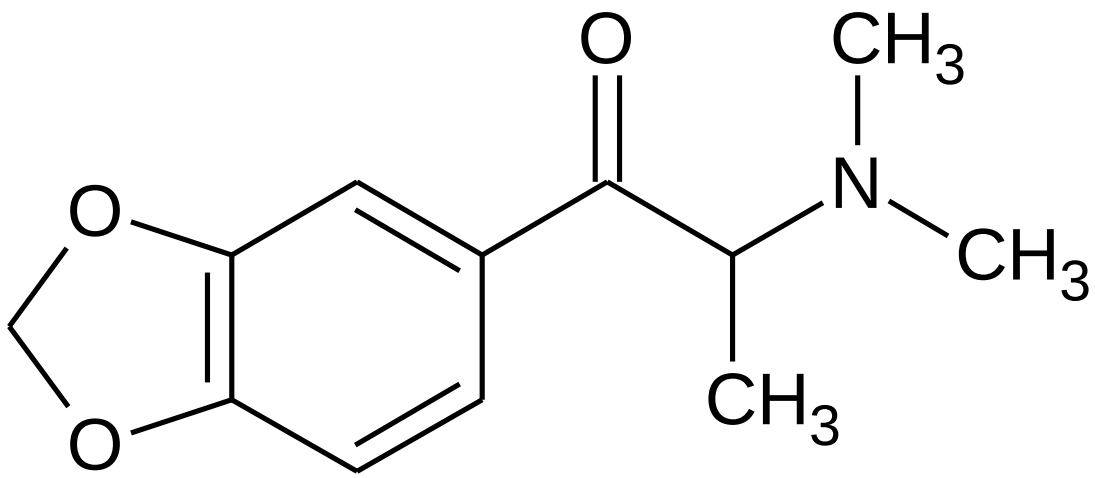


1. GENERAL INFORMATION

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-methylenedioxycathinone, *N*,*N*-Dimethyl-β-keto-3,4-methylenedioxyamphetamine

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max}: Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{12}H_{15}NO_3$	221	Not Determined
HCl	$C_{12}H_{15}NO_3 \cdot HCl$	257	260.9

3. ADDITIONAL RESOURCES

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

4. QUALITATIVE DATA

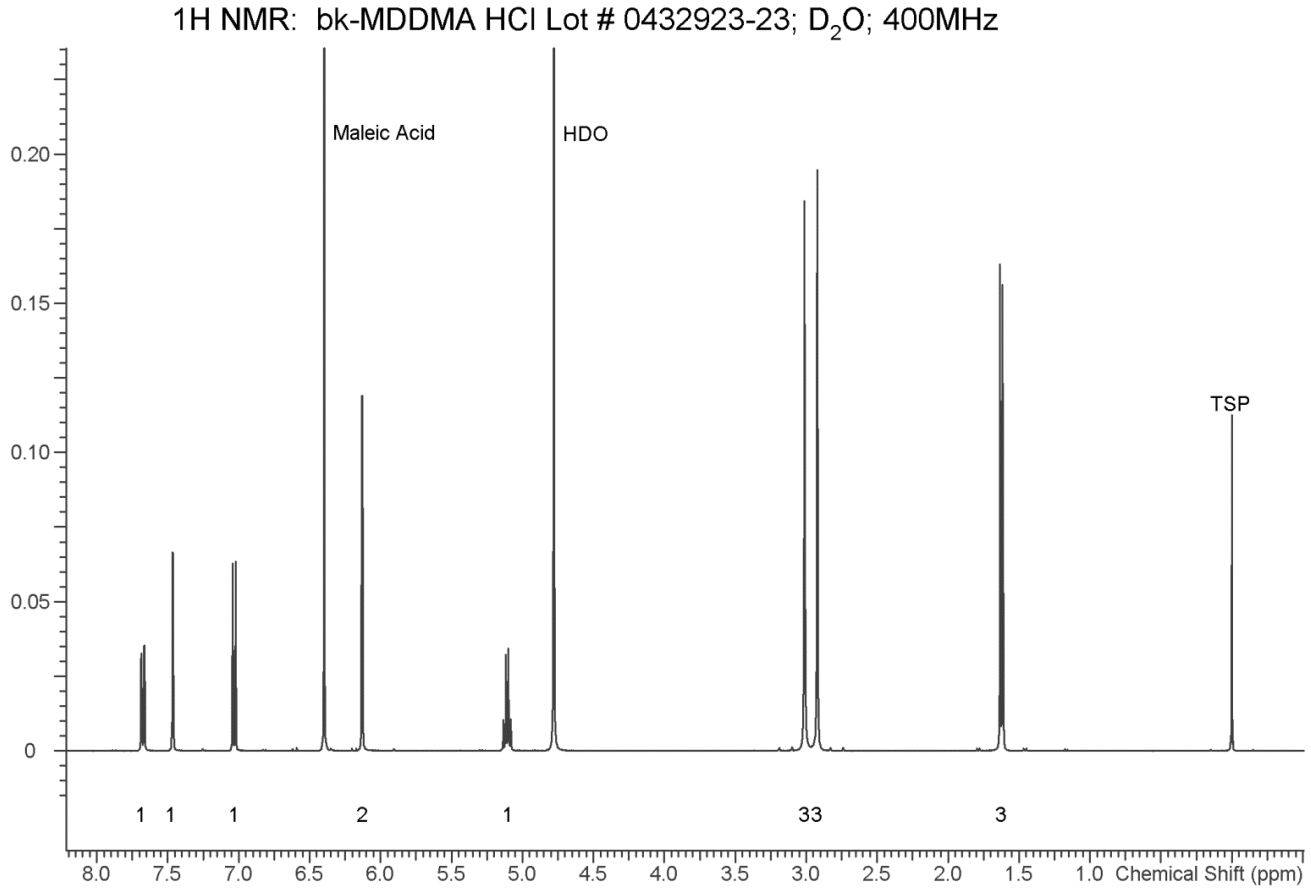
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

