

## GC/MS BATCH NUMBER: C90111

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**ESSENTIAL OIL:** CHAMOMILE ROMAN  
**BOTANICAL NAME:** CHAMAEMELUM NOBILE  
**ORIGIN:** UNITED KINGDOM

KEY CONSTITUENTS PRESENT IN THIS BATCH OF CHAMOMILE ROMAN OIL	%
3-METHYLAMYL ANGELATE	13.3
METHALLYL ANGELATE	12.8
ISOBUTYL ANGELATE	11.5
2-METHYLBUTYL ANGELATE	11.2
trans-PINOCARVEOL	5.7
3-METHYLAMYL ISOBUTYRATE	4.1
$\alpha$ -PINENE	3.3
PINOCARVONE	2.7
ISOAMYL METHACRYLATE + 2- METHYLBUTYL METHACRYLATE	2.2
2-METHYLBUTYL ISOBUTYRATE	2.1
3-METHYLAMYL METHACRYLATE	1.8
ISOBUTYL ISOBUTYRATE	1.7
ISOBUTYL METHACRYLATE	1.3

Comments from Robert Tisserand: Light, intense apple-fruity odor profile. Constituents are in expected amounts for UK Roman Chamomile oil.

**Date :** November 6, 2017

*SAMPLE IDENTIFICATION*

**Internal code :** 17K03-PTH1-1-CC

**Customer identification :** Chamomile Roman - UK - C9011177R

**Type :** Essential oil

**Source :** *Chamaemelum nobile*

**Customer :** Plant Therapy

*ANALYSIS*

**Method :** PC-PA-001-15E06, "Analysis of the composition of a liquid essential oil by GC-FID" (in French).

Identifications double-checked by GC-MS

**Analyst :** Alexis St-Gelais, M. Sc., chimiste

**Analysis date :** 2017-11-03

Checked and approved by :



