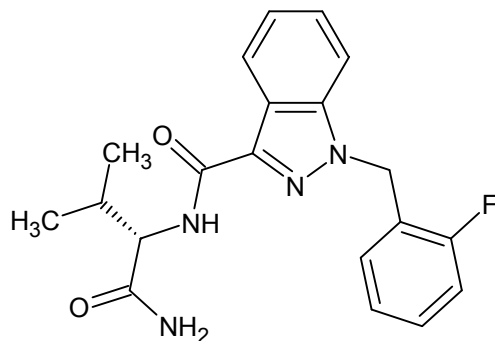




## AB-FUBINACA 2-fluorobenzyl isomer

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



### 1. GENERAL INFORMATION

**IUPAC Name:** *N*-[(2*S*)-1-amino-3-methyl-1-oxobutan-2-yl]-1-[(2-fluorophenyl)methyl]-1*H*-indazole-3-carboxamide

**CAS#:** 1185282-16-9

**Synonyms:** N/A

**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>20</sub> H <sub>21</sub> FN <sub>4</sub> O <sub>2</sub>	368	197.9



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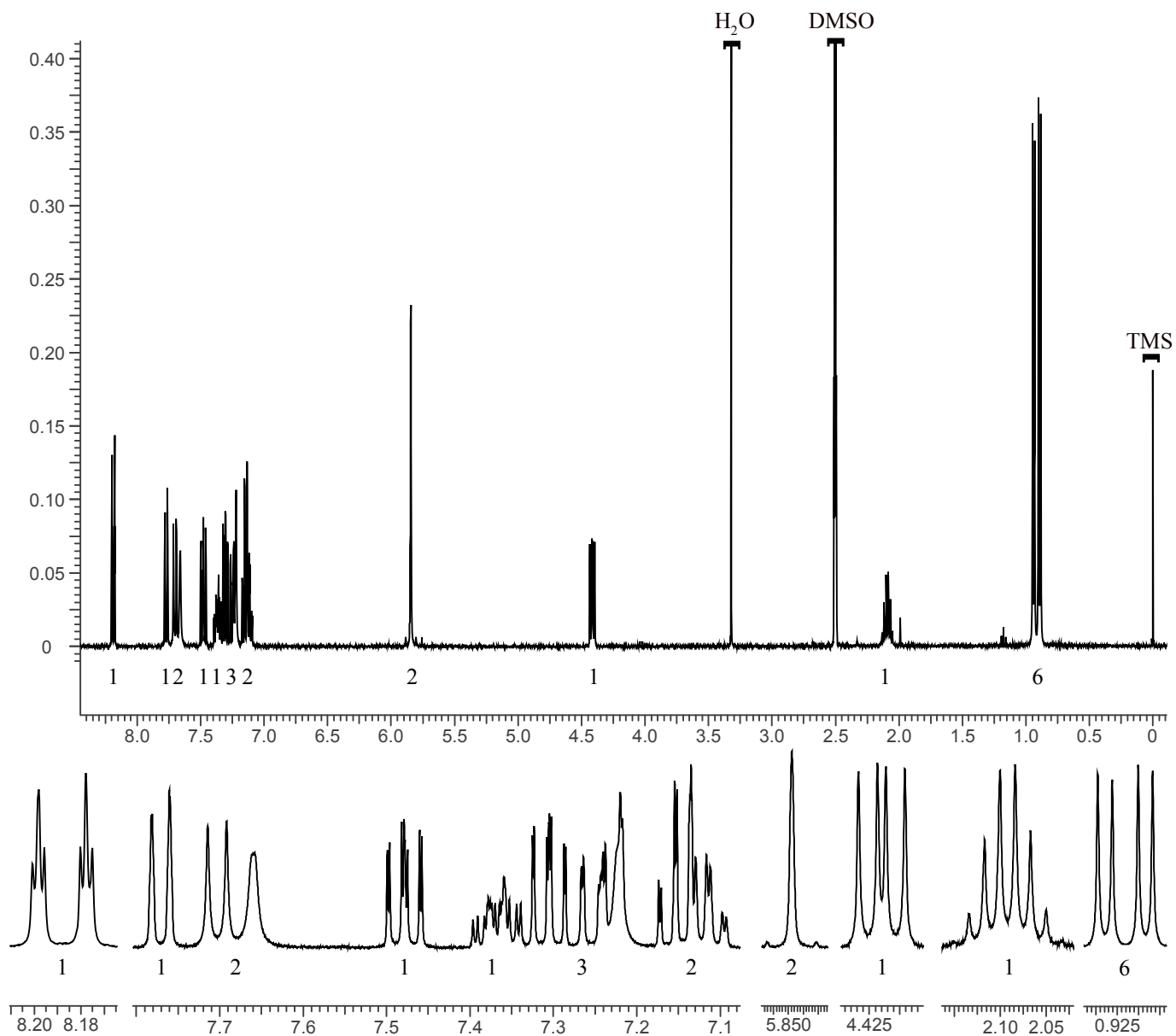
### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~5 mg/mL in DMSO- $d_6$  containing TMS for 0 ppm reference.

