

## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-(1,3-benzodioxol-5-yl)-2-(methylamino)propan-1-one
<b>CFR:</b>	Schedule I
<b>CAS#:</b>	186028-79-5 (base), 186028-80-8 (HCl)
<b>Synonyms:</b>	bk-MDMA, $\beta$ -ketone-MDMA, bk-methylenedioxyamphetamine, MDMC, 3,4-methylenedioxyamphetaminone, N-methyl-MDC, 3,4-methylenedioxy-N-methylcathinone, N-methyl-3,4-methylenedioxcathinone
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder (HCl)
<b>Kovat's Index:</b>	Pending
<b>UV<sub>max</sub> (nm):</b>	234.0, 281.9, 320.1

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>11</sub> H <sub>13</sub> NO <sub>3</sub>	207	Not Determined
HCl	C <sub>11</sub> H <sub>13</sub> NO <sub>3</sub> · HCl	243	248.4

## 3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

## 4. QUALITATIVE DATA

### 4.1 NUCLEAR MAGNETIC RESONANCE

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

*Sample Preparation:* Dilute analyte to ~25 mg/mL in deuterium oxide (D<sub>2</sub>O) containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

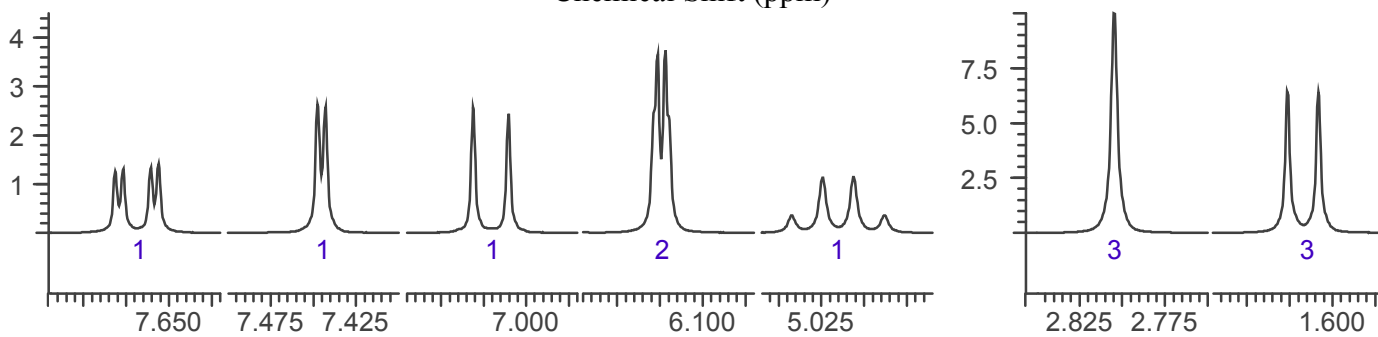
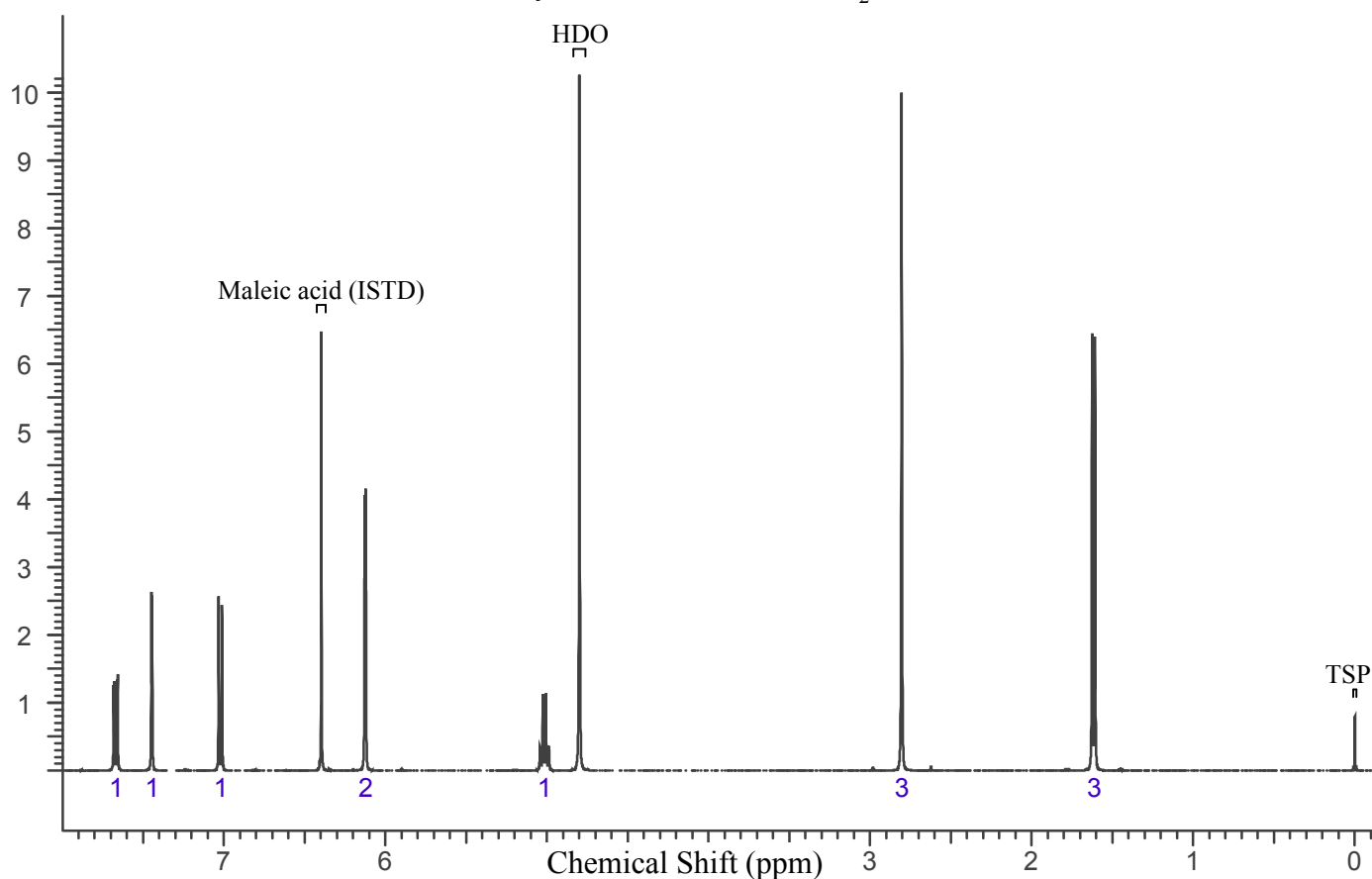
*Instrument:* 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 45 seconds

