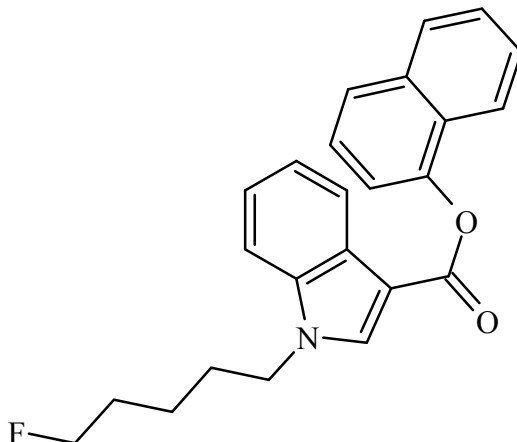




## 5-Fluoro-SDB-005 Indole

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	Naphthalen-1-yl 1-(5-fluoropentyl)-1H-indole-3-carboxylate
<b>CAS#:</b>	Not Available
<b>Synonyms:</b>	NM2201
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	Light Gray Powder
<b>UV<sub>max</sub>(nm):</b>	Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>24</sub> H <sub>22</sub> FNO <sub>2</sub>	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  $\text{CDCl}_3$  containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

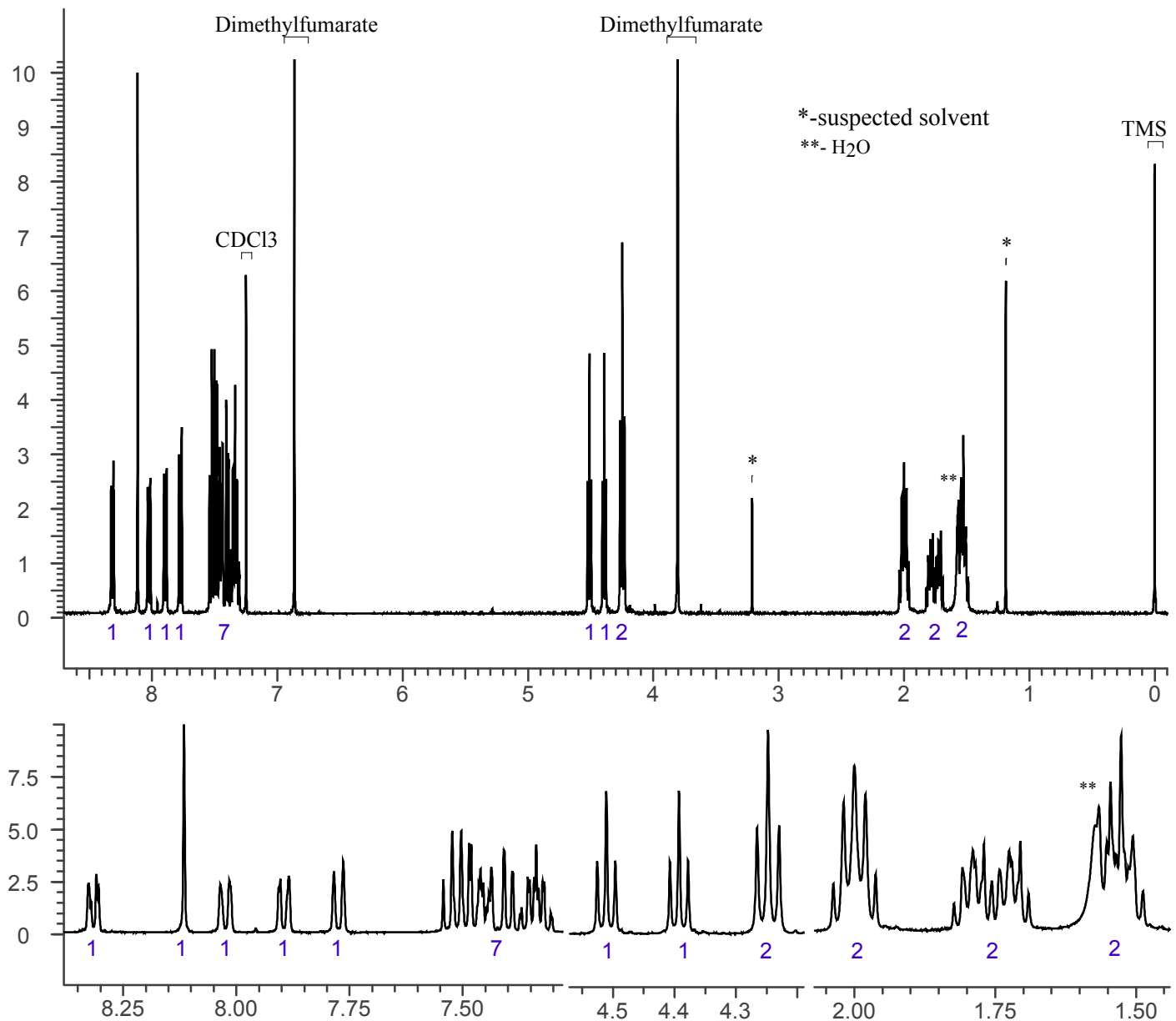
**Instrument:** 400 MHz NMR spectrometer

