

## 1. GENERAL INFORMATION

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

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>11</sub> H <sub>15</sub> NO	177	Not Determined
HCl	C <sub>11</sub> H <sub>15</sub> 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

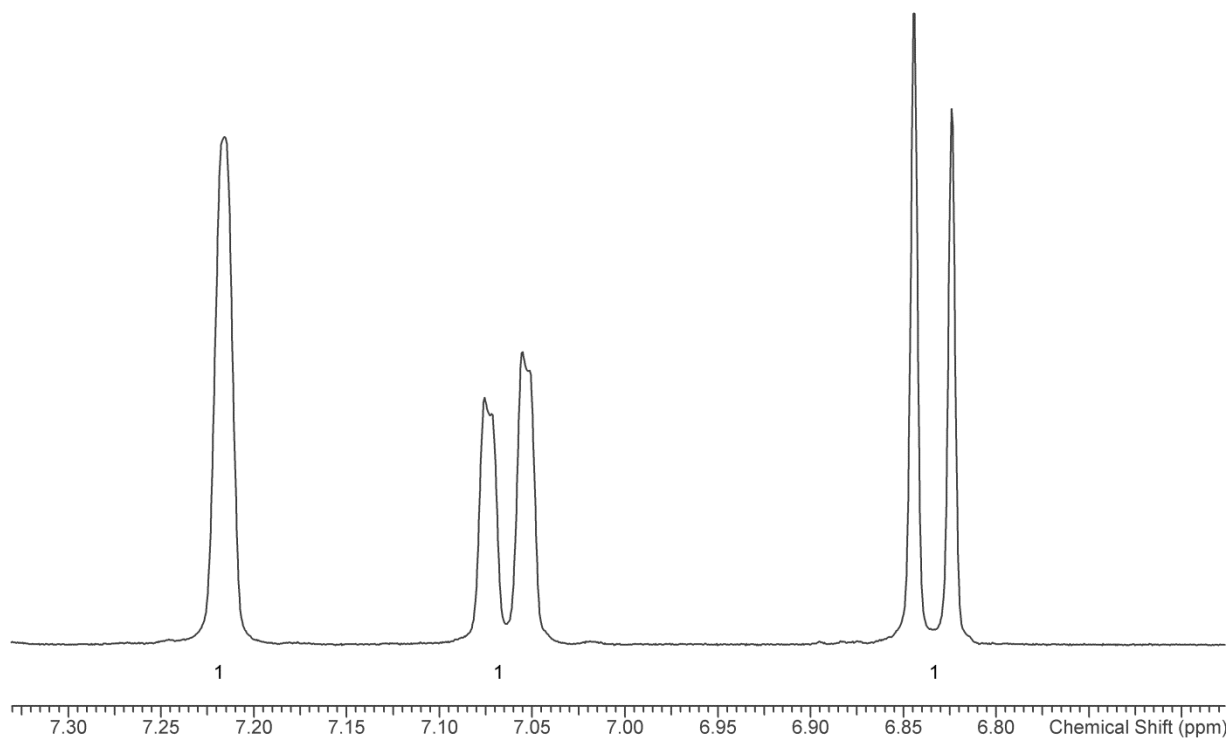
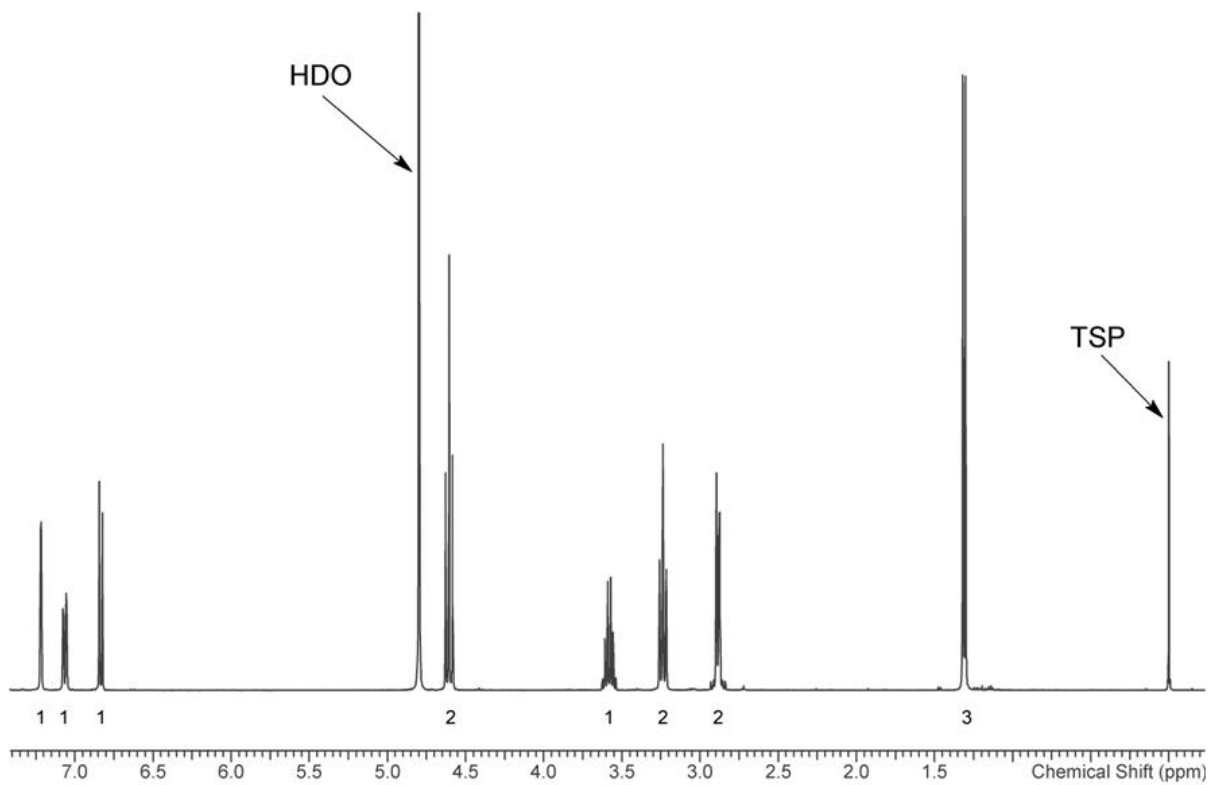
##### *Method NMR D<sub>2</sub>O*

