

### 1. GENERAL INFORMATION

**IUPAC Name:** 2-(ethylamino)-1-(3-methylphenyl)propan-1-one

**CFR:** Not Scheduled (4/2013)

**CAS#:** Not Available

**Synonyms:** 3-MEC, 3-methyl-N-ethylcathinone

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV<sub>max</sub>:** 254.8, 294.2

### 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	212.9

### 3. ADDITIONAL RESOURCES

Lopez-Avila V, Gao W, Urdahl R. Mass spectral fragmentation of cathinones by high-resolution TOFMS using a soft ionization source. *J Pharm Sci Innov.* 2012; 1(6): 44-53.

## 4. QUALITATIVE DATA

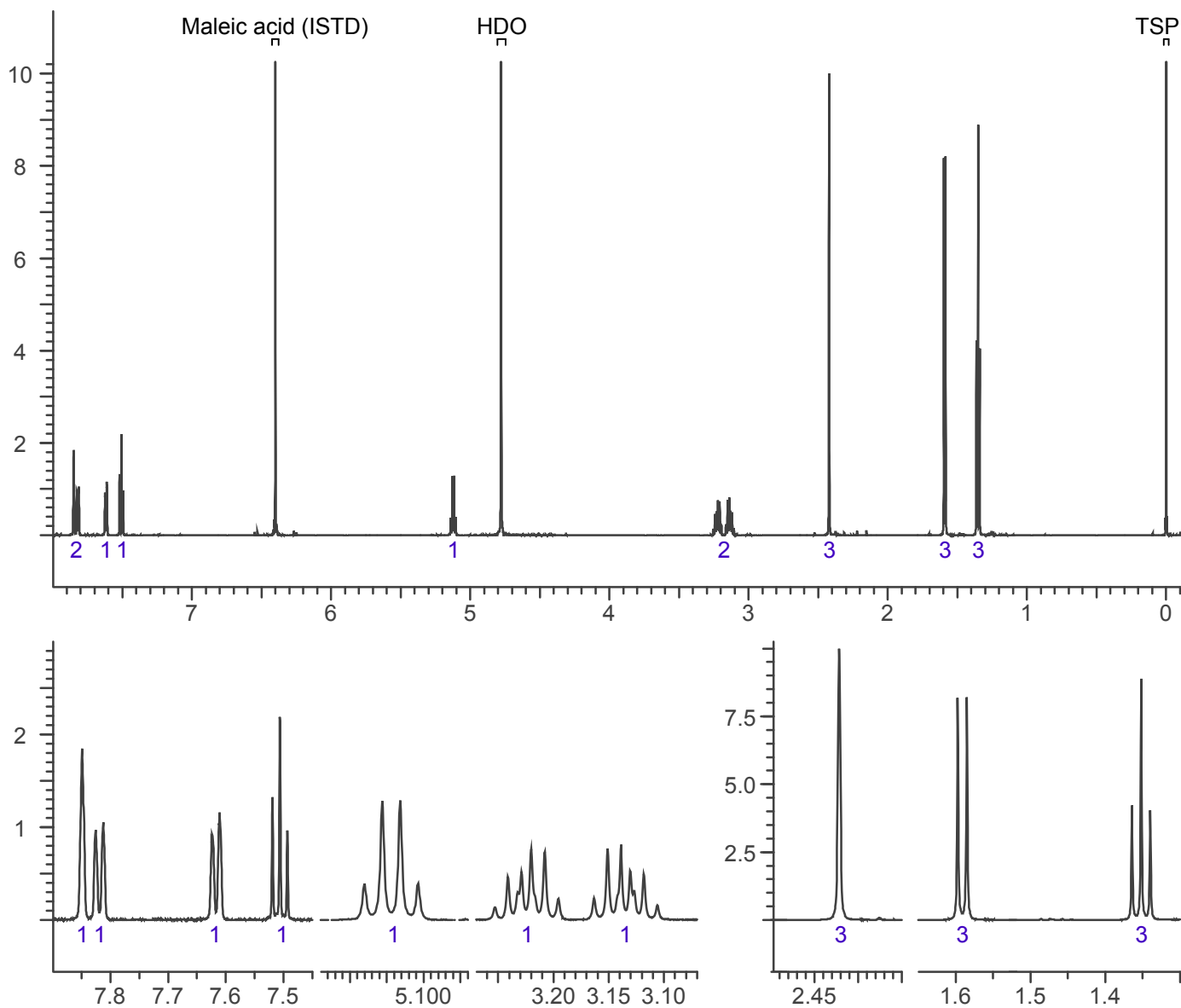
### 4.1 NUCLEAR MAGNETIC RESONANCE

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

*Sample Preparation:* Dilute analyte to ~5 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

