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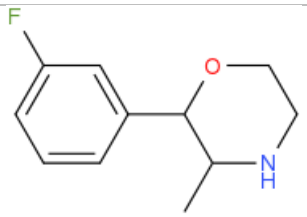
ANALYTICAL REPORT

3F-phenmetrazine, (C11H14FNO)

2-(3-fluorophenyl)-3-methylmorpholine

Remark – other NPS detected: none

Sample ID:	1172-15
Sample description:	powder - white
Sample type:	P- purchased
Date of entry:	4/17/2015

Substance identified-structure[i] (base form)	 HCl
Systematic name	2-(3-fluorophenyl)-3-methylmorpholine
Other names	3-FPM
Formula (per base form)	C11H14FNO
M_w (g/mol)	195.23
Salt form	salt HCl
Other compounds detected	none
Smiles	FC=1C=C(C=CC1)C1OCCNC1C
Compound Class	Others

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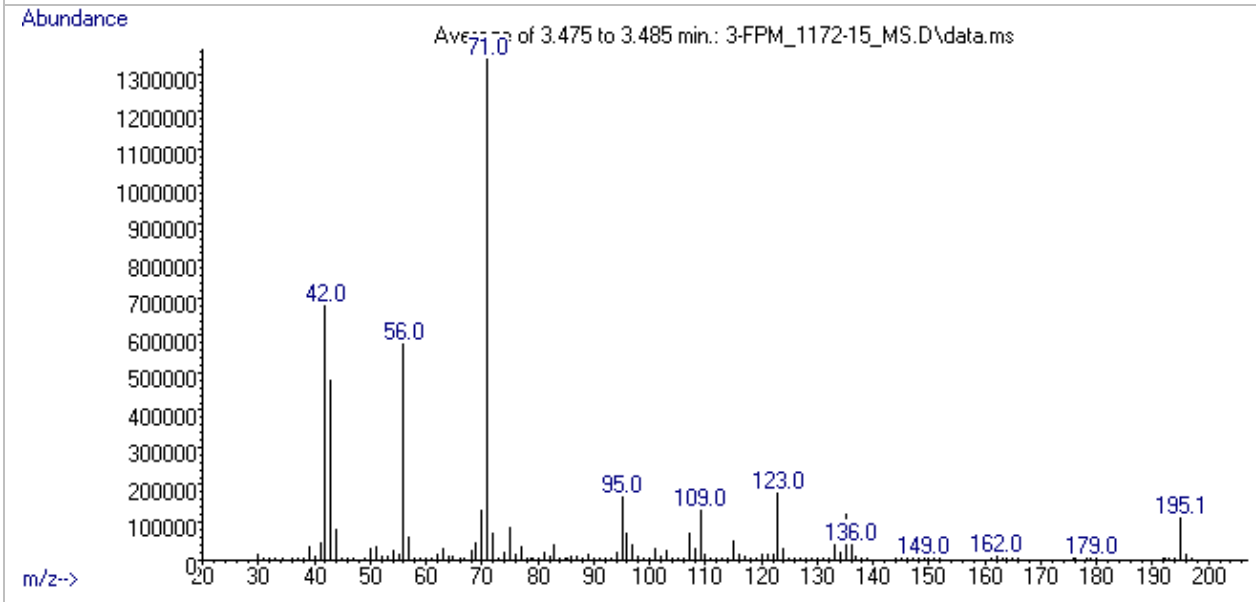
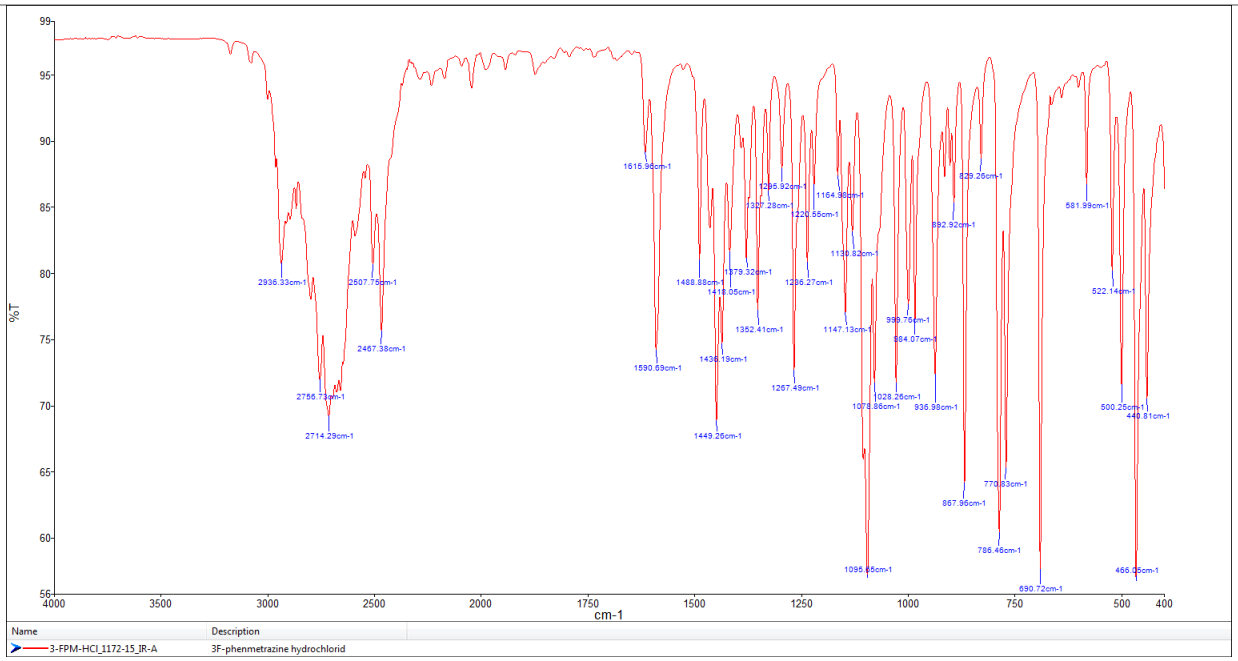
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 71; BP(2): 42,BP(3) :56
FTIR-ATR	+	salt HCl
FTIR (condensed phase)		
HPLC-TOF	+	Exact mass: 195.1059, measured/ Δppm:-2.15; 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