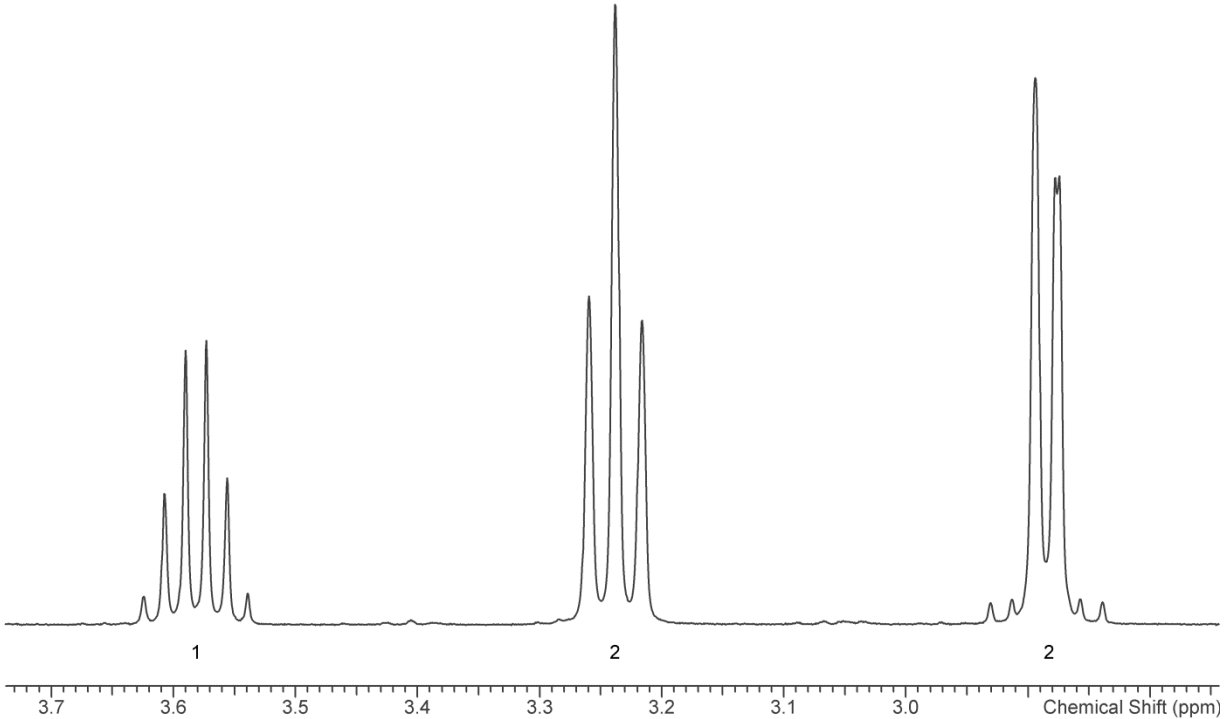
*Sample Preparation:* Dilute analyte to ~10 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference.

