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S podporo skladov Evropske unije
na področju notranjih zadev

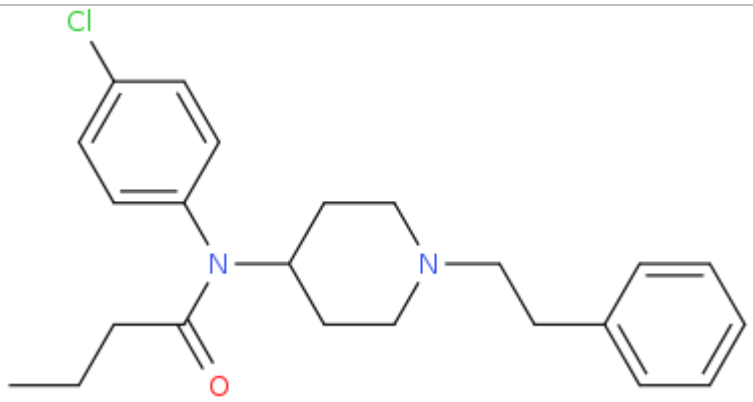
# ANALYTICAL REPORT

## 4Cl-butyryl fentanyl (C23H29ClN2O)

**N-(4-chlorophenyl)-N-[1-(2-phenylethyl)piperidin-4-yl]butanamide**

Remark – other active cpd. detected: none

| | |
|---|---|
| Sample ID: | 1876-17 |
| Sample description: | powder - white |
| Sample type: | RM-reference material |
| Comments: | CAY Lot#0512747-2, |
| Date of entry (DD/MM/YYYY): | 10/11/2017 |

| | |
|---|---|
| Substance identified-structure[1] (base form) |  |
| Systematic name: | N-(4-chlorophenyl)-N-[1-(2-phenylethyl)piperidin-4-yl]butanamide |
| Other names: | para-Chlorobutyryl fentanyl; N-(4-chlorophenyl)-N-[1-(2-phenylethyl)-4-piperidinyl]-butanamide |
| Formula (per base form) | C23H29ClN2O |
| $M_w$ (g/mol) | 384,95 |
| Salt form: | HCl |
| StdInChIKey (per base form) | YRAMWTYYYLTADR-UHFFFAOYSA-N |
| Other active cpd. detected | none |
| Add.info (purity..) | 100 % |

[1] 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): 12,84 BP(1): 293; BP(2): 180,BP(3) :223, |
| FTIR-ATR | + | direct measurement |
| GC-IR (condensed phase) | + | always as base form |
| HPLC-TOF | + | exact monoisotopic mass: 384,1968<br>Δppm (difference from calculated): -2,24 |

**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 0C. 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 $^0$C for 1 min, followed by heating up to 190 $^0$C at rate 8 $^0$C/min, then heating up to 293 0C at a rate of 18 $^0$C/min, hold for 7.1 min, then heating at 50 $^0$C/min up to 325 $^0$C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235$^0$C, source and quadropole temperatures 280$^0$C and 180$^0$C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

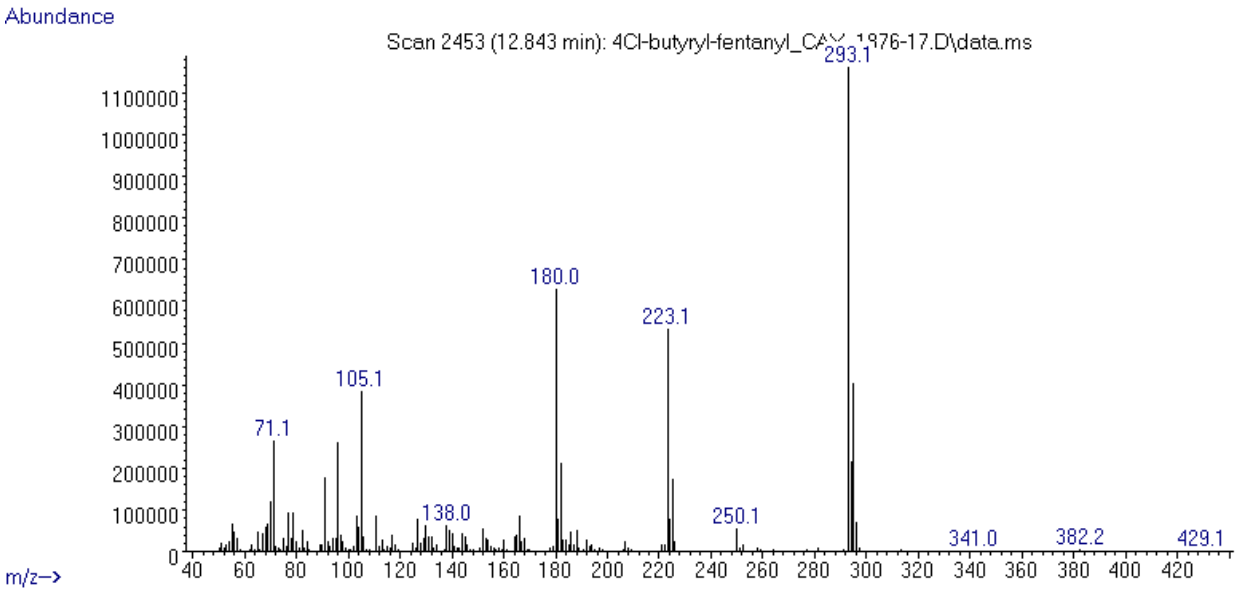
**2. FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm$^{-1}$; resolution 4cm$^{-1}$

