## ANALYTICAL REPORT

**beta-Methylfentanyl (C23H30N2O)**

**N-phenyl-N-[1-(2-phenylpropyl)piperidin-4-yl]propanamide**

Remark – other active cpd. detected: none

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1810-17</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description:</td>
<td>powder - white</td>
</tr>
<tr>
<td>Sample type:</td>
<td>RM-reference material</td>
</tr>
<tr>
<td>Comments:</td>
<td>CAY Lot#0494309-5; RESPONSE -purchasing</td>
</tr>
<tr>
<td>Date of entry (DD/MM/YYYY):</td>
<td>13/04/2017</td>
</tr>
</tbody>
</table>

### Substance identified-structure (base form)

![Structure](attachment:image.png)

### Systematic name:
N-phenyl-N-[1-(2-phenylpropyl)piperidin-4-yl]propanamide

### Other names:
N-[3-methyl-1-(2-phenylethyl)piperidin-4-yl]-N-phenylbutanamide; 3-MBF; beta-methyl Fentanyl; β-Methylfentanyl

### Formula (per base form)
C23H30N2O

### M\text{w} (g/mol)
350,51

### Salt form:
HCl

### StdInChIKey (per base form)
UXIGUKSHASXDNIIUHFFFAOYSA-N

### Other active cpd. detected
none

### Add.info (purity..)
98%

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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
Supporting information

<table>
<thead>
<tr>
<th>Analytical 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): 10,96 BP(1): 245; BP(2): 146, BP(3): 189,</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>
</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 quadropole 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)


   MSD source EI = 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 until 6 min) amu.

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

4. HPLC-TOF for exact monoisotopic mass and empirical formula control - results are not shown in the report.
ANALYTICAL RESULTS

MS (EI)

Scan 2123 (10.955 min): Beta-methylisobuteryl_1810-17_15AY D'olata.ms
FTIR-ATR - sample as received

IR (condensed phase – after chromatographic separation)

NOTE: This is condensed phase IR (per base form of substance)
Instrument (DiscovIR-GC)