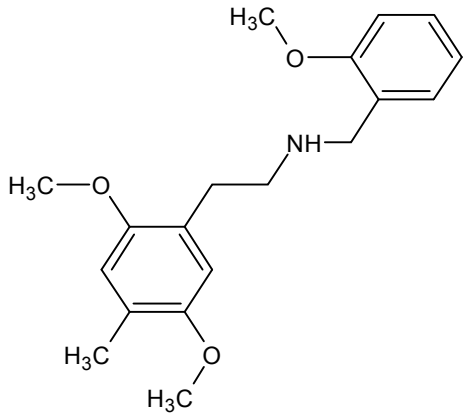
25D-NBOMe

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



1. GENERAL INFORMATION

IUPAC Name: 2-(2,5-dimethoxy-4-methylphenyl)-*N*-(2-methoxybenzyl)ethanamine

CAS#: 1354632-02-2 (base), 1539266-35-7 (HCl)

Synonyms: 25D-NB2OMe, 2C-D-NBOMe

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

UV_{max} (nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{19}H_{25}NO_3$	315	Not Determined
HCl	$C_{19}H_{25}NO_3 \cdot HCl$	351	169.0

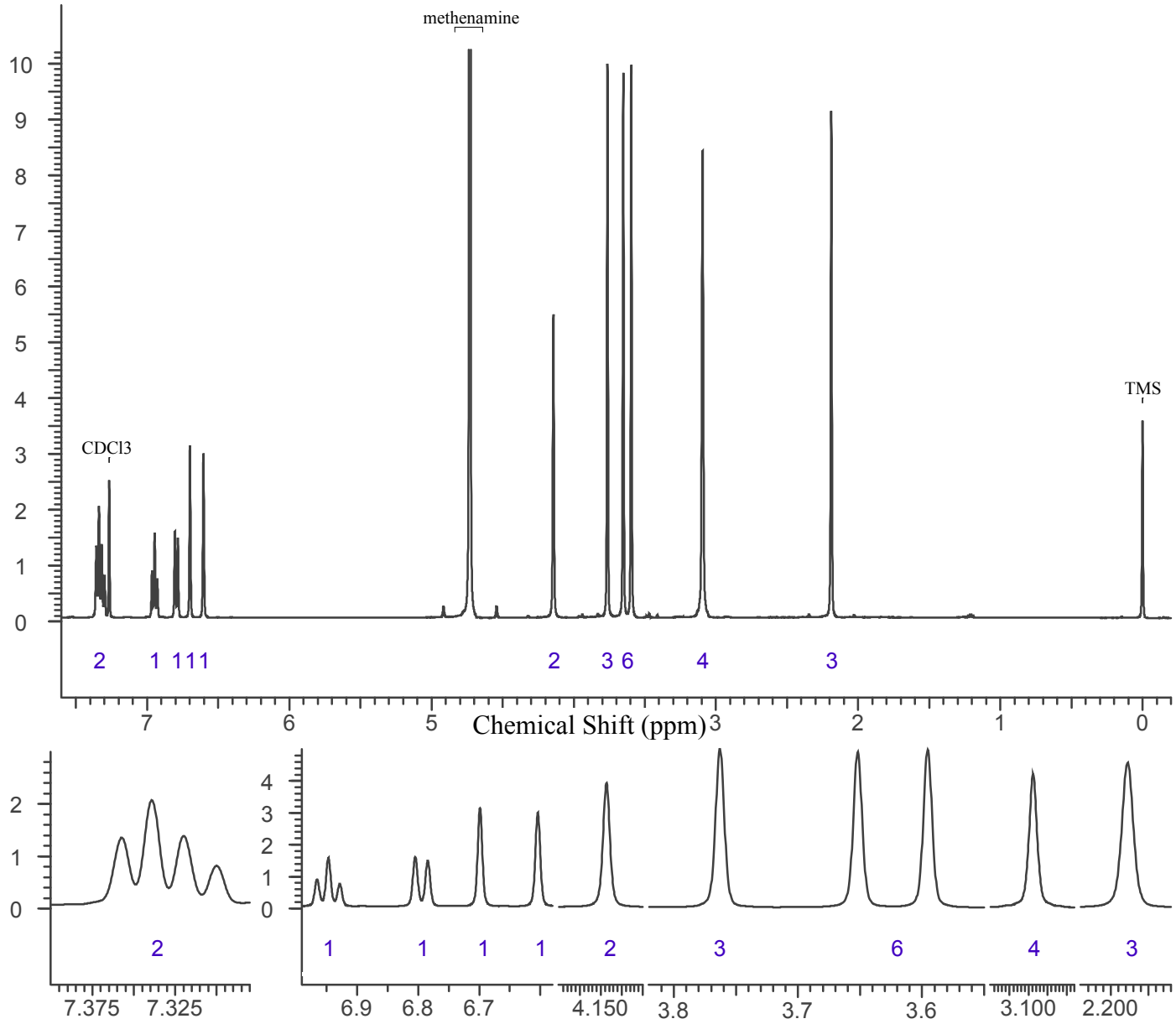
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~7 mg/mL in deuterium chloroform ($CDCl_3$) containing TMS for 0 ppmreferenceandmethenamineasquantitativeinternalstandard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}H NMR: 25D-NBOMe HCl Lot# N17-P88C; $CDCl_3$; 400MHz

