1. GENERAL INFORMATION

**IUPAC Name:** N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(5-fluoropentyl)-1H-indazole-3-carboxamide

**CFR:** Not Scheduled (10/2013)

**CAS#:** Not Available

**Synonyms:** 5-Fluoro-AB-PINACA

**Source:** DEA Reference Material Collection

**Appearance:** White powder (base)

**Kovat's Index:** Pending

**UV$_{max}$ (nm):** 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$<em>{18}$H$</em>{25}$FN$<em>{4}$O$</em>{2}$</td>
<td>348</td>
<td>85.3</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES

No resources identified as of 10/2013.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CD$_3$OD

Sample Preparation: Dilute analyte to ~10 mg/mL in methanol-$d_4$ (CD$_3$OD) 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

$^1$H NMR: 5F-AB-PINACA; Lot RM-130816-02; CD$_3$OD; 400 MHz

* = Impurity

Maleic acid (ISTD)  CD3OH/HOD

CD2HOD

TMS
4.2 Gas Chromatography/Mass Spectrometry

*Sample Preparation:* Dilute analyte ~ 1 mg/mL in methanol

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

**Column:** HP-5 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) 90°C initial temperature for 2.0 min
  2) Ramp to 300°C at 14 °C/min
  3) Hold final temperature for 17.0 min

**Injection Parameters:** Split Ratio = 25:1, 1 μL injected

**MS Parameters:**
- Mass scan range: 29-750 amu
- Threshold: 50
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:** 18.218 min
EI Mass Spectrum: 5F-AB-PINACA; Lot RM-130816-02
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