

1. GENERAL INFORMATION

IUPAC Name: 1-amino-1-(4-fluorophenyl)propan-2-one

CFR: Not Scheduled (7/2013)

CAS#: Not Available

Synonyms: 4-FIC

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 FNO	167	Not Determined
HCl	C ₉ H ₁₀ FNO · HCl	203	211.1

3. ADDITIONAL RESOURCES

[Forendex](#)

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.

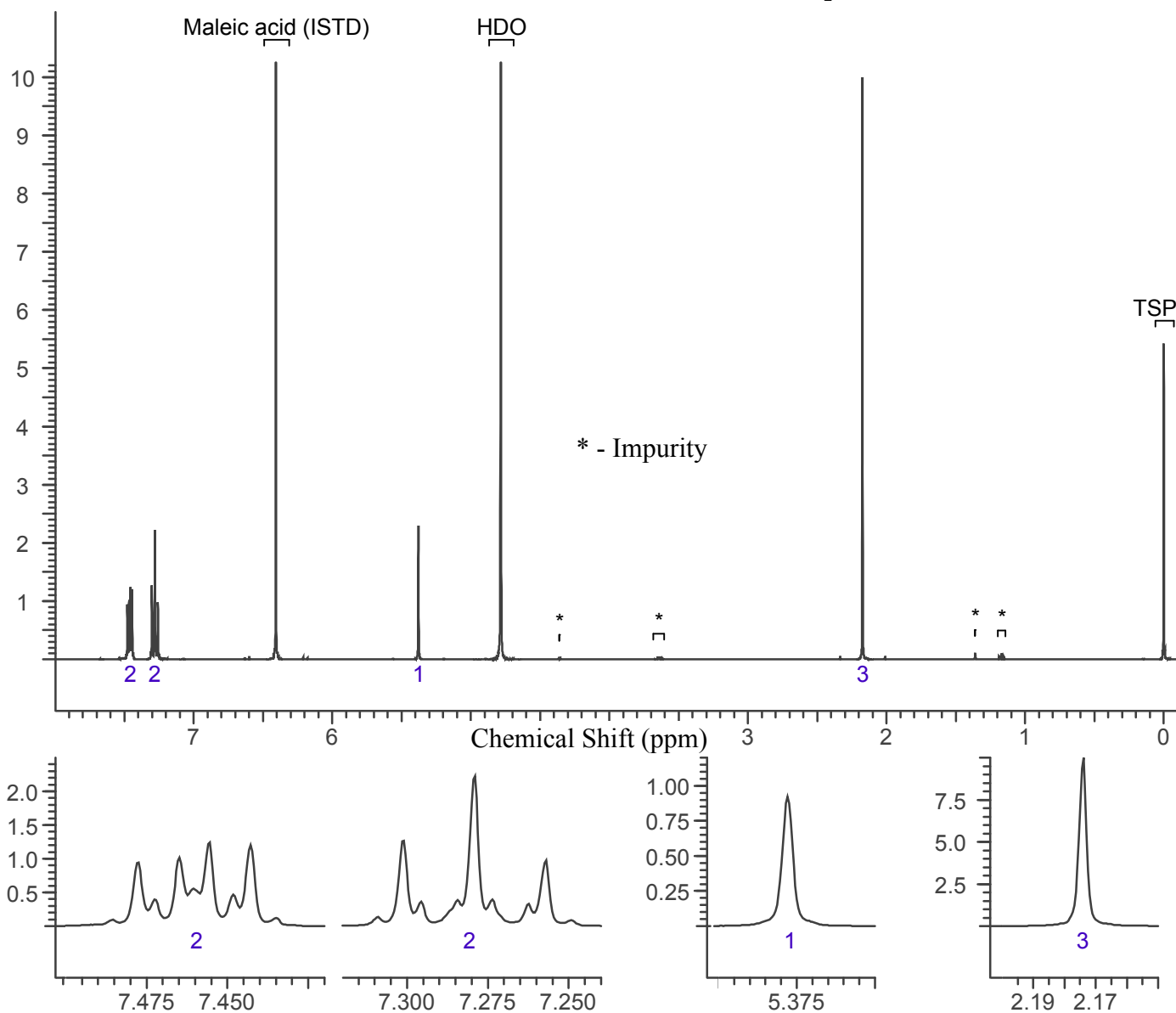
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 45 seconds

