

## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-pentyl-N-(tricyclo[3.3.1.1 <sup>3,7</sup> ]dec-1-yl)-1H-indazole-3-carboxamide
<b>CFR:</b>	Not Scheduled (11/2012)
<b>CAS #:</b>	1345973-53-6
<b>Synonyms:</b>	APINACA N-adamantyl-1-pentylindazole-3-carboxamide N-adamantyl-1-pentyl-1H-indazole-3-carboxamide
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<b>Kovat's Index:</b>	Pending
<b>UV<sub>max</sub>:</b>	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>31</sub> N <sub>3</sub> O	365	63.6

### 3. *ADDITIONAL RESOURCES*

[Forendex](#)

[Wikipedia](#)

### 4. *QUALITATIVE DATA*

#### 4.1 NUCLEAR MAGNETIC RESONANCE

##### *Method NMR CDCl<sub>3</sub>*

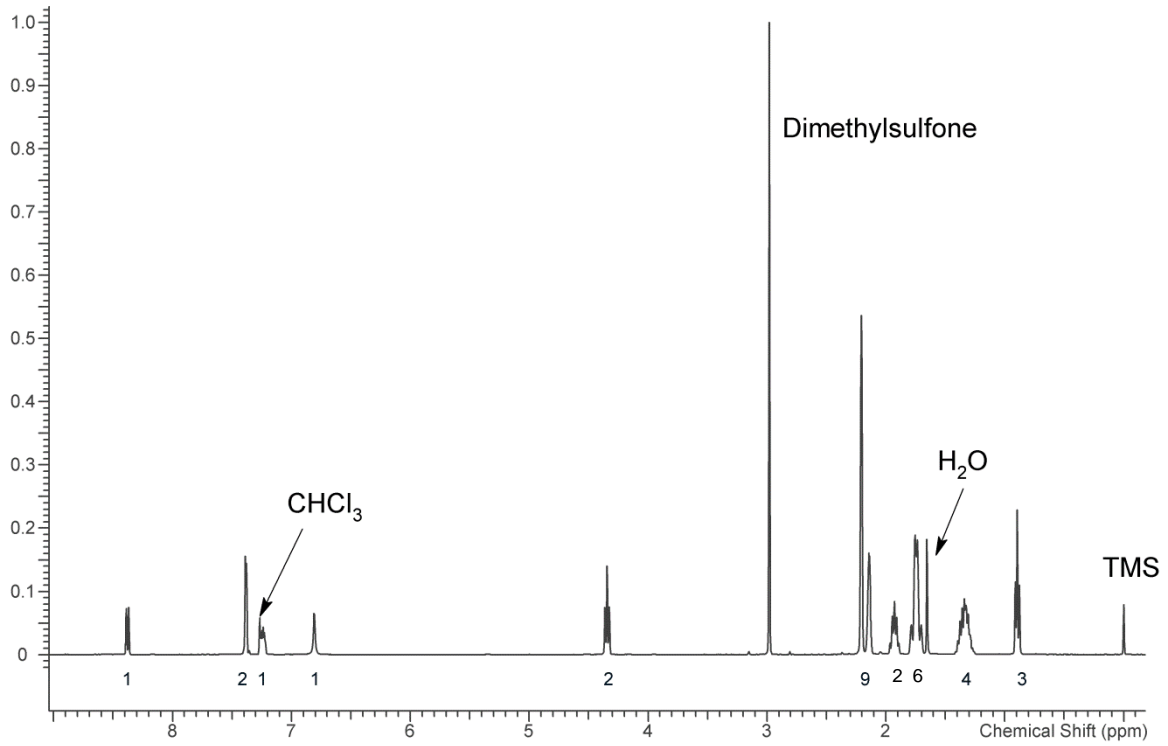
*Sample Preparation:* Dilute analyte to ~10 mg/mL in CDCl<sub>3</sub> containing TMS for 0 ppm reference and dimethylsulfone as quantitative ISTD

*Instrument:* Varian Mercury 400 MHz NMR spectrometer with proton detection probe

