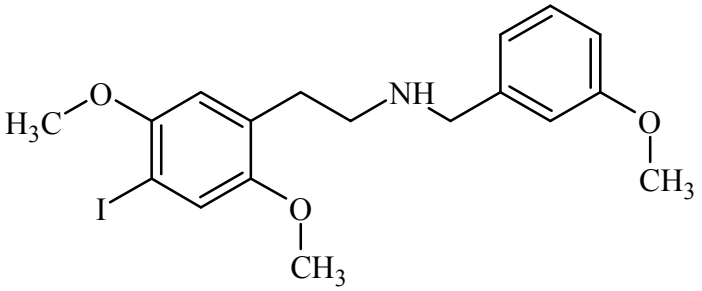
25I-NB3OMe

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)ethylamine

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 (^{o}C)
Base	$C_{18}H_{22}INO_3$	427	Not Determined
HCl	$C_{18}H_{22}INO_3$ HCl	463	99-102.5

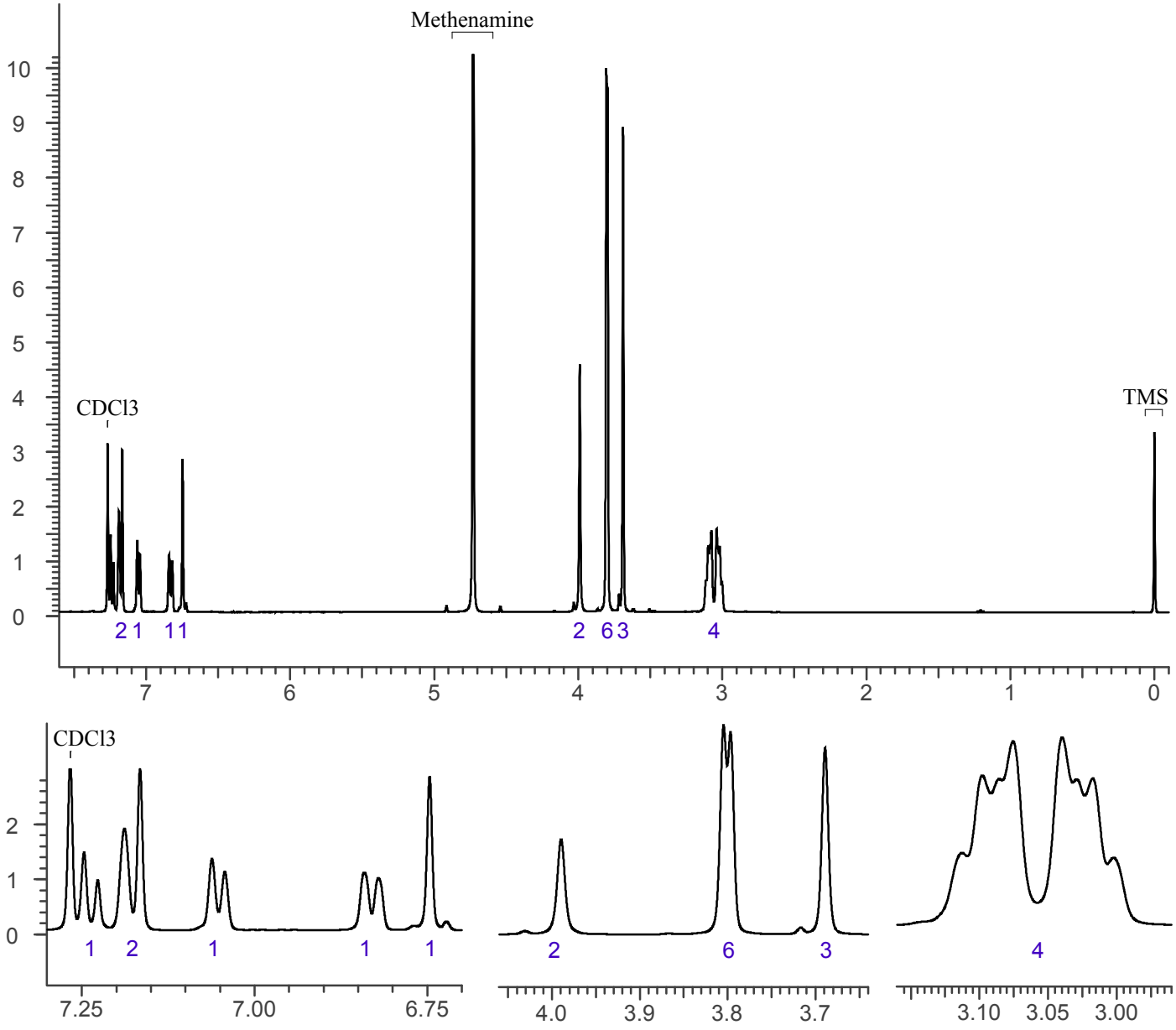
3. QUALITATIVE DATA

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

1H NMR: 25I-NB3OMe HCl Lot N17-P74D, $CDCl_3$, 400MHz

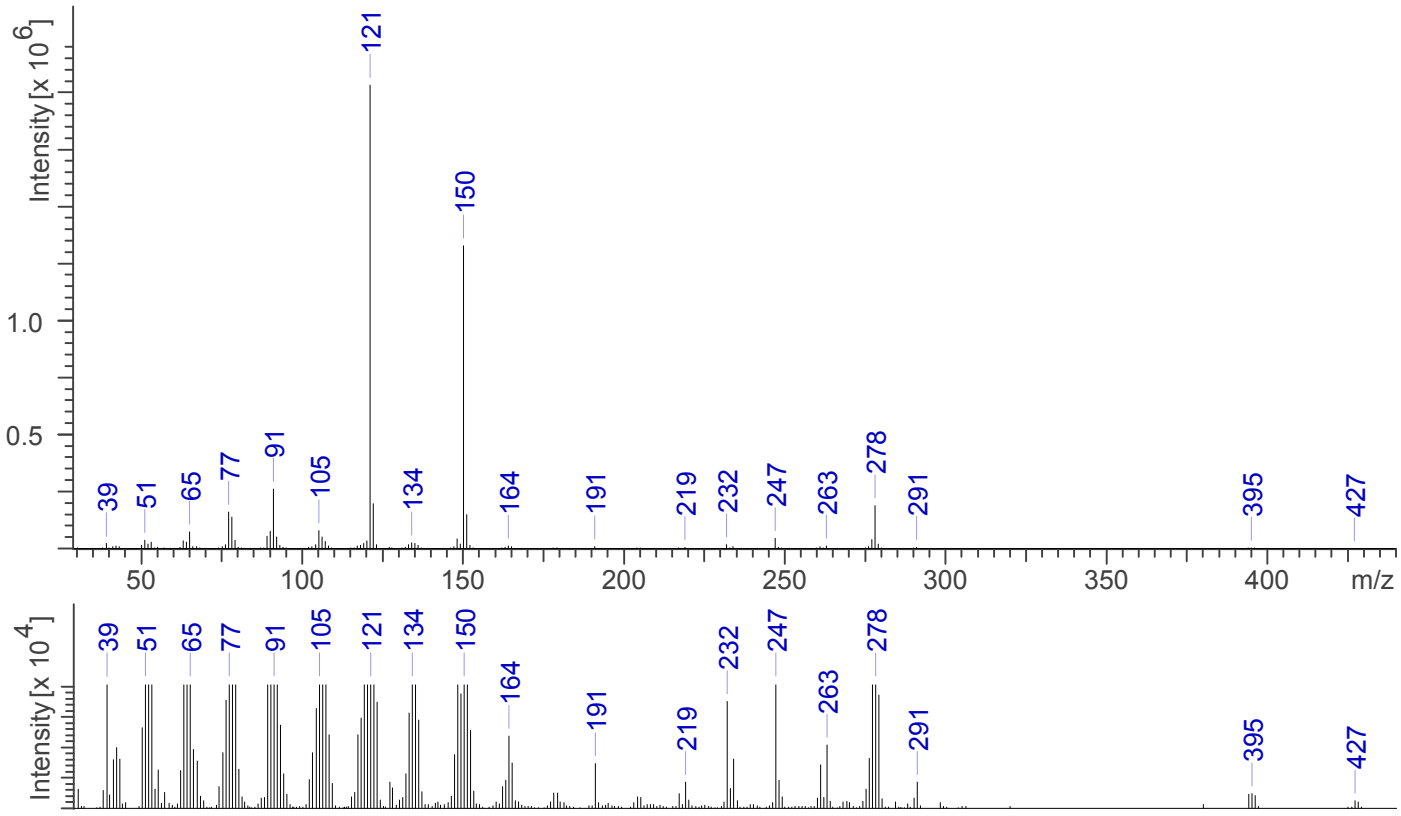


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in $CHCl_3$.

