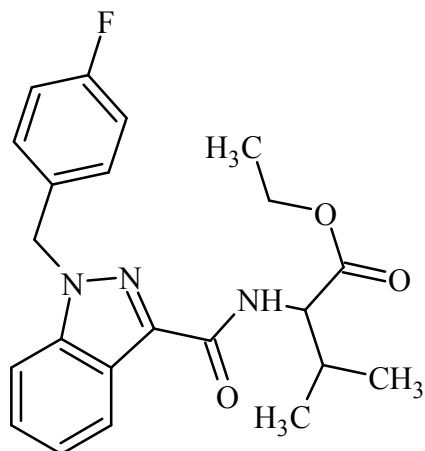




## EMB-FUBINACA

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>	ethyl <i>N</i> -{1-[(4-fluorophenyl)methyl]-1 <i>H</i> -indazole-3-carbonyl} valinate
<b>CAS#:</b>	NA
<b>Synonyms:</b>	AEB-FUBINACA, FU-AEB, 5-fluoro EMB-FUBINACA, ethyl (1-(4-fluorobenzyl)-1 <i>H</i> -indazole-3-carbonyl)-L-valinate
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	white powder
<b>UV<sub>max</sub>(nm):</b>	NA

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>22</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>3</sub>	397.45	66



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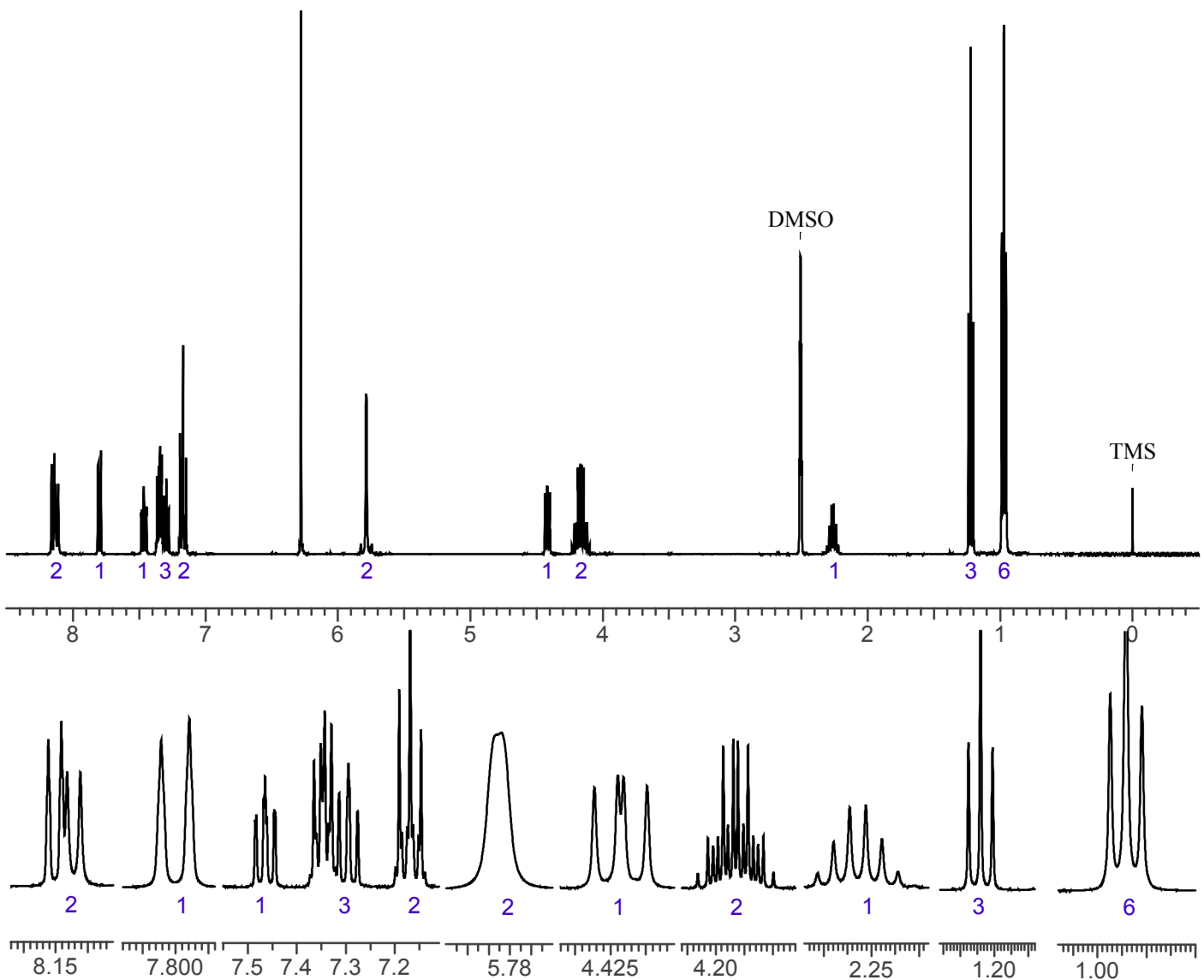
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~11 mg/mL in DMSO containing TMS for 0 ppm reference and maleic acid 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

