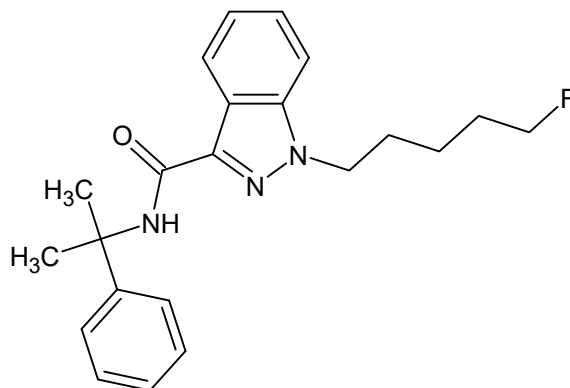




5-Fluoro-CUMYL-PINACA

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)-N-(2-phenylpropan-2-yl)-1H-indazole-3-carboxamide
CAS#:	1400742-16-6
Synonyms:	CUMYL-5F-PINACA
Source:	DEA Reference Material Collection
Appearance:	Colorless viscous liquid
UV_{max}(nm):	Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₂ H ₂₆ FN ₃ O	367.46	Not Determined



5-Fluoro-CUMYL-PINACA

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



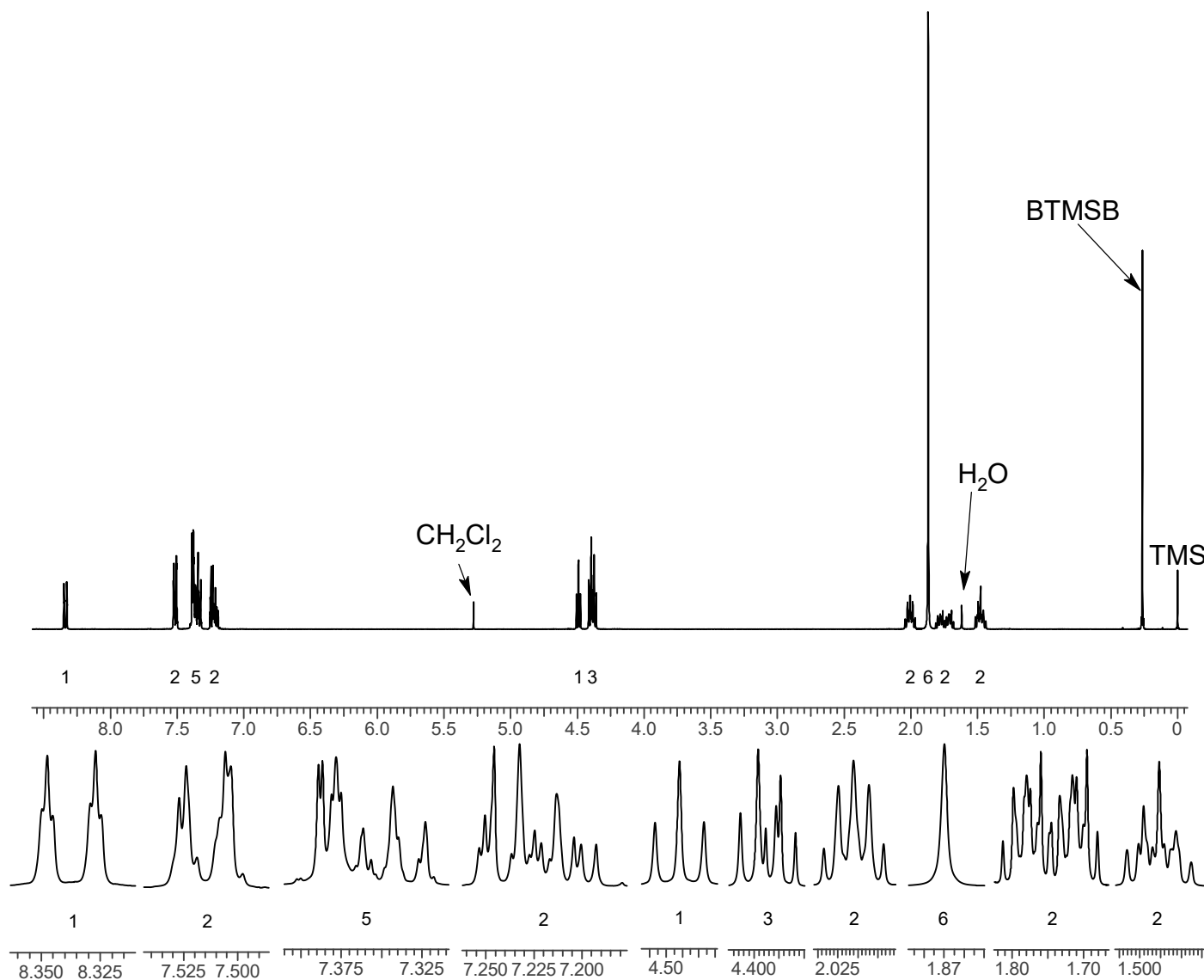
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~24 mg/mL in CDCl_3 containing TMS for 0 ppm reference and 1,4-BTMSB- d_4 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-Fluoro-CUMYL-PINACA; Lot# 0546719-1; CDCl_3 ; 400MHz





