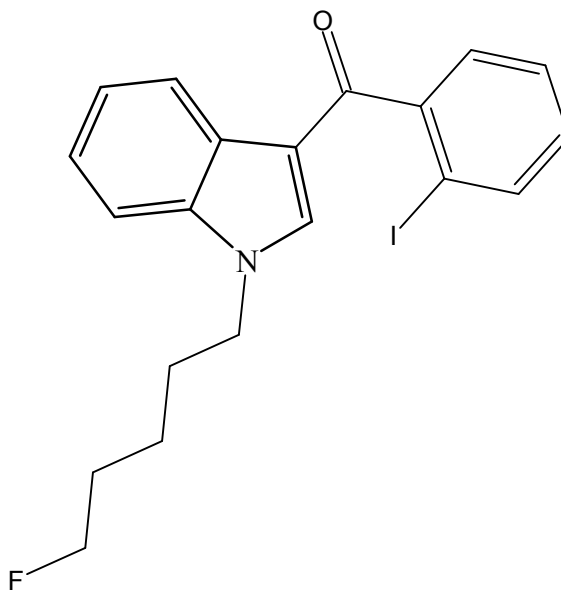




AM694

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



1. GENERAL INFORMATION

IUPAC [1-(5-fluoropentyl)-1H-indol-3-yl](2-iodophenyl)methanone

CAS#: 335161-03-0

Synonyms: N/A

Source: DEA Reference Material Collection

Appearance: White powder

UV_{max}(nm): 213.3, 251.1, 314.6

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

| Form | Chemical Formula | Molecular Weight | Melting Point (°C) |
|------|--------------------------------------|------------------|--------------------|
| Base | C ₂₀ H ₁₉ FINO | 435 | 107.7 |



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3. QUALITATIVE DATA

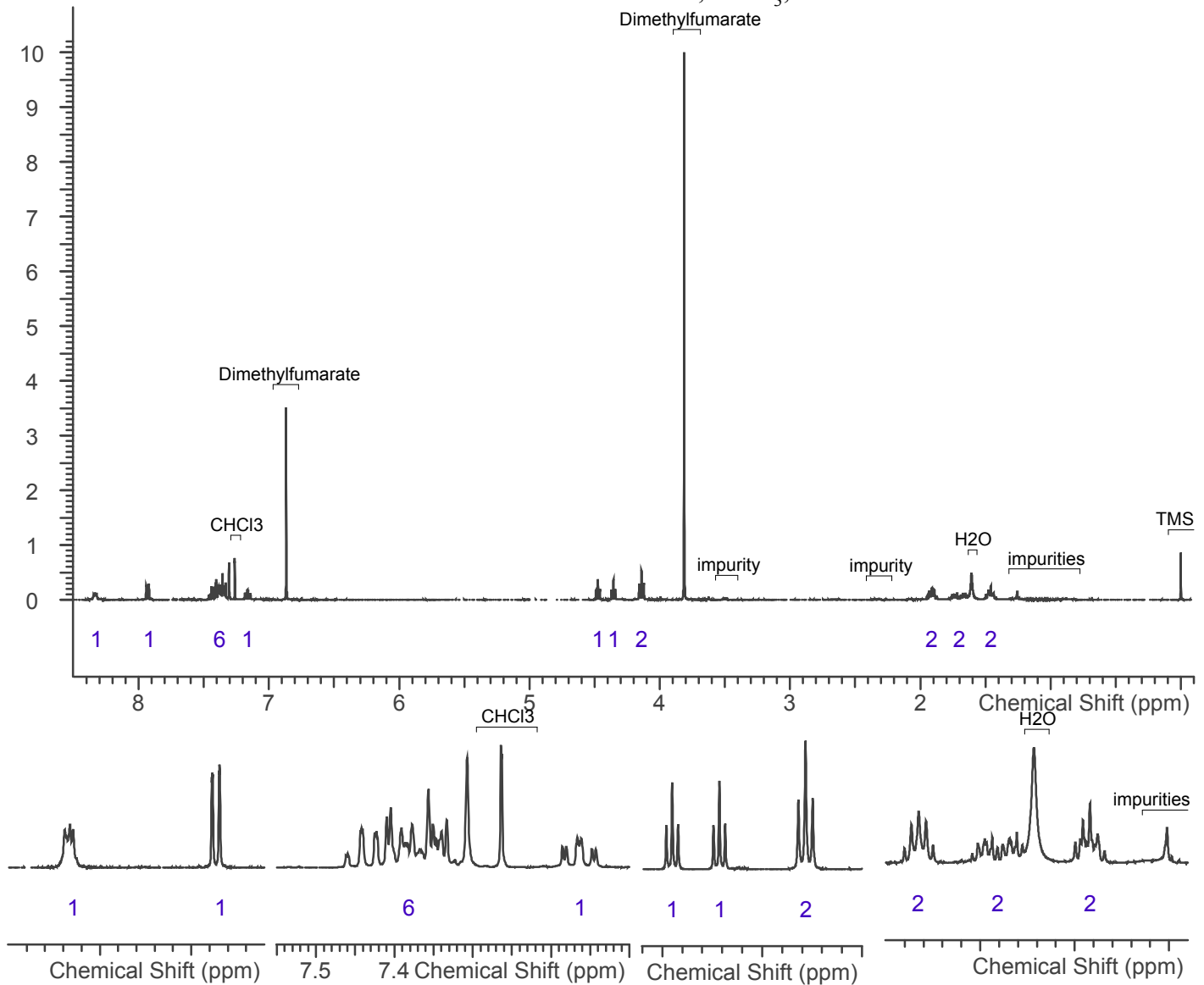
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~10 mg/mL in CDCl₃ containing TMS for 0 ppm reference and dimethylfumurate 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: AM694 Lot # K8H81108; CDCl₃; 400MHz





