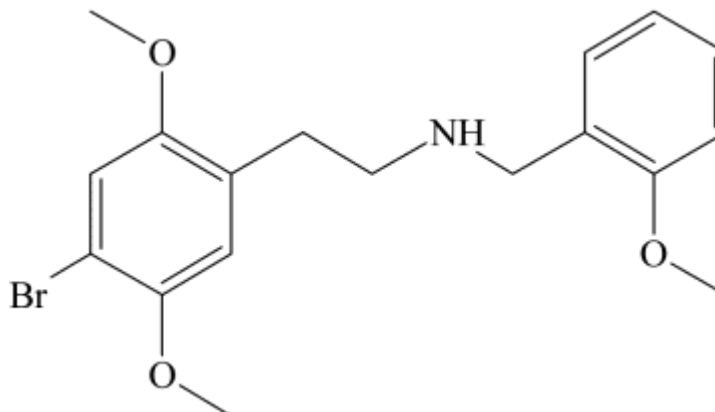




25B-NBOMe



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-bromo-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine
CFR:	Schedule 1 (Temporary, as of 11/15/2013)
CAS #:	1026511-90-9 (Base)
Synonyms:	2C-B-NBOMe, NBOMe-2C-B, Cimbi-36
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
UV_{max}:	205.1, 297.0

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₈ H ₂₂ NO ₃ Br	380	Not Determined
HCl	C ₁₈ H ₂₂ NO ₃ Br · HCl	416	175.8



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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

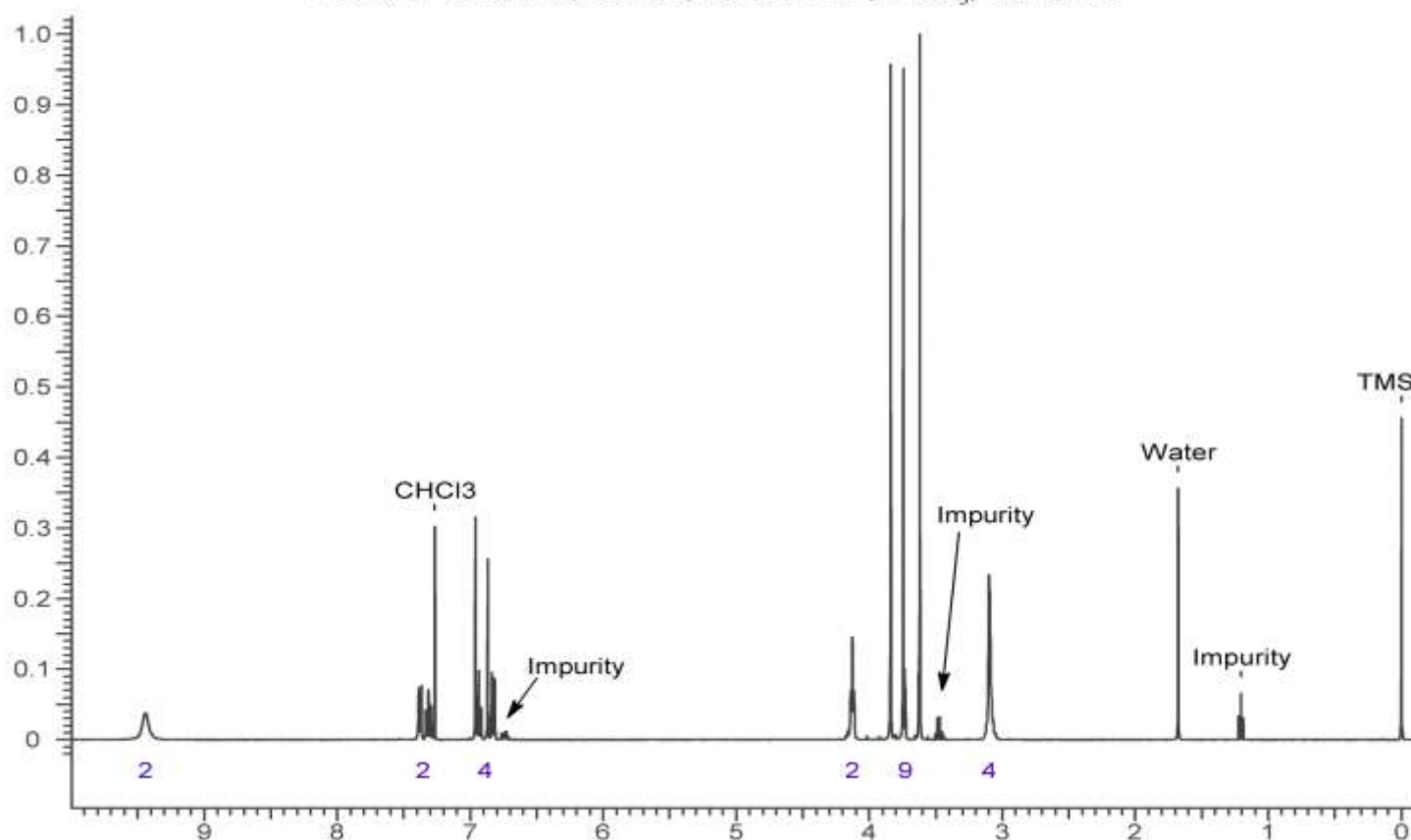
Sample Preparation: Dilute analyte to ~10 mg/mL in CDCl₃ containing TMS for 0 ppm reference.

