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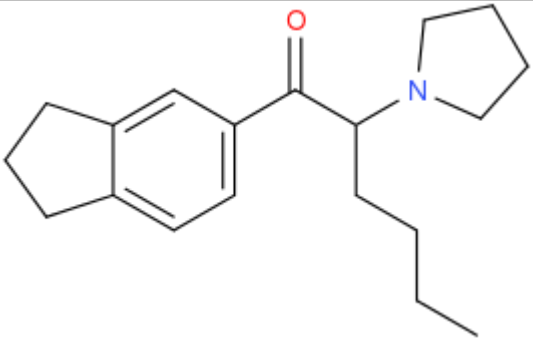
ANALYTICAL REPORT

5-BPDi, (C19H27NO)

1-(2,3-dihydro-1H-inden-5-yl)-2-(pyrrolidin-1-yl)hexan-1-one

Remark – other NPS detected: none

Sample ID:	1183-15
Sample description:	powder - off white
Sample type:	P- purchased
Date of entry:	7/11/2015

Substance identified-structure[i] (base form)	
Systematic name	1-(2,3-dihydro-1H-inden-5-yl)-2-(pyrrolidin-1-yl)hexan-1-one
Other names	
Formula (per base form)	C19H27NO
M_w (g/mol)	285,42
Salt form	HCl
Smiles	C1CCC2=CC(=CC=C12)C(C(CCCC)N1CCCC1)=O
Compound Class	Cathinones
Other NPS detected	none
Add.info (purity..)	pure

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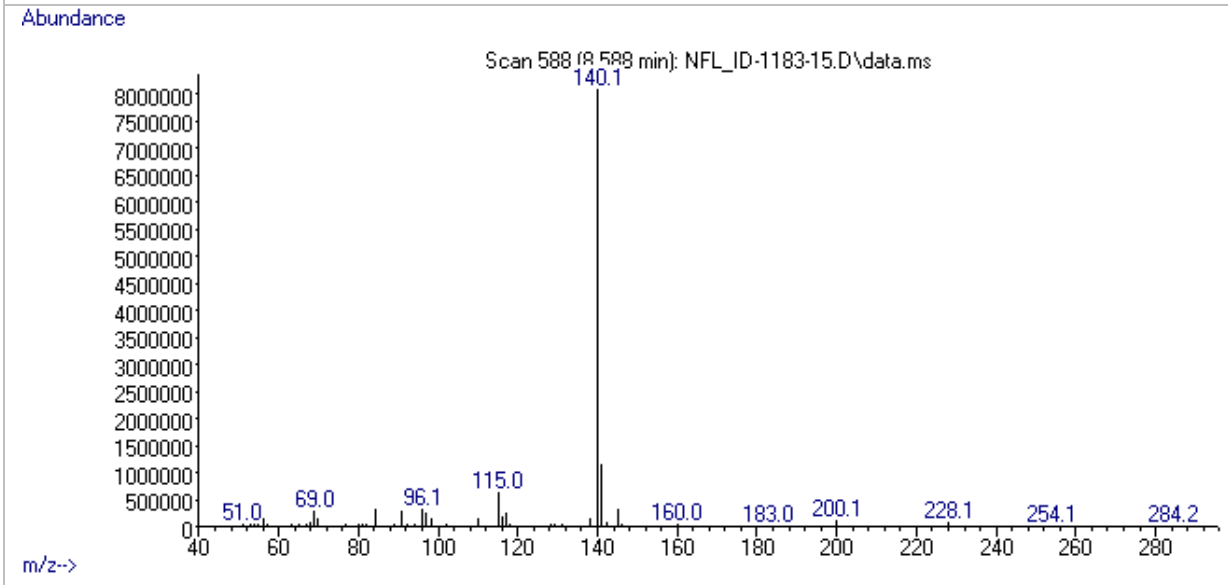
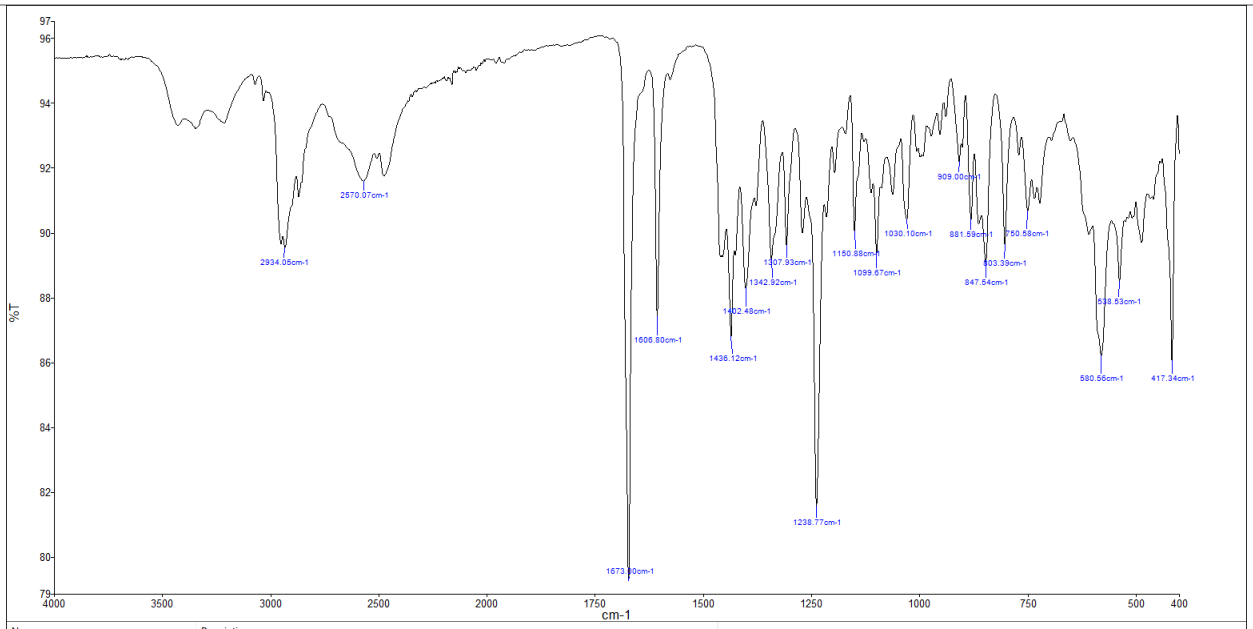
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 140; BP(2): 115,BP(3) :96,
FTIR-ATR	+	HCl
FTIR (condensed phase)	/	
HPLC-TOF	+	Exact mass: 285,2093, measured/ Δppm:-0,59; formula:C19H27NO
NMR-confirmed	+	
validation		
other		

