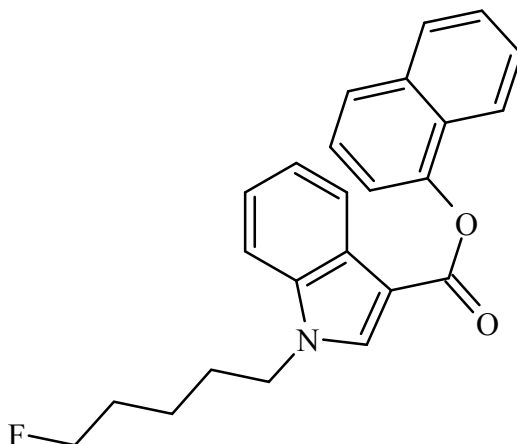




5-Fluoro-SDB-005 Indole

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



1. GENERAL INFORMATION

IUPAC Name:	Naphthalen-1-yl 1-(5-fluoropentyl)-1H-indole-3-carboxylate
CAS#:	Not Available
Synonyms:	NM2201
Source:	DEA Reference Material Collection
Appearance:	Light Gray 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 ₂₄ H ₂₂ FNO ₂	375	83.7-85.9



5-Fluoro-SDB-005 Indole

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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/mL in CDCl_3 containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

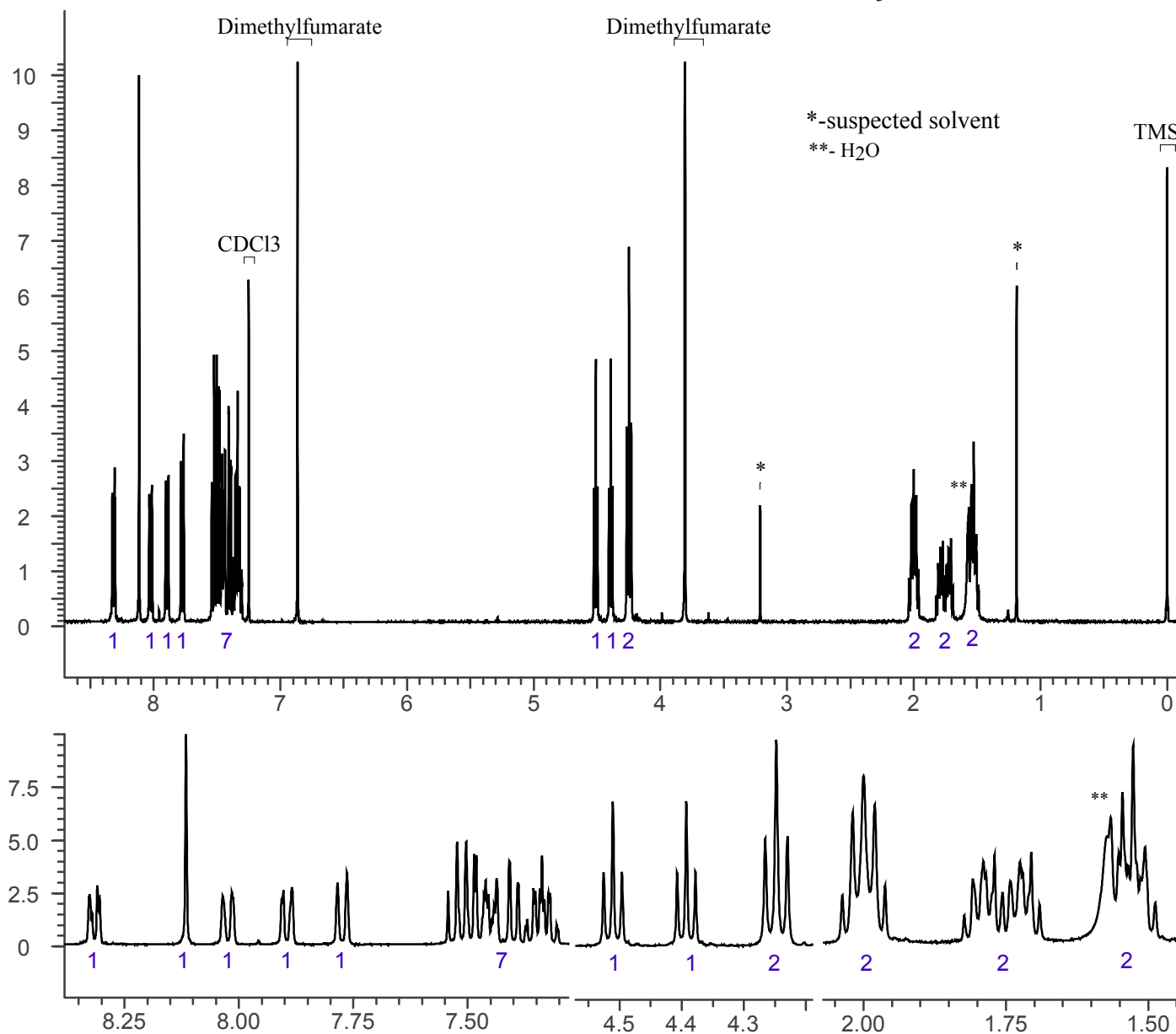
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