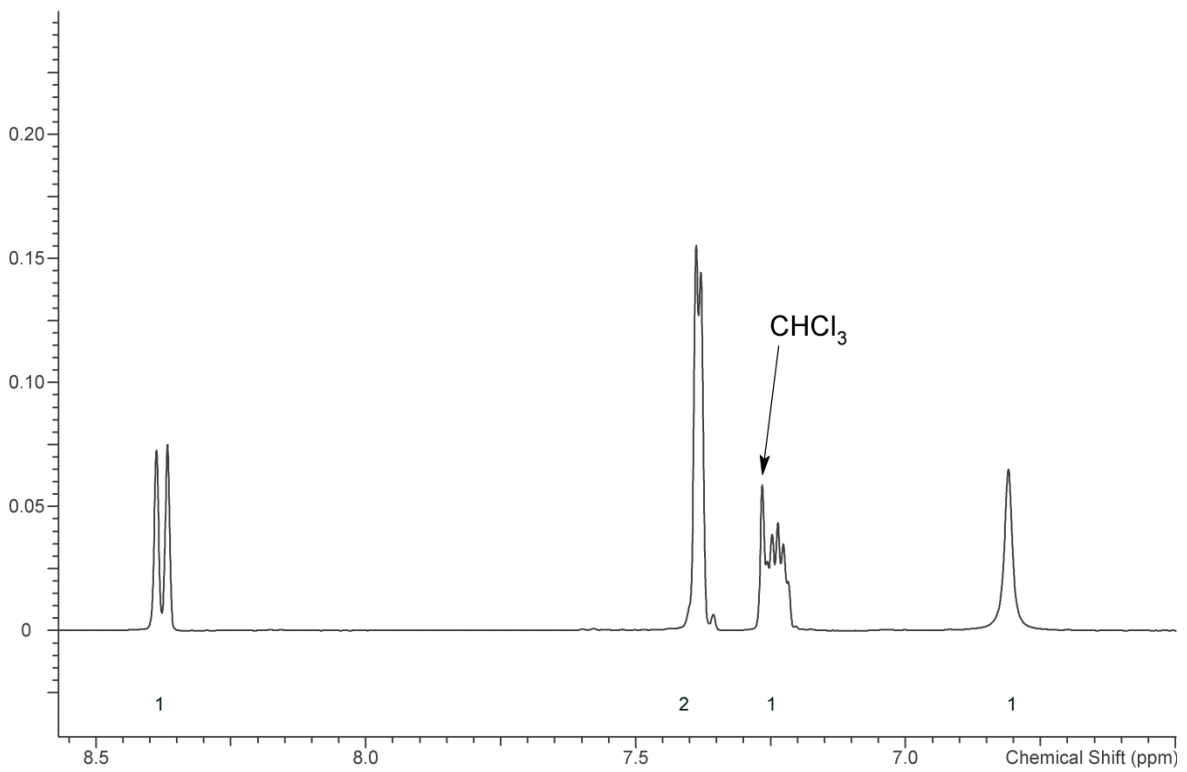
*Parameters:*

- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

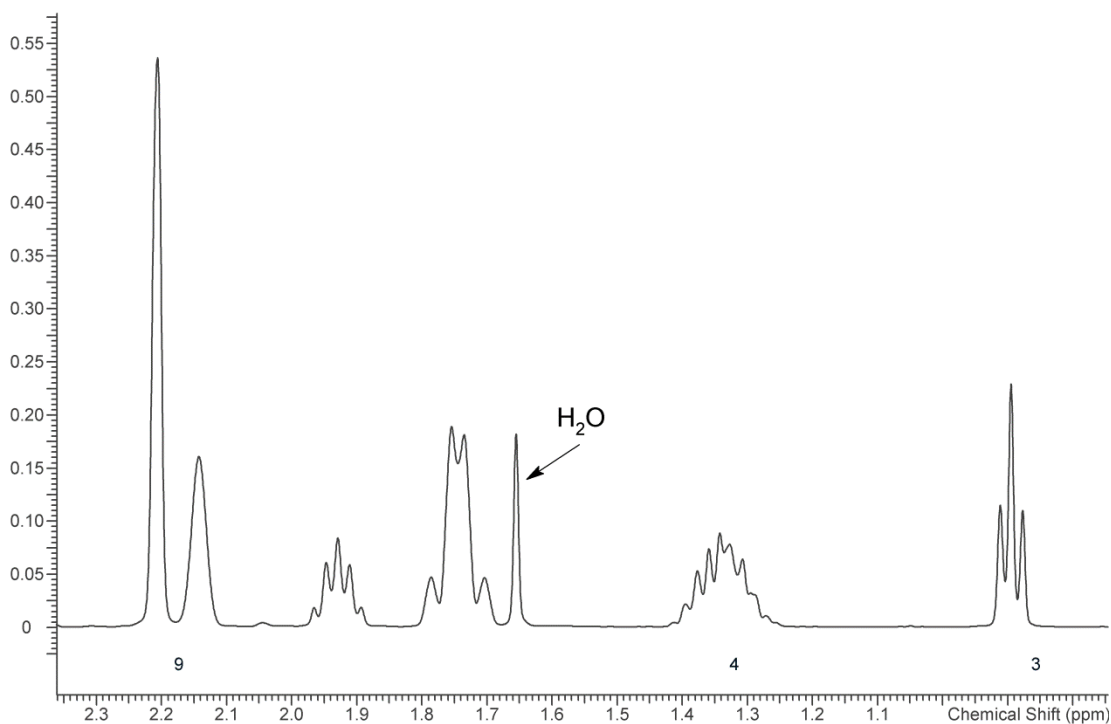
1H NMR: AKB-48 Lot # ALB222-12; CDCl<sub>3</sub>; 400MHz



