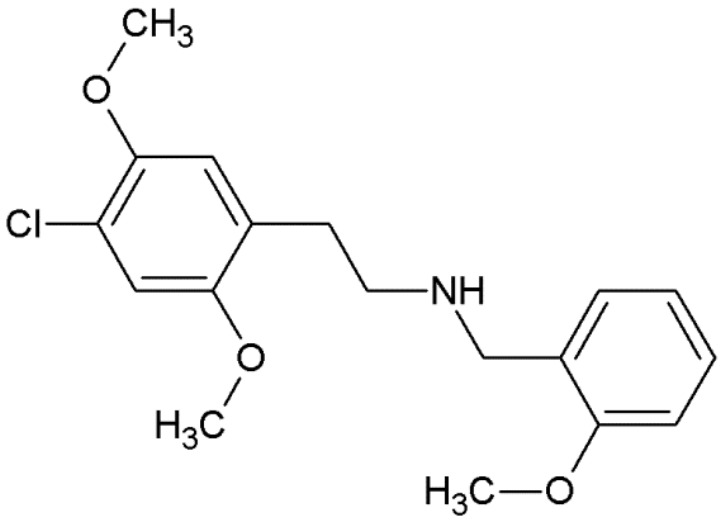


1. GENERAL INFORMATION

IUPAC Name: 2-(4-chloro-2,5-dimethoxyphenyl)-N-(2-methoxybenzyl)ethanamine

CFR: Not Scheduled (12/2012)

CAS #: 1227608-02-7

Synonyms: 2C-C-NBOMe, NBOMe-2C-C, Cimbi-82, Pandora, Dime

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	$C_{18}H_{22}ClNO_3$	335	Not Determined
HCl	$C_{18}H_{22}ClNO_3$.HCl	372	183.1

3. ADDITIONAL RESOURCES

Forendex

Wikipedia

4. QUALITATIVE DATA

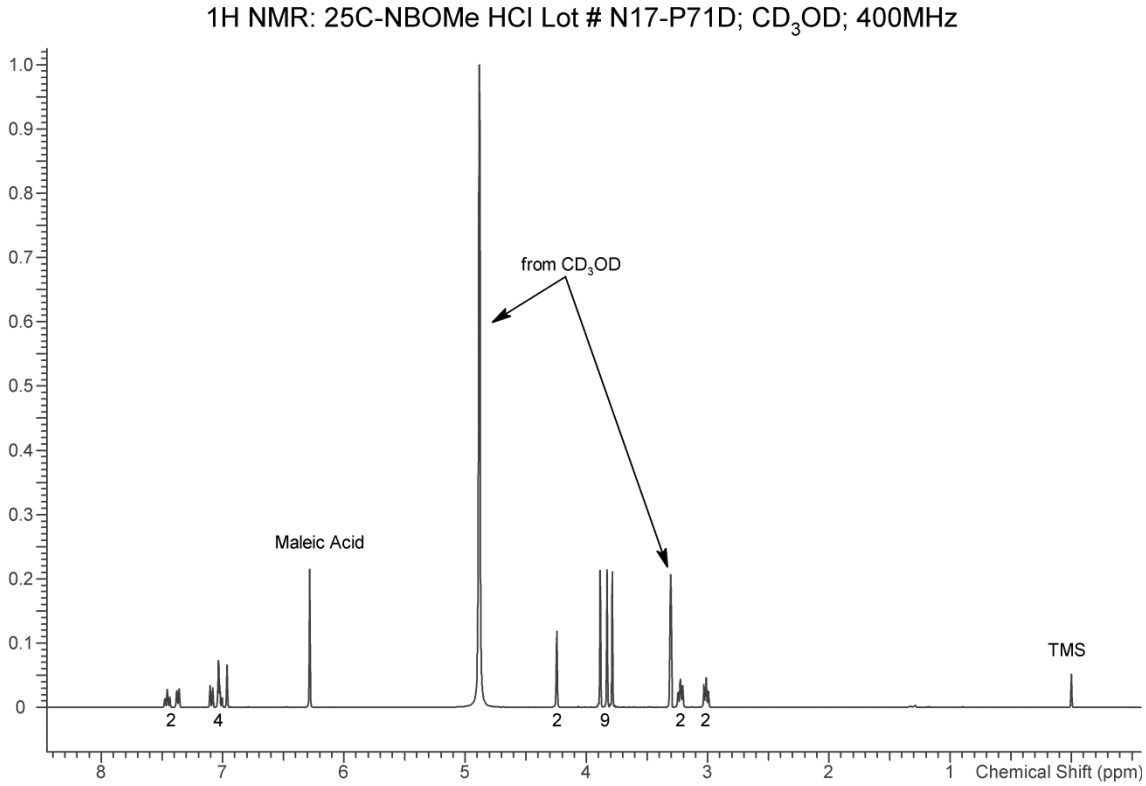
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CD_3OD

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterated methanol (CD_3OD) containing TMS for 0 ppm reference and maleic acid as quantitative internal standard.

