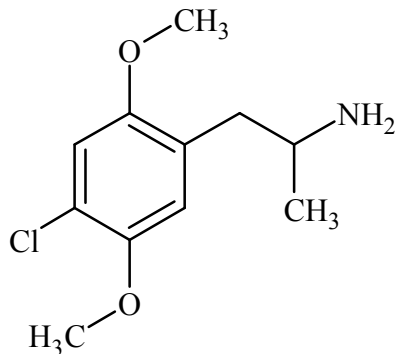




4-Chloro-2,5-Dimethoxyamphetamine

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



1. GENERAL INFORMATION

IUPAC Name:	1-(4-chloro-2,5-dimethoxyphenyl)propan-2-amine
CAS#:	123431-31-2 (base), 42203-77-0 (HCl)
Synonyms:	DOC, 4-Cl-2,5-DMA, 2,5-dimethoxy-4-chloroamphetamine
Source:	DEA Reference Material Collection
Appearance:	White powder
UV_{max} (nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₁ H ₁₆ ClNO ₂	229	Not Determined
HCl	C ₁₁ H ₁₆ ClNO ₂ · HCl	266	194.6



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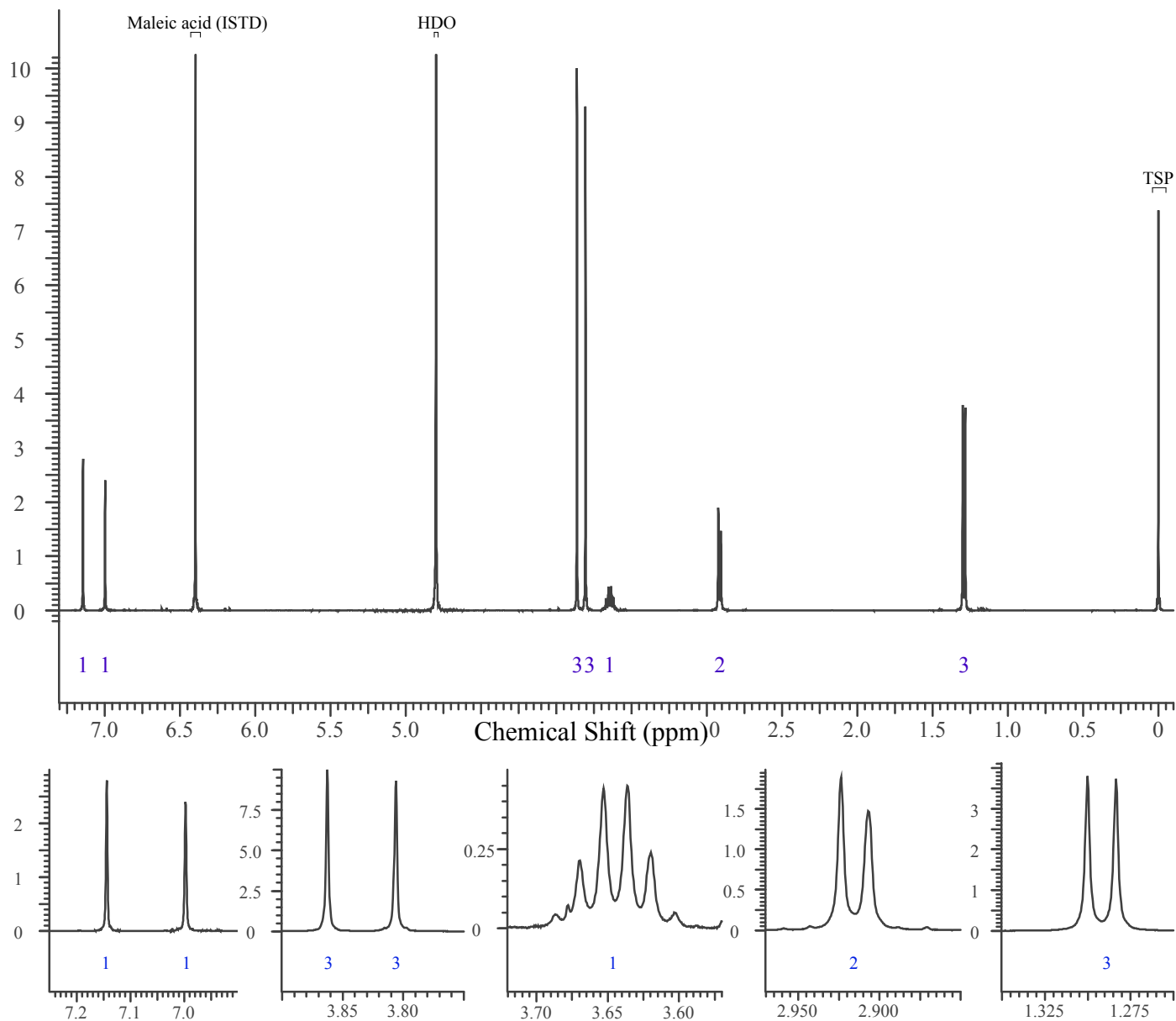
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterium oxide (D₂O) containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

