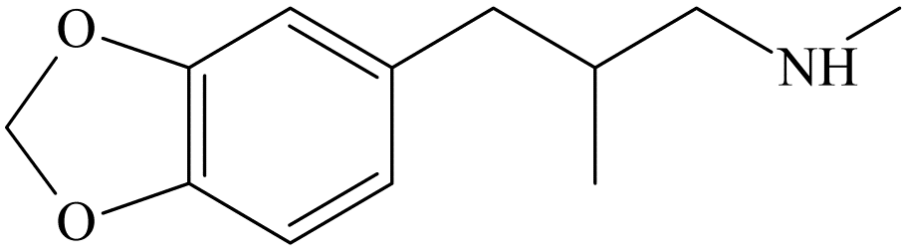
3,4-MDMA methylene homolog

Latest Revision: February 15, 2013



1. GENERAL INFORMATION

IUPAC Name: 3-(1,3-benzenodioxol-5-yl)-*N*,2-dimethylpropan-1-amine

CFR: Not Scheduled (as of 2/2013)

CAS #: N/A

Synonyms: 3,4-methylenedioxymethamphetamine methylene homolog, 3,4-methylenedioxymethamphetamine methyl homolog, Heliomethylamine

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max} (nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{12}H_{17}NO_2$	207	Not Determined
HCl	$C_{12}H_{17}NO_2 \cdot HCl$	243	144.9

3. ADDITIONAL RESOURCES

No resources identified as of 02/15/2013.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

