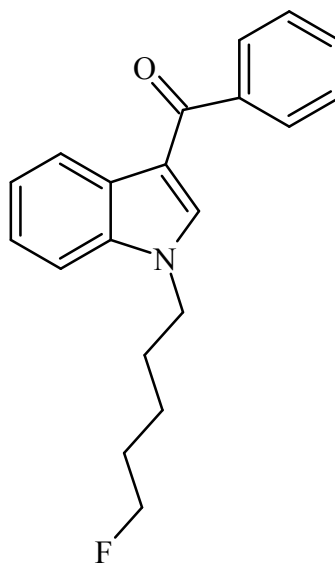




5-Fluoropentyl-3-pyridinoylindole

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



1. GENERAL INFORMATION

IUPAC Name: [1-(5-fluoropentyl)-1H-indol-3-yl](pyridin-3-yl)methanone

CAS#: Not Available

Synonyms: Not Available

Source: DEA Reference Material Collection

Appearance: Pale pink 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 ₁₉ H ₁₉ FN ₂ O	310	Not Determined
HCl	C ₁₉ H ₁₉ FN ₂ O HCl	346	174-176



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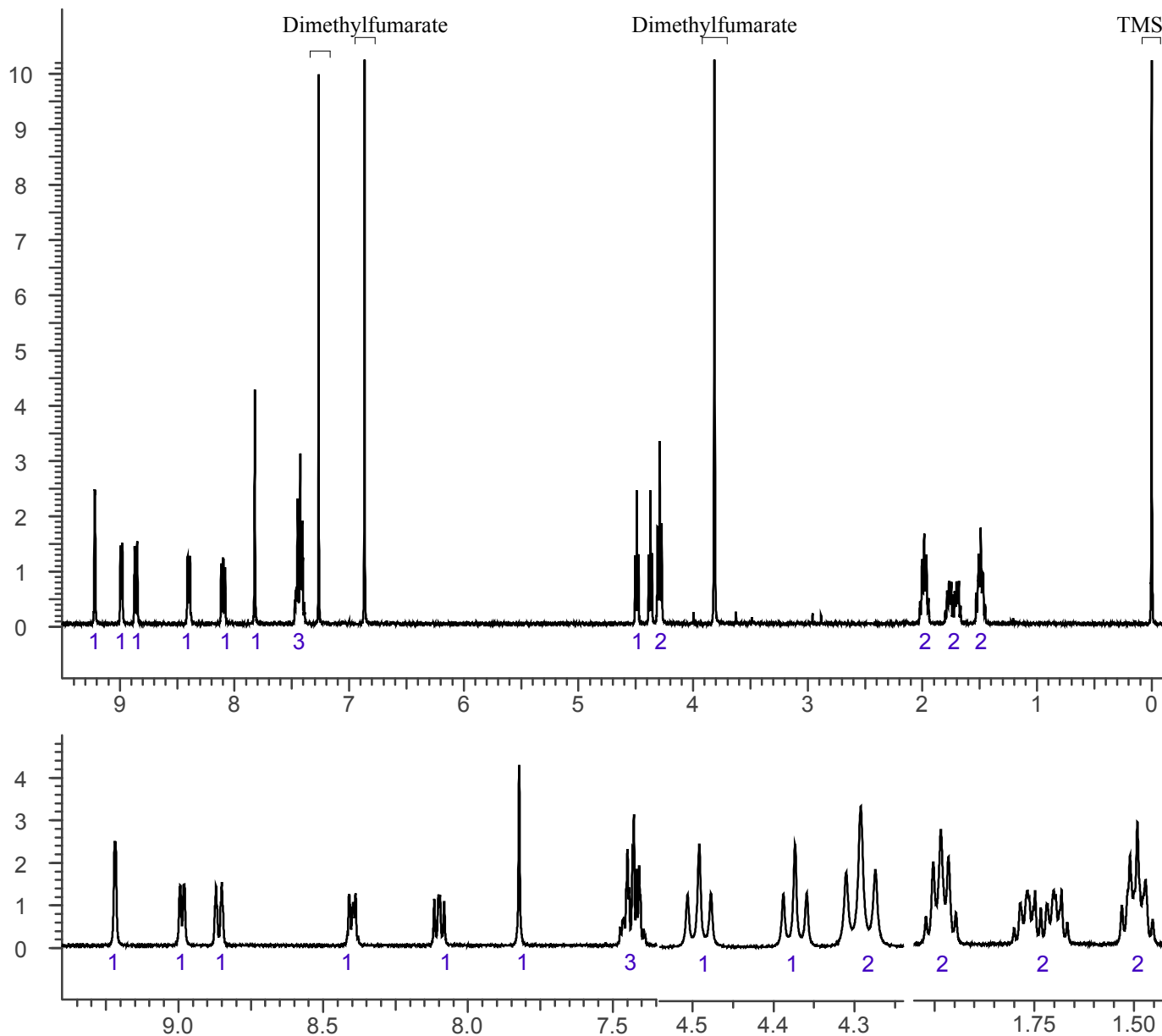
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~4 mg/mL in CDCl₃ 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: 5-Fluoropentyl-3-pyridinoylindole HCl, Lot 0465894-1, 400MHz, CDCl₃





