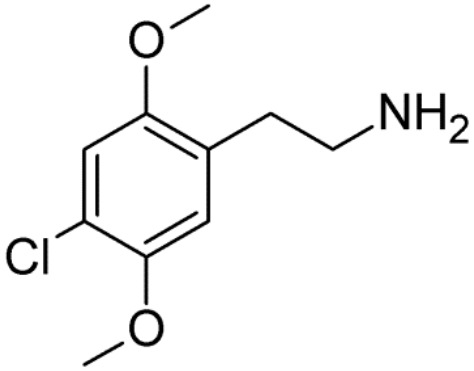
2C-C

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

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

CAS #: 88441-14-9 (Base)

Synonyms: 2,5-dimethoxy-4-chlorophenethylamine
4-chloro-2,5-dimethoxy-benzeneethanamine
1-(4-chloro-2,5-dimethoxyphenyl)-2-aminoethane
2-(4-chloranyl-2,5-dimethoxy-phenyl)ethanamine
2-(4-chloro-2,5-dimethoxy-phenyl)ethylamine

Source: DEA Reference Material Collection

Appearance: Beige powder (HCl)

UV_{max}: 248.7, 294.2

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{10}H_{14}ClNO_2$	215	Not Determined
HCl	$C_{10}H_{14}ClNO_2 \cdot HCl$	252	223.3

3. QUALITATIVE DATA

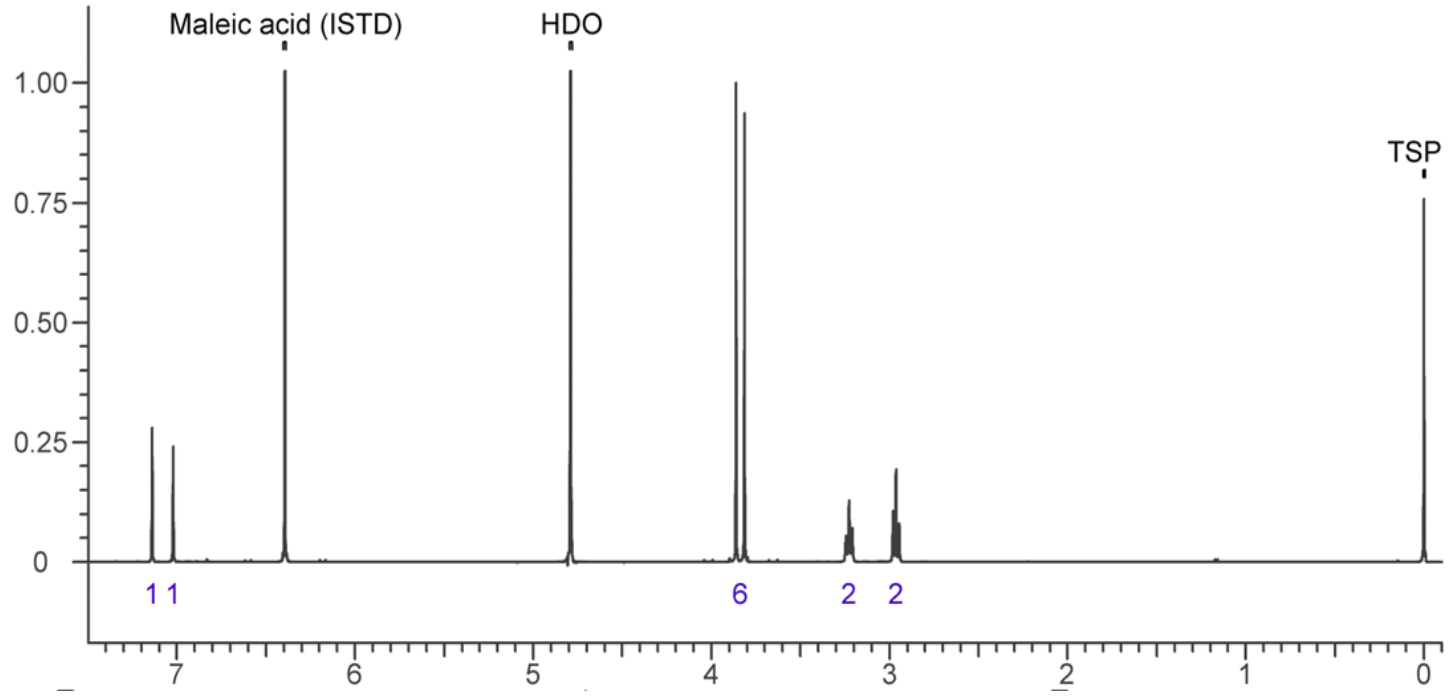
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

