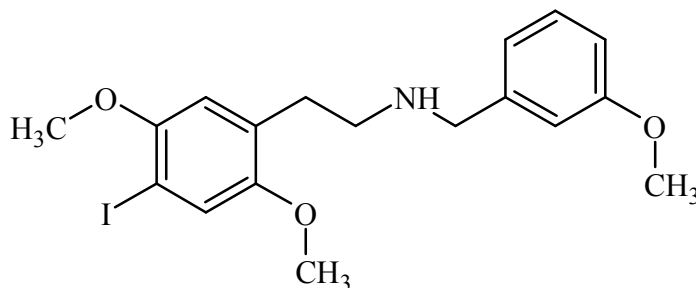




## 25I-NB3OMe

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	2-(4-iodo-2,5-dimethoxyphenyl)-N-(3-methoxybenzyl)ethanamine
<b>CAS#:</b>	Not Available
<b>Synonyms:</b>	3-Methoxy-25I-NBOMe HCl, N-(3-methoxybenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethylaniline
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<b>UV<sub>max</sub>(nm):</b>	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> INO <sub>3</sub>	427	Not Determined
HCl	C <sub>18</sub> H <sub>22</sub> INO <sub>3</sub> HCl	463	99-102.5



## 25I-NB3OMe

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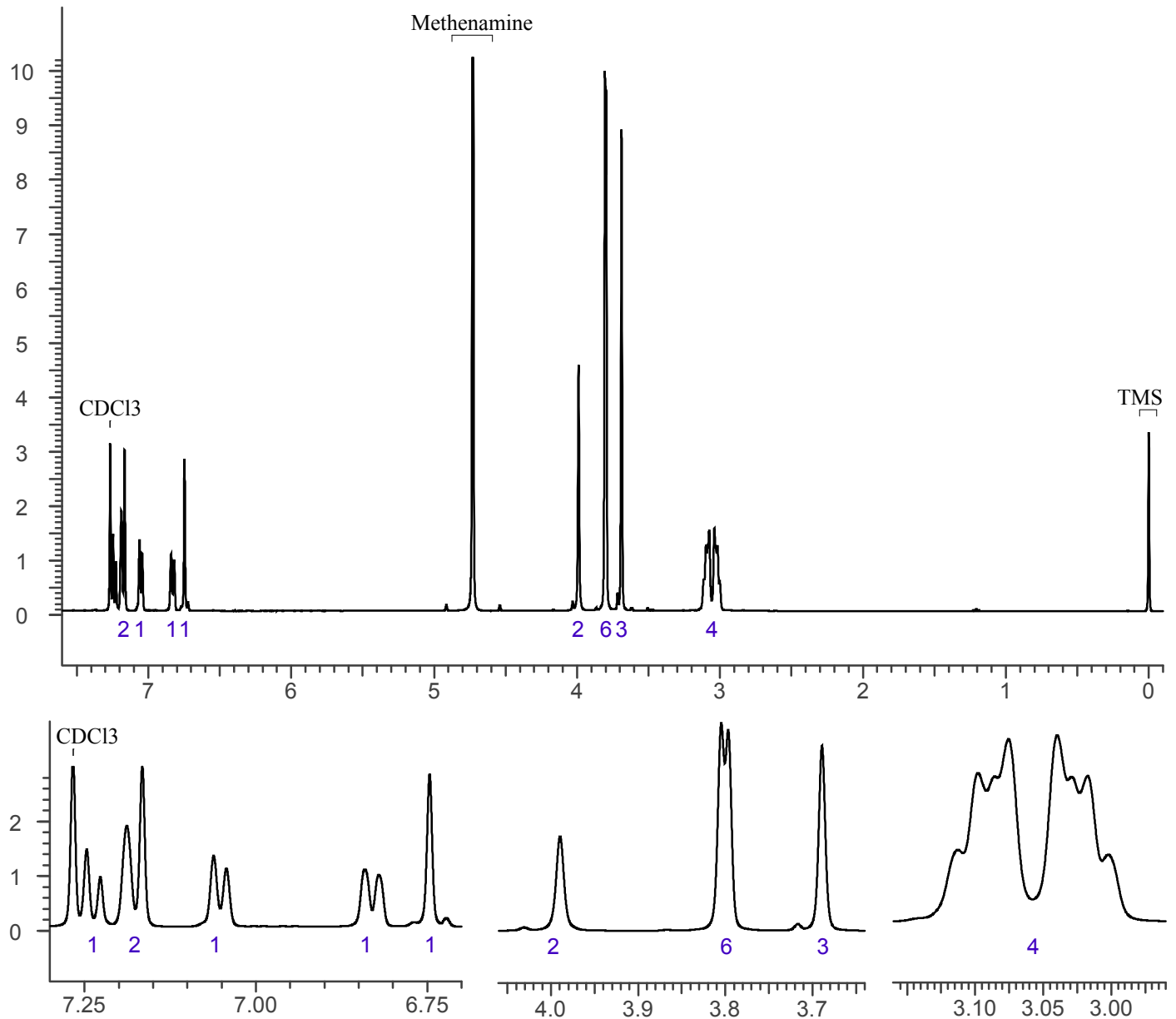


