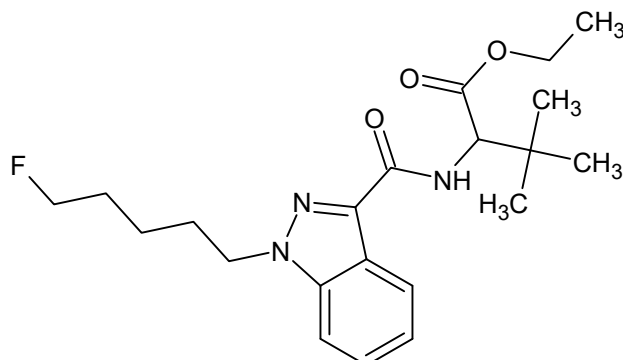




5-Fluoro-EDMB-PINACA

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



1. GENERAL INFORMATION

IUPAC Name:	ethyl 2-(1-(5-fluoropentyl)-1H-indazole-3-carboxamido)-3,3-dimethylbutanoate
CAS#:	NA
Synonyms:	NA
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 ₂₁ H ₃₀ FN ₃ O ₃	391.48	69.88



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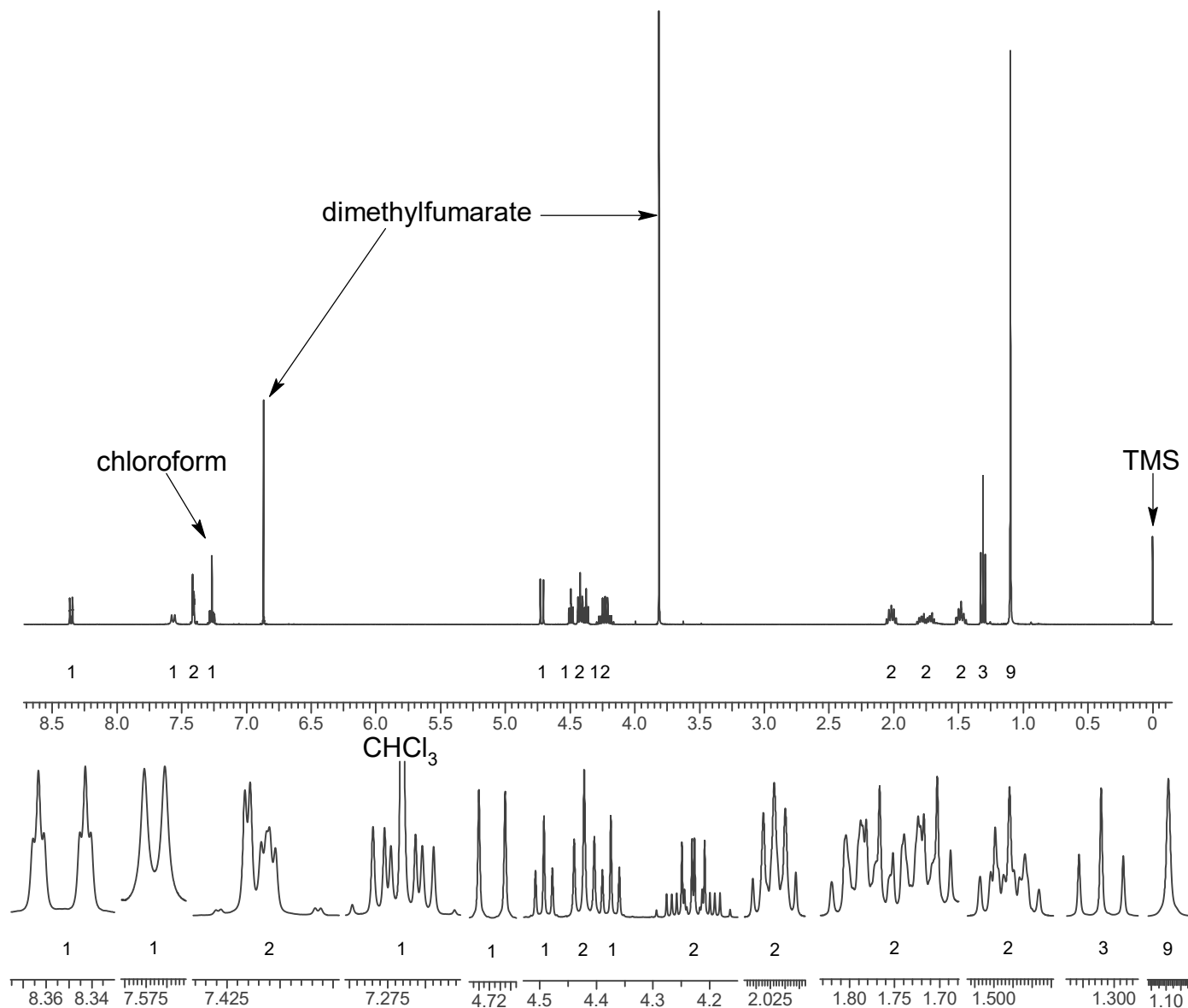
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/mL in chloroform-*d* 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

