

SLOVENIJA



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#### ANALYTICAL REPORT

### 3-Methylbutyrylfentanyl (C24H32N2O)

#### N-[(3R,4S)-3-methyl-1-(2-phenylethyl)piperidin-4-yl]-N-phenylbutanamide

Remark – other active cpd. detected: none

Sample ID:	1809-17		
Sample description:	powder - white		
Sample type:	RM-reference material		
Comments <sup>1</sup> :	CAY Lot#0496754-4; RESPONSE -purchasing		
Date of entry (DD/MM/YYYY):	13/04/2017		

Substance identified- structure <sup>2</sup> (base form)	N IIIIII			
Systematic name:	N-[(3R,4S)-3-methyl-1-(2-phenylethyl)piperidin-4-yl]-N-phenylbutanamide			
Other names:	N-[3-methyl-1-(2-phenylethyl)piperidin-4-yl]-N-phenylbutanamide (stereochemistry not defined);			
Formula (per base form)	C24H32N2O			
M <sub>w</sub> (g/mol)	364,53			
Salt form:	HCI			
StdInChIKey (per base form)	ZPAOSKLOFZWBLS-UHFFFAOYSA-N			
Other active cpd. detected	none			
Add.info (purity)	98%			

<sup>&</sup>lt;sup>1</sup> 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.

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<sup>&</sup>lt;sup>2</sup> Created by OPSIN free tool: <a href="http://opsin.ch.cam.ac.uk/">http://opsin.ch.cam.ac.uk/</a> **DOI:** 10.1021/ci100384d

## Report updates

date	comments (explanation)

## Supporting information

Analytical technique:	applied	remarks
GC-MS (El ionization)	+	NFL GC-RT (min): 11,86 BP(1): 273; BP(2): 160,BP(3):105,
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 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25  $\mu$ m. 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 0C 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  $^{\circ}$ C. Chromatographic separation as above (1). Split MS: IR = 1:9.

MSD source EI = 70 eV. GC-MS transfer line T=  $235^{\circ}$ C, source and quadropole temperatures  $280^{\circ}$ C and  $180^{\circ}$ C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

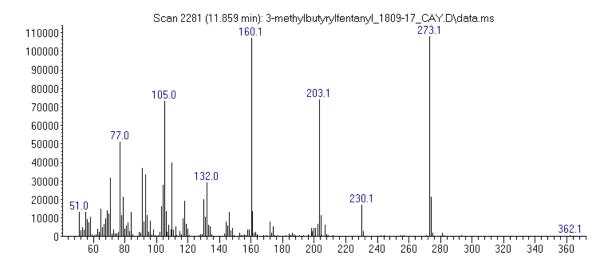
IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm<sup>-1</sup>.

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

#### **ANALYTICAL RESULTS**

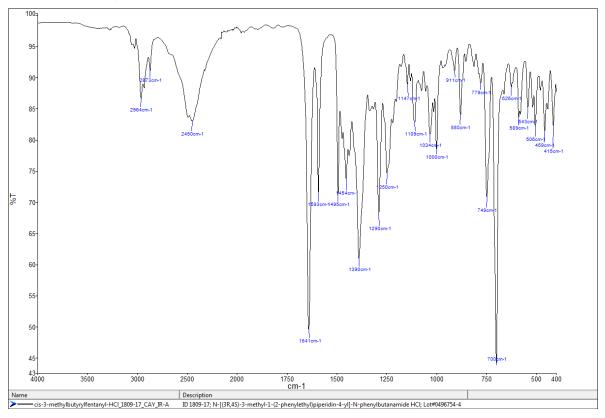
# MS (EI)

#### Abundance



m/z->

# FTIR-ATR - sample as received



# IR (condensed phase – after chromatographic separation)

