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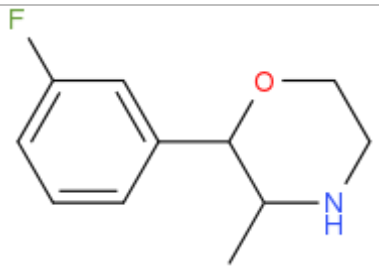
ANALYTICAL REPORT

3F-phenmetrazine (crystal), (C11H14FNO)

2-(3-fluorophenyl)-3-methylmorpholine

Remark – other NPS detected: none

Sample ID:	1173-15
Sample description:	crystal - white
Sample type:	P- purchased
Date of entry:	5/13/2015

Substance identified-structure[i] (base form)	 *HCl
Systematic name	2-(3-fluorophenyl)-3-methylmorpholine
Other names	3-FMP
Formula (per base form)	C11H14FNO
M_w (g/mol)	195,23
Salt form	HCl
Smiles	FC=1C=C(C=CC1)C1OCCNC1C
Compound Class	Others
Other NPS detected	none
Add.info (purity..)	pure

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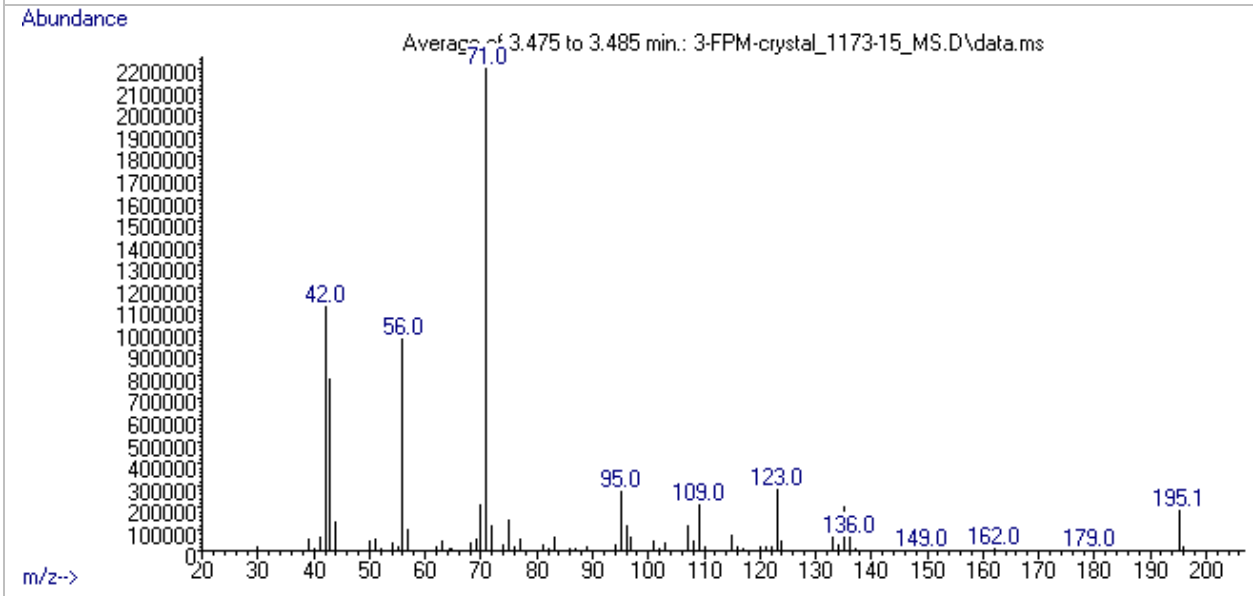
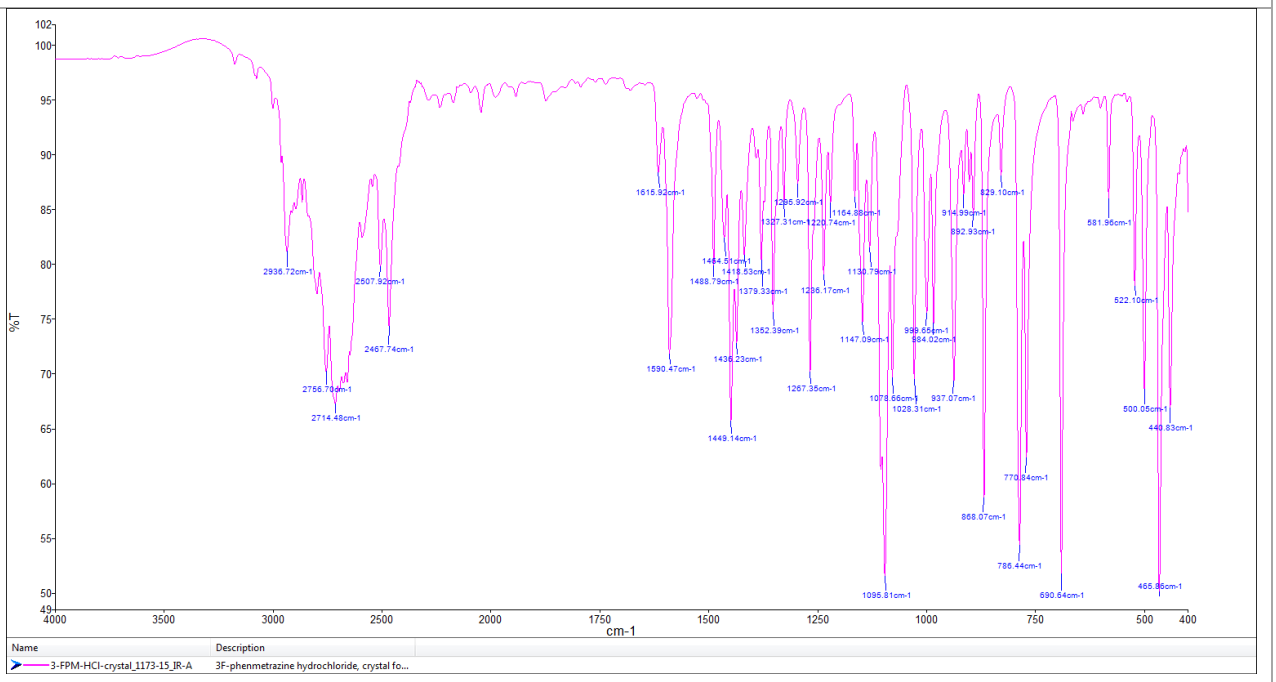
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 71; BP(2): 42,BP(3) :56,
FTIR-ATR	+	HCl
FTIR (condensed phase)	/	pending
HPLC-TOF	+	Exact mass: 195,1059, measured/ Δppm:-3,76; formula:C11H14FNO
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

