

## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	<i>N</i> -(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1 <i>H</i> -indazole-3-carboxamide
<b>CFR:</b>	Not Scheduled (7/2013)
<b>CAS#:</b>	1185282-01-2
<b>Synonyms:</b>	N/A
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<b>Kovat's Index:</b>	Pending
<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>20</sub> H <sub>21</sub> FN <sub>4</sub> O <sub>2</sub>	368	166.3

## 3. ADDITIONAL RESOURCES

Uchiyama, N; Matsuda, S; Wakana, D; Kikura-Hanajiri, R; Goda, Y. New cannabimimetic indazole derivatives, *N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1*H*-indazole-3-carboxamide (AB-PINACA) and *N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indazole-3-carboxamide (AB-FUBINACA) identified as designer drugs in illegal products. *Forensic Toxicol.* **2013**, *31* (1), 93-100.

[Forendex](#)

[Wikipedia](#)

#### 4. QUALITATIVE DATA

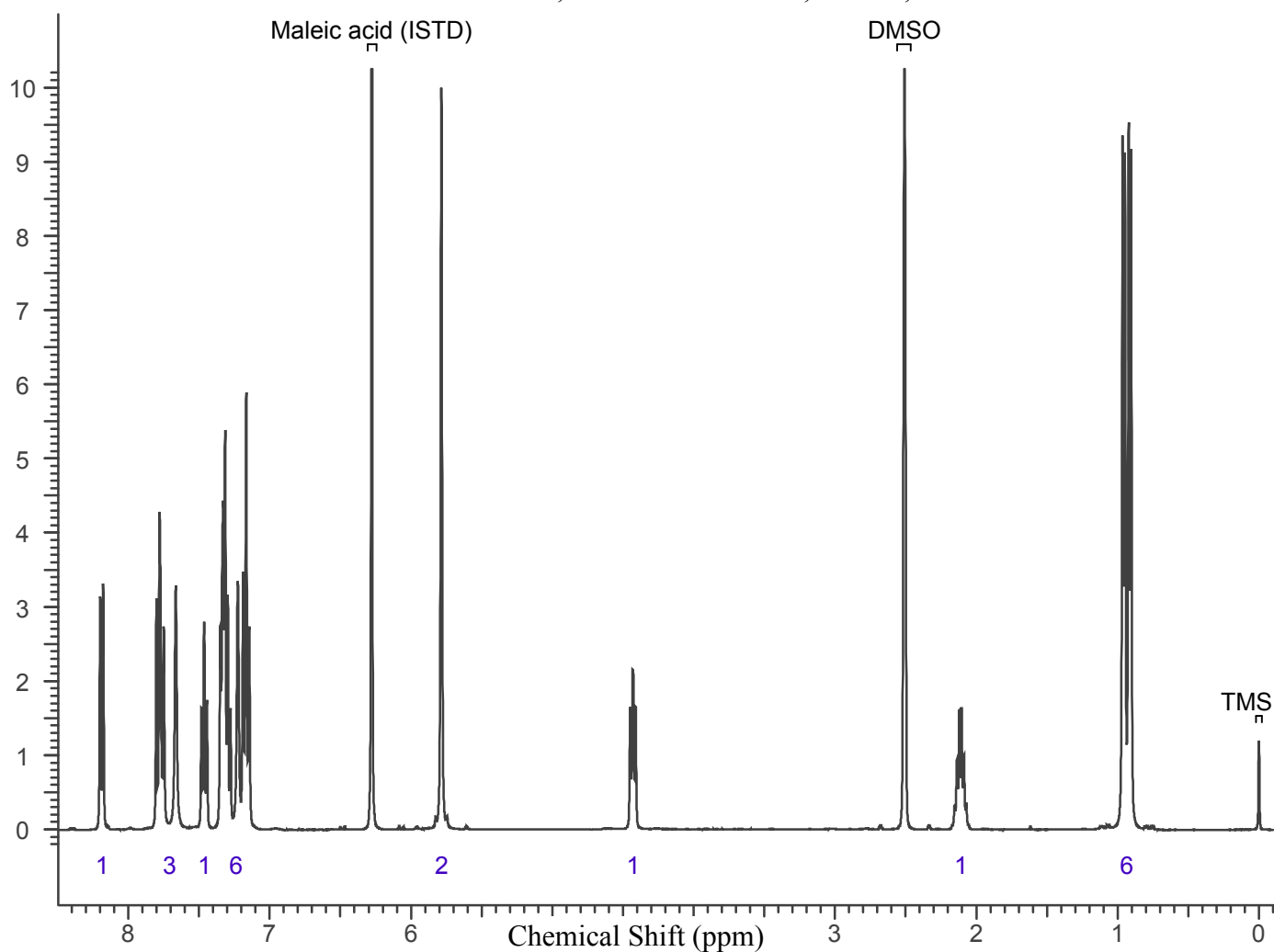
##### 4.1 NUCLEAR MAGNETIC RESONANCE

###### Method NMR DMSO

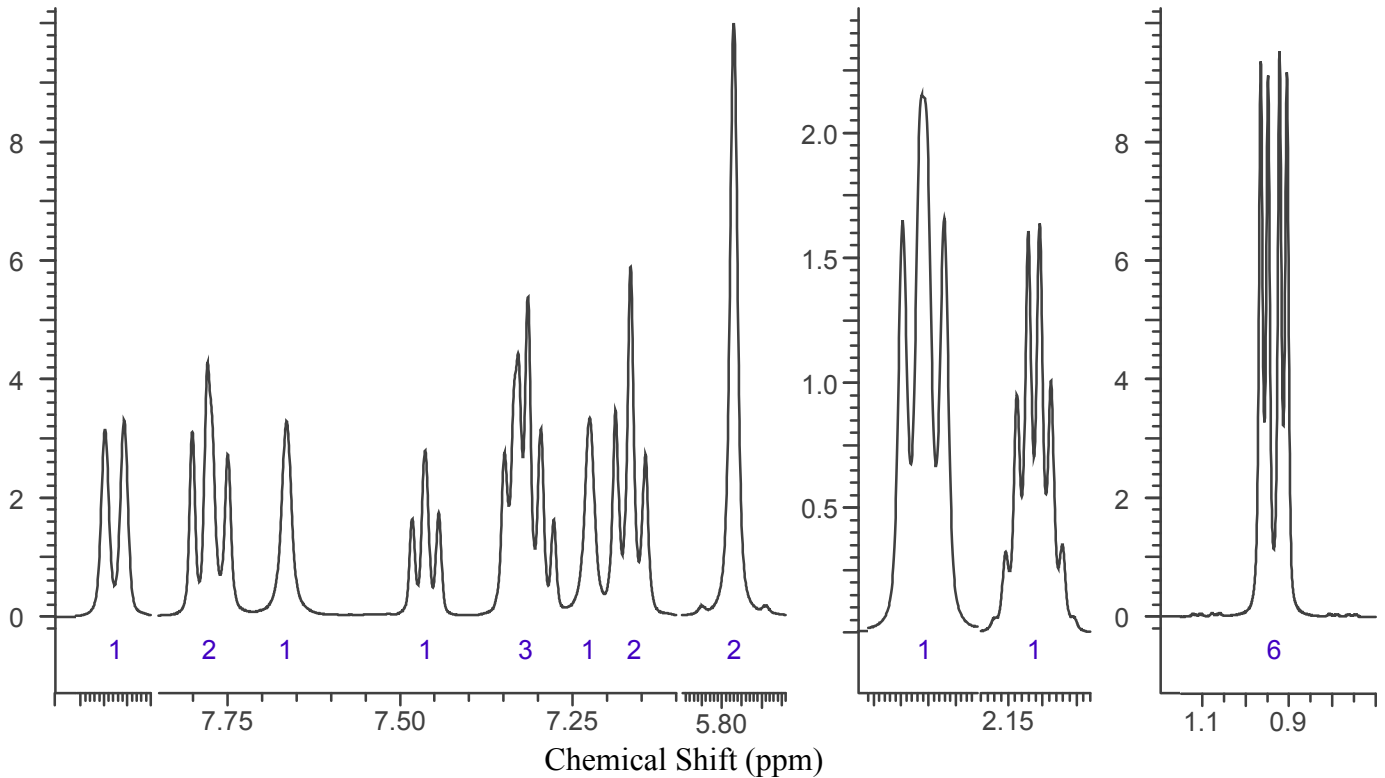
*Sample Preparation:* Dilute analyte to ~10 mg/mL in DMSO containing TMS for 0 ppm reference and maleic acid as quantitative internal standard.

