

1. GENERAL INFORMATION

IUPAC Name:	2-(2,5-dimethoxyphenyl)ethanamine
CFR:	Schedule I
CAS #:	3600-86-0
Synonyms:	2,5-dimethoxyphenethylamine
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Kovat's 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 · HCl	217	138.9

3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

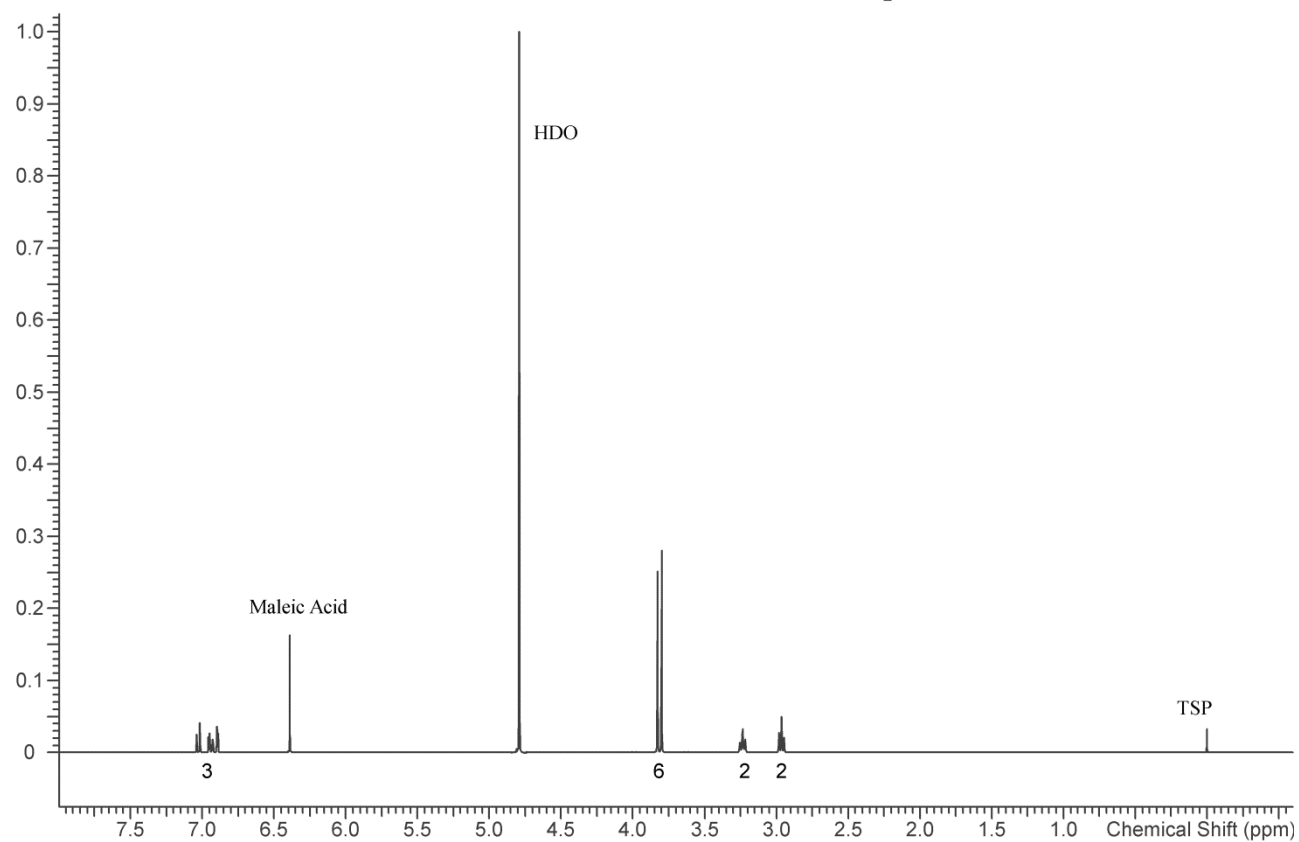
Method NMR D₂O

Sample Preparation: Dilute analyte to ~20 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

