1. GENERAL INFORMATION

**IUPAC Name:** methyl 2-(1-(cyclohexylmethyl)-1H-indole-3-carboxamido)-3,3-dimethylbutanoate

**CAS#:** 1971007-95-0

**Synonyms:** MMB-CHMINACA, methyl 2-[[1-(cyclohexylmethyl)-1H-indole-3-carbonyl]amino]-3,3-dimethylbutanoate

**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$<em>{23}$H$</em>{32}$N$_2$O$_3$</td>
<td>384.51</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in CDCl$_3$ 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: MDMB-CHMICA; Lot #0490914-16; CDCl$_3$; 400MHz
MDMB-CHMICA
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~3 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: 20.34 min

EI Mass Spectrum: MDMB-CHMICA; Lot #0490914-16
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR Thermo-Scientific iS-10, Smart iTX

Scan Parameters:
- Number of scans: 4
- Number of background scans: 4
- Resolution: 4 cm\(^{-1}\)
- Sample gain: 1
- Aperture: 150

FTIR Thermo-Scientific iS-10, Smart iTX; MDMB-CHMICA; Lot #0490914-16