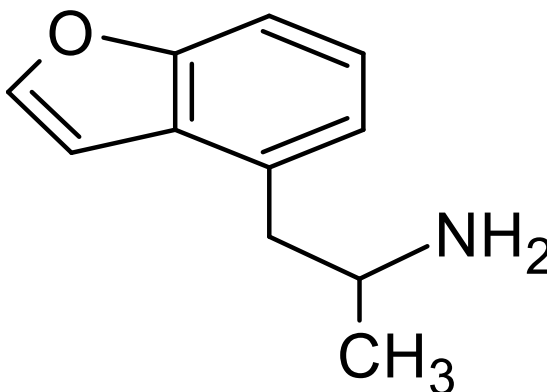




4-APB

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



1. GENERAL INFORMATION

IUPAC Name: 1-(1-benzofuran-4-yl)propan-2-amine

CAS#: Not Available

Synonyms: 4-(2-aminopropyl)benzofuran

Source: DEA Reference Material Collection

Appearance: Tan powder (HCl)

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 ₁₃ NO | 175 | Not Determined |
| HCl | C ₁₁ H ₁₃ NO · HCl | 211 | Not Determined |



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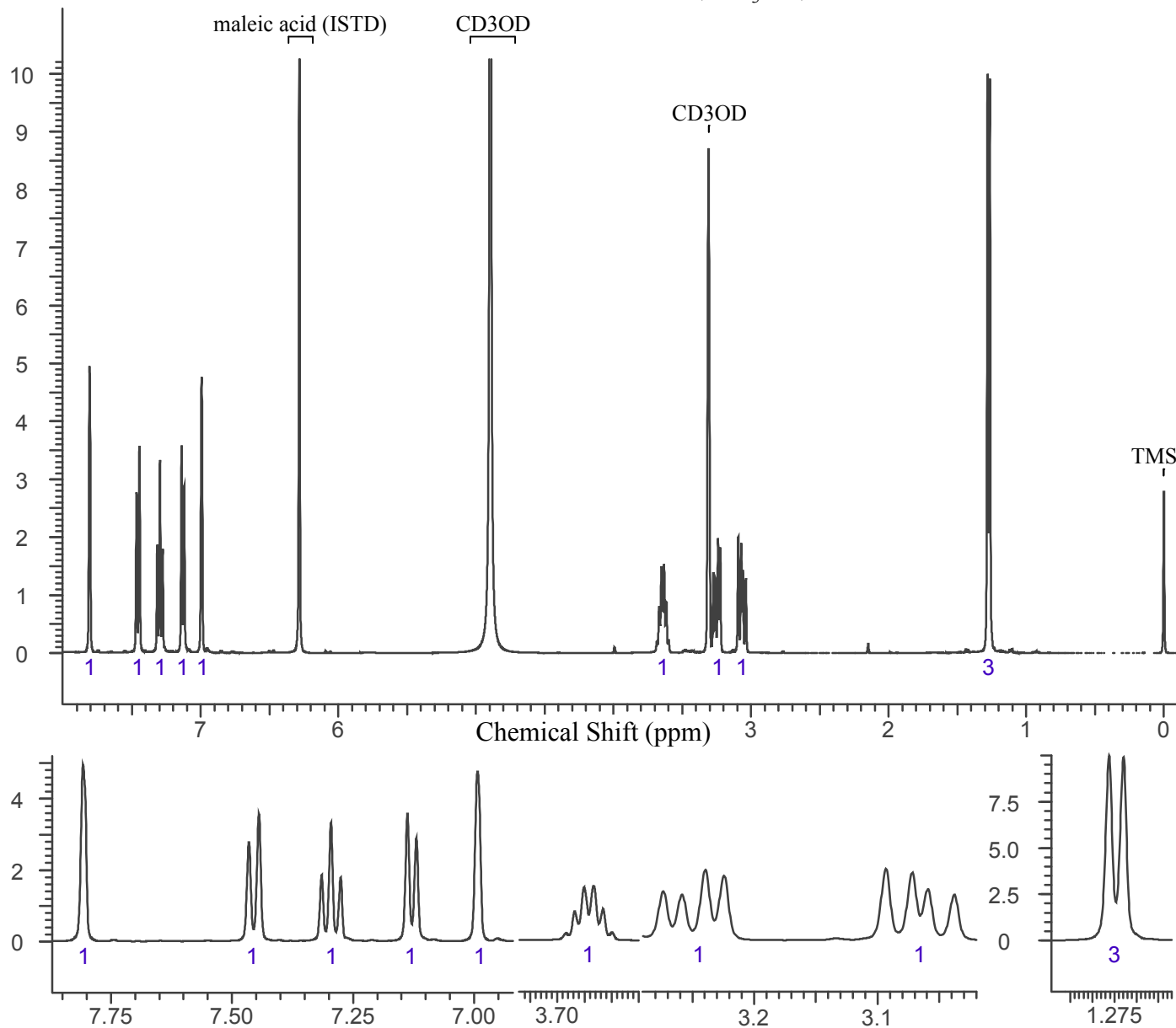
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterated methanol (CD₃OD) containing TMS 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-APB HCl Lot # N17-P87B; CD₃OD; 400MHz





