



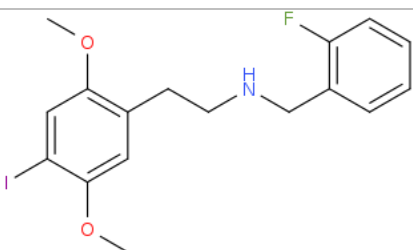
## ANALYTICAL REPORT

### 25I-NBF (C17H19FINO2)

#### N-(2-fluorobenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine, monohydrochloride

Remark – other active cpd. detected: possibly trace of 25-NBF

Sample ID:	1376-16
Sample description:	crystalline - brownish
Sample type:	RM-reference material
Comments <sup>1</sup> :	Cayman #0474616; RESPONSE -purchasing
Date of entry:	3/4/2015

Substance identified- structure <sup>2</sup> (base form)	
Systematic name:	N-(2-fluorobenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine, monohydrochloride
Other names:	25I-NB2F, 2C-I-NBF, NBF-2C-I, Cimbi-21
Formula (per base form)	C17H19FINO2
M <sub>w</sub> (g/mol)	415.24
Salt form:	HCl
StdInChIKey	LPBKNBHMWRBPHT-UHFFFAOYSA-N
Compound Class	Phenethylamines
Other active cpd. detected	(by HPLC-TOF impurity (most probably 25-NBF) was detected cca 1%)
Add.info (purity..)	>98 %

<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.

<sup>2</sup> Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

## Report updates

date	comments (explanation)
13 April 2018	compound class corrected

## Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 10.13 BP(1): 109; BP(2): 138,BP(3) :278,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	

### GC-MS (Agilent):

GC-method is RT locked to tetracosane (RT=9.53 min).

Injection volume 1 ml and split mode (1:50) .

Injector temperature: 280 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 2.8 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) amu.

**FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**GC- (MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

GC-method:

Injection volume 1 ml and split mode (1:5) .

Injector temperature: 280 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

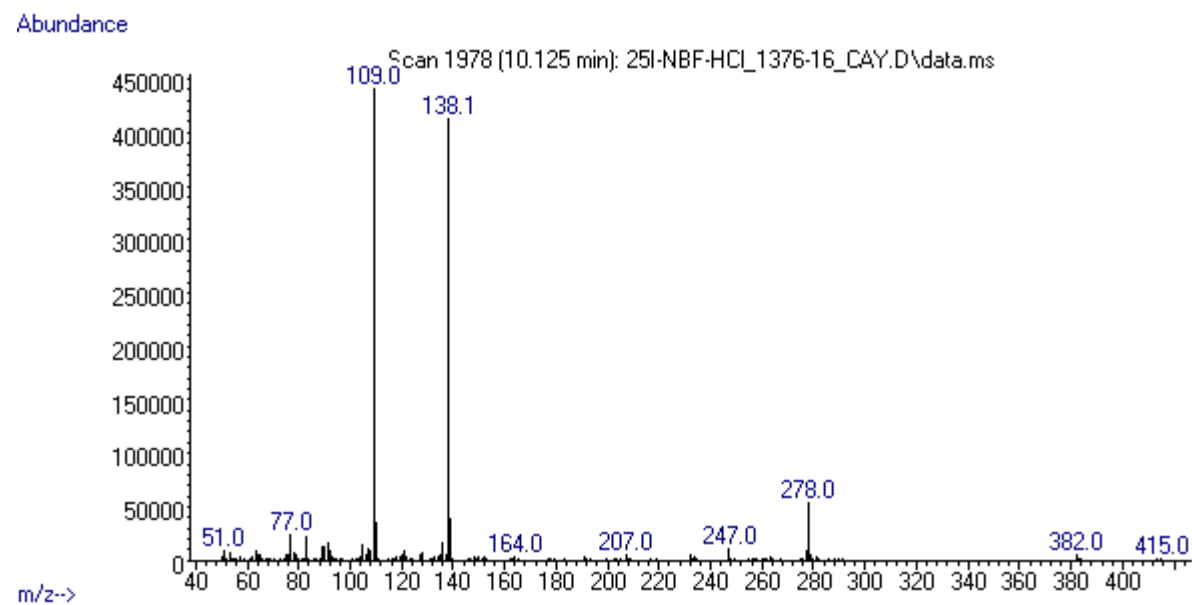
Split MS : IR : (1:9)

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) amu.

