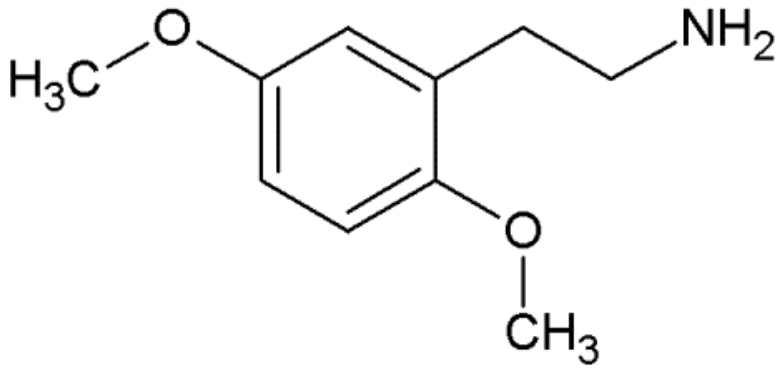
2C-H

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-dimethoxyphenyl)ethanamine
CAS #:	3600-86-0
Synonyms:	2,5-dimethoxyphenethylamine
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Retention Index:	Pending
UV_{max}:	225.0, 288.7 nm

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{10}H_{15}NO_2$	181	Not Determined
HCl	$C_{10}H_{15}NO_2 \cdot HCl$	217	138.9

