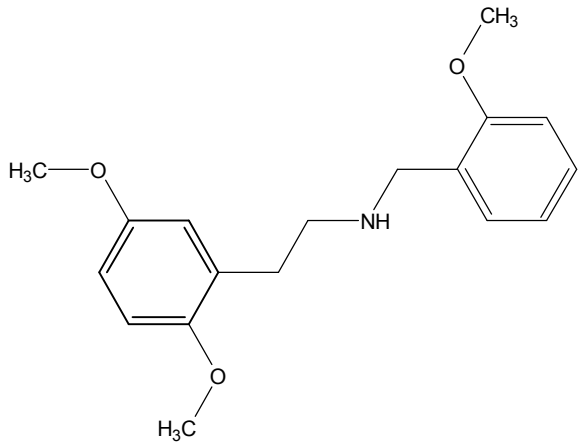
25H-NBOMe

Latest Revision: August 23, 2013



1. GENERAL INFORMATION

IUPAC Name: 2-(2,5-dimethoxyphenyl)-*N*-(2-methoxybenzyl)ethanamine

CFR: Not Scheduled (7/2013)

CAS#: Not Available

Synonyms: 25H-NB2OMe

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max}(nm): 281.6

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{18}H_{23}NO_3$	301	Not Determined
HCl	$C_{18}H_{23}NO_3 \cdot HCl$	337	118.2

3. ADDITIONAL RESOURCES

No resources identified as of 7/26/2013.

4. QUALITATIVE DATA

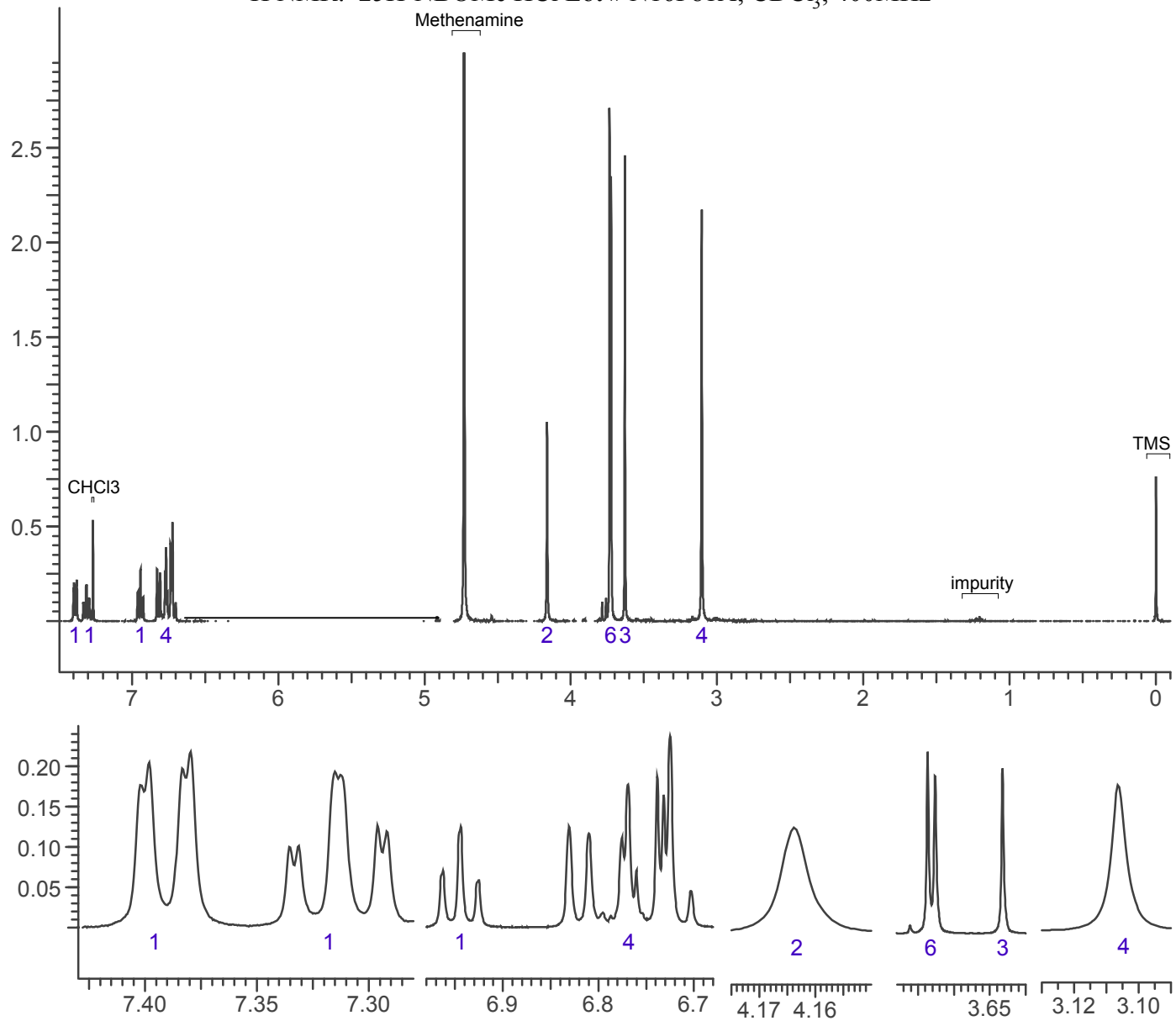
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $CDCl_3$

