

SERVICE DE SPECTROMETRIE DE MASSE DE L'ISIC (SSMI)

Dr. Laure Menin
Francisco Sepulveda
EPFL-SB-ISIC
SSMI, BCH 1524
CH-1015 Lausanne
Suisse
Phone: +41 21 693 94 64
Fax: +41 21 693 97 50
Laure.menin@epfl.ch

Pr. Yury O. Tsybin, Directeur
EPFL-SB-ISIC
LSMB, BCH 4312
CH-1015 Lausanne
Suisse
Phone: +41 21 693 97 51
Fax: +41 21 693 97 00
Yury.tsybin@epfl.ch



ANALYSES GC-MS

Le 12 Juillet 2012

Objet: Analyse d'une huile essentielle par GC-MS
Nom: **Camomille Romaine**
Lot: **CMARB195022**
Destinataire : Entreprise Gedane (Lausanne, Suisse)
Composés majoritaires: **Isobutyl Angelate ; Isoamyl Angelate; Methallyle Angelate**

CONDITIONS EXPERIMENTALES

Type d'instrument : GC CP-3800 couplé au 1200L Triple quadrupole MS/MS (Varian)
Mode d'ionisation : Impact électronique (IE), 70 eV (mode positif)
Gamme de masse : m/z 50-300 en 0.5 sec
Colonne : FactorFour VF-5ms (5% phenyl-methyl 95% dimethyl polysiloxane, 0.25mm x 30 m)
Débit : 1 mL/min
Gradient : 50°C pendant 3 min; Montée à 150°C en 20 min; Montée à 250°C en 7 min
Calibrant : FC43
Echantillons : Huile essentielle diluée 1:500 dans l'éther. Injection de 1 μ L.

Figure 1 – Chromatogramme TIC-GC/MS d'huile essentielle de Camomille (CMARB195022) analysée sur colonne capillaire

FactorFour VF-5ms (5% phenyl-methyl 95% dimethylpolysiloxane, 0.25mm x 30 m). Les numéros des pics sont reportés dans la Table 1.