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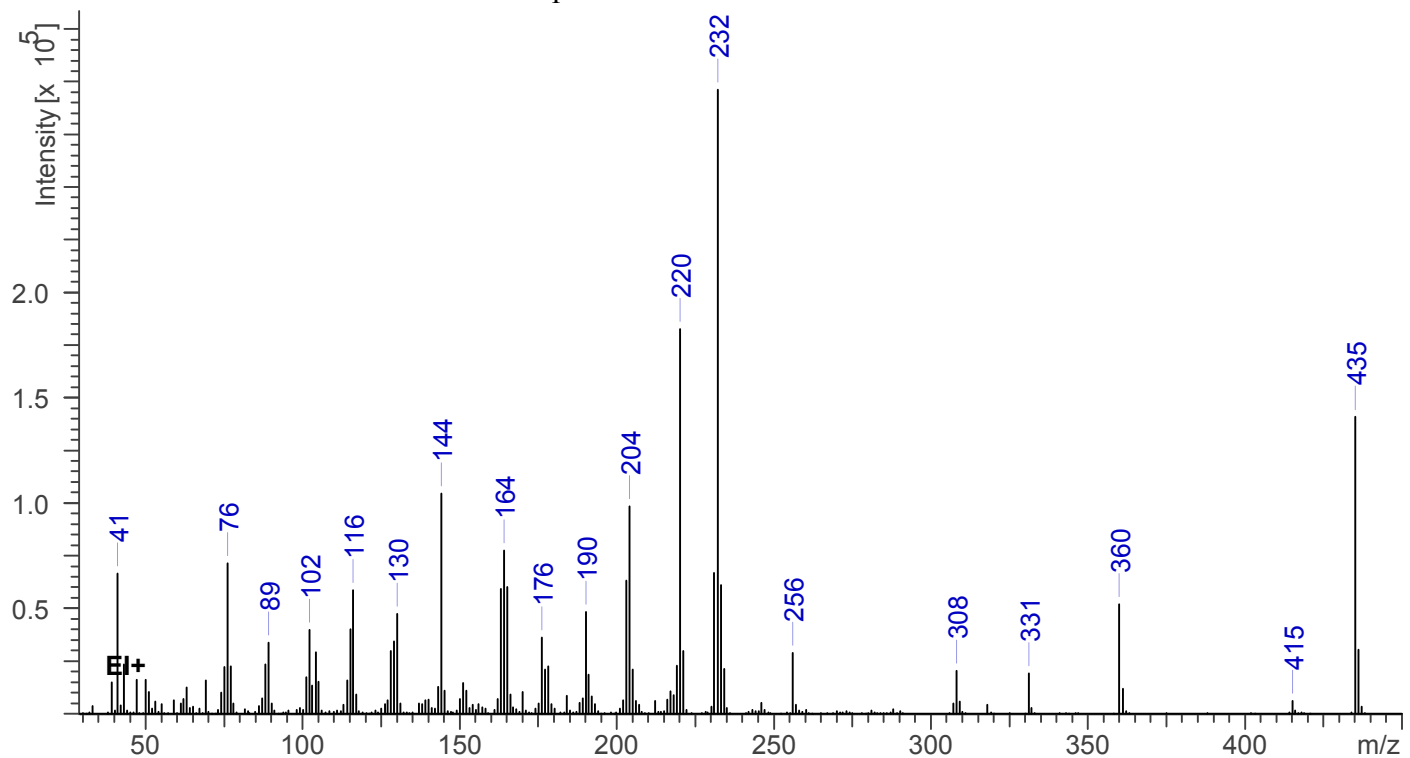


3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~1 mg/mL in methanol.

