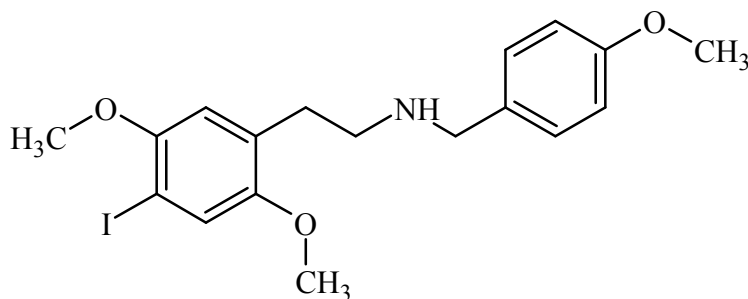




25I-NB4OMe HCl

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-(4-methoxybenzyl)ethanamine

CAS#: Not Available

Synonyms: N-(4-methoxybenzyl)-2-(4-iodo-2,5-dimethoxyphenyl)ethanamine
4-Methoxy-25I-NBOMe

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	170.4



25I-NB4OMe HCl

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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 mg/mL in CDCl_3 containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

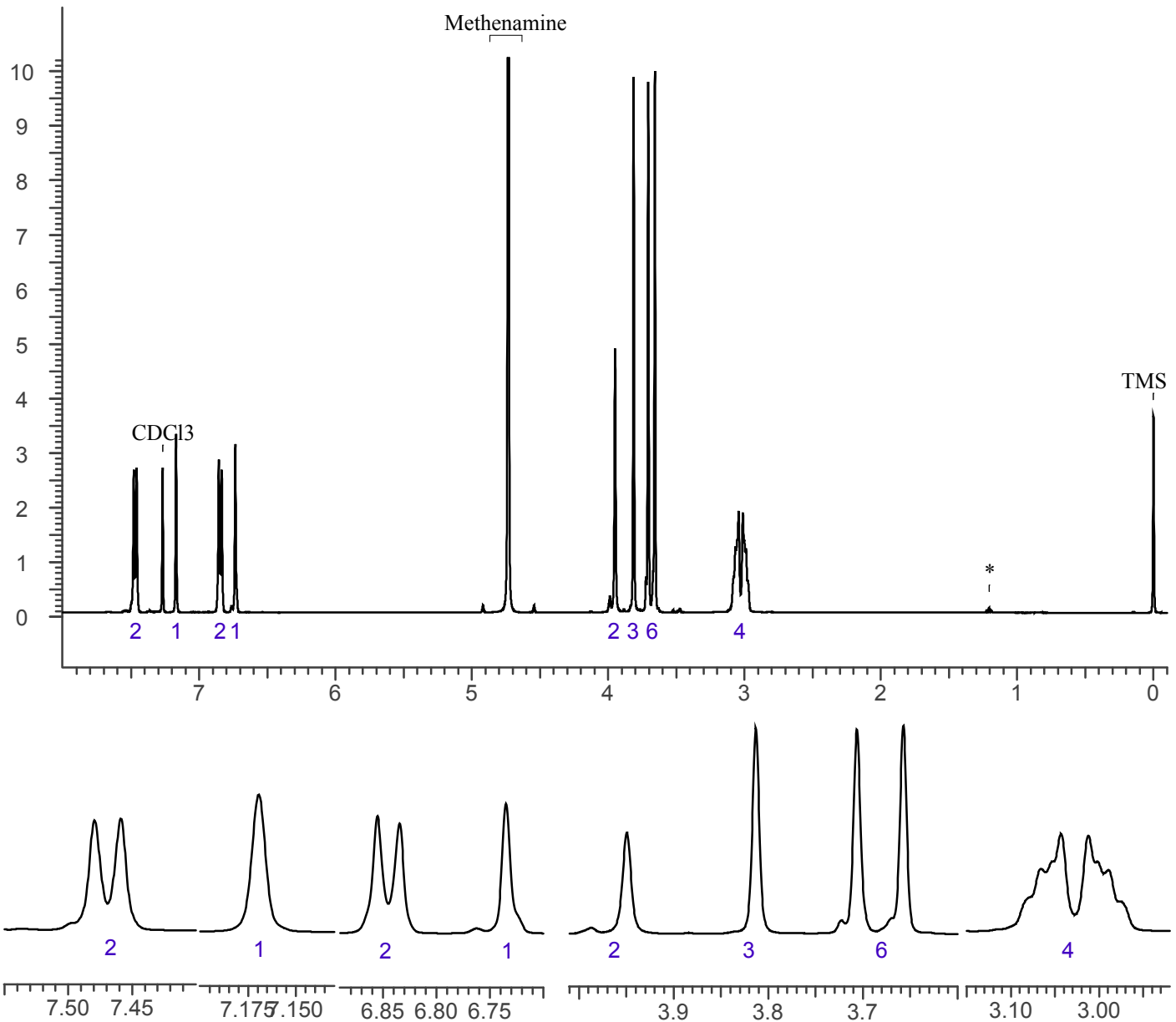
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 45 seconds

