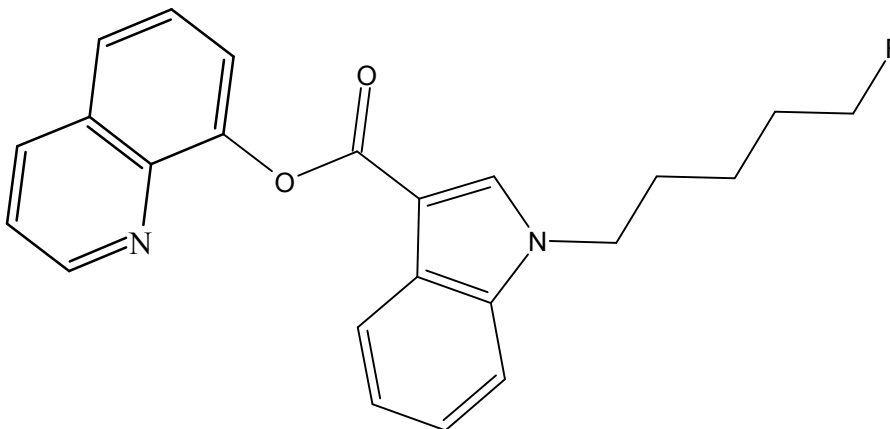




5-Fluoro-PB-22

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



1. GENERAL INFORMATION

IUPAC Name: quinolin-8-yl 1-(5-fluoropentyl)-1H-indole-3-carboxylate

CAS#: 1400742-41-7

Synonyms: 5F-PB-22

Source: DEA Reference Material Collection

Appearance: White powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₃ H ₂₁ FN ₂ O ₂	376	117.4



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3. QUALITATIVE DATA

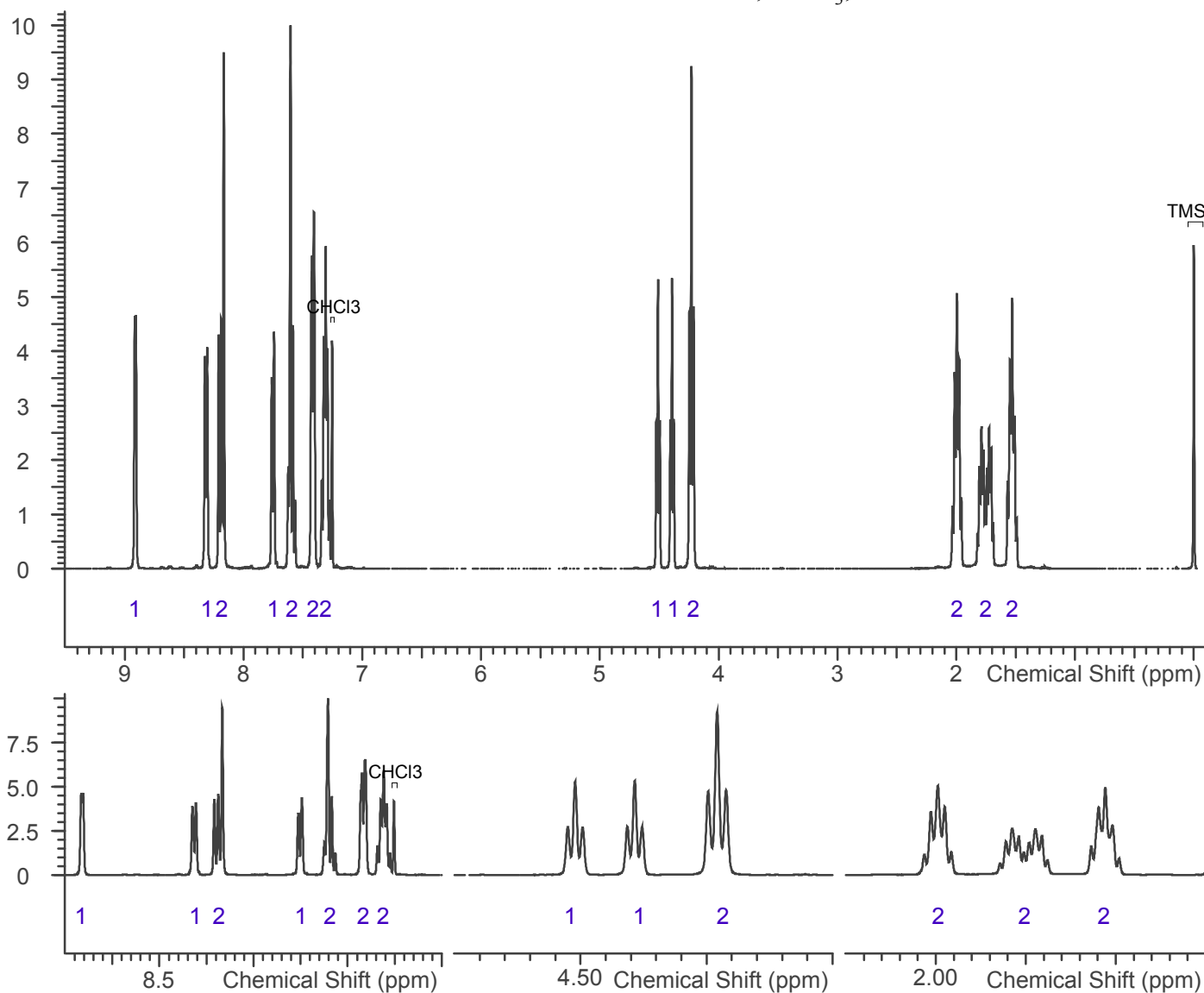
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