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: 19.372 min

EI Mass Spectrum: AM694 Lot # SL227B3





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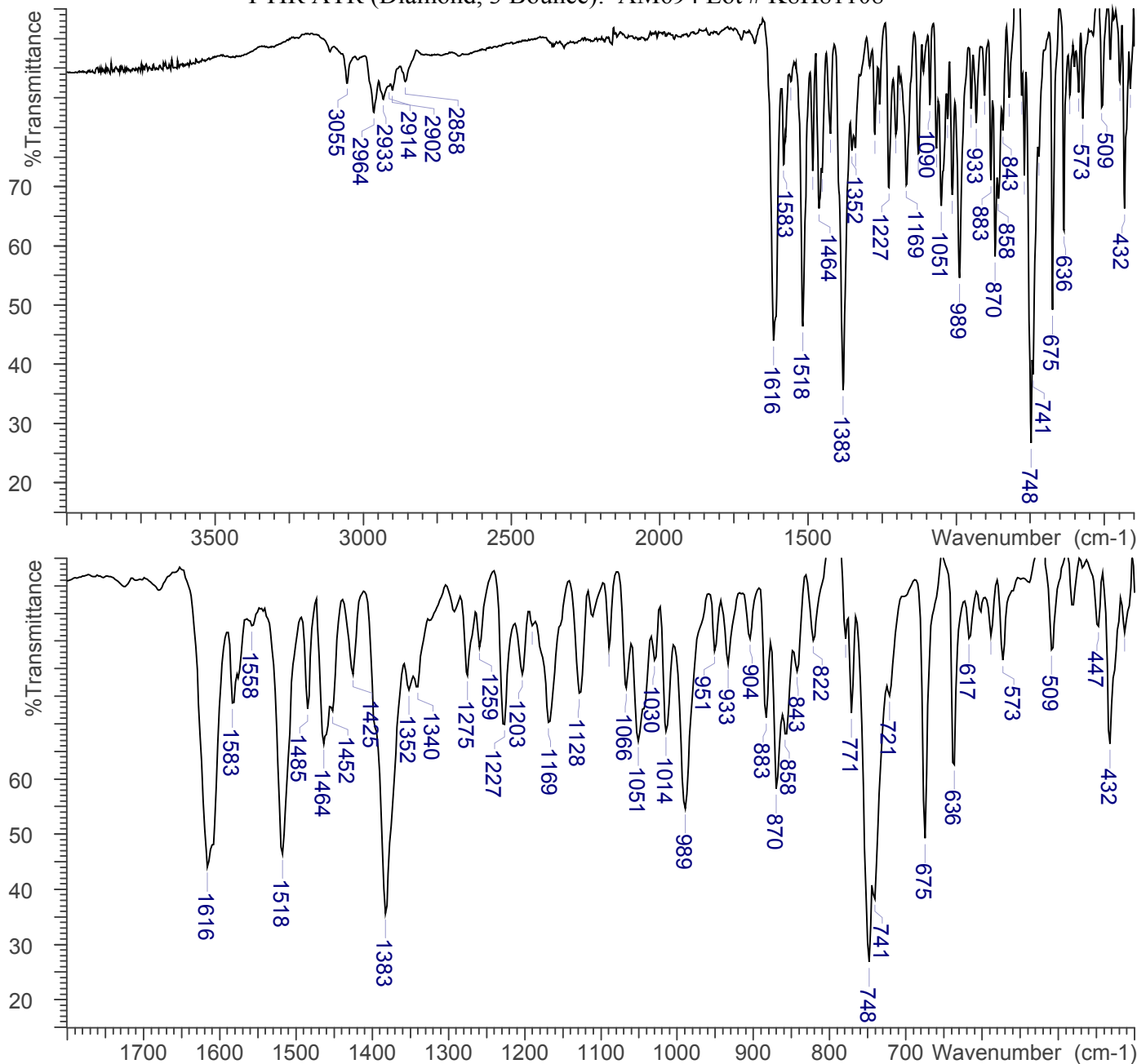


3.3 INFRARED SPECTROSCOPY (FTIR)

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): AM694 Lot # K8H81108





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3. **ADDITIONAL RESOURCES**

[Forendex](#)

[Wikipedia](#)