

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

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ANALYSES GC-MS

Le 27 Mai 2011

Objet: Analyse d'une huile essentielle par GC-MS
Nom: **Géranium**
Lot: **GERB445N63**
Destinataire : Entreprise Gedane (Lausanne, Suisse)
Composés majoritaires: **Citronellyl Formate ; Guaia-6,9-diene ; Isomenthone**

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 50-250 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 Géranium (GERB445N63) 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.

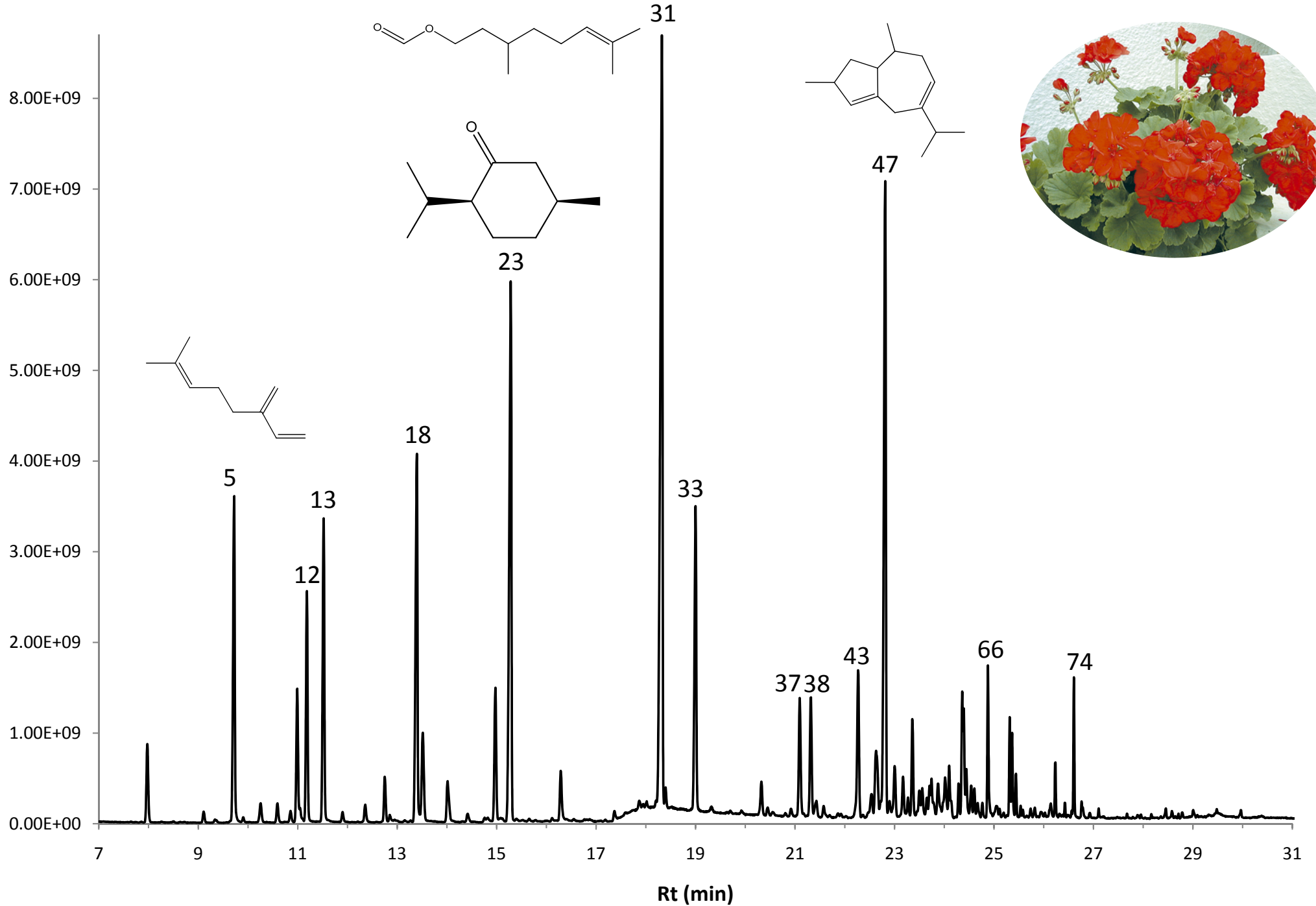


Table 1 – Composition de l'huile essentielle de Géranium (GERB445N63)

