

1. GENERAL INFORMATION

IUPAC Name:	1-(2,3-Dihydro-1-benzofuran-5-yl)propan-2-amine
CFR:	Not Scheduled (3/2013)
CAS #:	152623-94-4
Synonyms:	5-APDB; 3-Desoxy-MDA; EMA-4
Source:	DEA Reference Material Collection
Appearance:	White powder (HCl)
Kovat's Index:	Pending
UV_{max}:	228.5, 282.5 nm

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₁ H ₁₅ NO	177	Not Determined
HCl	C ₁₁ H ₁₅ NO·HCl	213	227.2

3. ADDITIONAL RESOURCES

[Wikipedia](#)

Casale JF, Hays PA. The Characterization of 5- and 6-(2-Aminopropyl)-2,3-dihydrobenzofuran. Microgram Journal 2011; 8(2):62-74.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

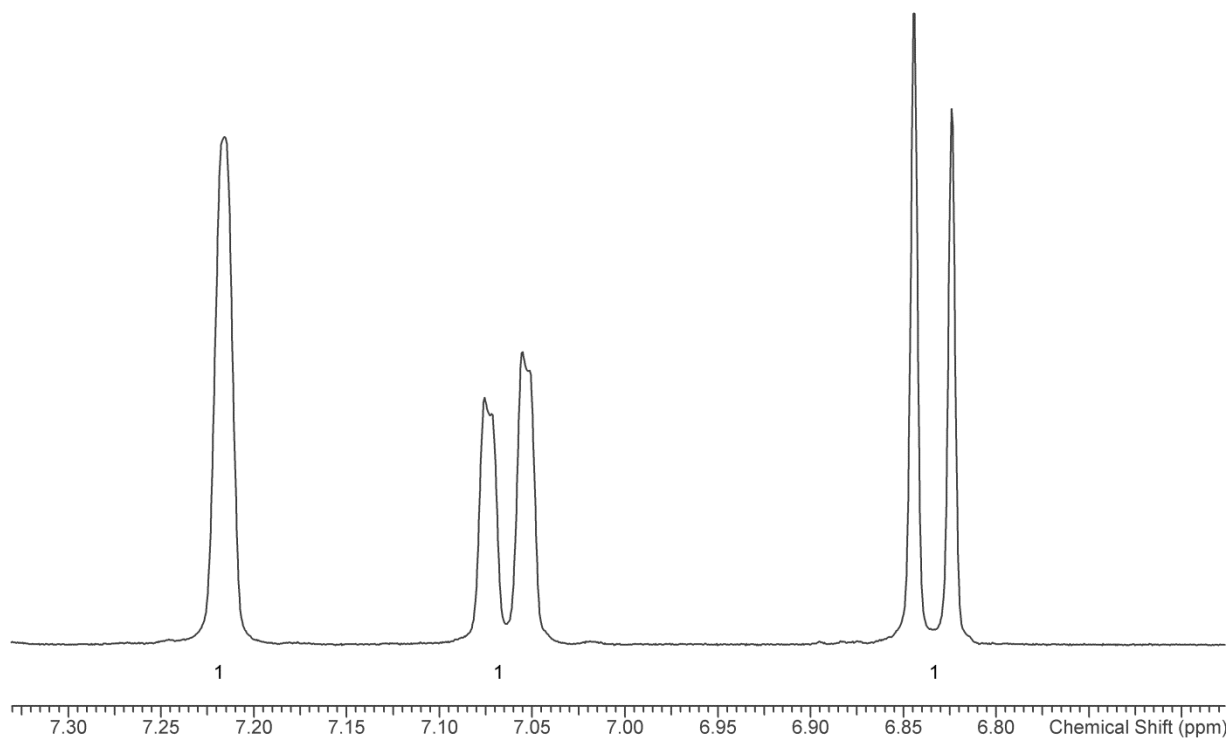
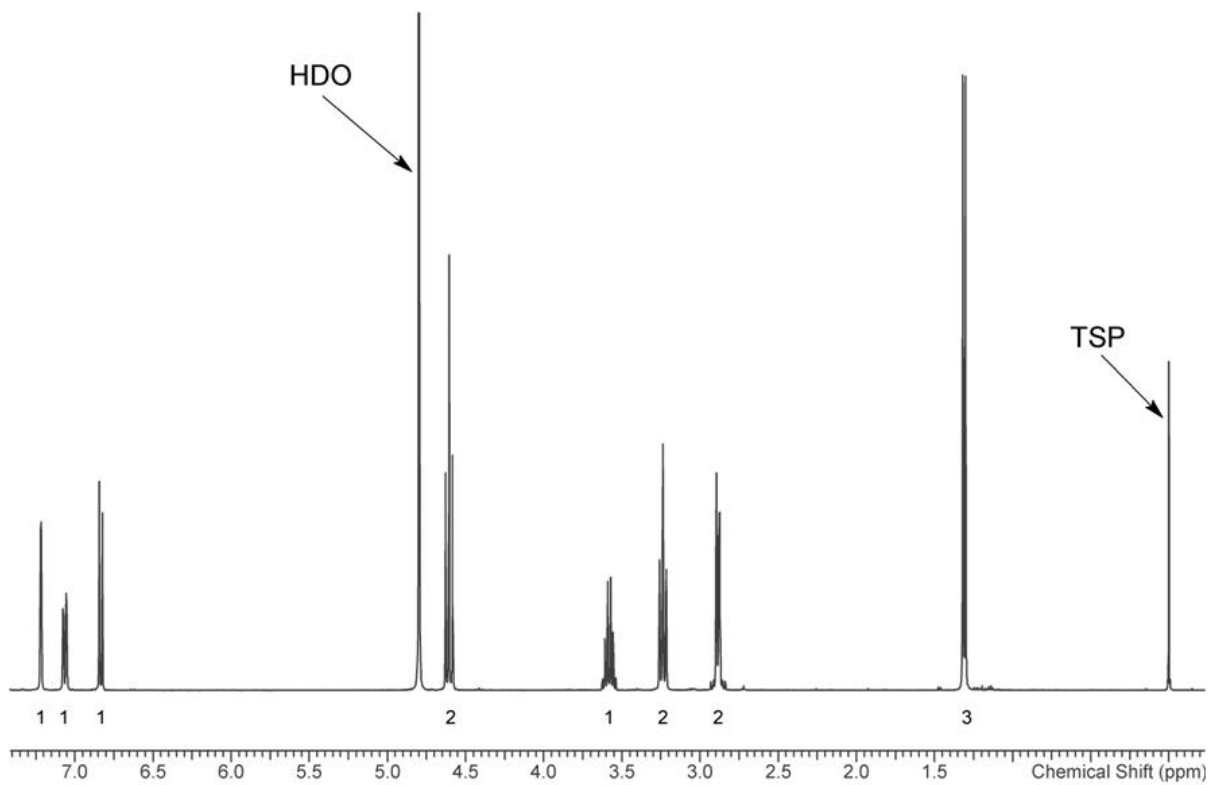
Method NMR D₂O

