

### 1. GENERAL INFORMATION

**IUPAC Name:** 1-(3,4-dimethylphenyl)-2-(methylamino)propan-1-one

**CFR:** Not Scheduled (7/2013)

**CAS#:** 1081772-06-6 (HCl)

**Synonyms:** 3,4-DMMC

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV<sub>max</sub> (nm):** Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>12</sub> H <sub>17</sub> NO	191	Not Determined
HCl	C <sub>12</sub> H <sub>17</sub> NO · HCl	227	216.4

### 3. ADDITIONAL RESOURCES

Locos, O; Reynolds, D. The Characterization of 3,4-Dimethylmethcathinone (3,4-DMMC). *J. Forensic Sci.* **2012**, 57(5), 1303-1306.

[Forendex](#)

[Wikipedia](#)

## 4. QUALITATIVE DATA

### 4.1 NUCLEAR MAGNETIC RESONANCE

#### Method NMR D<sub>2</sub>O

*Sample Preparation:* Dilute analyte to ~10 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

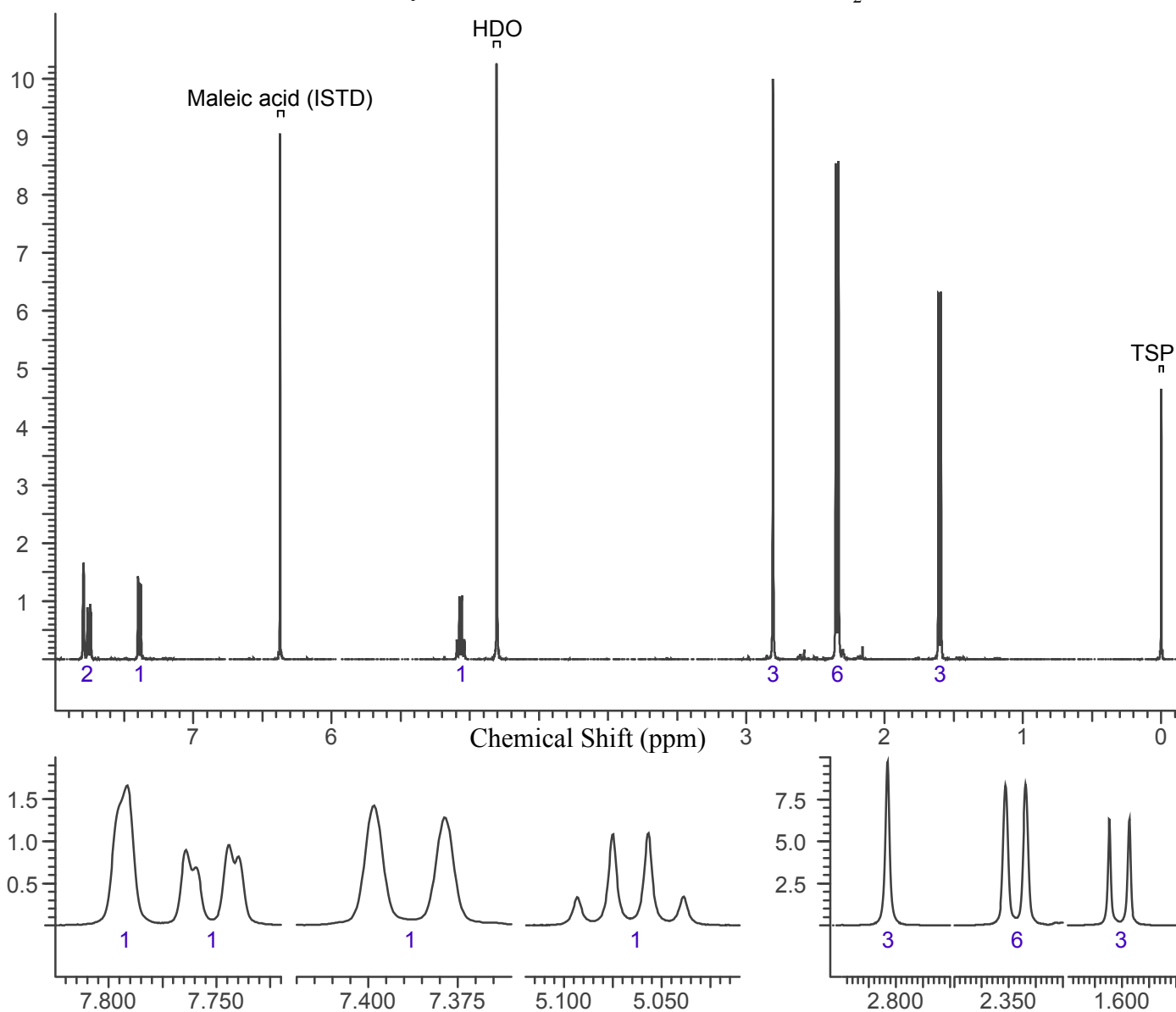
*Instrument:* 400 MHz NMR spectrometer

*Parameters:* Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

<sup>1</sup>H NMR: 3,4-Dimethylmethcathinone HCl; Lot N17-P79A; D<sub>2</sub>O; 400 MHz



## 4.2 Gas Chromatography/Mass Spectrometry

*Sample Preparation:* Dilute analyte ~ 1 mg/mL base extracted into chloroform.