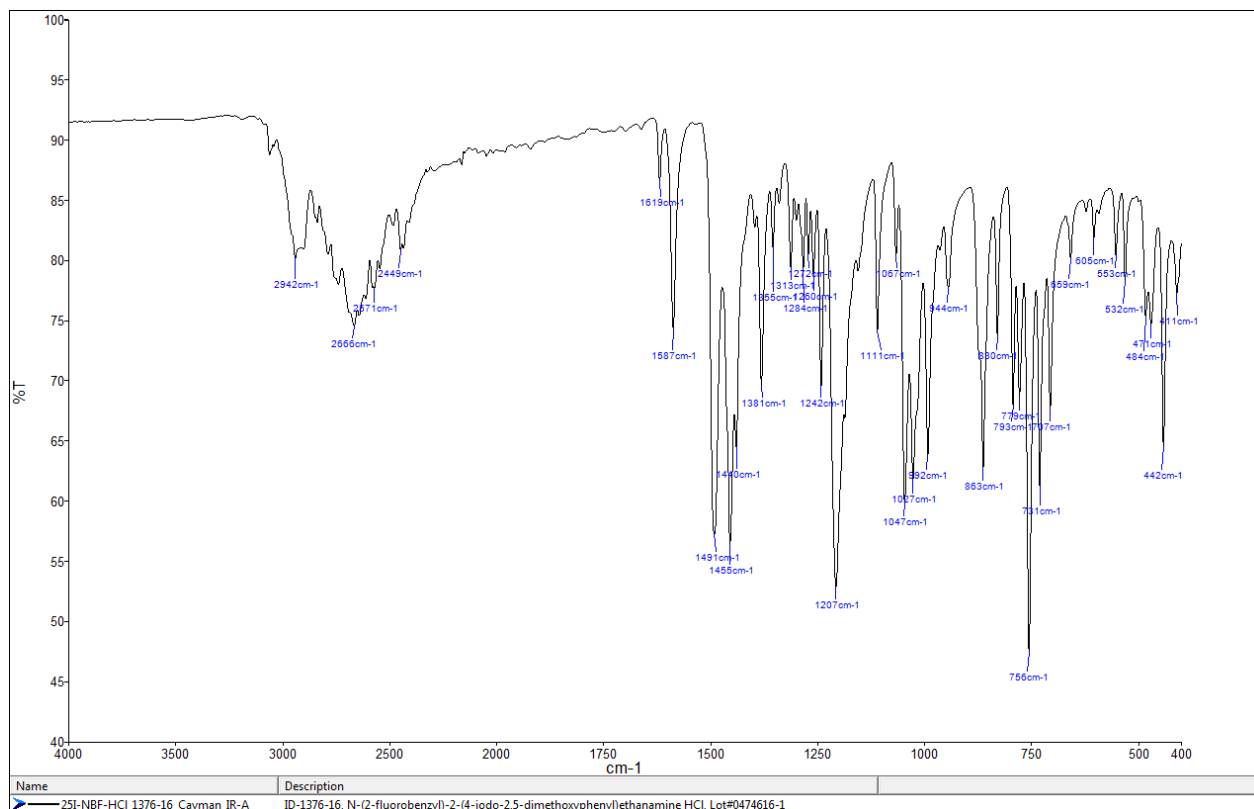
IR (condensed phase): IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

# FIGURES OF SPECTRA

MS (EI)



# FTIR-ATR



# IR-Condensed phase