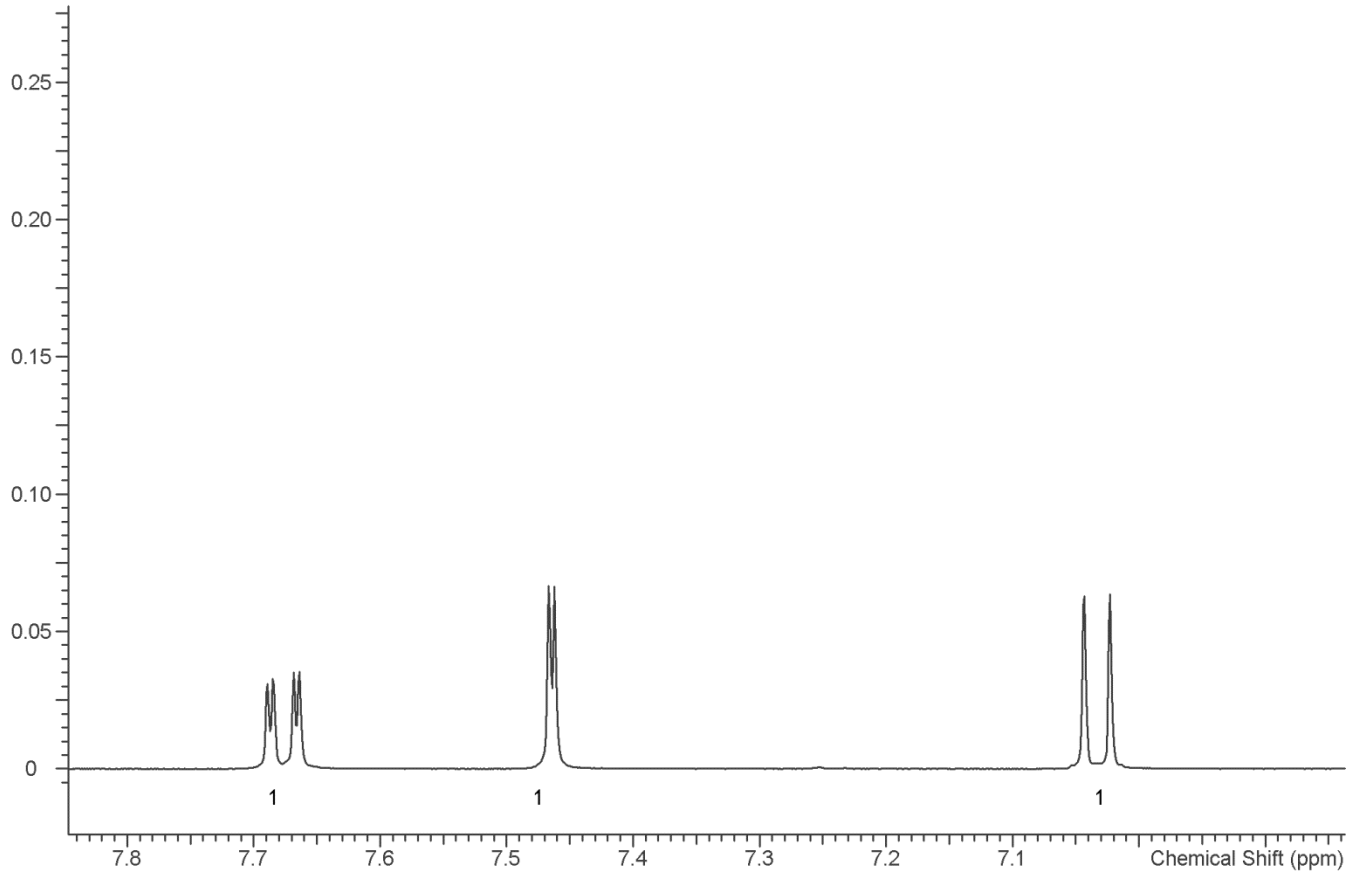
Sample Preparation: Dilute analyte to ~5 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