1H NMR: AKB-48 Aromatic Region Lot # ALB222-12; CDCl<sub>3</sub>; 400MHz



1H NMR: AKB-48 Lot # ALB222-12; CDCl3; 400 MHz



## 4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte to ~1 mg/mL in MeOH.

***Instrument:*** Gas chromatograph operated in split mode with MS detector

***Column:*** DB-1 MS 30m x .25mm x .25 $\mu$ m

***Carrier gas:*** Helium at 1 mL/min

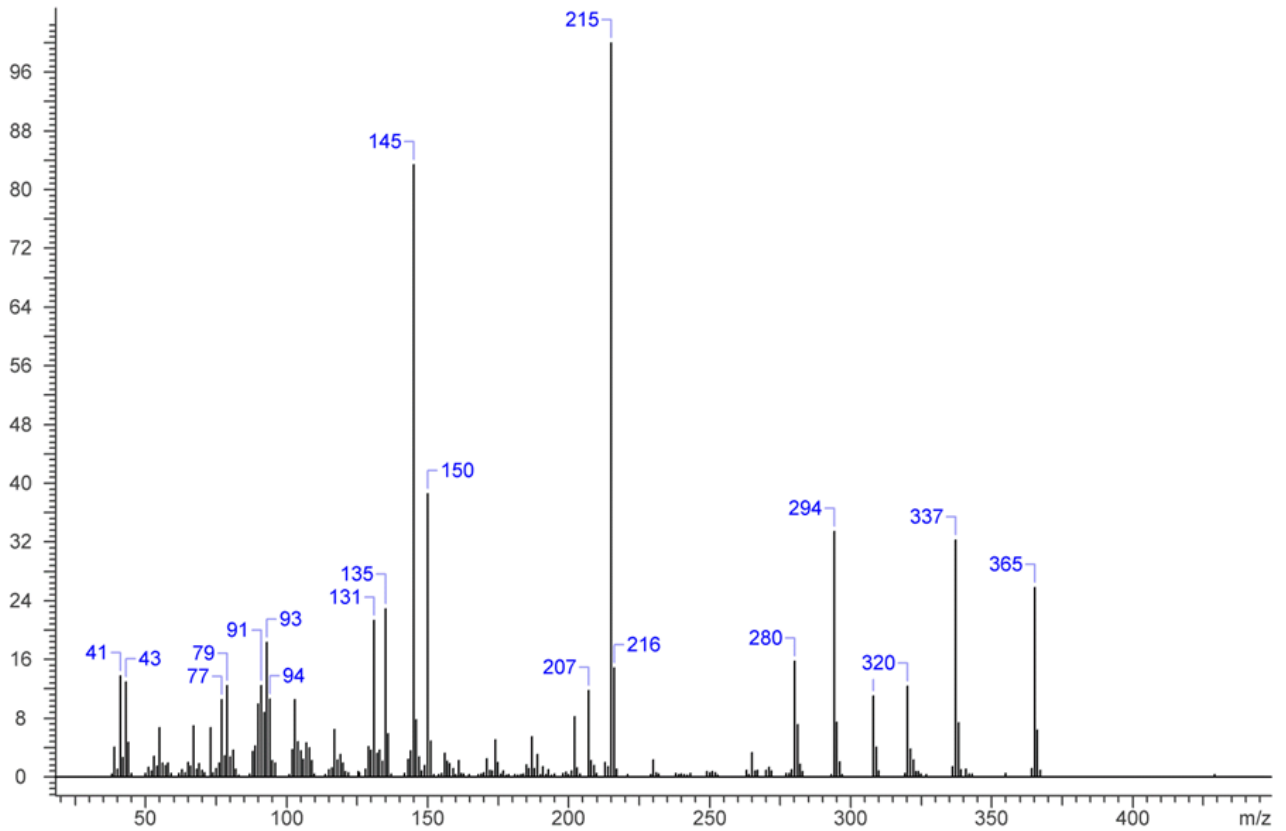
***Temperatures:*** Injector: 280°C  
MSD transfer line: 280°C  
MS Source: 230°C  
MS Quad: 150°C  
Oven program:  
1) 100°C initial temperature for 1.0 min  
2) Ramp to 300°C at 12°C/min  
3) Hold final temperature for 9.0 min

