

1. GENERAL INFORMATION

IUPAC Name:	5-iodo-2,3-dihydro-1H-inden-2-amine
CFR:	Not Scheduled (7/2013)
CAS#:	132367-76-1
Synonyms:	5IAI; 5-IAI; 2,3-dihydro-5-iodo-1H-inden-2-amine
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 ₉ H ₁₀ IN	259	Not Determined
HCl	C ₉ H ₁₀ IN · HCl	295	299-301

3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

Sample Preparation: Dilute analyte to ~5 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

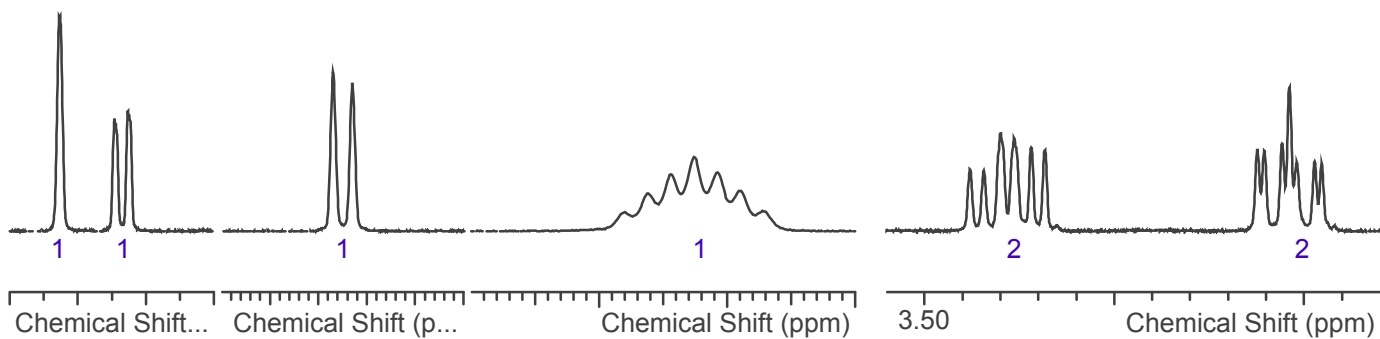
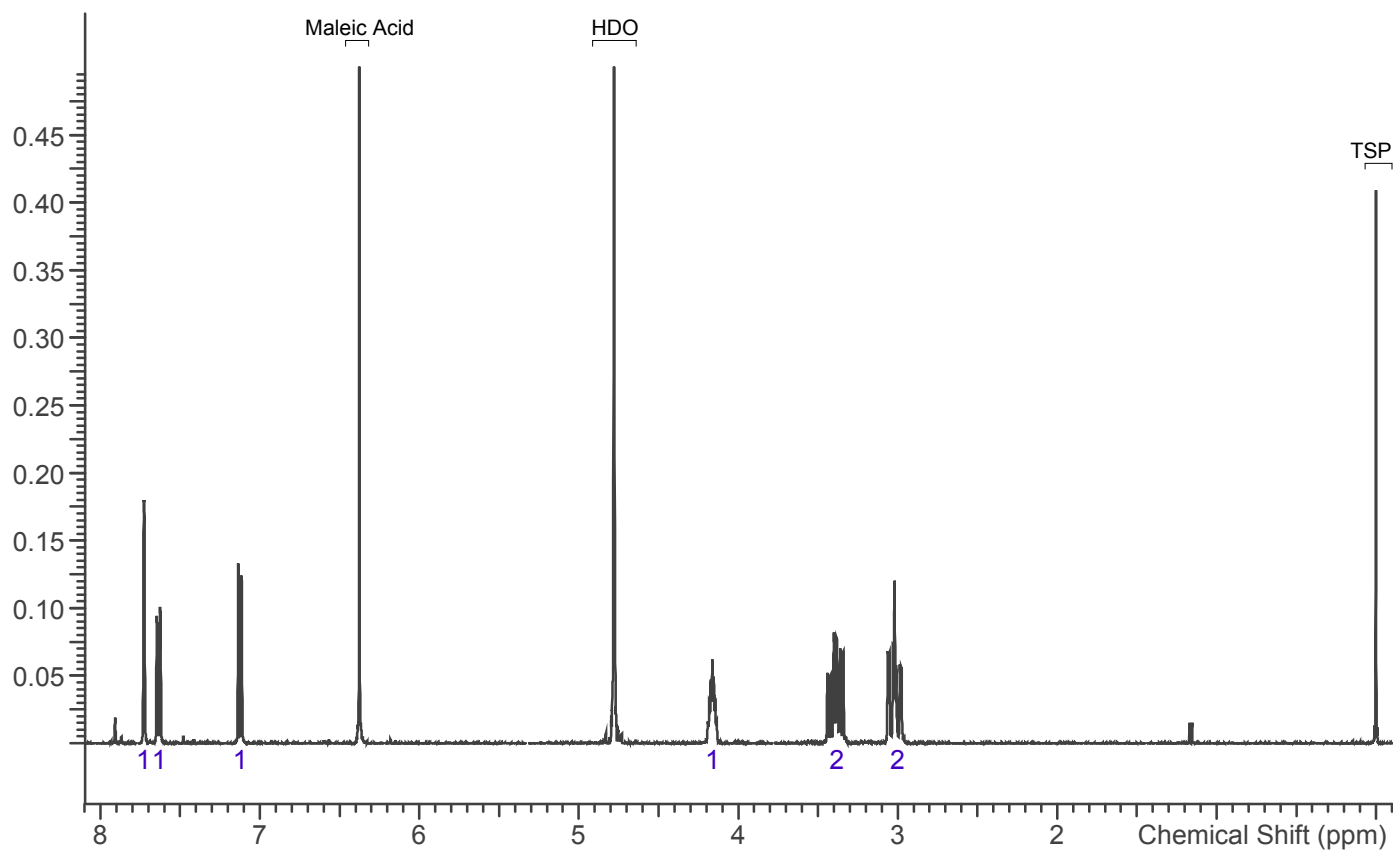
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 45 seconds