¹H NMR: 4-Chloro-2,5-dimethoxyamphetamine HCl; Lot MP193-194; D₂O; 400 MHz





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3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 mg/mL base extracted into chloroform

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m

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 μ L injected

MS Parameters: Mass scan range: 34-550 amu

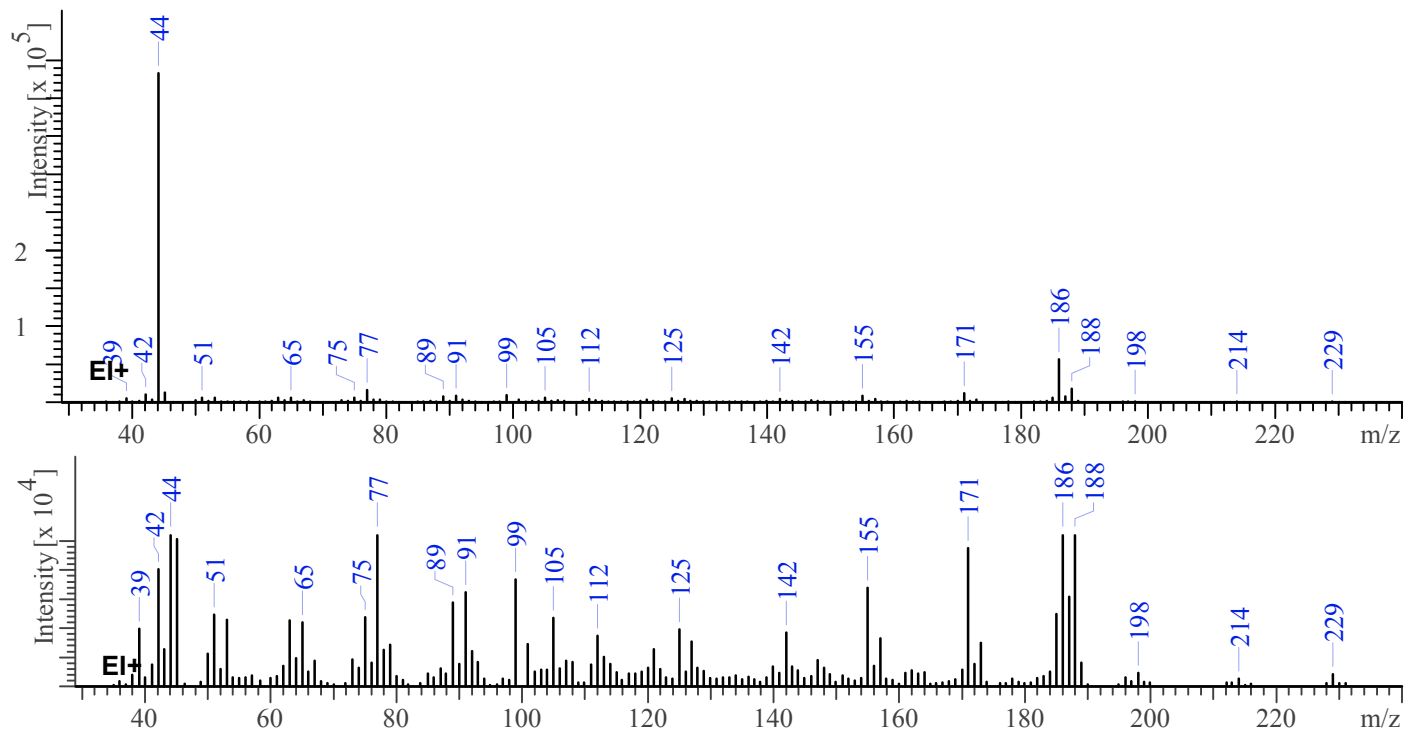
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 9.420 min