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

Pulse angle:  $90^\circ$

Delay between pulses: 45 seconds

$^1\text{H}$  NMR 5-Fluoro-SDB-005 Indole Lot RM-140318-06,  $\text{CDCl}_3$ , 400MHz





## 5-Fluoro-SDB-005 Indole

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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

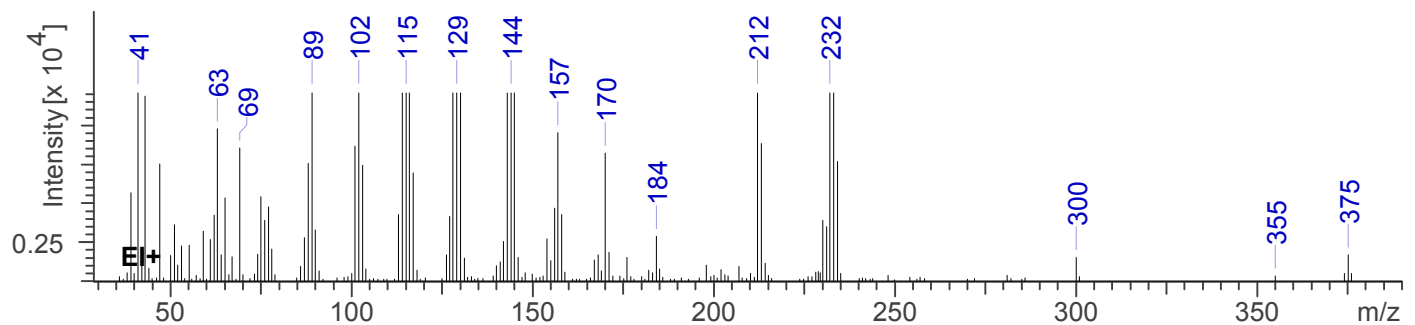
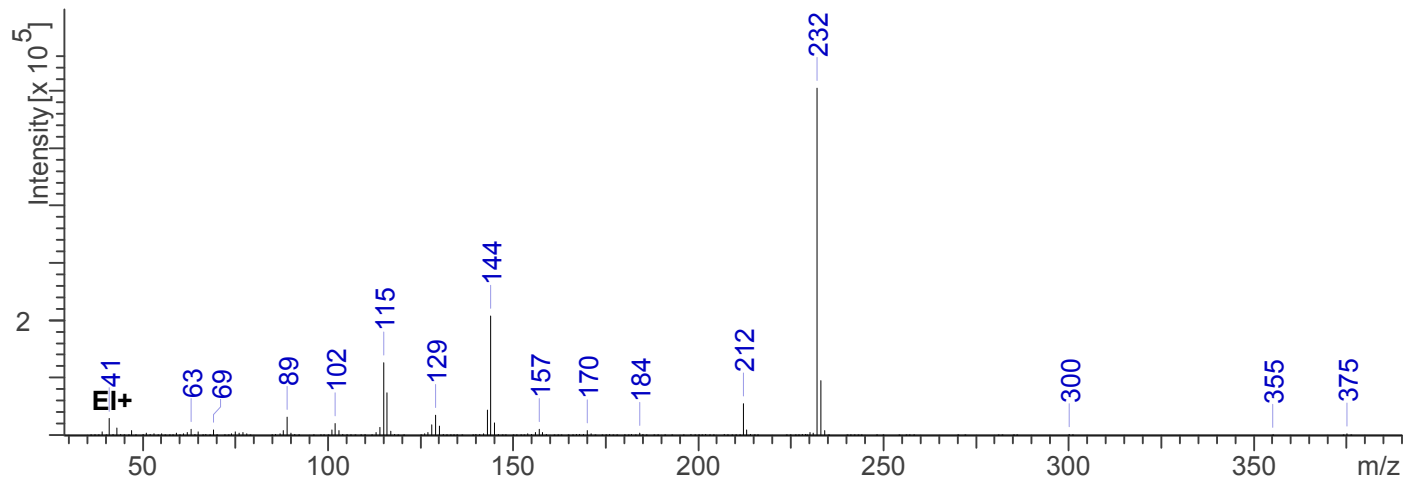
**Sample Preparation:** Dilute analyte ~4 mg/mL in CHCl<sub>3</sub>.