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

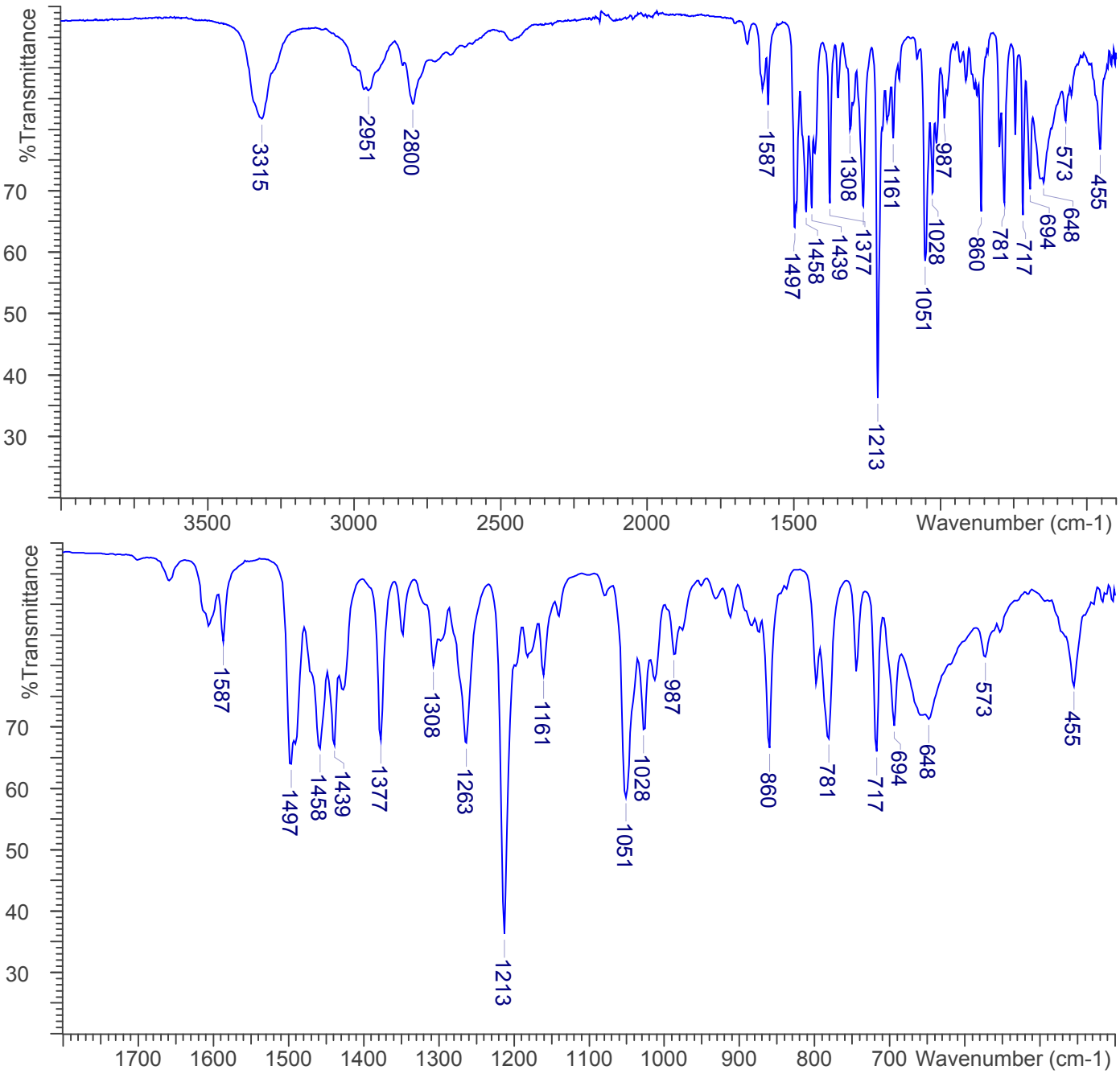


3.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: 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



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