Alexis St-Gelais, M. Sc., chimiste 2013-174

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IDENTIFIED COMPOUNDS

Identification	Column: BP5			Column: WAX			Molecular Class
	R.T.	R.I.	%	%	R.I.	R.T.	
Isovaleral	0.65	671	0.08	0.11	735	0.63*	Aliphatic aldehyde
2-Methylbutyral	0.66	673	0.05	[0.11]	735	0.63*	Aliphatic aldehyde
Isoamyl alcohol	1.11	732	0.17	3.72	1147	2.97*	Aliphatic alcohol
2-Methylbutyl alcohol	1.13	735	0.27	[3.72]	1147	2.97*	Aliphatic alcohol
Ethyl isobutyrate	1.22	746	0.02				Aliphatic ester
3-Methylvaleraldehyde	1.30	756	0.01				Aliphatic aldehyde
Methyl 2-methylbutyrate	1.39	768	0.03	0.03	922	1.04*	Aliphatic ester
Butyric acid	1.55	790	0.08				Aliphatic acid
Hexanal	1.70	804	0.06	0.10	1011	1.54	Aliphatic aldehyde
Methyl angelate	1.94	823	0.06	0.06	1048	1.91	Aliphatic ester
Ethyl 2-methylbutyrate	2.24	846	0.06	0.09	991	1.36	Aliphatic ester
3-Methylpentanol	2.34	853	0.76	0.90	1270	4.69	Aliphatic alcohol
cis-Hex-3-en-1-ol	2.47	863	0.12	12.75	1321	5.47*	Aliphatic alcohol
Isoamyl acetate	2.68	878	0.20	0.38	1056	1.99*	Aliphatic ester
2-Methylbutyl acetate	2.71	881	0.13	0.07	1062	2.06*	Aliphatic ester
Propyl methacrylate	2.74	883	0.06	[0.38]	1056	1.99*	Aliphatic ester
Isovaleric acid	2.80	888	0.01				Aliphatic acid
Ethyl angelate?	2.97	900	0.08				Aliphatic ester
Isobutyl isobutyrate	3.23*	915	1.40	1.67	1033	1.74*	Aliphatic ester
Tricyclene	3.23*	915	[1.40]	[0.03]	922	1.04*	Monoterpene
α-Pinene	3.42	926	3.32	3.12	944	1.13	Monoterpene
Prenyl acetate	3.51*	932	0.49	0.16	1190	3.53	Aliphatic ester
Angelic acid	3.51*	932	[0.49]				Aliphatic acid
Isobutyl methacrylate	3.66	941	1.25	1.28	1115	2.54*	Aliphatic ester
Camphene	3.70	943	0.85	0.82	999	1.43	Monoterpene
Thuja-2,4(10)-diene	3.79	949	0.07	[0.07]	1062	2.06*	Monoterpene
Methallyl methacrylate	3.94	957	0.92	1.11	1203	3.70	Aliphatic ester
Sabinene	4.13	969	0.06	[0.07]	1062	2.06*	Monoterpene
β-Pinene	4.19	972	0.30	[1.67]	1033	1.74*	Monoterpene
Isoamyl propionate	4.23	975	0.07				Aliphatic ester
Methallyl isobutyrate	4.43	986	0.31	0.33	1181	3.41	Aliphatic ester
Myrcene	4.52	992	0.11	[1.28]	1115	2.54*	Monoterpene
Propyl angelate	4.61	997	0.80	0.66	1197	3.62	Aliphatic ester
Isobutyl 2-methylbutyrate	4.74	1004	0.35	0.82	1128	2.71*	Aliphatic ester
Isoamyl isobutyrate	4.94	1015	0.75	[3.72]	1147	2.97*	Aliphatic ester
2-Methylbutyl isobutyrate	5.00	1018	2.11	[3.72]	1147	2.97*	Aliphatic ester
meta-Cymene	5.04	1020	0.10	[0.82]	1128	2.71*	Monoterpene
para-Cymene	5.13	1025	0.12	0.15	1210	3.80	Monoterpene
Limonene	5.17	1027	0.08	[3.72]	1147	2.97*	Monoterpene
β-Phellandrene	5.20	1029	0.07	[3.72]	1147	2.97*	Monoterpene
1,8-Cineole	5.22	1030	0.09	[3.72]	1147	2.97*	Monoterp. ether