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

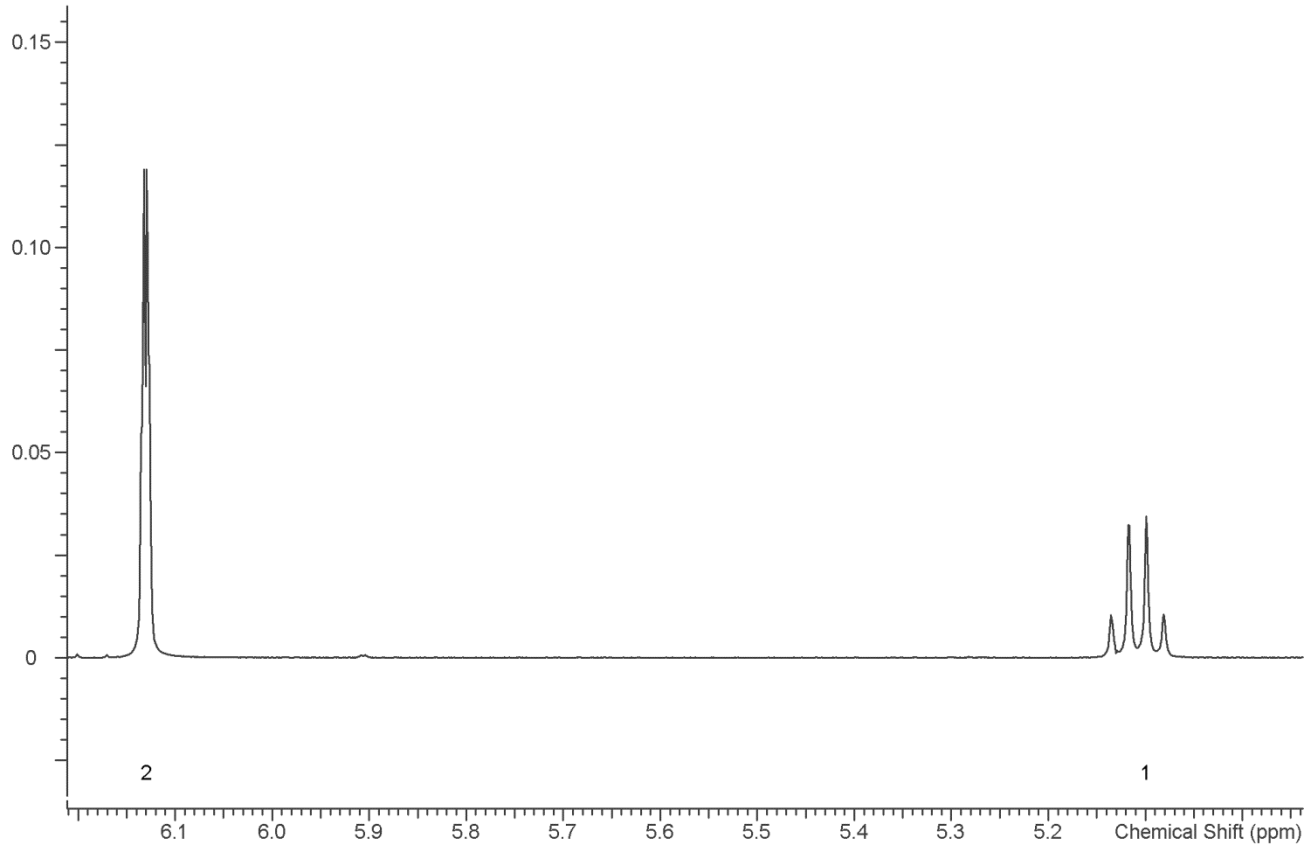
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