<sup>1</sup>H NMR: Methylone HCl; Lot N1P25; 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

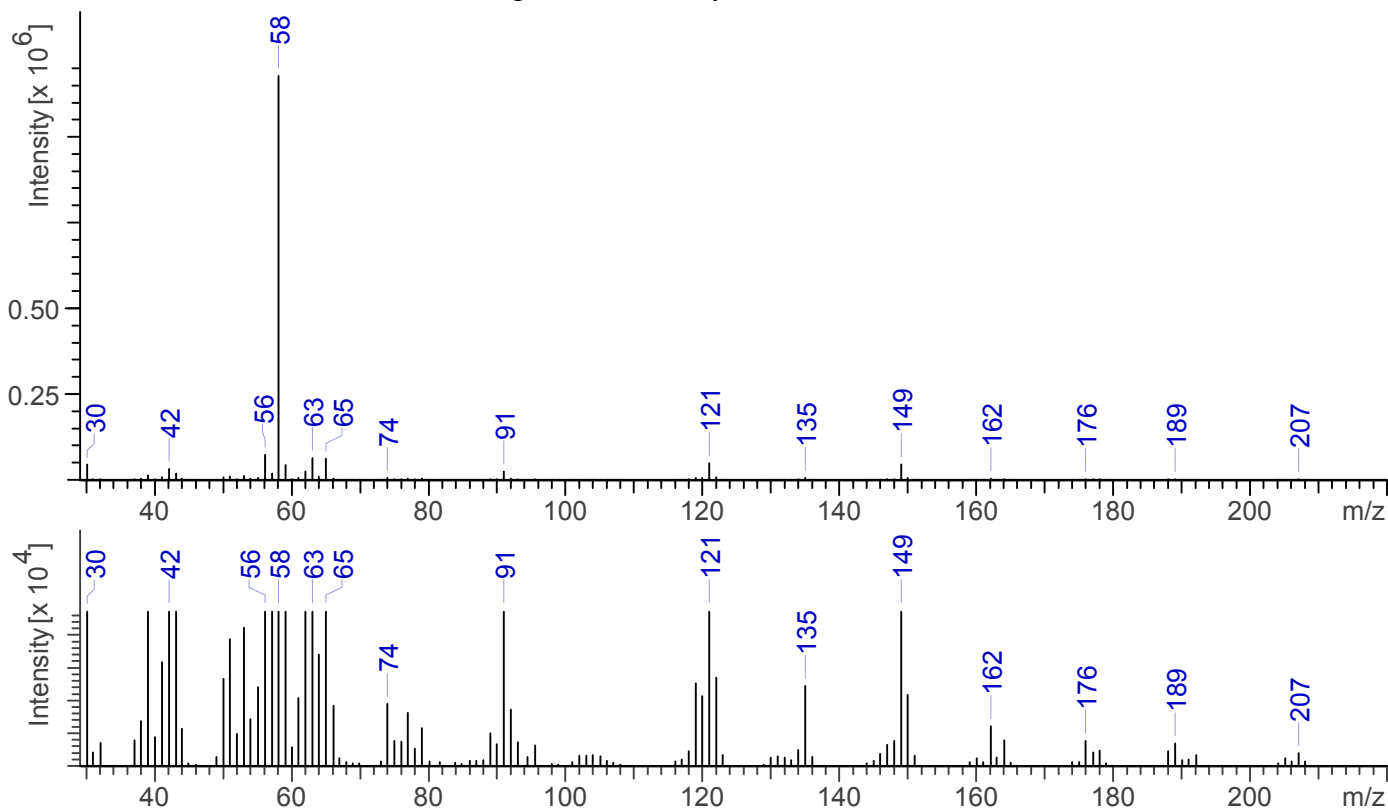
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

*Retention Time:* 9.462 min

EI Mass Spectrum: Methylone HCl; Lot N1P25



### 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: 150

FTIR ATR (Diamond, 3 Bounce): Methylene HCl; Lot N1P25