5-Fluoro-CUMYL-PINACA

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

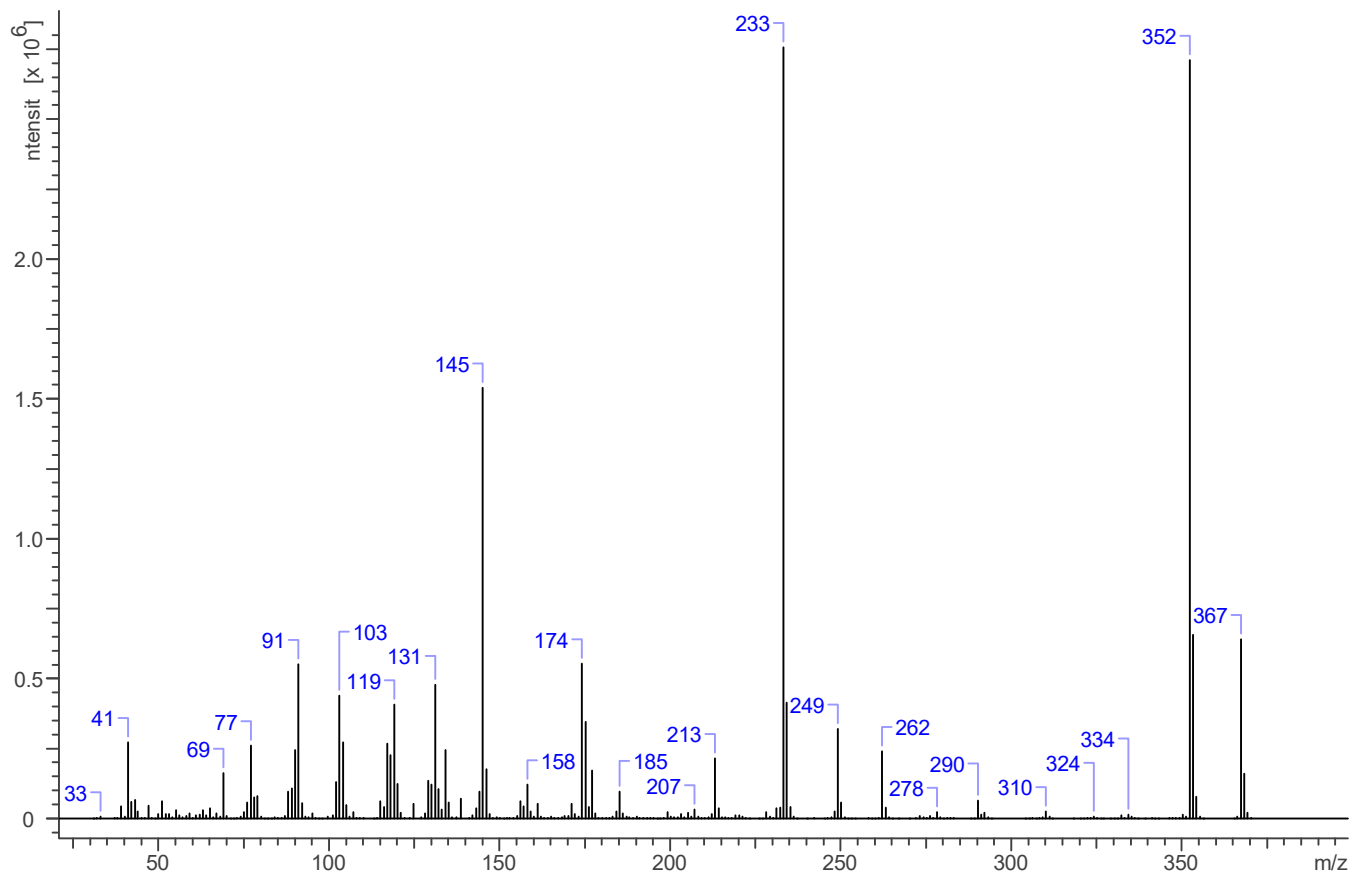


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~8 mg/2mL 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 9.0 min
Injection Parameters: Split Ratio = 25:1, 1 μ L injected
MS Parameters: Mass scan range: 30-550 amu Threshold: 250
Tune file: stune.u Acquisition mode: scan
Retention Time: 18.03 min

