

1. GENERAL INFORMATION

IUPAC Name:	1-(1-benzofuran-5-yl)propan-2-amine
CFR:	Not Scheduled (12/2012)
CAS #:	286834-80-8
Synonyms:	5-(2-aminopropyl)benzofuran, alpha-methyl-5-benzofuranethanamine, 1-(benzofuran-5-yl)propan-2-amine, 1-(5-benzofuranyl)-2-propanamine, [2-(benzofuran-5-yl)-1-methyl-ethyl]amine
Source:	DEA Reference Material Collection
Appearance:	White powder
Kovat's Index:	Pending
UVmax:	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

3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

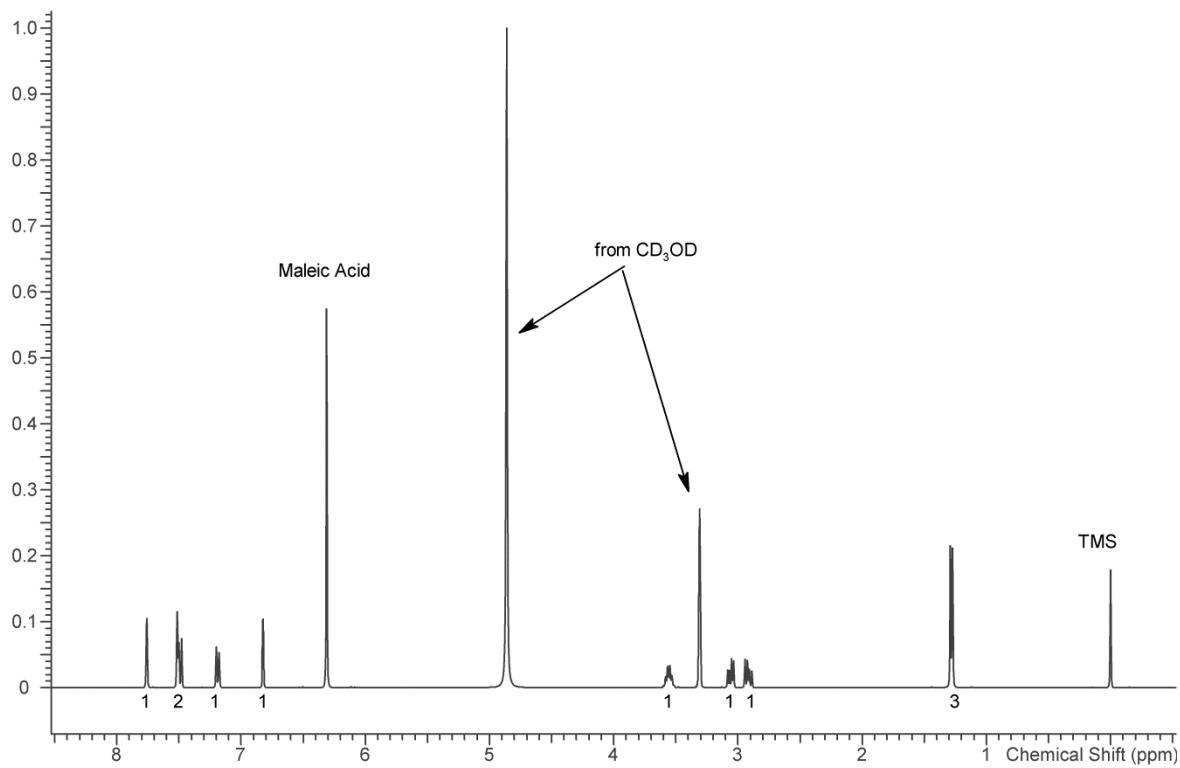
Method NMR CD₃OD

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated methanol (CD₃OD) containing TMS for 0 ppm reference and maleic acid as quantitative internal standard.

