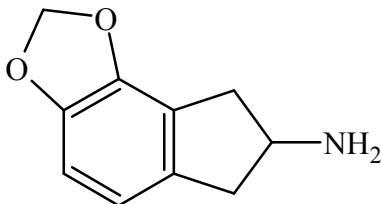




4,5-MDAI

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

IUPAC Name:	7,8-dihydro-6H-indeno[4,5-d][1,3]dioxol-7-amine
CFR:	Not Scheduled (11/2013)
CAS#:	Unavailable
Synonyms:	4,5-methylenedioxy-2-aminoindane
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Retention Index:	Pending
UV_{max} (nm):	202.3, 283.7

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₀ H ₁₁ NO ₂	177	Not Determined
HCl	C ₁₀ H ₁₁ NO ₂ · HCl	213	243.0



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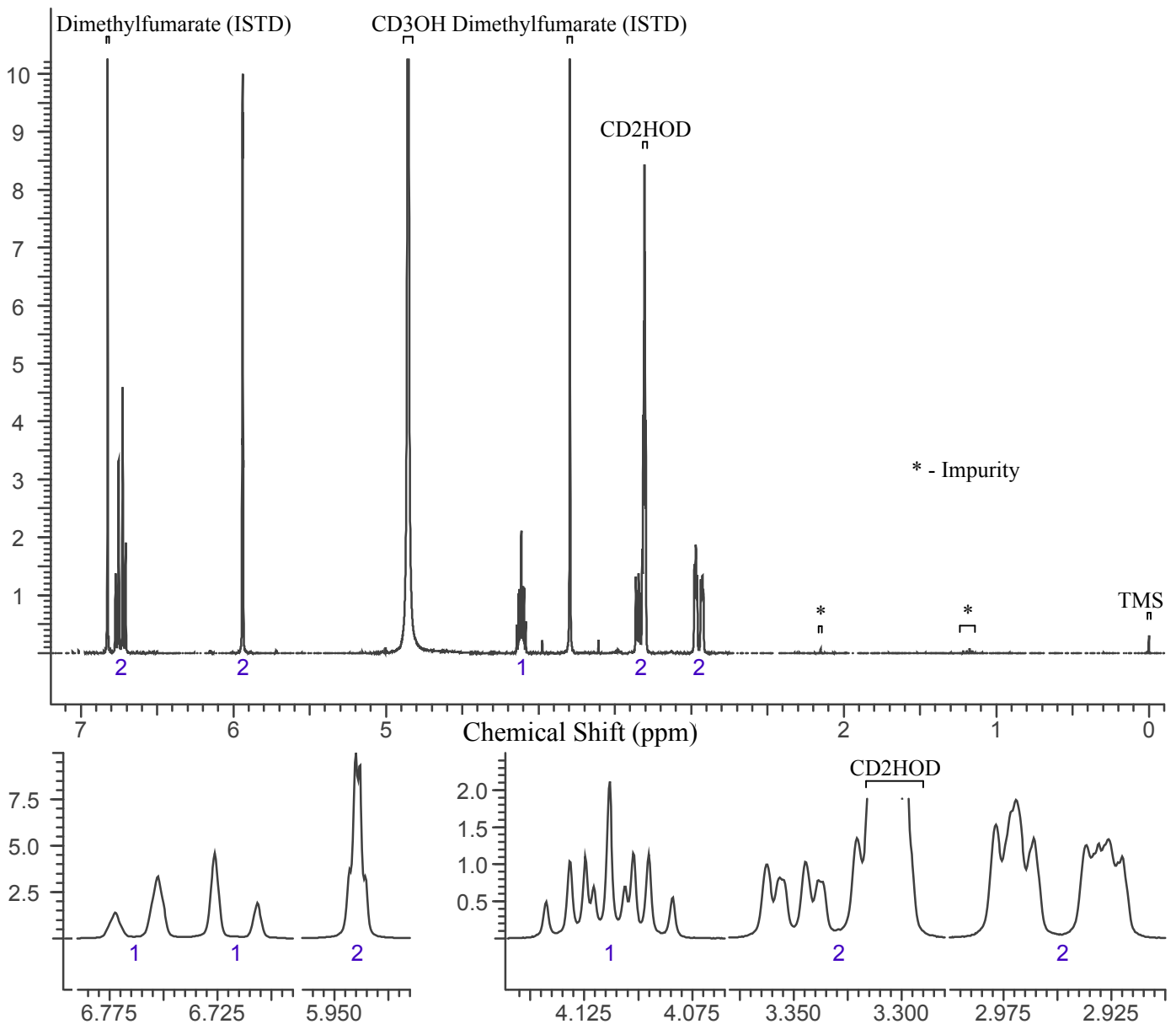


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterated methanol (CD₃OD) 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: 4,5-MDAI HCl; Lot N16-P75C; CD₃OD; 400 MHz





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3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 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 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