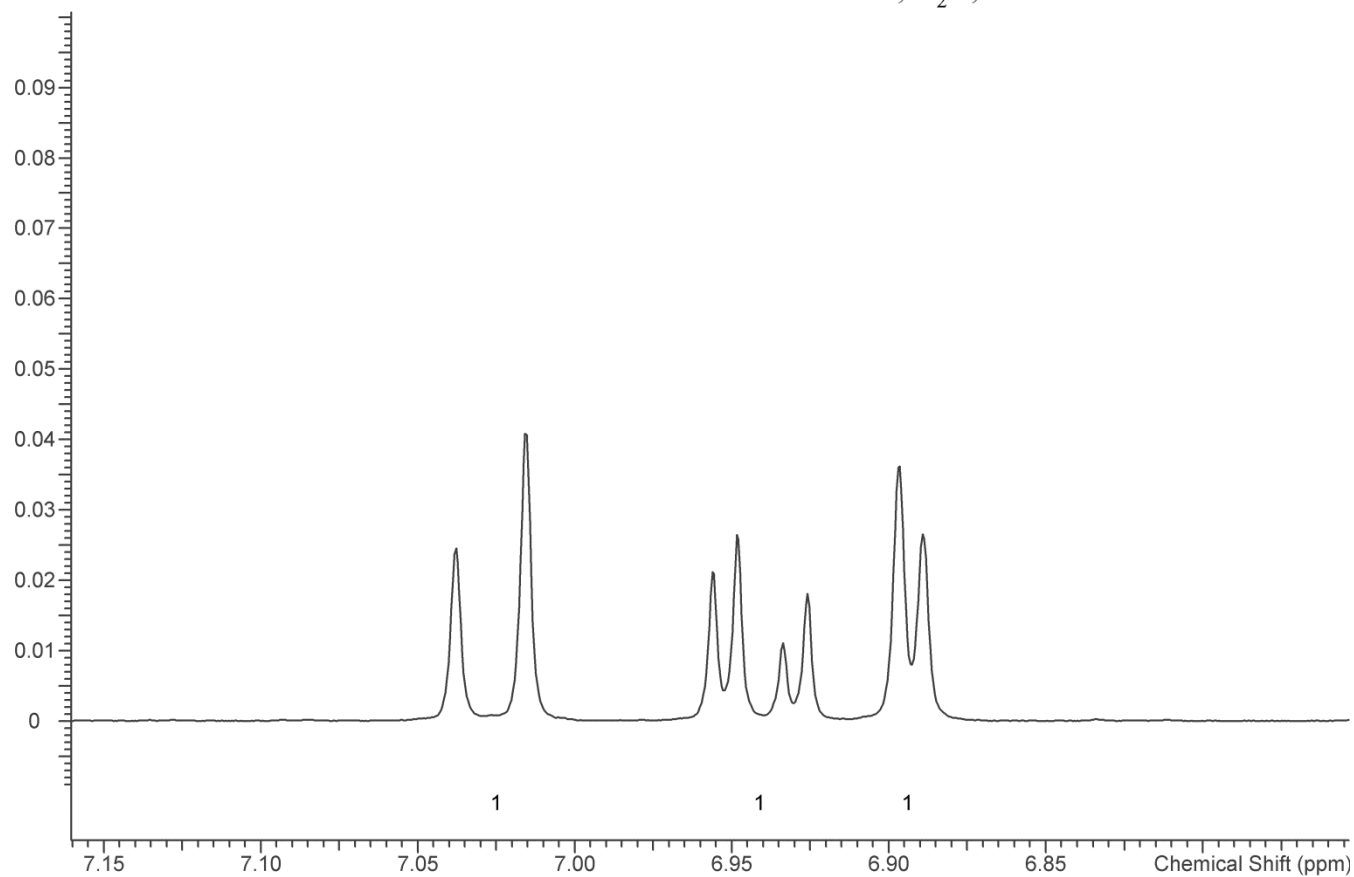
Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

