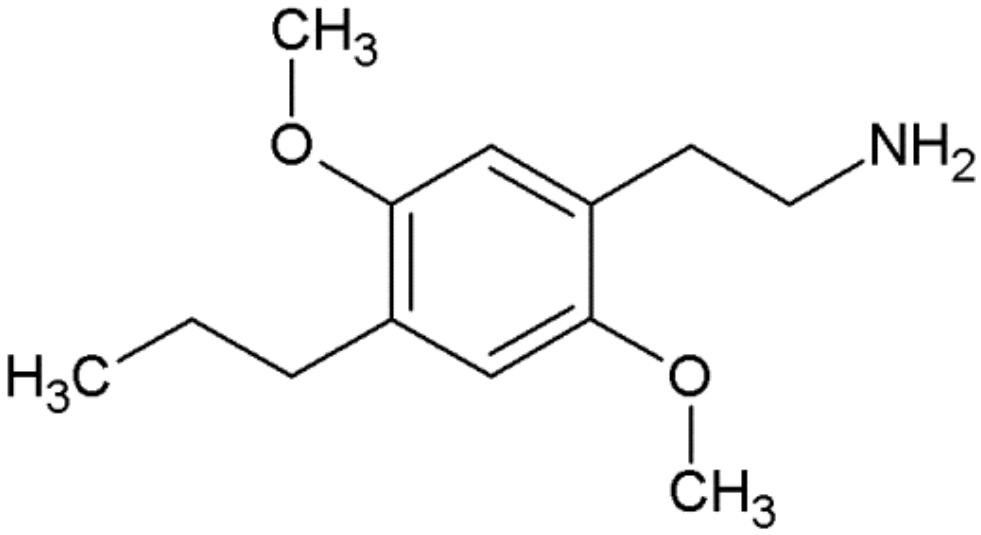


1. GENERAL INFORMATION

IUPAC Name: 2-(2,5-dimethoxy-4-propylphenyl)ethanamine

CFR: 1308.11; Schedule I

CAS #: 207740-22-5

Synonyms: 2,5-dimethoxy-4-propylphenethylamine

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max}: 289.9 nm

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{13}H_{21}NO_2$	223	Not Determined
HCl	$C_{13}H_{21}NO_2 \cdot HCl$	259	213.3

3. ADDITIONAL RESOURCES

Forendex

Wikipedia

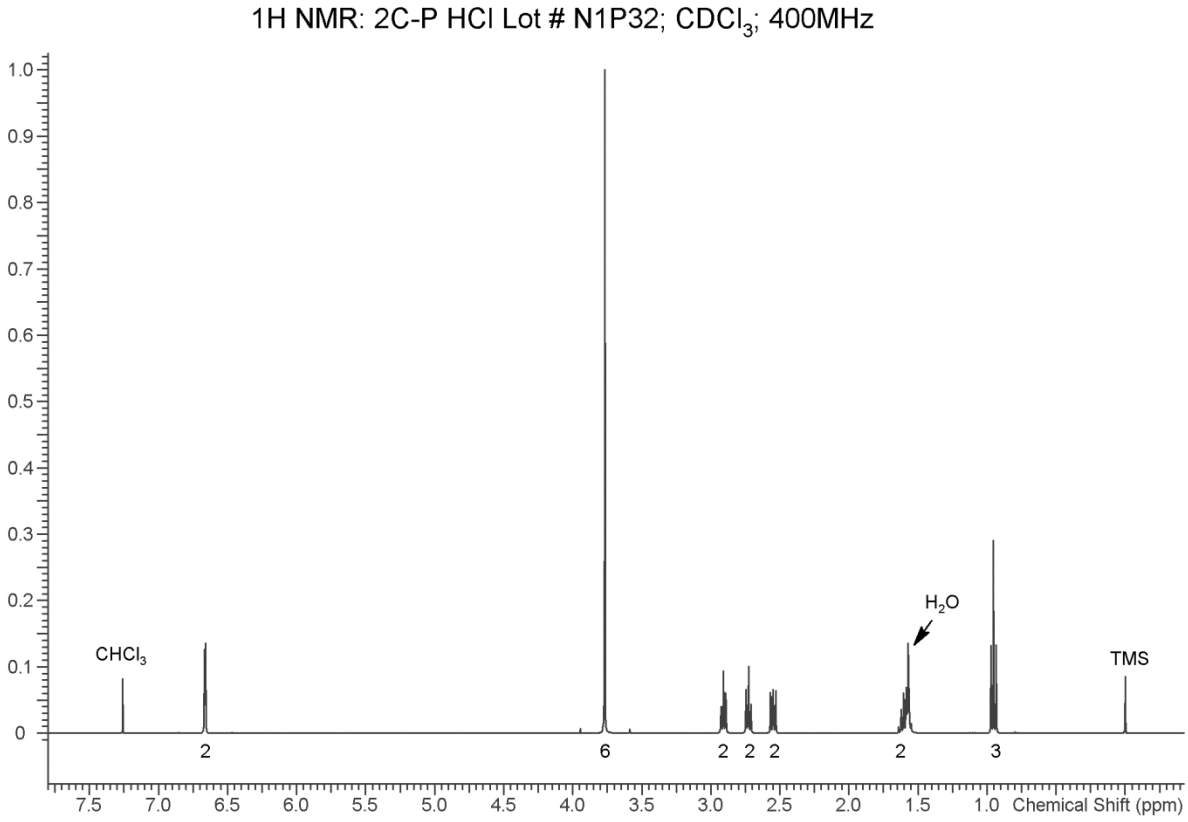
4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

