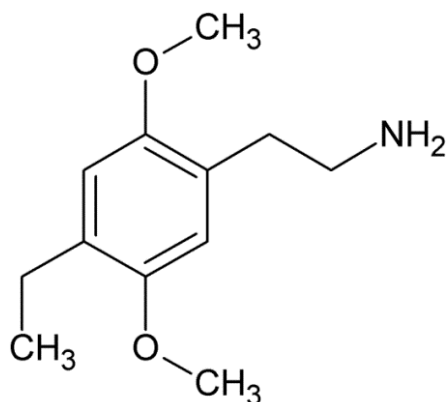




## 2C-E



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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	2-(4-ethyl-2,5-dimethoxyphenyl)ethanamine
<b>CAS #:</b>	71539-34-9 (Base)
<b>Synonyms:</b>	2,5-dimethoxy-4-ethylphenethylamine 2-(2,5-dimethoxy-4-ethylphenyl)ethanamine 1-(2,5-dimethoxy-4-ethylphenyl)-2-aminoethane
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder (HCl)
<b>UV<sub>max</sub>:</b>	289.3

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>12</sub> H <sub>19</sub> NO <sub>2</sub>	209	Not Determined
HCl	C <sub>12</sub> H <sub>19</sub> NO <sub>2</sub> · HCl	245	210.0



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### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

##### Method NMR D<sub>2</sub>O

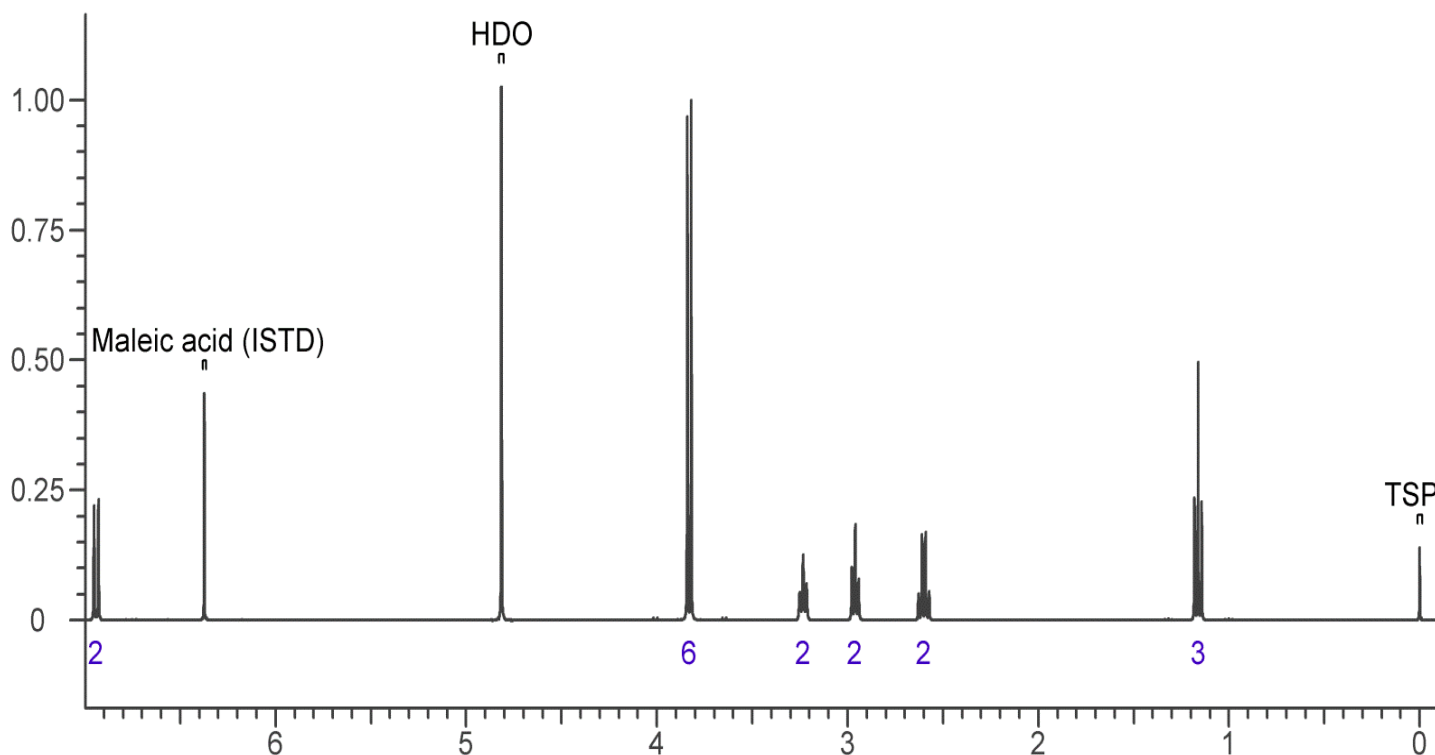
**Sample Preparation:** Dilute analyte to ~10 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