Isoamyl methacrylate + 2-Methylbutyl methacrylate	5.49	1045	2.22	2.33	1224	4.01	Aliphatic ester
Isobutyl angelate	5.68	1055	11.53	12.21	1239	4.24*	Aliphatic ester
Prenyl isobutyrate	5.76	1060	0.26	4.47	1260	4.53*	Aliphatic ester
Methallyl angelate	5.97	1071	12.84	[12.75]	1321	5.47*	Aliphatic ester
3-Methylamyl propionate?	6.09	1077	0.19	0.22	1251	4.41	Aliphatic ester
Unknown (m/z = 69, 41 (59), 67 (32), 68 (27), 53 (12)... 154 (5))	6.30	1089	0.25				Oxygenated monoterp.
Butyl angelate	6.38	1093	0.46	0.61	1292	5.02	Aliphatic ester
Isobutyl tiglate	6.44	1097	0.16	0.16	1305	5.20	Aliphatic ester
Isoamyl 2-methylbutyrate	6.55	1101	0.14	[12.21]	1239	4.24*	Aliphatic ester
2-Methylbutyl 2-methylbutyrate	6.62	1103	0.38	[12.21]	1239	4.24*	Aliphatic ester
$\alpha$ -Thujone	6.79	1110	0.04	0.10	1360	6.07	Monoterp. ketone
Methallyl tiglate?	6.84	1111	0.16	0.18	1391	6.55	Aliphatic ester
3-Methylamyl isobutyrate	6.93	1115	4.05	[4.47]	1260	4.53*	Aliphatic ester
$\alpha$ -Campholenal	7.27	1127	0.11				Monoterp. aldehyde
<i>trans</i> -Pinocarveol	7.71*	1143	7.57	5.73	1566	11.45	Monoterp. alcohol
3-Methylamyl methacrylate	7.71*	1143	[7.57]	20.65	1346	5.84*	Aliphatic ester
Isoamyl angelate	7.81	1147	6.28	[20.65]	1346	5.84*	Aliphatic ester
2-Methylbutyl angelate	7.94	1151	11.23	[20.65]	1346	5.84*	Aliphatic ester
Camphene hydrate	8.08	1156	0.33	0.43	1517	9.65*	Monoterp. alcohol
<i>C. nobile</i> biomarker	8.15	1159	0.58	0.96	1408	6.89*	Aliphatic ester
Pinocarvone	8.26	1163	2.68	2.53	1472	8.41	Monoterp. ketone
Isopinocampnone	8.44	1170	0.14	0.31	1506	9.22*	Monoterp. alcohol
Borneol	8.65	1177	0.56	0.48	1616	13.48*	Monoterp. alcohol
Terpinen-4-ol	8.82	1183	0.06	[0.43]	1517	9.65*	Monoterp. alcohol
$\alpha$ -Terpineol	9.20*	1197	0.99	1.27	1621	13.70*	Monoterp. alcohol
Isobutyl 3-hydroxy-2-methylenebutyrate	9.20*	1197	[0.99]	0.39	1703	17.98	Aliphatic ester
Prenyl angelate	9.33	1200	0.75	0.94	1452	7.93	Aliphatic ester
Isoamyl tiglate	9.47*	1203	1.03	[0.96]	1408	6.89*	Aliphatic ester
Myrtenal	9.47*	1203	[1.03]	0.82	1527	10.01	Monoterp. aldehyde
3-Methylamyl valerate	9.80	1211	0.06	0.06	1398	6.67	Aliphatic ester
Verbenone	9.86	1212	0.03	0.05	1602	12.77	Monoterp. ketone
3-Methylamyl angelate	11.68	1252	13.27	13.32	1448	7.82	Aliphatic ester
Bornyl acetate	12.87	1278	0.13	[0.31]	1506	9.22*	Monoterp. ester
Isoamyl 3-hydroxy-2-methylenebutyrate	13.57	1293	0.21	0.20	1820	25.68	Aliphatic ester
3-Methylamyl tiglate	14.03	1302	0.09	[0.31]	1506	9.22*	Aliphatic ester
<i>C. nobile</i> biomarker	20.31	1397	0.18	0.15	1933	33.46	
$\beta$ -Caryophyllene	20.60	1400	0.07	[0.43]	1517	9.65*	Sesquiterpene
Phenylethyl isobutyrate	21.18	1407	0.12	0.07	1808	24.86	Phenolic ester

<i>trans</i> - $\beta$ -Farnesene	24.52	1447	0.21	[0.48]	1616	13.48*	Sesquiterpene
Germacrene D	25.65	1460	0.92	[1.27]	1621	13.70*	Sesquiterpene
$\beta$ -Selinene	26.25	1468	0.16	[1.27]	1621	13.70*	Sesquiterpene
( <i>E,E</i> )- $\alpha$ -Farnesene	29.11	1502	0.31	0.43	1694	17.53	Sesquiterpene
( <i>E,E</i> )-Matricaria ester?	32.51	1550	0.08	0.10	2204	42.62	Polyne
Copaborneol	35.79	1596	0.10				Sesquiterp. alcohol
Phytone	44.39	1843	0.05	0.06	2075	39.07	Aliphatic ketone
<b>Total identified</b>			<b>96.85%</b>	<b>97.56%</b>			

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken account in the identified total