MS spectrum (EI)



FTIR - ATR



[i] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

Target Compound Screening Report

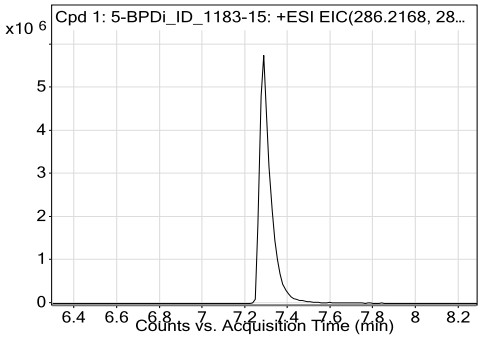
Data File	5-BPDi_1183-15_TOF.d	**Sample Name**	5-BPDi
Sample Type	Sample	**Position**	P1-E4
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-13-5-2015-XDB-C18-ESI-poz.m	**Acquired Time**	6/8/2015 10:26:43 AM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment	extract in MeOH		

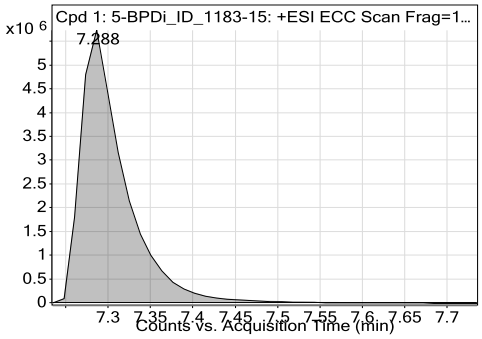
Compound Table

Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 1: 5-BPDi_ID_1183-15	5-BPDi_ID_1183-15	C19 H27 N O	C19 H27 N O	7.288	285.2094