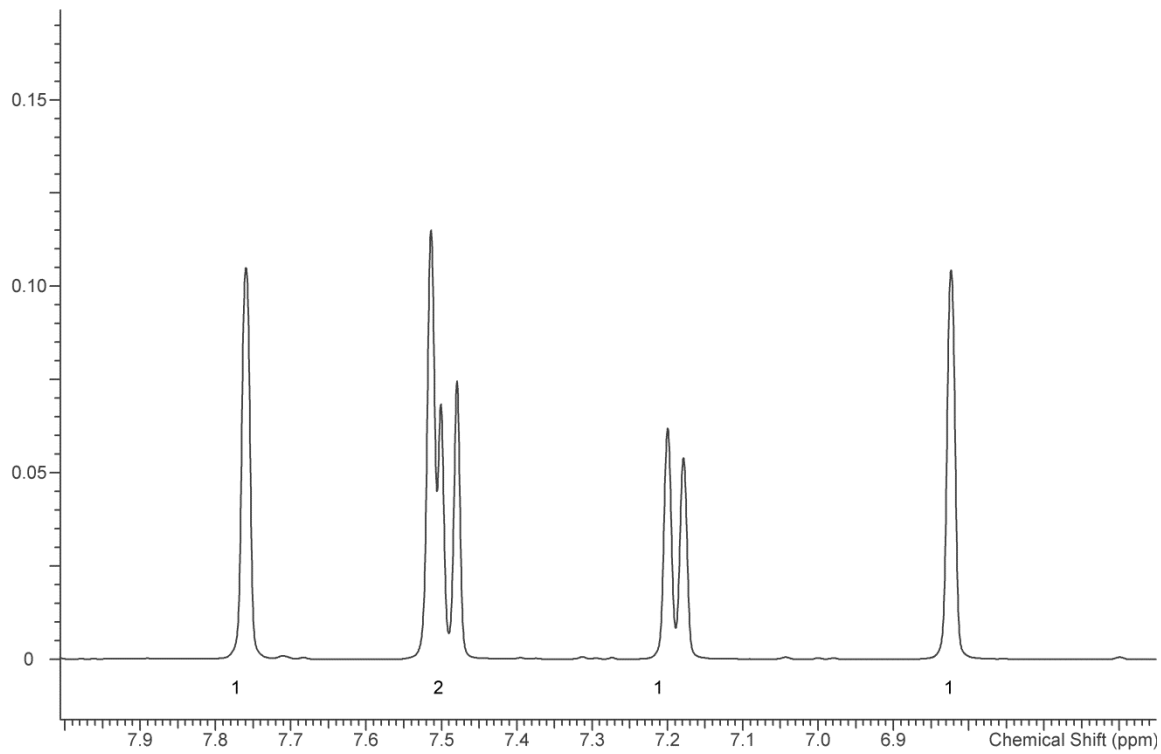
Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

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

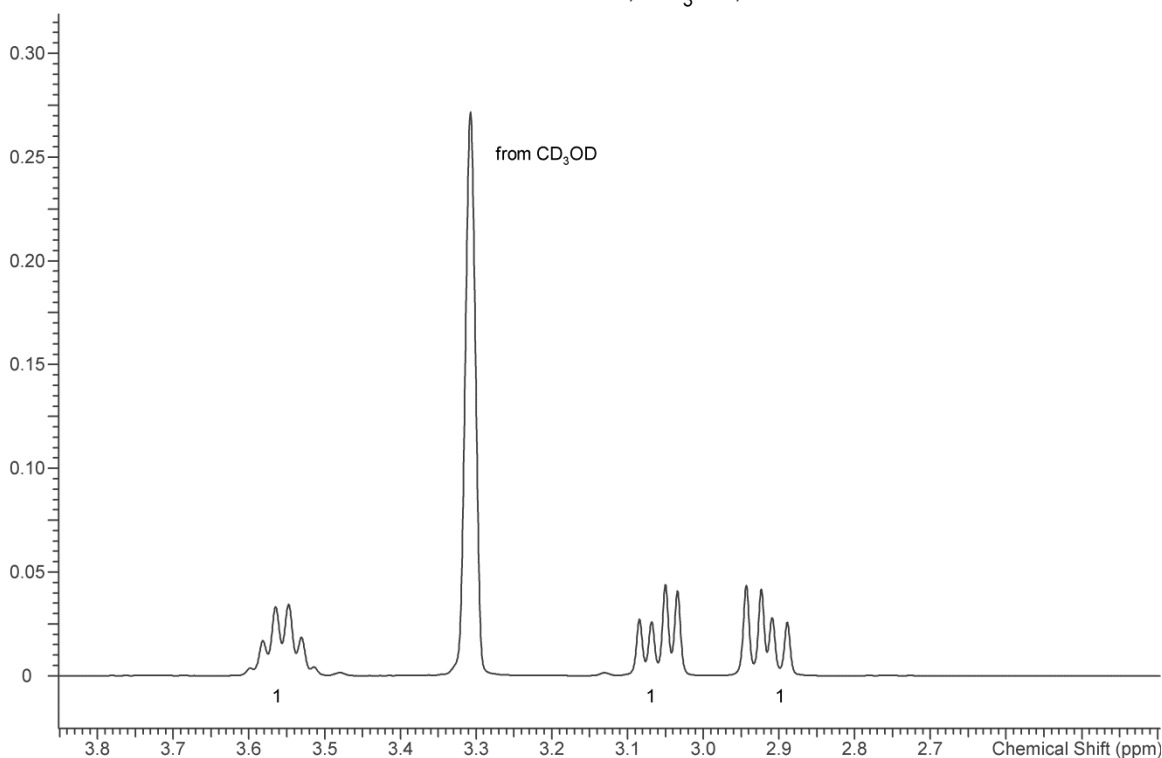
1H NMR: 5-APB HCl Lot # N17-P64B; CD₃OD; 400 MHz