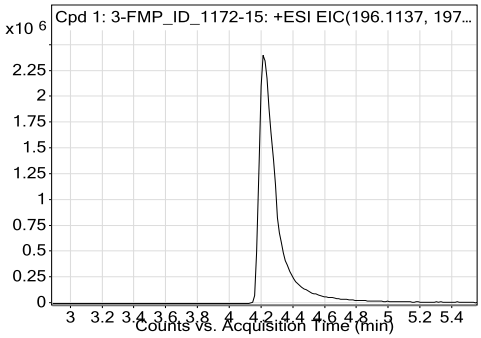
Data File	3-FPM-crystal_ID_1173-15-TOF.d	**Sample Name**	3-FPM
Sample Type	Sample	**Position**	P1-F6
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-2-4-2015-XDB-C18-ESI-poz.m	**Acquired Time**	4/10/2015 9:48:57 AM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment	crystal form, extract in MeOH		

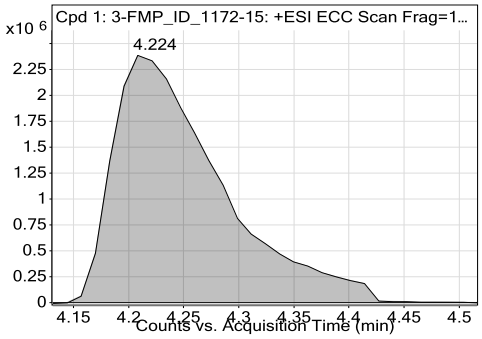
Compound Table

Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 1: 3-FMP_ID_1172-15	3-FMP_ID_1172-15	C11 H14 F N O	C11 H14 F N O	4.224	195.1065

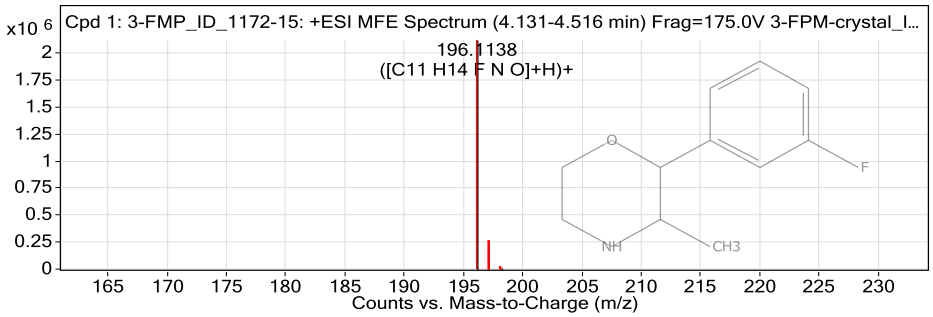
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpds Algorith
3-FMP_ID_1172-15	196.1138	4.224	195.1065	4.211	C11 H14 F N O	195.1059	-2.96	C11 H14 F N O	Find by Molecular Feature