¹H NMR: 5-iodo-2-aminoindan HCl Lot N17-P44A; D₂O; 400MHz

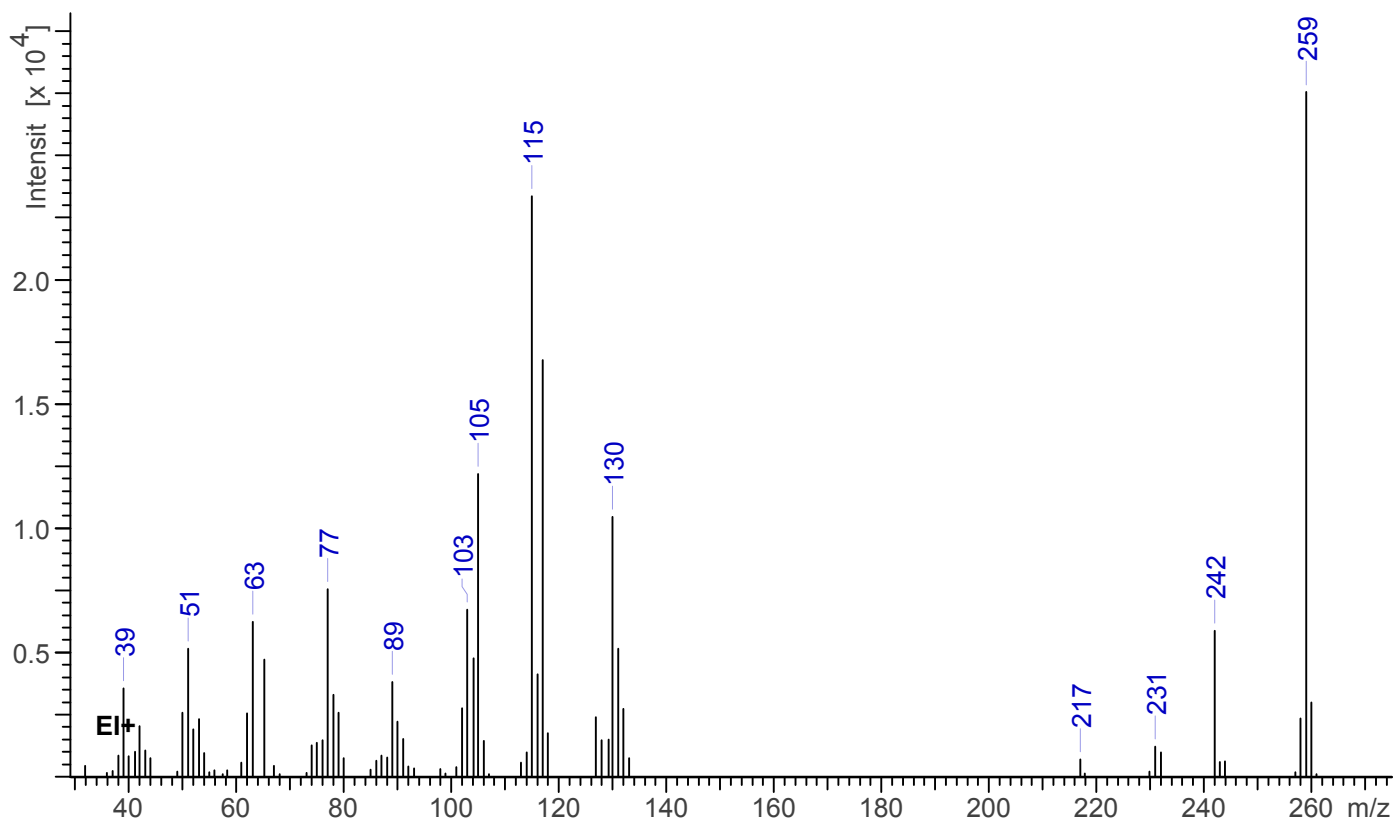


4.2 Gas Chromatography/Mass Spectrometry

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: 8.932 min

EI Mass Spectrum: 5-iodo-2-aminoindan HCl Lot N17-P44A



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): 5-iodo-2-aminoindan HCl Lot N17-P44A