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

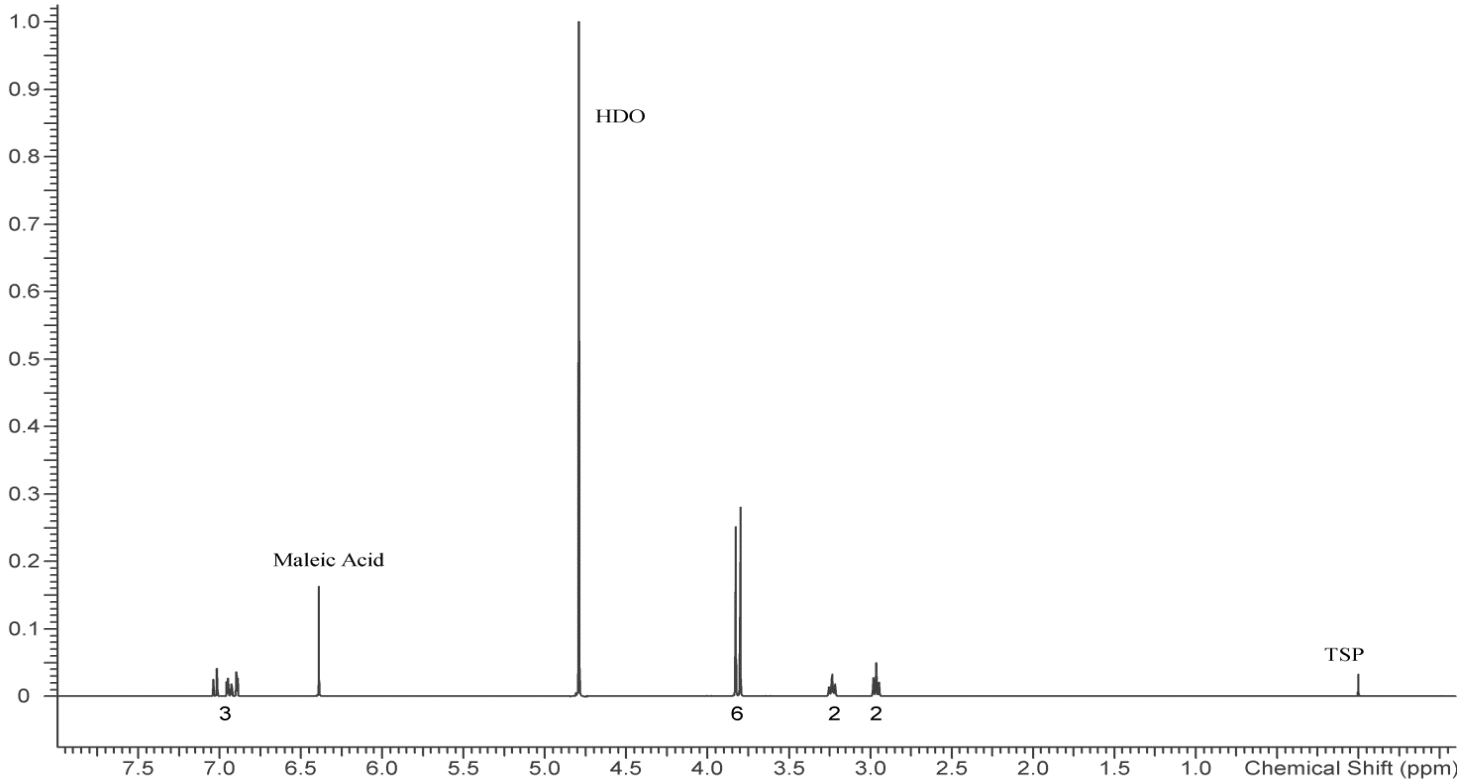
Method NMR D_2O

Sample Preparation: Dilute analyte to ~20 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

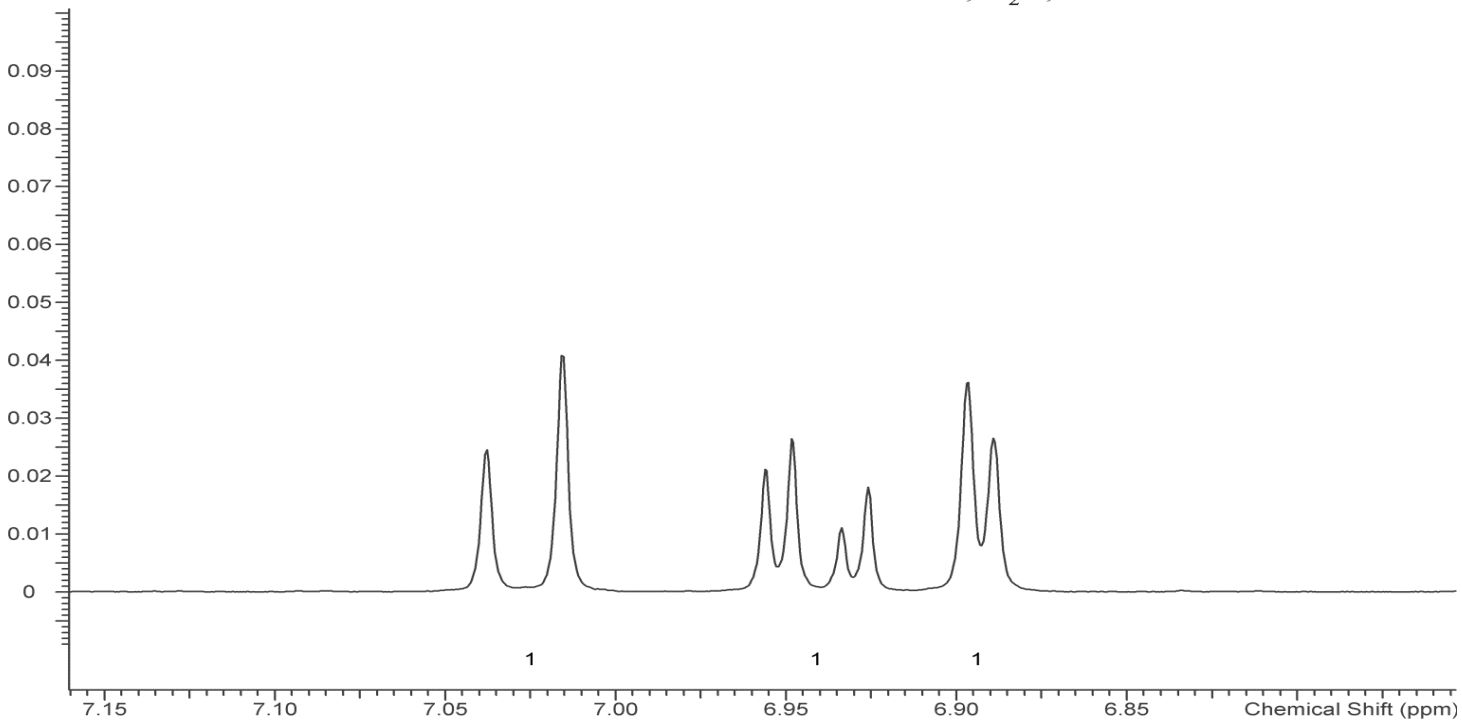
Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