**Instrument:** 600 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-methylethcathinone HCl; lot 0435404-15; D<sub>2</sub>O; 600 MHz



## 4.2 Gas Chromatography/Mass Spectrometry

*Sample Preparation:* Dilute analyte ~ 4 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 30.0 min

**Injection Parameters:** Split Ratio = 25:1, 1  $\mu$ L injected

**MS Parameters:** Mass scan range: 34-550 amu

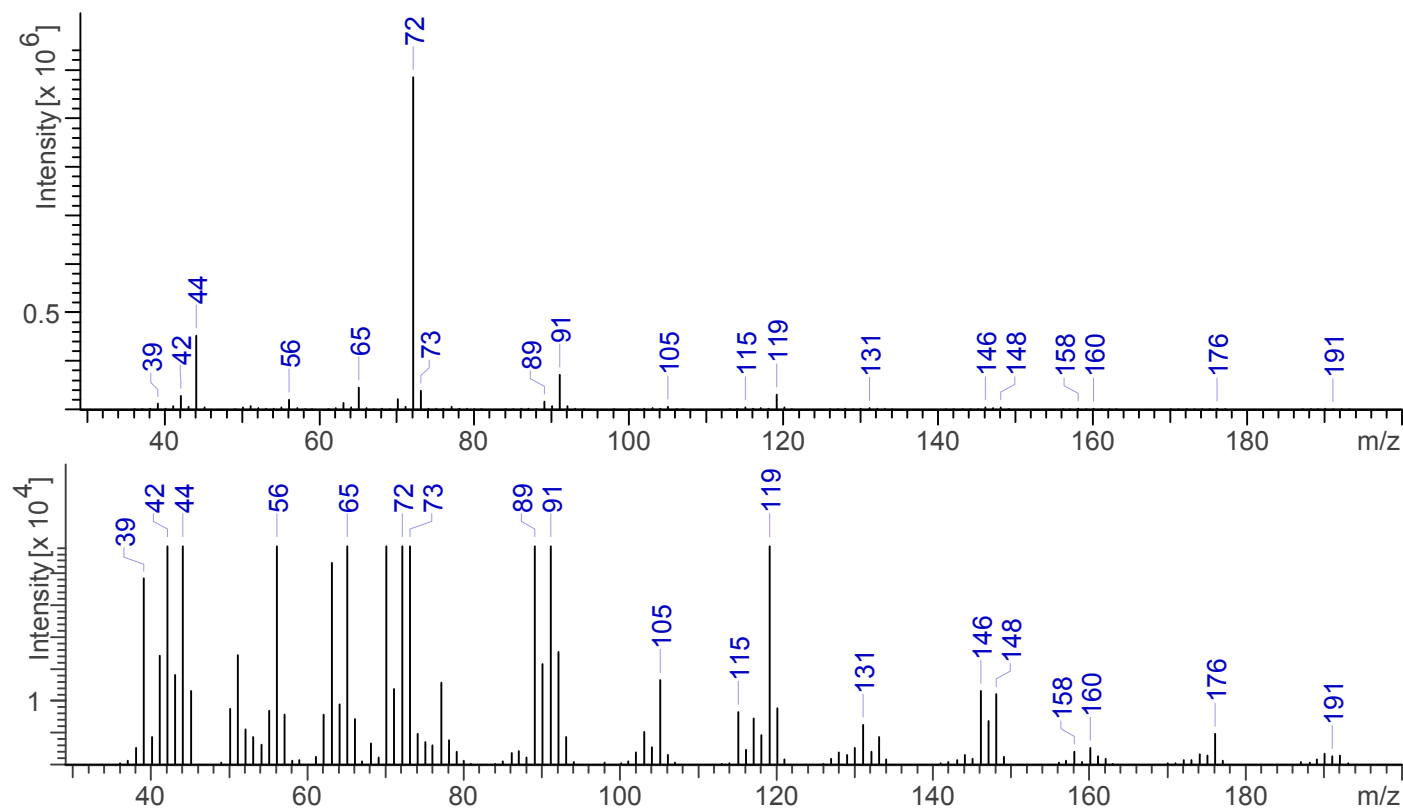
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 7.654 min

EI Mass Spectrum: 3-methylethcathinone HCl; lot 0435404-15



### 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): 3-methylethcathinone HCl; lot 0435404-15