**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

<sup>1</sup>H NMR: 2C-E HCl; Lot H0407, D<sub>2</sub>O, 400 MHz



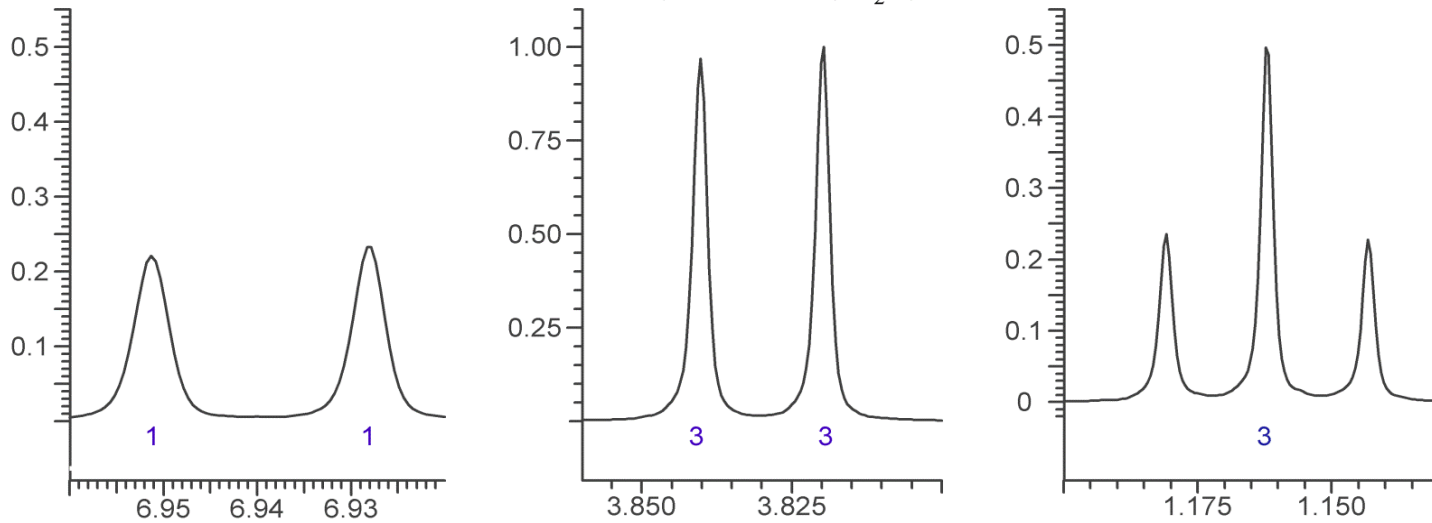


## 2C-E

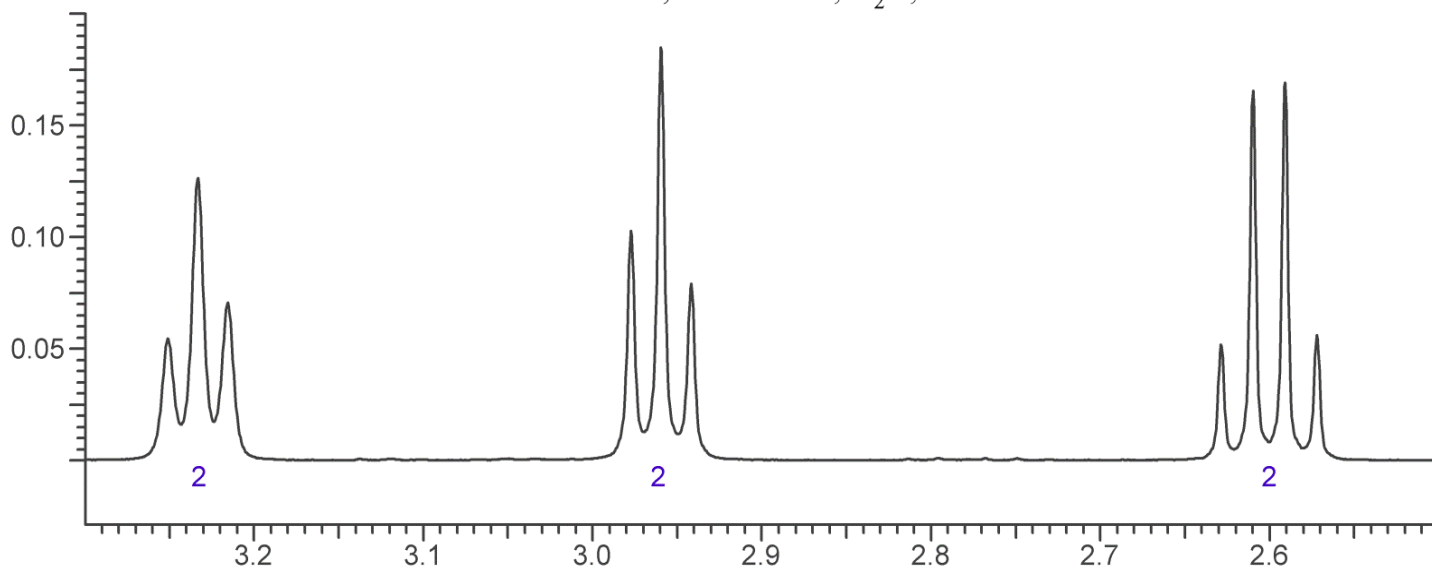
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$^1\text{H}$  NMR: 2C-E HCl; Lot H0407,  $\text{D}_2\text{O}$ , 400 MHz



$^1\text{H}$  NMR: 2C-E HCl; Lot H0407,  $\text{D}_2\text{O}$ , 400 MHz





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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte to ~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 0.25 $\mu$ 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  $\mu$ L injected

