3.19]
Eudesma- 2,4(15),11-triene	11.29	1758.9	0.12	11.60*	1495.7	[3.19]
δ-Guaiene	10.18*	1666.4	[18.71]	11.73*	1505.4	[18.41]
Pentadecane	8.03	1497.7	0.05	11.73*	1505.4	[18.41]
Nootkatene	11.15	1747.1	0.01	11.80*	1510.5	[0.30]
γ-Cadinene	10.58	1699.6	0.49	11.80*	1510.5	[0.30]
7-epi-α-Selinene	10.64	1704.6	0.15	11.82	1512.0	0.21
Unknown POCA XLV [m/z 159, 91 (81), 117 (68), 131 (51), 105 (46)... 202 (37)]	9.79	1635.0	0.17	11.88	1516.9	0.08
Unknown POCA IX [m/z 41, 67 (95), 93 (92), 107 (91), 55 (77), 81 (77), 79 (73)... 205 (17)...	11.53	1779.7	0.02	11.92	1519.9	0.01
Unknown POCA X	11.48*	1775.4	[0.08]	11.95	1522.6	0.02

[m/z 161, 119 (92), 91 (69), 105 (52), 145 (49)... 218 (6)]						
Unknown POCA XI [m/z 91, 105 (98), 108 (83), 93 (82), 133 (79), 77 (64), 79 (57), 41 (56), 145 (55)... 218? (5)]				12.02	1527.8	0.13
Unknown POCA XII [m/z 91, 105 (78), 93 (77), 107 (71), 79 (64), 41 (63), 77 (63), 145 (60)... 218 (17)]				12.04	1529.7	0.10
Unknown POCA LIII [m/z 133, 105 (70), 146 (69), 145 (61), 91 (55), 131 (45), 187 (42), 159 (39), 119 (33), 202 (30)...]	11.48*	1775.4	[0.08]	12.08	1532.8	0.01
Unknown POCA XIII [m/z 145, 131 (91), 91 (86), 105 (68), 146 (66), 43 (54)... 220? (5)]				12.12	1535.7	0.01
Norpatchoulénol	14.29	2028.6	0.57	12.24	1545.0	0.58
Unknown POCA XIV [m/z 191, 159 (66), 133 (53), 91 (45), 41 (42), 177 (35), 105 (33), 220 (32)]	13.86	1988.2	0.02	12.36	1554.7	0.01
Unknown POCA XV [m/z 41, 67 (90), 55 (87), 79 (85), 107 (84), 81 (84), 93 (84), 121 (77), 91 (74)... 220 (7)]				12.46	1562.5	0.06
Unknown POCA XVI [m/z 43, 107	12.53	1866.8	0.16	12.54	1568.7	0.17

(94), 81 (71), 41 (63), 67 (58), 111 (58), 93 (55), 83 (54)... 205 (8), 220 (1)]						
Unknown POCA XIV isomer	14.62	2060.1	0.02	12.61*	1574.2	[0.32]
Caryophyllene oxide isomer	12.90	1899.6	0.07	12.61*	1574.2	[0.32]
Caryophyllene oxide	12.98	1906.5	0.26	12.61*	1574.2	[0.32]
Unknown POCA XVII [m/z 43, 79 (44), 81 (41), 93 (40), 91 (40)... 220 (5)]	14.53	2052.0	0.36	12.72	1583.2	0.52
Unknown POCA XVIII [m/z 43, 105 (77), 91 (71), 93 (68), 41 (62), 107 (6)... 205 (41), 220 (7)]	14.85	2082.8	0.23	12.88	1595.0	0.05
Hexadecane	9.28	1594.0	0.04	12.94	1600.4	0.04
Humulene epoxide II	13.57	1961.0	0.04	12.96	1602.0	0.08
Unknown POCA XIX [m/z 43, 161 (73), 91 (53), 95 (52), 79 (46), 119 (45)... 205 (29), 220? (1)]	15.02*	2098.5	[28.06]	13.03	1607.6	0.09
Unknown POCA XX [m/z 41, 91 (92), 55 (81), 93 (81), 79 (74), 43 (71), 95 (68), 123 (65)... 220 (17)]	15.07	2104.3	0.20	13.07	1610.3	0.24
Unknown POCA XXI [m/z 43, 79 (41), 93 (39), 41 (39), 91 (38), 81 (36)... 220 (3)]				13.12	1614.8	0.23
Unknown POCA XXII [m/z 41, 55 (92), 95 (80), 81	15.02*	2098.5	[28.06]	13.22	1623.0	0.59

