

## 1. GENERAL INFORMATION

**IUPAC Name:** 1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)propan-1-one

**CFR:** Not Scheduled (03/2013)

**CAS #:** 109367-07-9

**Synonyms:** 3,4-methylenedioxy-N,N-dimethylcathinone, dimethylone, *N,N*-Dimethyl MDCATH, *N,N*-Dimethyl-3,4-methylenedioxcathinone, *N,N*-Dimethyl- $\beta$ -keto-3,4-methylenedioxyamphetamine

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV<sub>max</sub>:** 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>15</sub> NO <sub>3</sub>	221	Not Determined
HCl	C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub> · HCl	257	260.9

### 3. ADDITIONAL RESOURCES

Zaitso K, Katagi M, Kamata HT, Miki A, Tsuchihashi H. Discrimination and identification of regioisomeric  $\beta$ -keto analogues of 3,4-methylenedioxyamphetamines by gas chromatography-mass spectrometry. *Forensic Toxicology* 2008; 26:45-51.

### 4. QUALITATIVE DATA

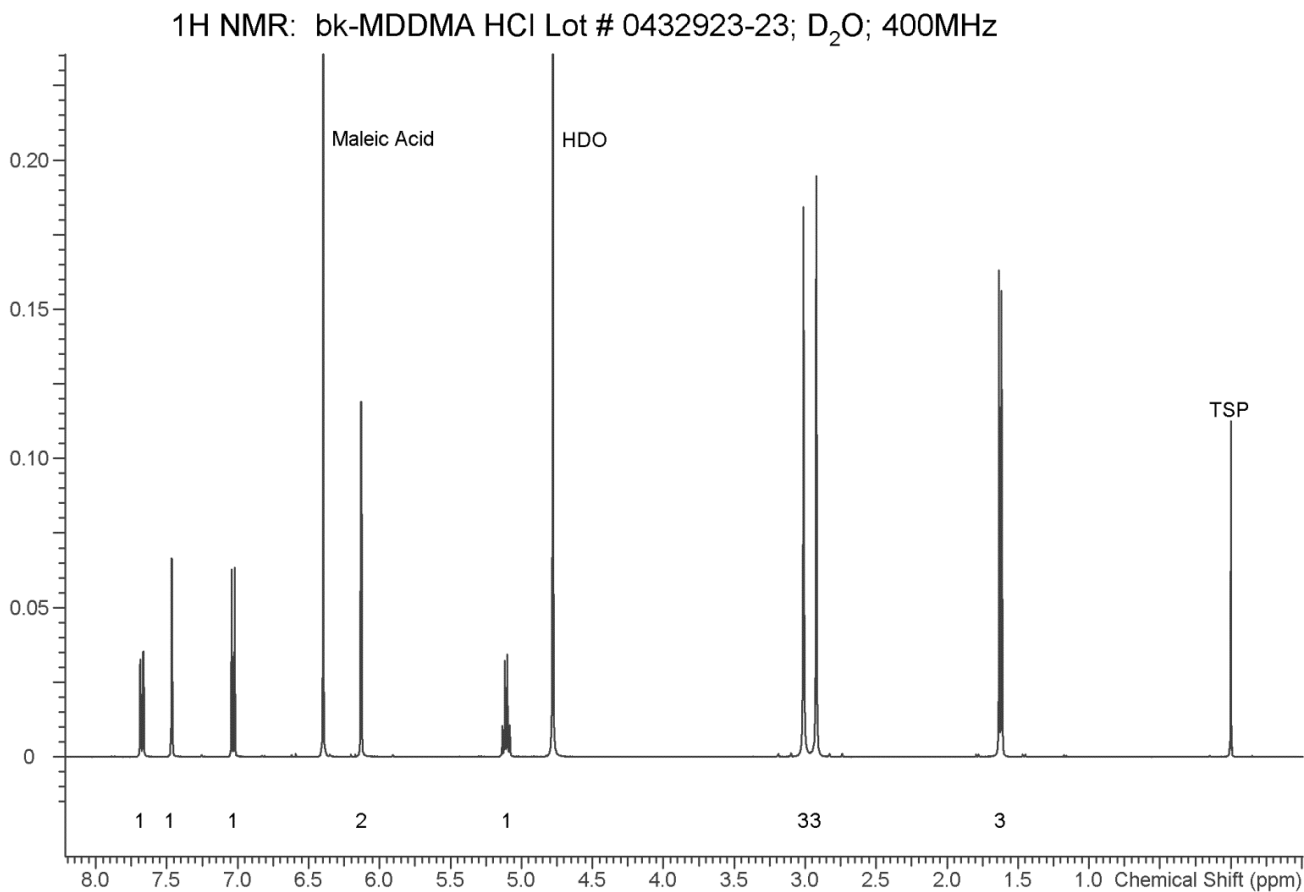
#### 4.1 NUCLEAR MAGNETIC RESONANCE

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

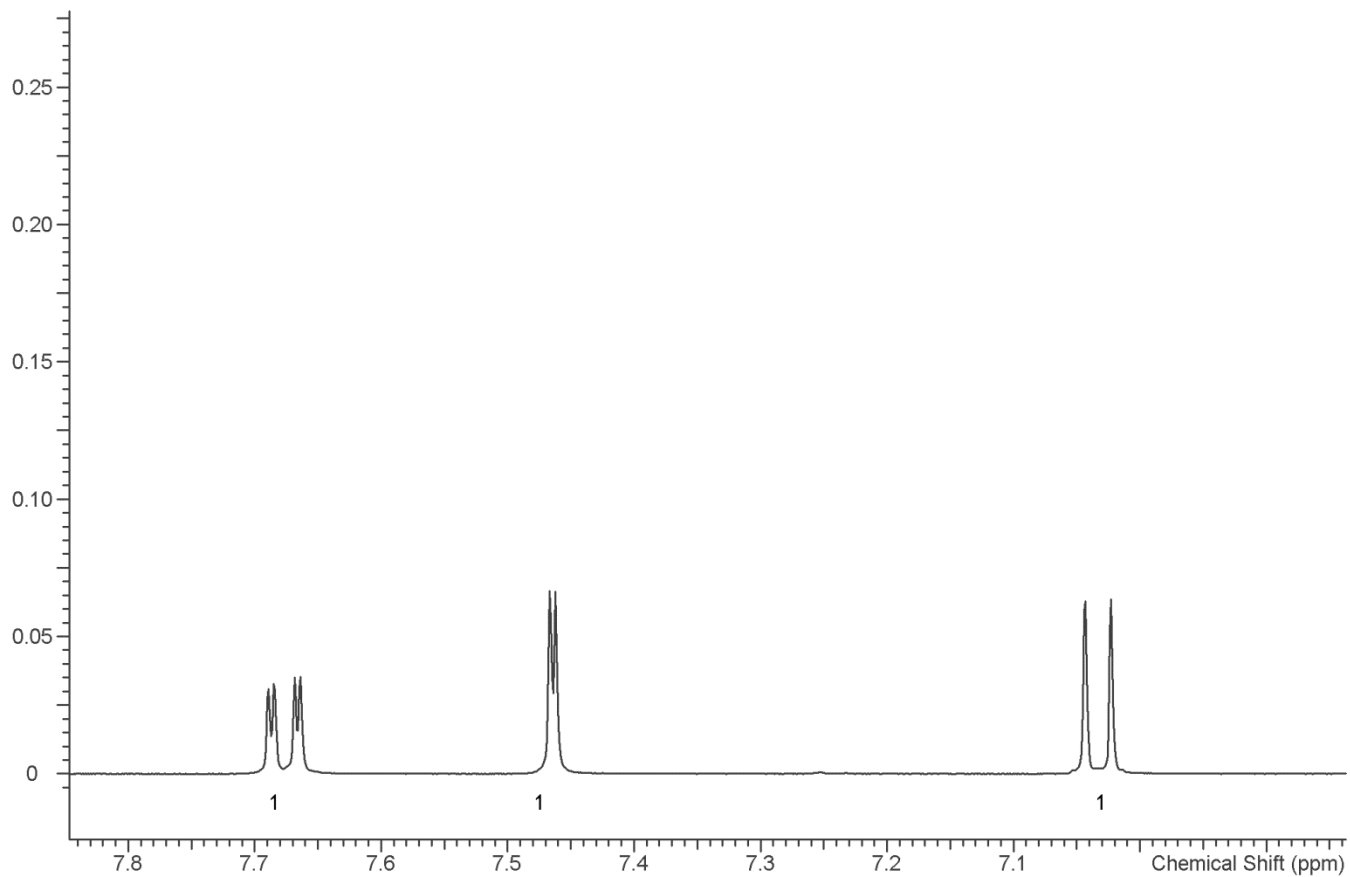
*Sample Preparation:* Dilute analyte to ~5 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