**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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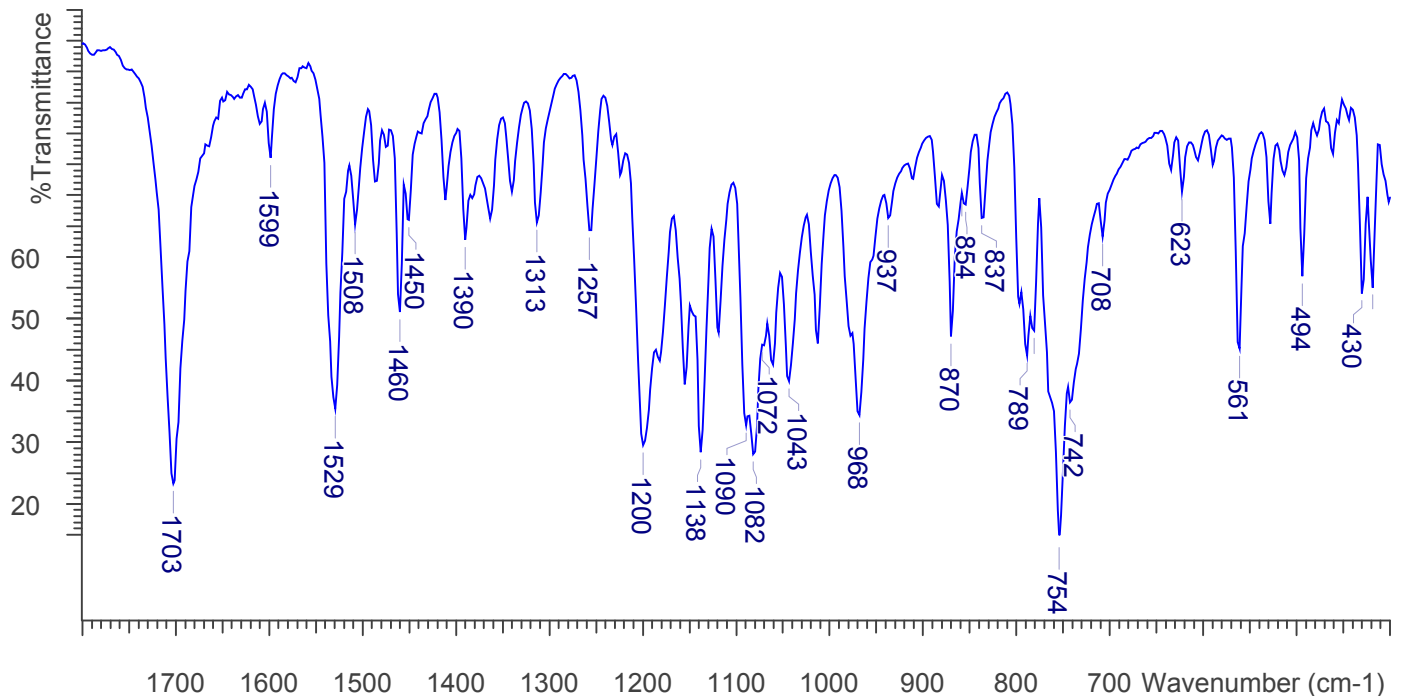
