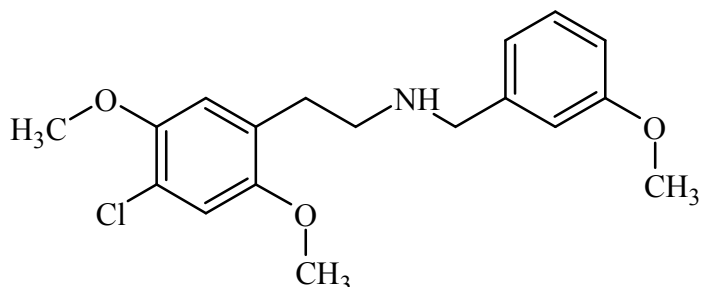




## 25C-NB3OMe

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



### 1. GENERAL INFORMATION

**IUPAC Name:** 2-(4-chloro-2,5-dimethoxyphenyl)-N-(3-methoxybenzyl)ethanamine

**CAS#:** Not Available

**Synonyms:** N-(3-methoxybenzyl)-2-(4-chloro-2,5-dimethoxyphenyl)ethanamine  
3-Methoxy-25C-NBOMe

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV<sub>max</sub>(nm):** Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>18</sub> H <sub>22</sub> ClNO <sub>3</sub>	335	Not Determined
HCl	C <sub>18</sub> H <sub>22</sub> ClNO <sub>3</sub> HCl	372	161.5



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### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~10 mg/mL in CDCl<sub>3</sub> containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

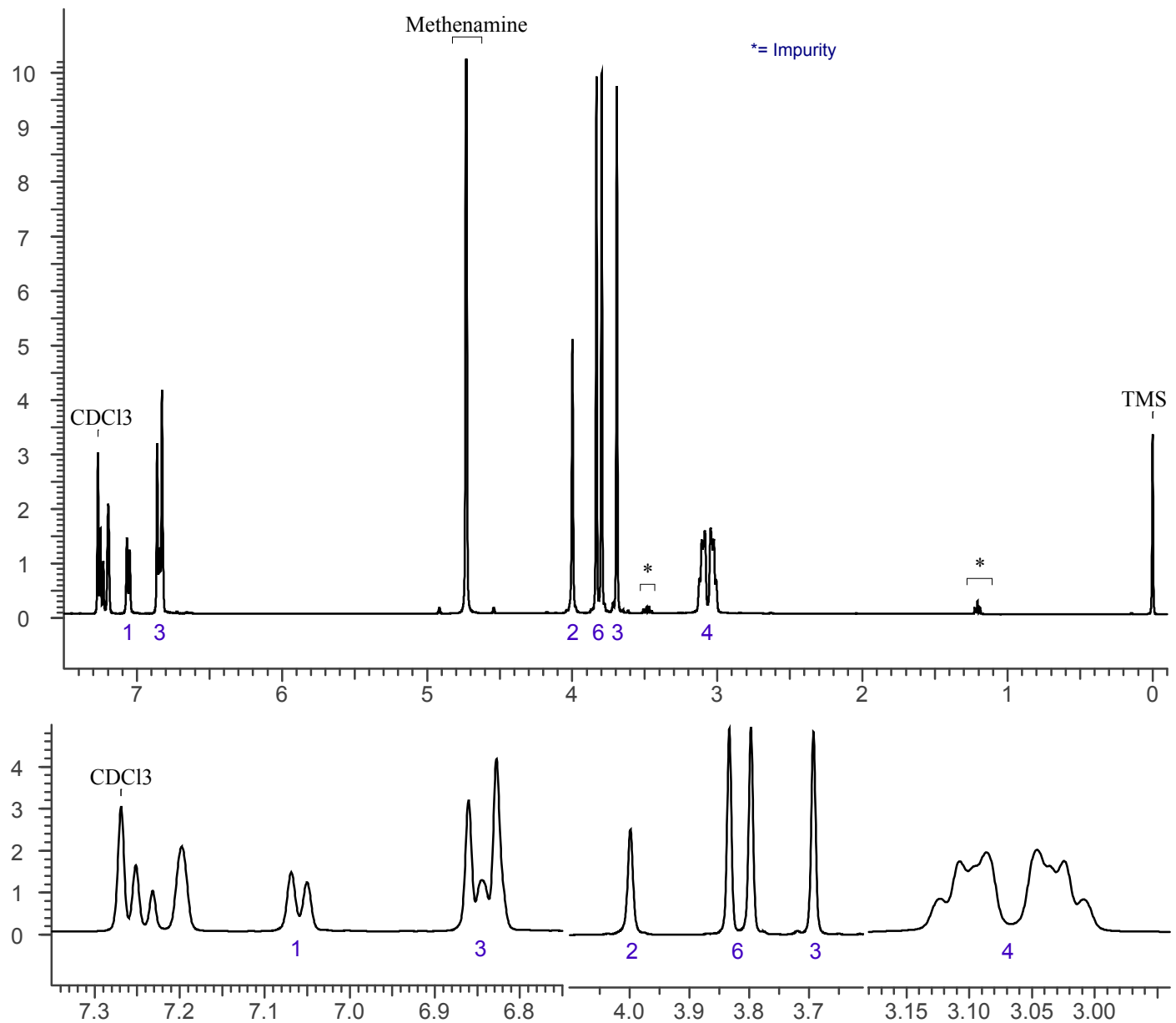
**Instrument:** 400 MHz NMR spectrometer

**Parameters:** Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

<sup>1</sup>H NMR: 25C-NB3OMe HCl Lot N17-P72C, CDCl<sub>3</sub>, 400MHz





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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~4 mg/mL in CHCl<sub>3</sub>.