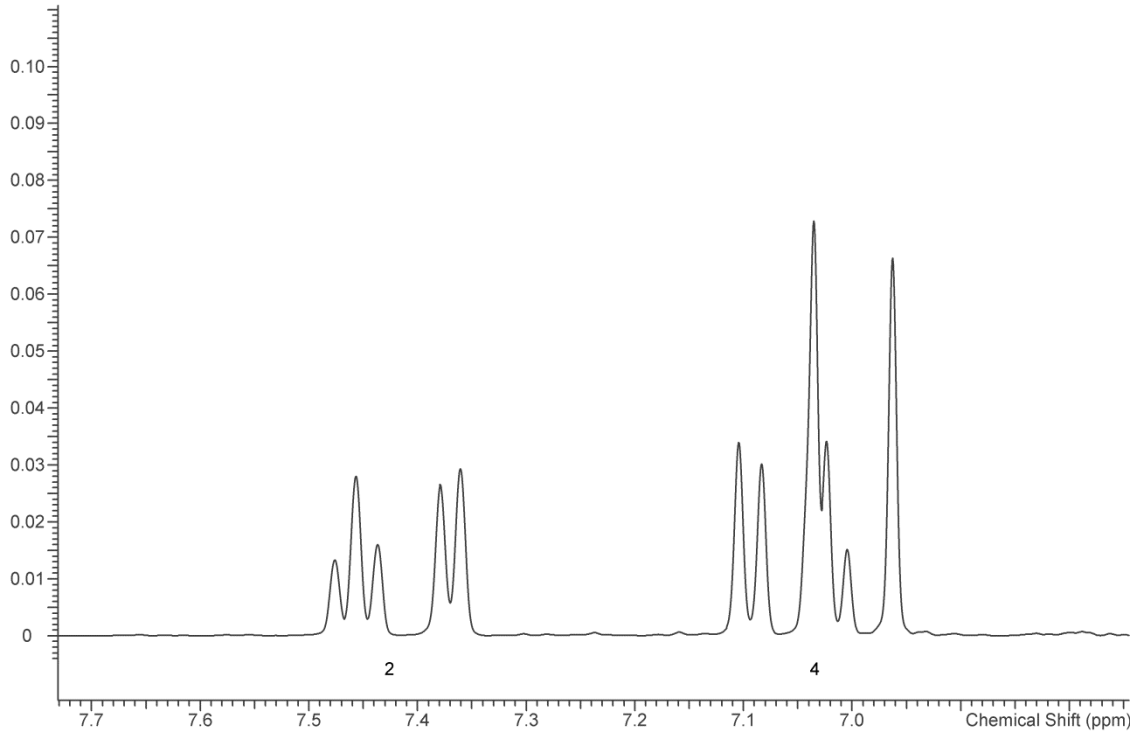
Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

