

1. GENERAL INFORMATION

IUPAC Name:	4-methylhexan-2-amine
CFR:	Not Scheduled (4/2013)
CAS #:	105-41-9
Synonyms:	1,3-dimethylamylamine, methylhexanamine, 2-amino-4-methylhexane, 1,3-dimethylpentylamine, 4-methyl-2-hexylamine
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 ₇ H ₁₇ N	115	Not Determined
HCl	C ₇ H ₁₇ N · HCl	151	122.9

3. ADDITIONAL RESOURCES

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

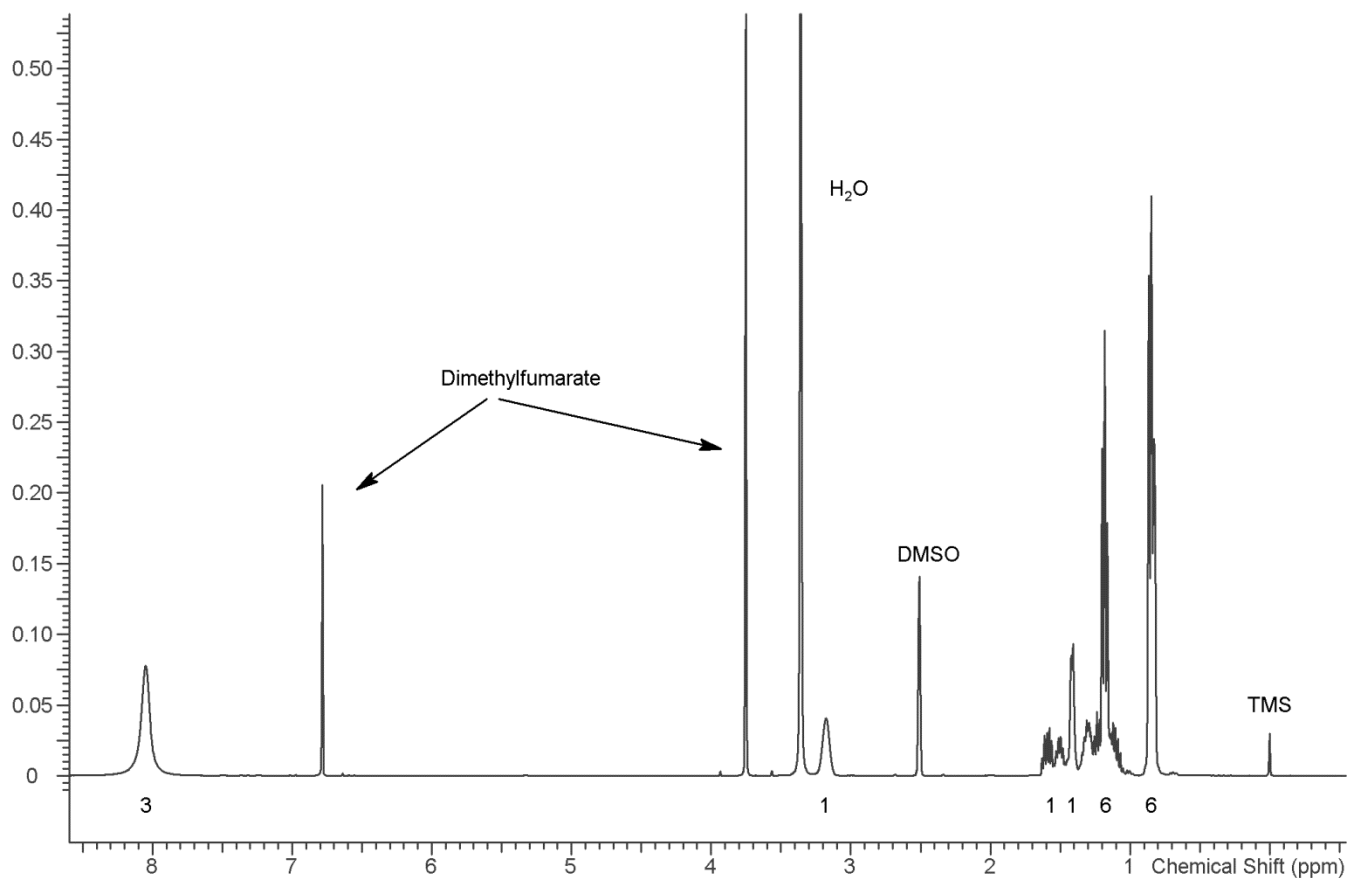
Method NMR Dimethylfumarate/DMSO

Sample Preparation: Dilute analyte to ~10 mg/mL in DMSO containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

