1. GENERAL INFORMATION

**IUPAC Name:** 2-(4-chloro-2,5-dimethoxyphenyl)-N-(4-methoxybenzyl)ethanamine

**CAS#:** Not Available

**Synonyms:** N-(4-methoxybenzyl)-2-(4-chloro-2,5-dimethoxyphenyl)ethylamine

4-Methoxy-25C-NBOMe

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\textsubscript{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 (ºC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C\textsubscript{18}H\textsubscript{22}ClNO\textsubscript{3}</td>
<td>335</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{18}H\textsubscript{22}ClNO\textsubscript{3}HCl</td>
<td>372</td>
<td>189.1</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 methenamine 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

![NMR Spectrogram](attachment:image.png)
25C-NB4OMe

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 ~4 mg/mL in CHCl₃.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm
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 = 20:1, 1 µL injected

MS Parameters:
- Mass scan range: 30-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 15.534 min

EI Mass Spectrum 25C-NB4OMe HCl Lot N17-P73C
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

FTIR ATR (Diamond, 3 Bounce) 25C-NB4OMe HCl Lot N17-P73C
4. ADDITIONAL RESOURCES