^1H NMR 25I-NB4OMe HCl Lot N17-P75C, CDCl_3 , 400MHz





25I-NB4OMe HCl

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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~6 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

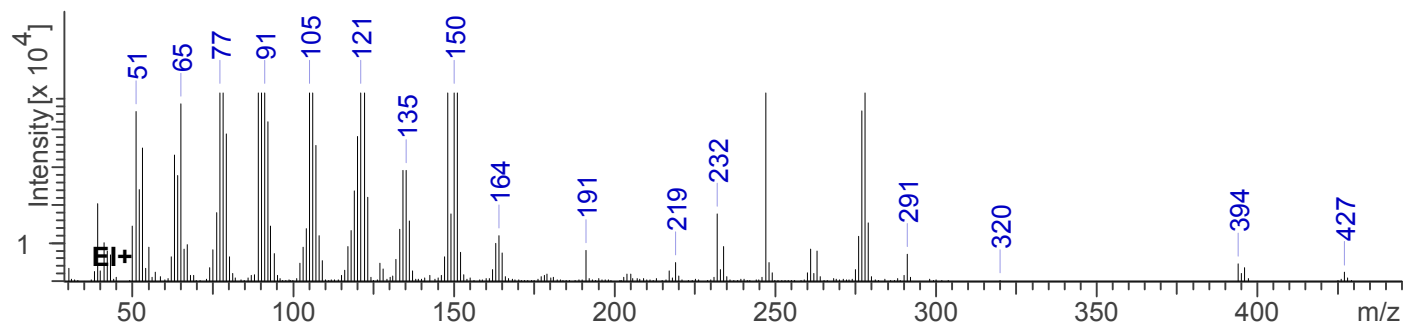
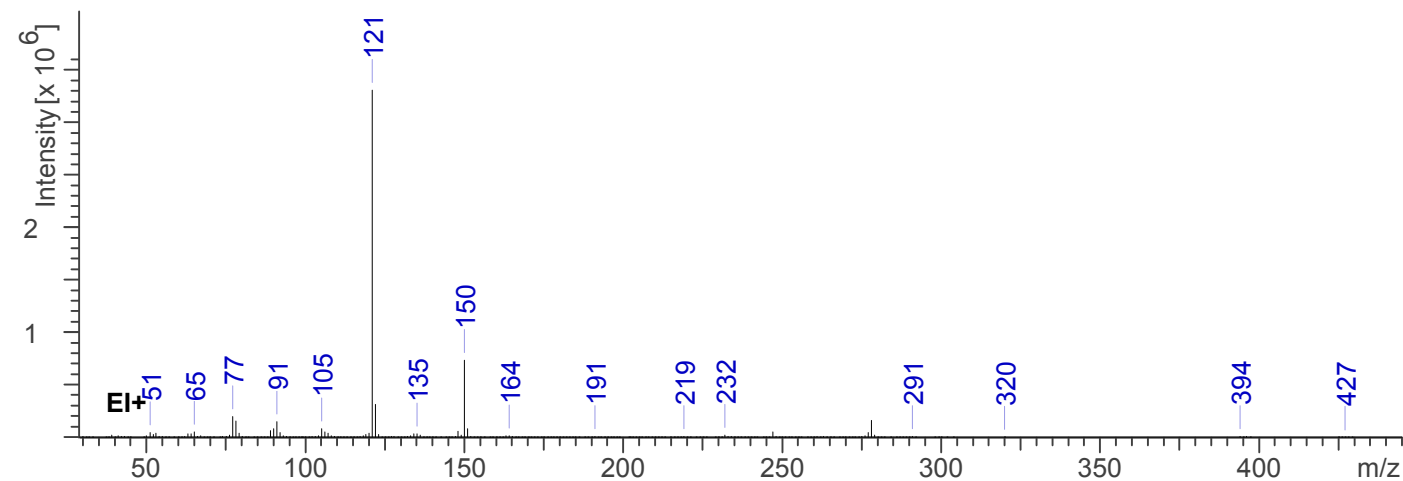
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 16.739 min

