ANALYTICAL REPORT

2C-T-7-NBOMe (C21H29NO3S)

{2-[2,5-dimethoxy-4-(propylsulfanyl)phenyl]ethyl}[(2-methoxyphenyl)methyl]amine

Remark – other active cpd. detected: none

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1336-16</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description:</td>
<td>crystalline - white</td>
</tr>
<tr>
<td>Sample type:</td>
<td>RM-reference material</td>
</tr>
<tr>
<td>Comments:</td>
<td>Lipomed Lot# 1567.1B1.1; RESPONSE -purchasing</td>
</tr>
<tr>
<td>Date of entry:</td>
<td>3/8/2016</td>
</tr>
</tbody>
</table>

Substance identified-structure\(^2\) (base form)

Systematic name:       [2-[2,5-dimethoxy-4-(propylsulfanyl)phenyl]ethyl][(2-methoxyphenyl)methyl]amine

Other names:           25T7-NB2OMe

Formula (per base form): C21H29NO3S

\(M_w\) (g/mol): 375.53

Salt form:            HCl

StdInChIKey:           CPVMNHOHOSNFOP-UHFFFAOYSA-N

Compound Class:        Phenethylamines

Other active cpd. detected: none

Add.info (purity..):   > 98.5 % (as HCL)

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\(^1\) This report has been produced with the financial support of the Prevention of and Fight against Crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

\(^2\) Created by OPSIN free tool: [http://opsin.ch.cam.ac.uk/](http://opsin.ch.cam.ac.uk/) DOI: 10.1021/ci100384d
Report updates

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
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<tbody>
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Supporting information

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
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<tbody>
<tr>
<td>GC-MS (El ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 11.89\nBP(1): 121; BP(2): 150; BP(3) :91,</td>
</tr>
<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
</tr>
<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

**GC-MS (Agilent):**
GC-method is RT locked to tetracosane (RT=9.53 min).
Injection volume 1 ml and split mode (1:50).
Injector temperature: 280 °C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
MSD source El = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min) to 550 (300) amu.

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

**GC- (MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm-1
GC-method:
Injection volume 1 ml and split mode (1:5).
Injector temperature: 280 °C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
Split MS : IR : (1:9)
MSD source El = 70 eV. GC-MS transfer line T= 235°C, source and quadropole 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 phase): IR scan range 4000 to 700, resolution 4cm-1
FIGURES OF SPECTRA

MS (EI)
Abundance

Scan 2297 [11.893 min]: 2C-T-7-NBOMe-HCl_1336-1S_LIP.D\data.ms

Scan 2373 [12.385 min]: 2C-T-7-NBOMe-HCl_1336-16_LIP-TFAden.D\data.ms

MS (EI)-TFA derivative
Abundance