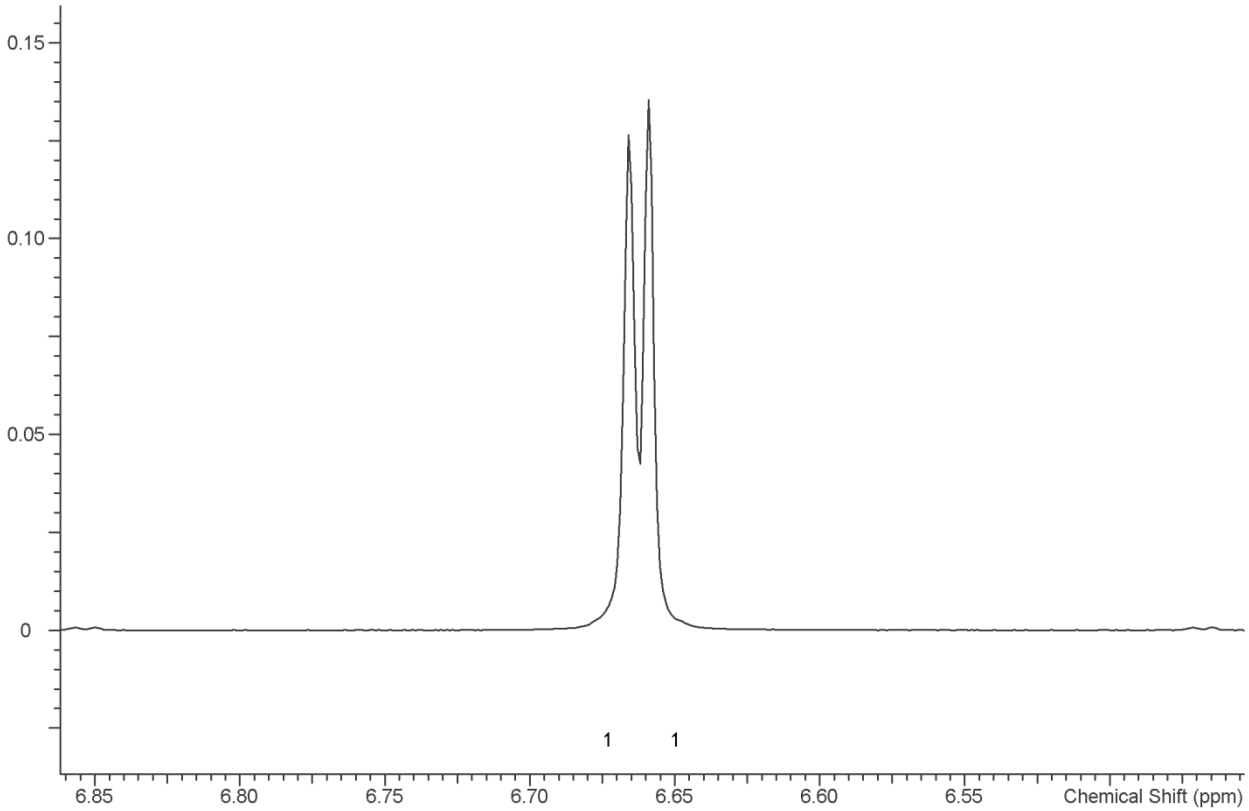
Method NMR $CDCl_3$

Sample Preparation: Extract analyte with saturated sodium bicarbonate in D_2O and deuterochloroform ($CDCl_3$) to ~10mg/mL.

