



## ANALYTICAL REPORT

4F-PV8

### Acknowledgement

**Analytically evaluated sample was kindly provided by the Forensic Science Institute (FSI) Zurich, Switzerland. NMR analyses were performed in Dr. Stefan Höck, ZHAW Wädenswil Institute of Chemistry and Biological Chemistry and are enclosed in this report by the permission of Dr. Michael Bovens.**

MS and FTIR measurements shown in this report were done in NFL.

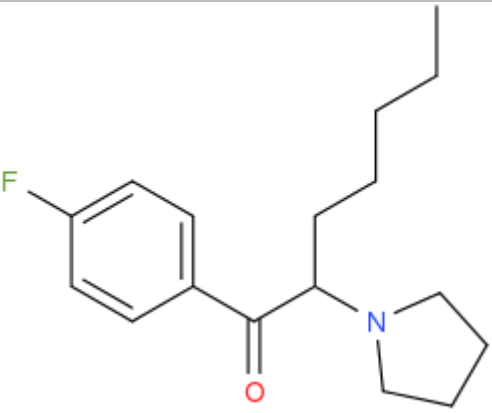
# ANALYTICAL REPORT

## 4F-PV8 (C17H24FNO)

### 1-(4-fluorophenyl)-2-(pyrrolidin-1-yl)heptan-1-one

Remark – other active cpd. detected: **none**

Sample ID:	1432-16
Sample description:	powder - white-pale
Sample type:	collected/Kindly provided by Forensic Science Institute Zurich, Switzerland (NMR confirmed);
Comments <sup>1</sup> :	
Date of entry:	1/15/2016

Substance identified-structure <sup>2</sup> (base form)	
Systematic name:	1-(4-fluorophenyl)-2-(pyrrolidin-1-yl)heptan-1-one
Other names:	
Formula (per base form)	C17H24FNO
M <sub>w</sub> (g/mol)	277,38
Salt form:	HCl
StdInChIKey	YAFFHHPPQAYLLA-UHFFFAOYSA-N
Compound Class	Cathinones
Other active cpd. detected	none
Add.info (purity..)	app. 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)
08/12/2016	Compound class changed.

## Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 6,65 BP(1): 154; BP(2): 155,BP(3) :95,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	spectrum consistent by the one from FSI Zurich (QM>0.99)

### 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 quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 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)

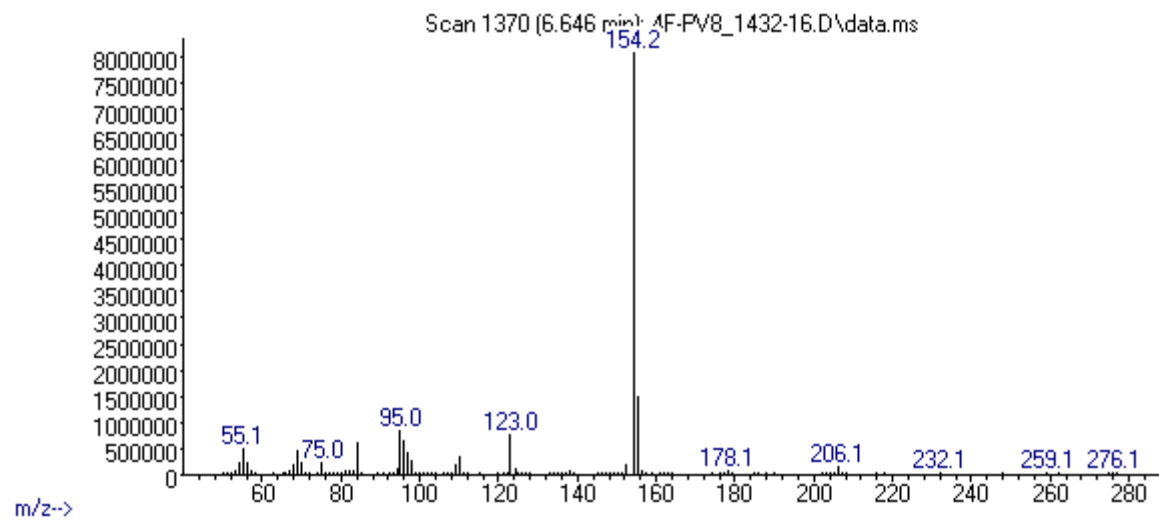
MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