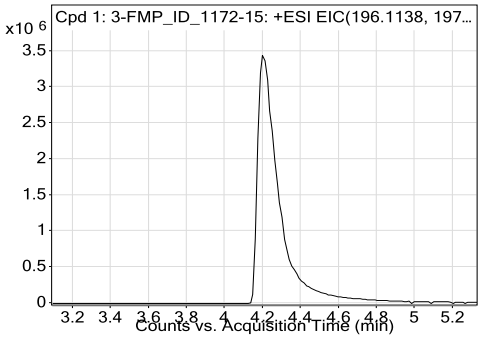
Data File	3-FPM_ID_1172-15_TOF.d	**Sample Name**	3-FPM
Sample Type	Sample	**Position**	P1-F5
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-2-4-2015-XDB-C18-ESI-poz.m	**Acquired Time**	4/10/2015 9:34:24 AM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment	white powder, extract in MeOH		

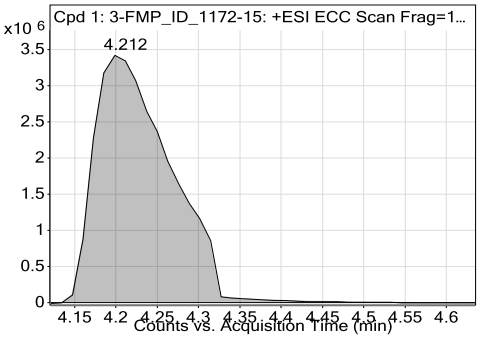
Compound Table

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	4.212	195.1067

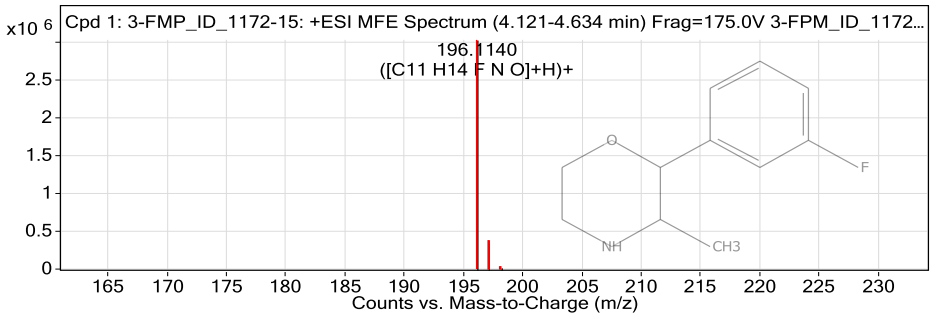
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpds Algorith
3-FMP_ID_1172-15	196.114	4.212	195.1067	4.211	C11 H14 F N O	195.1059	-3.76	C11 H14 F N O	Find by Molecular Feature

Compound Chromatograms

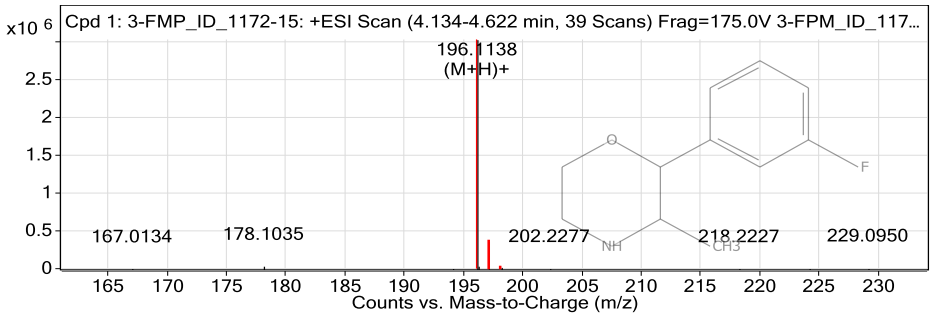




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
196.114	1	3034731.25	C11 H14 F N O	(M+H)+