4-APB

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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 = 20:1, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu

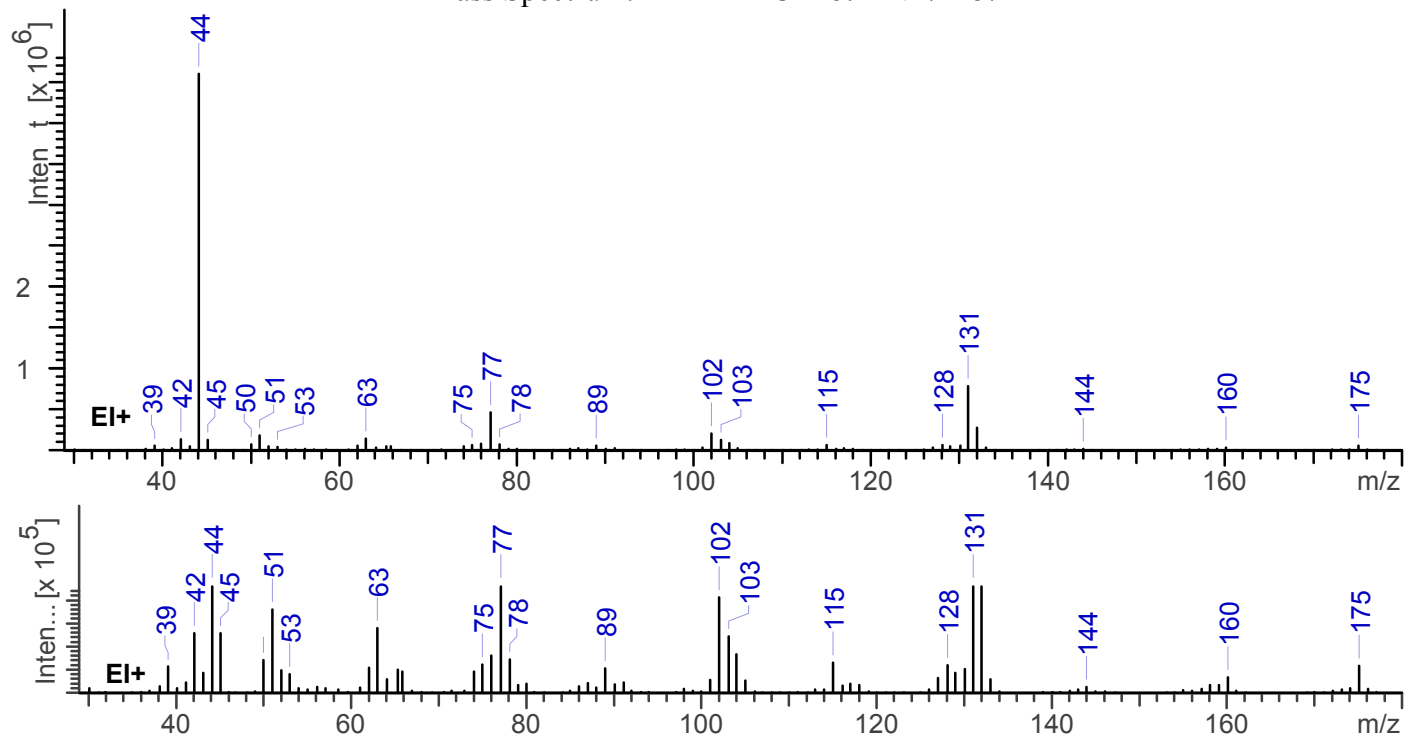
Threshold: 90

Tune file: stune.u

Acquisition mode: scan

Retention Time: 7.018 min

EI Mass Spectrum: 4-APB HCl Lot # N17-P87B





4-APB

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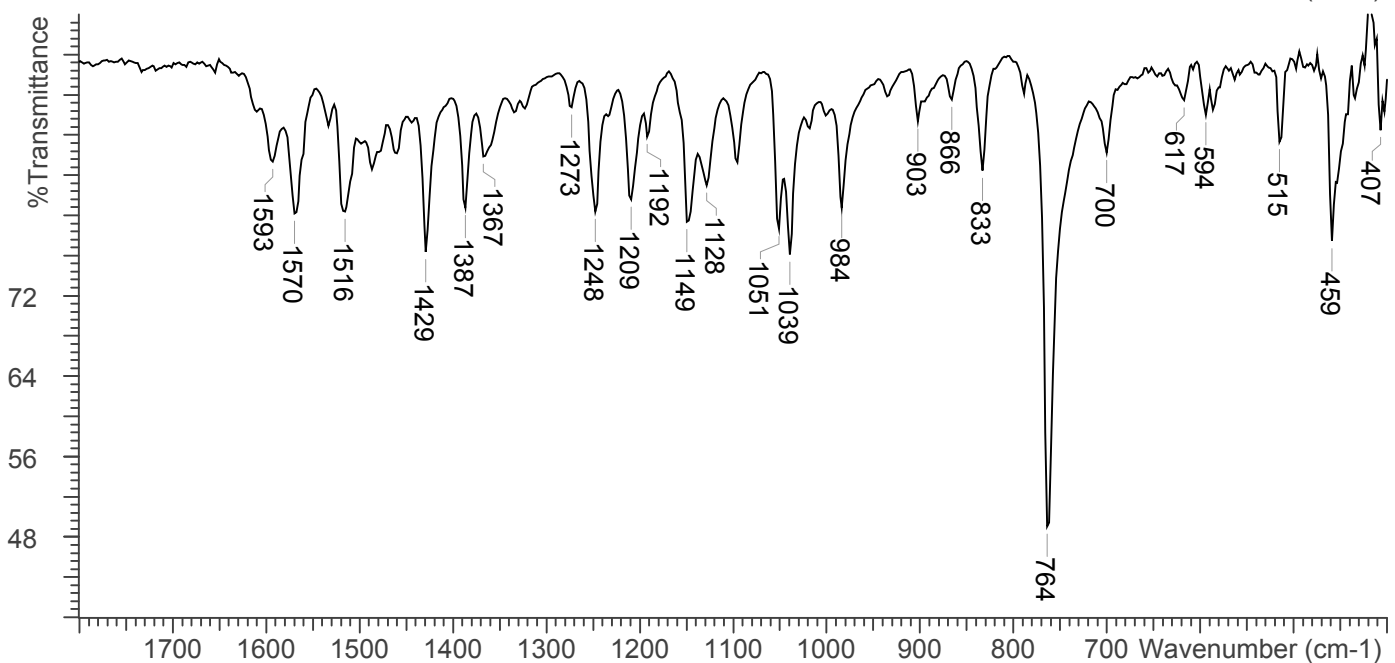