N°	Retention Time (min.)	Area	% of Total	Identification (NIST 08/MassFinder)	Prob (%)
1	7.97	2.19E+09	1.22	α -Pinene	80
2	9.11	3.03E+08	0.17	2H,pyran, 2-ethenyltetrahydro-2,6,6-trimethyl	80
3	9.33	1.36E+08	0.08	Sabinene	83
4	9.44	1.25E+08	0.07	β -Pinene	84
5	9.72	8.66E+09	4.81	Myrcene	82
6	9.91	1.22E+08	0.07	D2- Carene	79
7	10.25	6.16E+08	0.34	α -Phellandrene	82
8	10.59	5.42E+08	0.30	α -Terpinene	78
9	10.85	3.11E+08	0.17	p-Cymene	78
10	10.99	3.57E+09	1.98	D-Limonene	30
11	11.04	3.68E+08	0.20	β -Phellandrene	77
12	11.18	5.93E+09	3.29	β-(Z)-Ocimene	72
13	11.52	7.99E+09	4.44	β-(E)-Ocimene	64
14	11.90	2.91E+08	0.16	γ -Terpinene	85
15	12.36	5.47E+08	0.30	Trans-Linalool Oxide	74
16	12.75	1.18E+09	0.66	Terpinolene	36
17	12.85	1.54E+08	0.09	Cis-Linalool Oxide	72
18	13.39	1.12E+10	6.21	Linalool	82
19	13.51	2.99E+09	1.66	Cis-Rose Oxide	91
20	14.01	1.40E+09	0.78	Trans-Rose Oxide	75
21	14.42	2.76E+08	0.15	(4E,6Z)-allo-Ocimene	77
22	14.97	3.68E+09	2.04	Menthone	71
23	15.28	1.80E+10	10.01	Isomenthone	74
24	16.12	6.85E+07	0.04	Isomenthol	78
25	16.29	1.47E+09	0.82	α -Terpineol	74
26	17.37	2.60E+08	0.14	Geranial	66
27	17.87	3.44E+08	0.19	Piperitone	66
28	17.95	2.01E+08	0.11	Menthyl Formate	70
29	18.02	2.81E+08	0.16	α -Citronellol	48
30	18.20	2.71E+08	0.15	Neral	64
31	18.32	2.78E+10	15.46	Citronellyl Formate	48
32	18.40	4.97E+08	0.28	Neryl Formate	69
33	19.00	8.62E+09	4.79	Geranyl Formate	98
34	20.32	9.71E+08	0.54	Citronellyl Acetate	38
35	20.45	2.10E+08	0.12	Phenehyl Propionate	83
36	20.92	2.21E+08	0.12	α -Ylangene	79
37	21.09	3.38E+09	1.88	Isodauca-6,9-diene	10
38	21.32	3.34E+09	1.86	β-Bourbonene	73

Table 1 – Composition de l'huile essentielle de Géranium (GERB445N63) (suite)

N°	Retention Time (min.)	Area	% of Total	Identification (NIST 08/MassFinder)	Prob (%)
39	21.43	5.87E+08	0.33	β -Elemene	15
40	21.57	3.43E+08	0.19	2-Phenylethyl Butyrate	87
41	21.86	1.22E+08	0.07	Isocaryophyllene	22
42	21.92	1.90E+08	0.11	α -Gurgujene	10
43	22.27	4.40E+09	2.44	β-Caryophyllene	48
44	22.54	9.07E+08	0.50	Trans- α -Bergamotene	61
45	22.63	2.92E+09	1.62	α -Guaiene	70
46	22.72	2.95E+08	0.16	Cis- β -Guaiene / α -Gurgujene	61/ 20
47	22.81	2.01E+10	11.15	Guaia-6,9-diene	81
48	22.90	5.18E+08	0.29	Carota-5,8-diene	62
49	23.00	1.61E+09	0.89	5-epi-Aritolochene	62
50	23.17	1.14E+09	0.63	α -Humulene	79
51	23.27	5.54E+08	0.31	allo-Aromadendrene	25
52	23.36	2.57E+09	1.43	Neryl butanoate	41
53	23.50	7.27E+08	0.40	γ -Amorphene	85
54	23.65	4.99E+08	0.28	α -Murolene	89
55	23.71	7.01E+08	0.39	D-Germacrene	33
56	23.78	3.89E+08	0.22	γ -Guaiene	10
57	23.88	1.28E+09	0.71	α -Selinene	15
58	24.02	1.61E+09	0.89	α -Amorphene / α -Cadinene	90 / 80
59	24.10	1.55E+09	0.86	Geranyl Burytate	94
60	24.29	6.95E+08	0.39	γ -Cadinene	65
61	24.36	2.52E+09	1.40	ω -Amorphene	70
62	24.39	2.06E+09	1.14	Citronellyl isobutyrate	33
63	24.61	6.26E+08	0.35	w-Cadinene / Cubenene	72 / 20
64	24.67	4.25E+08	0.24	α -Cadinene	76
65	24.77	3.20E+08	0.18	β -Calacorene / γ -Calacorene	84 / 74
66	24.88	3.18E+09	1.76	Geranyl Burytate	98
67	25.32	1.79E+09	0.99	Unknown	
68	25.36	1.67E+09	0.93	Phenylethyl tiglate	73
69	25.44	7.31E+08	0.41	cis-Sesquisabinene hydrate	87
70	25.54	1.93E+08	0.11	trans-Sesquisabinene hydrate	79
71	25.82	2.33E+08	0.13	1-epi-Cubenol	25
72	26.14	4.55E+08	0.25	Cubenol	61
73	26.23	1.00E+09	0.56	Citronellyl Tiglate	10
74	26.61	2.14E+09	1.19	Geranyl Tiglate	93
75	26.76	2.56E+08	0.14	Farnesol	30
76	26.92	9.80E+07	0.05	Nerolidyl Acetate	15
77	27.10	1.41E+08	0.08	Geranyl Caproate	16