**Instrument:** 400 MHz NMR spectrometer  
**Parameters:** Spectral width: at least containing -3 ppm through 13 ppm  
Pulse angle: 90°  
Delay between pulses: 45 seconds

$^1\text{H}$ NMR: AB-FUBINACA 2-fluorobenzyl isomer; Lot# 0455357-18; DMSO- $d_6$ ; 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); 15m x 0.25 mm x 0.25  $\mu$ m

**Carrier Gas:** Helium at 1.5 mL/min

**Temperatures:** Injector: 280°C                      MSD transfer line: 280°C

MS Source: 250°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 9.0 min

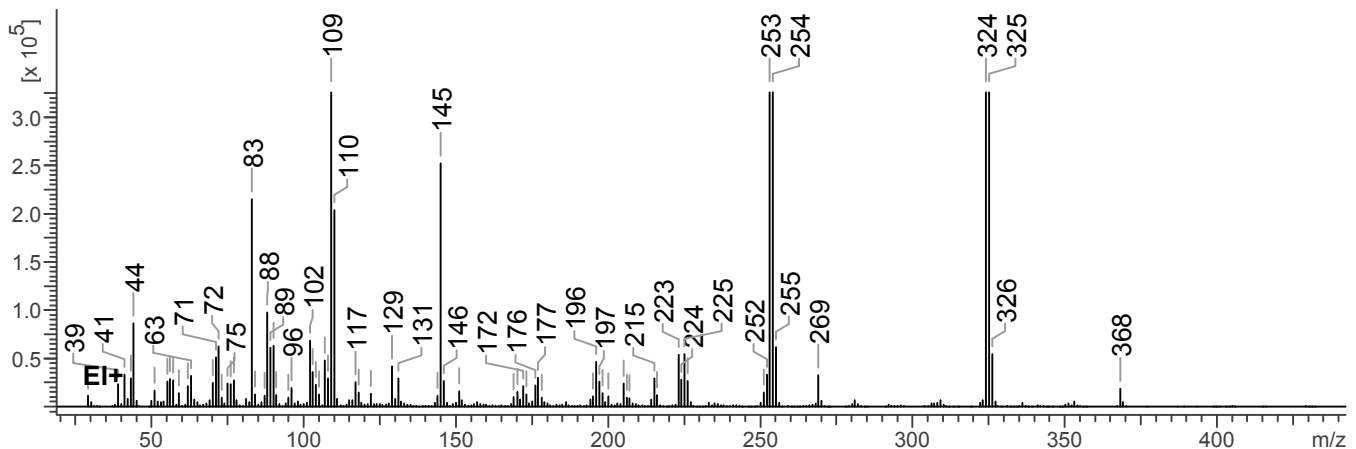
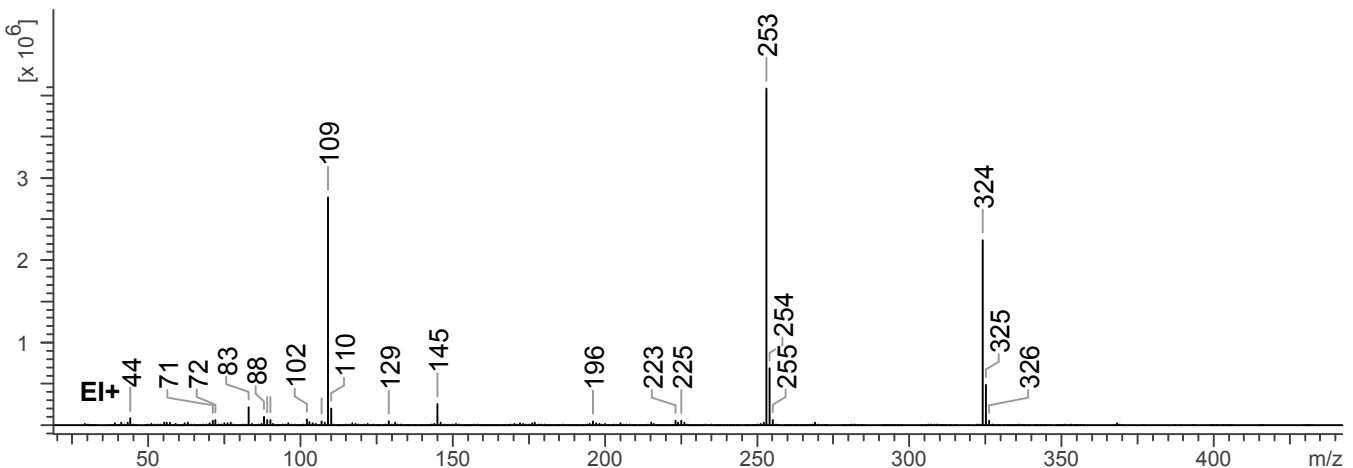
**Injection Parameters:** Split Ratio = 25:1, 2  $\mu$ L injected