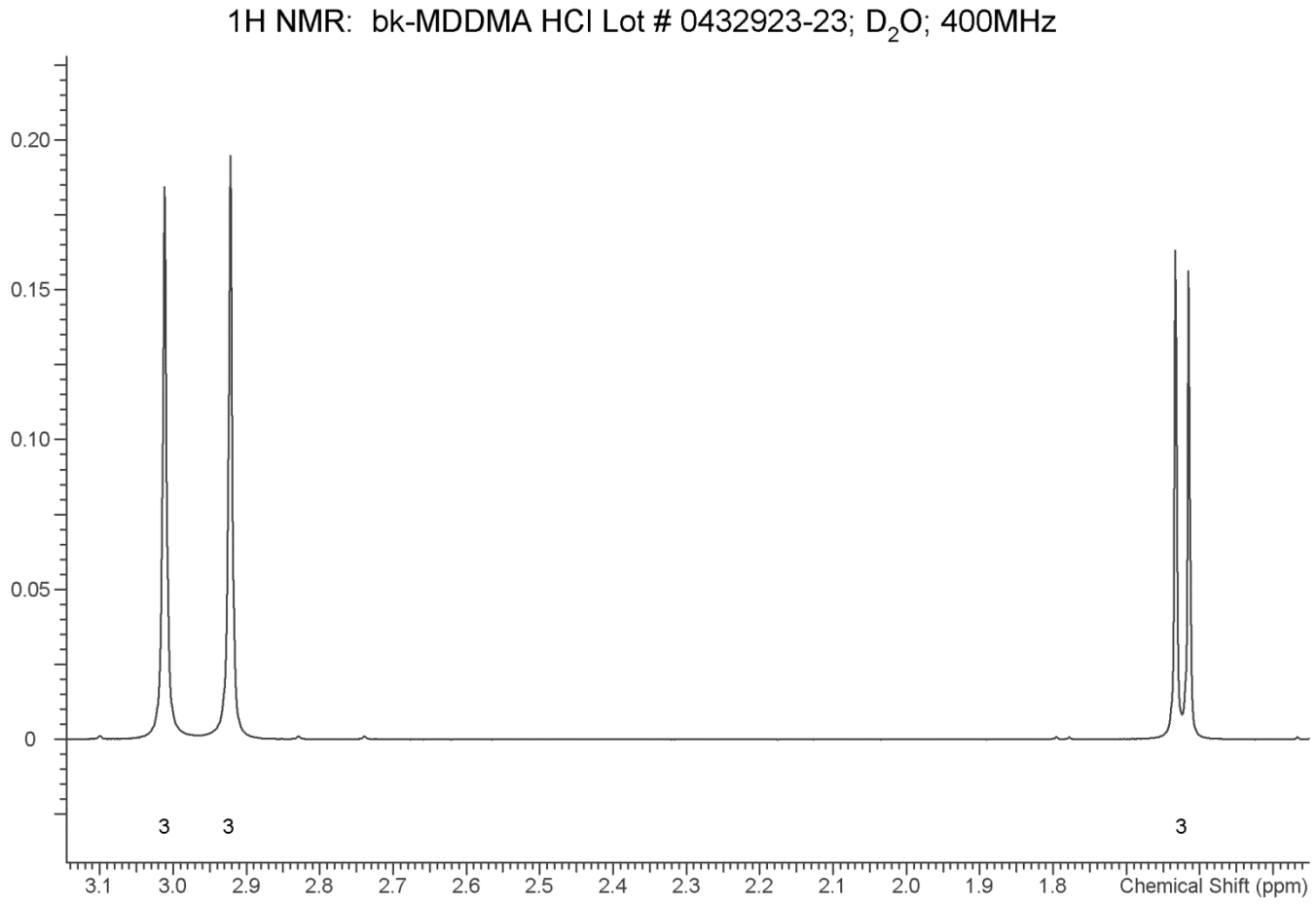


1H NMR: bk-MDDMA HCl Lot # 0432923-23; D_2O; 400MHz



1H NMR: bk-MDDMA HCl Lot # 0432923-23; D_2O; 400MHz



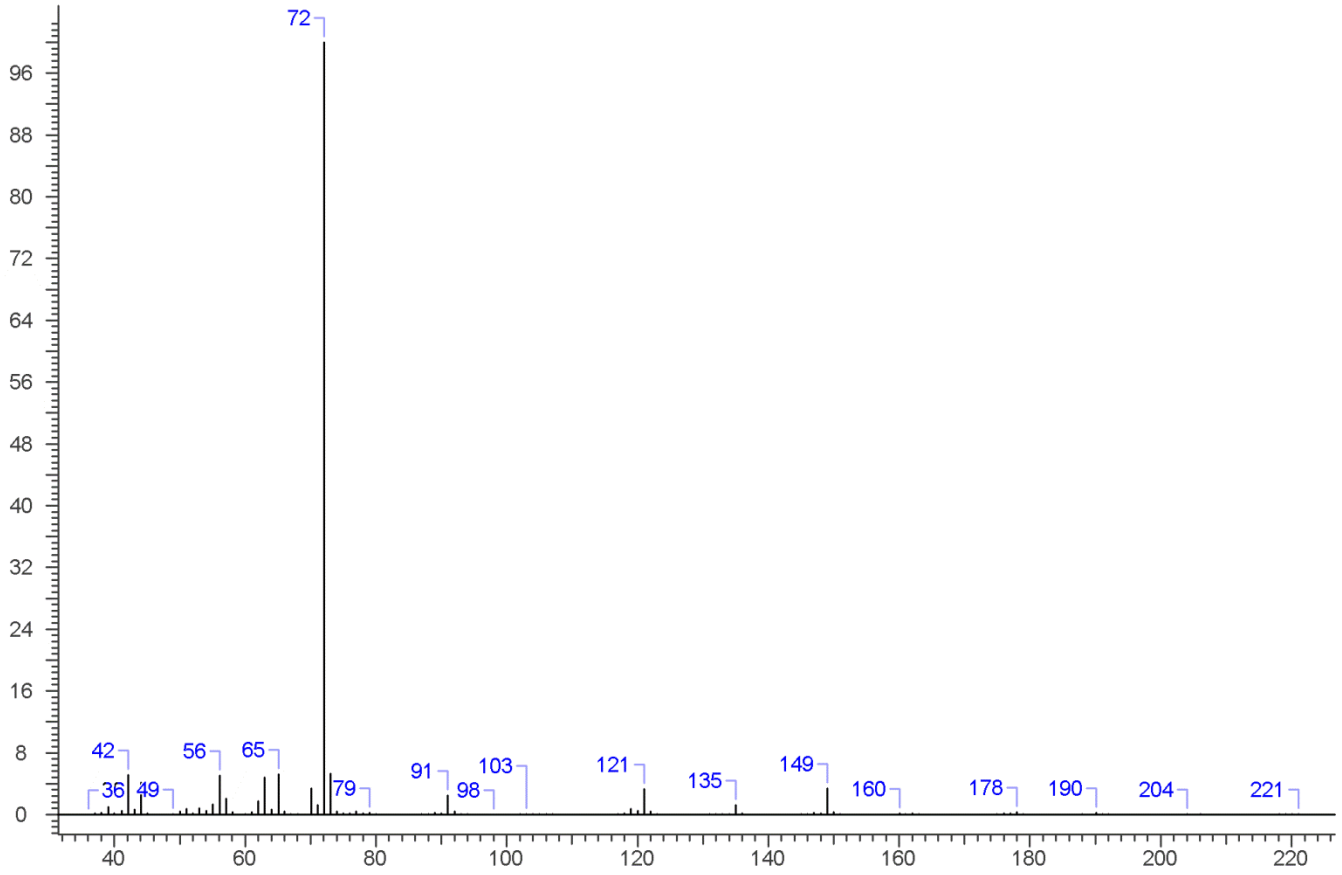


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~4 mg/mL base extracted into $CHCl_3$.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x .25mm x .25μm
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 µL 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