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

Parameters:

- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

¹H NMR: 25B-NBOMe HCl; lot N18-P1C, CDCl₃, 400 MHz



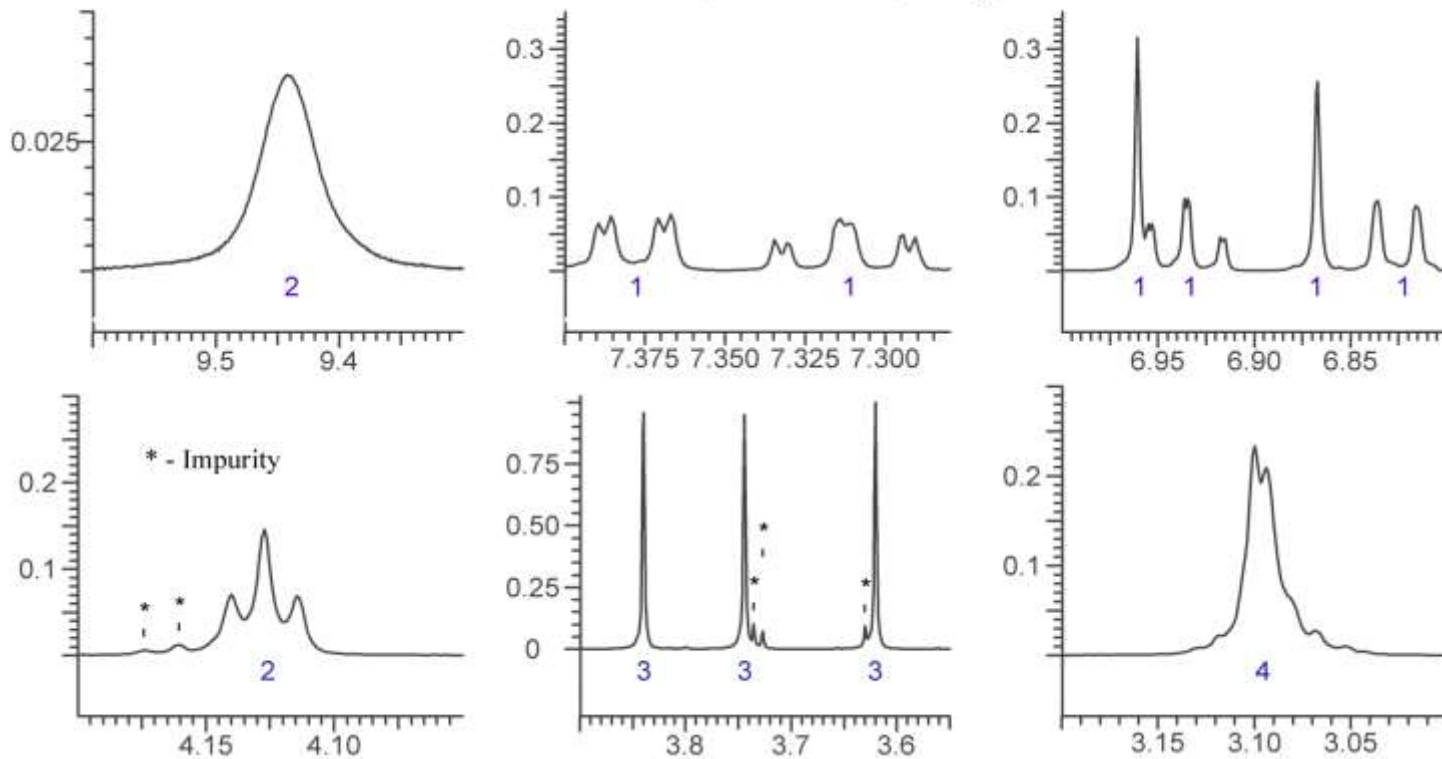


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^1H NMR: 25B-NBOMe HCl; lot N18-P1C, CDCl_3 , 400 MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 1 mg/mL into methanol.