**Instrument:** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

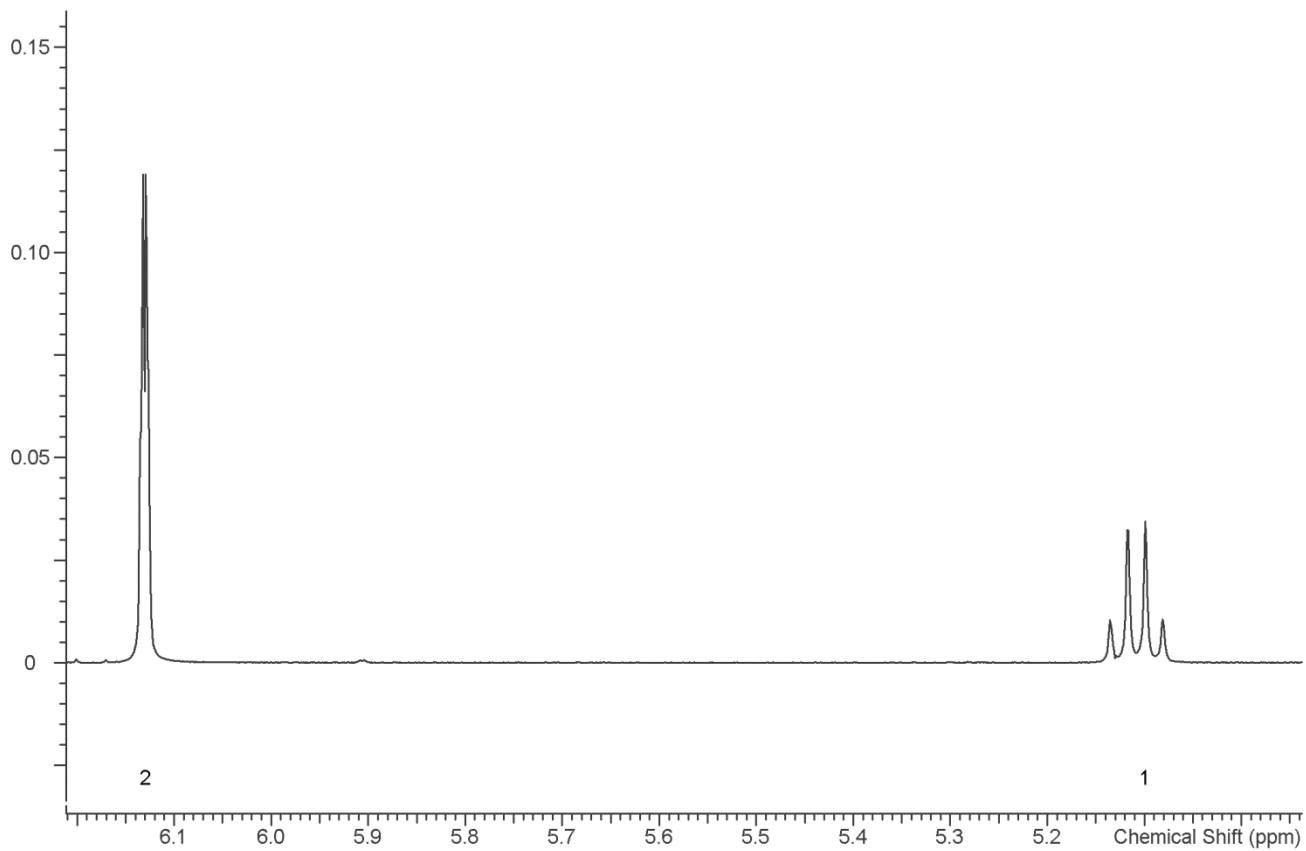
**Parameters:** Spectral width: at least containing -3 ppm through 13 ppm  
Pulse angle: 90°  
Delay between pulses: 45 seconds