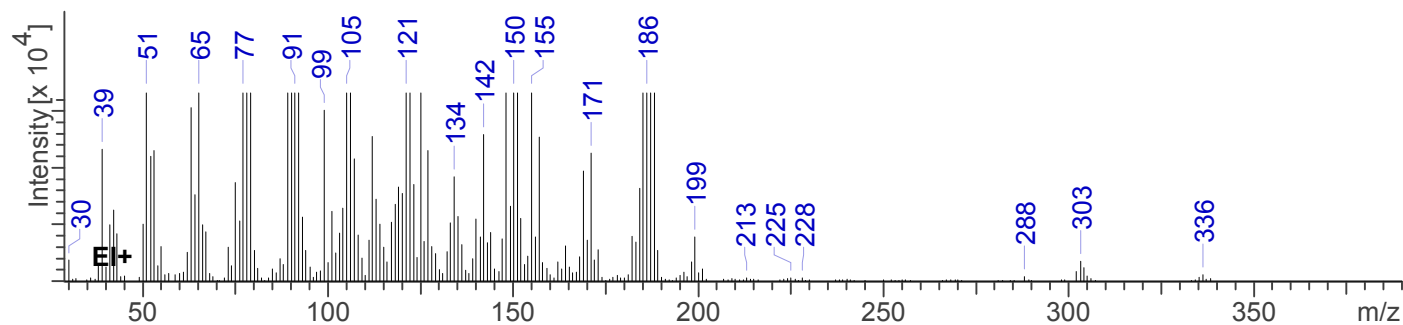
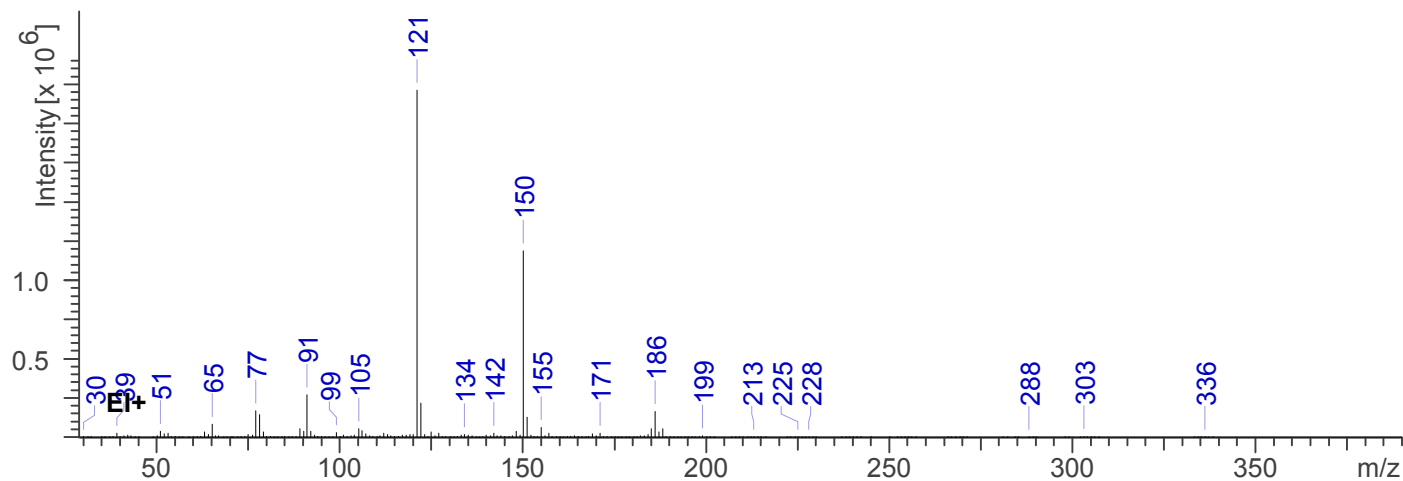
**Instrument:** Agilent gas chromatograph operated in split mode with MS detector  
**Column:** DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μm  
**Carrier Gas:** Helium at 1 mL/min  
**Temperatures:** Injector: 280°C  
MSD transfer line: 280°C  
MS Source: 230°C  
MS Quad: 150°C  
Oven program:  
1) 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:** 15.387 min

EI Mass Spectrum, 25C-NB3OMe HCl Lot N17-P72C







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### 4. ADDITIONAL RESOURCES

Casale, J. and Hays, P. Characterization of Eleven 2,5-Dimethoxy-N-(2-methoxybenzyl)phenethylamine (NBOME) Derivatives and Differentiation from their 3- and 4- methoxybenzyl analogs. Part 1. *Microgram Journal*, 2012; 9(2):84-109.