**MS Parameters:** Mass scan range: 30-550 amu                      Threshold: 150

Tune file: stune.u                      Acquisition mode: scan

**Retention Time:** 20.399 min

EI Mass Spectrum: AB-FUBINACA 2-fluorobenzyl isomer; Lot# 0455357-18





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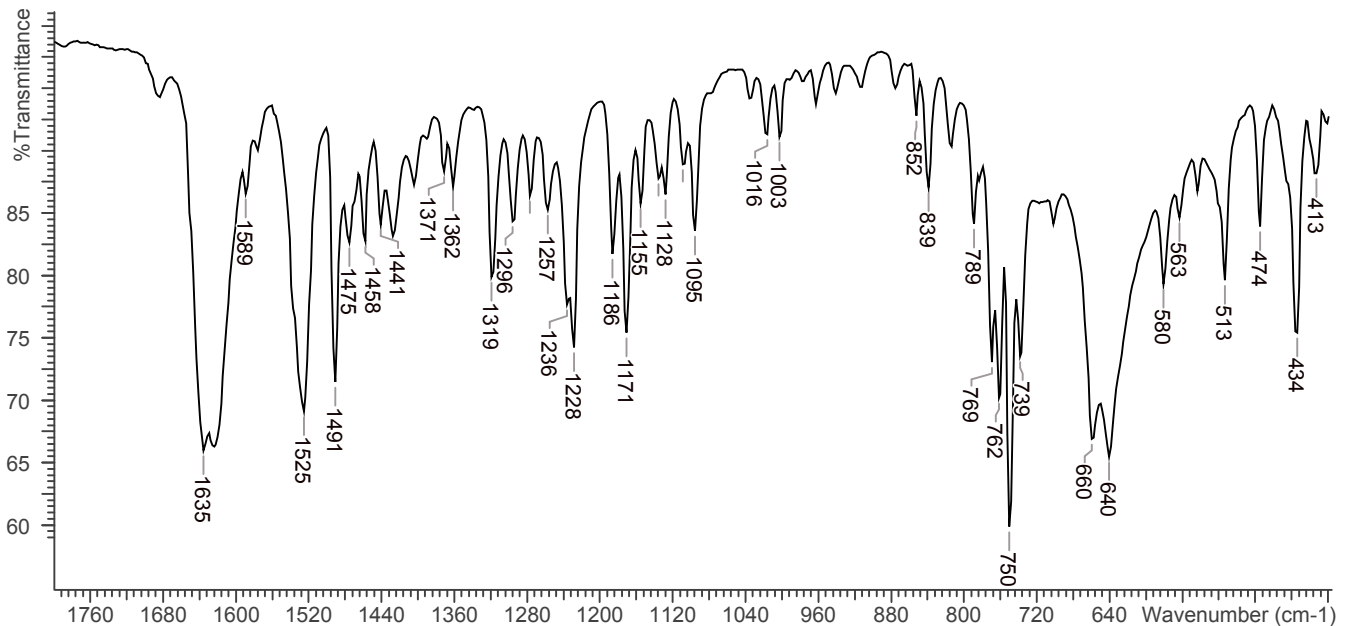
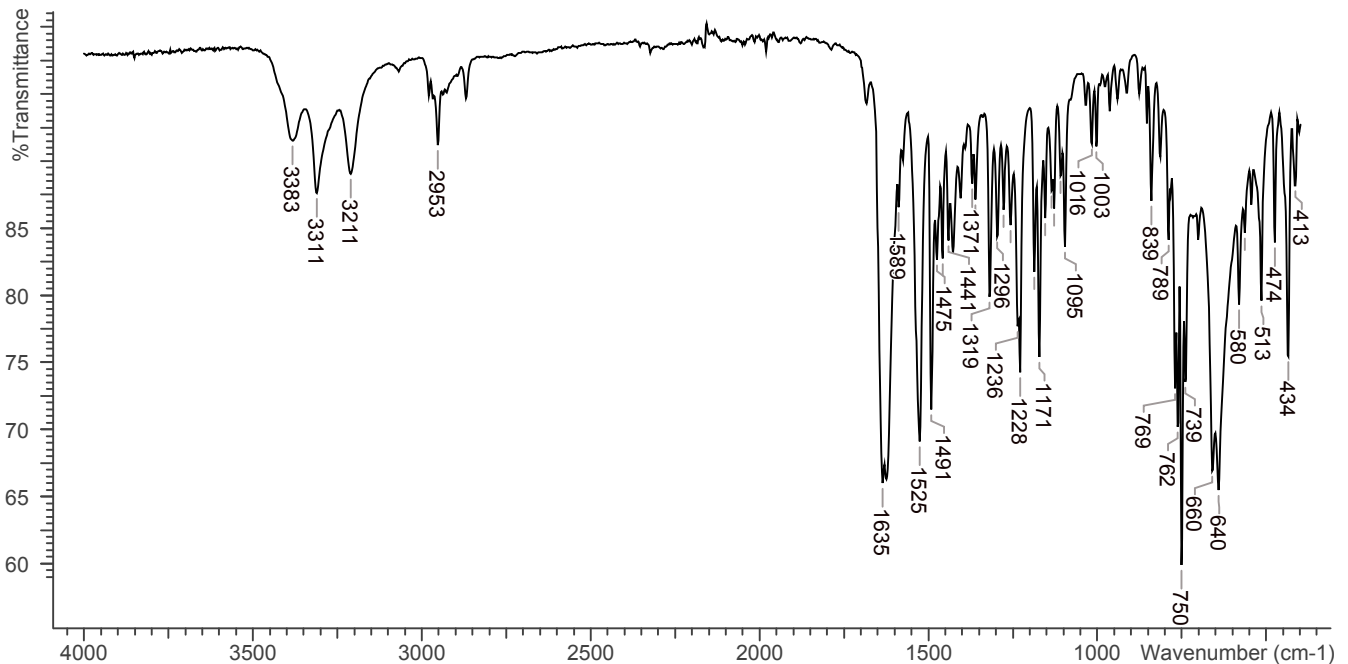


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (1 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 1  
Aperture: 150

FTIR ATR (Diamond 1 Bounce): AB-FUBINACA 2-fluorobenzyl isomer; Lot# 0455357-18





## AB-FUBINACA 2-fluorobenzyl isomer

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### 4. ADDITIONAL RESOURCES

No additional resources as of 03/2016