

1. GENERAL INFORMATION

IUPAC Name:	3,4-dichloro- <i>N</i> -{[1-(dimethylamino)cyclohexyl]methyl}benzamide
CFR:	Not Scheduled (5/2013)
CAS#:	55154-30-8 (base)
Synonyms:	N/A
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	$C_{16}H_{22}Cl_2N_2O$	329*	Not Determined
HCl	$C_{16}H_{22}Cl_2N_2O \cdot HCl$	365	219.6

*Monoisotopic mass: 328

3. ADDITIONAL RESOURCES

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~10 mg/mL in CDCl₃ containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

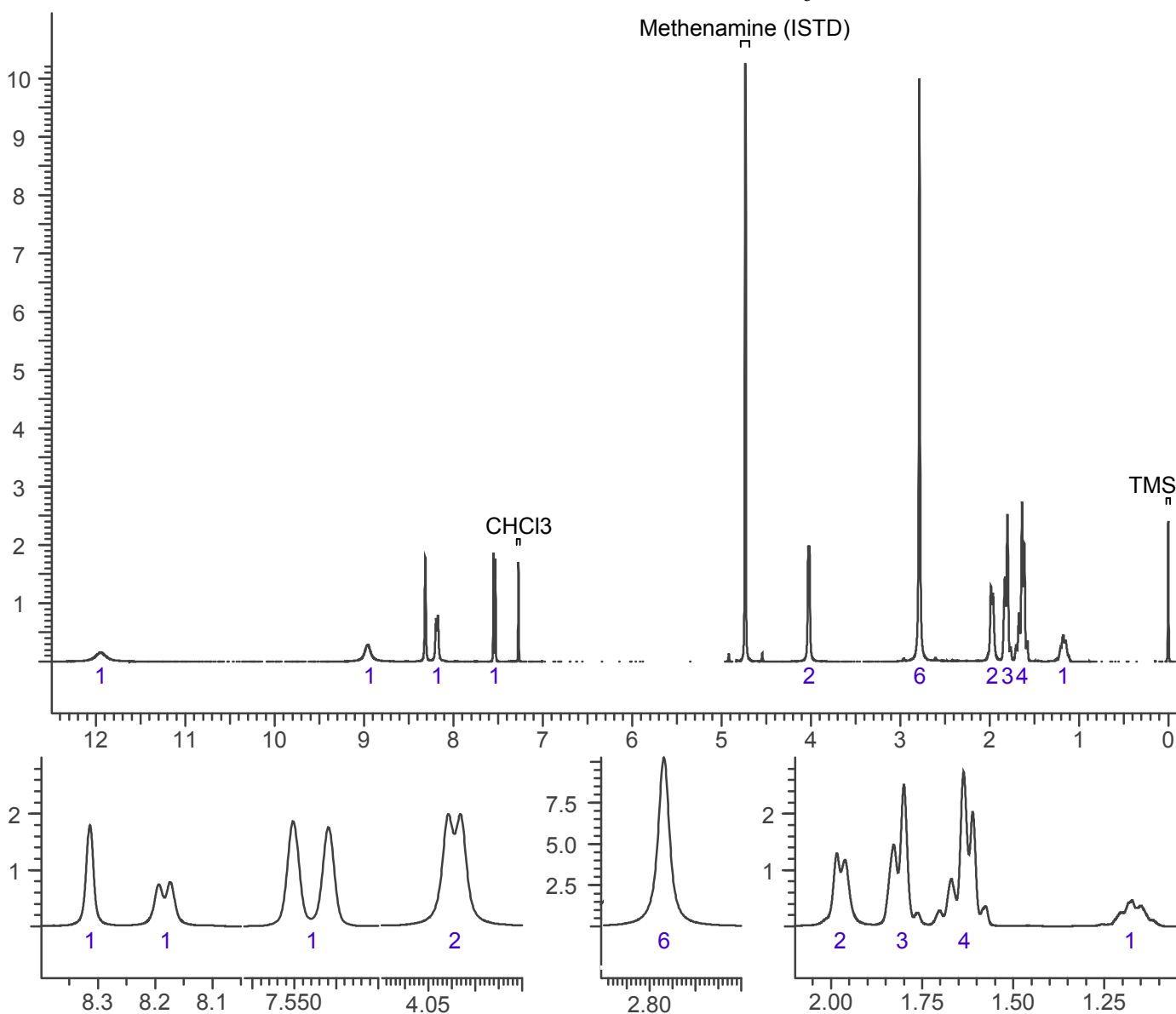
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

¹H NMR: AH-7921 HCl; Lot RM-022813-2; CDCl₃; 400 MHz



4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 1 mg/mL in chloroform.