EI Mass Spectrum: 4-Chloro-2,5-dimethoxyamphetamine HCl; Lot MP193-194





4-Chloro-2,5-Dimethoxyamphetamine

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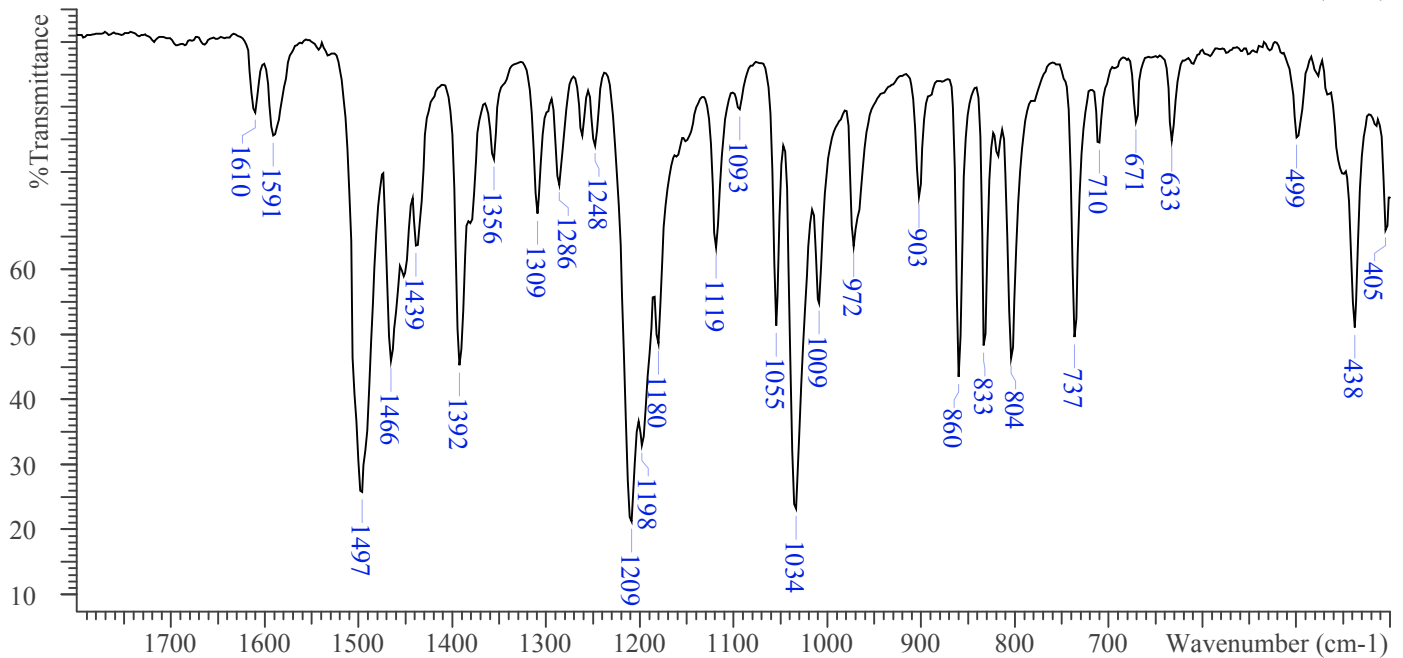
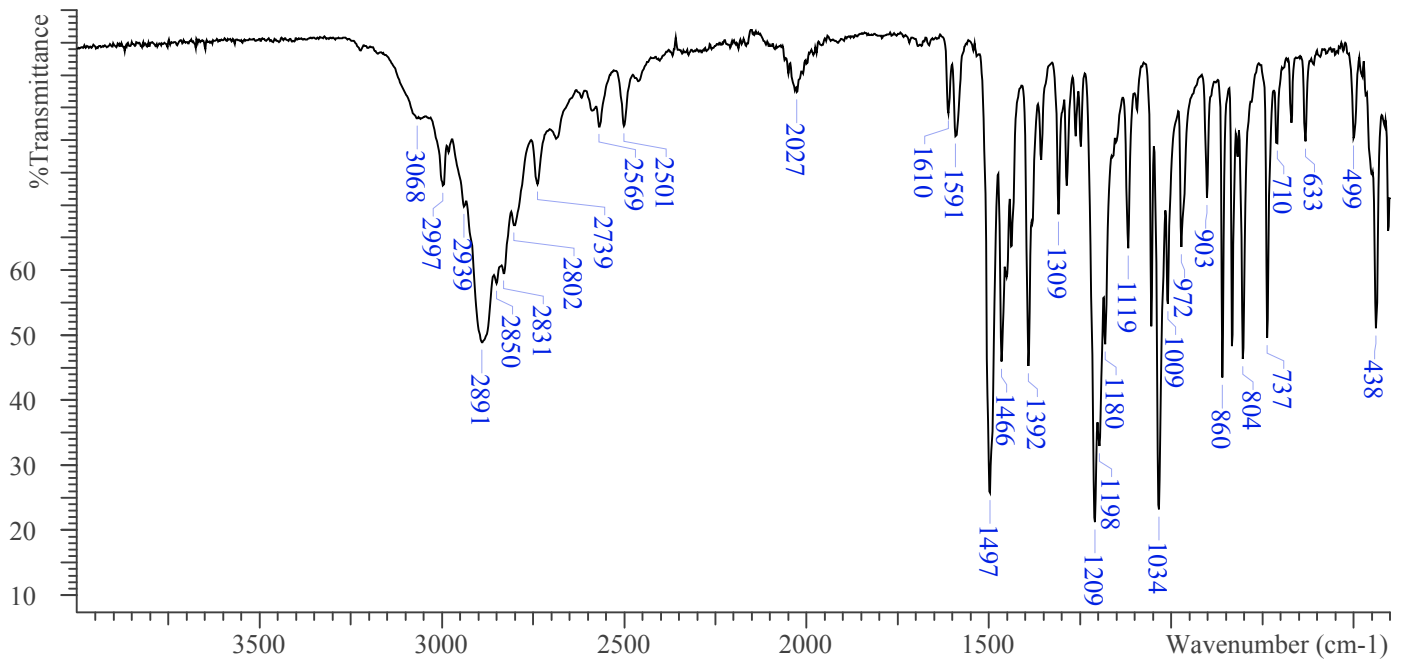


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 4-Chloro-2,5-dimethoxyamphetamine HCl; Lot MP193-194





4-Chloro-2,5-Dimethoxyamphetamine

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4. **ADDITIONAL RESOURCES**

[Forendex](#)

[Wikipedia](#)