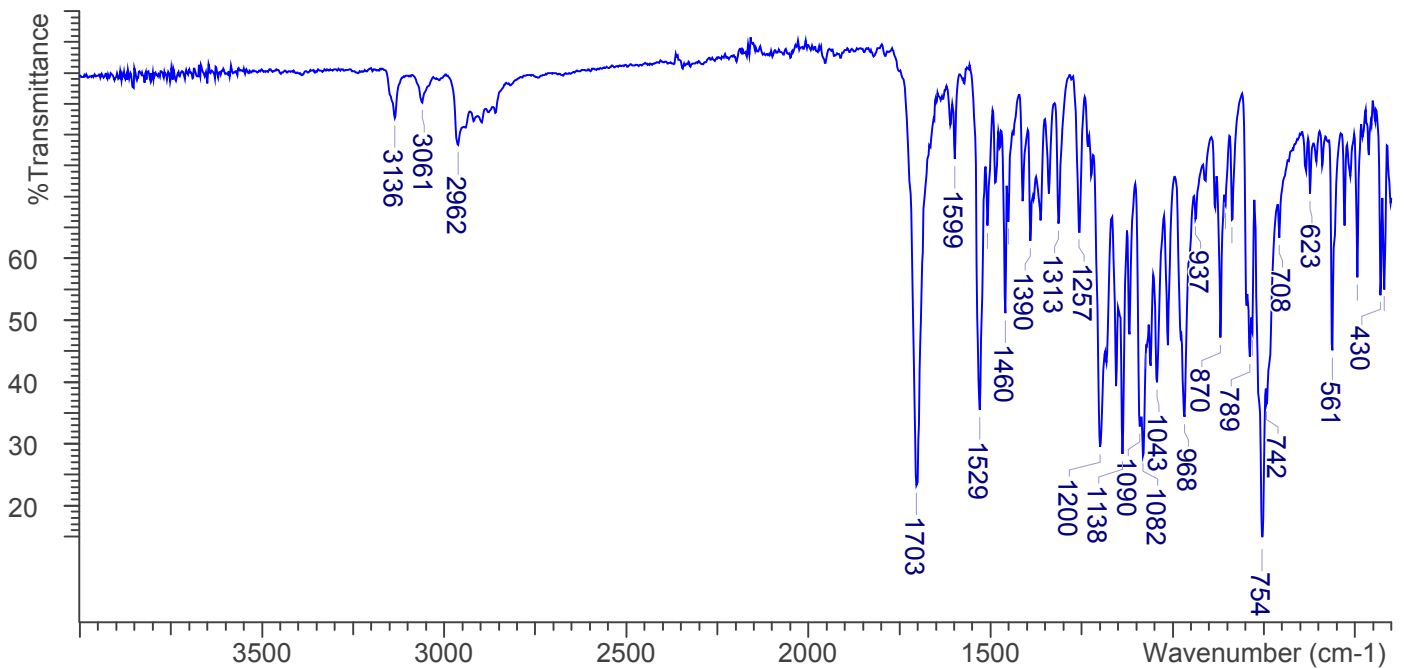


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
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.