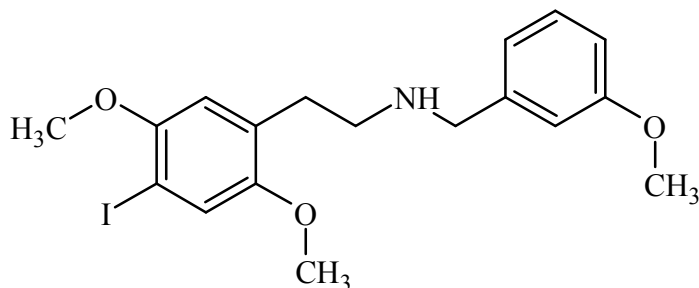




25I-NB3OMe

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-iodo-2,5-dimethoxyphenyl)-N-(3-methoxybenzyl)ethanamine
CAS#:	Not Available
Synonyms:	3-Methoxy-25I-NBOMe HCl, N-(3-methoxybenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethylaniline
Source:	DEA Reference Material Collection
Appearance:	White powder
UV_{max}(nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₈ H ₂₂ INO ₃	427	Not Determined
HCl	C ₁₈ H ₂₂ INO ₃ HCl	463	99-102.5



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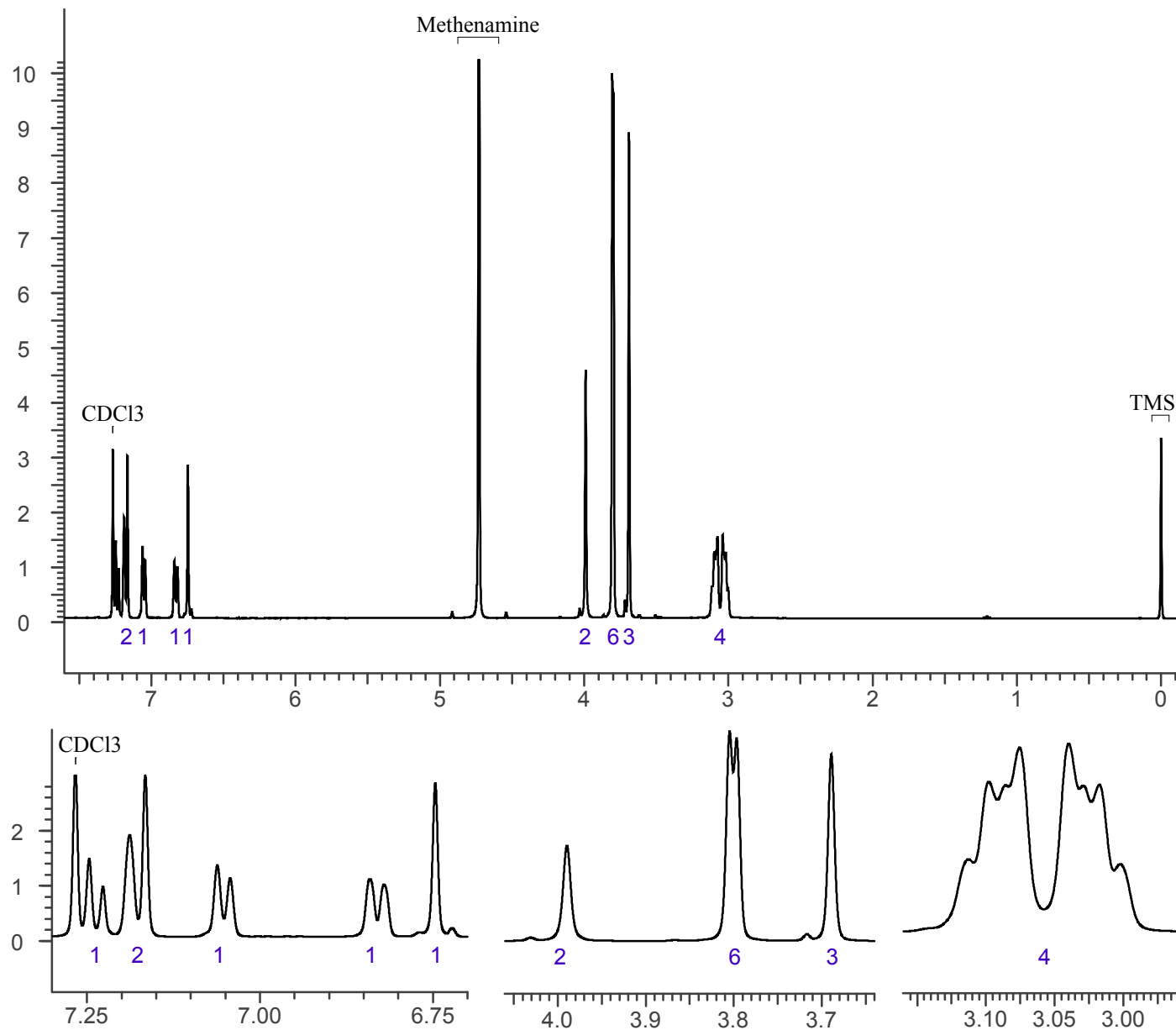