### 3. QUALITATIVE DATA

#### 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  
1H NMR: 25I-NB3OMe HCl Lot N17-P74D, CDCl<sub>3</sub>, 400MHz





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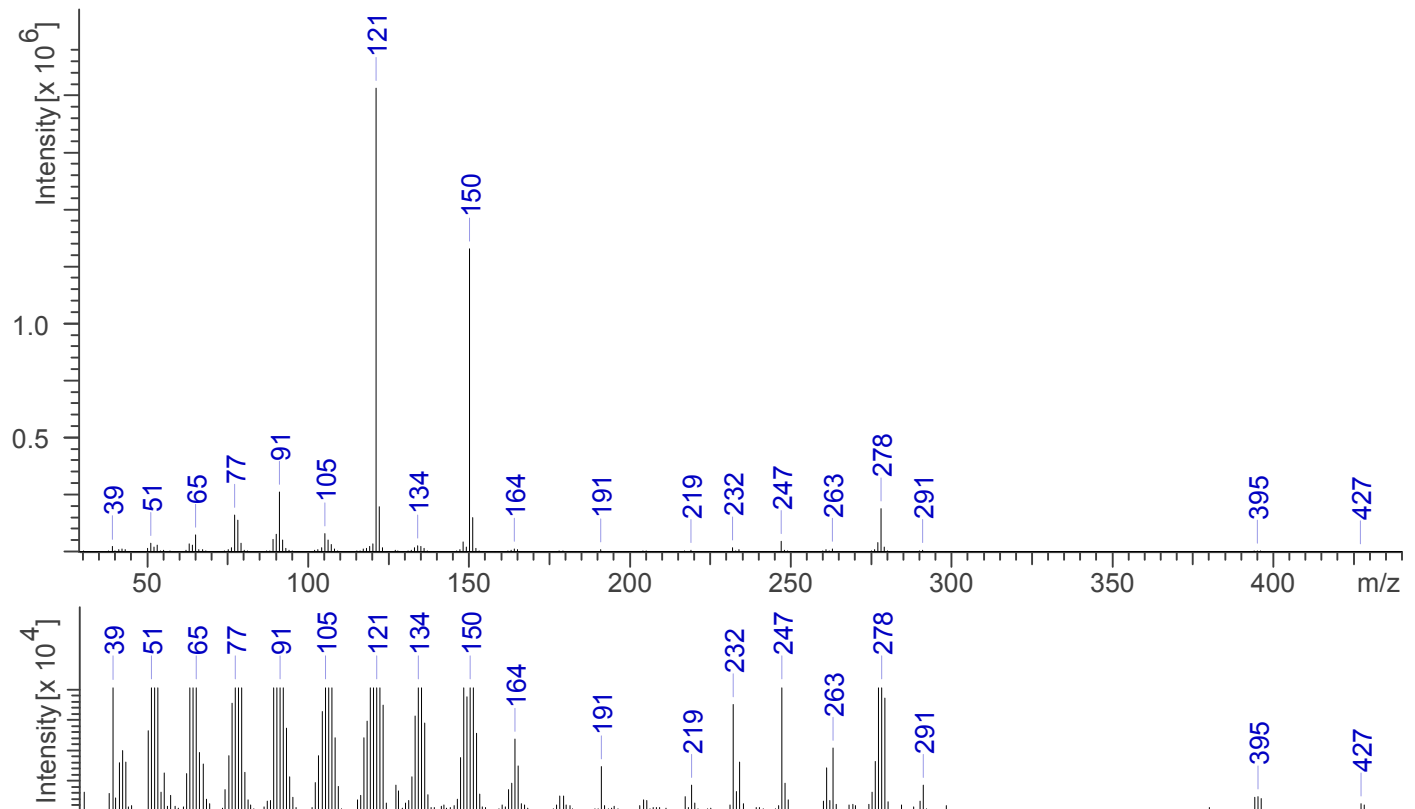
### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~5 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:** 16.594 min

