

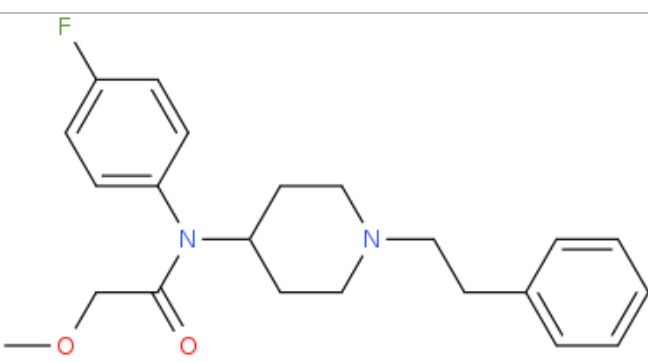
## ANALYTICAL REPORT

4-Fluoro Methoxyacetyl fentanyl (C<sub>22</sub>H<sub>27</sub>FN<sub>2</sub>O<sub>2</sub>)

## N-(4-fluorophenyl)-2-methoxy-N-[1-(2-phenylethyl)piperidin-4-yl]acetamide

Remark – other active cpd. detected: none

|                             |                       |
|-----------------------------|-----------------------|
| Sample ID:                  | 1846-17               |
| Sample description:         | powder - white        |
| Sample type:                | RM-reference material |
| Comments:                   | CAY Lot#0503688-6,    |
| Date of entry (DD/MM/YYYY): | 18/08/2017            |

|   |   |
|---|---|
| Substance identified-structure <sup>1</sup> (base form) |  |
| Systematic name:  | N-(4-fluorophenyl)-2-methoxy-N-[1-(2-phenylethyl)piperidin-4-yl]acetamide           |
| Other names:  | para-fluoro Methoxyacetyl fentanyl; 4F-Methoxyacetyl fentanyl                       |
| Formula (per base form)                                 | C <sub>22</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>2</sub>                      |
| M <sub>w</sub> (g/mol)                                  | 370,47  |
| Salt form:  | HCl   |
| StdInChIKey (per base form)                             | KDXSBALZECTNCT-UHFFFAOYSA-N   |
| Other active cpd. detected                              | none  |
| Add.info (purity..)                                     | 100,0%  |

<sup>1</sup> Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d



## Report updates

| date | comments (explanation) |
|------|------------------------|
|      |                        |
|      |                        |
|      |                        |
|      |                        |

## Supporting information

| Analytical technique:   | applied | remarks  |
|-------------------------|---------|--|
| GC-MS (EI ionization)   | +       | NFL GC-RT (min): 11,49 BP(1): 279; BP(2): 105,BP(3) :96, |
| FTIR-ATR                | +       | direct measurement                                       |
| GC-IR (condensed phase) | +       | always as base form                                      |

**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<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**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 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 (solid) phase): IR scan range 4000 to 650, resolution 4 cm<sup>-1</sup>.

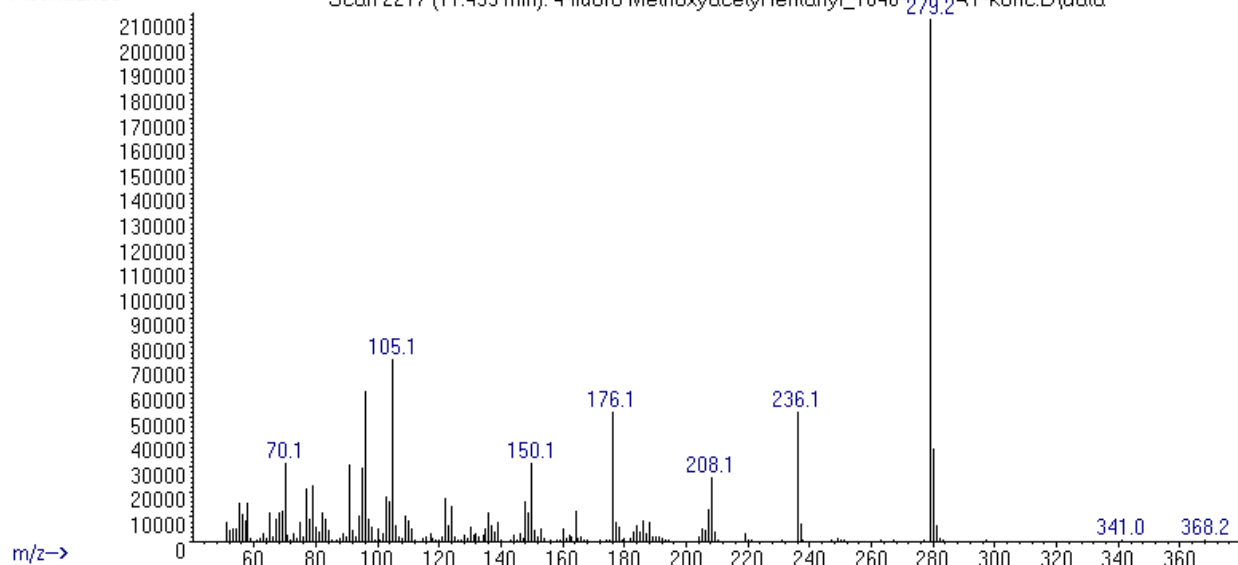
4. HPLC-TOF for exact monoisotopic mass and empirical formula control - results are not shown in the report.

