

### 1. GENERAL INFORMATION

|                               |  |
|-------------------------------|--|
| <b>IUPAC Name:</b>            | 2-(ethylamino)-2-(3-methoxyphenyl)-cyclohexanone |
| <b>CFR:</b>                   | Not Scheduled (5/2013)                           |
| <b>CAS#:</b>                  | 1239943-76-0 (base), 1239908-48-5 (HCl)          |
| <b>Synonyms:</b>              | MXE, 3-MeO-2-Oxo-PCE                             |
| <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> | 278.8  |

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

| Form | Chemical Formula                                      | Molecular Weight | Melting Point (°C) |
|------|---|------------------|--------------------|
| Base | C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>       | 247              | Not Determined     |
| HCl  | C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub> · HCl | 283              | 244.9              |

### 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 ~10 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

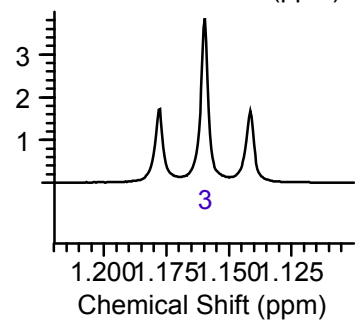
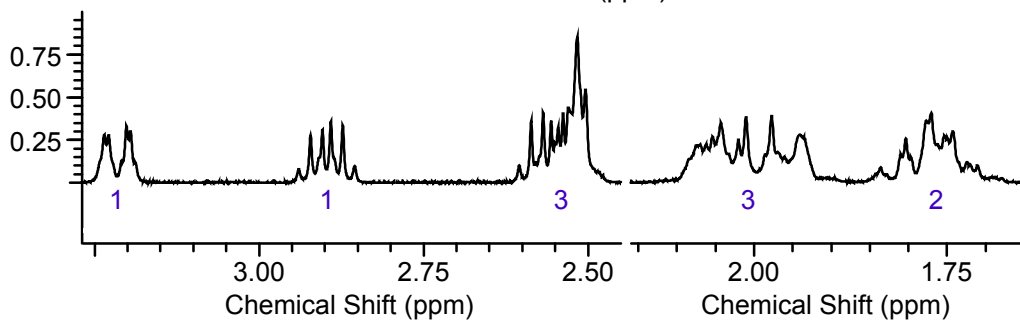
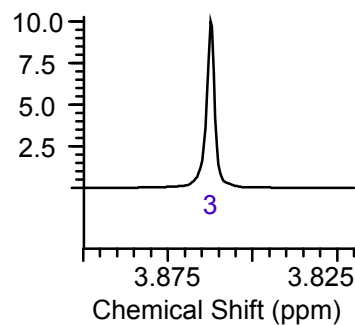
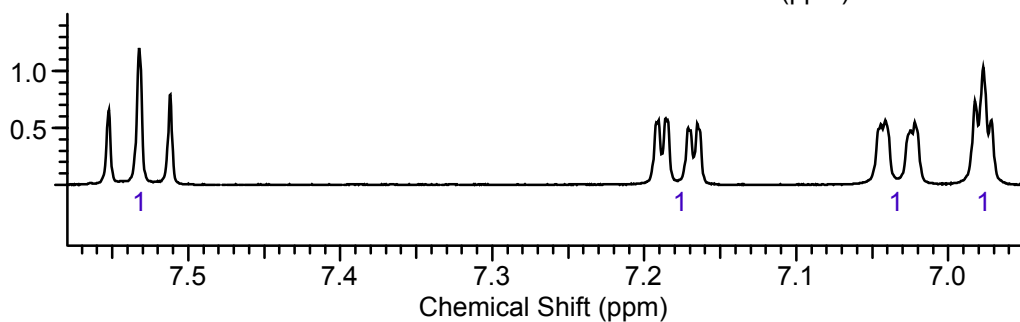
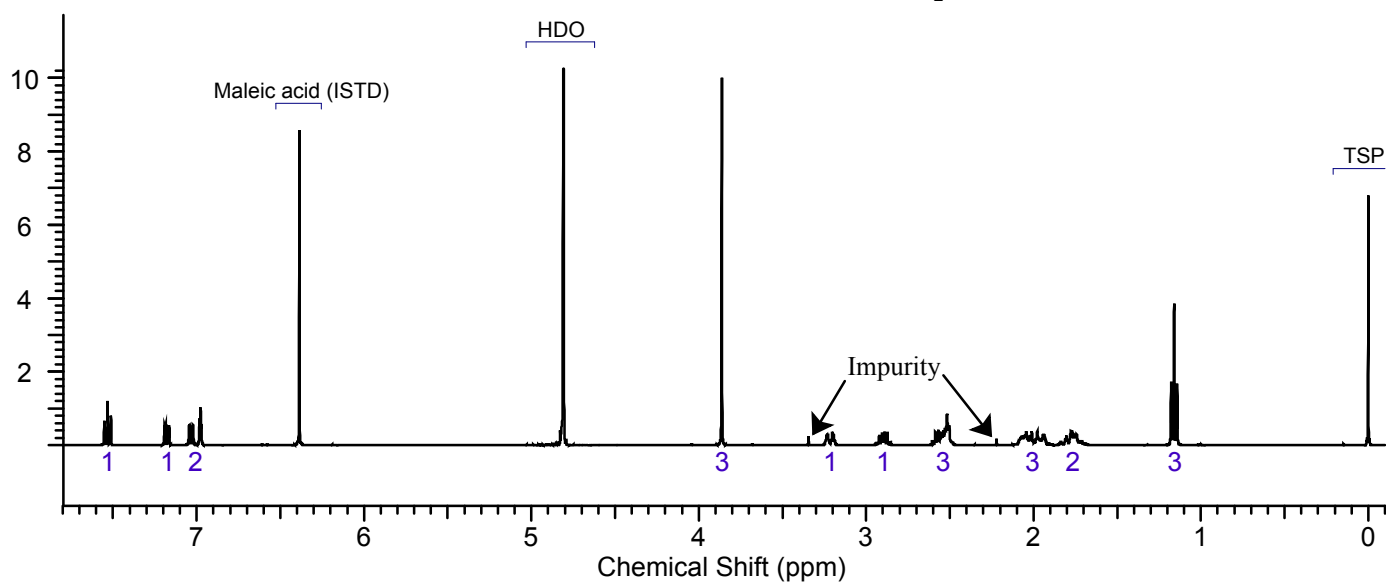
**Instrument:** 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 45 seconds