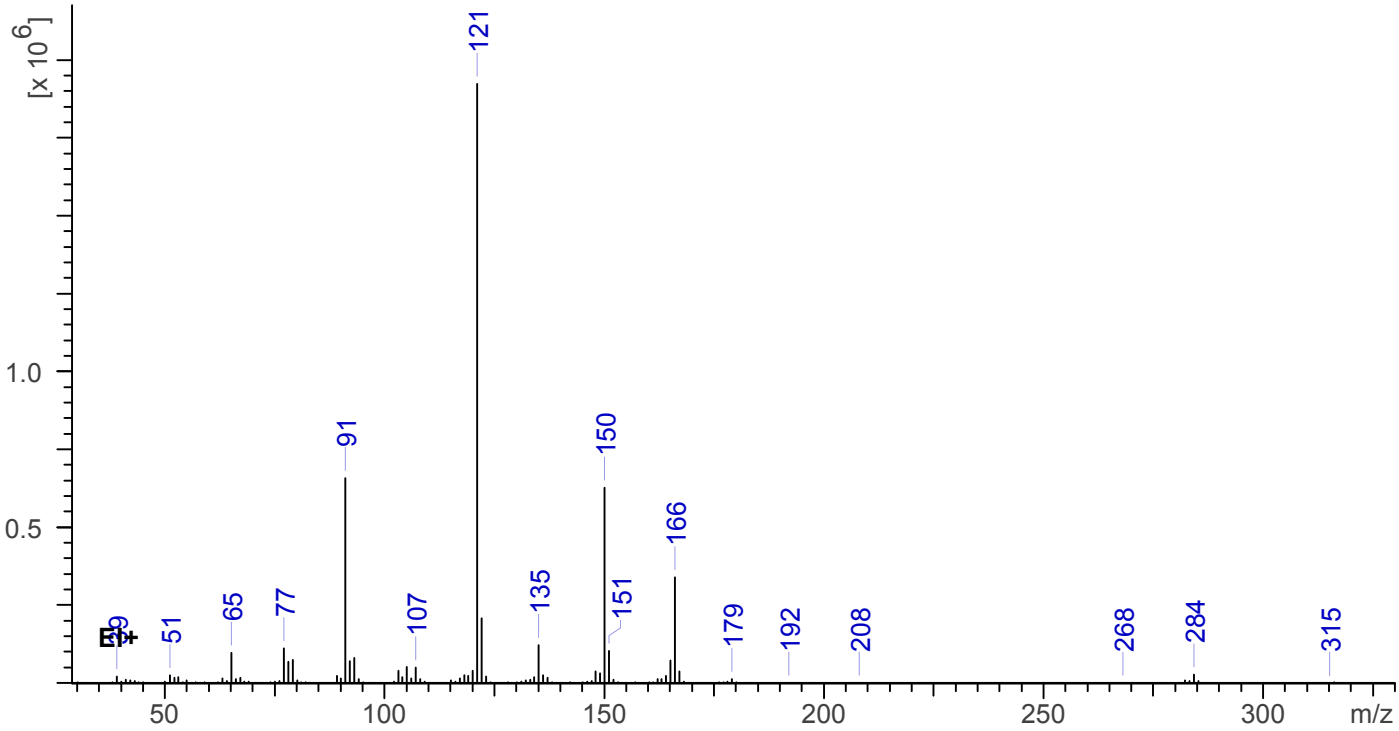


3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 mg/mL in methanol

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: 34-550 amu Threshold: 90 Tune file: stune.u Acquisition mode: scan
Retention Time:	15.455 min