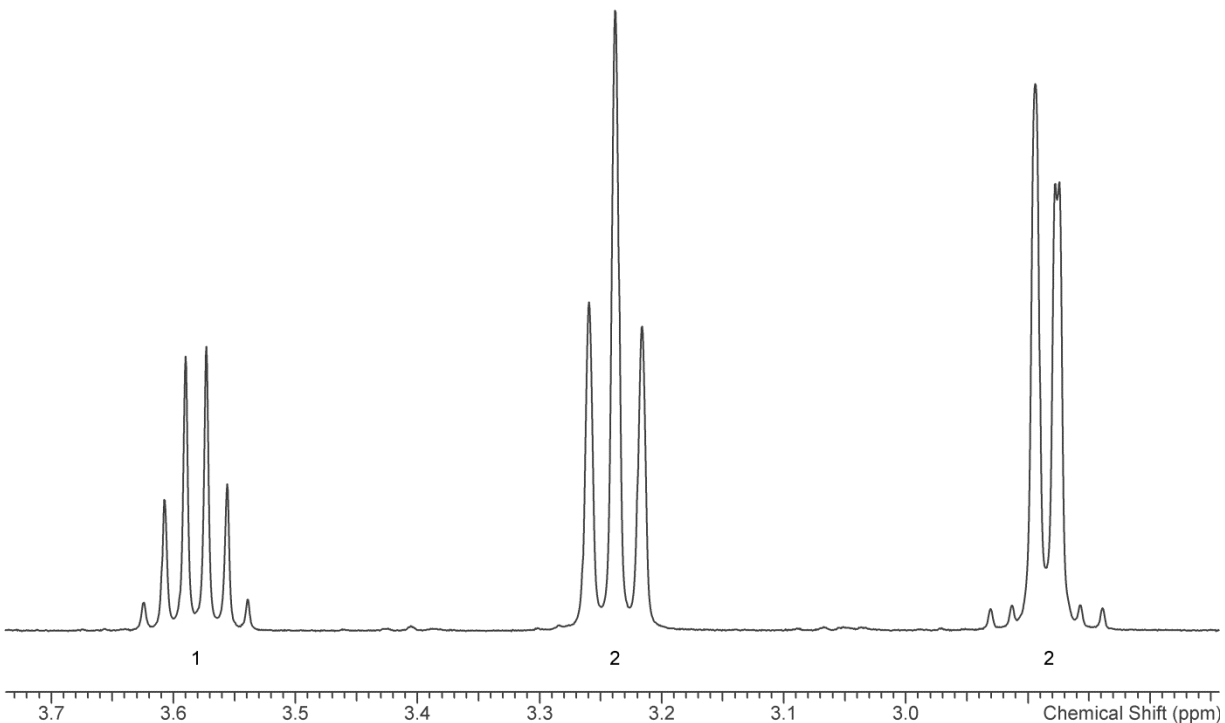
Sample Preparation: Dilute analyte to ~10 mg/mL in D₂O containing TSP for 0 ppm reference.