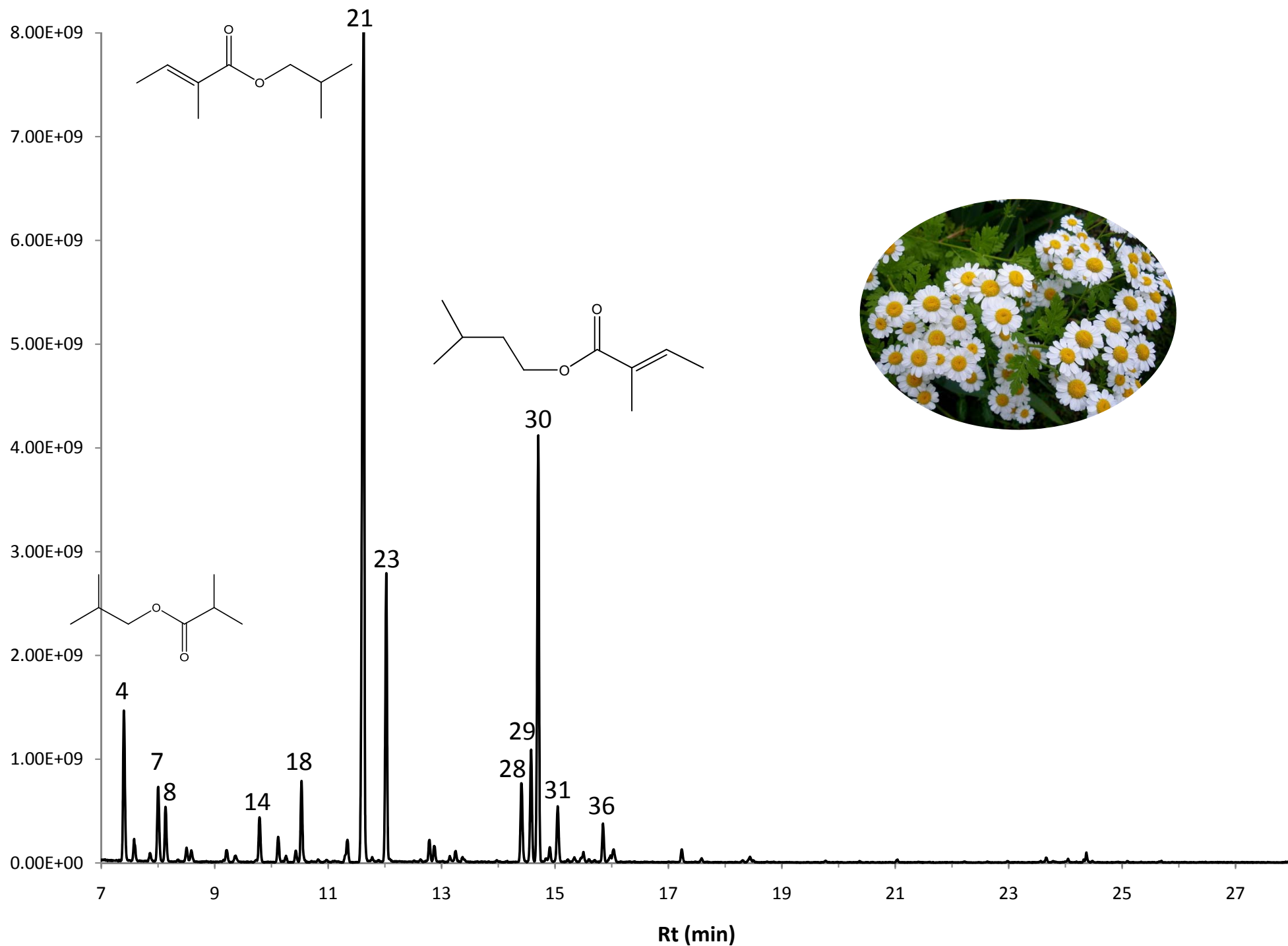


Table 1 – Composition de l'huile essentielle de Camomille Romaine (CMARB195022)

N°	Retention Time (min.)	Area	% of Total	Identification (NIST 08/MassFinder)	Prob (%)
1	5.76	5.14E+07	0.1	Isopropyl Butyrate	15
2	6.32	7.11E+07	0.1	Amyl Acetate	37
3	6.37	9.57E+07	0.2	2-Methylbutyl Acetate	75
4	7.40	3.28E+09	5.5	Isobutyl Isobutyrate (=isobutyl isobutanoate)	60
5	7.58	5.00E+08	0.8	Dimethylallyl Acetate	68
6	7.86	1.89E+08	0.3	2-Butyltetrahydrofuran	17
7	8.00	1.79E+09	3.0	α-Pinene	67
8	8.13	1.18E+09	2.0	Isobutyl Methacrylate	36
9	8.35	2.24E+07	0.0	Propyl2-methylbutyrate	17
10	8.50	3.10E+08	0.5	Camphene	62
11	8.59	2.80E+08	0.5	Glycidol Methacrylate	12
12	9.21	2.57E+08	0.4	Sabinene	86
13	9.37	1.95E+08	0.3	β -Pinene	67
14	9.79	9.59E+08	1.6	Propyl Angelate	*
15	10.12	5.48E+08	0.9	Isobutyl 2-methylbutanoate	68
16	10.26	1.16E+08	0.2	Isobutyl isovalerate	66
17	10.43	2.03E+08	0.3	iso-Amyl iso-butyrate (= 3-methylbutyl isobutyrate)	28
18	10.53	1.72E+09	2.9	2-Methylbutyl Isobutyrate	69
19	10.82	5.38E+07	0.1	p-Cymene	52
20	11.34	4.92E+08	0.8	3-Methylbutyl methacrylate	75
21	11.63	2.30E+10	38.5	Isobutyl Angelate	57
22	11.78	1.33E+08	0.2	Butanoic acid, 3-methylbut-2-enyl ester	68
23	12.02	6.08E+09	10.2	Methallyle Angelate	*
24	12.79	4.97E+08	0.8	Butyl 3-methyl-2-butanoate	40
25	12.87	1.84E+08	0.3	Isobutyl tiglate	59
26	13.15	4.41E+07	0.1	3-Methylbutyl 2-methylbutyrate	10
27	13.25	2.25E+08	0.4	2-Methylbutyl 2-methylbutyrate	62
28	14.41	1.91E+09	3.2	trans Pinocarveol	30
29	14.58	2.50E+09	4.2	3-Methylbutyl Angelate	66
30	14.70	9.28E+09	15.5	Isoamyl Angelate	*
31	15.05	1.35E+09	2.3	Pinocarvone	63
32	15.34	9.82E+07	0.2	Borneol	63
33	15.46	5.94E+07	0.1	Cis-Pinocamphone	50
34	15.50	2.22E+08	0.4	Isobutyl 3-hydroxy-2-methylenebutanoate	82
35	15.59	3.18E+07	0.1	4-Terpeneol	66
36	15.85	7.93E+08	1.3	3-Methyl-2-butenic acid, 3-methylbut-2-enyl ester	68
37	15.98	1.50E+08	0.3	isoamyl Tiglate	30
38	16.03	3.46E+08	0.6	Myrtenal	41
39	17.23	2.37E+08	0.4	2-Hydroxy-2-methyl-but-3-enyl 2-methyl-2(Z)-butenoate	89
40	17.59	7.46E+07	0.1	Hexyl 3-methyl-2-butenate	50
41	18.31	4.56E+07	0.1	Z)-Hex-3-enyl (E)-2-methylbut-2-enoate	22
42	18.44	1.63E+08	0.3	Isopentyl 3-hydroxy-2-methylenebutanoate	71
43	21.03	5.57E+07	0.1	Geranyl Acetate	52
44	23.67	1.20E+08	0.2	α -Muuroleone	63
45	24.04	3.34E+07	0.1	α -Farnesene	37