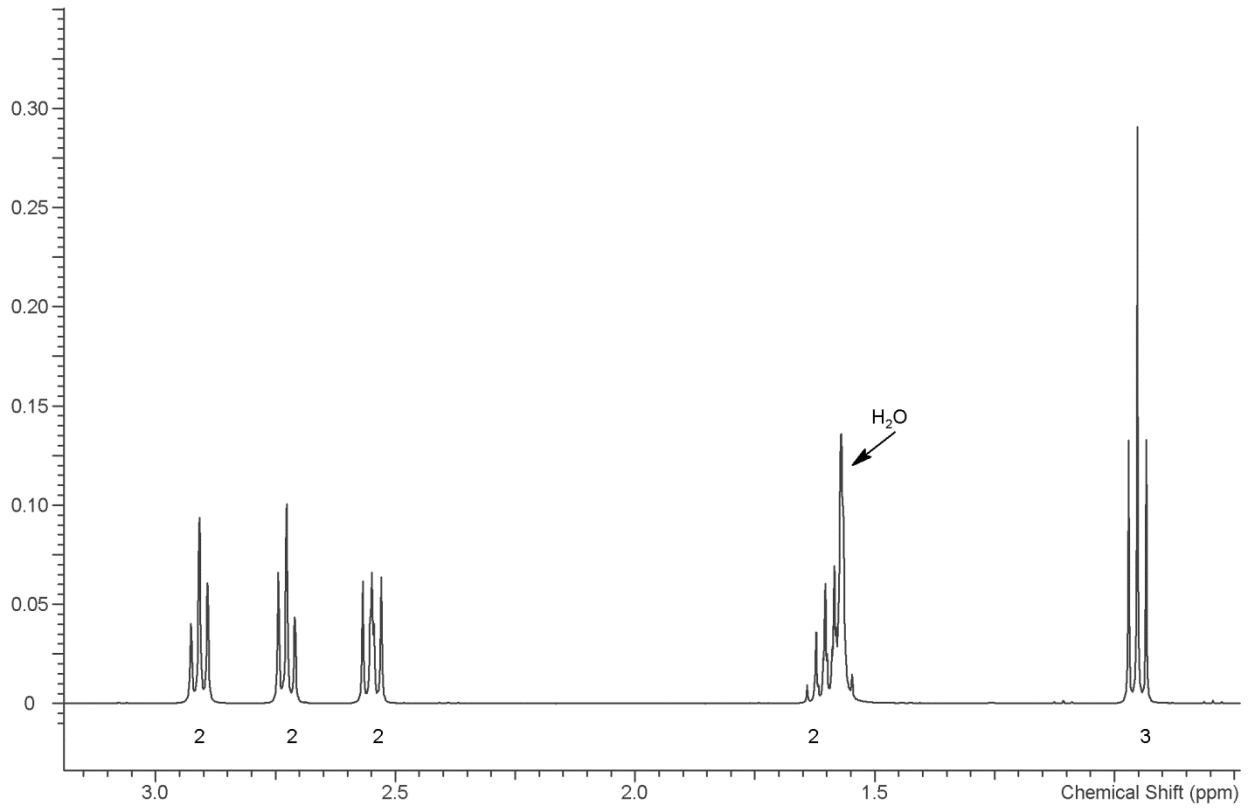
Instrument:	Varian Mercury 400 MHz NMR spectrometer with proton detection probe
Parameters:	Spectral width: at least containing -3 ppm through 13 ppm Pulse angle: 90° Delay between pulses: 45 seconds Number of scans (NT): 8 Number of steady state scans: 0 Oversampling: 4 or more Shimming: automatic gradient shimming of Z1-4 shims Phasing, Drift Correction: automatic or manual



