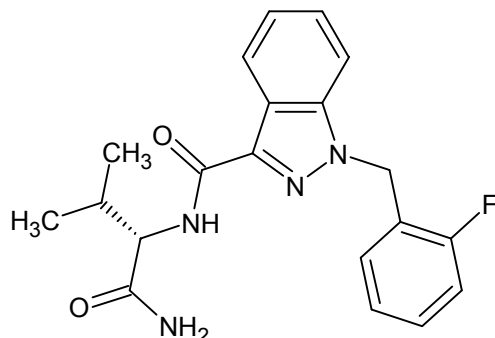




AB-FUBINACA 2-fluorobenzyl isomer

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



1. GENERAL INFORMATION

IUPAC Name:	<i>N</i> -[(2 <i>S</i>)-1-amino-3-methyl-1-oxobutan-2-yl]-1-[(2-fluorophenyl)methyl]-1 <i>H</i> -indazole-3-carboxamide
CAS#:	1185282-16-9
Synonyms:	N/A
Source:	DEA Reference Material Collection
Appearance:	White 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 ₂₀ H ₂₁ FN ₄ O ₂	368	197.9



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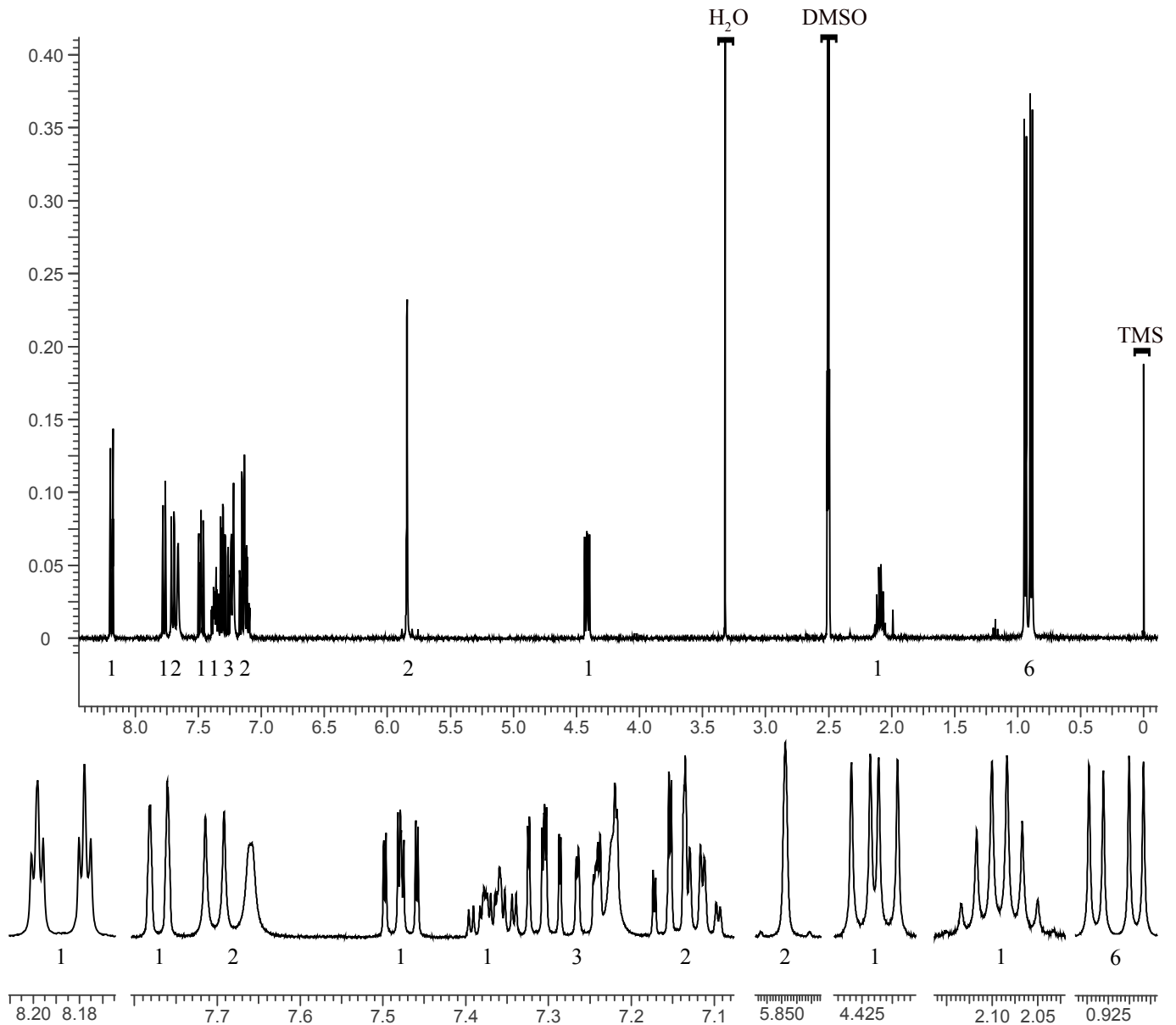
3. QUALITATIVE DATA