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

Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 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

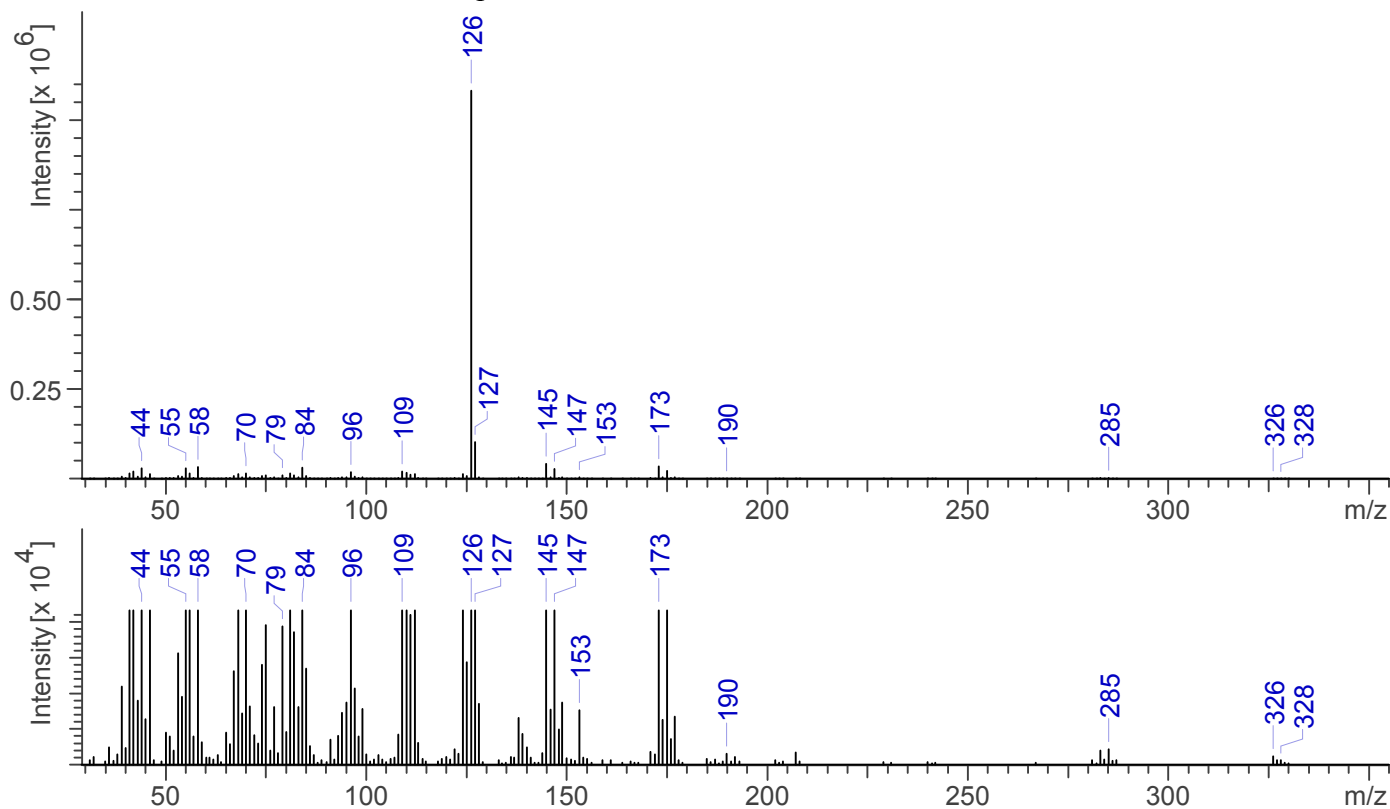
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 16.385 min

EI Mass Spectrum: AH-7921 HCl; Lot RM-022813-2



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 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 bounce): AH-7921 HCl; Lot RM-022813-2

