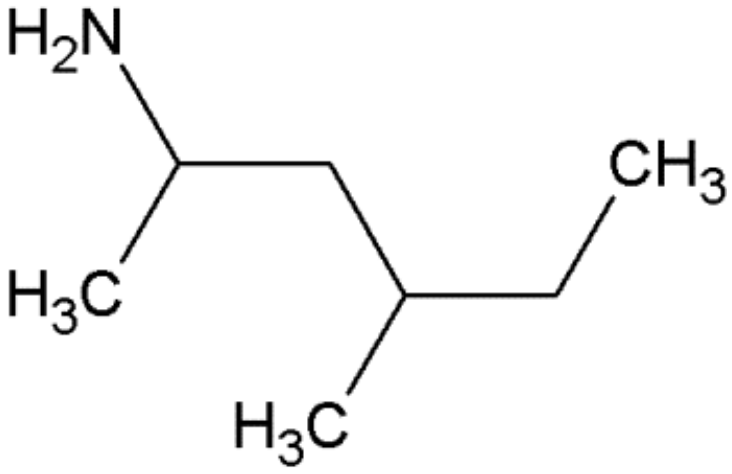


1. GENERAL INFORMATION

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	$C_7H_{17}N$	115	Not Determined
HCl	$C_7H_{17}N \cdot HCl$	151	122.9

