1. GENERAL INFORMATION

**IUPAC Name:** methyl 2-(1-(4-fluorobenzyl)-1H-indole-3-carboxamido)pentanoate

**CAS#:** NA

**Synonyms:** methyl N-{1-[(4-fluorophenyl)methyl]-1H-indole-3-carbonyl}norvalinate; MMB-FUBICA isomer 1

**Source:** DEA Reference Material Collection

**Appearance:** white powder

**UV\textsubscript{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\textsubscript{22}H\textsubscript{23}FN\textsubscript{2}O\textsubscript{3}</td>
<td>382.43</td>
<td>148.45</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in 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

$^1$HNMR: MEP-FUBICA; LOT # 0502952-7; CD$_3$OD; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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 30.0 min
Injection Parameters:
- Split Ratio = 25:1, 1 µL injected
MS Parameters:
- Mass scan range: 30-550 amu
- Tune file: stune.u
- Threshold: 150
- Acquisition mode: scan
Retention Time: 20.422 min

EI Mass Spectrum: MEP-FUBICA; LOT # 0502952-7
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): MEP-FUBICA; LOT # 0502952-7