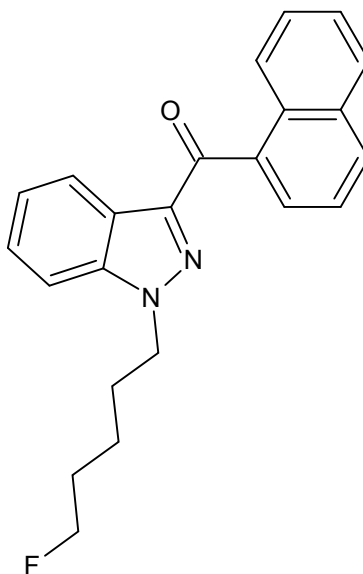




## AM-2201 Indazole

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)-1H-indazol-3-yl](naphthalen-1-yl)methanone

**CAS#:** N/A

**Synonyms:** THJ-2201, Fluoropentyl-JWH-018 indazole, 5-Fluoro-THJ-018

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV<sub>max</sub>(nm):** Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>23</sub> H <sub>21</sub> FN <sub>2</sub> O	360	79.6



# AM-2201 Indazole

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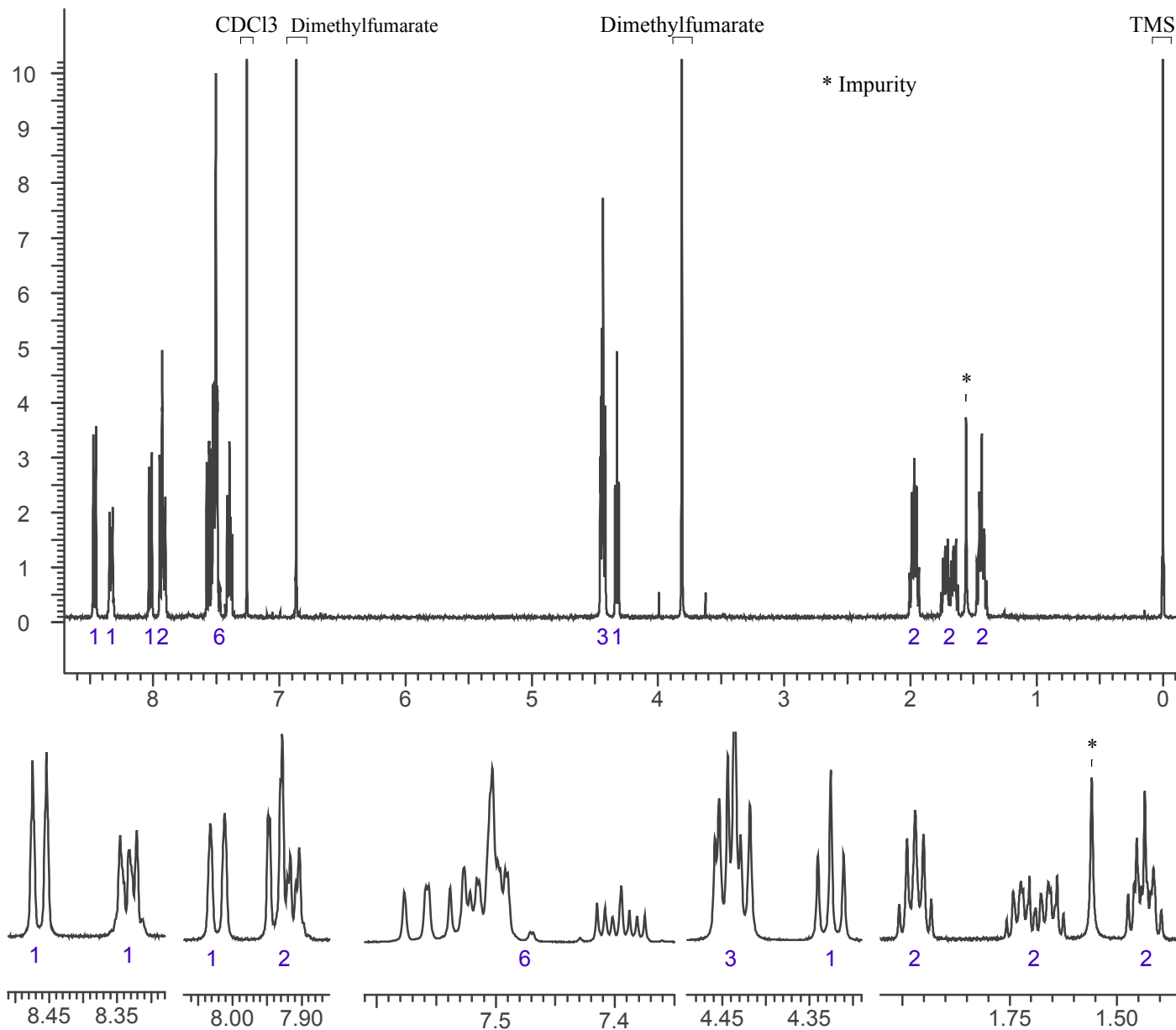


## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~7 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: AM-2201 Indazole; Lot 0454101-23;  $\text{CDCl}_3$ ; 400MHz





## AM-2201 Indazole

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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

**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  $\mu$ 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 30.0 min

**Injection Parameters:** Split Ratio = 20:1, 1  $\mu$ L injected

**MS Parameters:** Mass scan range: 30-550 amu

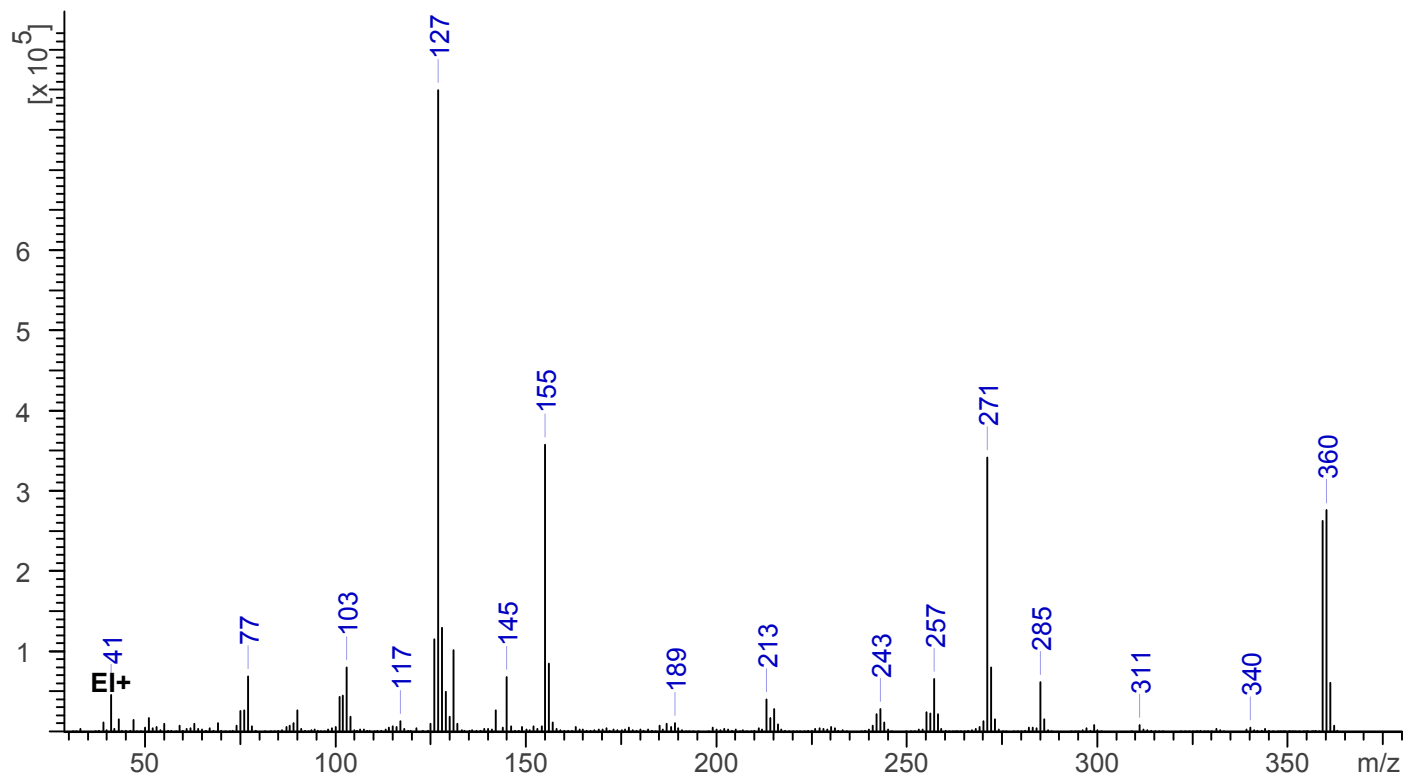
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 18.218min