***Instrument:*** Agilent gas chromatograph operated in split mode with MS detector

***Column:*** DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25  $\mu$ m

***Carrier Gas:*** Helium at 1 mL/min

***Temperatures:*** Injector: 280°C

MSD transfer line: 280°C

MS Source: 230°C

MS Quad: 150°C

Oven program:

1) 100°C initial temperature for 1.0 min

2) Ramp to 300°C at 12 °C/min

3) Hold final temperature for 9.0 min

***Injection Parameters:*** Split Ratio = 20:1, 1  $\mu$ L injected

***MS Parameters:*** Mass scan range: 30-550 amu

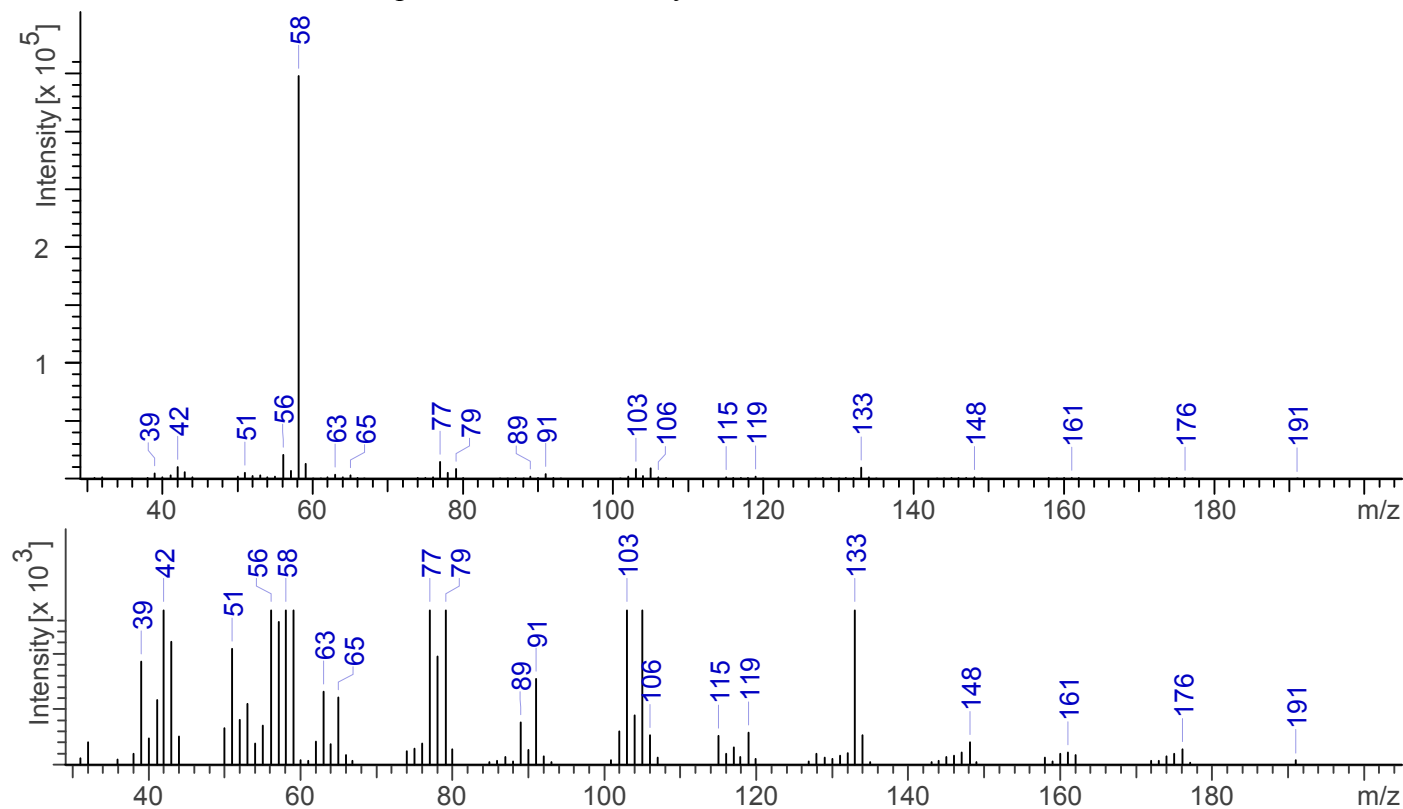
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

***Retention Time:*** 8.337 min

EI Mass Spectrum: 3,4-Dimethylmethcathinone HCl; Lot N17-P79A



### 4.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:** Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 100

FTIR ATR (Diamond, 3 Bounce): 3,4-Dimethylmethcathinone HCl; Lot N17-P79A