Instrument: Gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x 0.25mm x 0.25 μ m

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:

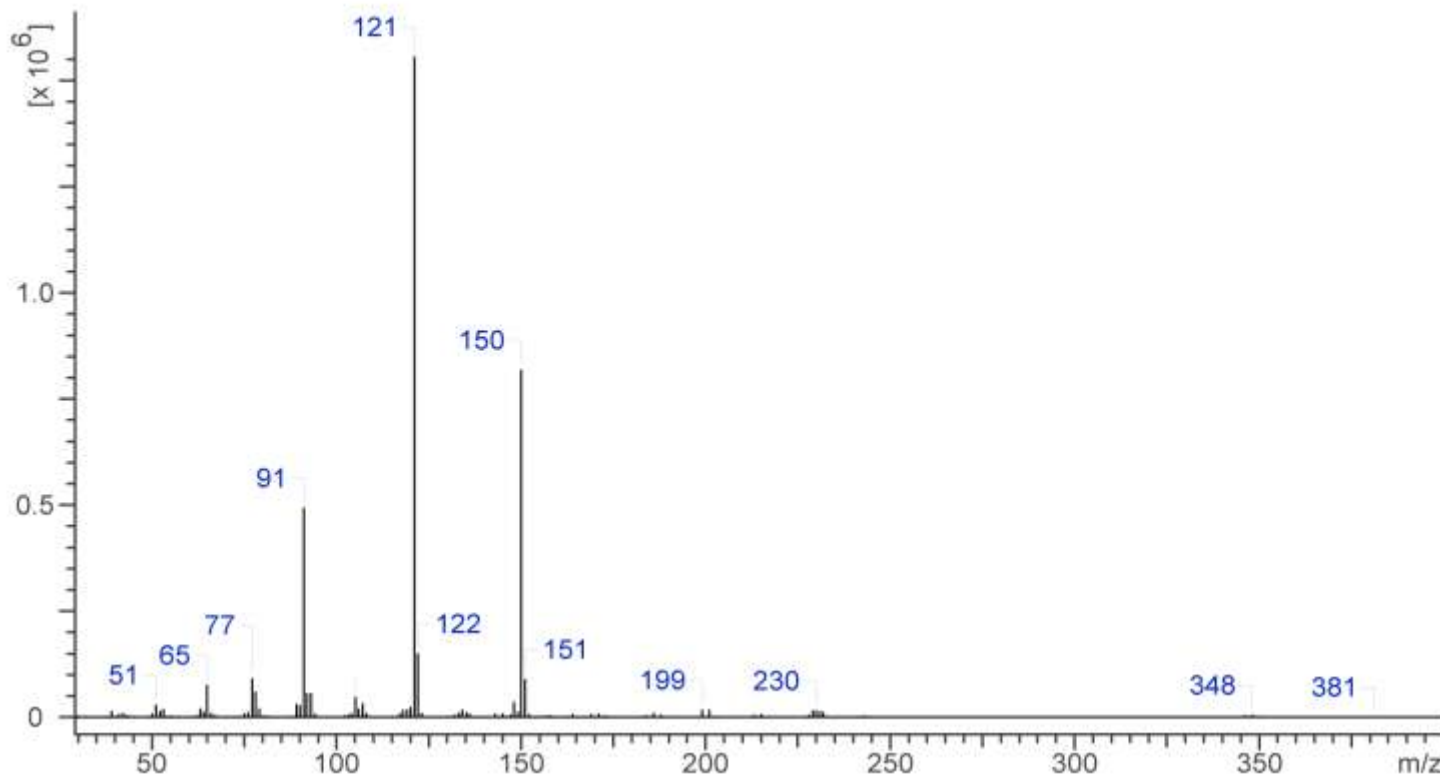
- 1) 100°C initial temperature for 1.0 min
- 2) Ramp to 300°C at 12°C/min
- 3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 μ L injected

MS Parameters:
Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 16.796 minutes