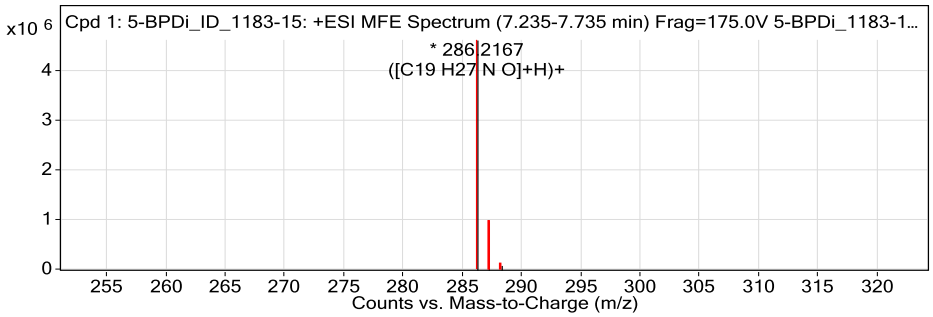
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpds Algorith
5-BPDi_ID_1183-15	286.2167	7.288	285.2094	7.288	C19 H27 N O	285.2093	-0.59	C19 H27 N O	Find by Molecular Feature

Compound Chromatograms

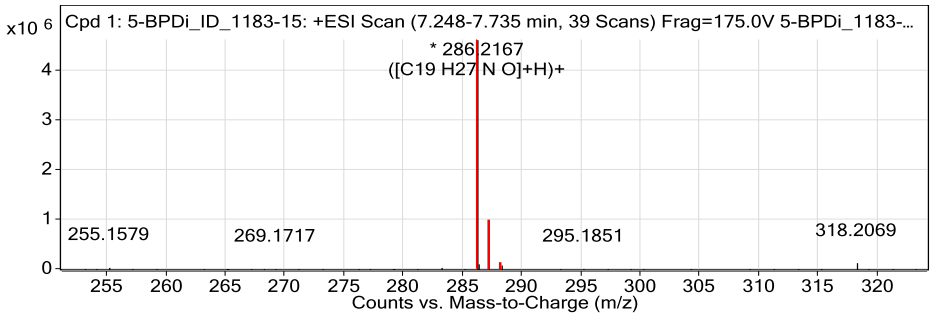




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
286.2167	1	4615733	C19 H27 N O	(M+H)+
287.2202	1	967276.57	C19 H27 N O	(M+H)+
288.223	1	100377.71	C19 H27 N O	(M+H)+
289.2248	1	8628.46	C19 H27 N O	(M+H)+

--- End Of Report ---

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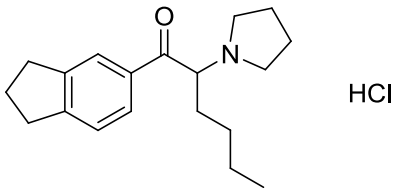
REPORT

Sample ID:	**1183-15**
Our notebook code:	P-1183-15
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^1H, ^{13}C, ^1H–^1H *gs*-COSY, ^1H–^{13}C *gs*-HSQC, ^1H–^{13}C *gs*-HMBC, ^1H–^{15}N *gs*-HMBC.
Proposed structure with chemical name:	 HCl 1-(2,3-dihydro-1*H*-inden-5-yl)-2-(pyrrolidin-1-yl)hexan-1-one hydrochloride
Comments:	- Structure elucidation based on 1D and 2D NMR spectra - Compound is pure by NMR
Supporting information:	Copies of ^1H and ^{13}C NMR spectra
Author:	Prof. Dr. Janez Košmrlj
Date of report:	July 11, 2015

