1. GENERAL INFORMATION

**IUPAC Name:** 1-pentyl-N-(tricyclo[3.3.1.1\(^3,7\)]dec-1-yl)-1H-indazole-3-carboxamide

**CFR:** Not Scheduled (11/2012)

**CAS #:** 1345973-53-6

**Synonyms:**
- APINACA
- N-adamantyl-1-pentylindazole-3-carboxamide
- N-adamantyl-1-pentyl-1H-indazole-3-carboxamide

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**Kovat’s Index:** Pending

**UV\(_{max} \):** Not Determined

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C(<em>{23})H(</em>{31})N(_3)O</td>
<td>365</td>
<td>63.6</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES

Forendex
Wikipedia

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~10 mg/mL in CDCl₃ 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
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 .25μm

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

**Retention Time:**
- 20.035 min
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$^{-1}$
- Sample gain: 8
- Aperture: 150