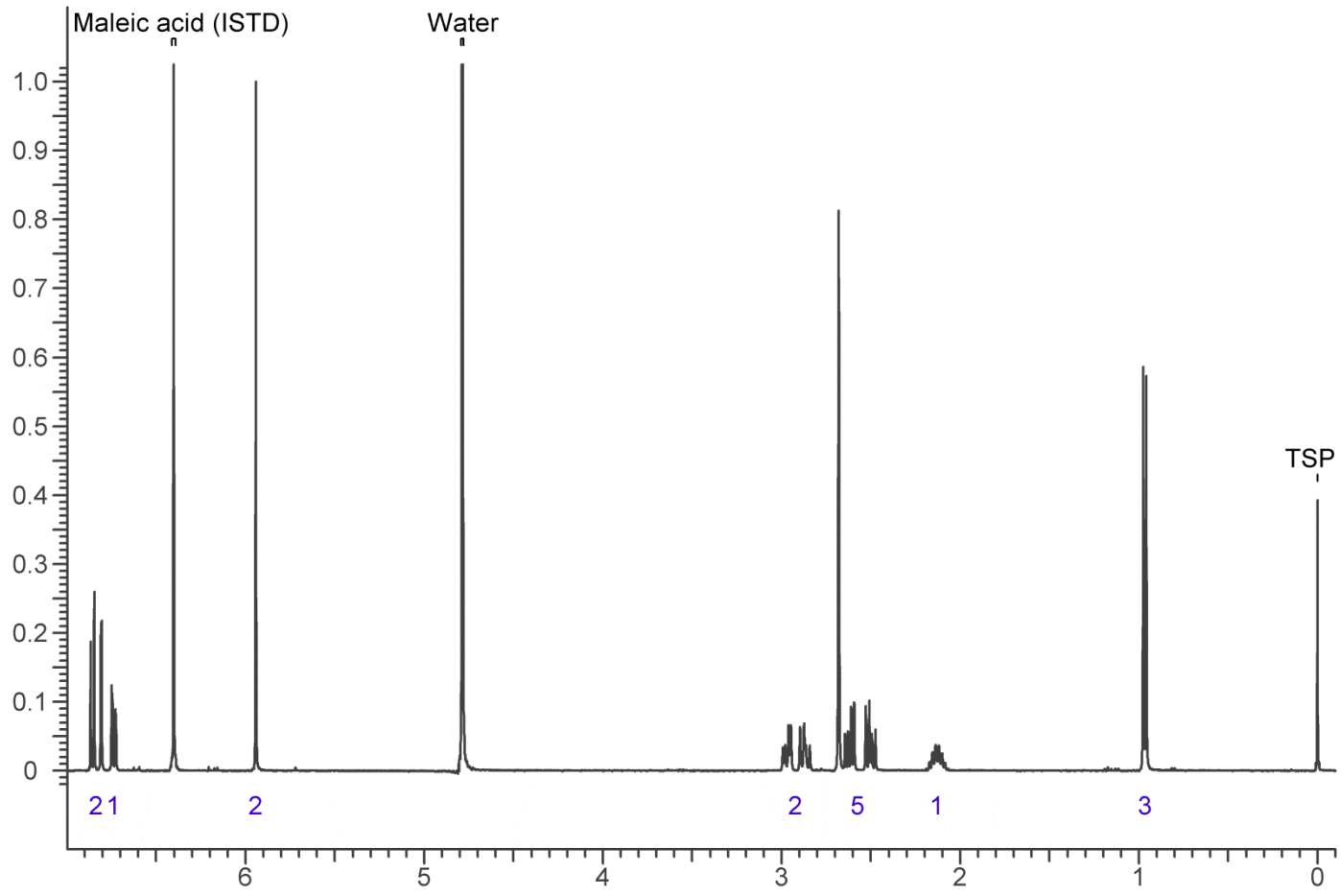
Method NMR D_2O

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
Number of scans (NT): 8
Number of steady state scans: 0
Oversampling: 4 or more
Shimming: automatic gradient shimming of Z1-4 shims
Phasing, Drift Correction: automatic or manual

^{1}H NMR: 3,4-MDMA methylene homolog HCl; lot 0430048-14, D_2O, 400 MHz



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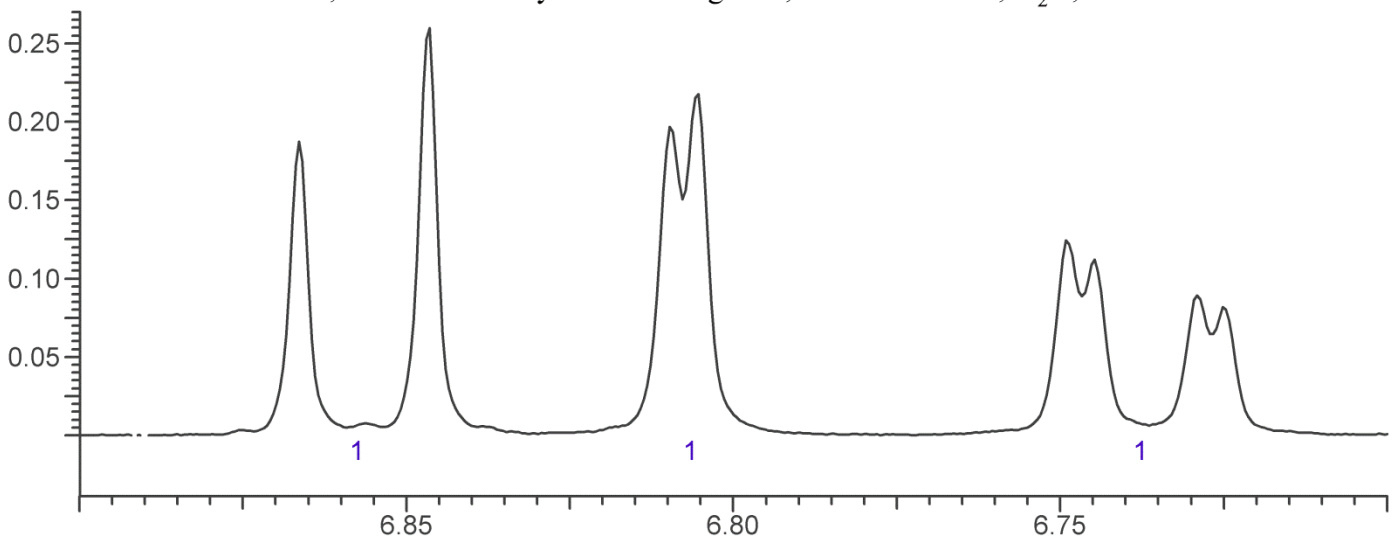

