1. GENERAL INFORMATION

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

*CFR:* Not Scheduled (03/2013)

*CAS #:* N/A

*Synonyms:* 4-ethyl-2,5-dimethoxy-N-(2-methoxybenzyl)phenethylamine

*Source:* DEA Reference Material Collection

*Appearance:* White powder (HCl)

*Kovat’s Index:* Pending

*UV*$_{max}$:* 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$<em>{20}$H$</em>{27}$NO$_3$</td>
<td>329</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{20}$H$</em>{27}$NO$_3$·HCl</td>
<td>365</td>
<td>161.6</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES

No resources identified as of 3/1/2013.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterochloroform (CDCl₃) containing TMS for 0 ppm reference.

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
1H NMR: 25E-NBOMe HCl Lot # N17P97B; CDCl₃, 400 MHz

1H NMR: 25E-NBOMe HCl Lot # N17P97B; CDCl₃, 400 MHz
4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in CHCl₃.

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x .25mm x .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) 90°C initial temperature for 2.0 min
  2) Ramp to 300°C at 14°C/min
  3) Hold final temperature for 10.0 min

Injection Parameters: Split Ratio = 25:1, 1 µL injected

MS Parameters:
- Mass scan range: 34-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 15.891 minutes

El Mass Spectrum: 25E-NBOMe HCl Lot # N17P97B
4.3 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