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in CDCl₃ 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, CDCl₃, 400MHz





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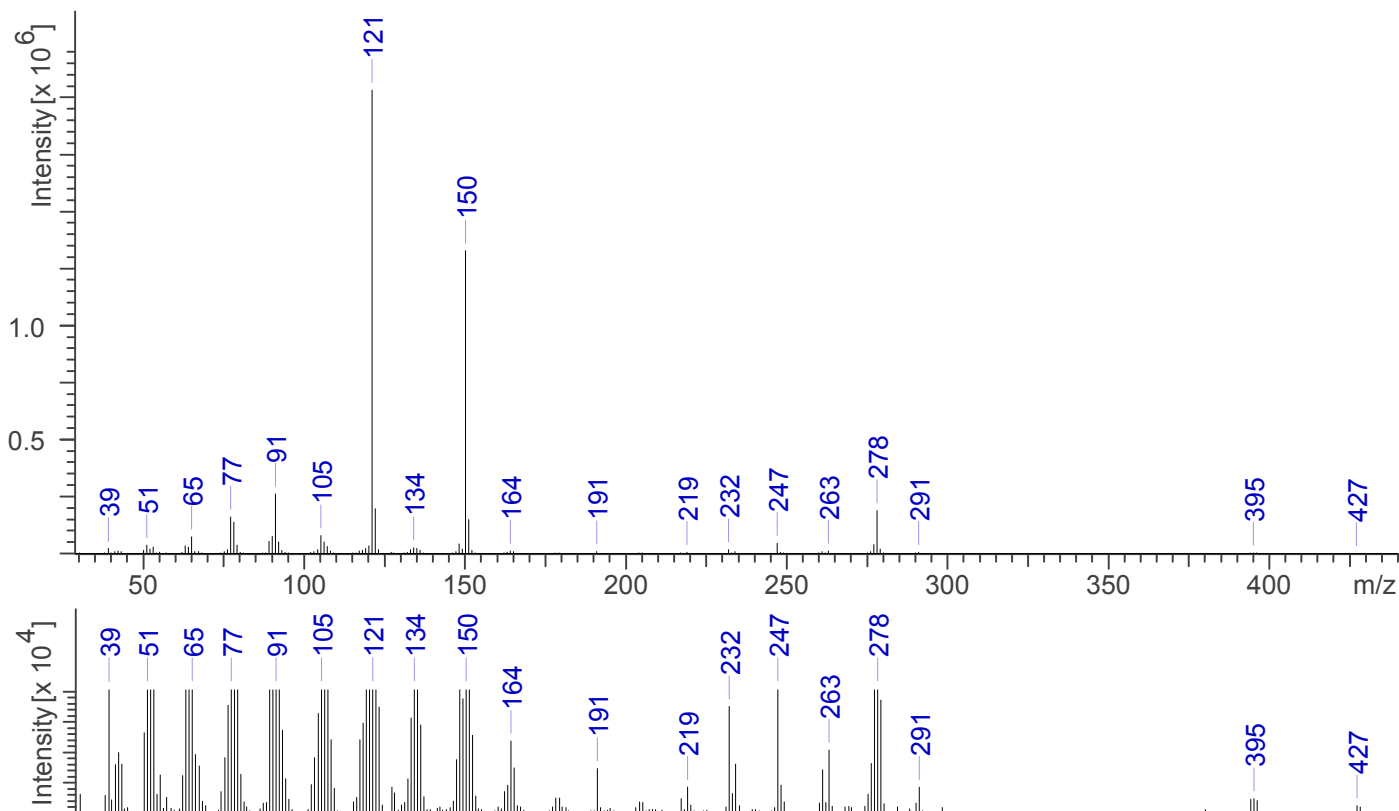
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 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: 16.594 min