**MS Parameters:** Mass scan range: 30-550 amu

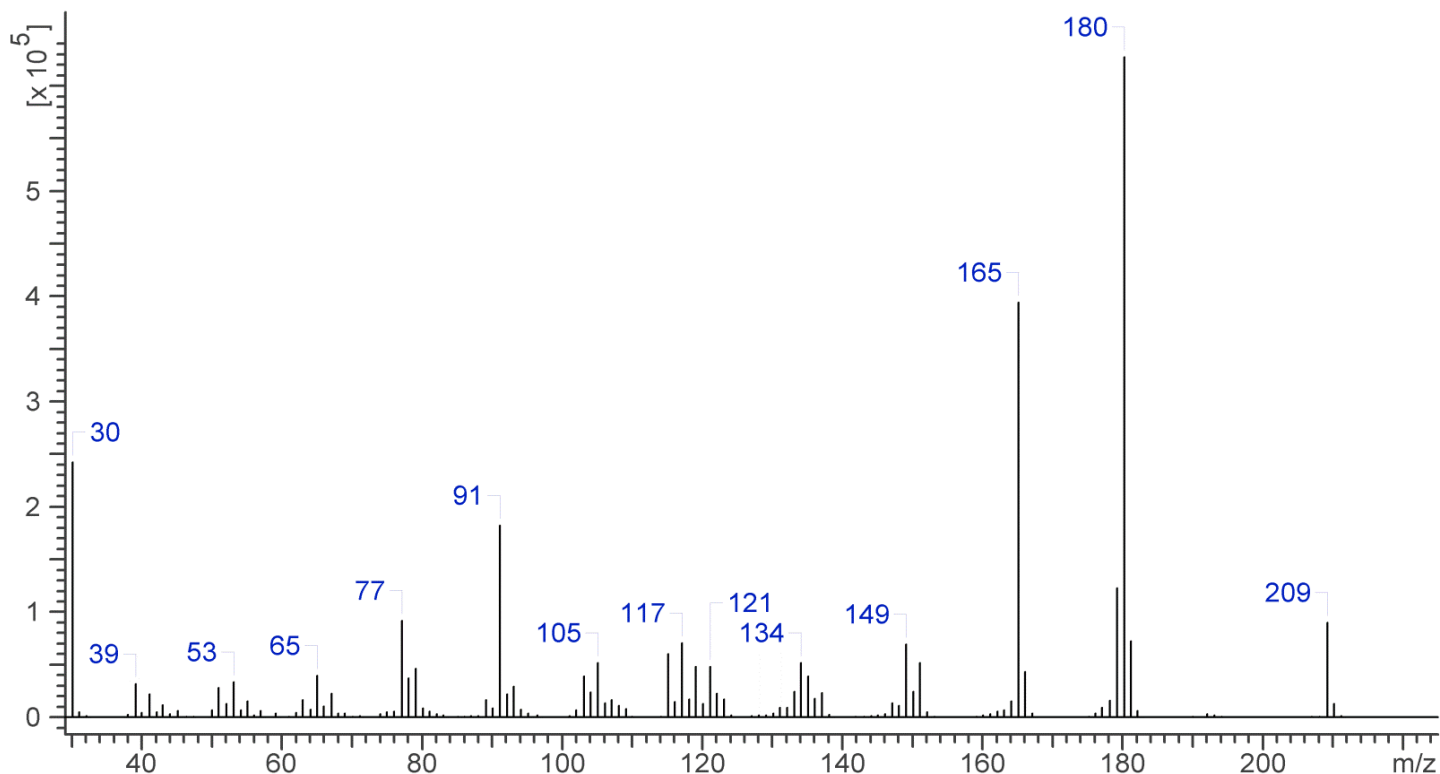
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 9.223 minutes

EI Mass Spectrum: 2C-E HCl, Lot H0407





## 2C-E

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### 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**