<sup>1</sup>H NMR: EMB-FUBINACA lot# 0473498-18, DMSO, 400MHz  
maleic acid





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## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector

**Column:** HP-5; 30m 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: 230°C

MS Quad: 150°C

Oven program:

1) 100°C initial temperature for 1.0 min

2) Ramp to 280°C at 12 °C/min

3) Hold final temperature for 9.0 min

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

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

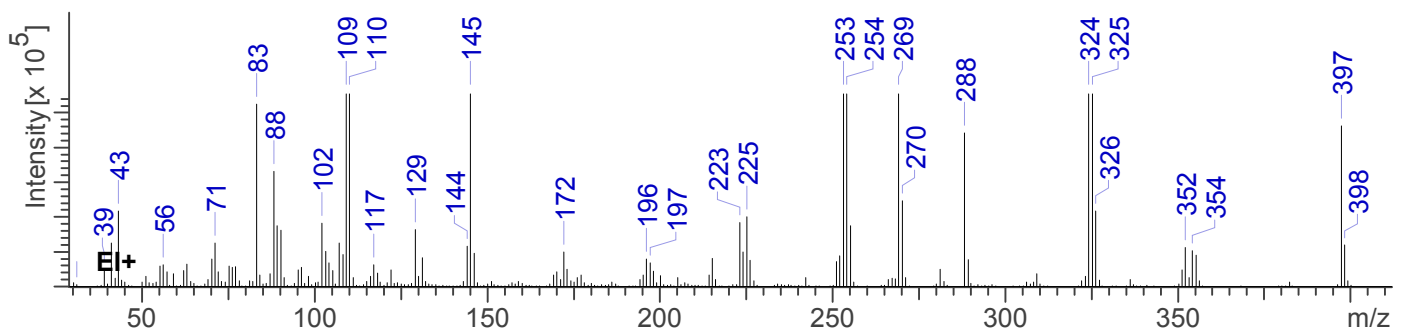
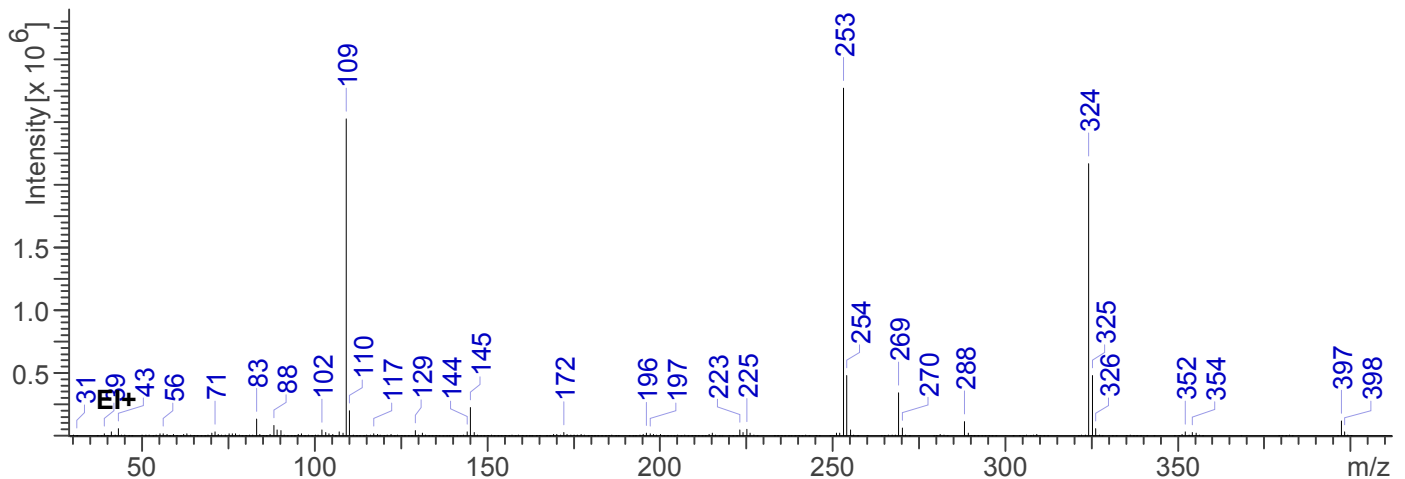
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 18.428 min