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

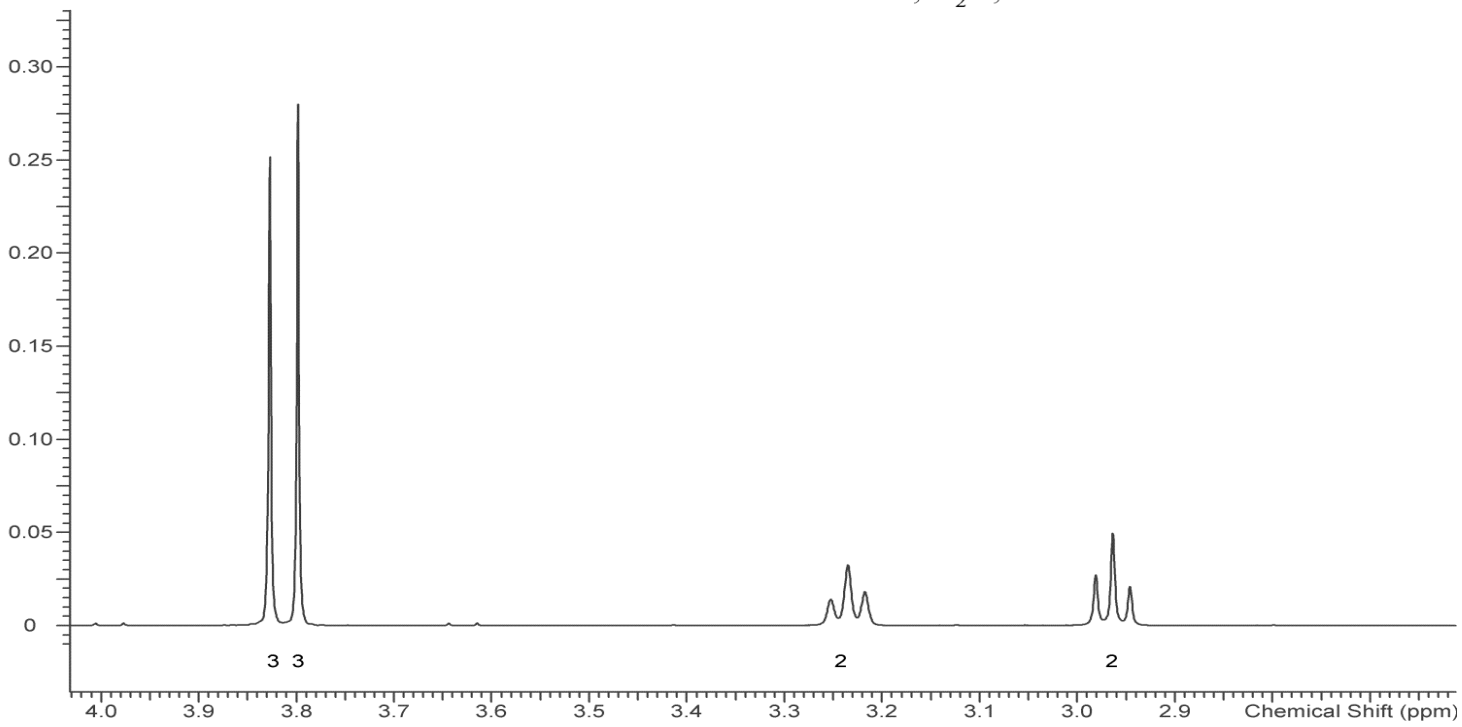
1H NMR: 2C-H HCl Lot # MP137-139, D_2O, 400MHz