EI Mass Spectrum: 25I-NB3OMe HCl, Lot N17-P74D





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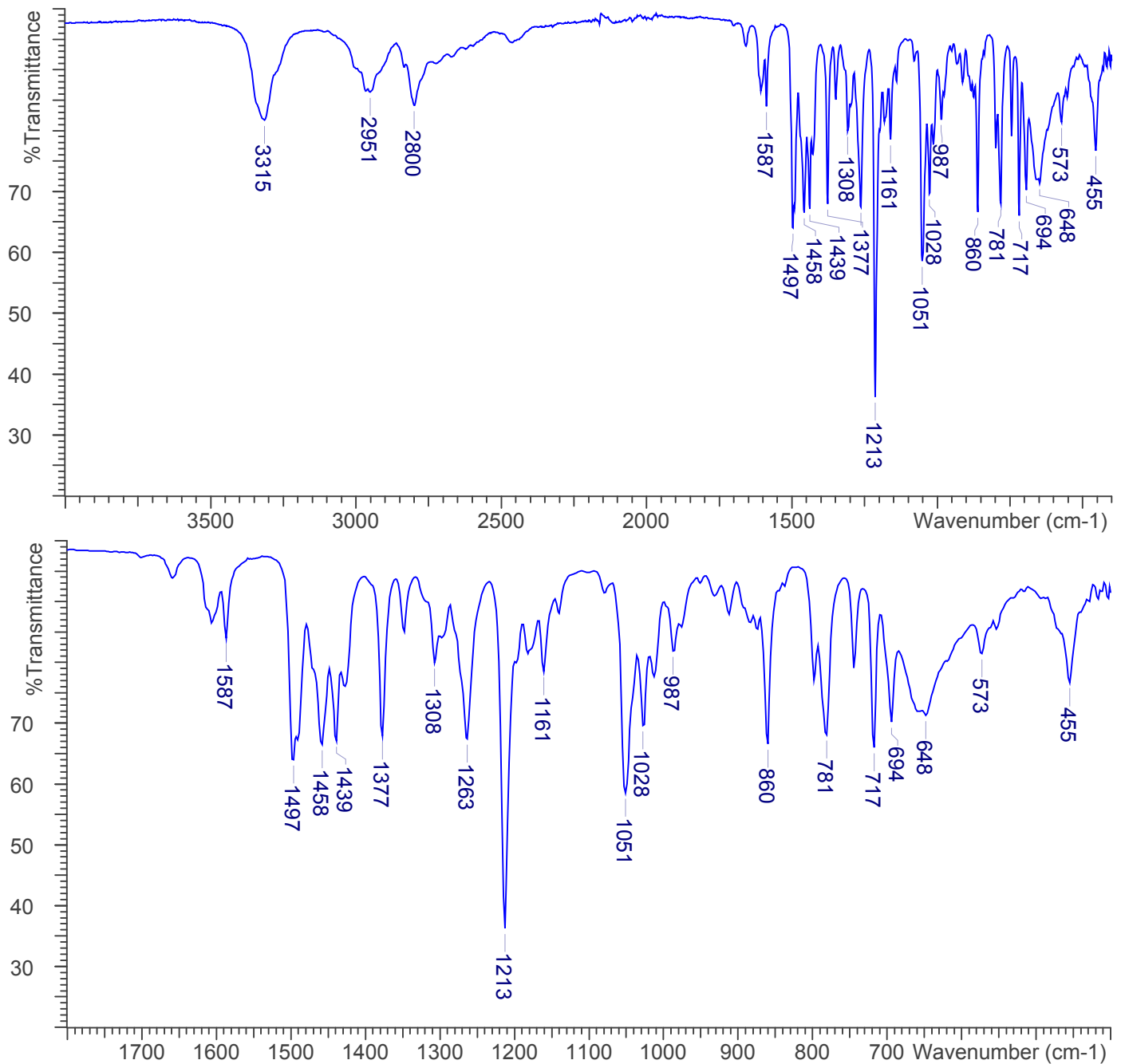


### 3.3 INFRARED SPECTROSCOPY (FTIR)

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

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 25I-NB3OMe HCl, Lot N17-P74D





## 25I-NB3OMe

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



### **4. ADDITIONAL RESOURCES**

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