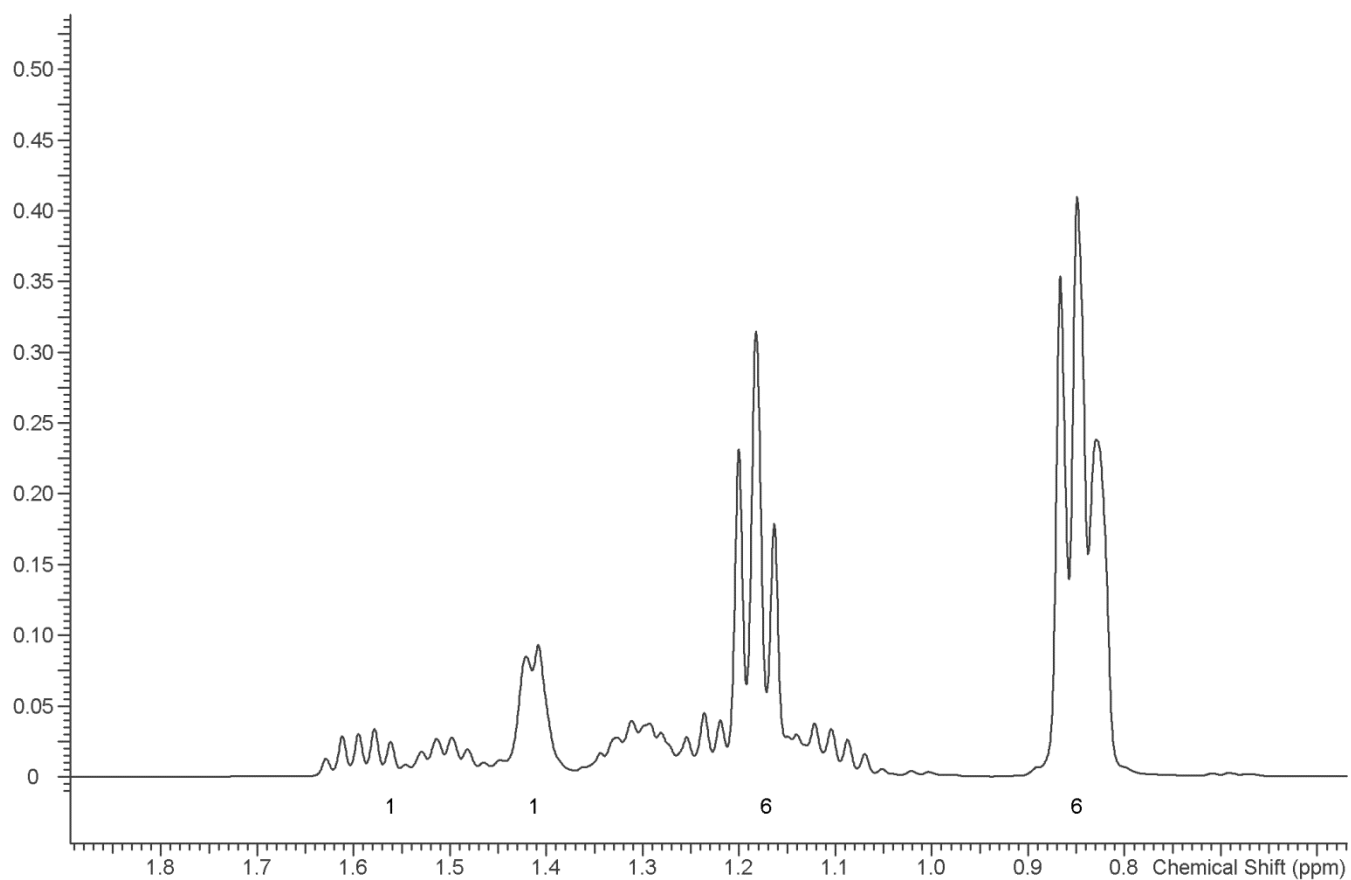
Instrument: 400 MHz NMR spectrometer

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

1H NMR: DMAA HCl Lot N1P7; DMSO; 400MHz

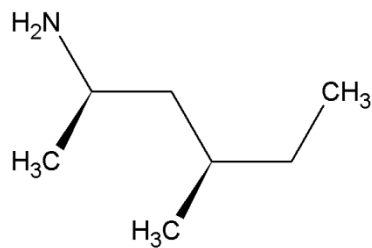
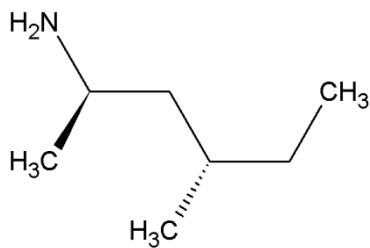