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

^1H 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 μ 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

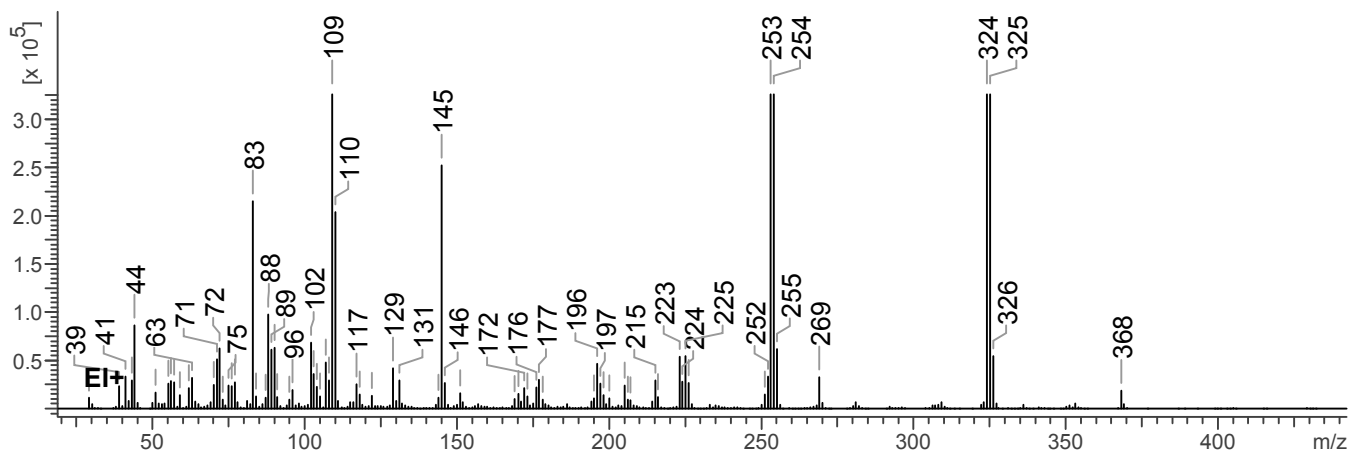
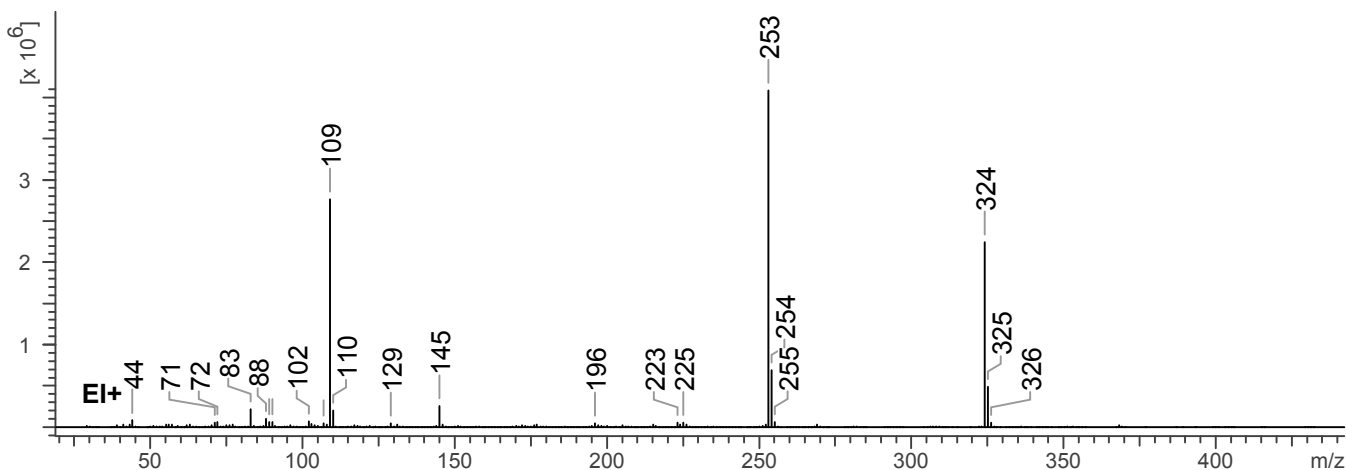
Injection Parameters: Split Ratio = 25:1, 2 μ L injected