***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 D<sub>2</sub>O, 400MHz





## 4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte to ~1 mg/ml in 0.5N NaOH/CHCl<sub>3</sub> 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

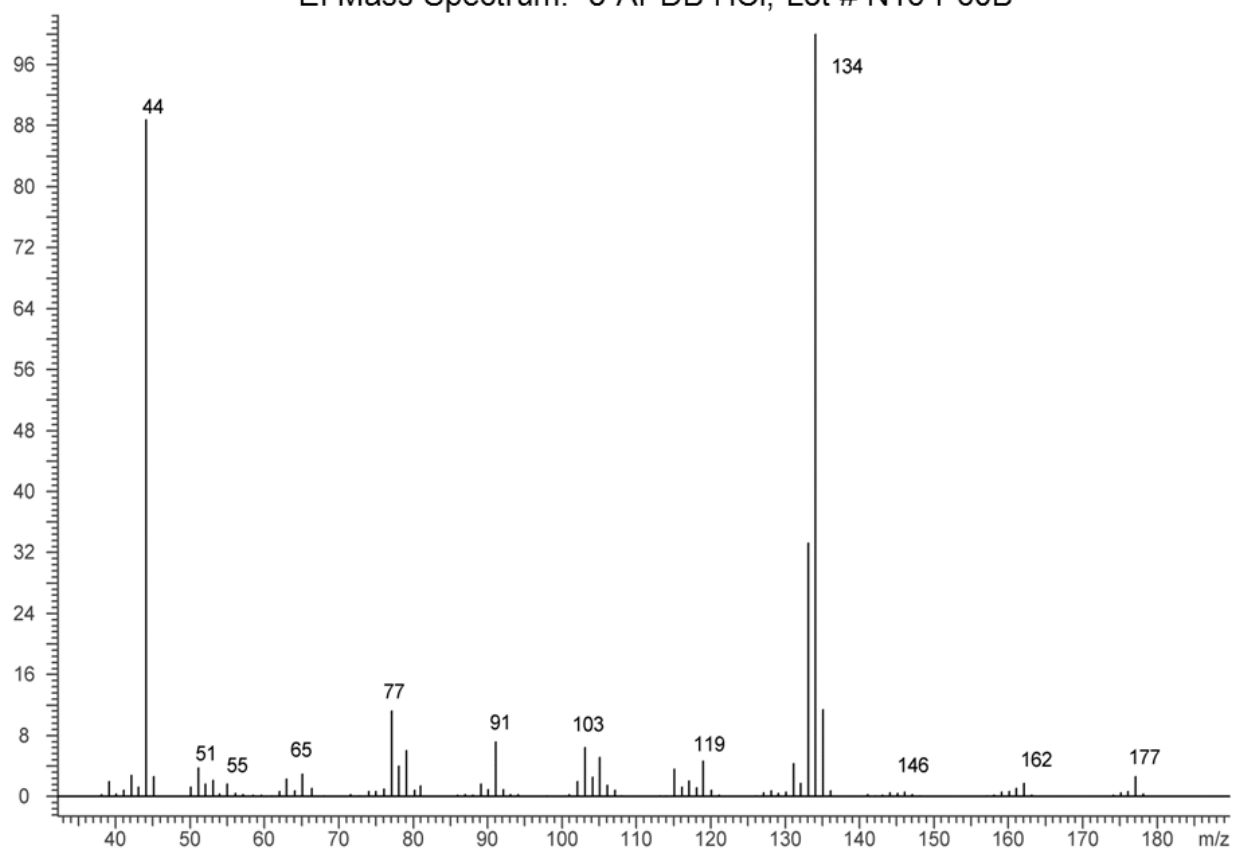
***Temperatures:*** Injector: 280°C  
MSD transfer line: 280°C  
MS Source: 230°C  
MS Quad: 150°C  
Oven program:  
1) 100°C initial temperature for 1.0 min  
2) Ramp to 300°C at 12°C/min  
3) Hold final temperature for 9.0 min

***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<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

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

