

1. GENERAL INFORMATION

IUPAC Name:	2-(4-ethyl-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine
CFR:	Not Scheduled (03/2013)
CAS #:	N/A
Synonyms:	4-ethyl-2,5-dimethoxy-N-(2-methoxybenzyl)phenethylamine
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Kovat's Index:	Pending
UV_{max}:	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₀ H ₂₇ NO ₃	329	Not Determined
HCl	C ₂₀ H ₂₇ NO ₃ · HCl	365	161.6

3. ADDITIONAL RESOURCES

No resources identified as of 3/1/2013.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

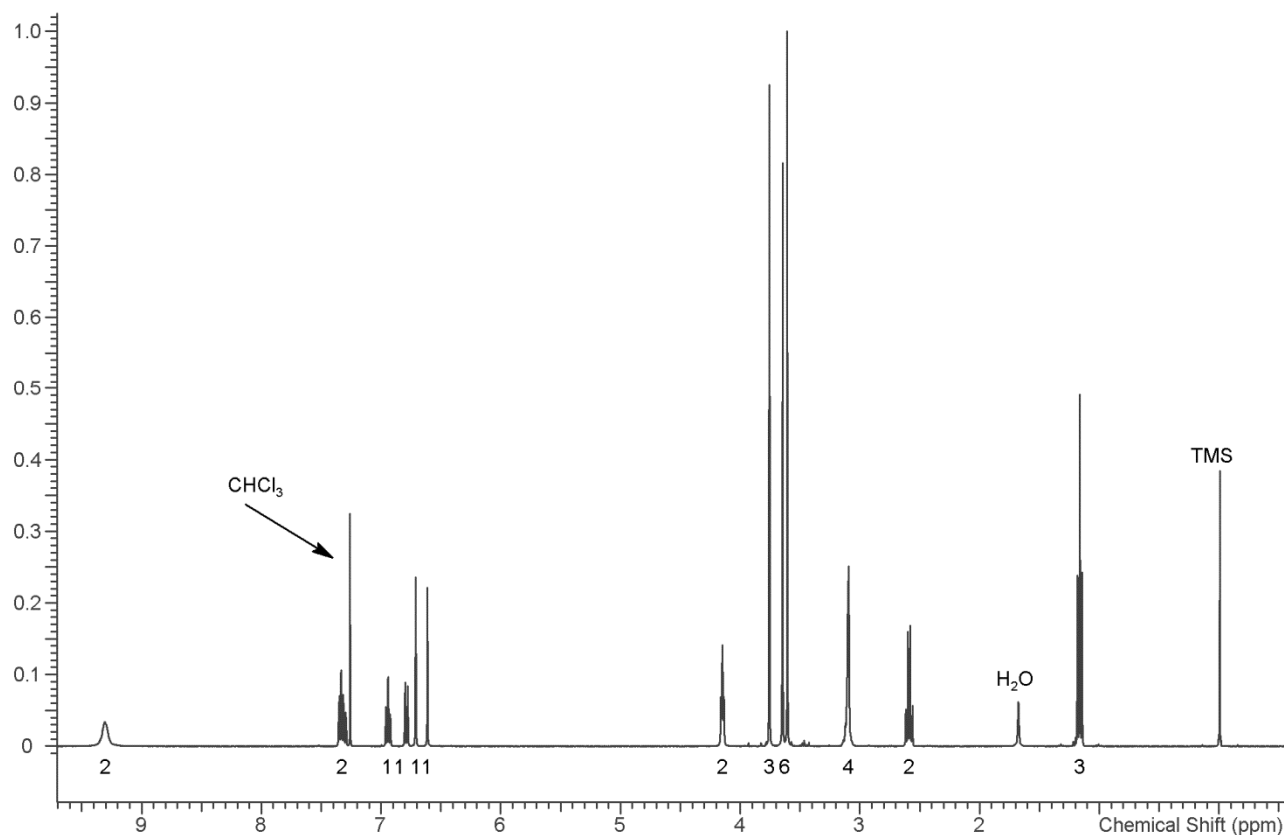
Method NMR CDCl₃

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

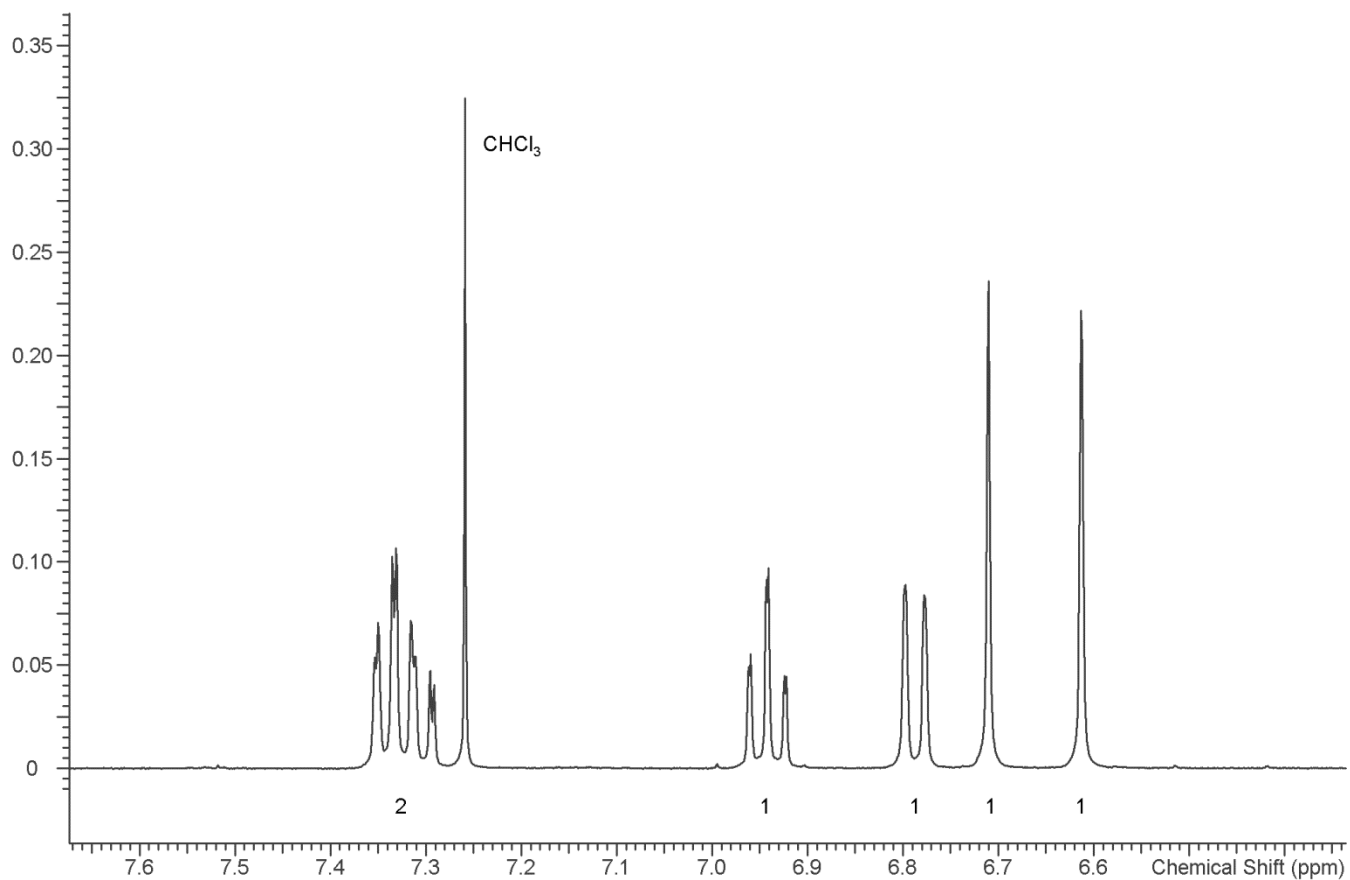
Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