¹HNMR: 5-Fluoro-EDMB-PINACA; Lot # 0516373-15; CDCl₃; 400MHz





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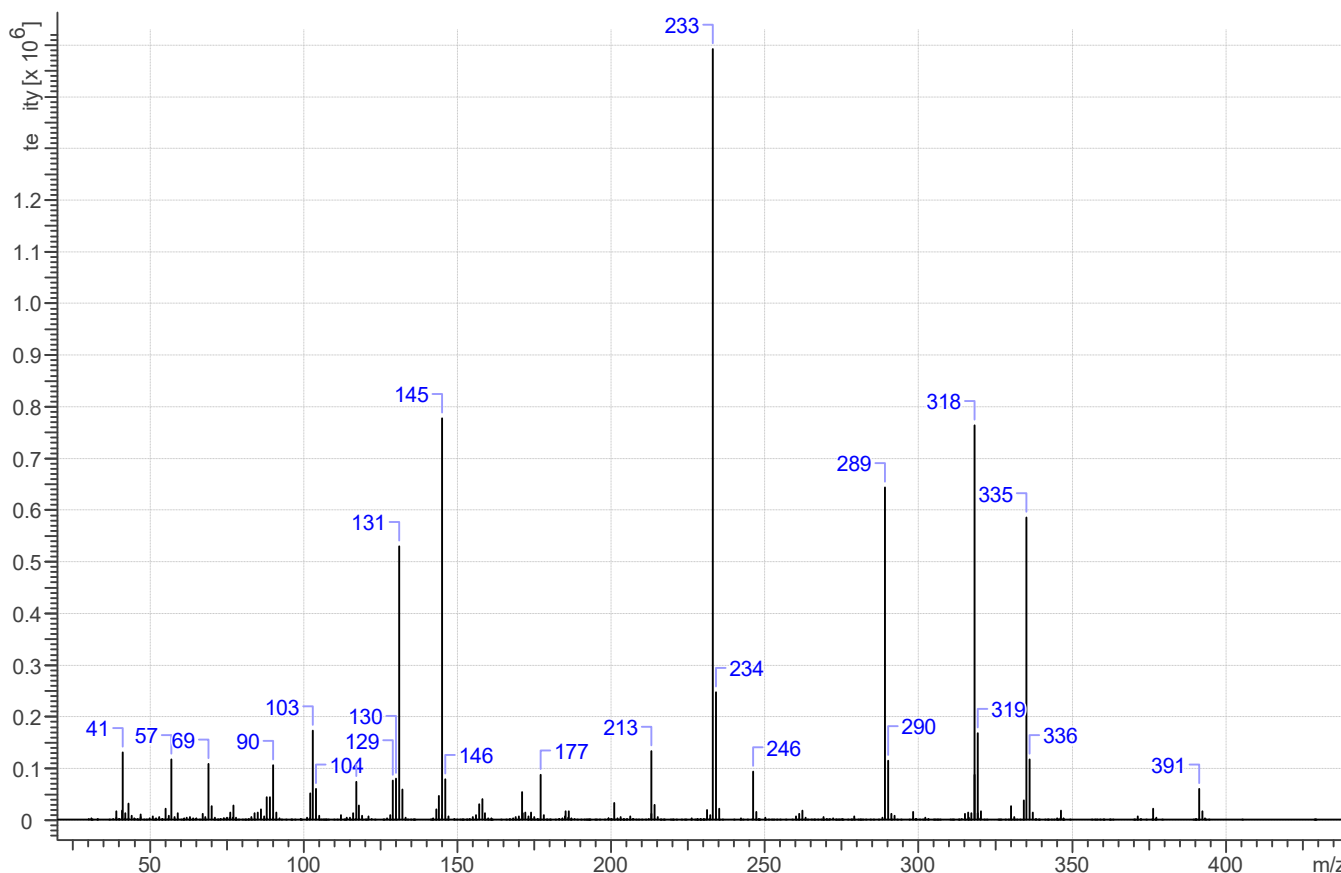


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in MeOH

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 μ m
Carrier Gas: Helium at 1.5 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 280°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: 30-550 amu Threshold: 150
Tune file: stune.u Acquisition mode: scan
Retention Time: 16.799 min