# ANALYTICAL RESULTS

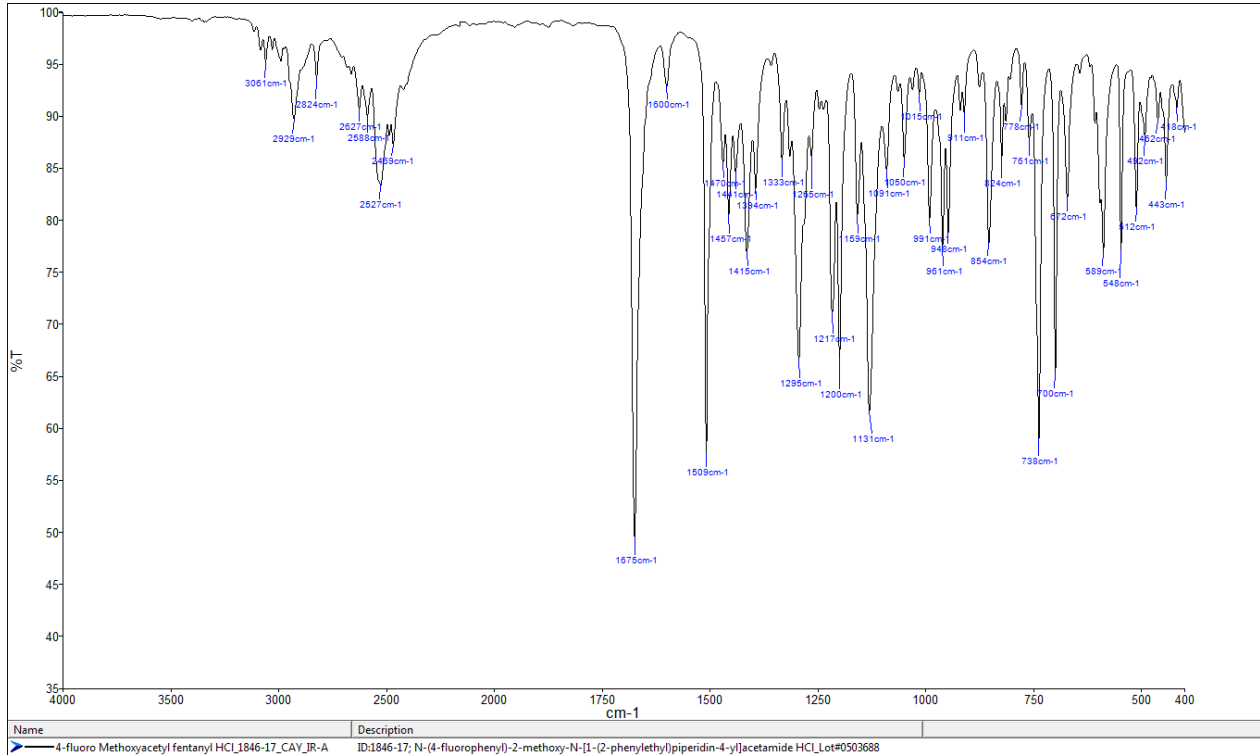
MS (EI)

Abundance

Scan 2217 (11.493 min): 4-fluoro Methoxyacetyl fentanyl\_1846-17\_CAY-konc.D\data



### FTIR-ATR - sample as received



### IR (condensed phase – after chromatographic separation)