197.1168	1	363243.04	C11 H14 F N O	(M+H)+
198.1196	1	28945.91	C11 H14 F N O	(M+H)+
199.1211	1	1569.9	C11 H14 F N O	(M+H)+

--- End Of Report ---

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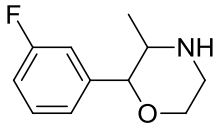
REPORT

Sample ID:	**1172-15**
Our notebook code:	P-1172-15
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^{1}H, ^{13}C, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{1}H–^{15}N *gs*-HMBC, ^{19}F
Proposed structure with chemical name:	 HCl 2-(3-fluorophenyl)-3-methylmorpholine hydrochloride
Comments:	- Structure elucidation based on 1D and 2D NMR spectra - Compound is pure by NMR
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra
Author:	Prof. Dr. Janez Košmrlj
Date of report:	April 30, 2015

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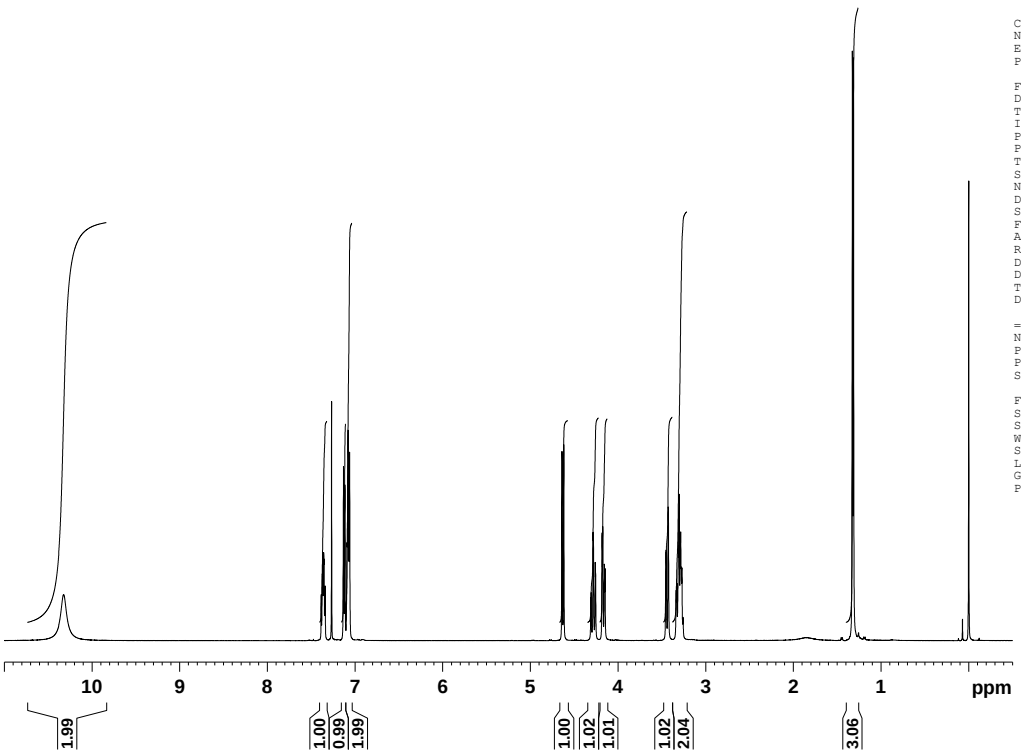
P-1172-15
1H