**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: AB-FUBINACA; Lot RM-130530-01; DMSO; 400 MHz



<sup>1</sup>H NMR: AB-FUBINACA; Lot RM-130530-01; DMSO; 400 MHz



## 4.2 Gas Chromatography/Mass Spectrometry

*Sample Preparation:* Dilute analyte ~ 1 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 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 9.0 min

***Injection Parameters:***

Split Ratio = 20:1, 1 μL injected

***MS Parameters:***

Mass scan range: 30-550 amu

Threshold: 100

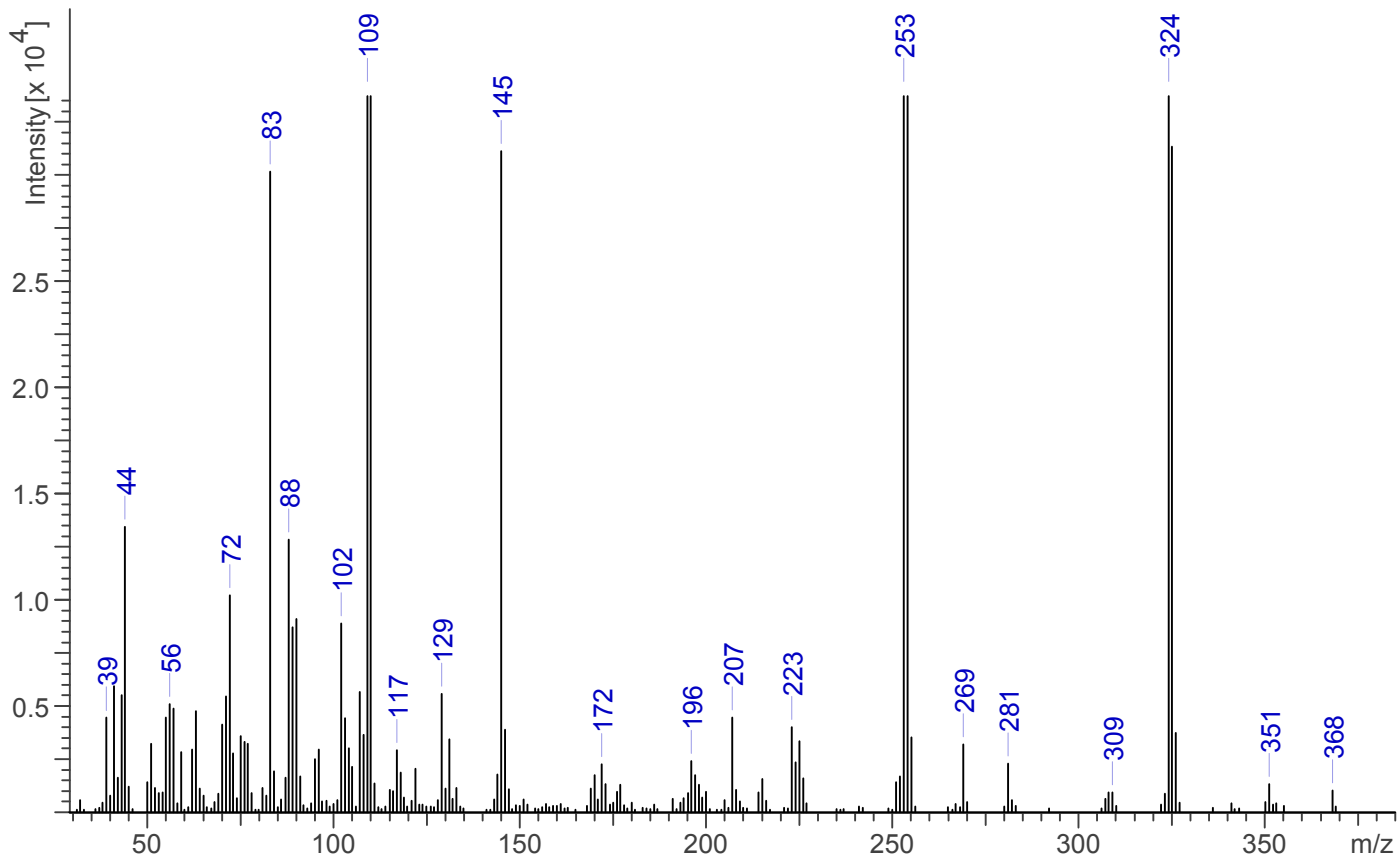
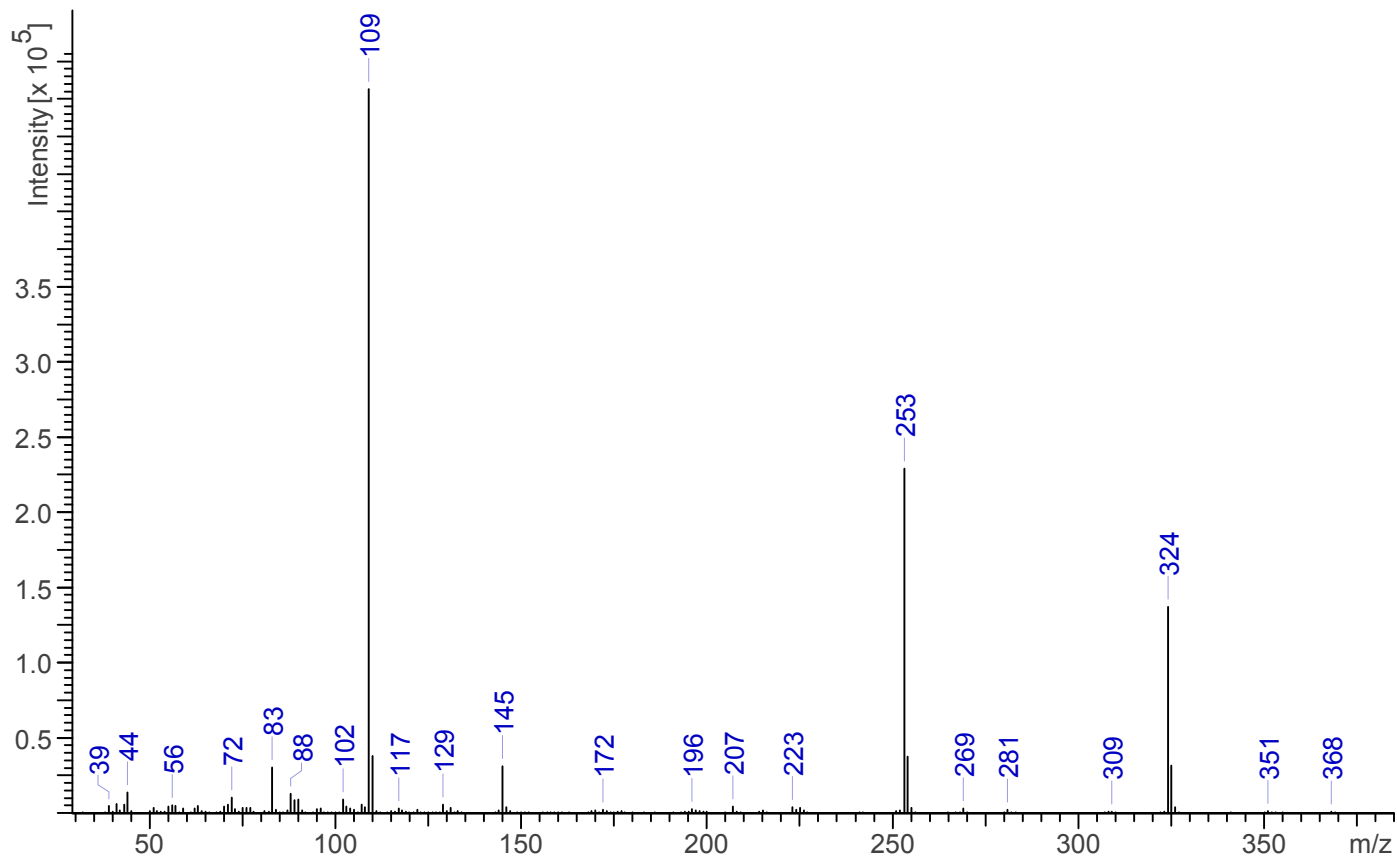
Tune file: stune.u

Acquisition mode: scan

***Retention Time:***

19.039 min

EI Mass Spectrum: AB-FUBINACA; Lot RM-130530-01



### 4.3 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): AB-FUBINACA; Lot RM-130530-01

