**ANALYTICAL REPORT**

*Methacrylfentanyl (C23H28N2O2)*

**2-methyl-N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]prop-2-enamide**

Remark – other active cpd. detected: none

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1896-17</th>
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<tbody>
<tr>
<td>Sample description:</td>
<td>powder - white</td>
</tr>
<tr>
<td>Sample type:</td>
<td>RM-reference material</td>
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<tr>
<td>Comments:</td>
<td>CAY Lot#0515141-3,</td>
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<tr>
<td>Date of entry (DD/MM/YYYY):</td>
<td>07/12/2017</td>
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**Systematic name:** 2-methyl-N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]prop-2-enamide

**Other names:** Methacrylic fentanyl; Methacrylic-F; N-(1-phenethylpiperidin-4-yl)-N-phenylmethacrylamide

**Formula (per base form):** C23H28N2O2

**M_w (g/mol):** 348,49

**Salt form:** base

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

**Other active cpd. detected:** none

**Add.info (purity..):** 100 %

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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
Report updates

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

Analytical technique: | applied remarks
---|---
GC-MS (EI ionization) | NFL GC-RT (min): 11,32 BP(1): 257; BP(2): 69,BP(3):214,

FTIR-ATR | direct measurement
GC-IR (condensed phase) | always as base form
HPLC-TOF | exact monoisotopic mass: 348,2202
\[\Delta ppn \text{ (difference from calculated): -1.22}\]

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 thickens 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
ANALYTICAL RESULTS

MS (EI)

Abundance

Scan 2186 (11.315 min): Methacrylfentanyl_1896-17_CAY.D\data.ms

m/z -->

69.0
105.1
158.1
186.1
214.1
257.2
279.1
316.2
FTIR-ATR - sample as received

IR (condensed phase – after chromatographic separation)

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