EI Mass Spectrum: AM2201 Indazole; Lot 0454101-23





# AM-2201 Indazole

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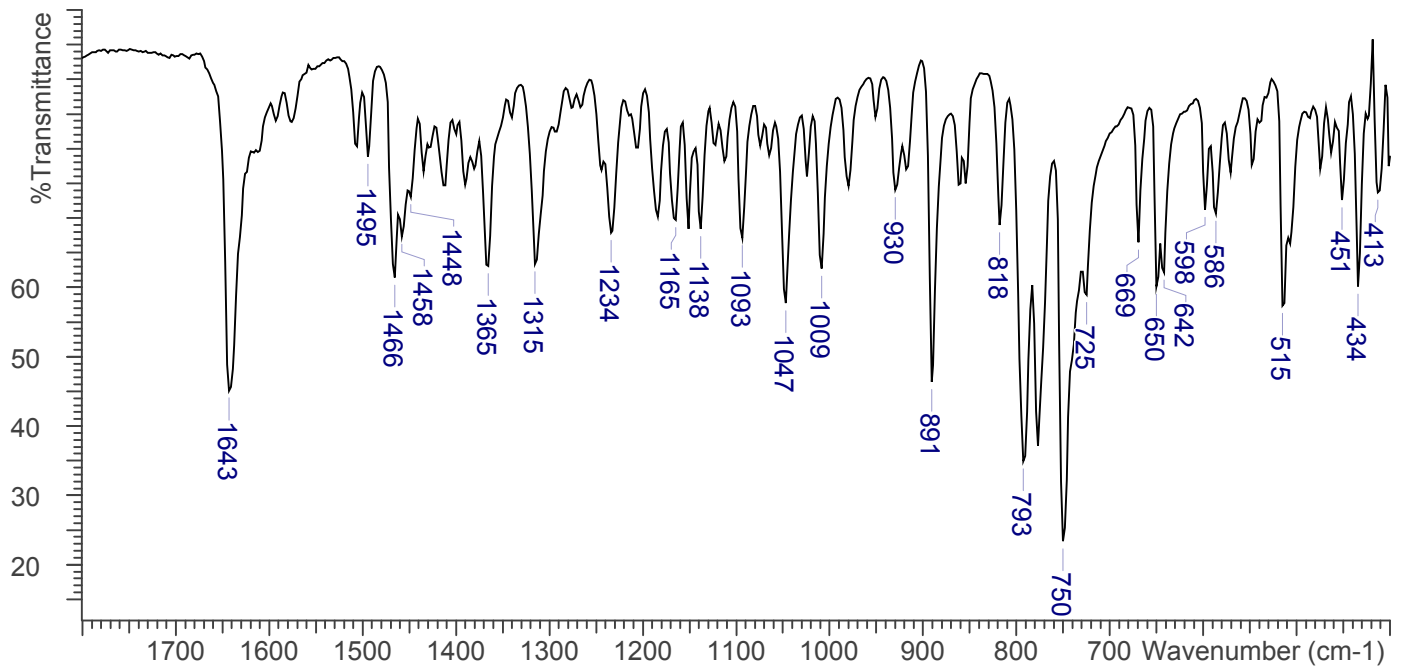
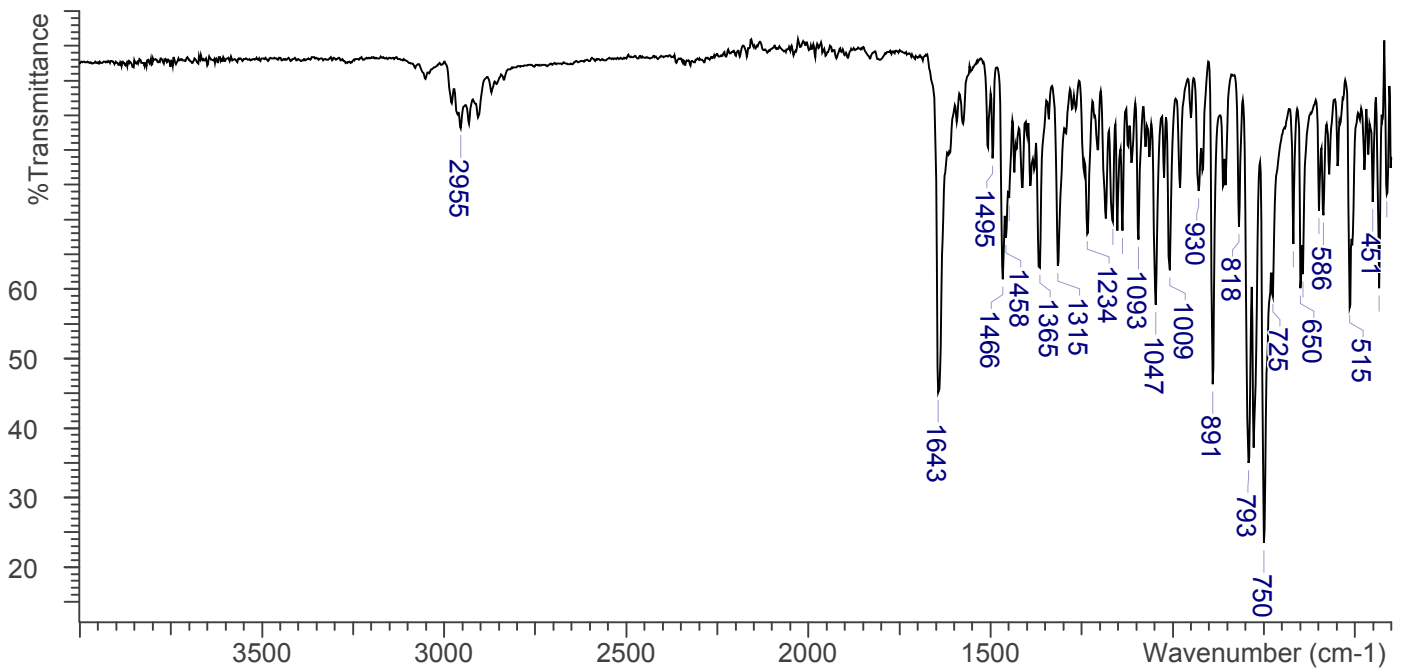


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**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): AM-2201 Indazole, Lot 0454101-23





## AM-2201 Indazole

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### **4. ADDITIONAL RESOURCES**

*No literature available as of 05/2014*