EI Mass Spectrum: 5-Fluoro-EDMB-PINACA; Lot # 0516373-15





5-Fluoro-EDMB-PINACA

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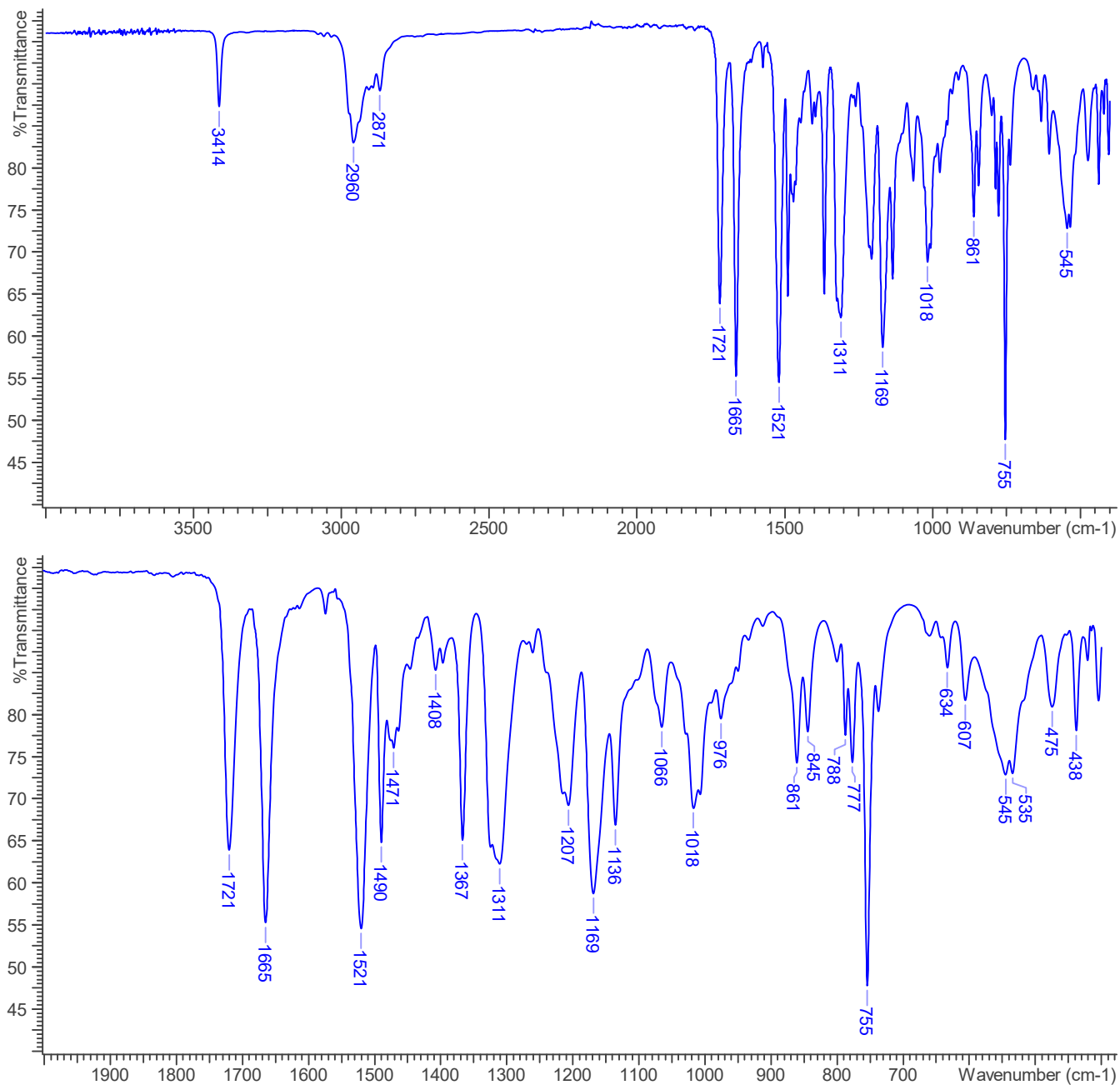


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 5-Fluoro-EDMB-PINACA; Lot # 0516373-15





5-Fluoro-EDMB-PINACA

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4. ADDITIONAL RESOURCES

Liu, C. et al. Identification and analytical characterization of six synthetic cannabinoids NNL-3, 5F-NPB-22-7N, 5F-AKB-48-7N, 5F-EDMB-PINACA, EMB-FUBINACA, and EG-018. Drug Test Anal. 9(8), 1251-1261 (2017).