^1H NMR 5-Fluoro-SDB-005 Indole Lot RM-140318-06, CDCl_3 , 400MHz





5-Fluoro-SDB-005 Indole

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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃.

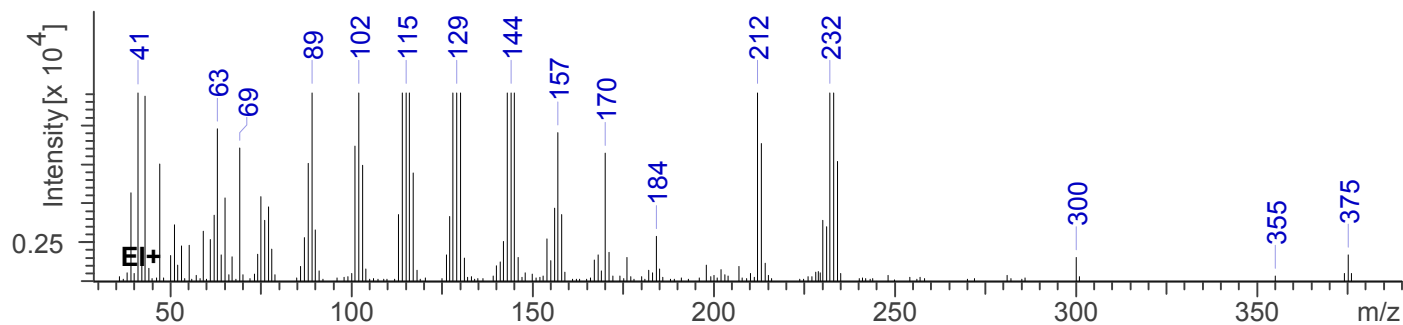
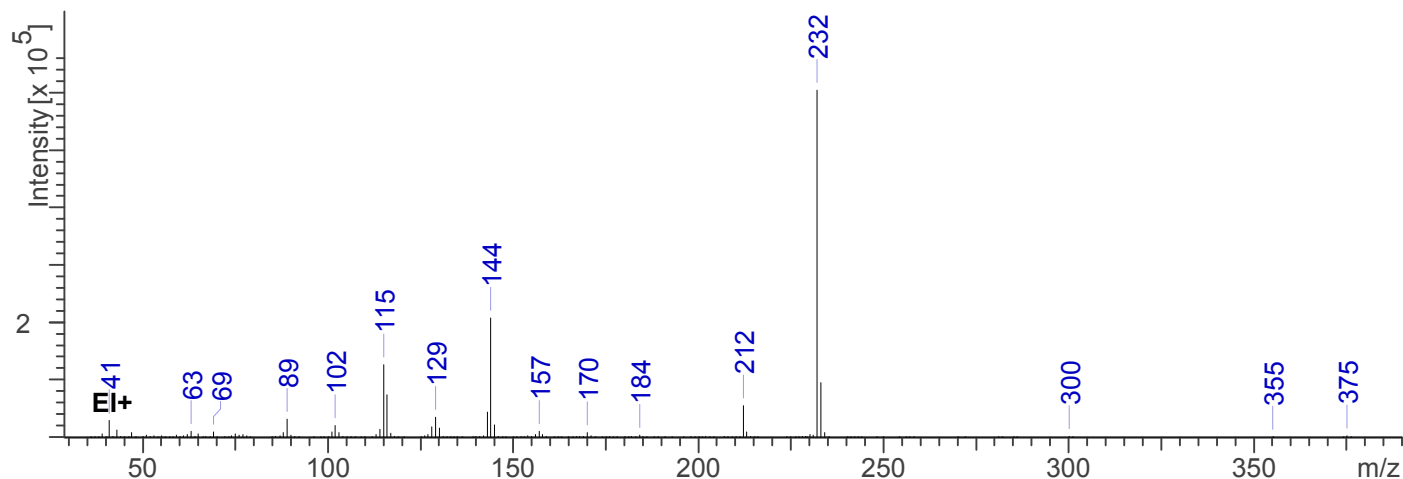
Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1 mL/min
Temperatures: Injector: 280°C
MSD transfer line: 280°C
MS Source: 230°C
MS Quad: 150°C
Oven program:
1) 100°C initial temperature for 1.0 min
2) Ramp to 300°C at 12 °C/min
3) Hold final temperature for 30.0 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: 20.654 min