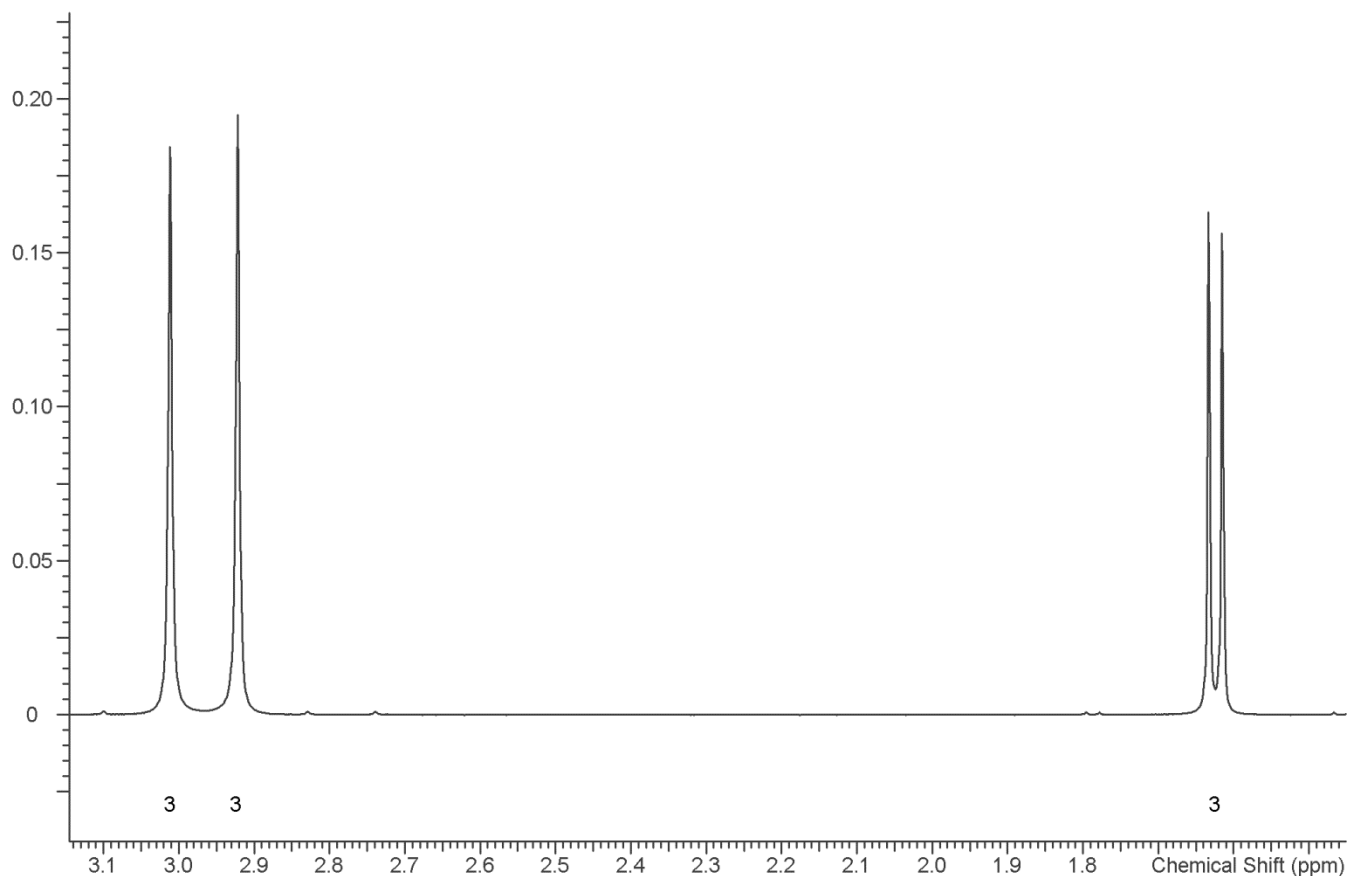
1H NMR: bk-MDDMA HCl Lot # 0432923-23; D<sub>2</sub>O; 400MHz



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## 4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte to ~4 mg/mL base extracted into CHCl<sub>3</sub>.

