1. GENERAL INFORMATION

**IUPAC Name:** methyl 2-(1-(4-fluoropentyl)-1H-indazole-3-carboxamido)-3,3-dimethylbutanoate

**CAS#:** NA

**Synonyms:** 4-Fluoro-MDMB-PINACA; methyl 2-{[1-(4-fluoropentyl)-1H-indazole-3-carbonyl]amino}-3,3-dimethylbutanoate

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**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_{20}H_{28}FN_{3}O_{3}</td>
<td>377.45</td>
<td>47.26</td>
</tr>
</tbody>
</table>
3. **QUALITATIVE DATA**

3.1 **NUCLEAR MAGNETIC RESONANCE**

*Sample Preparation:* Dilute analyte to ~11 mg/mL in methanol-$d_4$ containing TMS for 0 ppm reference and dimethylfumarate 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

$^1$HNMR: 4-Fluoro ADB; Lot # 0524165-1; CD$_3$OD; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃

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 1.5 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 280°C at 12 °C/min
3) Hold final temperature for 9.0 min

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

MS Parameters:
- Mass scan range: 30-550 amu
- Threshold: 250
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 16.044 min

EI Mass Spectrum: 4-Fluoro ADB; Lot # 0524165-1
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)
Scan Parameters:
- Number of scans: 32
- Number of background scans: 32
- Resolution: 4 cm⁻¹
- Sample gain: 1
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): 4-Fluoro ADB; Lot # 0524165-1