EI Mass Spectrum 5-Fluoro-SDB-005 Indole Lot RM-140318-06





5-Fluoro-SDB-005 Indole

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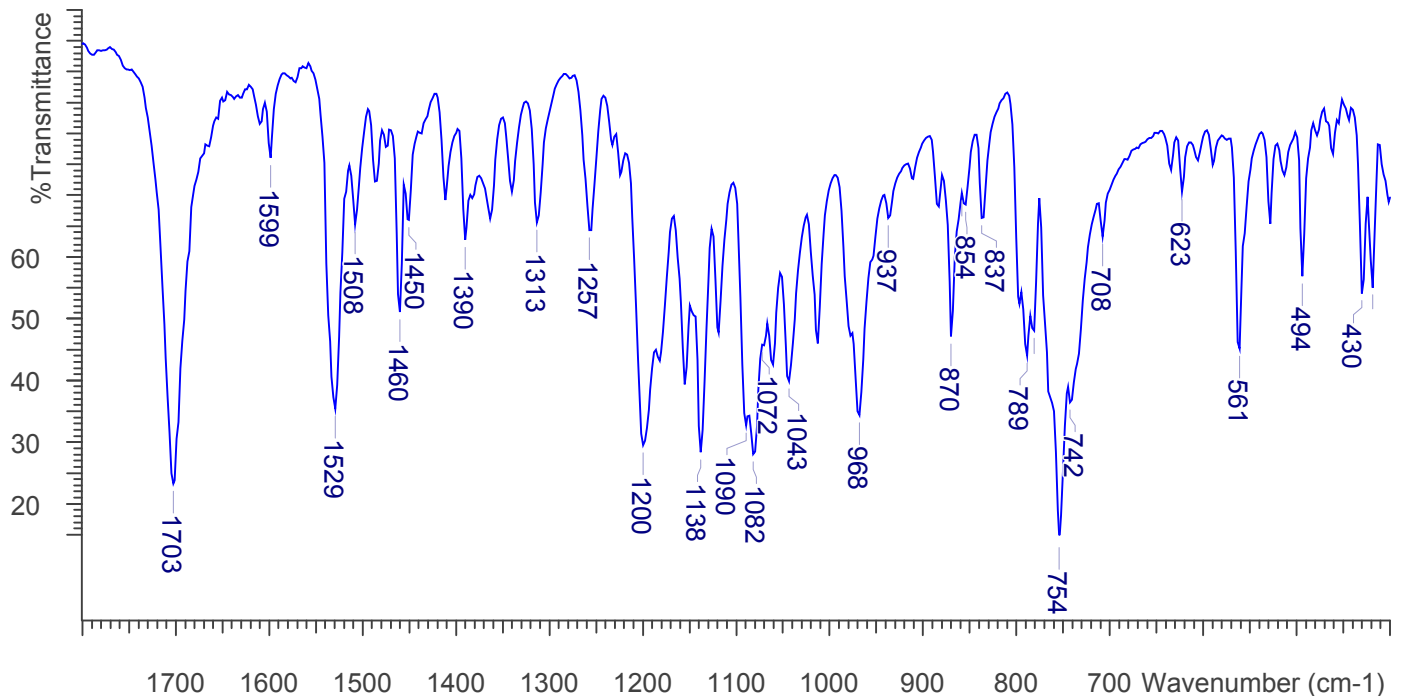
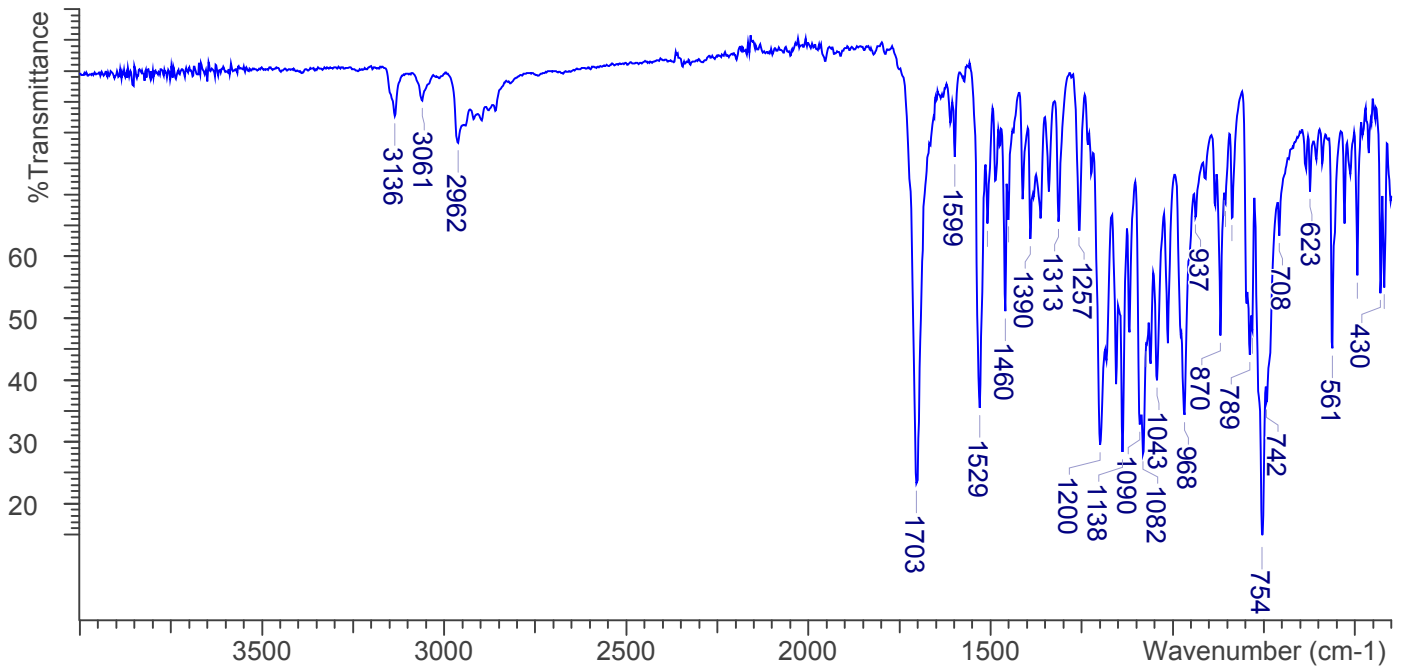


3.3 INFRARED SPECTROSCOPY (FTIR)

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-SDB-005 Indole Lot RM-140318-06





5-Fluoro-SDB-005 Indole

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4. ADDITIONAL RESOURCES

No Literature available as of 10/2014.