EI Mass Spectrum: 25B-NBOMe HCl; lot N18-P1C





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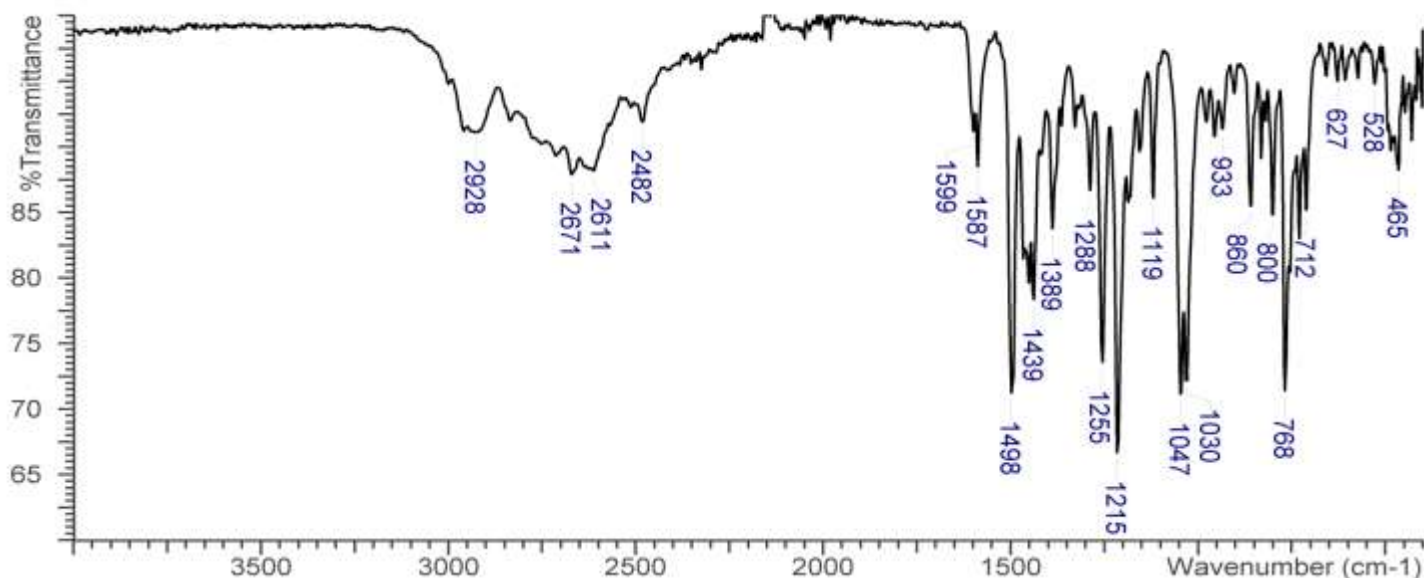
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

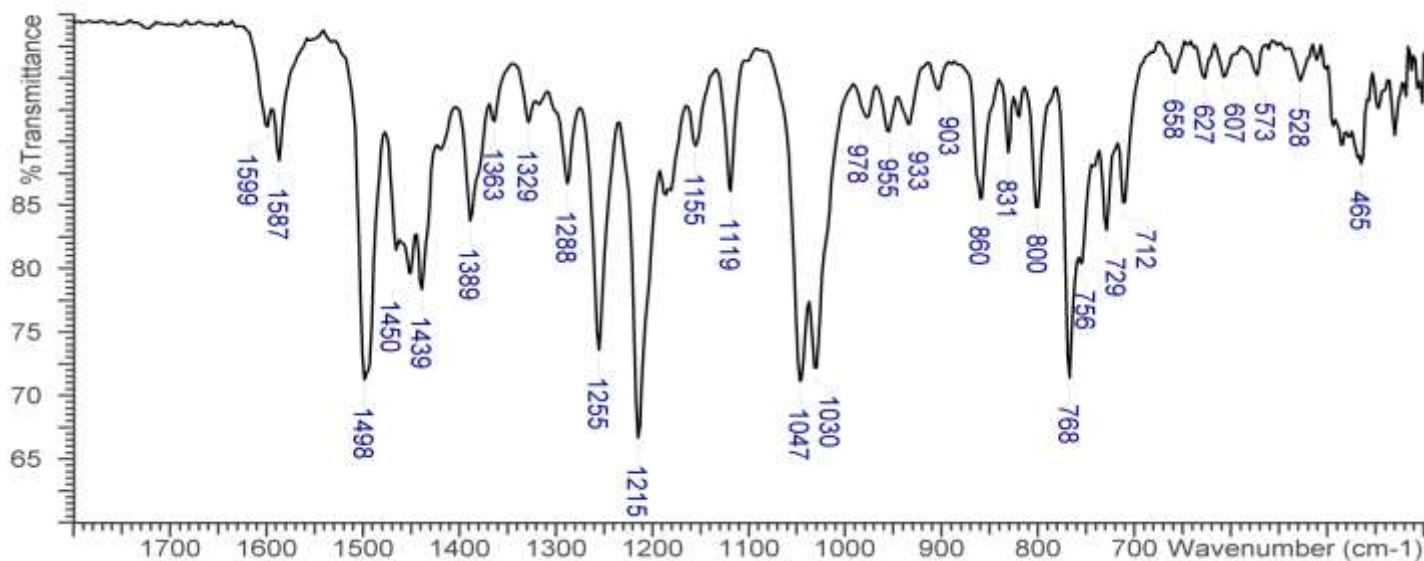
Scan Parameters:

Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 bounce): 25B-NBOMe HCl, lot N18-P1C



FTIR ATR (Diamond, 3 bounce): 25B-NBOMe HCl, lot N18-P1C





25B-NBOMe



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4. ADDITIONAL RESOURCES

[Wikipedia](#)