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4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~4 mg/mL in CHCl₃, base extracted with 5 drops 1 N NaOH.

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:

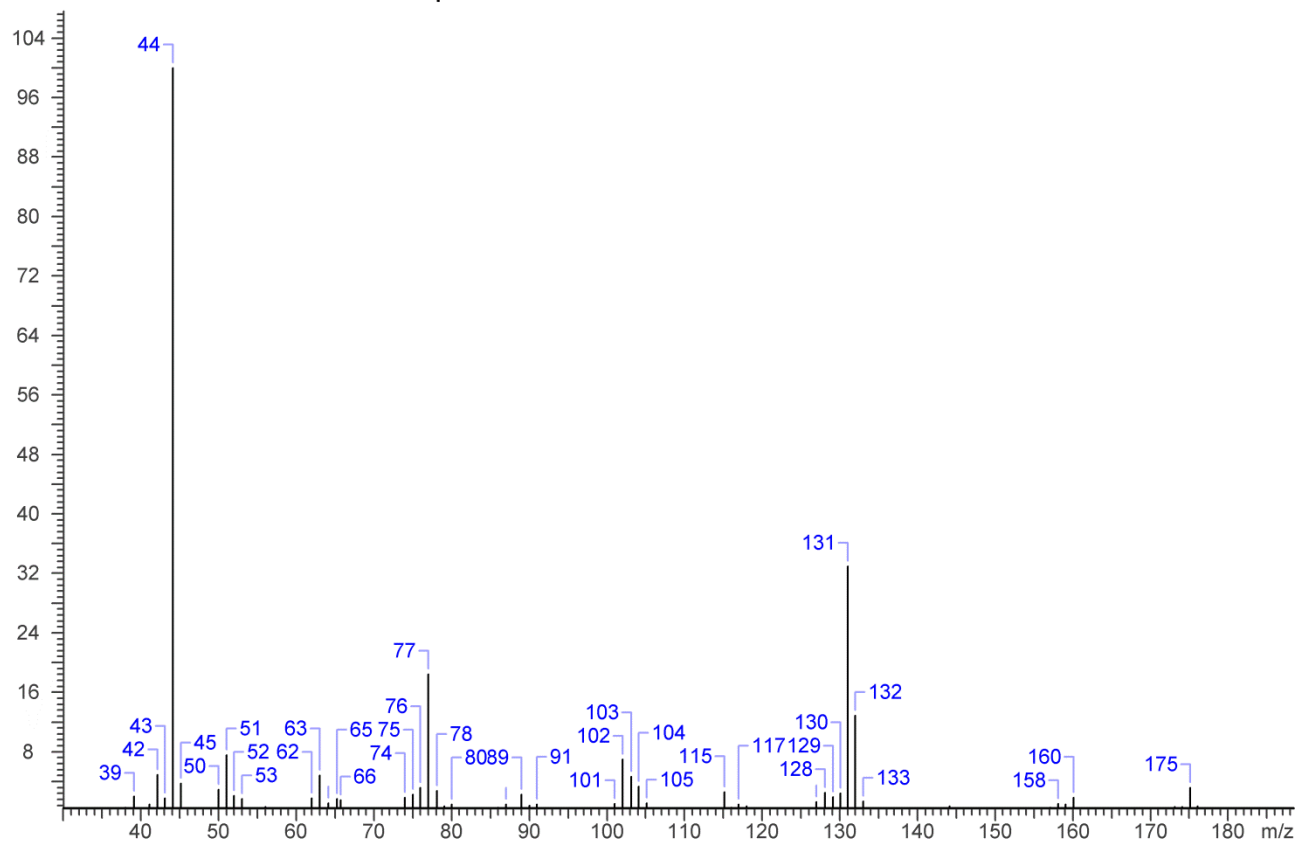
- 1) 100°C initial temperature for 1.0 min
- 2) Ramp to 300°C at 12°C/min
- 3) Hold final temperature for 9.0 min

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: 7.600 min.