¹H NMR: 4-Fluoroisocathinone HCl; Lot 0433668-11; D₂O; 400 MHz



4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 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 30.0 min

Injection Parameters: Split Ratio = 25:1, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu

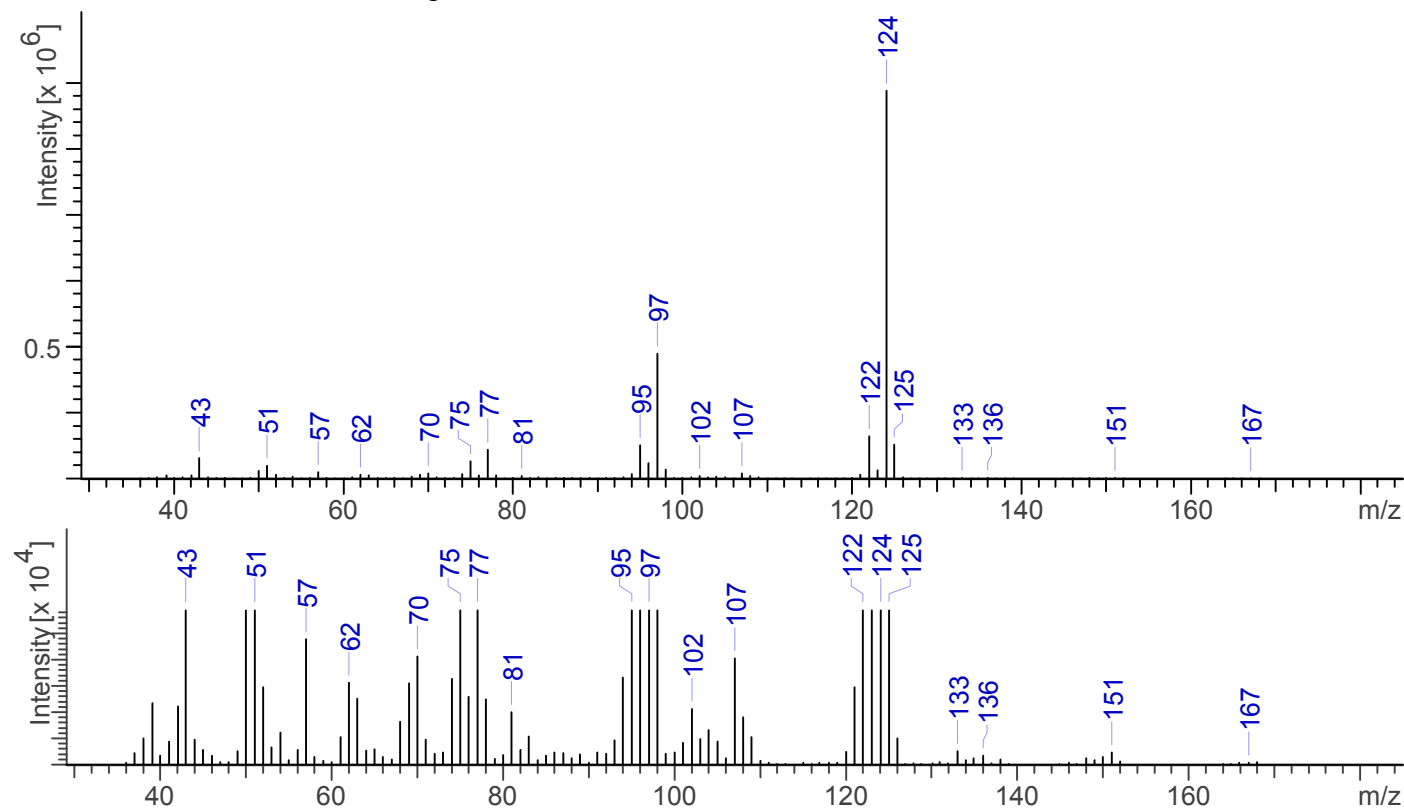
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 5.367 min

EI Mass Spectrum: 4-Fluoroisocathinone HCl; Lot 0433668-11



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): 4-Fluoroisocathinone HCl; Lot 0433668-11