* Identification manuelle

Table 1 – Composition de l'huile essentielle de Camomille Romaine (CMARB195022)

N°	Retention Time (min.)	Area	% of Total	Identification (NIST 08/MassFinder)
1	5.76	5.14E+07	0.1	Isopropyl Butyrate
2	6.32	7.11E+07	0.1	Amyl Acetate
3	6.37	9.57E+07	0.2	2-Methylbutyl Acetate
4	7.40	3.28E+09	5.5	Isobutyl Isobutyrate (=isobutyl isobutanoate)
5	7.58	5.00E+08	0.8	Dimethylallyl Acetate
6	7.86	1.89E+08	0.3	2-Butyltetrahydrofuran
7	8.00	1.79E+09	3.0	α-Pinene
8	8.13	1.18E+09	2.0	Isobutyl Methacrylate
9	8.35	2.24E+07	0.0	Propyl 2-methylbutyrate
10	8.50	3.10E+08	0.5	Camphene
11	8.59	2.80E+08	0.5	Glycidol Methacrylate
12	9.21	2.57E+08	0.4	Sabinene
13	9.37	1.95E+08	0.3	β -Pinene
14	9.79	9.59E+08	1.6	Propyl Angelate
15	10.12	5.48E+08	0.9	Isobutyl 2-methylbutanoate
16	10.26	1.16E+08	0.2	Isobutyl isovalerate
17	10.43	2.03E+08	0.3	iso-Amyl iso-butyrate (= 3-methylbutyl isobutyrate)
18	10.53	1.72E+09	2.9	2-Methylbutyl Isobutyrate
19	10.82	5.38E+07	0.1	p-Cymene
20	11.34	4.92E+08	0.8	3-Methylbutyl methacrylate
21	11.63	2.30E+10	38.5	Isobutyl Angelate
22	11.78	1.33E+08	0.2	Butanoic acid, 3-methylbut-2-enyl ester
23	12.02	6.08E+09	10.2	Methylallyl Angelate
24	12.79	4.97E+08	0.8	Butyl 3-methyl-2-butanoate
25	12.87	1.84E+08	0.3	Isobutyl tiglate
26	13.15	4.41E+07	0.1	3-Methylbutyl 2-methylbutyrate
27	13.25	2.25E+08	0.4	2-Methylbutyl 2-methylbutyrate
28	14.41	1.91E+09	3.2	trans Pinocarveol
29	14.58	2.50E+09	4.2	3-Methylbutyl Angelate
30	14.70	9.28E+09	15.5	Isoamyl Angelate
31	15.05	1.35E+09	2.3	Pinocarvone
32	15.34	9.82E+07	0.2	Borneol
33	15.46	5.94E+07	0.1	Cis-Pinocamphone
34	15.50	2.22E+08	0.4	Isobutyl 3-hydroxy-2-methylenebutanoate
35	15.59	3.18E+07	0.1	4-Terpineol
36	15.85	7.93E+08	1.3	3-Methyl-2-butenic acid, 3-methylbut-2-enyl ester
37	15.98	1.50E+08	0.3	isoamyl Tiglate
38	16.03	3.46E+08	0.6	Myrtenal
39	17.23	2.37E+08	0.4	2-Hydroxy-2-methyl-but-3-enyl 2-methyl-2(Z)-butenoate
40	17.59	7.46E+07	0.1	Hexyl 3-methyl-2-butenate
41	18.31	4.56E+07	0.1	Z)-Hex-3-enyl (E)-2-methylbut-2-enoate
42	18.44	1.63E+08	0.3	Isopentyl 3-hydroxy-2-methylenebutanoate
43	21.03	5.57E+07	0.1	Geranyl Acetate
44	23.67	1.20E+08	0.2	α -Muuroolene
45	24.04	3.34E+07	0.1	α -Farnesene