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

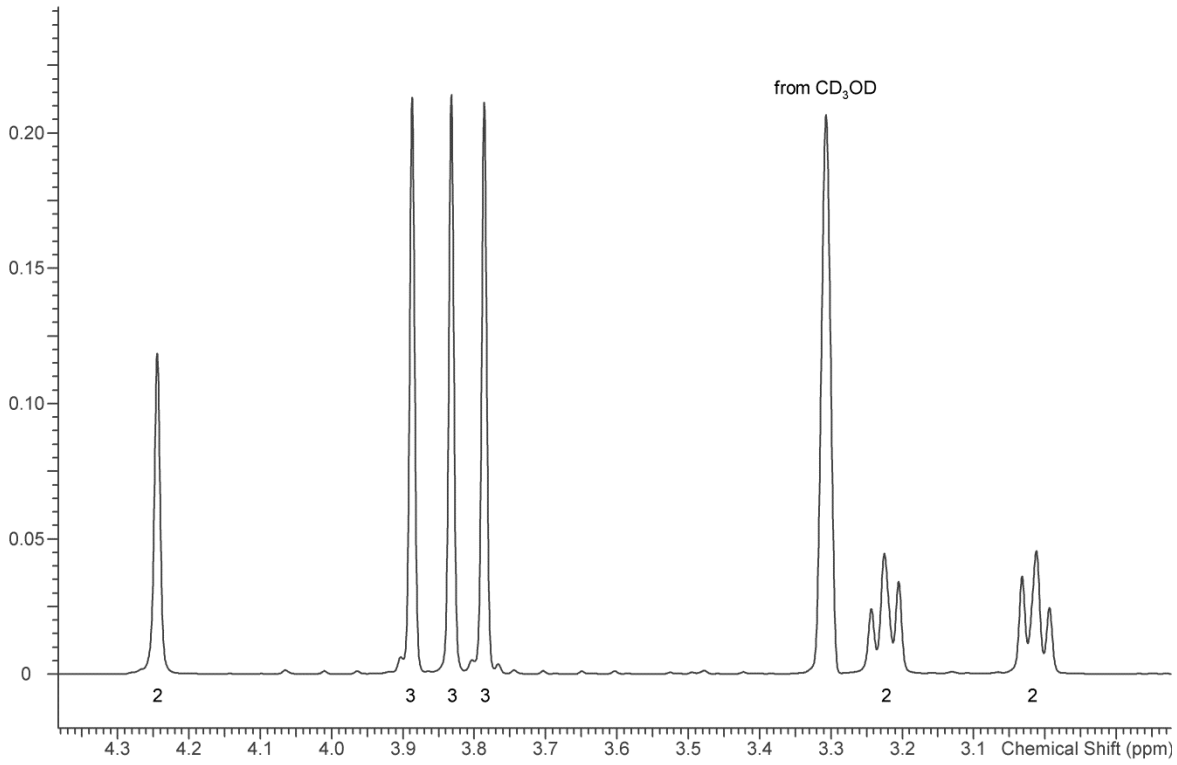


Note: The three singlets at 3.8-3.9 ppm in the above spectrum each represent 3 hydrogens. These are notated as 9 hydrogens total in the full spectrum due to the close proximity of the signals. The expanded view below shows the more detailed integration.

1H NMR: 25C-NBOMe HCl Lot # N17-P71D; CD_3OD; 400MHz



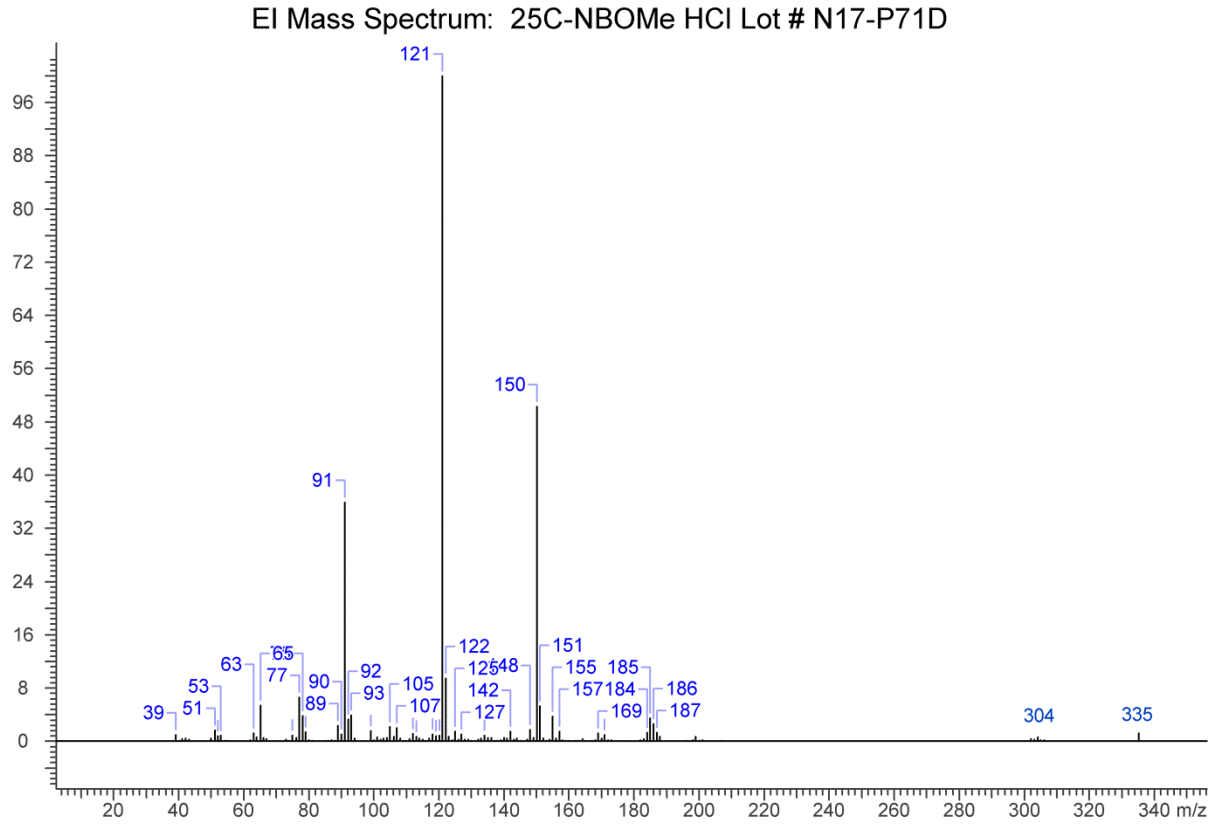
1H NMR: 25C-NBOMe HCl Lot # N17-P71D; CD_3OD; 400MHz