EI Mass Spectrum 25I-NB4OMe HCl, Lot N17-P75C





25I-NB4OMe HCl

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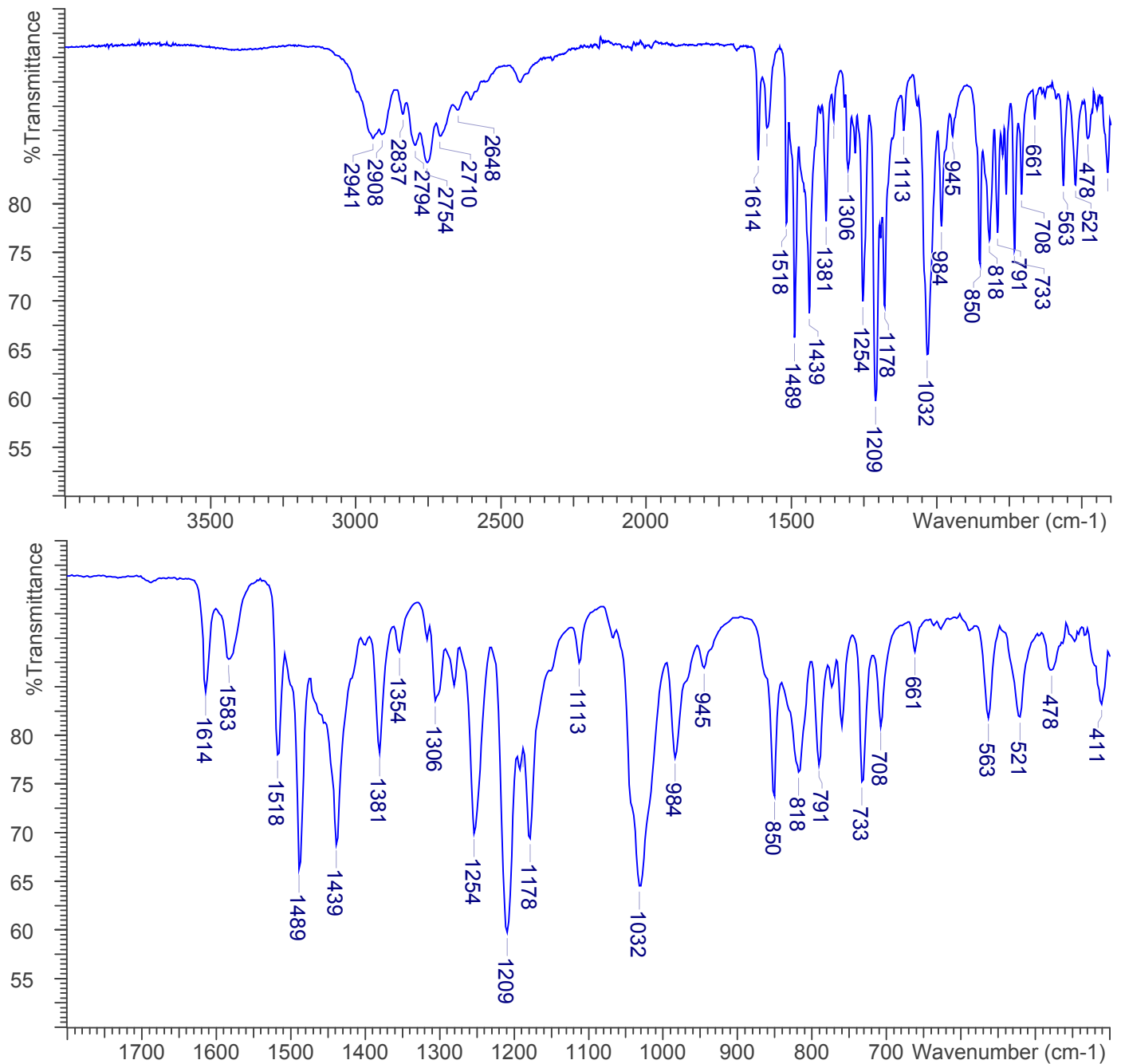


3.3 INFRARED SPECTROSCOPY (FTIR)

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-NB4OMe HCl (Lot N17-P75C)





25I-NB4OMe HCl

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 from their 3- and 4-methoxybenzyl analogs. Part 1. Microgram Journal, 2012; 9(2):84-109.