3. ADDITIONAL RESOURCES

Wikipedia

4. QUALITATIVE DATA

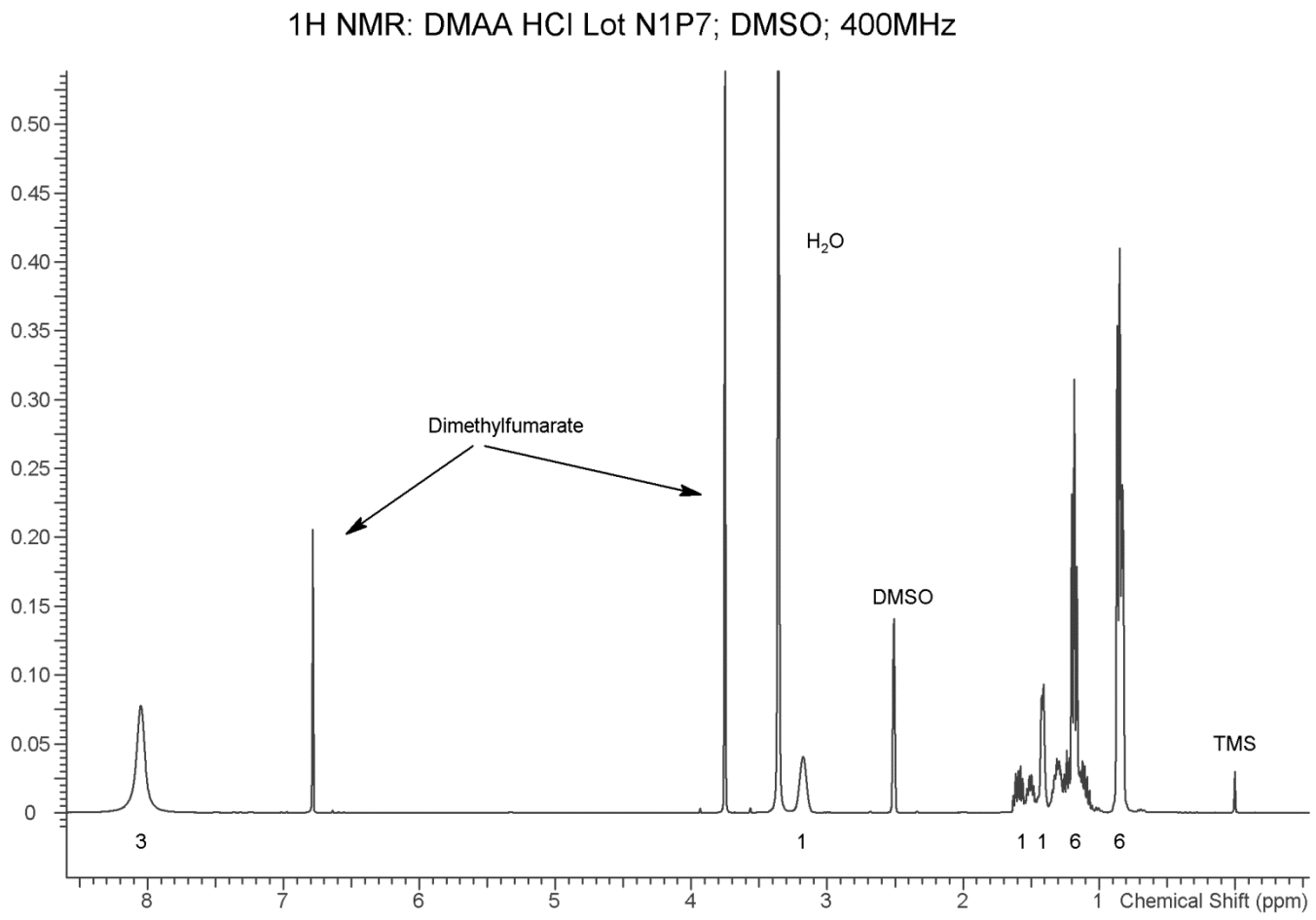
4.1 NUCLEAR MAGNETIC RESONANCE

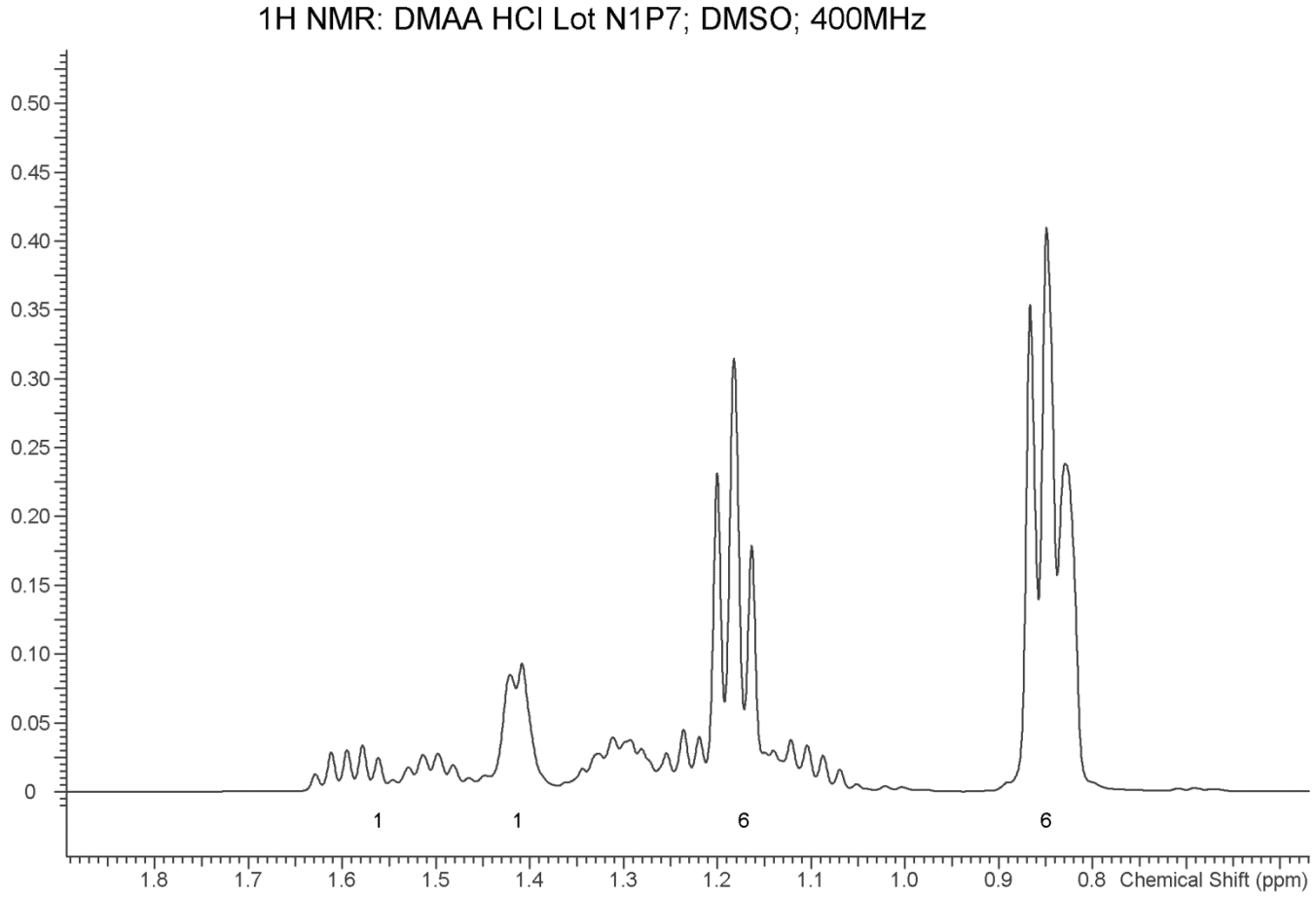
Method NMR Dimethylfumarate/DMSO

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

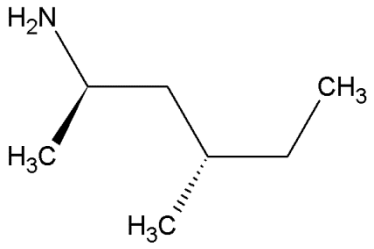
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