Compound Chromatograms

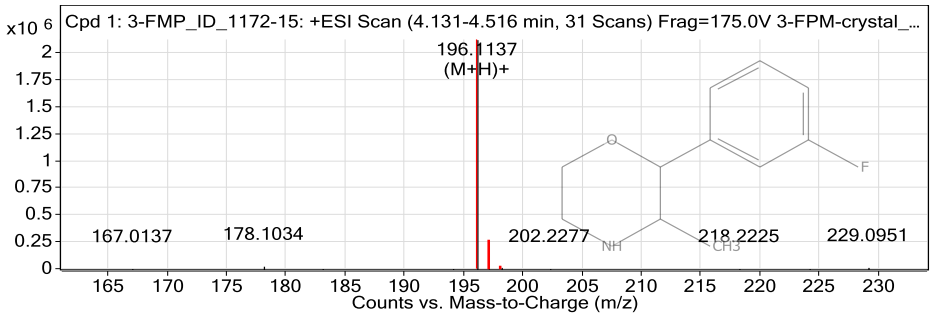




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
196.1138	1	2122623.75	C11 H14 F N O	(M+H)+
197.1168	1	261632.02	C11 H14 F N O	(M+H)+
198.1195	1	20288.99	C11 H14 F N O	(M+H)+
199.1229	1	1278.03	C11 H14 F N O	(M+H)+

--- End Of Report ---

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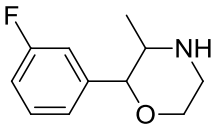
REPORT

Sample ID:	**1173-15**
Our notebook code:	P-1173-15
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^1H
Proposed structure with chemical name:	 HCl 2-(3-fluorophenyl)-3-methylmorpholine hydrochloride
Comments:	- Structure confirmed by comparing ^1H NMR spectra with that of 1172-15 (P-1172-15) - Compound is pure by NMR
Supporting information:	Copy of ^1H spectrum
Author:	Prof. Dr. Janez Košmrlj
Date of report:	April 30, 2015

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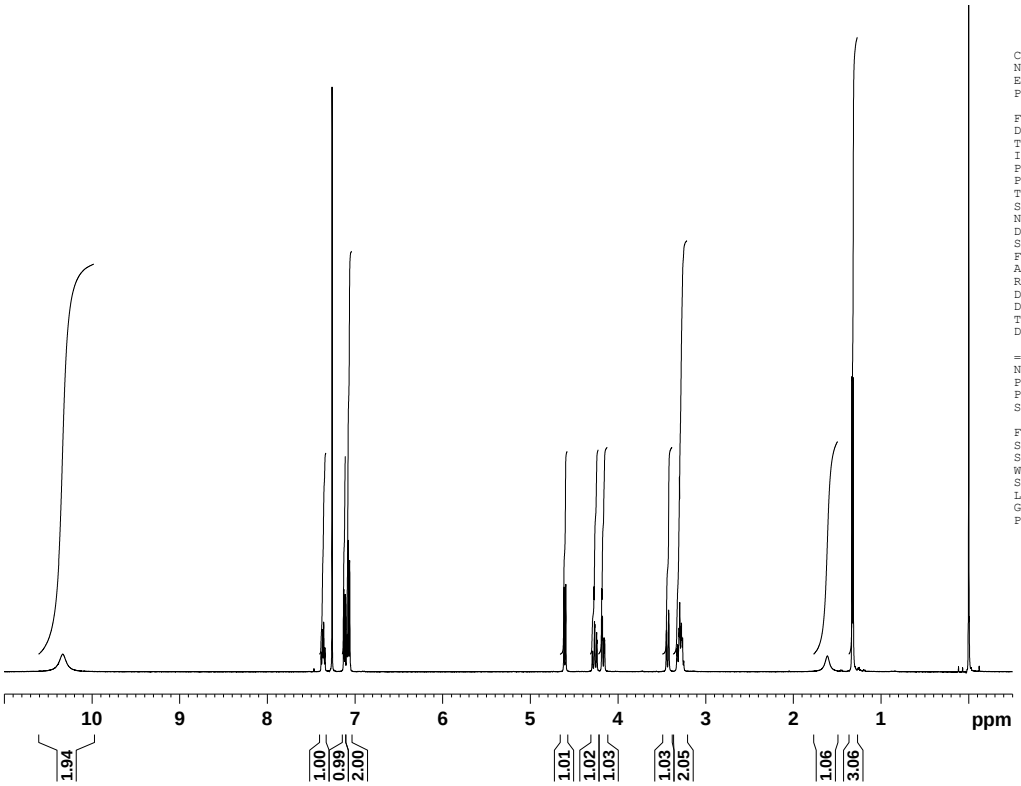
P-1173-15
1H




```
Current Data Parameters
NAME                 P-1173-15
EXPNO                       20
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150423
Time                   23.15
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                       181
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             500.1300120 MHz
WDW                       EM
SSB       0
LB                      0.30 Hz
GB        0
PC                      1.00
```