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

***MS Parameters:*** Mass scan range: 34-550 amu  
Threshold: 100  
Tune file: stune.u  
Acquisition mode: scan

***Retention Time:*** 20.035 min

EI Mass Spectrum: AKB-48 Lot # ALB222-12



### 4.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:**

FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**

Number of scans: 32

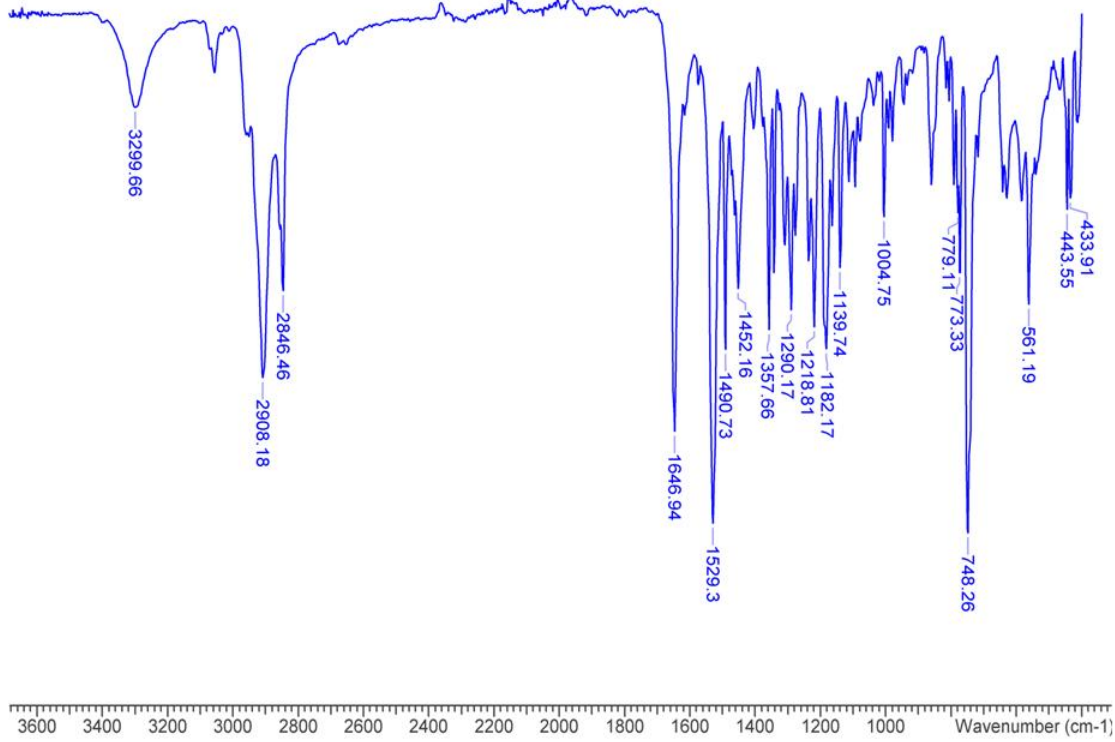
Number of background scans: 32

Resolution 4 cm<sup>-1</sup>

Sample gain: 8

Aperture: 150

FTIR: AKB-48 Lot # ALB222-12



FTIR: AKB-48 Lot # ALB222-12 (low cm⁻¹)