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





25I-NB3OMe

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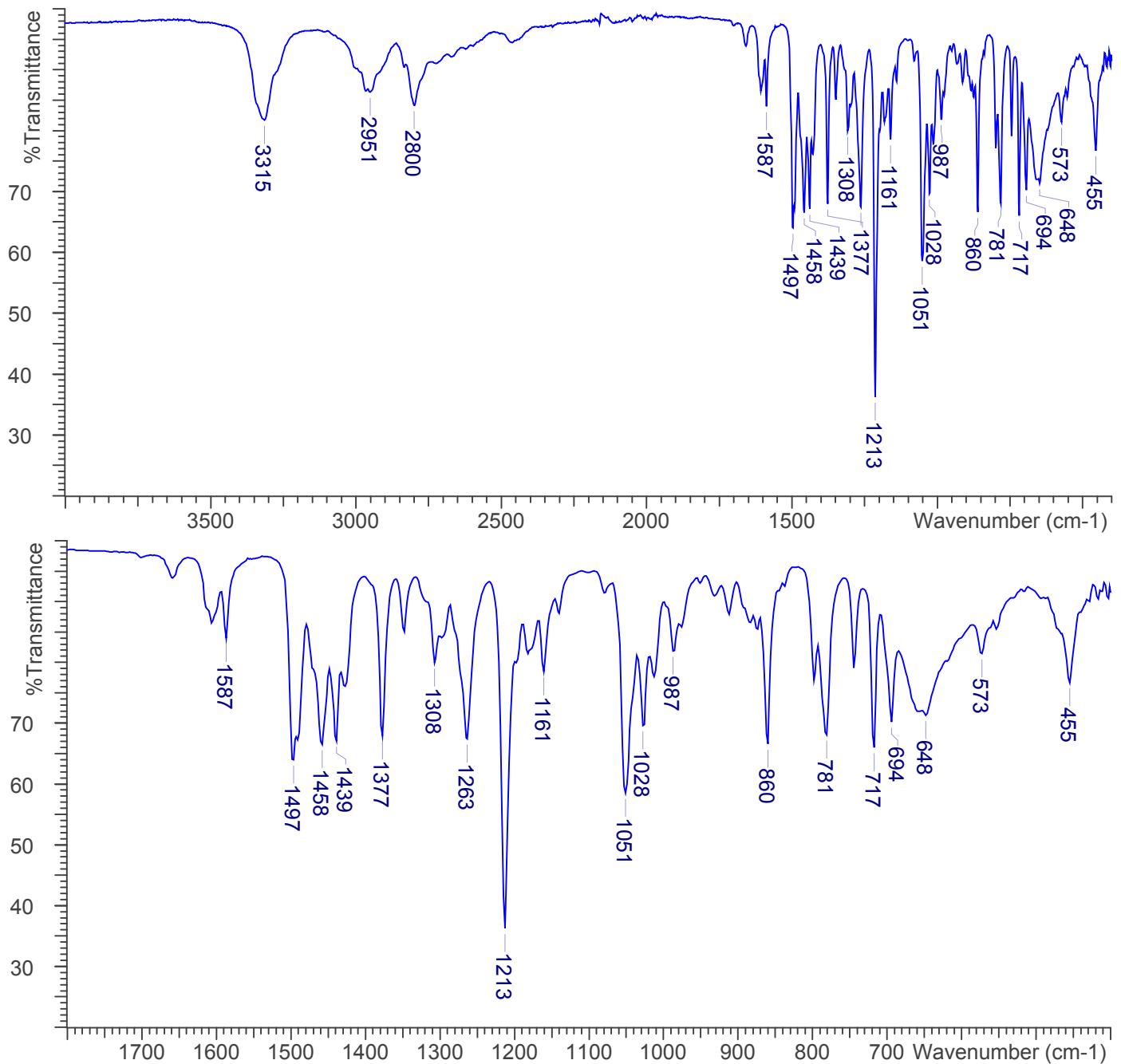


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

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





25I-NB3OMe

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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 of their 3- and 4-Methoxybenzyl Analogues - Part 1. *Microgram Journal* 2012; 9(2):84-109