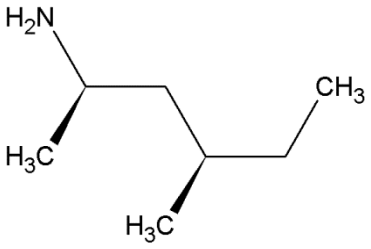




NMR Analytical Observation

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



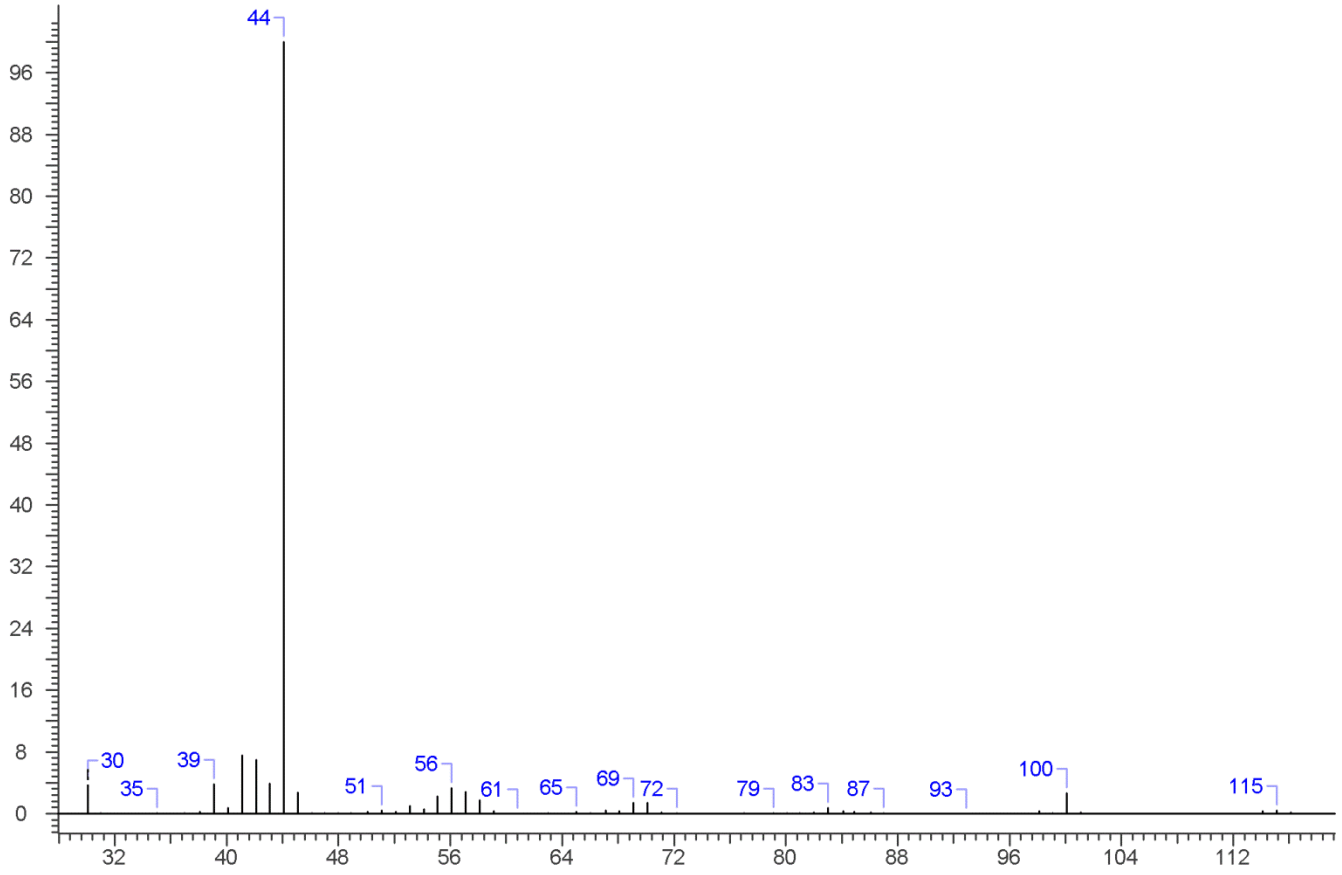


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL base extracted into chloroform