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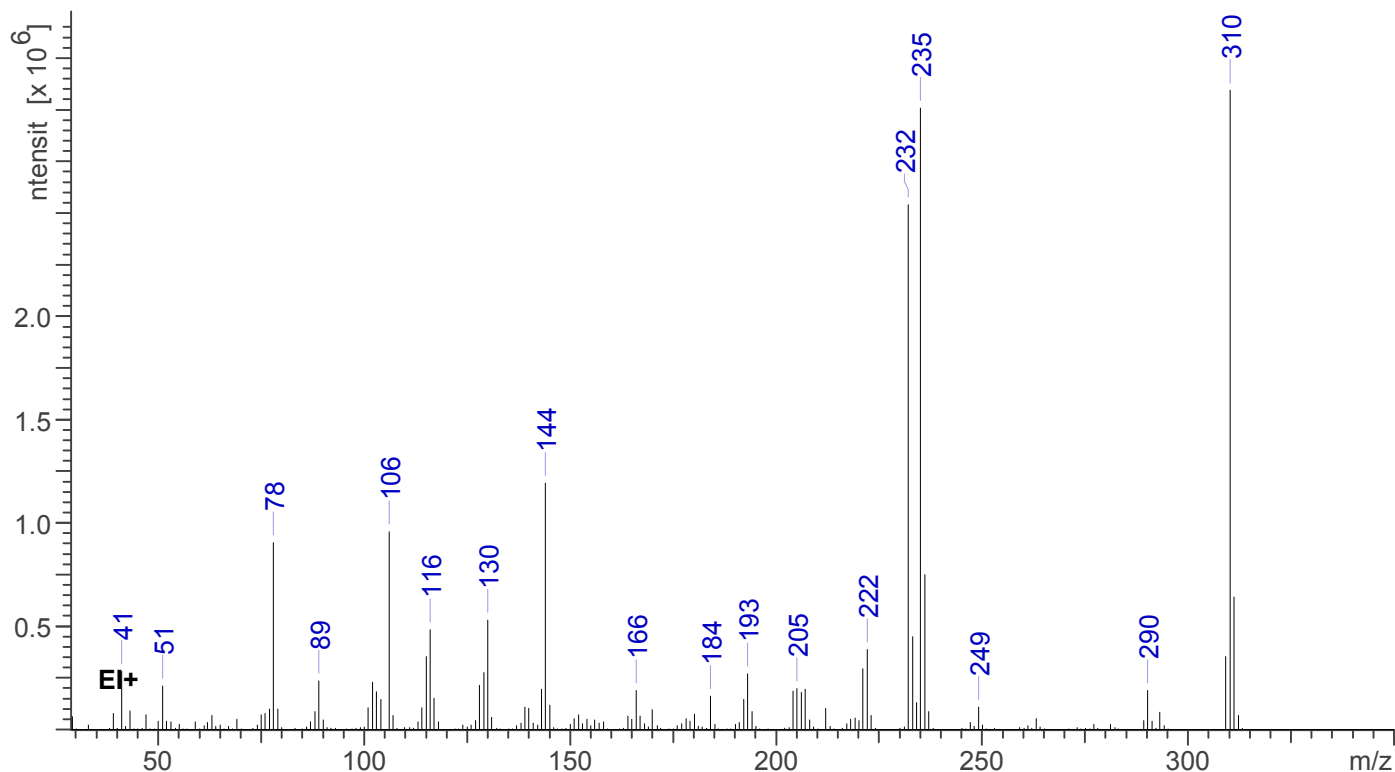
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~6 mg/mL in CHCl₃.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
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 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 18.870 min