<sup>1</sup>H NMR: Methoxetamine HCl; Lot N16-P100C; D<sub>2</sub>O; 400 MHz



## 4.2 Gas Chromatography/Mass Spectrometry

*Sample Preparation:* Dilute analyte ~ 1 mg/mL in methanol.

*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

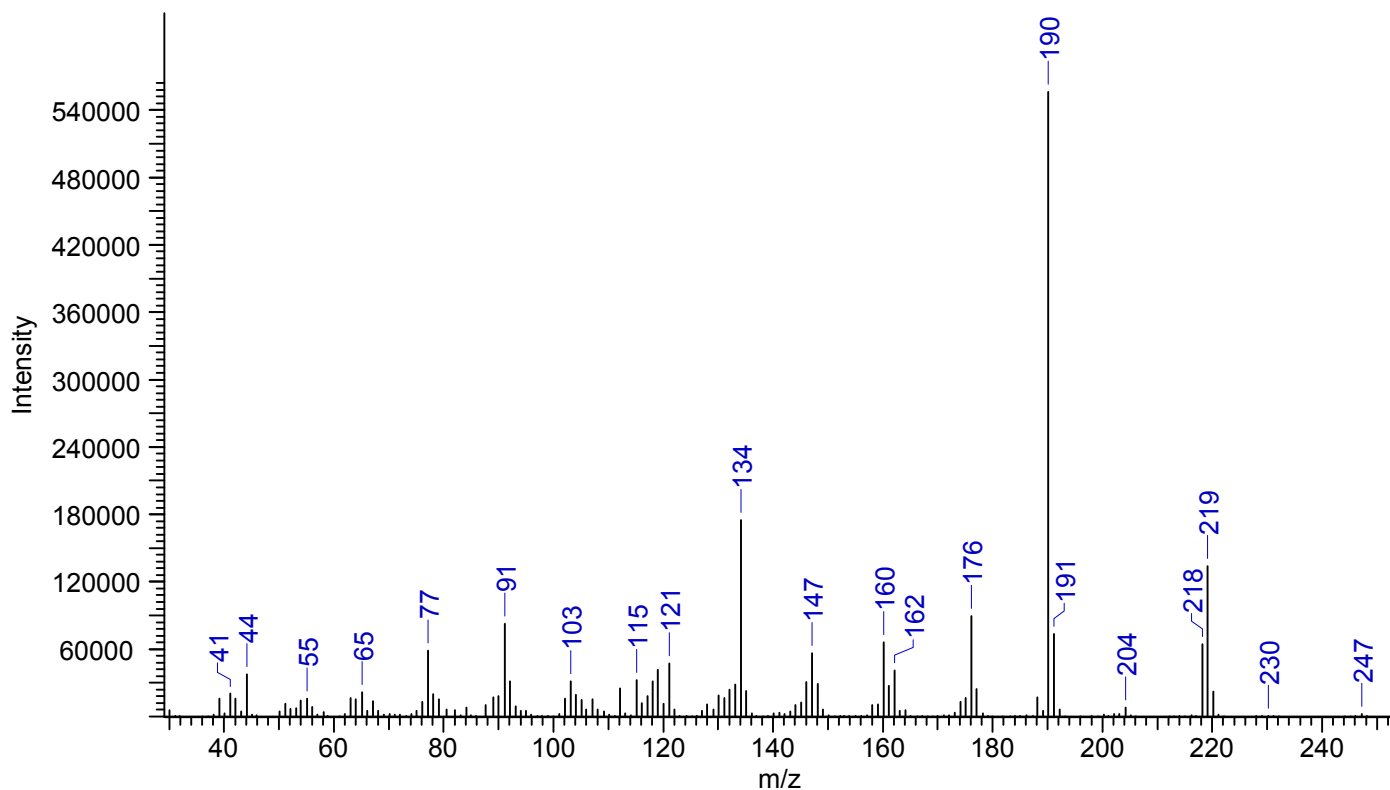
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

*Retention Time:* 11.280 min

EI Mass Spectrum: Methoxetamine HCl; Lot N16-P100C



### 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

IR ATR (Diamond, 3 bounce): Methoxetamine HCl; Lot N16-P100C

