

# 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 19 Mars 2013

**Objet:** Analyse d'une huile essentielle d'Ylang Ylang  
**Nom latin:** *Cananga odorata var. genuina, Unona odoratissima (Annoncées)*  
**Lot:** **LDB975N016**  
**Provenance:** Madagascar  
**Partie distillée:** Fleurs  
**Destinataire :** Entreprise Gedane (Lausanne, Suisse)  
**Composés majoritaires:**

Nom	N° CAS	N° CE (EINECS)	Caractéristiques
Germacrene D	37839-63-7		Non connue
$\alpha$ -Farnesene	502-61-4	242-582-0	Non connue
$\beta$ -Caryophyllene	87-44-5	201-746-1	Xi, R36

## *CONDITIONS EXPERIMENTALES*

**Type d'instrument :** 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 :** 3 min à 50°C ; Montée à 150°C en 20 min puis à 250°C en 7 min  
**Calibrant :** FC43  
**Echantillons :** Huile essentielle diluée 1:1000 dans l'éther. Injection de 1  $\mu$ L.

Figure 1 – Chromatogramme TIC-GC/MS d'huile essentielle de Ylang Ylang (YLDB975N016) analysée sur colonne capillaire FactorFour VF-5ms (5% phenyl-methyl 95% diméthylpolysiloxane, 0.25mm x 30 m). Les numéros des pics sont reportés dans la Table 1.

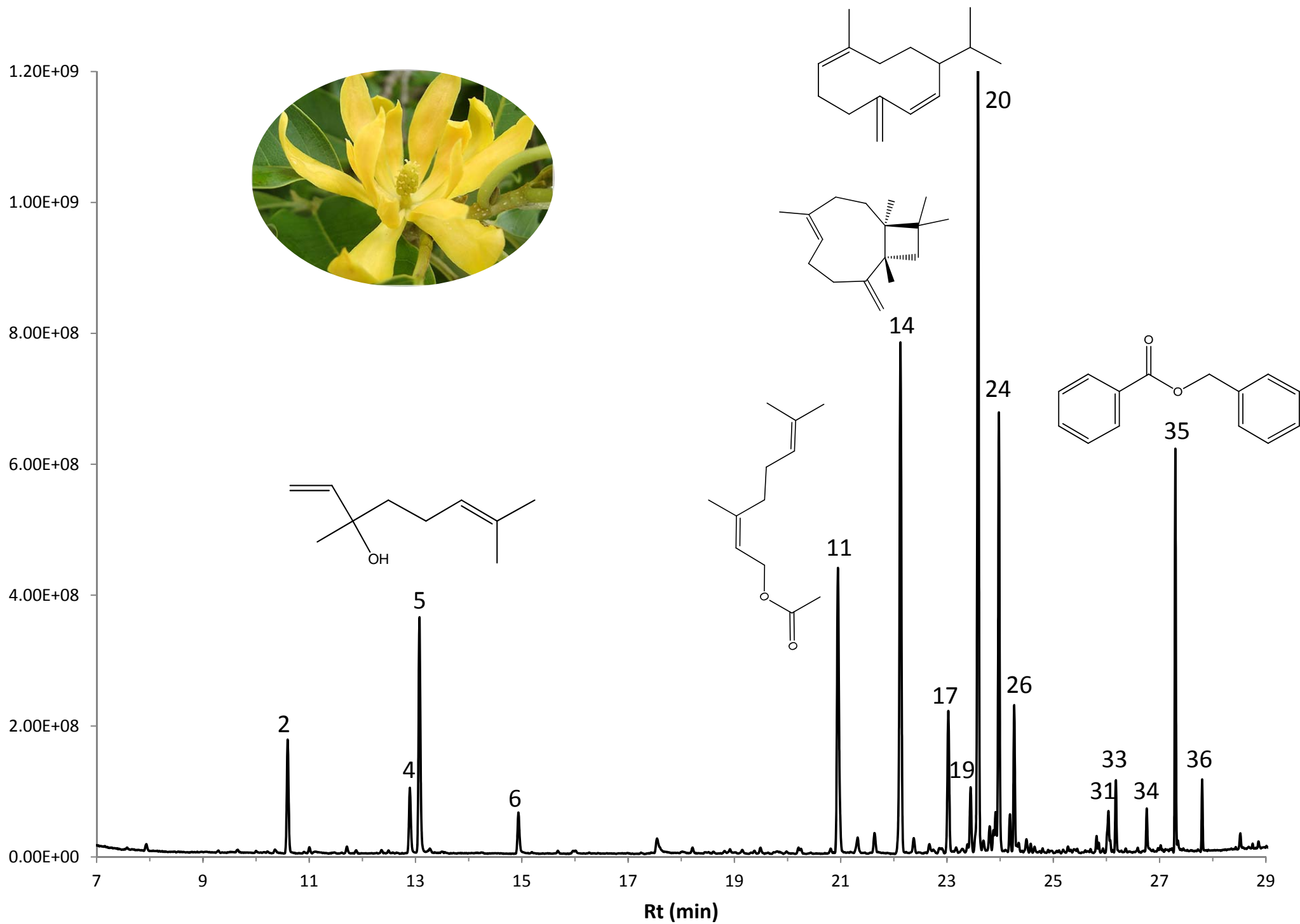


Table 1 – Composition de l'huile essentielle d'Ylang Ylang (LDB975N016)