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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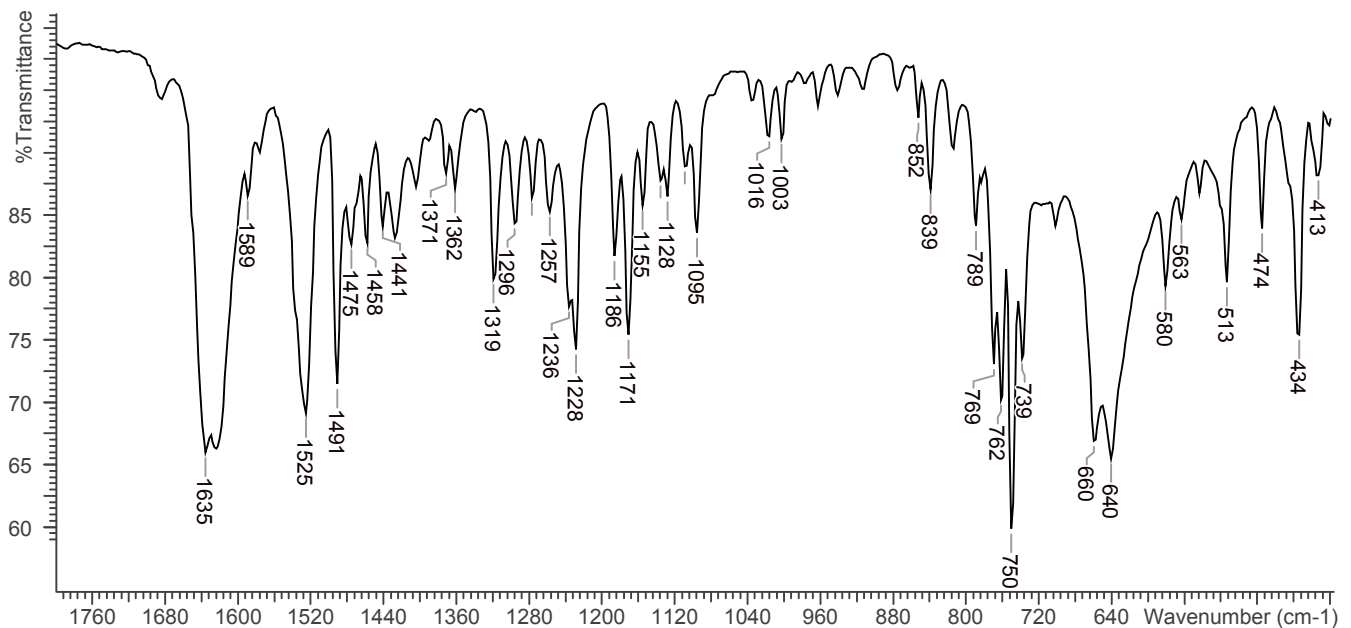
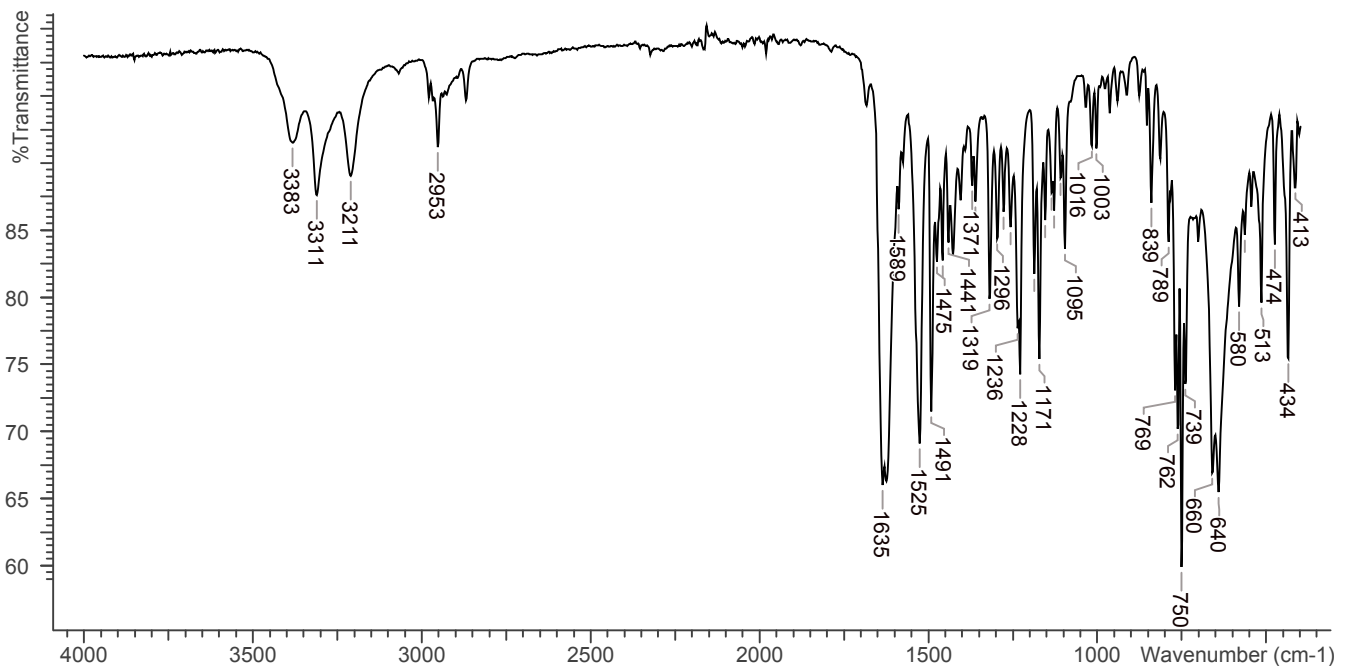


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
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