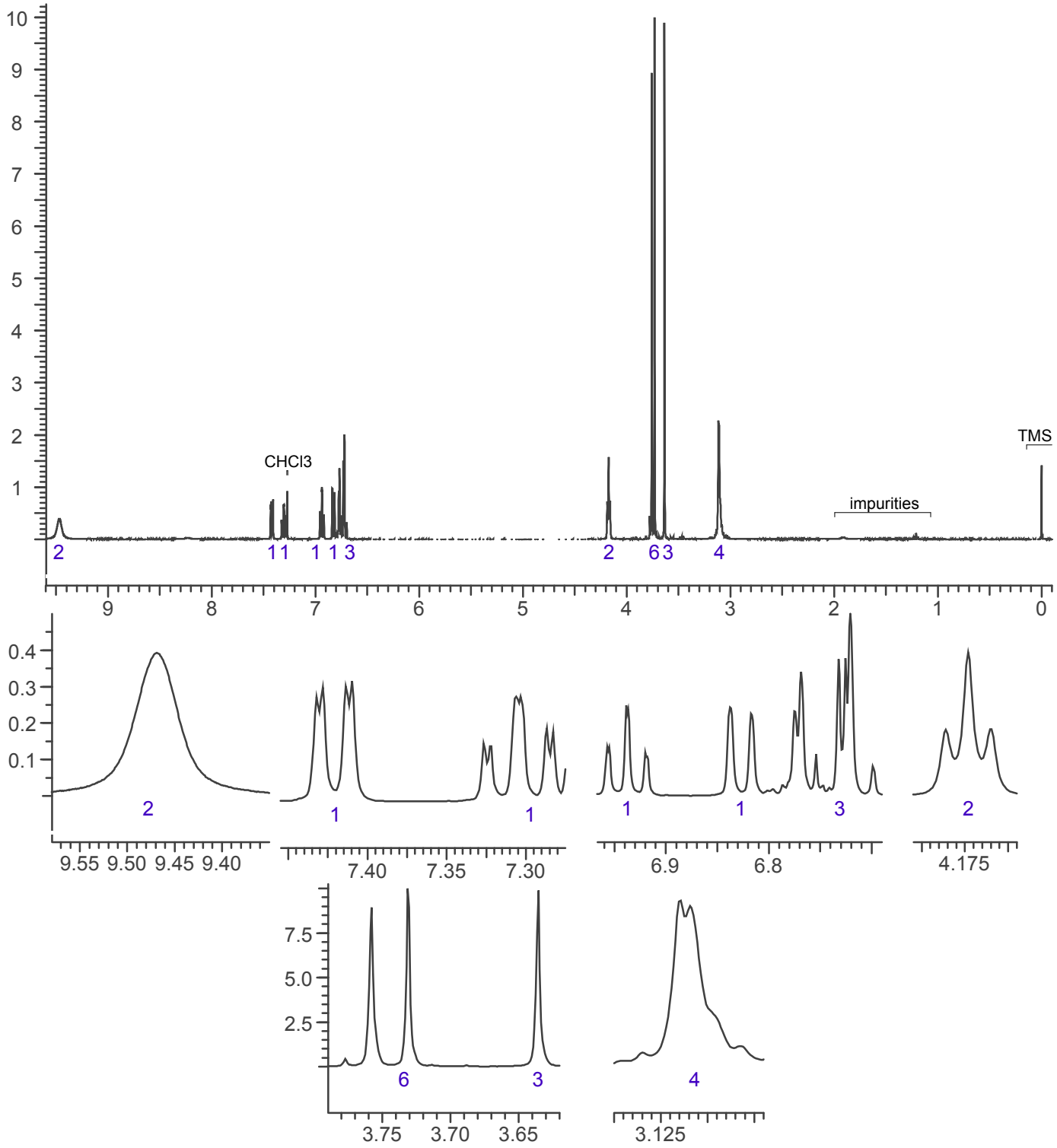
Sample Preparation: Dilute analyte to ~10 mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

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

^{1}H NMR: 25H-NBOMe HCl Lot # N16P81A; $CDCl_3$; 400MHz



^{1}H NMR: 25H-NBOMe HCl Lot N16P81A; $CDCl_3$; 400MHz



NMR Analytical Observation:

Due to the basic nature of the methenamine, the N-H peak above 9 ppm is not present when it is used as an internal standard. The methenamine interacts with the proton on the nitrogen.