1H NMR: 2C-H HCl Lot # MP137-139, D_2O, 400MHz



1H NMR: 2C-H HCl Lot # MP137-139, D_2O, 400MHz

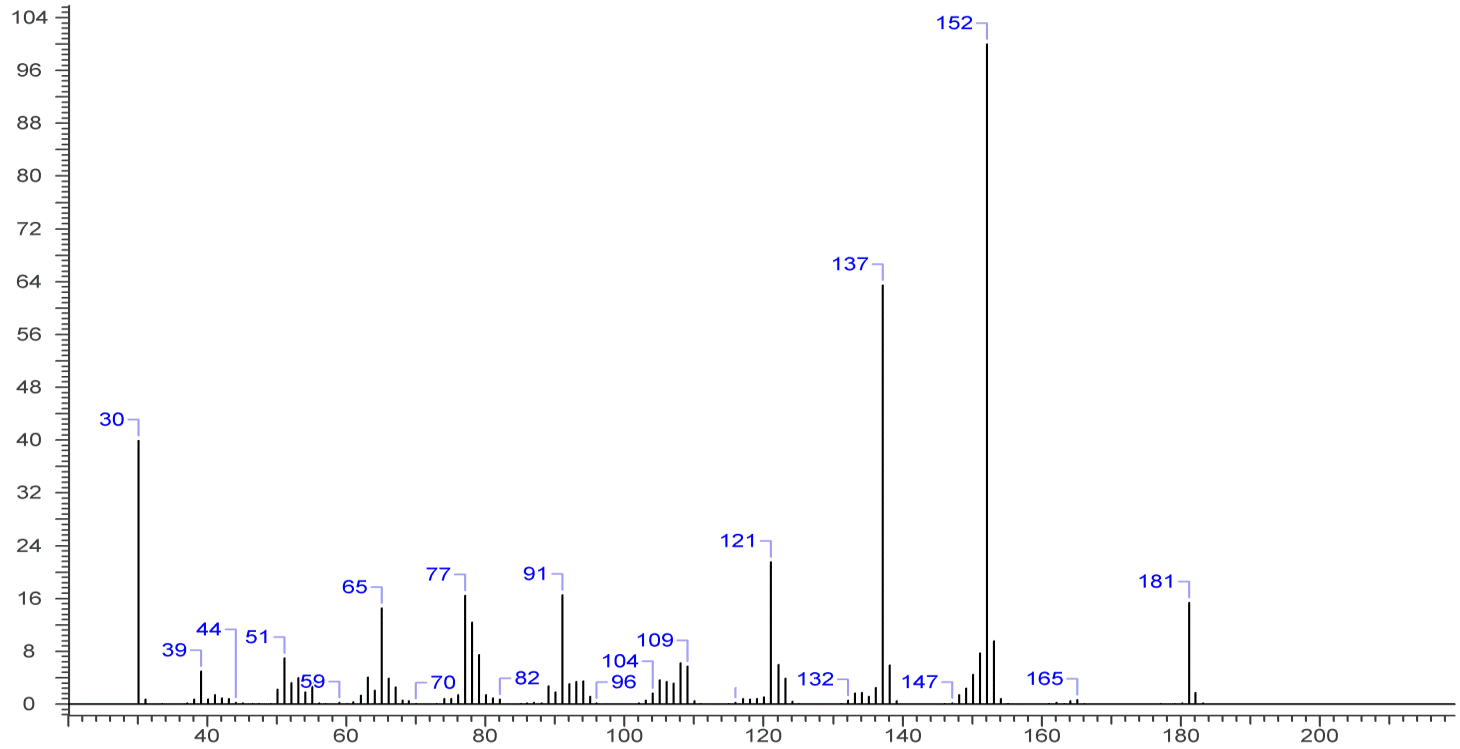


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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 0.25mm x 0.25µm
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:	8.036 minutes