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

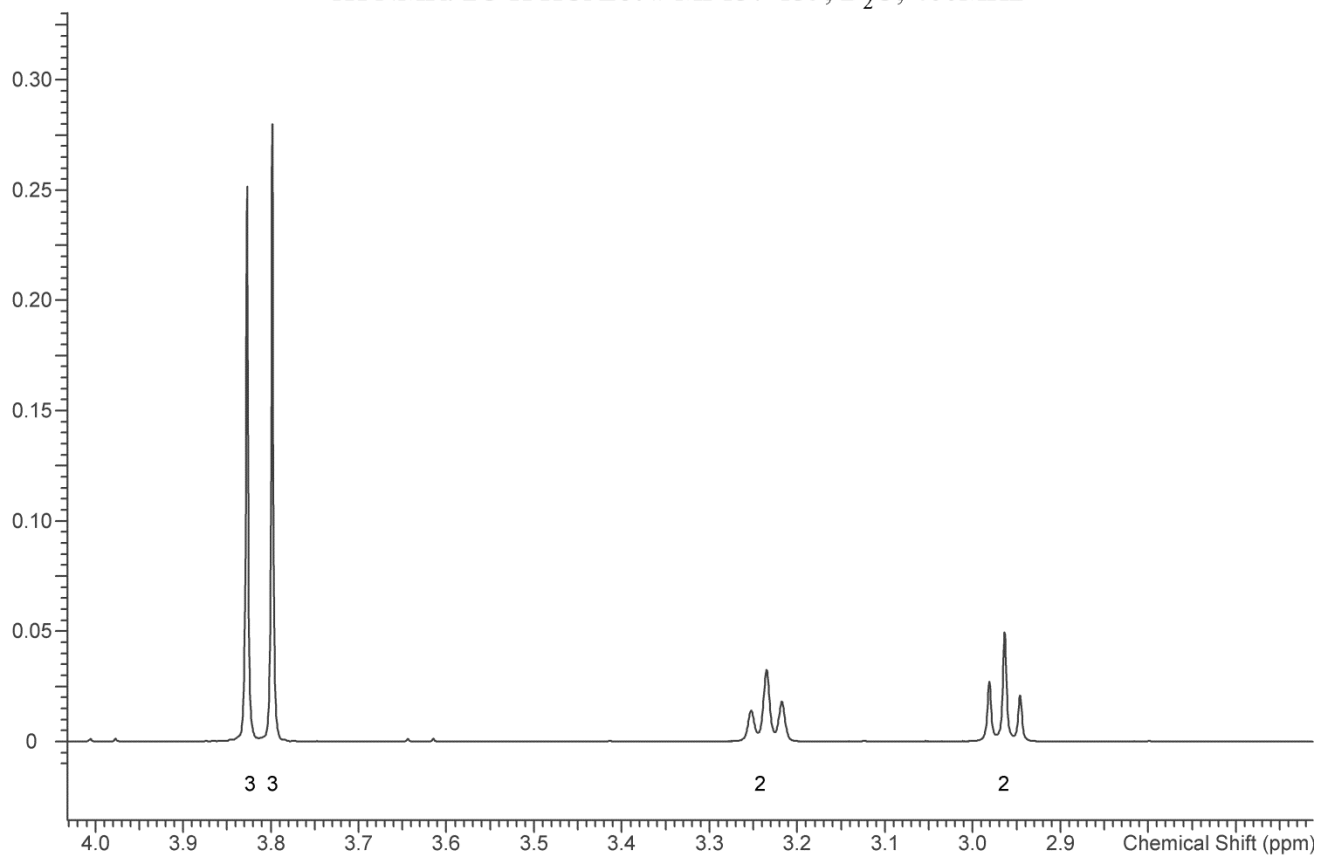
1H NMR: 2C-H HCl Lot # MP137-139, D₂O, 400MHz