EI Spectrum: 5-Fluoropentyl-3-pyridinoylindole HCl, Lot 0465894-1





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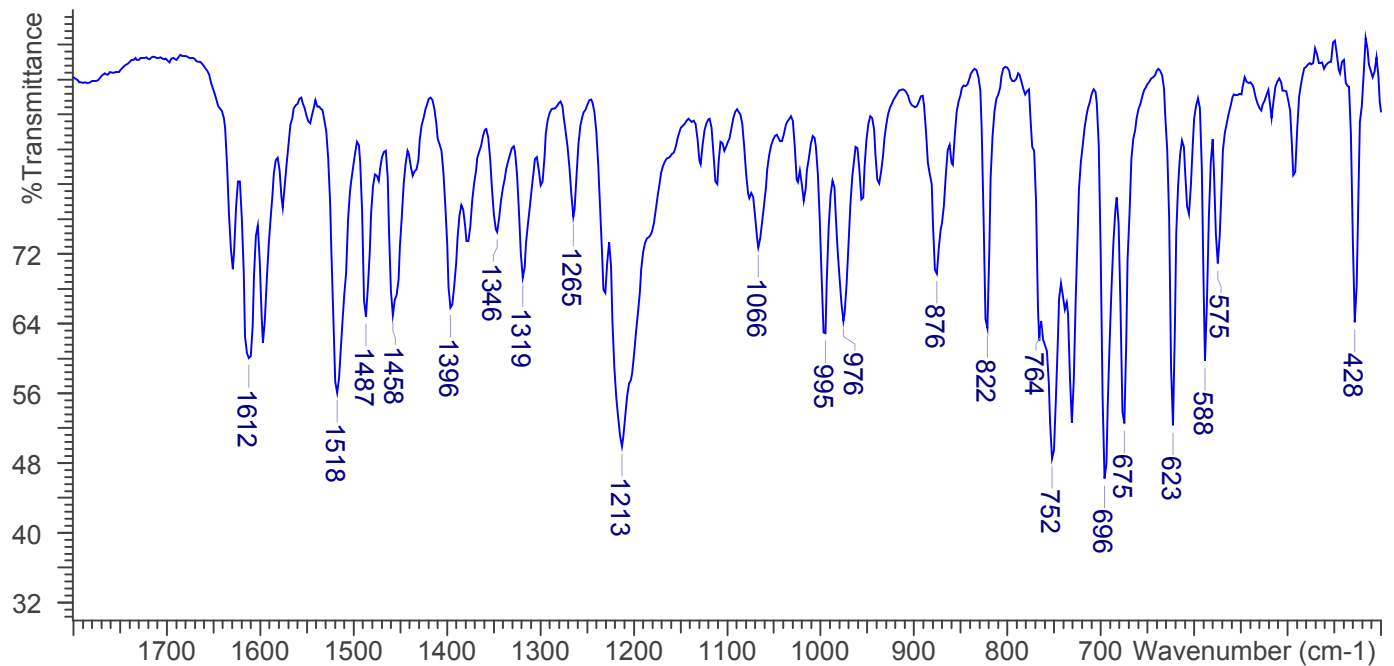
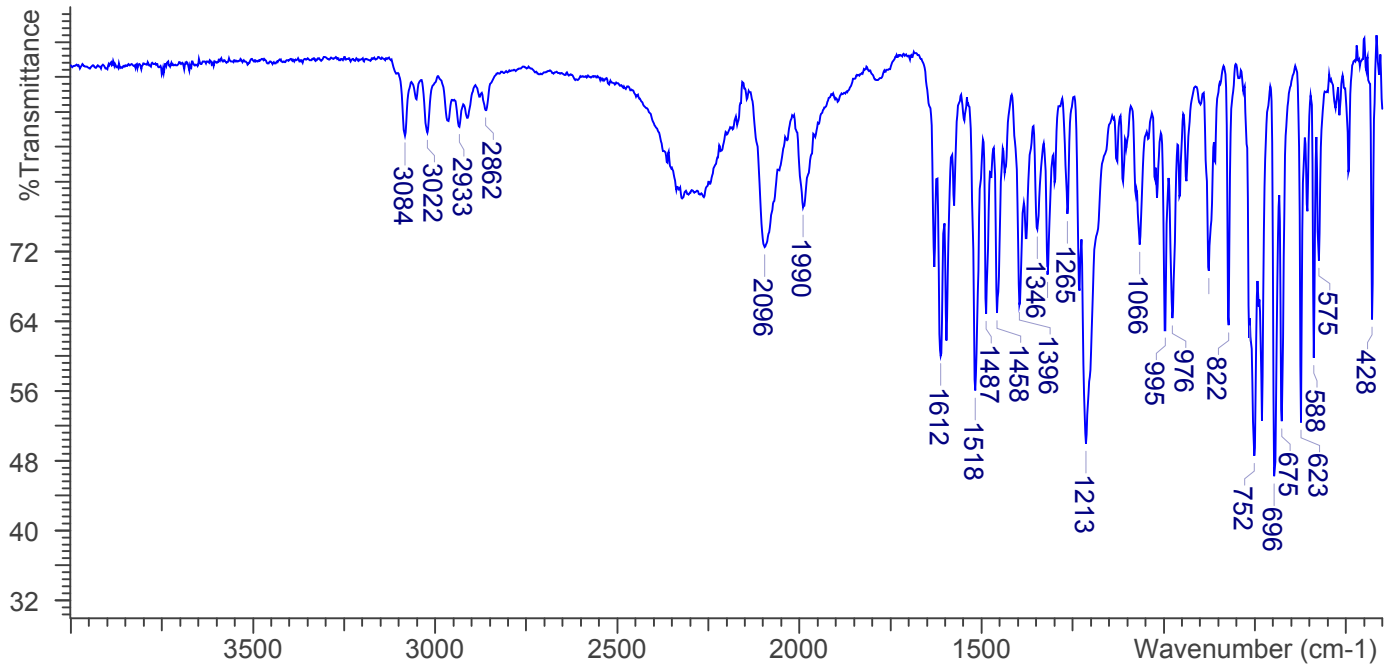


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): 5-Fluoropentyl-3-pyridinoylindole HCl, Lot 0465894-1





5-Fluoropentyl-3-pyridinoylindole

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4. ADDITIONAL RESOURCES

N. Uchiyama, et al., URB-754: A new class of designer drug and 12 synthetic cannabinoids detected in illegal products, *Forensic Sci. Int.* (2012), <http://dx.doi.org/10.1016/j.forsciint.2012.08.047>