EI Mass Spectrum: 5-Fluoro-CUMYL-PINACA; Lot# 0546719-1





5-Fluoro-CUMYL-PINACA

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

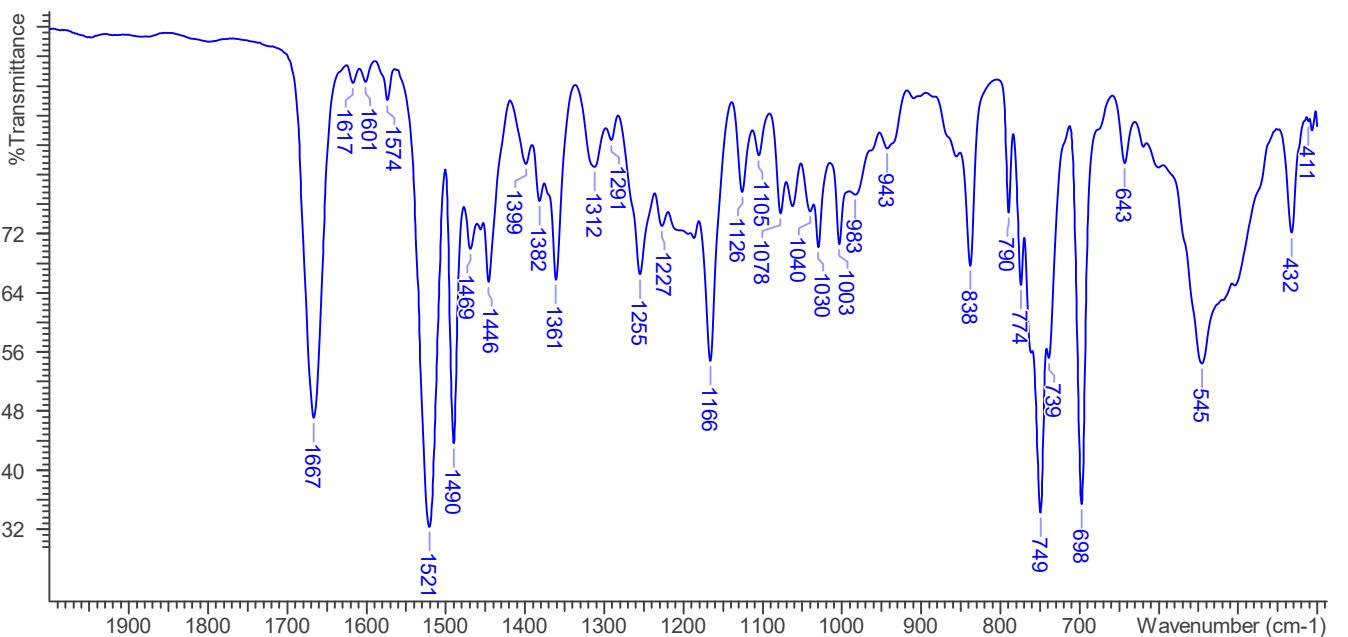
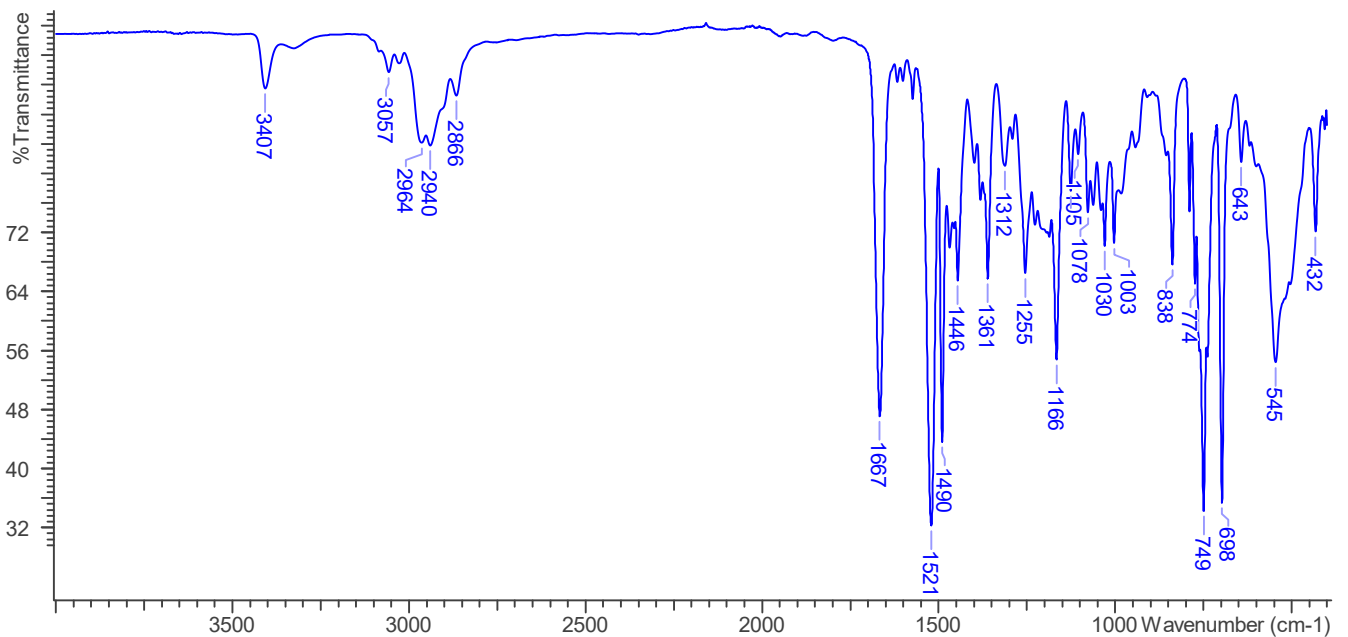


3.3 INFRARED SPECTROSCOPY (FTIR)

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-CUMYL-PINACA; Lot# 0546719-1





5-Fluoro-CUMYL-PINACA

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



4. ADDITIONAL RESOURCES

Asada, A.; Doi, T.; Tagami, T.; et al. Cannabimimetic activities of cumyl carboxamide-type synthetic cannabinoids. *Forensic Toxicology*. DOI 10.1007/s11419-017-0374-9.