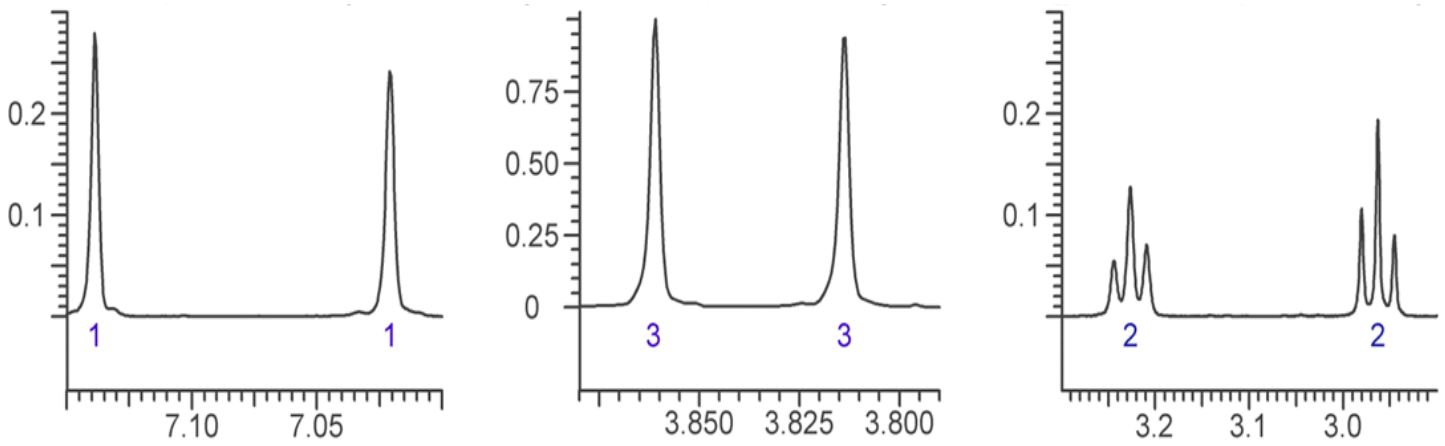
Sample Preparation: Dilute analyte to ~10 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