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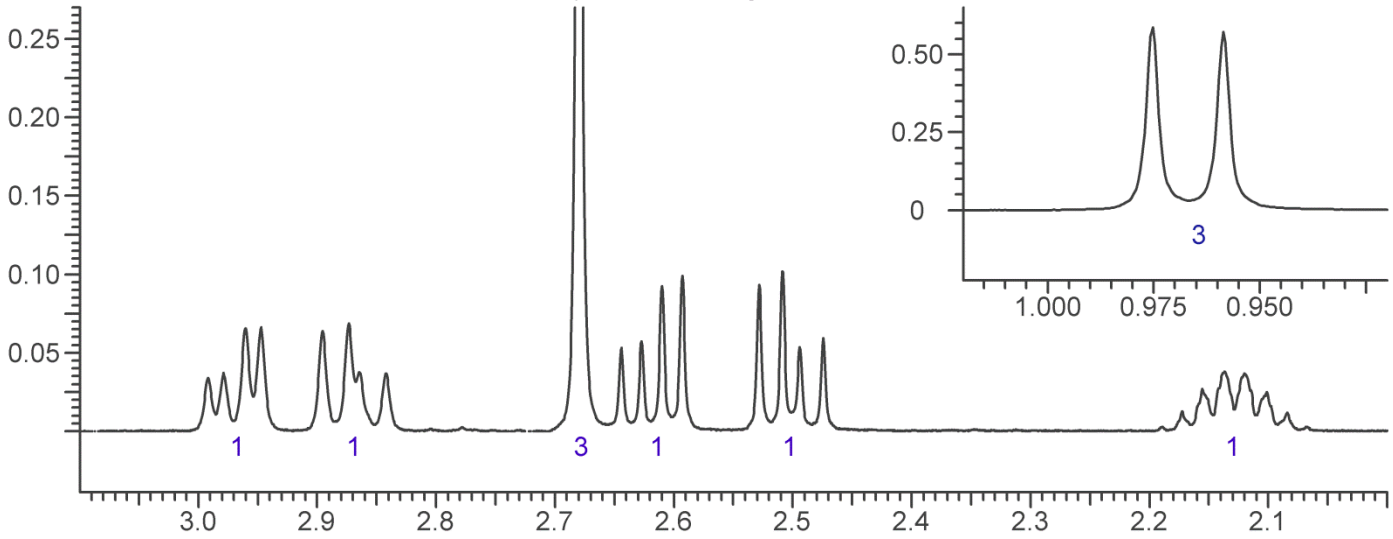
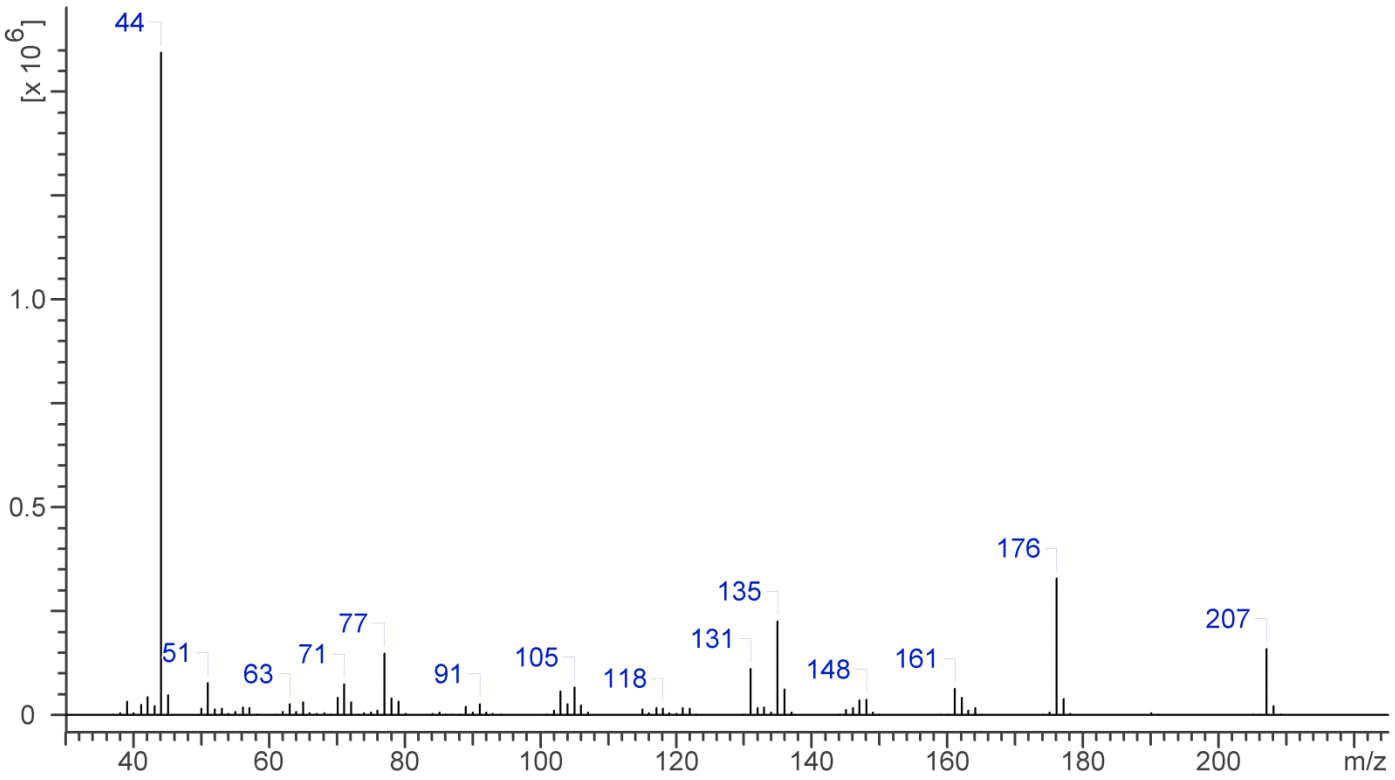