1H NMR: DMAA HCl Lot N1P7; DMSO; 400MHz



NMR Analytical Observation

DMAA has two chiral carbons; therefore, two diastereomers are possible. Diastereomers produce slightly different chemical shifts for proton and carbon. Both diastereomers are present in the above spectra.



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 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 .25mm x .25 μ 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 μ L injected

MS Parameters: Mass scan range: 30-550 amu

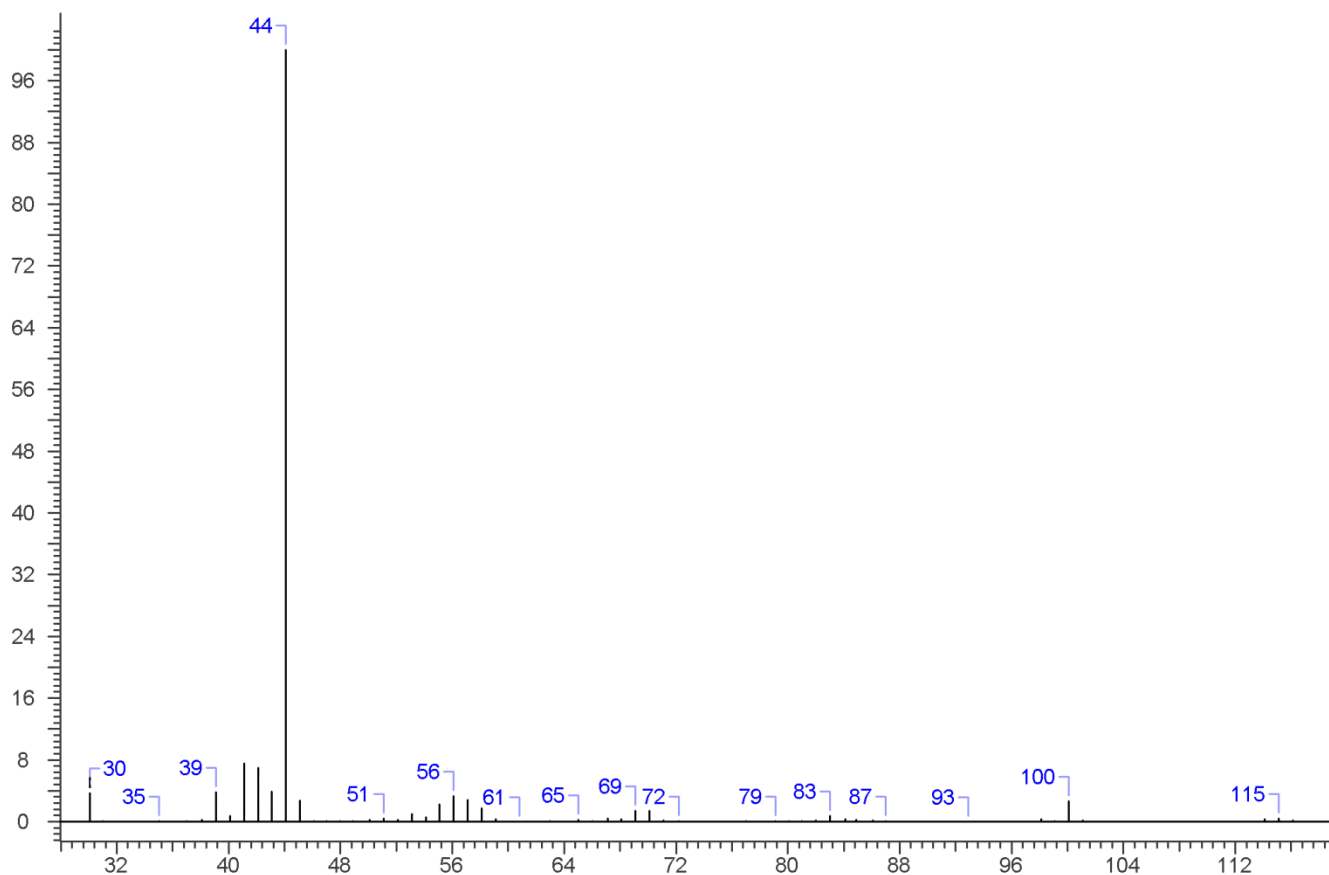
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 2.100 minutes

