# ANALYTICAL REPORT

Venlafaxine (C17H27NO2)

1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexan-1-ol

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### Remark – other active cpd. detected none

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1974-18</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description:</td>
<td>liquid - transparent</td>
</tr>
<tr>
<td>Sample type:</td>
<td>RM-reference material</td>
</tr>
<tr>
<td>Comments:</td>
<td>CAY Lot#0534039,</td>
</tr>
<tr>
<td>Date of entry (DD/MM/YYYY):</td>
<td>03/10/2018</td>
</tr>
</tbody>
</table>

### Substance identified-structure\(^1\) (base form)

![Structure Diagram]

### Systematic name:

1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexan-1-ol

### Other names:

**Formula (per base form)**: C17H27NO2

**M_\text{w} (g/mol)**: 277.41

**Salt form**: HCl

**StdInChIKey (per base form)**: PNVNHUZROJLTJ-UHFFFAOYSA-N

### Other active cpd. detected

- **none**

### Add.info (purity..)

- **99.43%**: 1mg/ml MeOH solution

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\(^1\) Created by OPSIN free tool: [http://opsin.ch.cam.ac.uk/](http://opsin.ch.cam.ac.uk/)  DOI: 10.1021/ci100384d
Supporting information

**Analytical technique:**

<table>
<thead>
<tr>
<th>Technique</th>
<th>Applied</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 7,68 BP(1): 58; BP(2): 134, BP(3): 121,</td>
</tr>
<tr>
<td>FTIR-ATR</td>
<td>-</td>
<td>direct measurement</td>
</tr>
<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
<td>always as base form</td>
</tr>
<tr>
<td>HPLC-TOF</td>
<td>+</td>
<td>exact mass theoretical: 277,2042 / measured Δppm: 5,7</td>
</tr>
</tbody>
</table>

1. **GC-MS** (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

2. **FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4cm⁻¹

3. **GC-(MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

   GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 °C. Chromatographic separation as above (1).

   Split MS: IR = 1 : 9.

   MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

   IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

4. **HPLC-TOF** (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AIS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.
ANALYTICAL RESULTS

MS (EI)

Detailed m/z labels

Stran 3 od 5

ID 1974-18
IR- (condensed (solid) phase – after chromatographic separation) - spectrum per base form
IR- (condensed (solid) phase – after chromatographic separation) - spectrum per base form (part of spectrum enlarged)