**3. GC- (MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 $^0$C. Chromatographic separation as above **(1).**
Split MS : IR = 1 : 9.
MSD source EI = 70 eV. GC-MS transfer line T= 235$^0$C, source and quadropole temperatures 280$^0$C and 180$^0$C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.
IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm$^{-1}$.

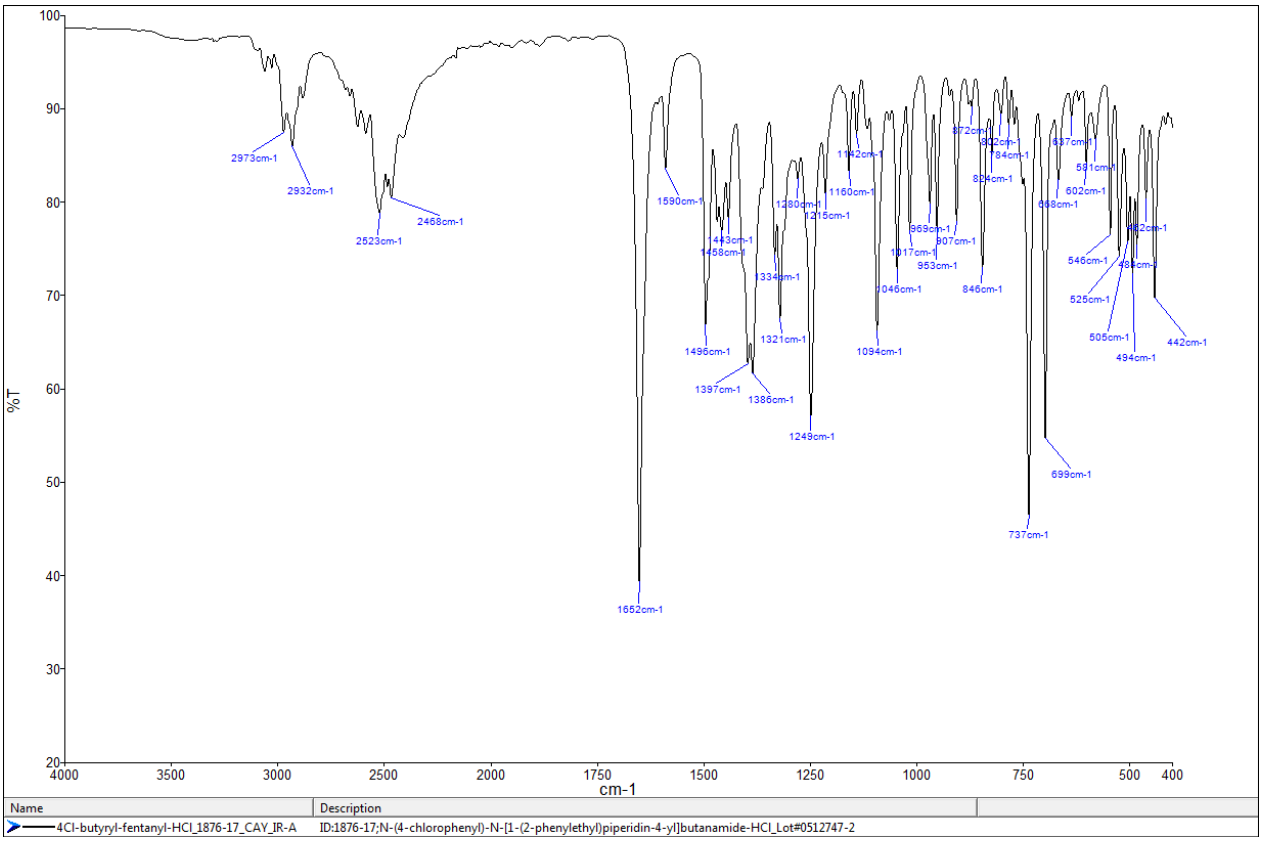
4. HPLC-TOF for exact monoisotopic mass and empirical formula control

## ANALYTICAL RESULTS

MS (EI)



FTIR-ATR - sample as received




IR (condensed phase – after chromatographic separation)