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

***Column:*** DB-1 MS or equivalent; 30m x .25mm x .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: 30-550 amu

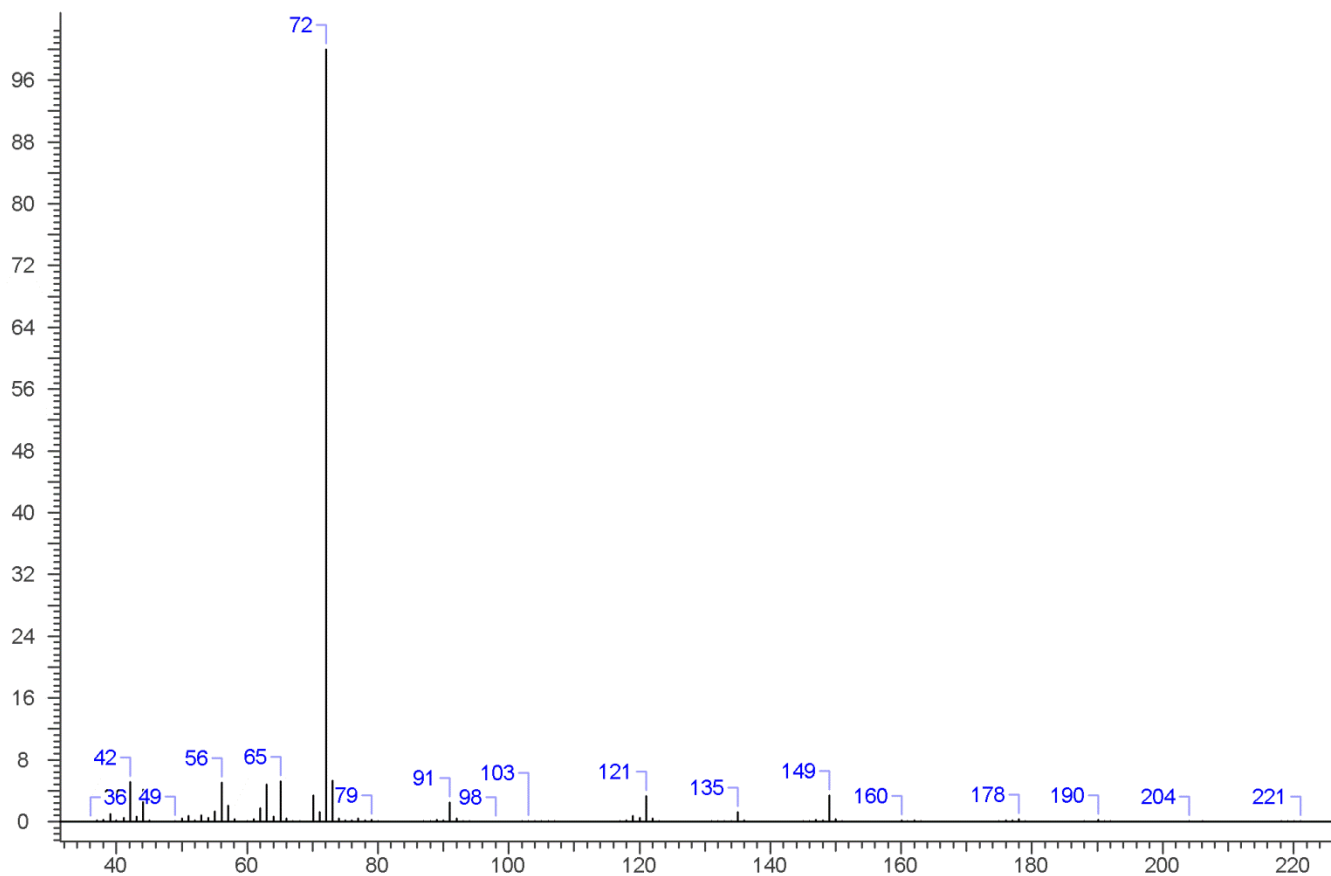
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