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

^{1}H NMR: 2C-C HCl; lot H-0408, D_2O, 400 MHz



^{1}H NMR: 2C-C HCl; lot H-0408, D_2O, 400 MHz

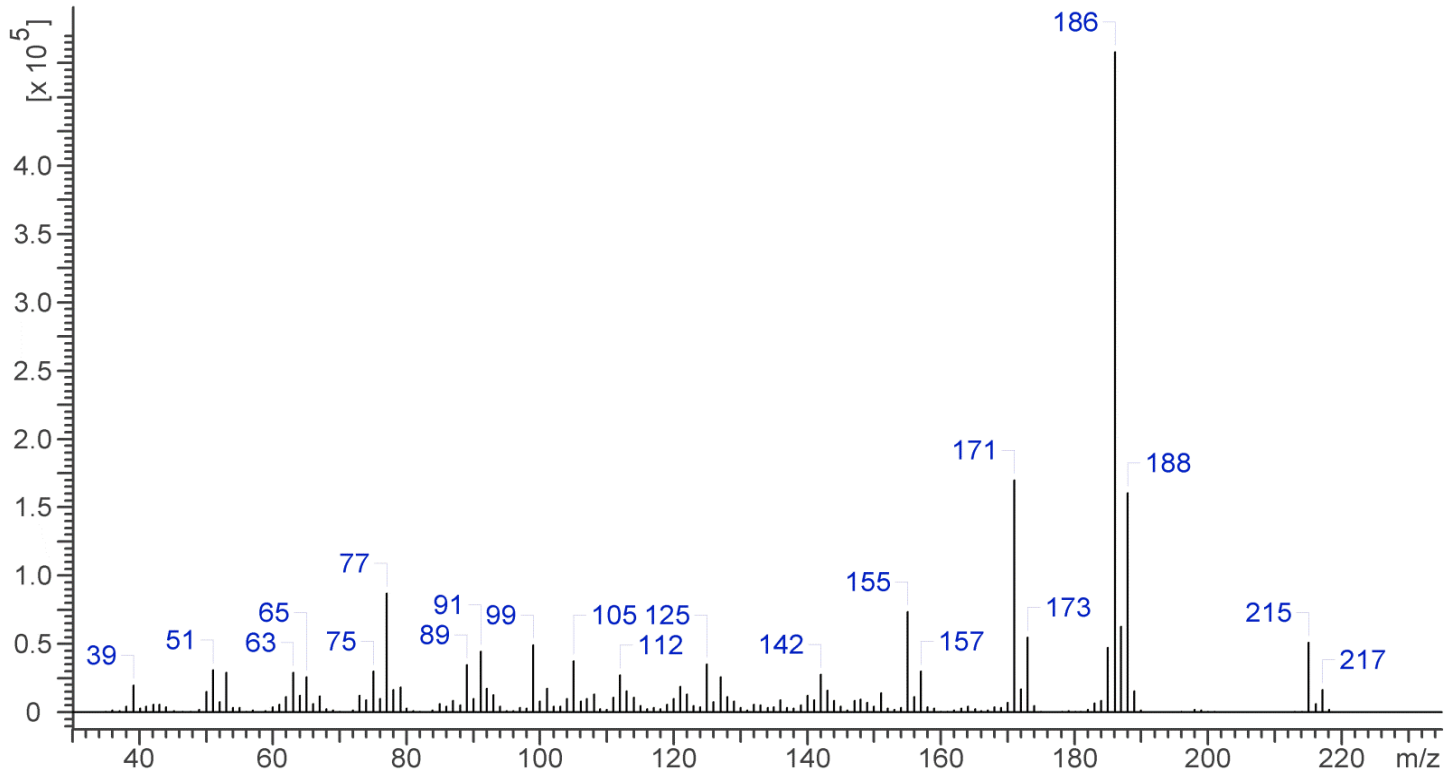


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 1 mg/mL base extracted into chloroform.

Instrument:	Gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 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 = 25:1, 1 µL injected
MS Parameters:	Mass scan range: 34-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	9.847 minutes