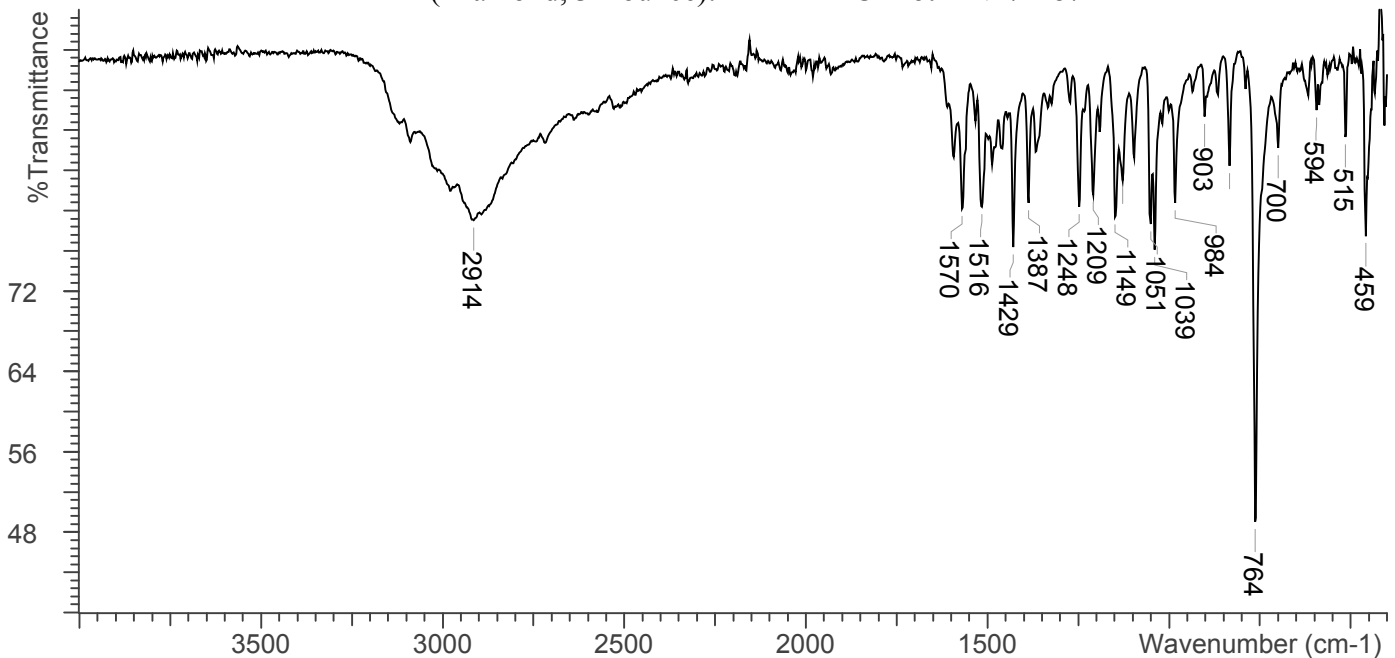


3.3 INFRARED SPECTROSCOPY (FTIR)

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-APB HCl Lot # N17-P87B





4-APB

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4. **ADDITIONAL RESOURCES**

Casale, J. F.; Hays, P. A. The Characterization of 6-(2-Aminopropyl)benzofuran and Differentiation from its 4-, 5-, and 7-Positional Analogues. *Microgram* **2012**, 9(2), 61-74.