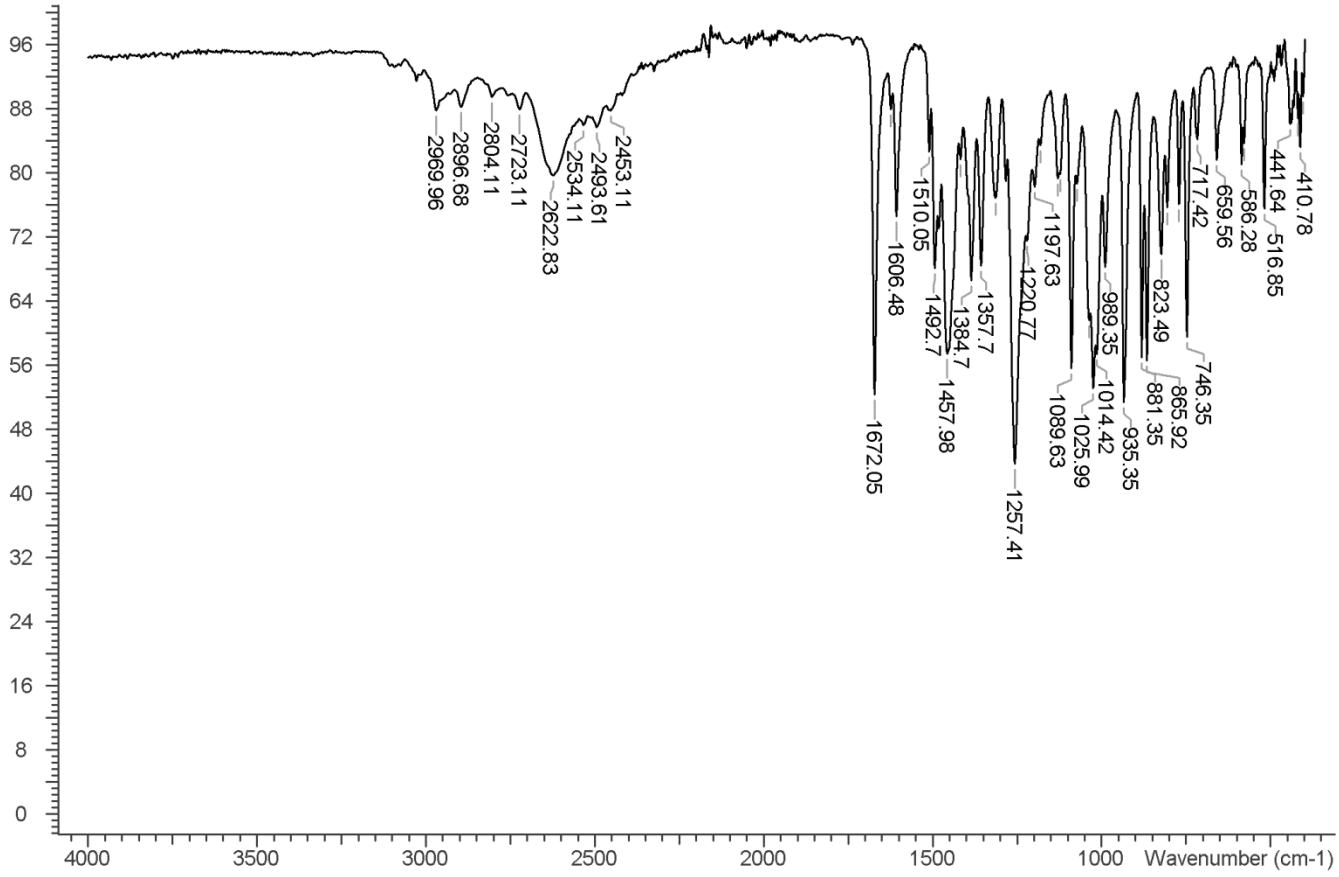


4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150

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



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