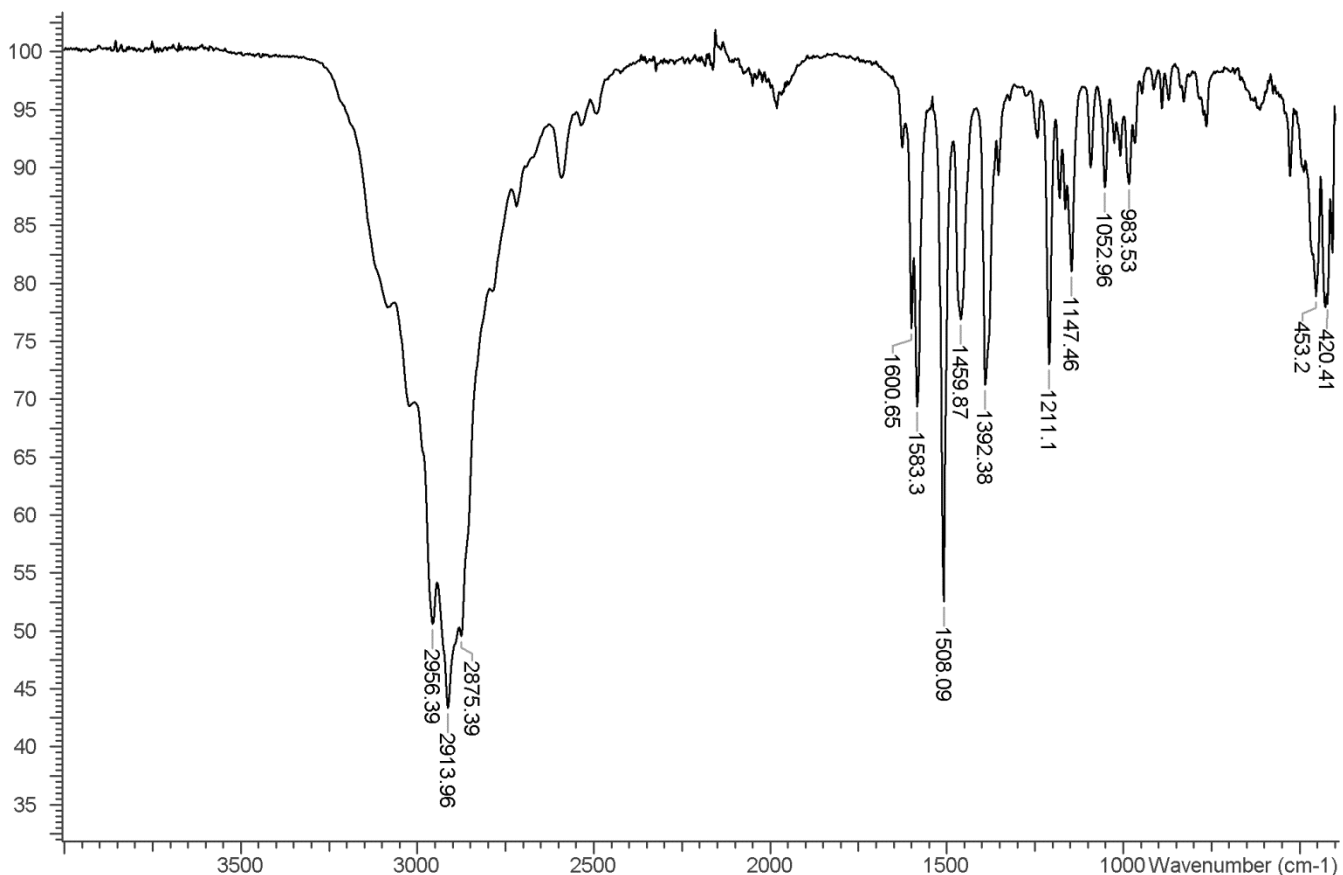
EI Mass Spectrum: DMAA HCl Lot N1P7



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): DMAA HCl Lot N1P7



FTIR ATR (Diamond, 3 Bounce): DMAA HCl Lot N1P7