EI Mass Spectrum: 5-APB HCl Lot # N17-P64B



4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument:

FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:

Number of scans: 32

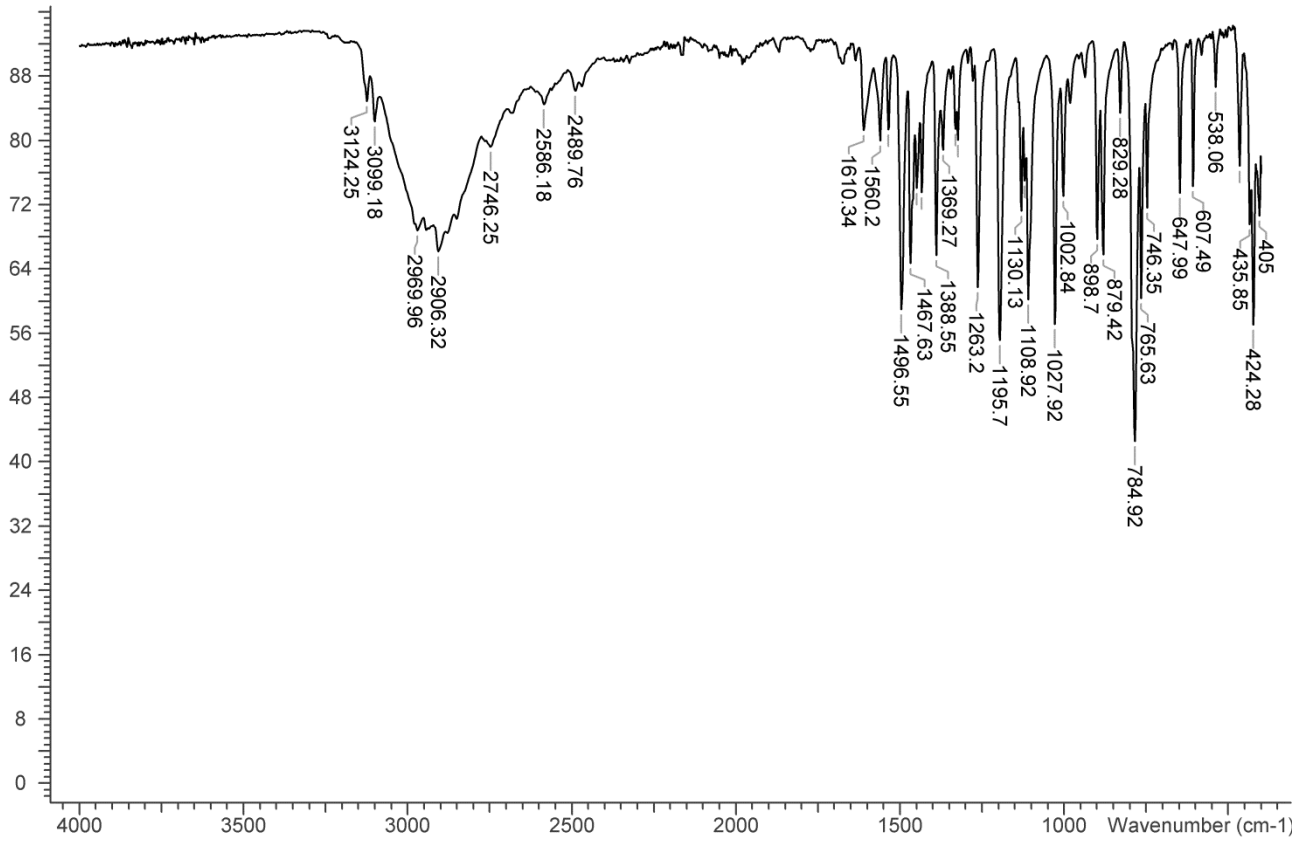
Number of background scans: 32

Resolution: 4cm^{-1}

Sample gain: 8

Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 5-APB HCl Lot # N17-P64B



FTIR ATR (Diamond, 3 Bounce): 5-APB HCl Lot # N17-P64B