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15	12.36	5.47E+08	0.30	Trans-Linalool Oxide
16	12.75	1.18E+09	0.66	Terpinolene
17	12.85	1.54E+08	0.09	Cis-Linalool Oxide
18	13.39	1.12E+10	6.21	Linalool
19	13.51	2.99E+09	1.66	Cis-Rose Oxide
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22	14.97	3.68E+09	2.04	Menthone
23	15.28	1.80E+10	10.01	Isomenthone
24	16.12	6.85E+07	0.04	Isomenthol
25	16.29	1.47E+09	0.82	α -Terpineol
26	17.37	2.60E+08	0.14	Geranial
27	17.87	3.44E+08	0.19	Piperitone
28	17.95	2.01E+08	0.11	Menthyl Formate
29	18.02	2.81E+08	0.16	α -Citronellol
30	18.20	2.71E+08	0.15	Neral
31	18.32	2.78E+10	15.46	Citronellyl Formate
32	18.40	4.97E+08	0.28	Neryl Formate
33	19.00	8.62E+09	4.79	Geranyl Formate
34	20.32	9.71E+08	0.54	Citronellyl Acetate
35	20.45	2.10E+08	0.12	Phenehyl Propionate
36	20.92	2.21E+08	0.12	α -Ylangene
37	21.09	3.38E+09	1.88	Isodauca-6,9-diene
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42	21.92	1.90E+08	0.11	α -Gurgujene
43	22.27	4.40E+09	2.44	β-Caryophyllene
44	22.54	9.07E+08	0.50	Trans- α -Bergamotene
45	22.63	2.92E+09	1.62	α -Guaiene
46	22.72	2.95E+08	0.16	Cis- β -Guaiene / α -Gurgujene
47	22.81	2.01E+10	11.15	Guaia-6,9-diene
48	22.90	5.18E+08	0.29	Carota-5,8-diene
49	23.00	1.61E+09	0.89	5-epi-Aritolochene
50	23.17	1.14E+09	0.63	α -Humulene
51	23.27	5.54E+08	0.31	allo-Aromadendrene
52	23.36	2.57E+09	1.43	Neryl butanoate
53	23.50	7.27E+08	0.40	γ -Amorphene
54	23.65	4.99E+08	0.28	α -Muurolene
55	23.71	7.01E+08	0.39	D-Germacrene
56	23.78	3.89E+08	0.22	γ -Guaiene
57	23.88	1.28E+09	0.71	α -Selinene
58	24.02	1.61E+09	0.89	α -Amorphene / α -Cadinene
59	24.10	1.55E+09	0.86	Geranyl Burytate
60	24.29	6.95E+08	0.39	γ -Cadinene
61	24.36	2.52E+09	1.40	ω -Amorphene
62	24.39	2.06E+09	1.14	Citronellyl isobutyrate
63	24.61	6.26E+08	0.35	w-Cadinene / Cubenene
64	24.67	4.25E+08	0.24	α -Cadinene
65	24.77	3.20E+08	0.18	β -Calacorene / γ -Calacorene
66	24.88	3.18E+09	1.76	Geranyl Burytate
67	25.32	1.79E+09	0.99	Unknown
68	25.36	1.67E+09	0.93	Phenylethyl tiglate
69	25.44	7.31E+08	0.41	cis-Sesquisabinene hydrate
70	25.54	1.93E+08	0.11	trans-Sesquisabinene hydrate
71	25.82	2.33E+08	0.13	1-epi-Cubenol
72	26.14	4.55E+08	0.25	Cubenol
73	26.23	1.00E+09	0.56	Citronellyl Tiglate
74	26.61	2.14E+09	1.19	Geranyl Tiglate
75	26.76	2.56E+08	0.14	Farnesol
76	26.92	9.80E+07	0.05	Nerolidyl Acetate
77	27.10	1.41E+08	0.08	Geranyl Caproate