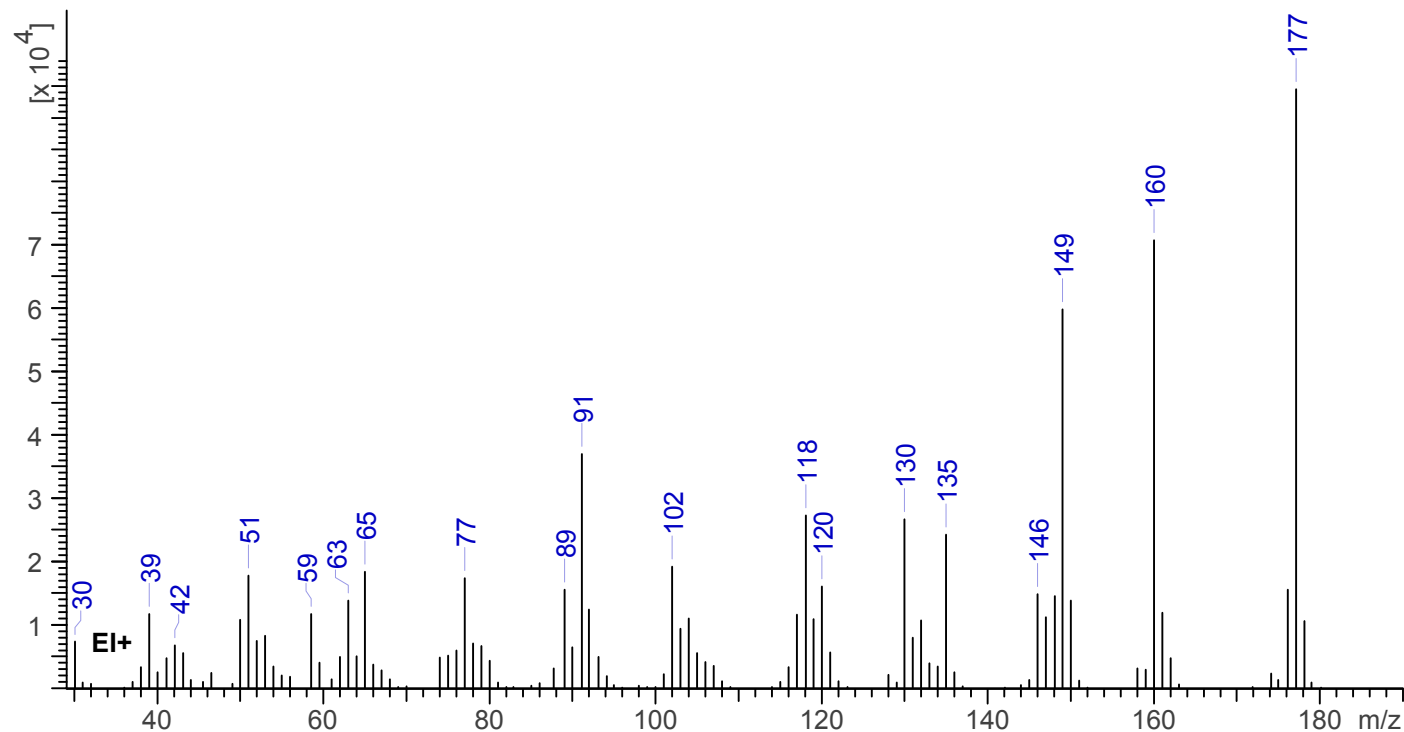
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 8.261 min