(76), 109 (76), 67 (66), 125 (65)... 220 (12)]						
Caryophylladienol II	16.28*	2225.9	[0.11]	13.27	1627.4	0.19
Hinesol	15.24*	2121.3	[0.29]	13.32	1630.9	0.29
Patchoulol	15.02*	2098.5	[28.06]	13.56*	1651.3	[30.48]
Pogostol	15.43	2139.9	2.03	13.56*	1651.3	[30.48]
Unknown POCA XXIII [m/z 175, 218 (59), 133 (49), 91 (43), 41 (38), 147 (36)]	15.24*	2121.3	[0.29]	13.64	1657.4	0.10
Unknown POCA XXV [m/z 95, 107 (99), 41 (85), 93 (82), 91 (82), 109 (71), 105 (71), 105 (71), 108 (66)... 220 (29)]	16.34	2232.2	0.02	13.87	1676.6	0.16
Unknown POCA XXVI [m/z 91, 41 (100), 107 (98), 108 (95), 95 (87), 93 (87), 105 (85), 79 (77), 119 (72)... 220? (15)]	16.25	2223.1	0.04	13.90	1679.0	0.04
Unknown POCA XXVII [m/z 43, 41 (95), 97 (89), 109 (71), 55 (71), 107 (70), 95 (69), 110 (65)... 222 (5)]	15.66	2162.7	0.07	13.99	1686.2	0.03
Rotundone	15.88	2185.3	0.10	14.16	1700.8	0.12
Unknown POCA LV [m/z 105, 107 (98), 91 (95), 166 (80), 248 (80), 93 (76)... 233 (66)]	13.29	1935.6	0.03	14.19*	1703.2	[0.11]
Unknown POCA XXVIII [m/z 43, 41 (82), 137 (78), 109 (76), 95 (75), 91 (72), 55 (67)... 220? (14)]				14.19*	1703.2	[0.11]

Pogostone	19.80	2615.8	0.80	14.29	1711.5	1.20
Unknown POCA XXIX [m/z 107, 93 (87), 41 (83), 81 (82), 67 (80), 55 (76)... 204 (53), 207 (34), 222 (9)]	17.12	2313.9	0.18	14.41*	1721.6	[0.29]
Unknown POCA XXX [m/z 83, 43 (85), 55 (39), 41 (29), 121 (27), 120 (25)... 218 (3)]	17.23	2325.7	0.08	14.41*	1721.6	[0.29]
Unknown POCA XXXI [m/z 133, 148 (68), 147 (59), 91 (56), 79 (45), 105 (44)... 218 (8)]	17.36	2340.2	0.02	14.49	1729.2	0.06
Unknown POCA XLIX [m/z 91, 108 (86), 107 (85), 93 (80), 120 (75), 105 (71), 95 (72)... 218 (37)]	16.28*	2225.9	[0.11]	14.53	1732.6	0.02
Unknown POCA XXXII [m/z 43, 83 (93), 55 (42), 41 (37), 121 (34), 111 (28)... 222? (1)]	17.70	2376.5	0.02	14.68	1745.4	0.02
Unknown POCA XXXIII [m/z 134, 107 (96), 91 (84), 93 (78), 79 (77), 41 (74), 43 (66), 77 (65)...]	17.59	2364.8	0.01	14.77	1753.0	0.01
Unknown POCA XXXIV [m/z 43, 191 (68), 41 (62), 91 (51), 95 (49), 110 (44)... 234 (22)]				14.80	1755.7	0.04
Unknown POCA XXXV [m/z 91, 105 (88), 95 (79), 93 (78), 81 (72), 79 (66)... 205 (33),				14.85	1760.4	0.10

220 (7)...						
Unknown POCA XXXVI [m/z 149, 131 (54), 105 (48), 91 (46), 41 (30), 93 (27)... 218 (23)]	17.54	2359.4	0.12	14.95	1768.9	0.07
Unknown POCA XXXVII [m/z 43, 95 (58), 67 (50), 41 (47), 55 (38), 109 (37)... 221 (9)... 236? (3)]	18.27*	2439.7	[0.09]	15.12	1783.7	0.02
Unknown POCA XXXVIII [m/z 219, 43 (67), 91 (46), 79 (42), 41 (41), 55 (36)... 234 (6)]	18.27*	2439.7	[0.09]	15.26	1795.8	0.03
Unknown POCA XL [m/z 43, 91 (77), 79 (74), 109 (73), 110 (71)... 218 (52), 234? (1)]	17.79	2386.1	0.01	15.33	1801.9	0.03
Unknown POCA XXXIX [m/z 43, 91 (43), 41 (37), 79 (32), 219 (31)... 234 (14)]				15.39*	1807.2	[0.02]
Unknown POCA XLII [m/z 91, 41 (79), 43 (74), 79 (72), 105 (65), 77 (64), 147 (64), 93 (61)... 218 (26), 234 (14)]	17.49	2354.0	0.01	15.39*	1807.2	[0.02]
Unknown POCA XLIV [m/z 41, 110 (77), 55 (75), 69 (74), 43 (74), 95 (71), 97 (71), 123 (71), 67 (63), 136 (56)... 236? (7)]				15.81	1844.8	0.02
Phytol	19.42	2571.0	0.03	18.59	2111.7	0.03
Total reported		95.24%			97.73%	

\*: 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