EI Mass Spectrum: 2C-H HCl Lot # MP137-139

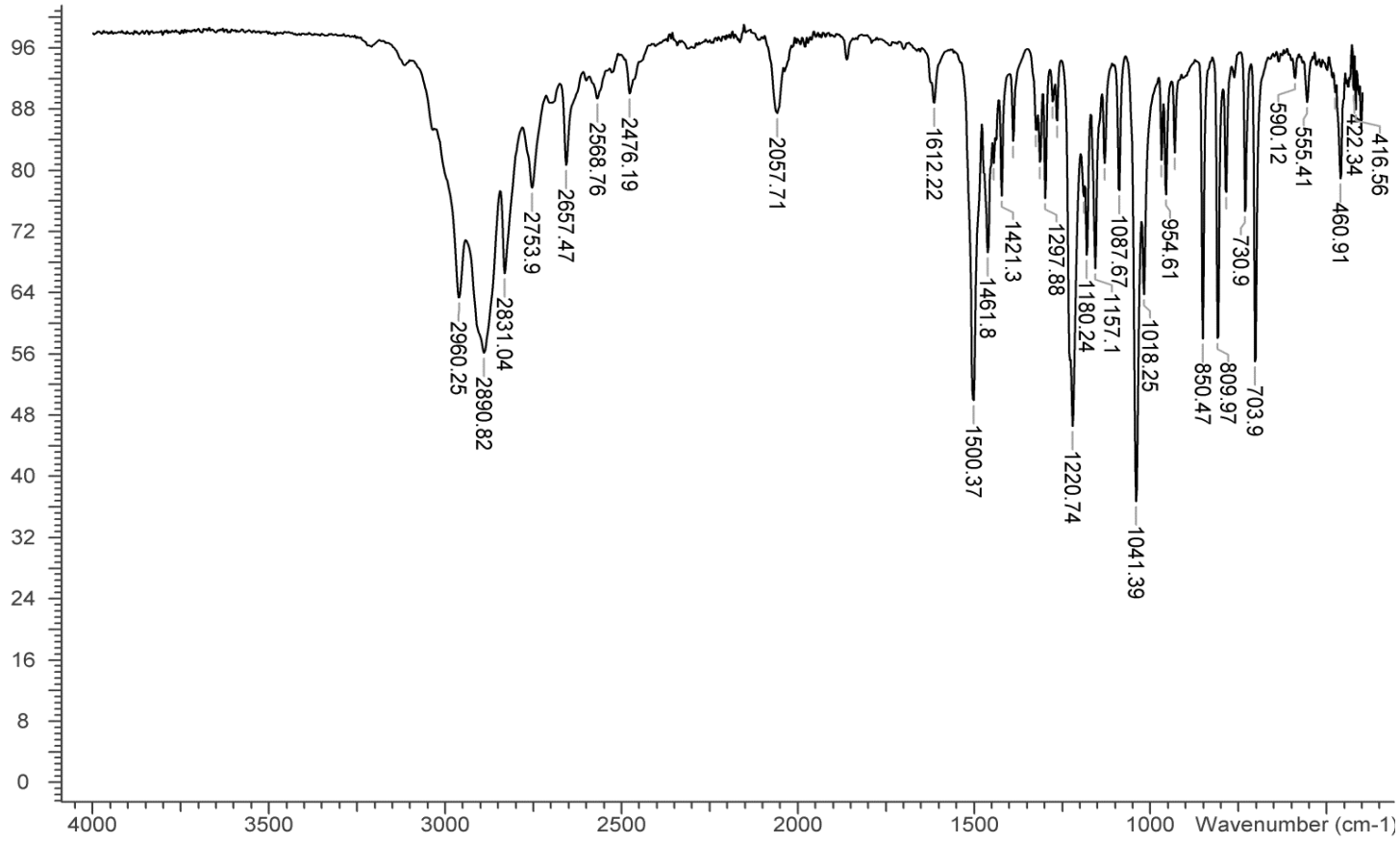


3.3 INFRARED SPECTROSCOPY (FTIR)

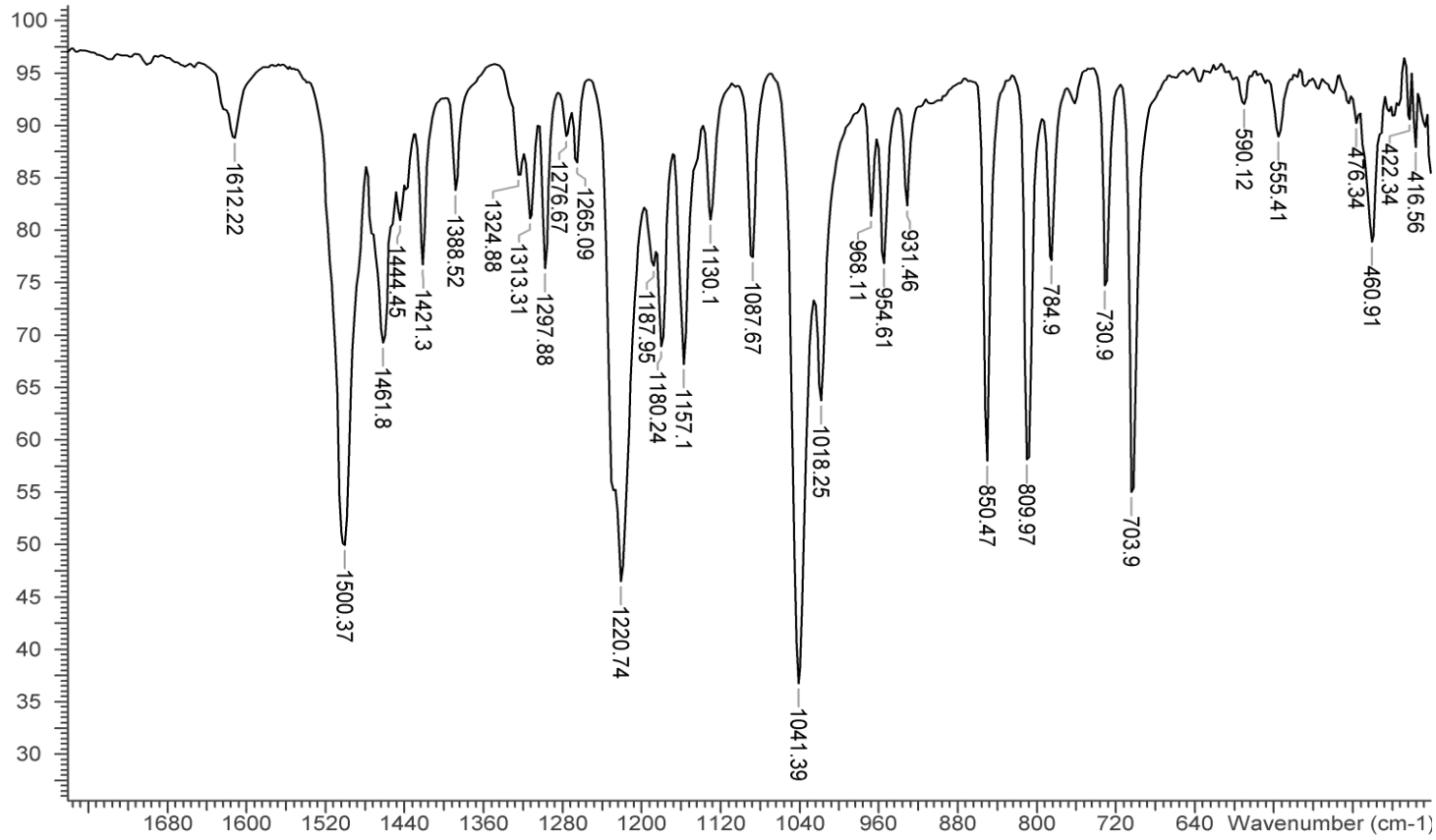
Instrument: FTIR with diamond ATR attachment (3 bounce)

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-H HCl Lot # MP137-139



FTIR ATR (Diamond, 3 Bounce): 2C-H HCl Lot # MP137-139



4. ADDITIONAL RESOURCES

Forendex

Wikipedia