Number of scans: 32

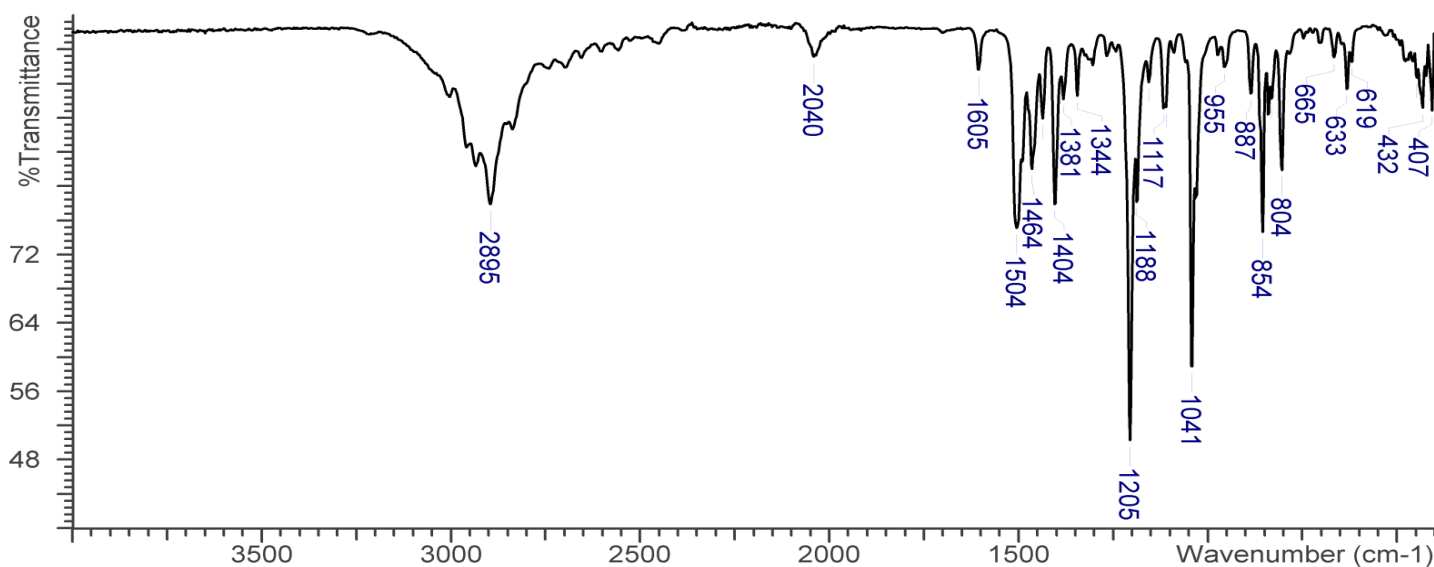
Number of background scans: 32

Resolution:  $4\text{cm}^{-1}$

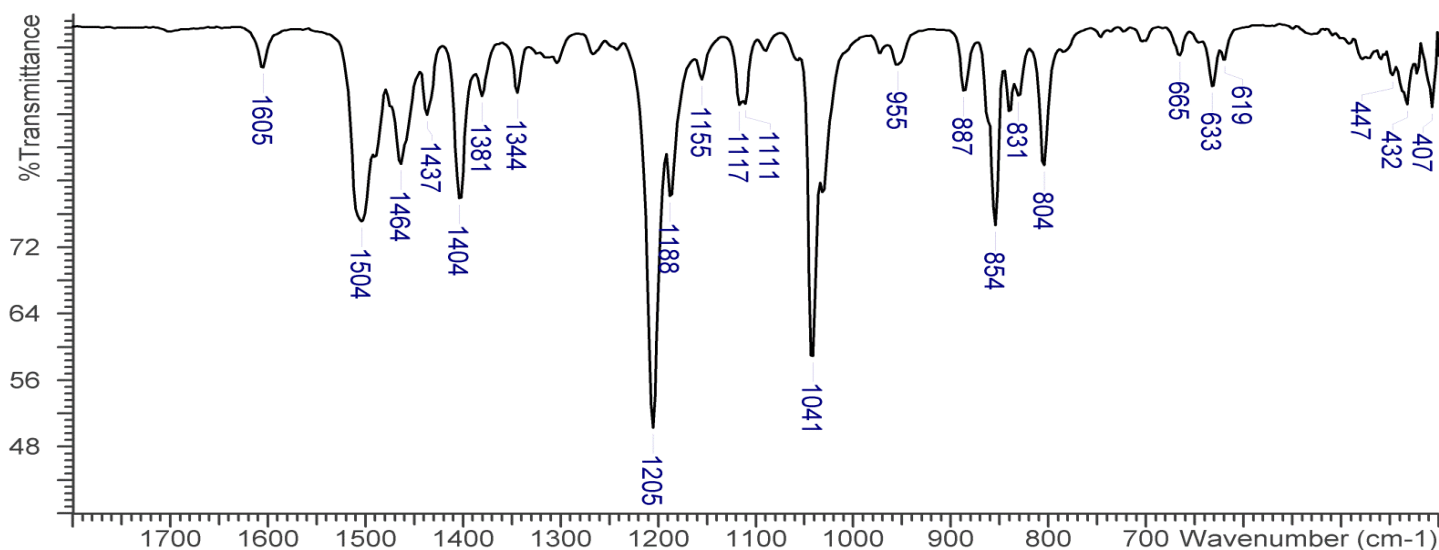
Sample gain: 8

Aperture: 150

FTIR ATR (Diamond, 3 bounce): 2C-E HCl, Lot H0407



FTIR ATR (Diamond, 3 bounce): 2C-E HCl, Lot H0407





## 2C-E

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#### **4. ADDITIONAL RESOURCES**

[Forendex](#)

[Wikipedia](#)