Note: no correction factor was applied

#### OTHER DATA

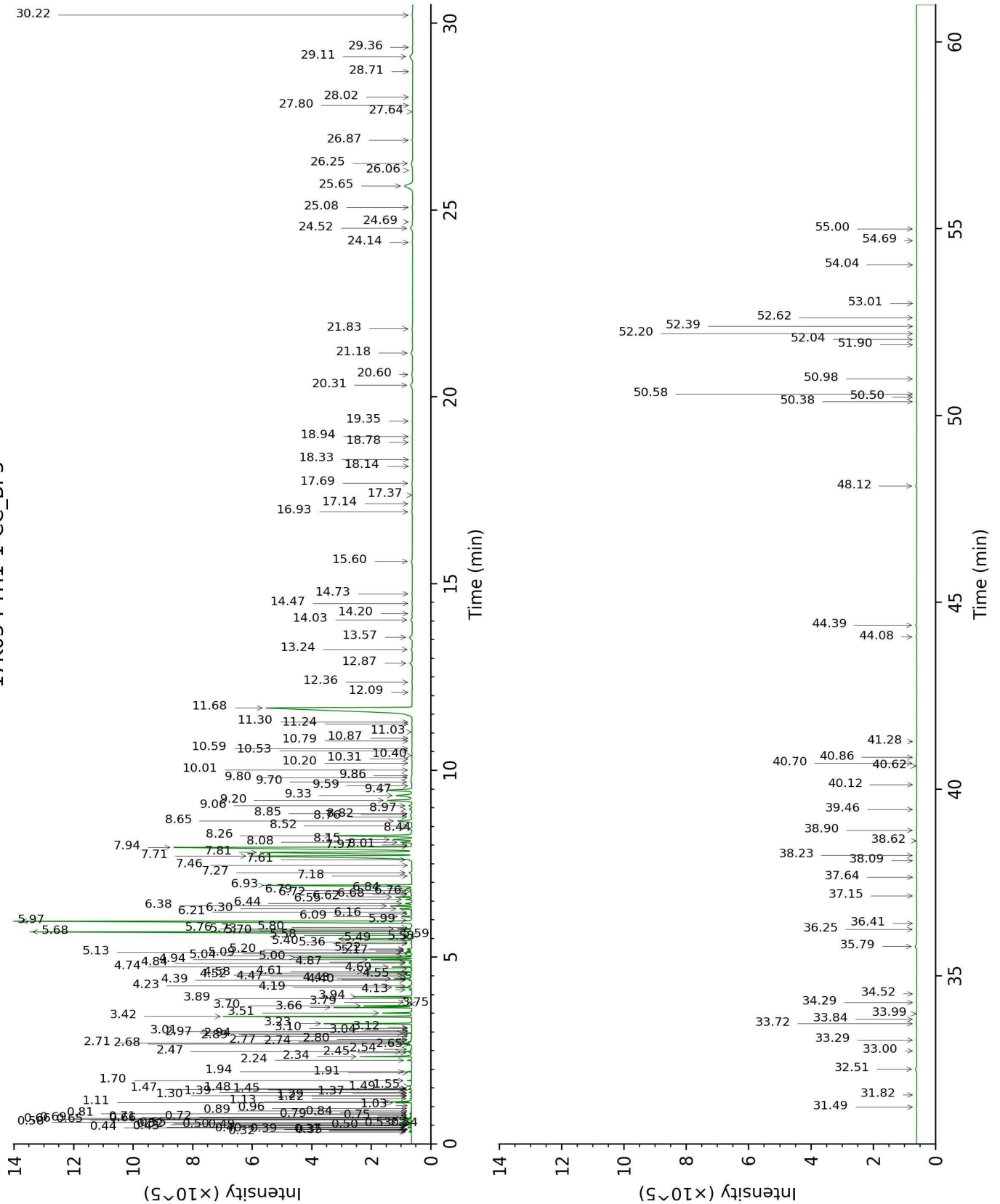
**Physical aspect :** Faintly green liquid

**Refractive index :**  $1.4455 \pm 0.0003$  (20 °C)

#### CONCLUSION

No adulterant, contaminant or diluent were detected using this method.

17K03-PTH1-1-CC\_BP5



17K03-PTH1-1-CC\_WAX

