AM2201

1. GENERAL INFORMATION

**IUPAC Name:** [1-(5-fluoropentyl)-1H-indol-3-yl](naphthalen-1-yl)methanone

**CAS #:** 335161-24-5

**Synonyms:** 1-(5-fluoropentyl)-3-(1-naphthoyl)indole

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**\(UV_{\text{max}}\):** 218.1, 314.0

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>(\text{C}<em>{24}\text{H}</em>{22}\text{FNO})</td>
<td>359</td>
<td>93.7</td>
</tr>
</tbody>
</table>

Latest Revision: 01/27/2014
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

_Method NMR CDCl₃_

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterochloroform (CDCl₃) containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

**Instrument:** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

**Parameters:**
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

\(^1\text{H} \text{NMR: AM2201 Lot SF0006; CDCl₃; 400 MHz}

[Graph showing NMR spectrum with peaks labeled CHCl₃, methenamine (ISTD), impurity, and TMS]
AM2201

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

$^1$H NMR: AM2201 Lot SF0006; CDCl$_3$; 400 MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in MeOH.

Instrument: Gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm

Carrier Gas: Helium at 1 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 300°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: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 21.093 minutes

EI Mass Spectrum: AM2201 Lot SF0006
3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:**
FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm\(^{-1}\)
Sample gain: 8
Aperture: 150
The Drug Enforcement Administration’s Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

4. ADDITIONAL RESOURCES

Forendex

Wikipedia