***Retention Time:*** 10.053 minutes

## EI Mass Spectrum: bk-MDDMA HCl Lot # 0432923-23



### 4.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:**

FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**

Number of scans: 32

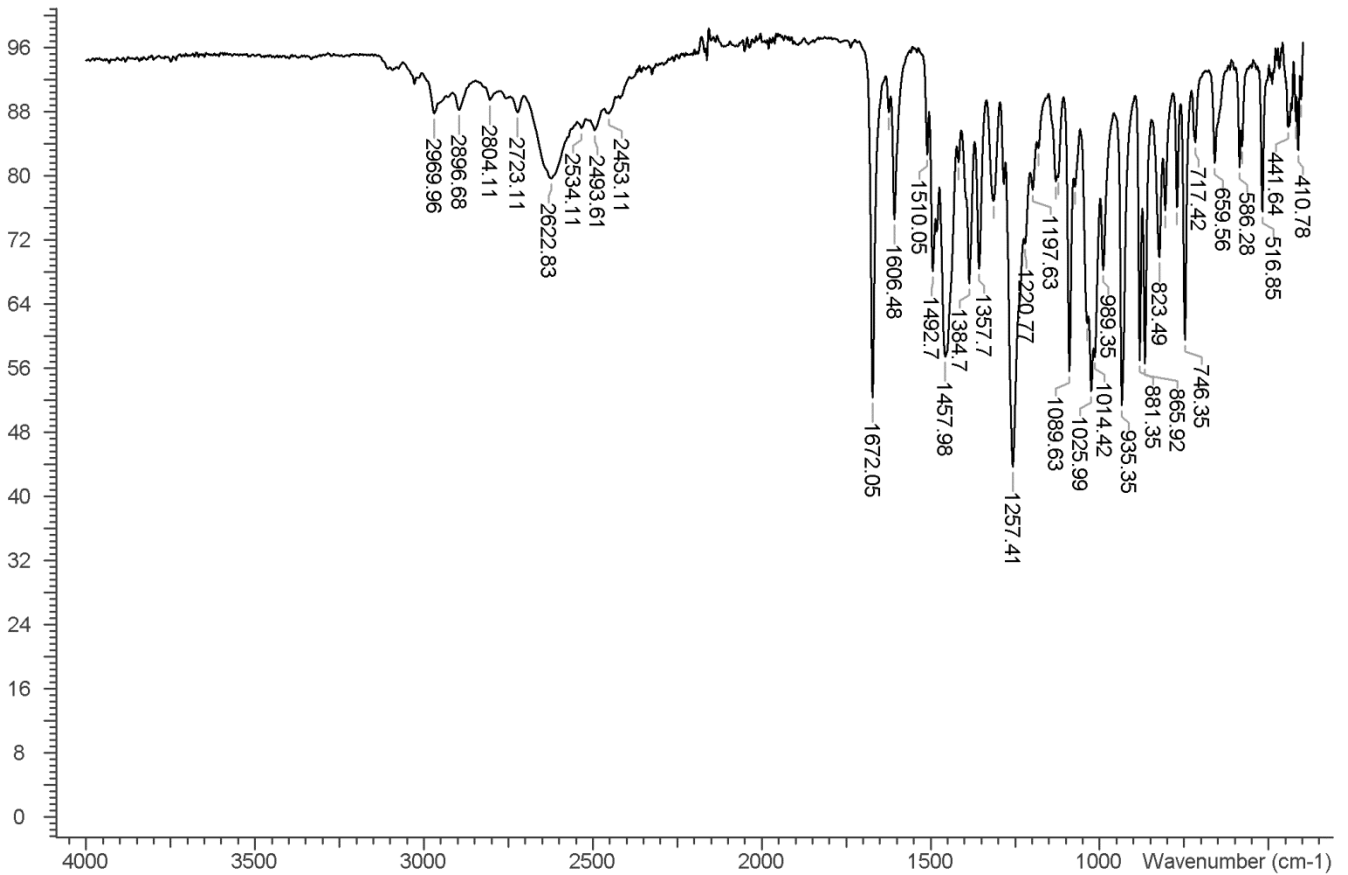
Number of background scans: 32

Resolution:  $4\text{cm}^{-1}$

Sample gain: 8

Aperture: 150

FTIR ATR (Diamond, 3 Bounce): bk-MDDMA HCl Lot # 0432923-23



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