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4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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

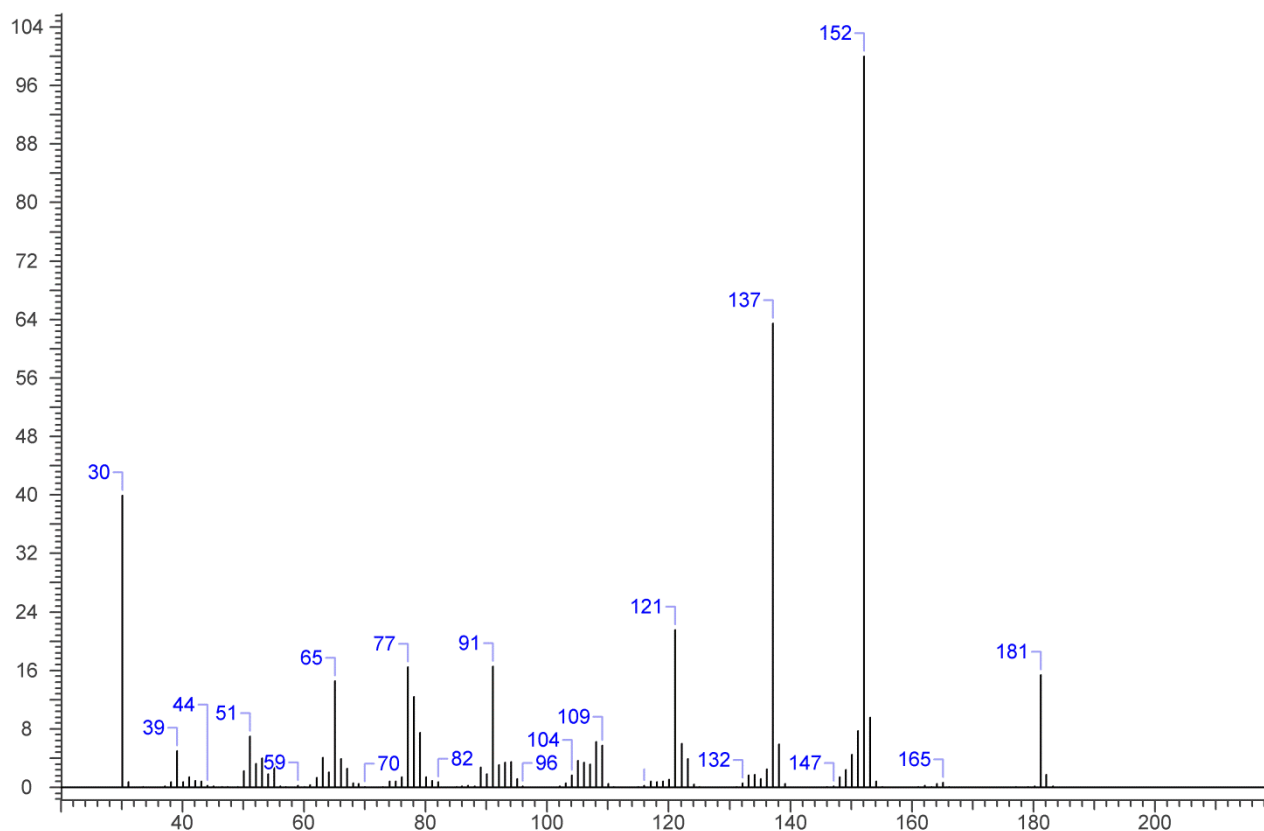
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 8.036 min