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

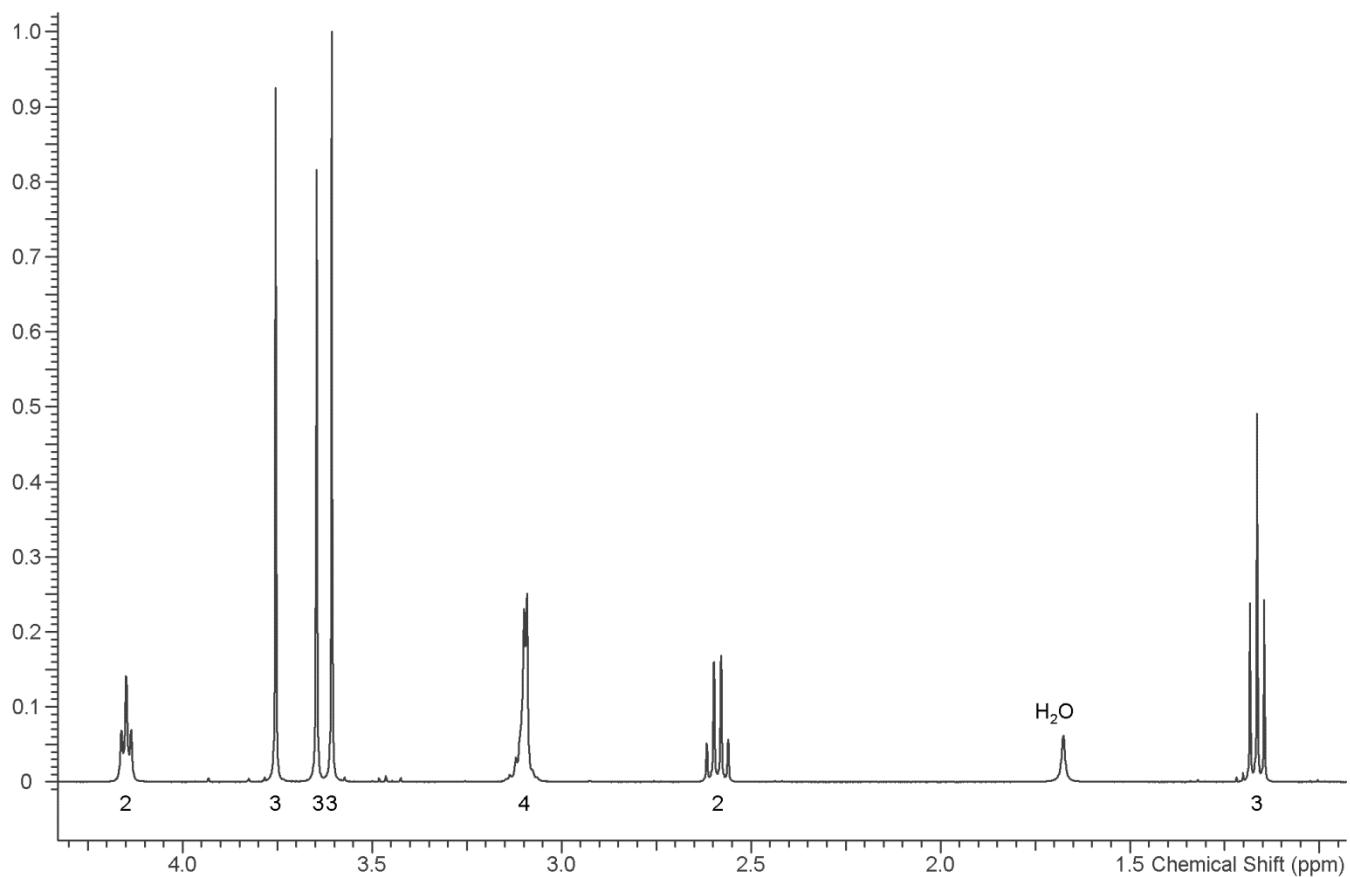
¹H NMR: 25E-NBOMe HCl Lot # N17P97B; CDCl₃; 400 MHz



1H NMR: 25E-NBOMe HCl Lot # N17P97B; CDCl₃; 400 MHz



1H NMR: 25E-NBOMe HCl Lot # N17P97B; CDCl₃; 400 MHz



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in CHCl₃.

