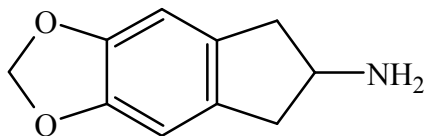




## 5,6-MDAI

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	6,7-dihydro-5H-indeno[5,6][1,3]dioxol-6-amine
<b>CFR:</b>	Not Scheduled (11/2013)
<b>CAS#:</b>	132741-81-2 (base), 155344-90-4 (HCl)
<b>Synonyms:</b>	5,6-methylenedioxy-2-aminoindane, MDAI
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	Beige powder (HCl)
<b>Retention Index:</b>	Pending
<b>UV<sub>max</sub> (nm):</b>	294.2

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>10</sub> H <sub>11</sub> NO <sub>2</sub>	177	Not Determined
HCl	C <sub>10</sub> H <sub>11</sub> NO <sub>2</sub> · HCl	213	256-275*

\* Charring occurred after 275 °C.



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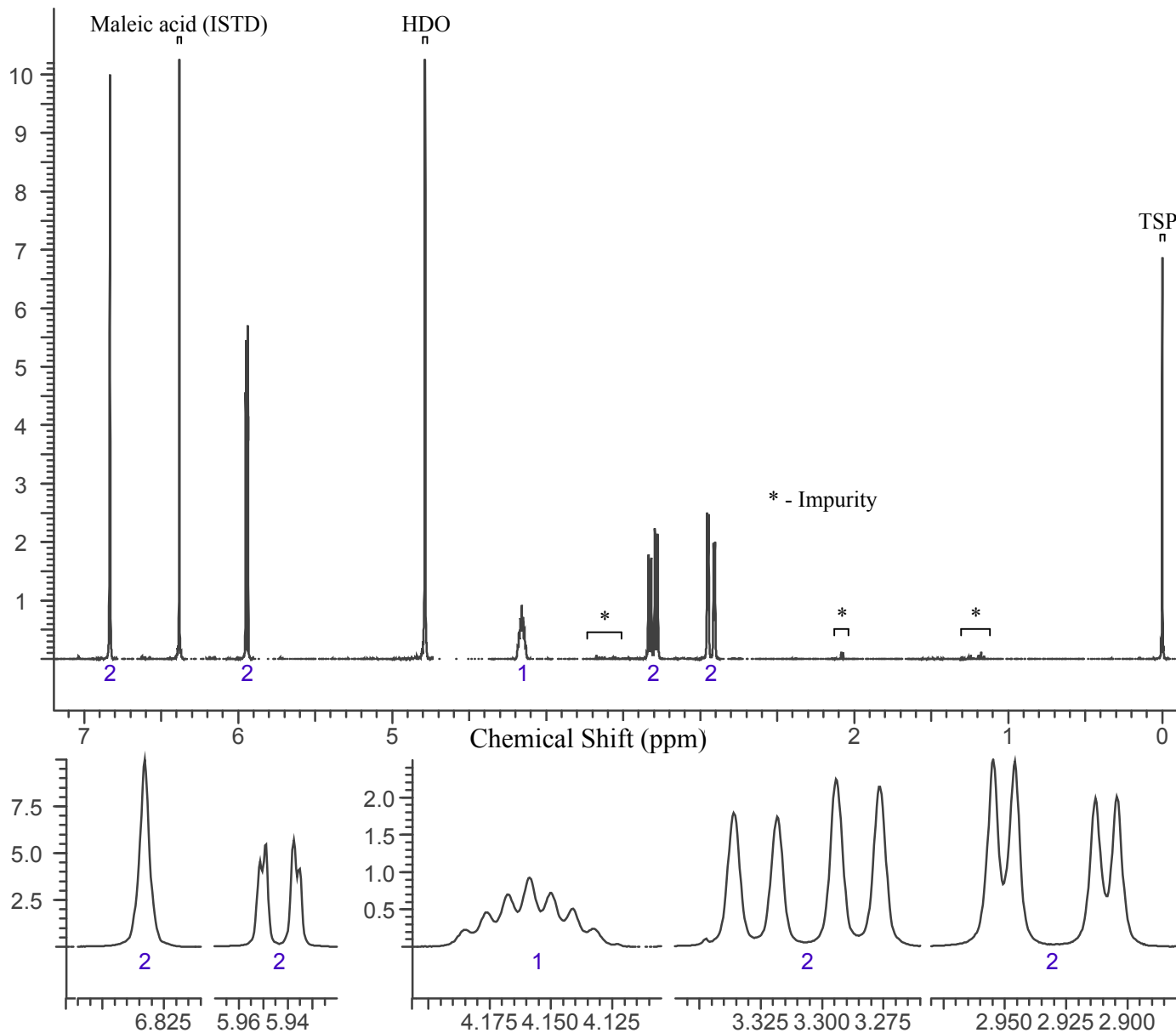


### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~10 mg/mL in deuterium oxide (D<sub>2</sub>O) containing TSP for 0 ppm reference and maleic acid 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  
<sup>1</sup>H NMR: MDAI HCl; Lot 2011DEA003-29A; D<sub>2</sub>O; 400 MHz





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### 3.2 Gas Chromatography/Mass Spectrometry

**Sample Preparation:** Dilute analyte ~ 4 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  $\mu$ 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  $\mu$ L injected

**MS Parameters:** Mass scan range: 34-550 amu

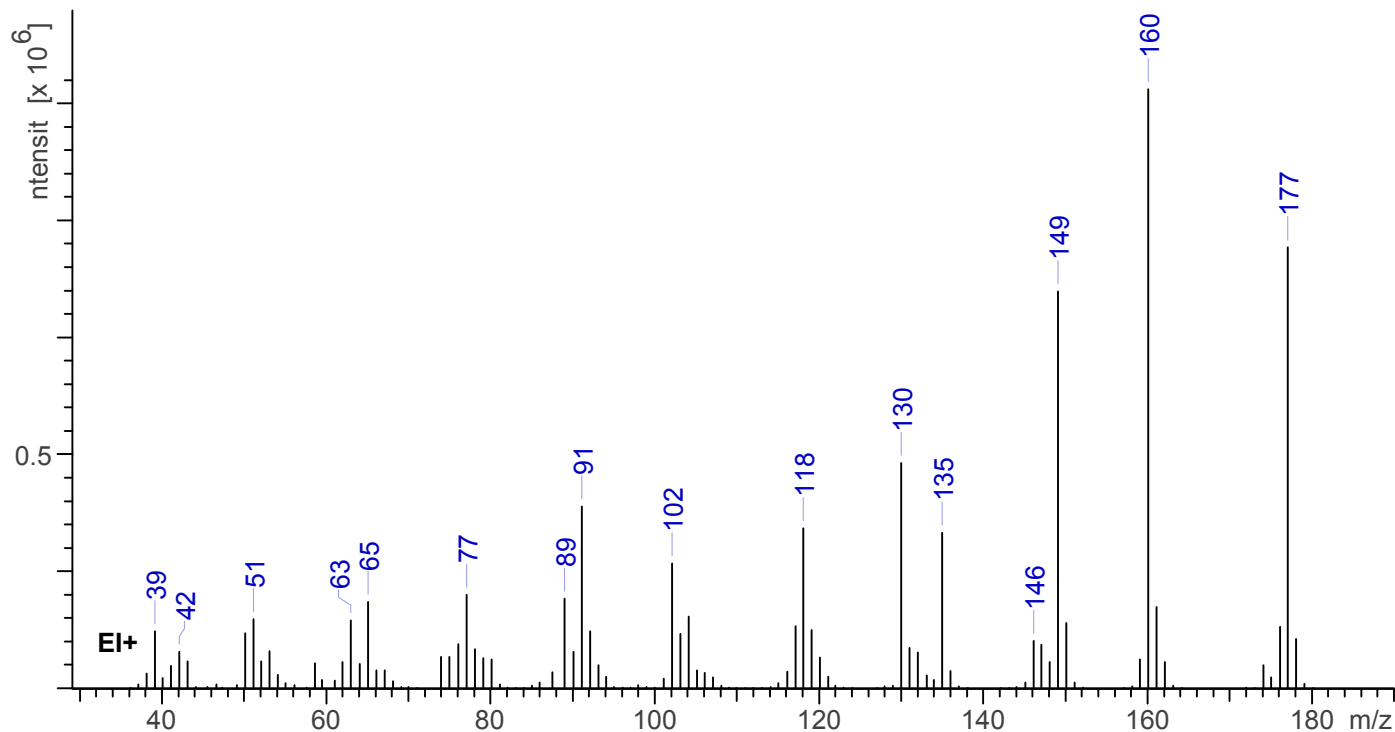
Threshold: 90

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 8.565 min

EI Mass Spectrum: MDAI HCl; Lot 2011DEA003-29A





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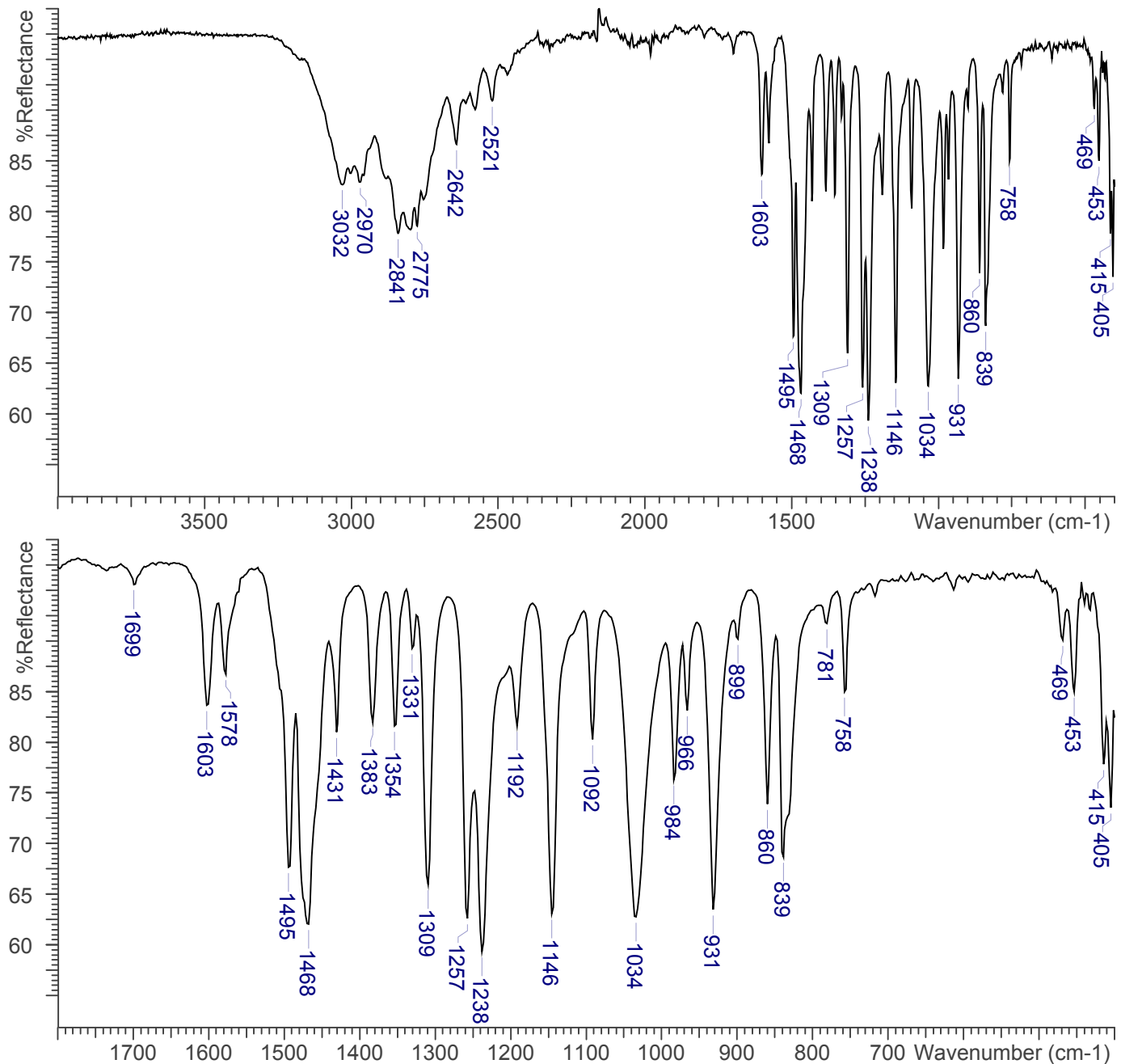


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): MDAI HCl; Lot 2011DEA003-29A





## 5,6-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.

[Forendex](#)

[Wikipedia](#)