MMB-2201

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

1. GENERAL INFORMATION

**IUPAC Name:** methyl N-[1-(5-fluoropentyl)-1H-indole-3-carbonyl]valinate

**CAS #:** 1616253-26-9

**Synonyms:** AMB-PICA, I-AMB, methyl 2-(1-(5-fluoropentyl)-1H-indole-3-carboxamido)-3-methylbutanoate

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV$_{\text{max}}$(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$<em>{20}$H$</em>{27}$FN$<em>{2}$O$</em>{3}$</td>
<td>362.44</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~7 mg/mL in CDCl₃ containing TMS for 0 ppm reference and BTMSB 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

¹HNMR: MMB-2201; Lot # 0457890-18; CDCl₃; 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:
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: 18.136 min

EI Mass Spectrum: MMB-2201; Lot # 0457890-18
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): MMB-2201; Lot # 0457890-18
4. ADDITIONAL RESOURCES

Wikipedia