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x .25mm x .25μm

Carrier Gas: Helium at 1 mL/min

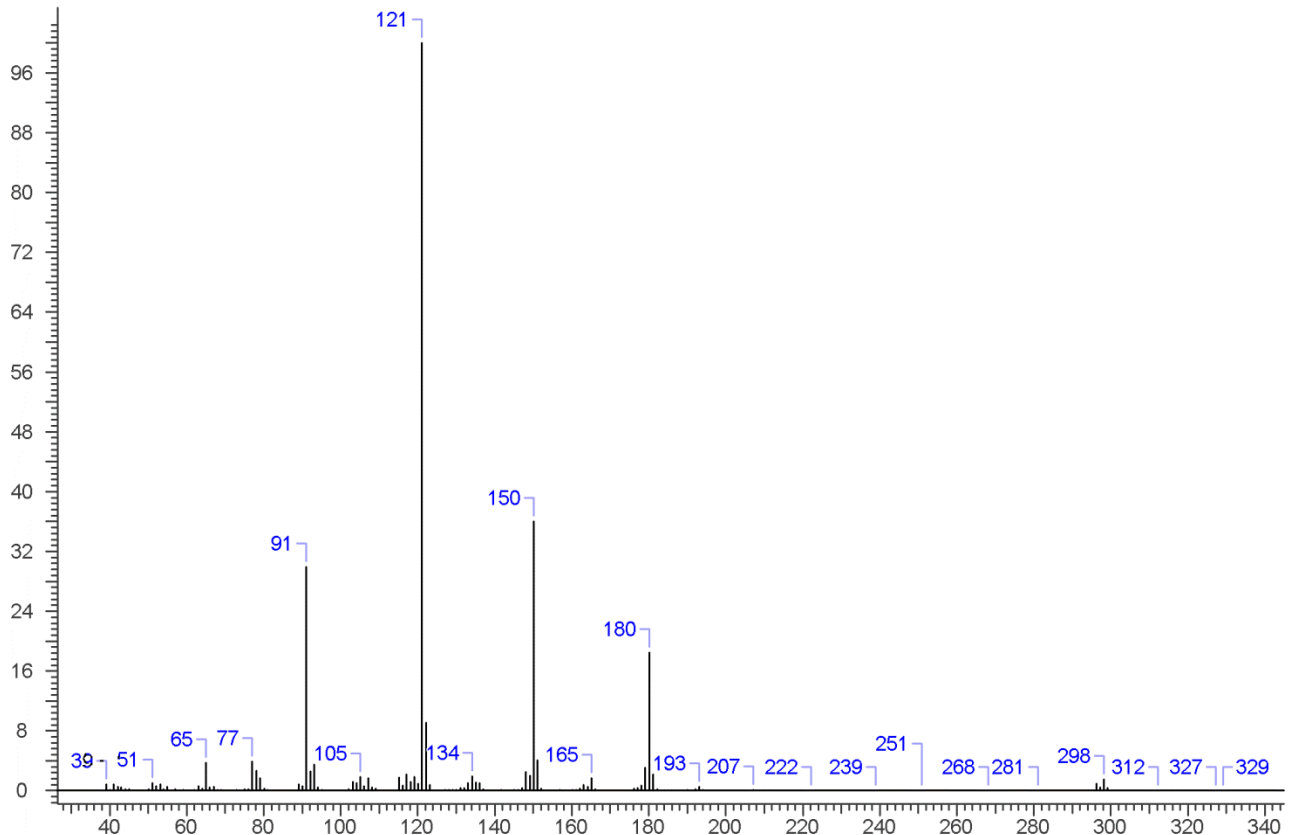
Temperatures:
Injector: 280°C
MSD transfer line: 280°C
MS Source: 230°C
MS Quad: 150°C
Oven program:
1) 90°C initial temperature for 2.0 min
2) Ramp to 300°C at 14°C/min
3) Hold final temperature for 10.0 min

Injection Parameters: Split Ratio = 25:1, 1 μL injected

MS Parameters:
Mass scan range: 34-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 15.891 minutes