1H NMR: 2C-P HCl Lot # N1P32; $CDCl_3$; 400MHz



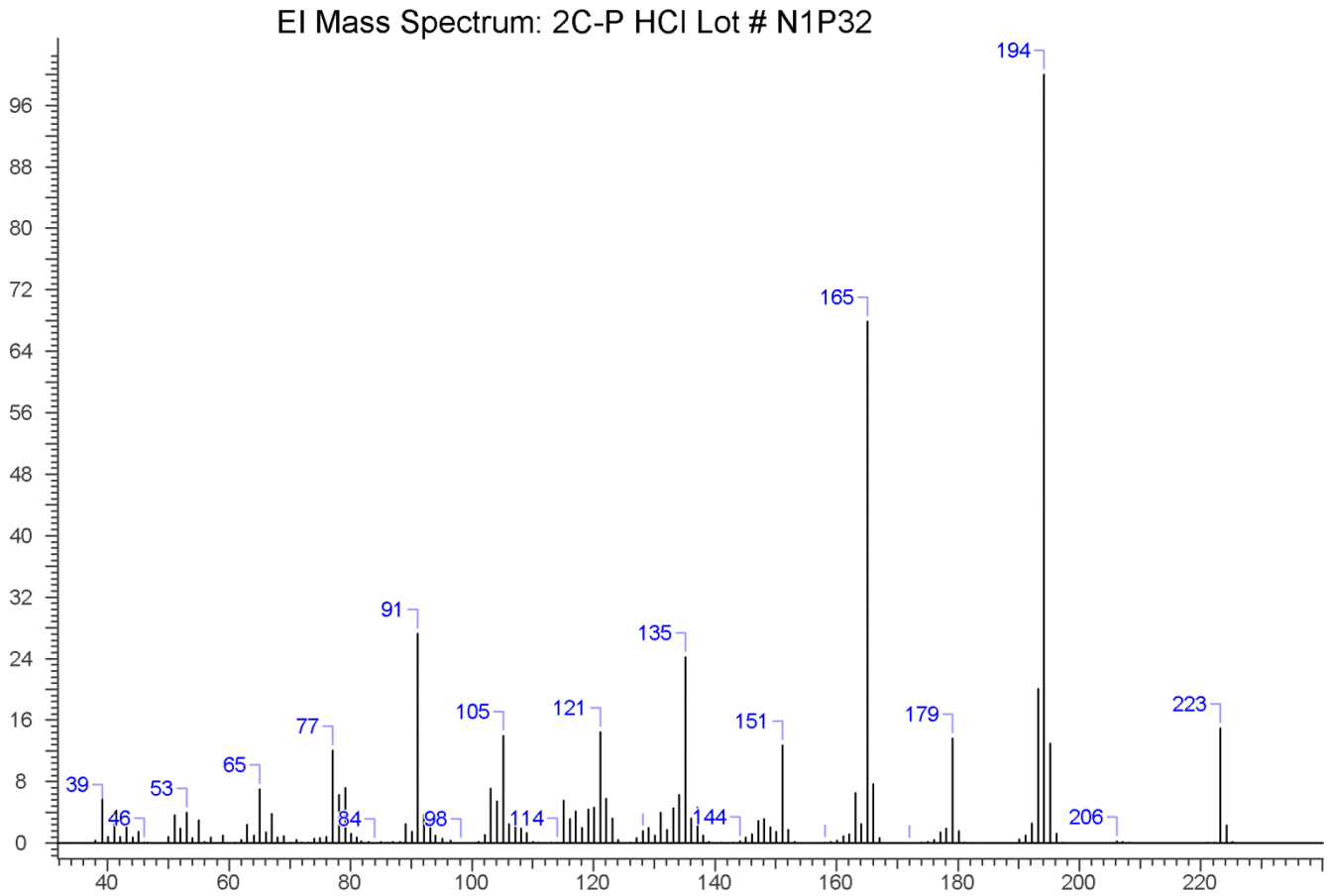
1H NMR: 2C-P HCl Lot # N1P32; $CDCl_3$; 400MHz