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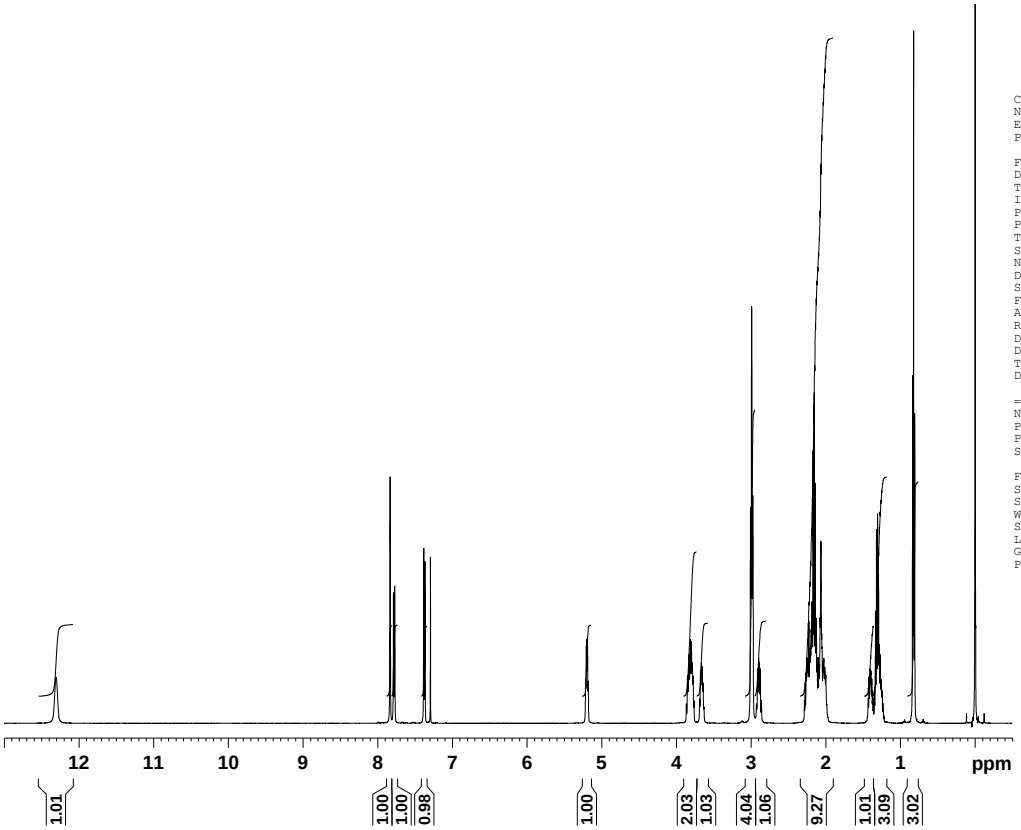


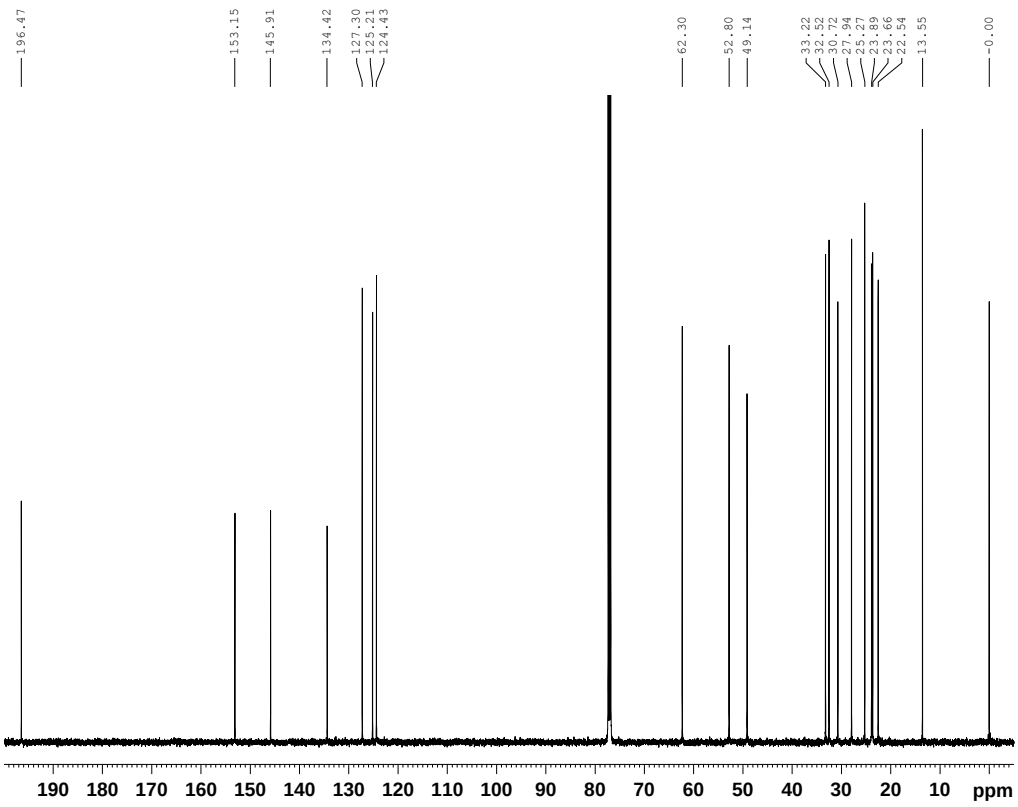
Current Data Parameters
NAME 1183-15
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150706
Time 22.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
PLW1 26.00000000 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 65536
SF 500.1299961 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P-1183-15



Current Data Parameters
NAME 1183-15
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150707
Time 1.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PLW1 122.00000000 W
SFO1 125.7703637 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 26.00000000 W
PLW12 0.32179001 W
PLW13 0.20595001 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577879 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40