ANALYTICAL REPORT

4F-iBF (C23H29FN2O)

N-(4-fluorophenyl)-2-methyl-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide

Remark – other active cpd. detected: none

Sample ID: 1710-16
Sample description: powder - white
Sample type: RM-reference material
Comments: CAY Lot#04907532; RESPONSE -purchasing
Date of entry: 1/6/2017

Substance identified-structure (base form)

\[
\begin{align*}
\text{Systematic name:} & \quad N-(4\text{-fluorophenyl})-2\text{-methyl-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide} \\
\text{Other names:} & \quad 4\text{-FIBF; FIBF; p-FIBF; 4-Fluoroisobutyrylfentanyl; para-Fluoroisobutyryl-fentanyl} \\
\text{Formula (per base form)} & \quad \text{C23H29FN2O} \\
M_w (g/mol) & \quad 368,5 \\
\text{Salt form:} & \quad \text{HCl} \\
\text{StdInChIKey (for base form)} & \quad \text{OZDOSQNUJXEOR-UHFFAOYSA-N} \\
\text{Other active cpd. detected} & \quad \text{none} \\
\text{Add.info (purity..)} & \quad 98\%
\end{align*}
\]

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/ DOI: 10.1021/ci100384d
Report updates

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
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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 (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 10,75 BP(1): 277; BP(2): 207, BP(3): 164,</td>
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<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
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<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
<td>always as base form</td>
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</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 4 cm⁻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 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.

   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)

Abundance

Scn 2031 (10.749min): FIEF+HCl_1710-16_CAY ara Data ms

m/z ->
FTIR-ATR - direct measurement (sample as received)

IR (condensed phase – after chromatographic separation)