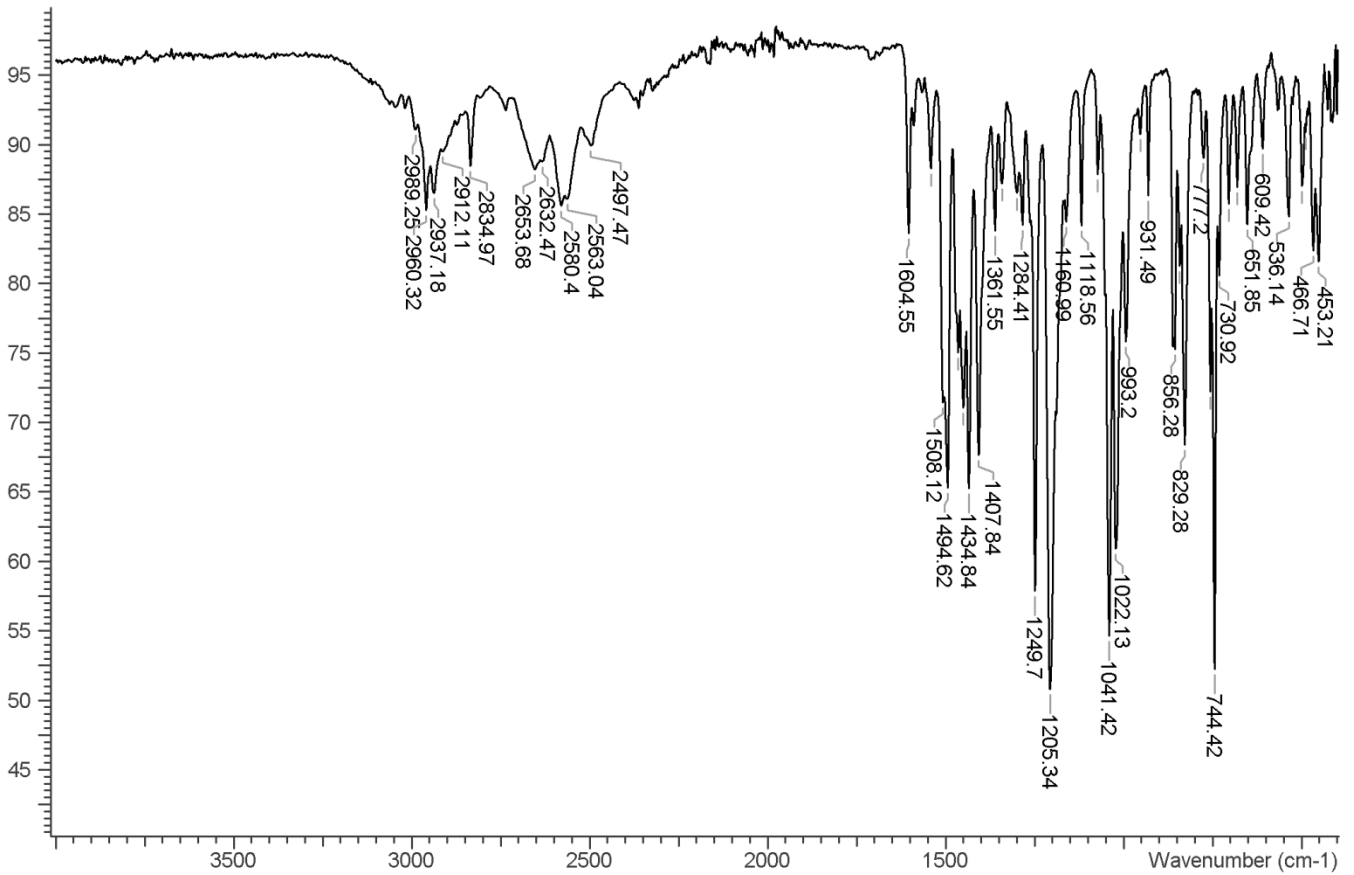
EI Mass Spectrum: 25E-NBOMe HCl Lot # N17P97B



4.3 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): 25E-NBOMe HCl Lot # N17P97B



FTIR ATR (Diamond, 3 Bounce): 25E-NBOMe HCl Lot # N17P97B

