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' (base form)

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

<table>
<thead>
<tr>
<th>Analytical technique</th>
<th>applied</th>
<th>remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>BP(1): 71; BP(2): 42; BP(3): 56</td>
</tr>
<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>salt HCl</td>
</tr>
<tr>
<td>FTIR (condensed phase)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HPLC-TOF</td>
<td>+</td>
<td>Exact mass: 195.1059, measured/Δppm: 2.15; formula: C11H14FNO</td>
</tr>
<tr>
<td>NMR-confirmed</td>
<td>+</td>
<td>validation</td>
</tr>
<tr>
<td>other</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### MS spectrum (EI)

Abundance of 3.475 to 3.485 min.: 3-FPN_1172-15_MS_D\data.ms
FTIR - ATR

![FTIR - ATR graph]

<table>
<thead>
<tr>
<th>Wave Number (cm⁻¹)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>-</td>
</tr>
<tr>
<td>2950</td>
<td>-</td>
</tr>
<tr>
<td>2927</td>
<td>-</td>
</tr>
<tr>
<td>2875</td>
<td>-</td>
</tr>
<tr>
<td>1600</td>
<td>-</td>
</tr>
<tr>
<td>1450</td>
<td>-</td>
</tr>
<tr>
<td>1440</td>
<td>-</td>
</tr>
<tr>
<td>1200</td>
<td>-</td>
</tr>
<tr>
<td>700</td>
<td>-</td>
</tr>
</tbody>
</table>

\[1\] 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 Type: Sample
Instrument Name: SG13170002
Acq Method: droge general-2-4-2015-XDB-C18-ESI-pos.m
IRM Calibration Status: Success
Comment: white powder, extract in MeOH

--- End Of Report ---
**REPORT**

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th><strong>1172-15</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Our notebook code:</td>
<td>P-1172-15</td>
</tr>
<tr>
<td>NMR sample preparation:</td>
<td>15 mg dissolved in 0.7 mL CDCl$_3$</td>
</tr>
<tr>
<td>NMR experiments:</td>
<td>$^1$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</td>
</tr>
<tr>
<td>Proposed structure with chemical name:</td>
<td><img src="image" alt="" /> 2-(3-fluorophenyl)-3-methylmorpholine hydrochloride</td>
</tr>
</tbody>
</table>
| 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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**Current Data Parameters**

**NAME**          P-1172-15

**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