1. GENERAL INFORMATION

**IUPAC Name:** 1-(5-fluoropentyl)-N-(tricyclo[3.3.1.1^3,7]dec-1-yl)-1H-indazole-3-carboxamide

**CFR:** Not Scheduled (2/2013)

**CAS #:** Not Available

**Synonyms:** 5F-APINACA; APINACA 5-Fluoropentyl analog; 5F-AKB-48

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**Kovat’s Index:** Pending

**UV\text{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_{23}H_{30}FN_{3}O</td>
<td>383</td>
<td>54.9</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES

No resources identified as of 02/08/2013.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~25 mg/mL in deuterochloroform (CDCl₃) containing TMS for 0 ppm reference and dimethylsulfone as quantitative internal standard.

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: 5-Fluoro-AKB-48 Lot # N1-P53EMG; CDCl₃; 400 MHz

1H NMR: 5-Fluoro-AKB-48 Lot # N1-P53EMG; CDCl₃; 400 MHz
4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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

Column: DB-1; 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: 30-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time:
- 20.913 minutes
GC/MS Analytical Observation:

Other laboratories have reported observing differences in the abundances of various fragment ions, similar to the variations seen in XLR11, and the cause has not yet been determined. No spectra are available.

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: 4cm⁻¹
- Sample gain: 8
- Aperture: 150
FTIR Analytical Observation:
Due to structural similarities with XLR11, polymorphic characteristics are expected in this compound.