N°	Retention Time (min.)	Area	% of Total	Identification (NIST 11 / Massfinder)	Prob (%)
1	7.94	2.44E+07	0.20	$\alpha$ -Pinene	62
2	<b>10.59</b>	<b>4.10E+08</b>	<b>3.35</b>	<b>p-Methylanisol</b>	<b>80</b>
3	11.00	2.12E+07	0.17	Eucalyptol	60
4	<b>12.89</b>	<b>2.52E+08</b>	<b>2.06</b>	<b>Methyl Benzoate</b>	<b>59</b>
5	<b>13.07</b>	<b>8.92E+08</b>	<b>7.30</b>	<b>Linalool</b>	<b>80</b>
6	<b>14.94</b>	<b>1.57E+08</b>	<b>1.28</b>	<b>Benzyl Acetate</b>	<b>83</b>
7	15.95	8.10E+06	0.07	$\alpha$ -Terpineol	20
8	16.02	1.22E+07	0.10	Estragole	56
9	17.54	8.68E+07	0.71	Geraniol	45
10	20.21	9.06E+06	0.07	$\alpha$ -Cubenene	25
11	<b>20.95</b>	<b>1.16E+09</b>	<b>9.53</b>	<b>Neryl Acetate</b>	<b>63</b>
12	21.32	6.98E+07	0.57	Cis- $\beta$ -Elemene	20
13	21.64	8.18E+07	0.67	Methyl 2,4-dichlorobenzoate	30
14	<b>22.12</b>	<b>1.96E+09</b>	<b>16.07</b>	<b><math>\beta</math>-Caryophyllene</b>	<b>75</b>
15	22.37	5.54E+07	0.45	$\beta$ -Copaene / Isogermacrene D	52/68
16	22.67	3.18E+07	0.26	Cinnamyl Acetate	61
17	<b>23.02</b>	<b>5.18E+08</b>	<b>4.24</b>	<b><math>\alpha</math>-Humulene</b>	<b>75</b>
18	23.38	2.31E+07	0.19	Cadina-1(6),4-diene trans	30
19	<b>23.44</b>	<b>2.13E+08</b>	<b>1.74</b>	<b><math>\alpha</math>-Amorphene / <math>\gamma</math>-Muurolene</b>	<b>20</b>
20	<b>23.58</b>	<b>2.63E+09</b>	<b>21.49</b>	<b>Germacrene D</b>	<b>20</b>
21	23.80	8.12E+07	0.66	$\gamma$ -Amorphene	63
22	23.87	2.59E+07	0.21	Bicyclogermacrene / Elixene	74/66
23	23.91	6.14E+07	0.50	$\alpha$ -Muurolene	57
24	<b>23.98</b>	<b>1.26E+09</b>	<b>10.31</b>	<b><math>\alpha</math>-Farnesene</b>	<b>67</b>
25	24.18	1.08E+08	0.88	$\gamma$ -Cadinene	67
26	<b>24.26</b>	<b>4.44E+08</b>	<b>3.64</b>	<b><math>\omega</math>-Cadinene / <math>\delta</math>-Cadinene</b>	<b>20</b>
27	24.49	4.90E+07	0.40	Cadina-1,4-diene	20
28	24.57	2.38E+07	0.20	$\alpha$ -Cadinene	67
29	25.85	2.68E+07	0.22	1-epi-Cubenol	15
30	25.94	1.41E+07	0.12	Cubenol	30
31	<b>26.04</b>	<b>1.48E+08</b>	<b>1.21</b>	<b><math>\tau</math>-Muurolol</b>	<b>55</b>
32	26.07	2.77E+07	0.23	$\alpha$ -Muurolol	23
33	<b>26.18</b>	<b>1.85E+08</b>	<b>1.51</b>	<b><math>\alpha</math>-Cadinol</b>	<b>60</b>
34	26.76	9.72E+07	0.80	Trans-Farnesol	25
35	<b>27.30</b>	<b>8.84E+08</b>	<b>7.24</b>	<b>Benzyl Benzoate</b>	<b>97</b>
36	<b>27.80</b>	<b>1.45E+08</b>	<b>1.19</b>	<b>Farnesol Acetate</b>	<b>40</b>
37	28.86	1.94E+07	0.16	Geranyl Benzoate	20

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