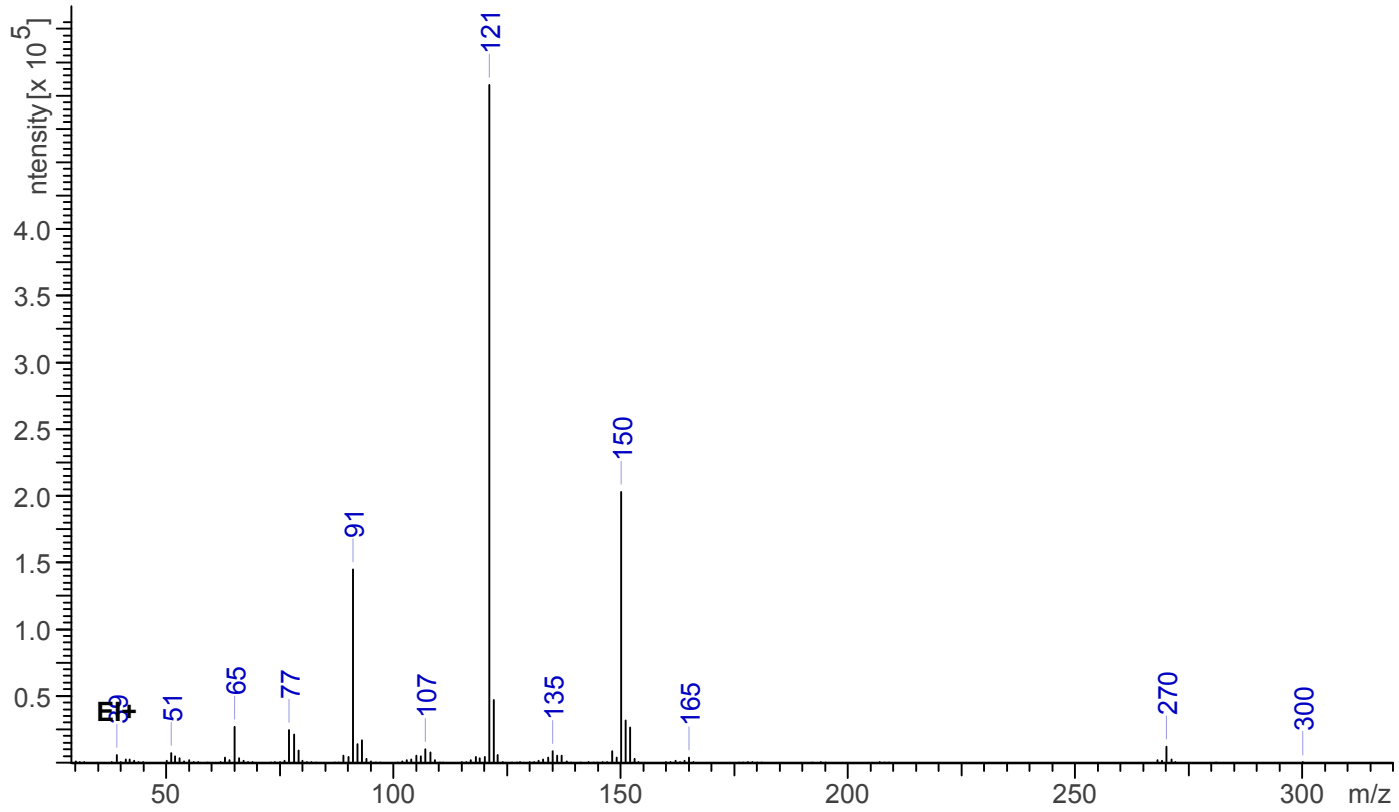
In the NMR spectra without methenamine, the N-H peak is integrated as 2 protons due to exchange with the HCl.

4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~1 mg/mL 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: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	14.998 min

EI Mass Spectrum: 25H-NBOMe HCl Lot N16P81A



4.3 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): 25H-NBOMe HCl Lot # N16P81A