EI Mass Spectrum: 2C-C, Lot H-0408



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

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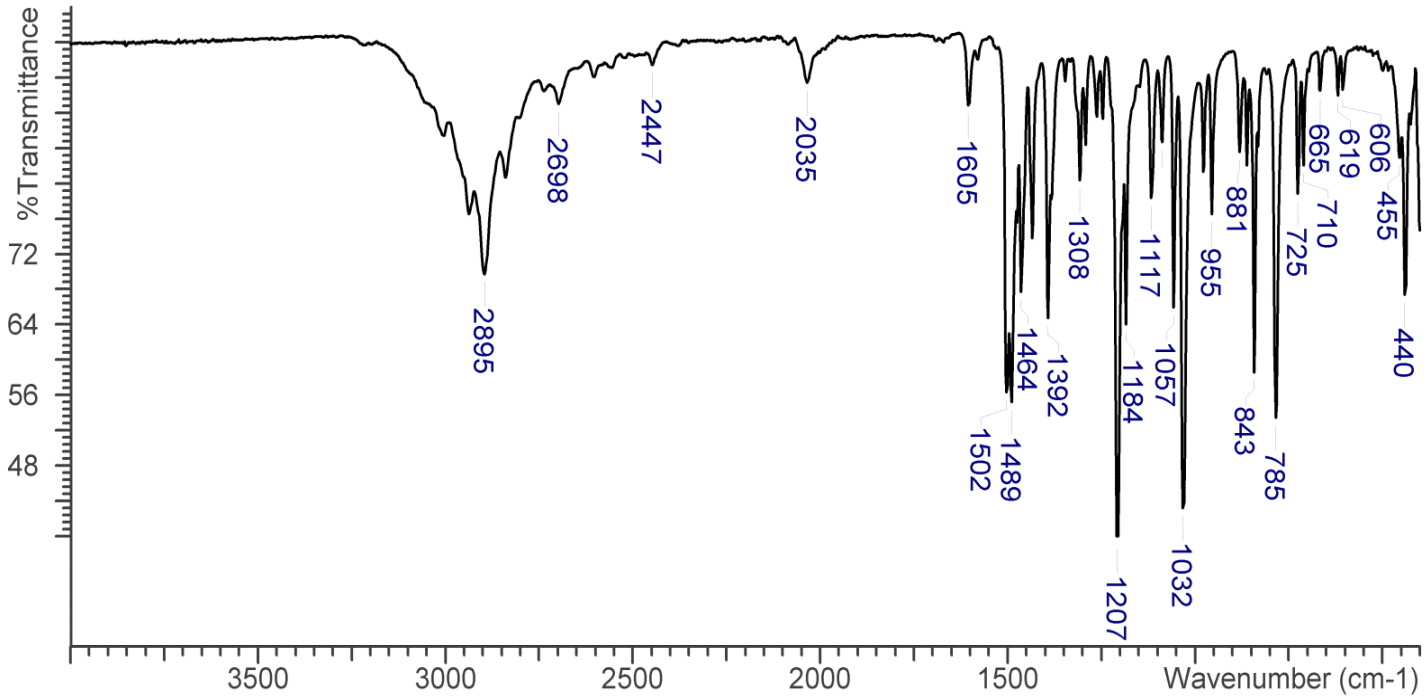
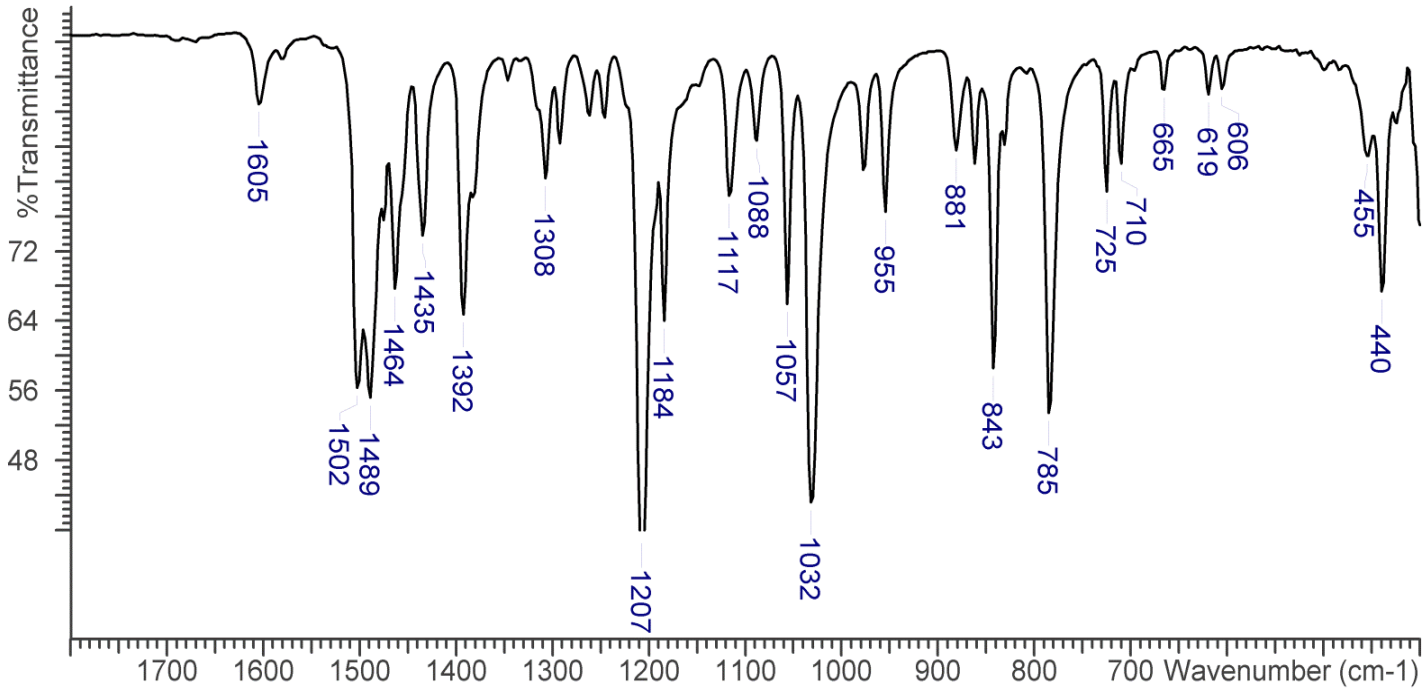
FTIR ATR (Diamond, 3 bounce): 2C-C HCl; lot H-0408



FTIR ATR (Diamond, 3 bounce): 2C-C HCl; lot H-0408



4. ADDITIONAL RESOURCES

Forendex

Wikipedia