EI Mass Spectrum: EMB-FUBINACA Lot# 0473498-18





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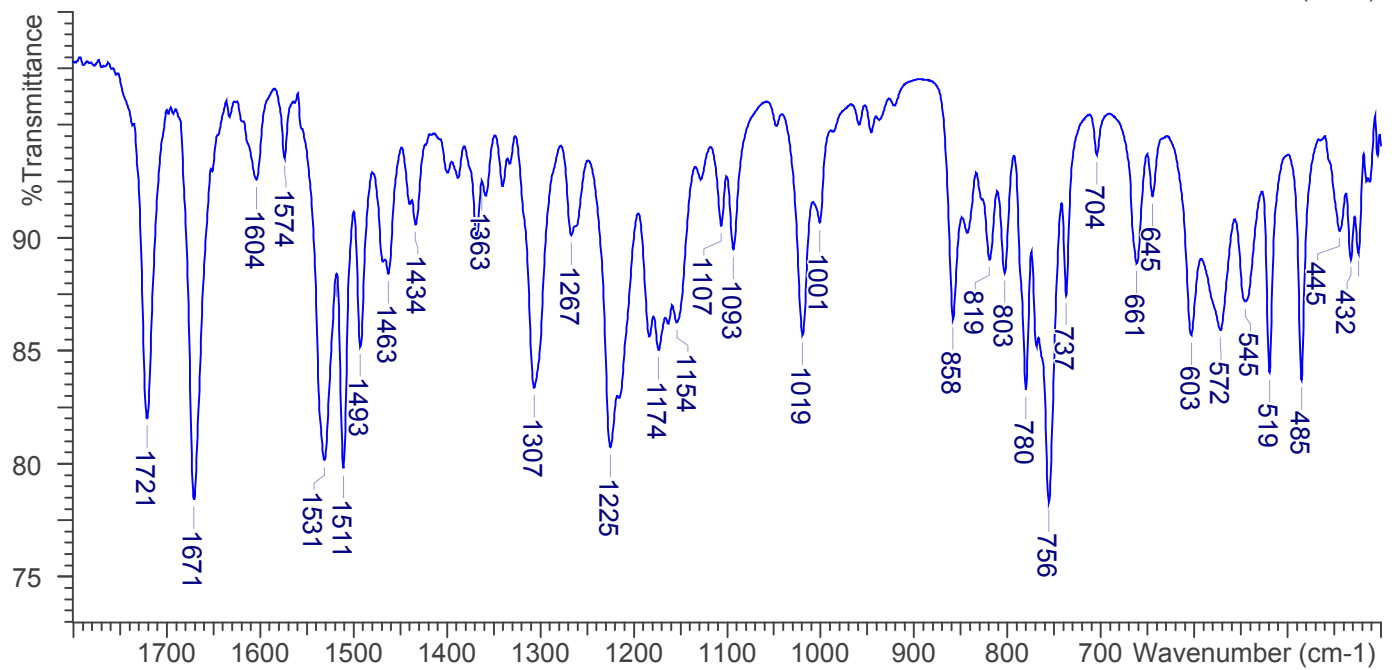
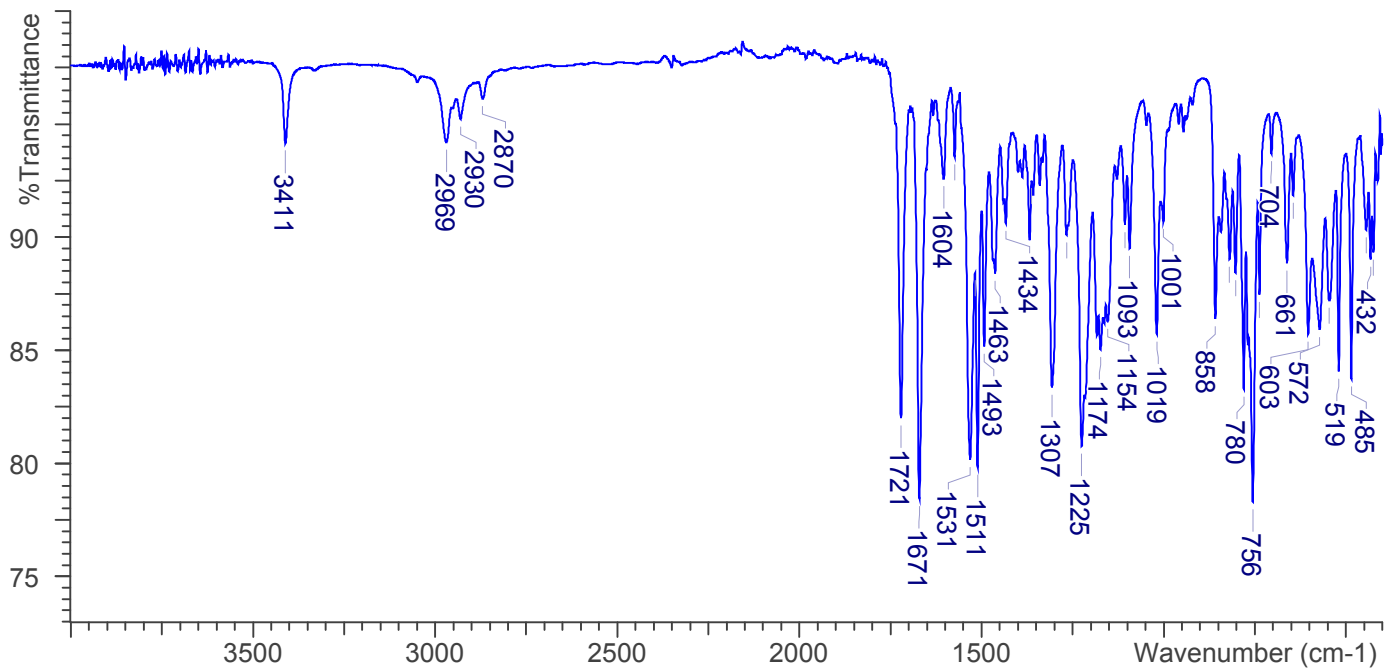


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**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): EMB-FUBINACA Lot# 0473498-18





## EMB-FUBINACA

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### **4. ADDITIONAL RESOURCES**

**Liu Cuimei, et.al Identification and analytical characterization of six synthetic cannabinoids NNL-3, 5F-NPB-22-7 N, 5F-AKB-48-7 N, 5F-EDMB-PINACA, EMB-FUBINACA, and EG-018, DOI: 10.1002/dta.2160**