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

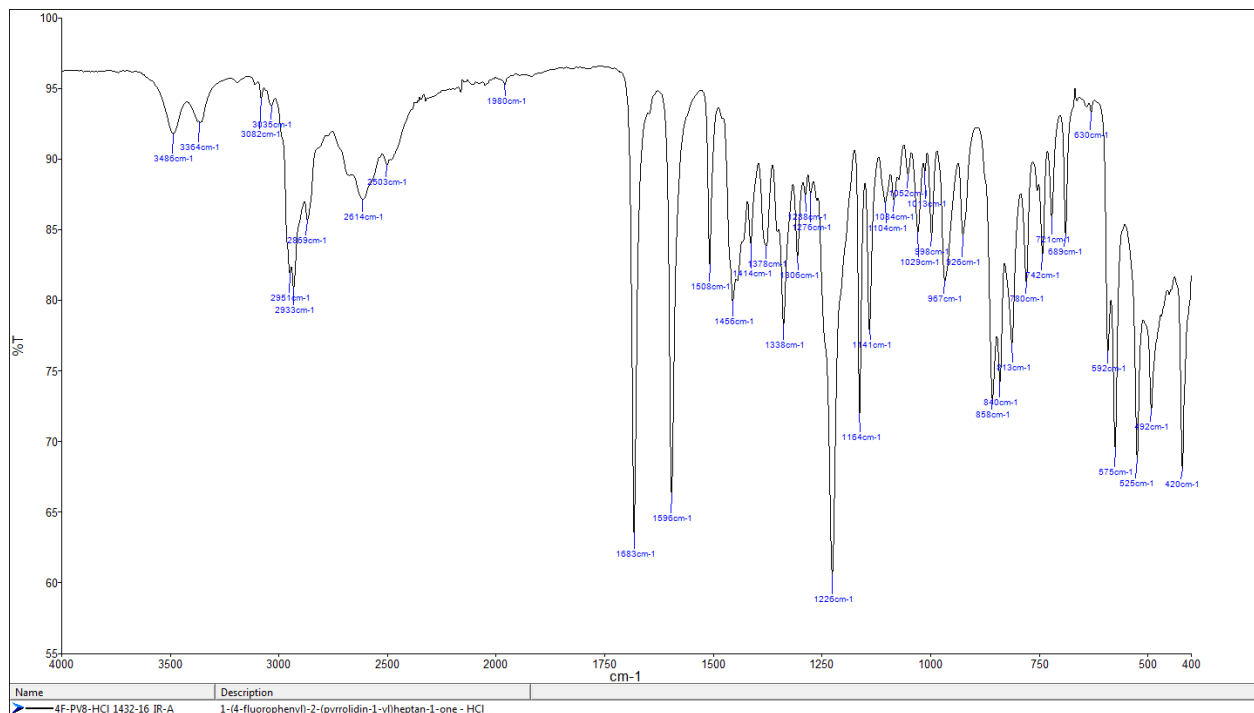
# FIGURES OF SPECTRA

MS (EI)