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-APDB HCl Lot # N16-P60B D₂O, 400MHz





4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/ml in 0.5N NaOH/CHCl₃ or MeOH.

Instrument: Gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x.25mm x .25µm

Carrier gas: Helium at 1 mL/min

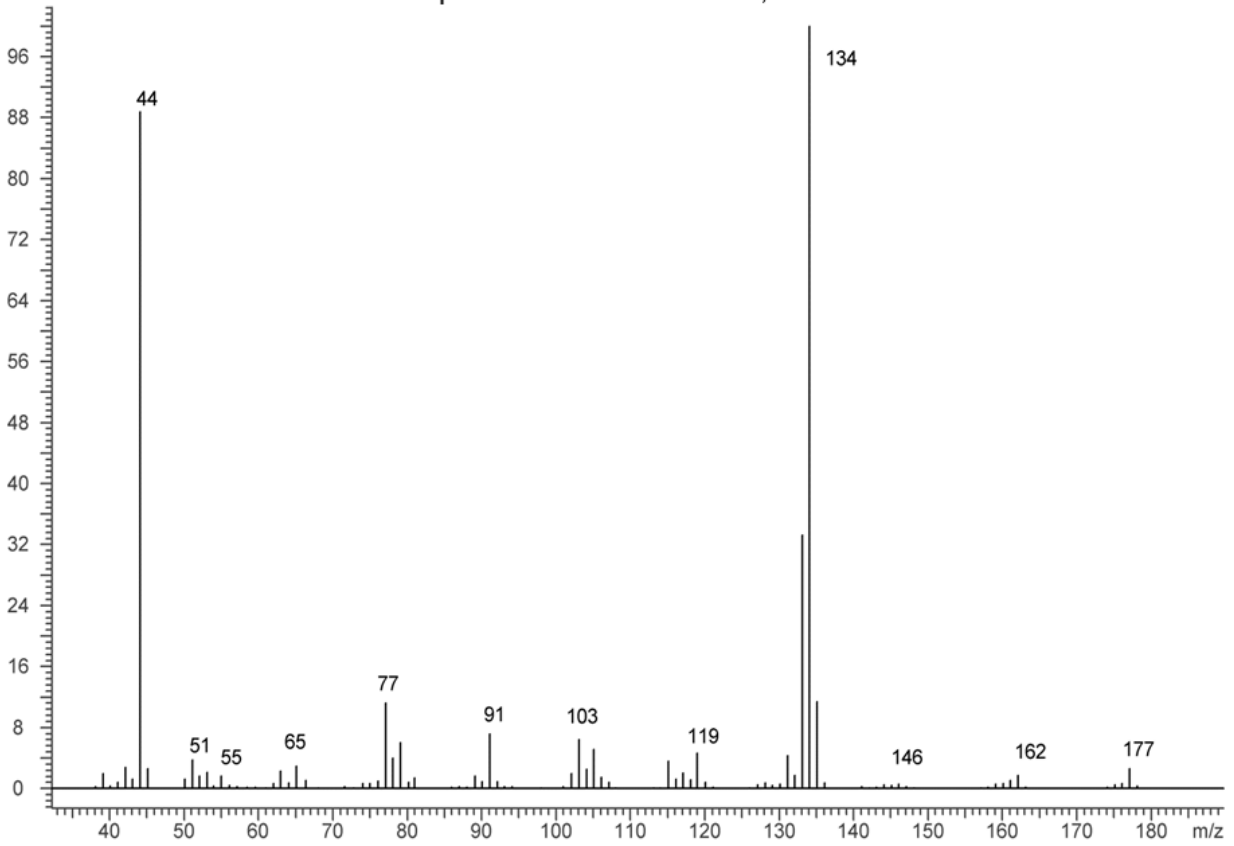
Temperatures:
 Injector: 280°C
 MSD transfer line: 280°C
 MS Source: 230°C
 MS Quad: 150°C
 Oven program:
 1) 100°C initial temperature for 1.0 min
 2) Ramp to 300°C at 12°C/min
 3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 µL injected

MS Parameters: Mass scan range: 34-550 amu
 Threshold: 100
 Tune file: stune.u
 Acquisition mode: scan

Retention time: 8.367 min

El Mass Spectrum: 5-APDB HCl, Lot # N16-P60B



4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ATR attachment
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR (Diamond ATR, 3 Bounce): 5-APDB HCl Lot # N16-P60B