Sample Preparation: Dilute analyte to ~15 mg/mL in CDCl₃ containing TMS for 0 ppm reference.

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-Fluoro-PB-22 Lot # RM-032013-2; CDCl₃; 400 MHz





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3.2 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

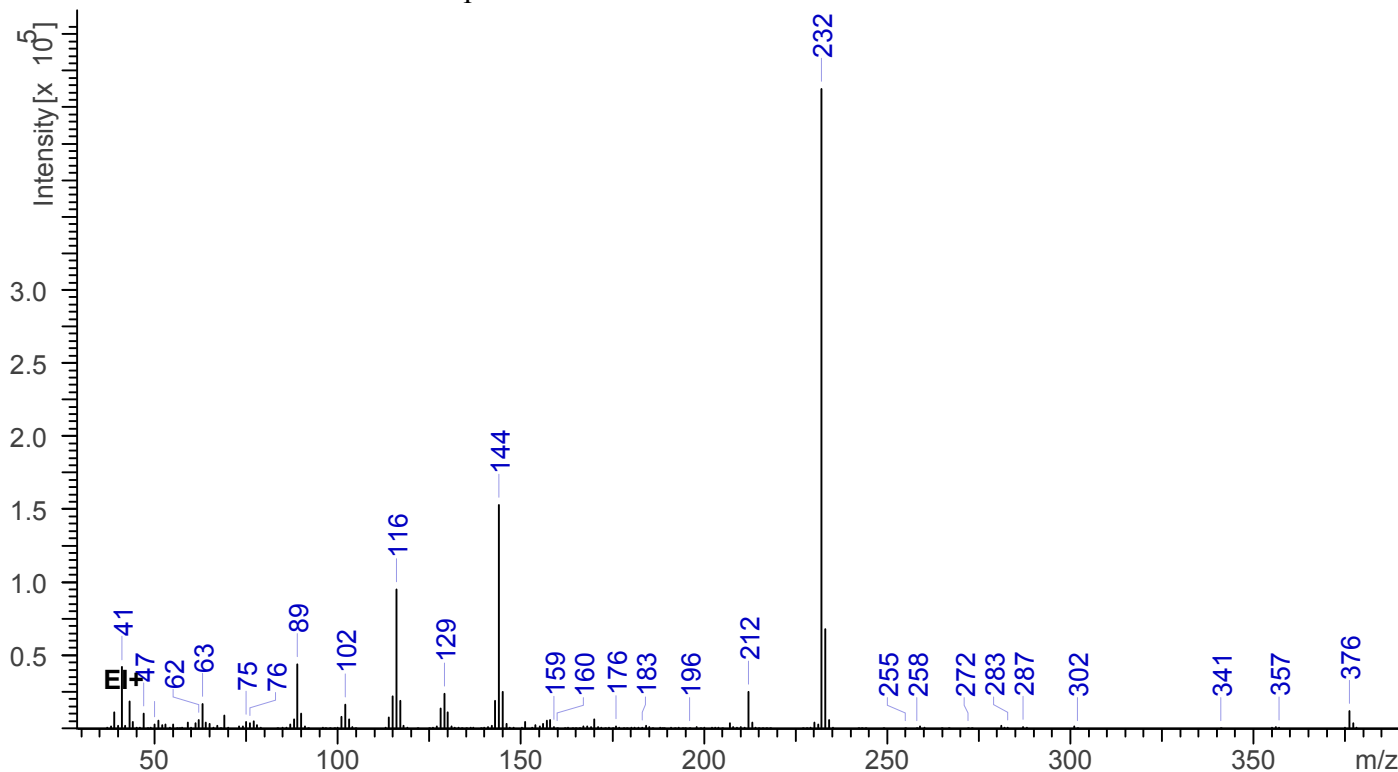
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 23.606 min