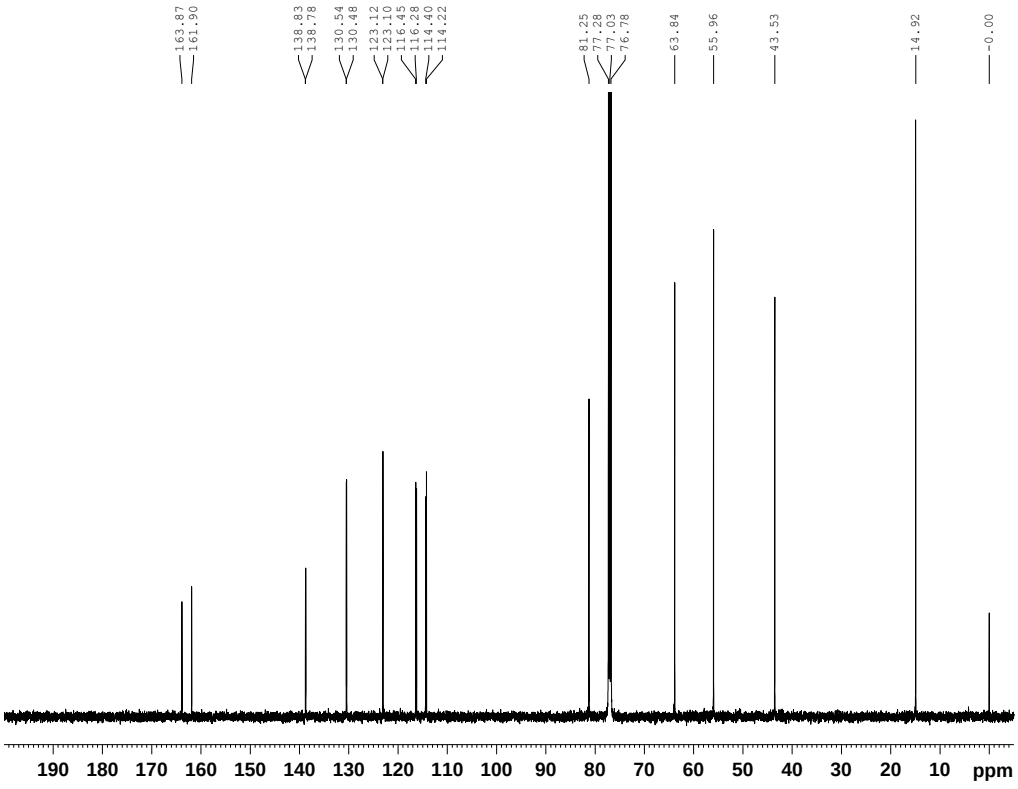

```
Current Data Parameters
NAME                  P-1172-15
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20150423
Time                      19.10
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                          114
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                500.1300095 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

P-1172-15
13C




```
Current Data Parameters
NAME                  P-1172-15
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20150423
Time                      21.39
INSTRUM                   spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         4096
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                125.7577899 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```