APP-BUTINACA

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

1. GENERAL INFORMATION

**IUPAC Name:**  
$N$-(1-amino-1-oxo-3-phenylpropan-2-yl)-1-butyl-$1H$-indazole-3-carboxamide

**CAS#:**  
N/A

**Synonyms:**  
APP-BINACA, $N\alpha$-(1-butyl-$1H$-indazole-3-carbonyl)phenylalaninamide

**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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>$C_{21}H_{24}N_{4}O_{2}$</td>
<td>364.44</td>
<td>133.64</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 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: APP-BUTINACA; Lot# 0552311-9; CDCl$_3$; 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:
   - 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
   - Tune file: stune.u
   - Acquisition mode: scan
   - Threshold: 250
Retention Time: 21.51 min

EI Mass Spectrum: APP-BUTINACA; Lot# 0552311-9
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): APP-BUTINACA; Lot# 0552311-9