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

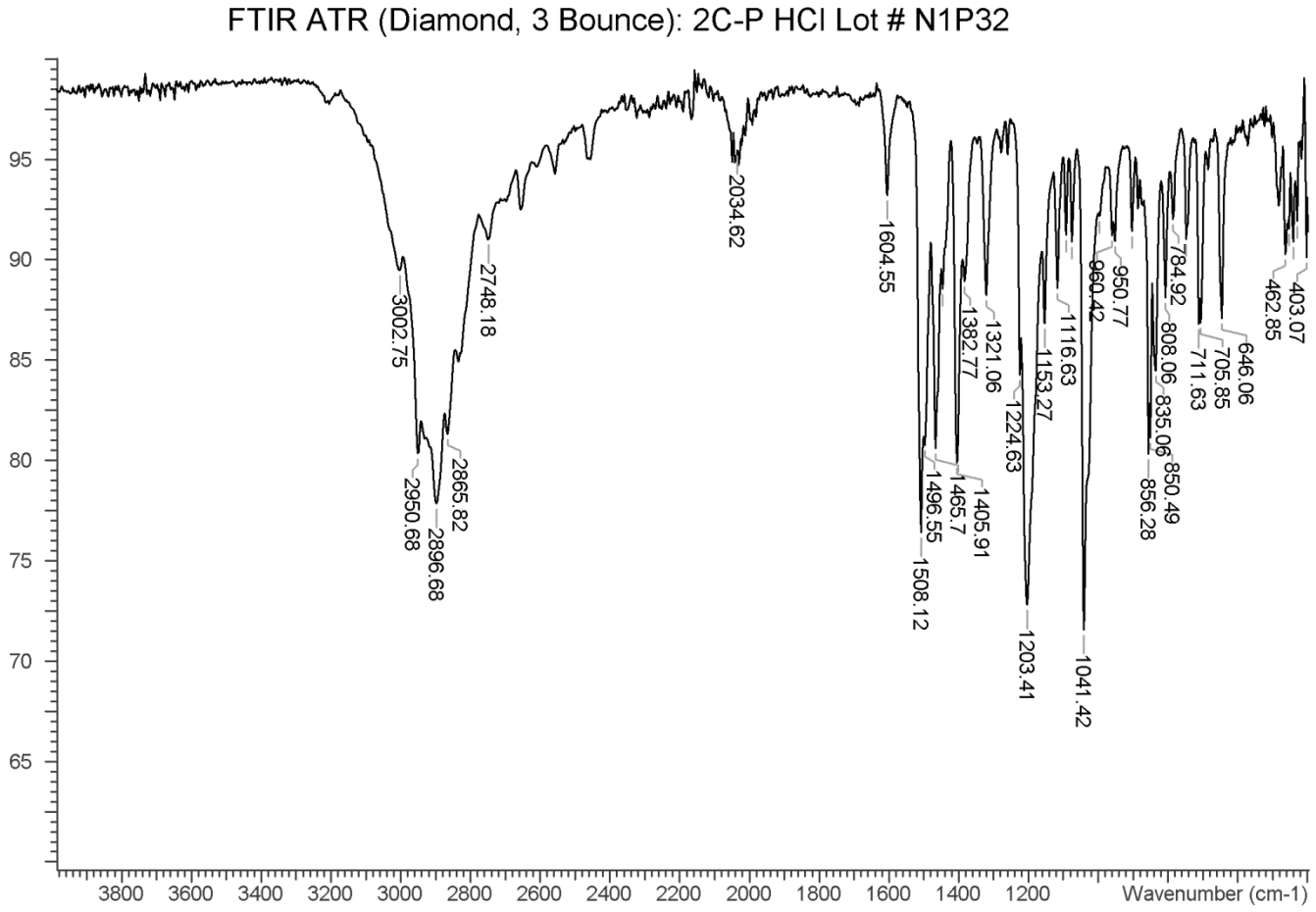
Sample Preparation: Dilute analyte to ~1 mg/mL base extracted in $CHCl_3$.