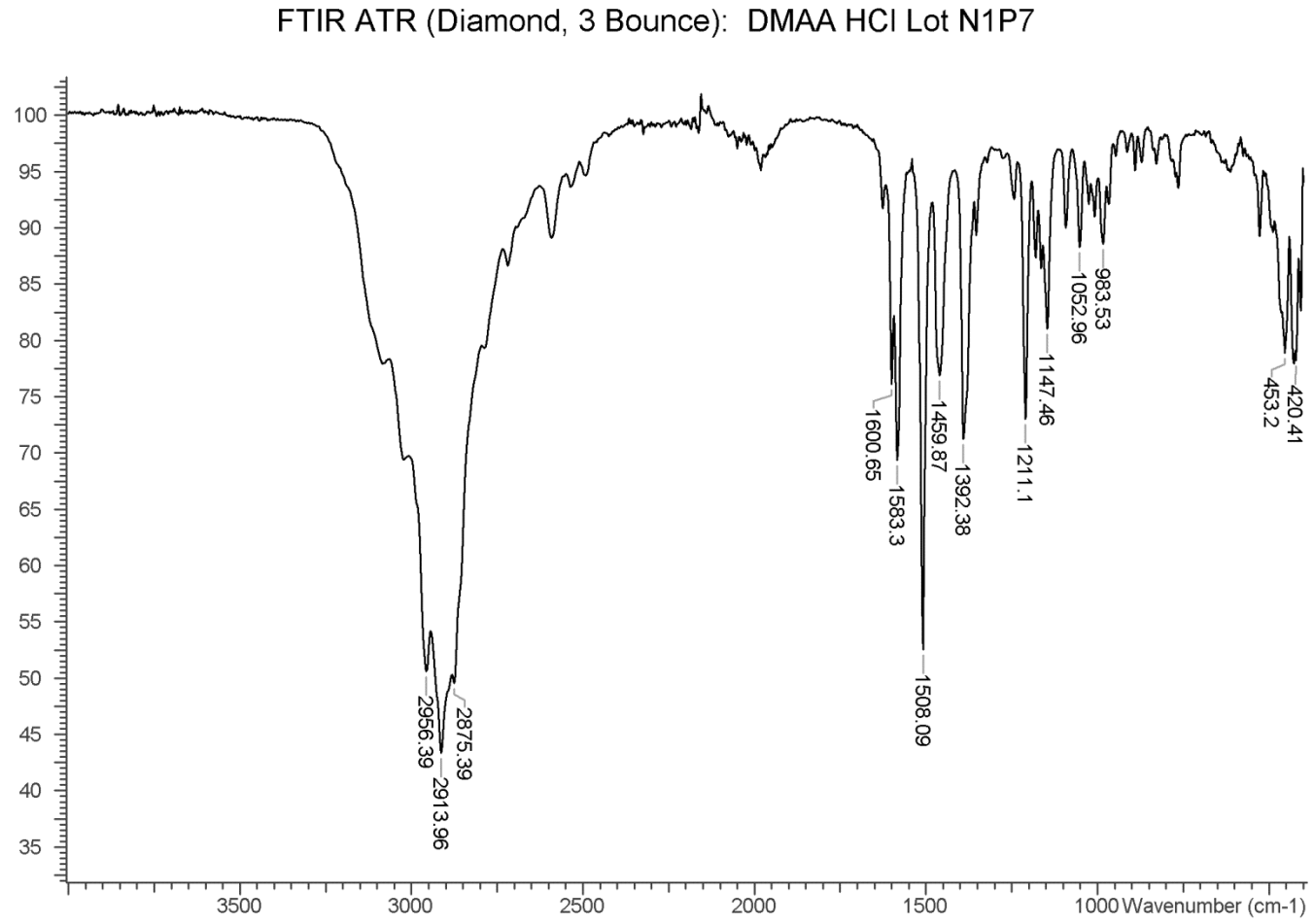
Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x .25mm x .25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp to 300°C at 12°C/min 3) Hold final temperature for 9.0 min
Injection Parameters:	Split Ratio = 20:1, 1 µL 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