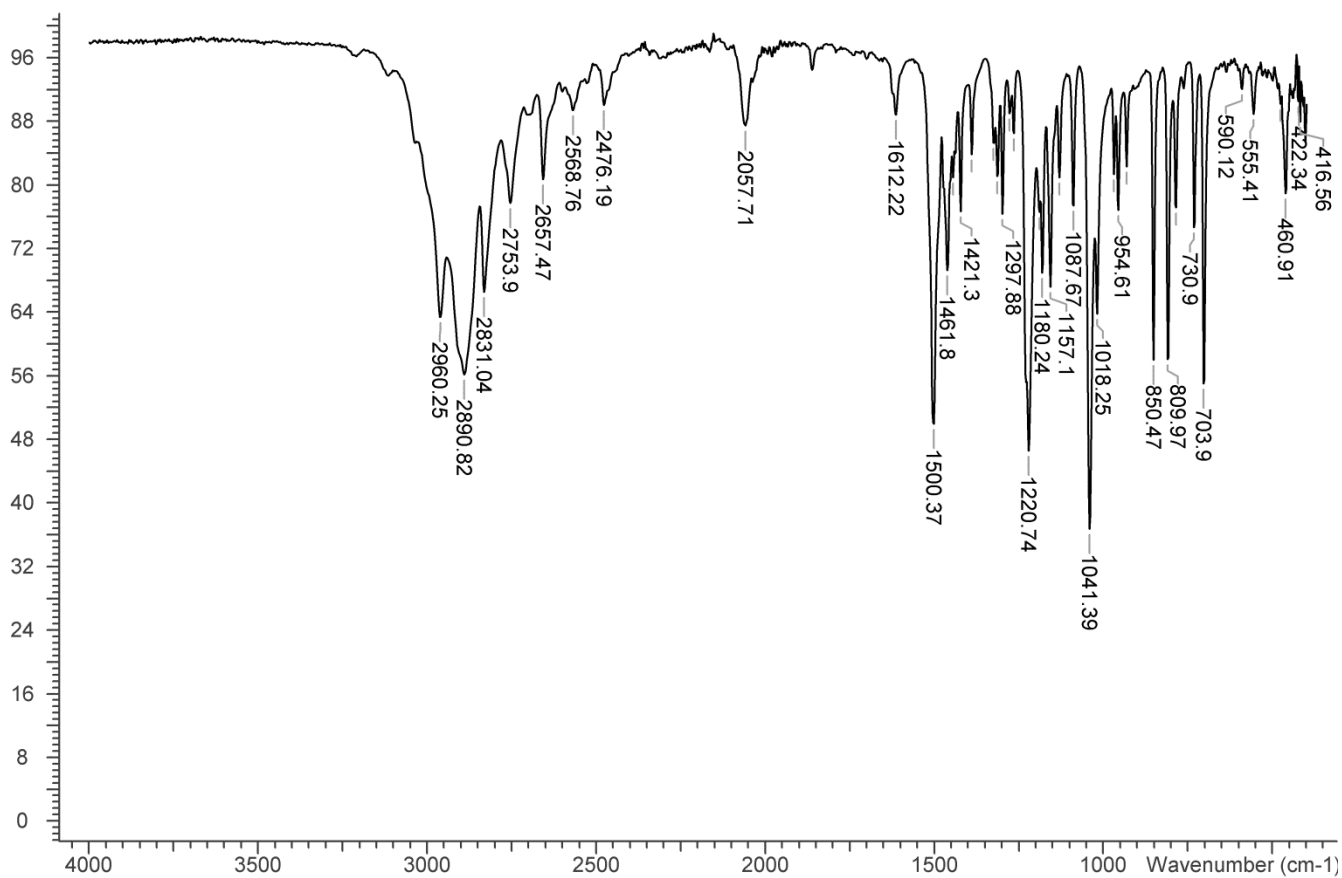
EI Mass Spectrum: 2C-H HCl Lot # MP137-139



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-H HCl Lot # MP137-139



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