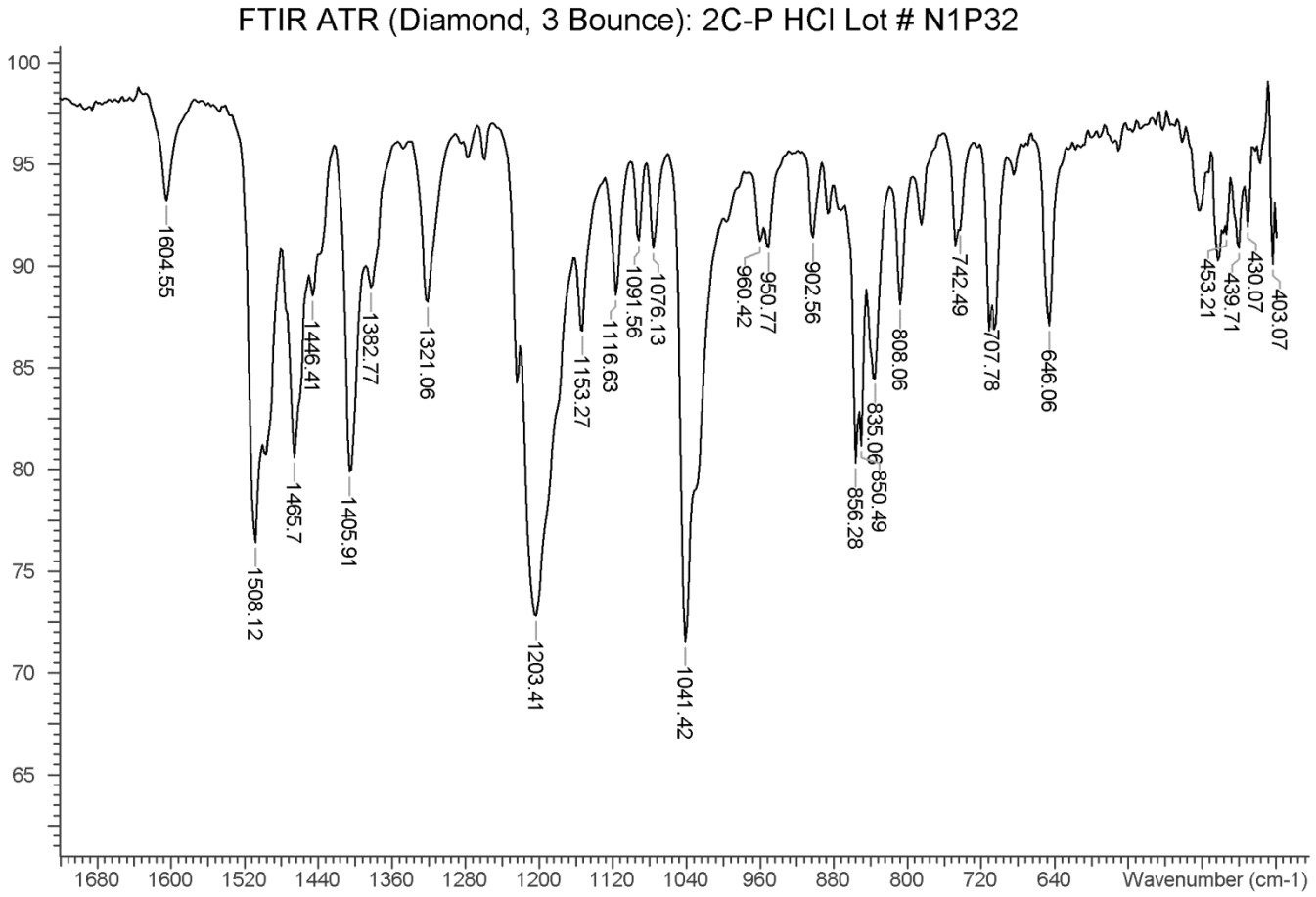
Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS; 30m x .25mm x .25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 90°C initial temperature for 2.0 min 2) Ramp to 300°C 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:	10.806 minutes



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): 2C-P HCl Lot # N1P32
100
95
90
85
80
75
70
65
1604.55
1508.12
1465.7
1446.41
1405.91
1382.77
1321.06
1203.41
1153.27
1116.63
1091.56
1076.13
1041.42
960.42
950.77
902.56
856.28
850.49
835.06
808.06
742.49
707.78
646.06
453.21
439.71
430.07
403.07
1680
1600
1520
1440
1360
1280
1200
1120
1040
960
880
800
720
640
Wavenumber (cm-1)