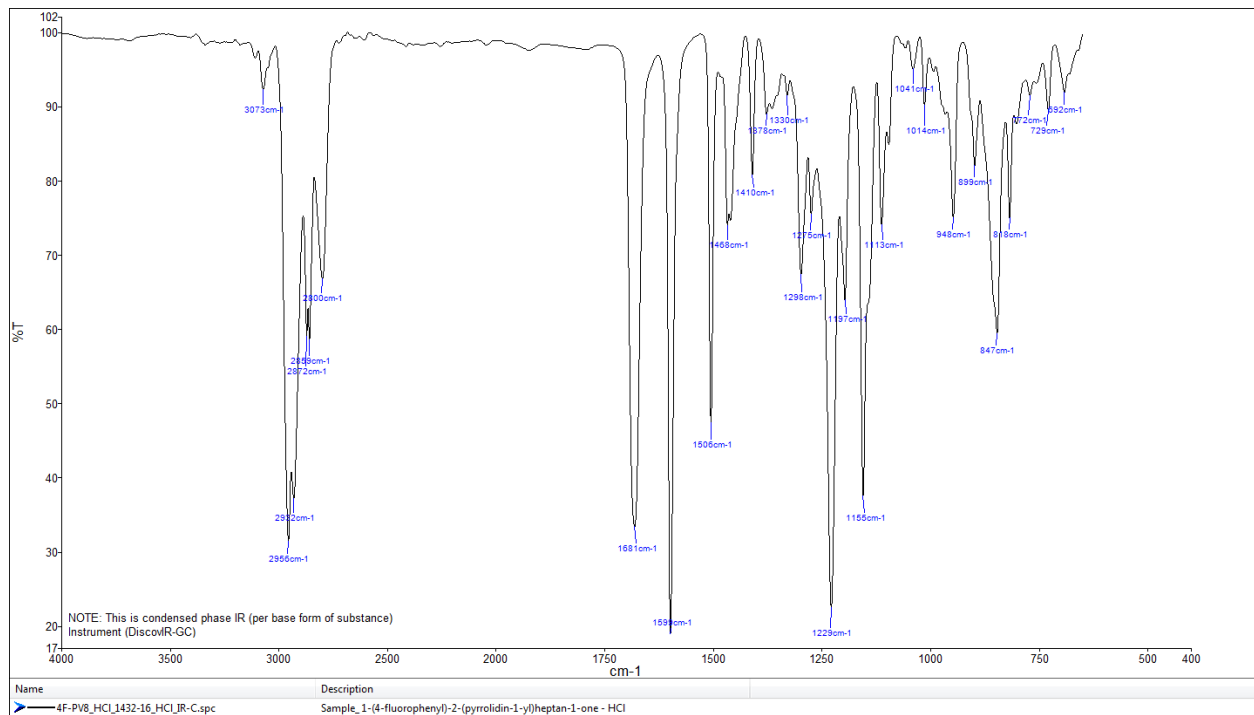
Abundance

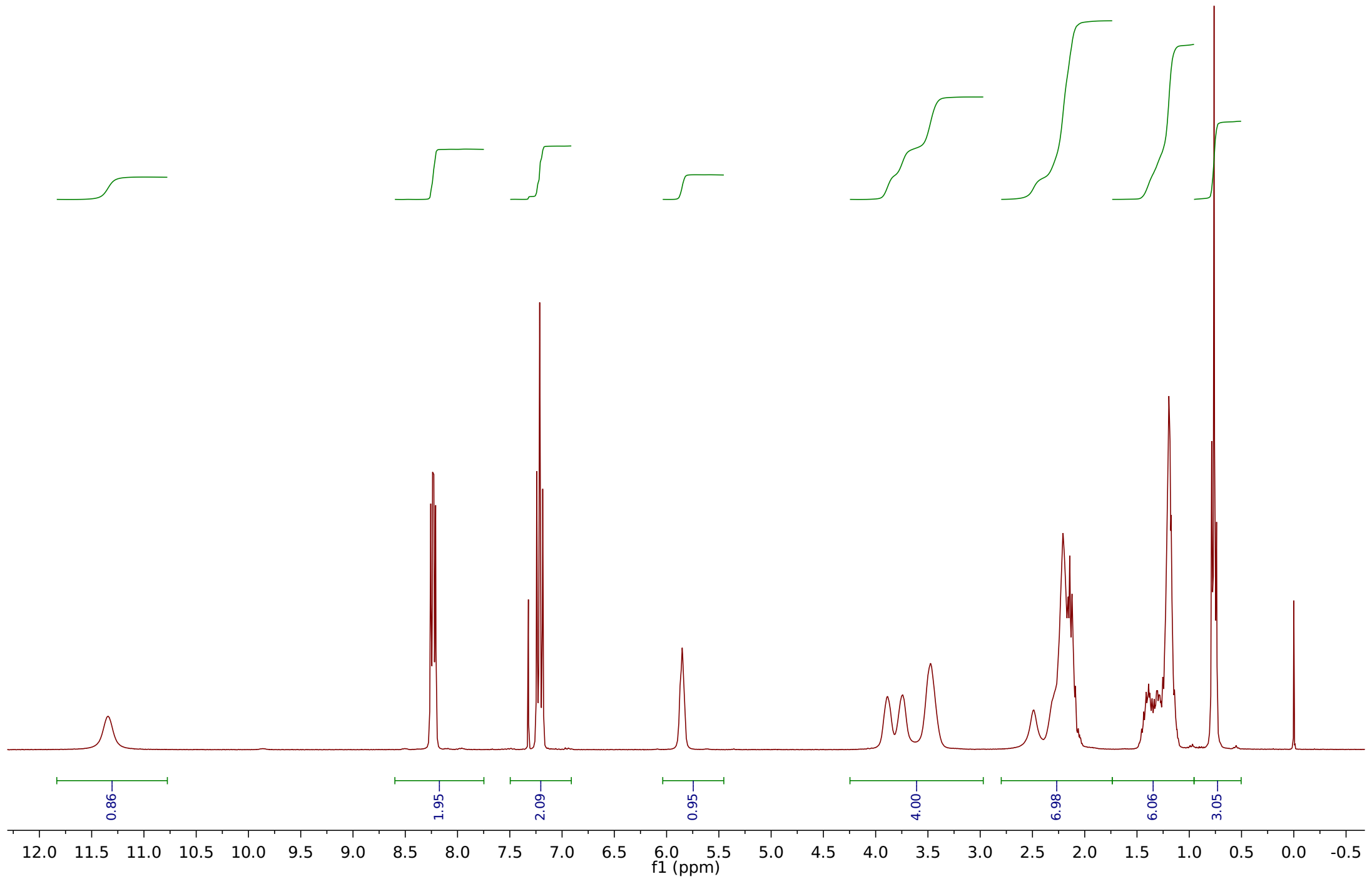


## FTIR-ATR



## IR-Condensed phase





4F-PV8.11.fid  
C13DEPT135 CDCl3 D:\\ hoeck 40