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~4 mg/mL in chloroform.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	HP-1 MS; 30m x 0.25 mm x 0.25 µm
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 µL injected
MS Parameters:	Mass scan range: 30-550 amu Threshold: 90 Tune file: stune.u Acquisition mode: scan
Retention Time:	9.471 min

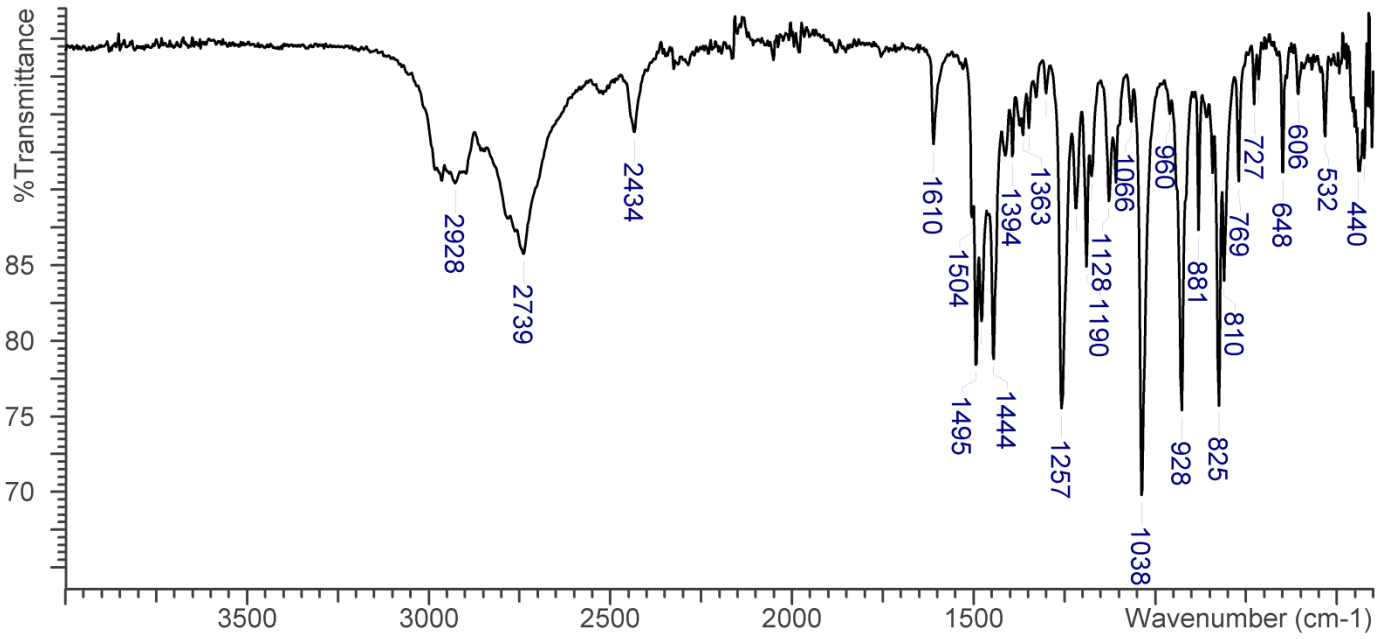
GC-MS: 3,4-MDMA methylene homolog HCl; lot 0430048-14



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): 3,4-MDMA methylene homolog HCl; lot 0430048-14



FTIR ATR (Diamond, 3 bounce): 3,4-MDMA methylene homolog HCl; lot 0430048-14