EI Mass Spectrum: 25D-NBOMe HCl Lot# N17-P88C

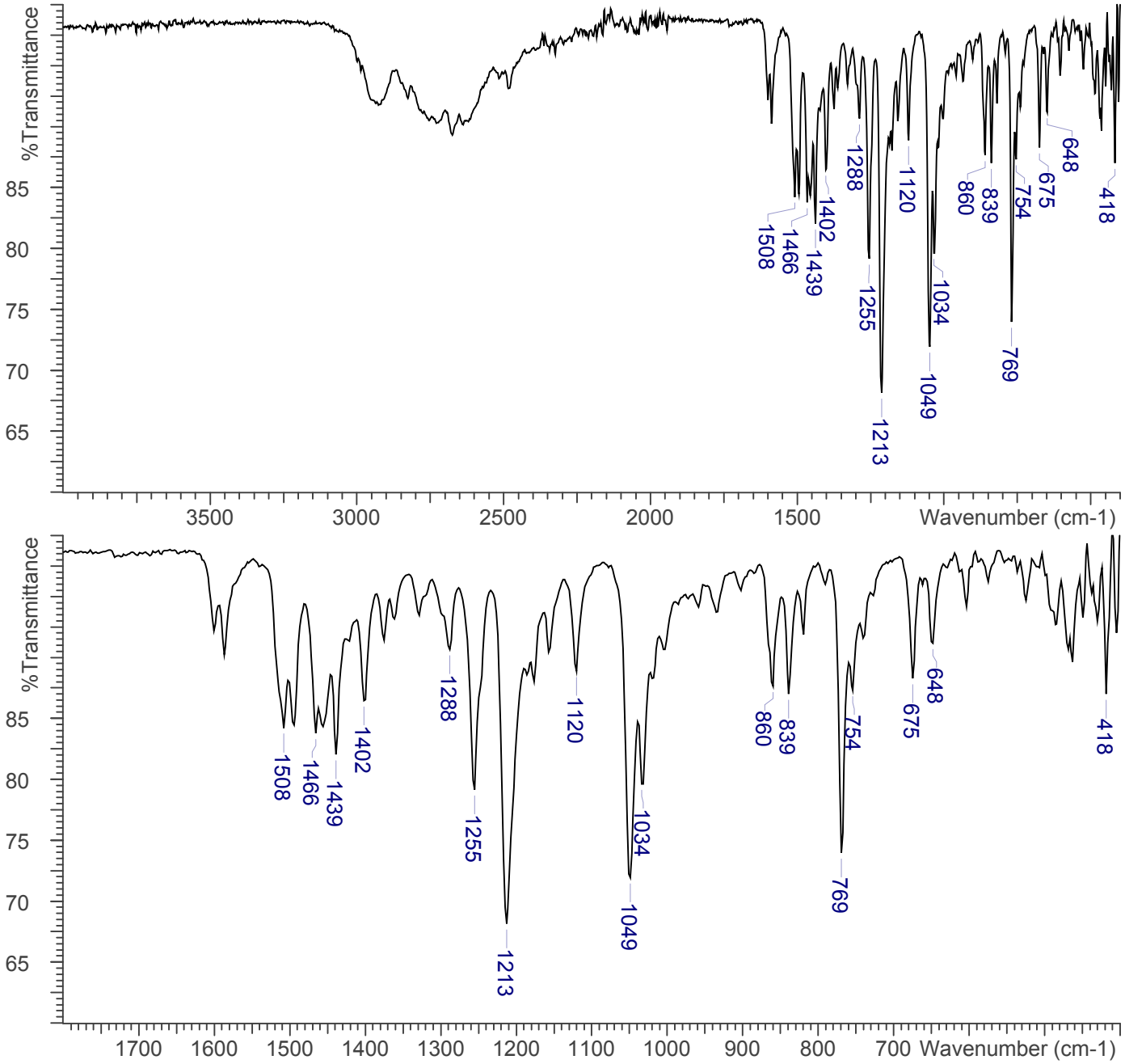


3.3 INFRARED SPECTROSCOPY (FTIR)

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): 25D-NBOMe HCl Lot# N17-P88C



4. ADDITIONAL RESOURCES

Forendex

Wikipedia