MMB-FUBICA

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

1. GENERAL INFORMATION

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

CAS#: 1971007-90-5

Synonyms: AMB-FUBICA

Source: DEA Reference Material Collection

Appearance: White powder

$UV_{max} (\text{nm})$: 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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C$<em>{22}$H$</em>{23}$FN$_2$O$_3$</td>
<td>382.43</td>
<td>149.53</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~19 mg/mL in methanol-d$_4$ 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: MMB-FUBICA; Lot # 0523265-1; CD$_3$OD; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in 9:1 CHCl₃: 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
  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: 150
- Tune file: stune.u
- Acquisition mode: scan
Retention Time: 19.833 min

EI Mass Spectrum: MMB-FUBICA; Lot # 0523265-1
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): MMB-FUBICA; Lot # 0523265-1