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

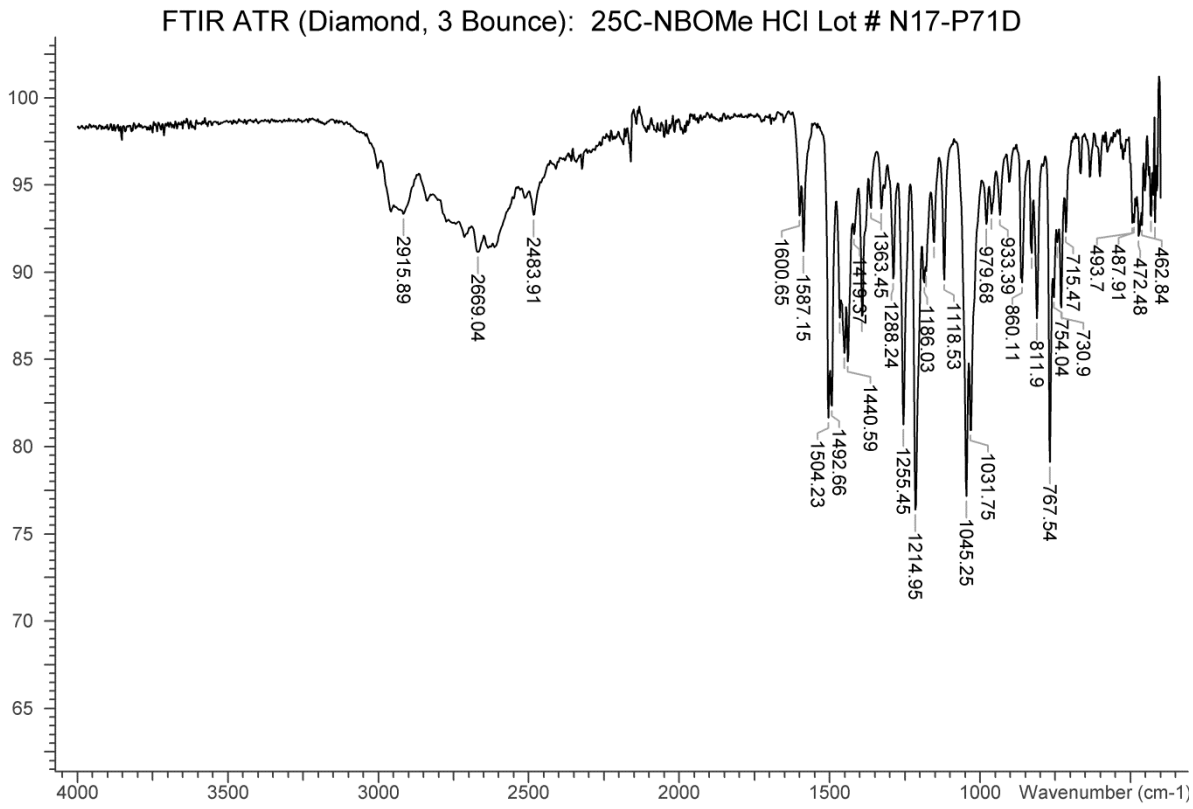
Sample Preparation: Dilute analyte to ~4 mg/mL in $CHCl_3$.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS; 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) 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:	16.372 min



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): 25C-NBOMe HCl Lot # N17-P71D