EI Mass Spectrum: 4,5-MDAI HCl; Lot N16-P75C





4,5-MDAI

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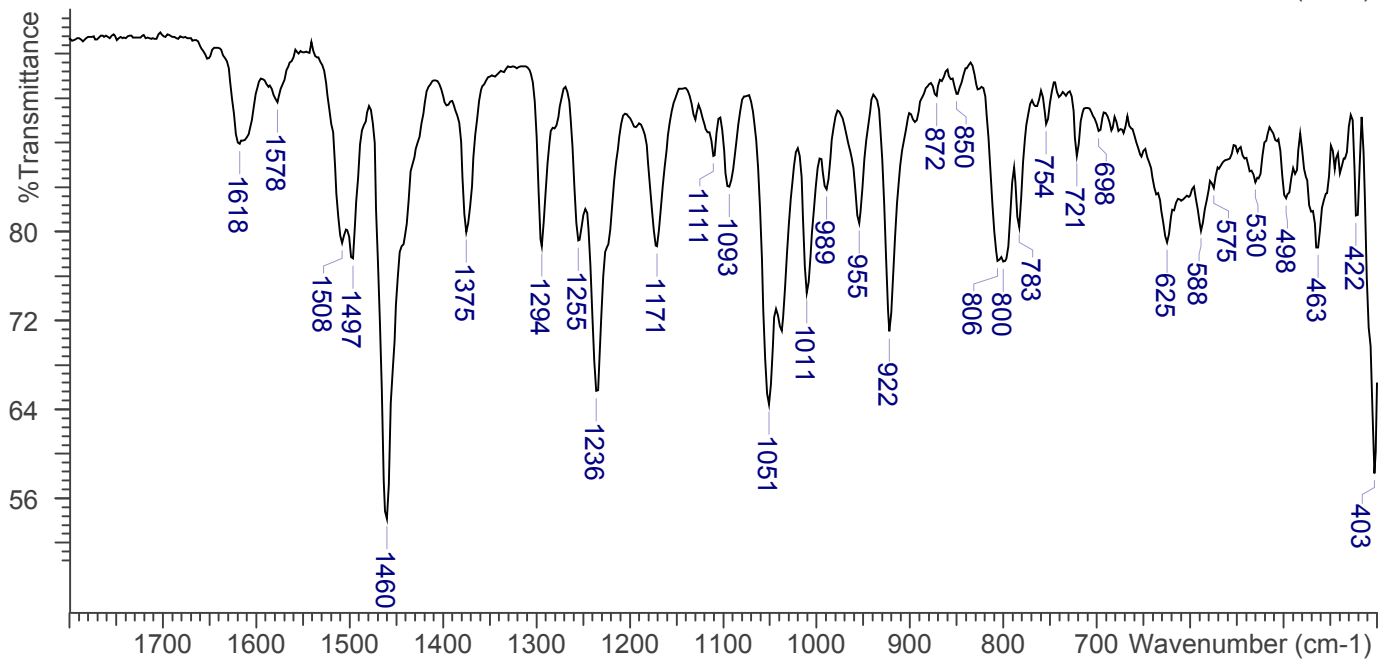
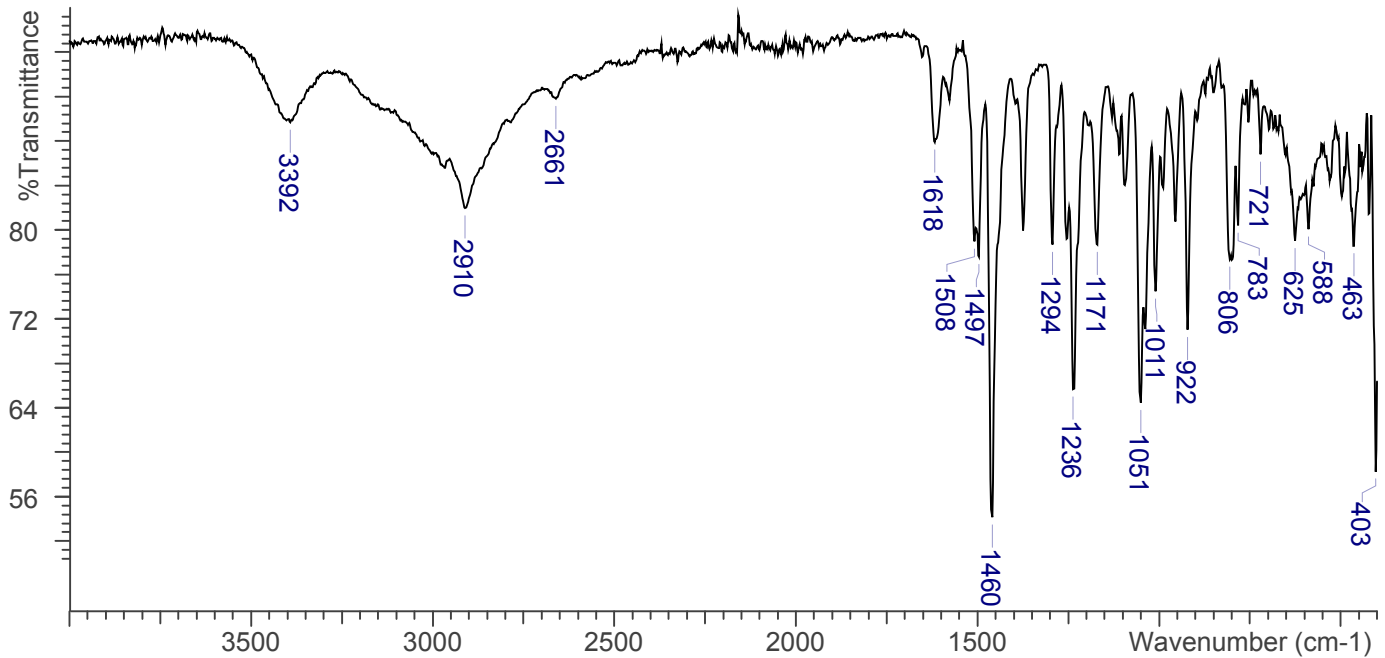


3.3 INFRARED SPECTROSCOPY (FTIR)

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): 4,5-MDAI HCl; Lot N16-P75C





4,5-MDAI

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4. **ADDITIONAL RESOURCES**

Casale, J. F.; Hays, P. A. Characterization of the "Methylenedioxy-2-aminoindans". *Microgram J.* **2011**, 8(2), 43-52.