EI Mass Spectrum: 5-Fluoro-PB-22 Lot # RM-032013-2





5-Fluoro-PB-22

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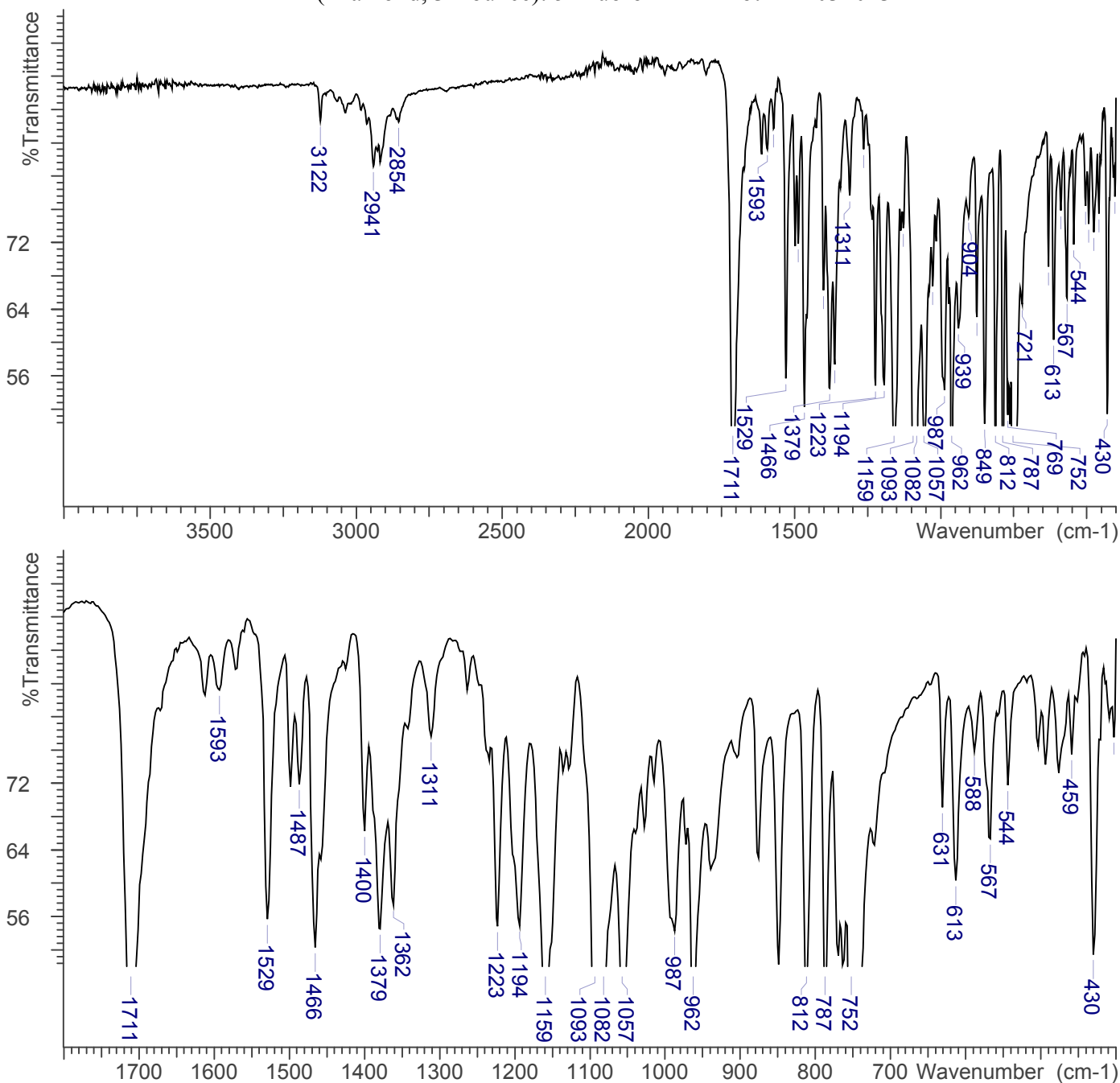


3.3 INFRARED SPECTROSCOPY (FTIR)

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): 5-Fluoro-PB-22 Lot RM-032013-2





5-Fluoro-PB-22

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4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)