

## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-(1-Benzofuran-6-yl)propan-2-amine
<b>CFR:</b>	Not Scheduled (3/2013)
<b>CAS #:</b>	Base: 286834-85-3; HCl: 286834-84-2
<b>Synonyms:</b>	6-APB; Benzo-Fury; Benfamine
<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>	245.6, 284.3 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>13</sub> NO	175	Not determined
HCl	C <sub>11</sub> H <sub>13</sub> NO·HCl	212	164.7

### 3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

### 4. QUALITATIVE DATA

#### 4.1 NUCLEAR MAGNETIC RESONANCE

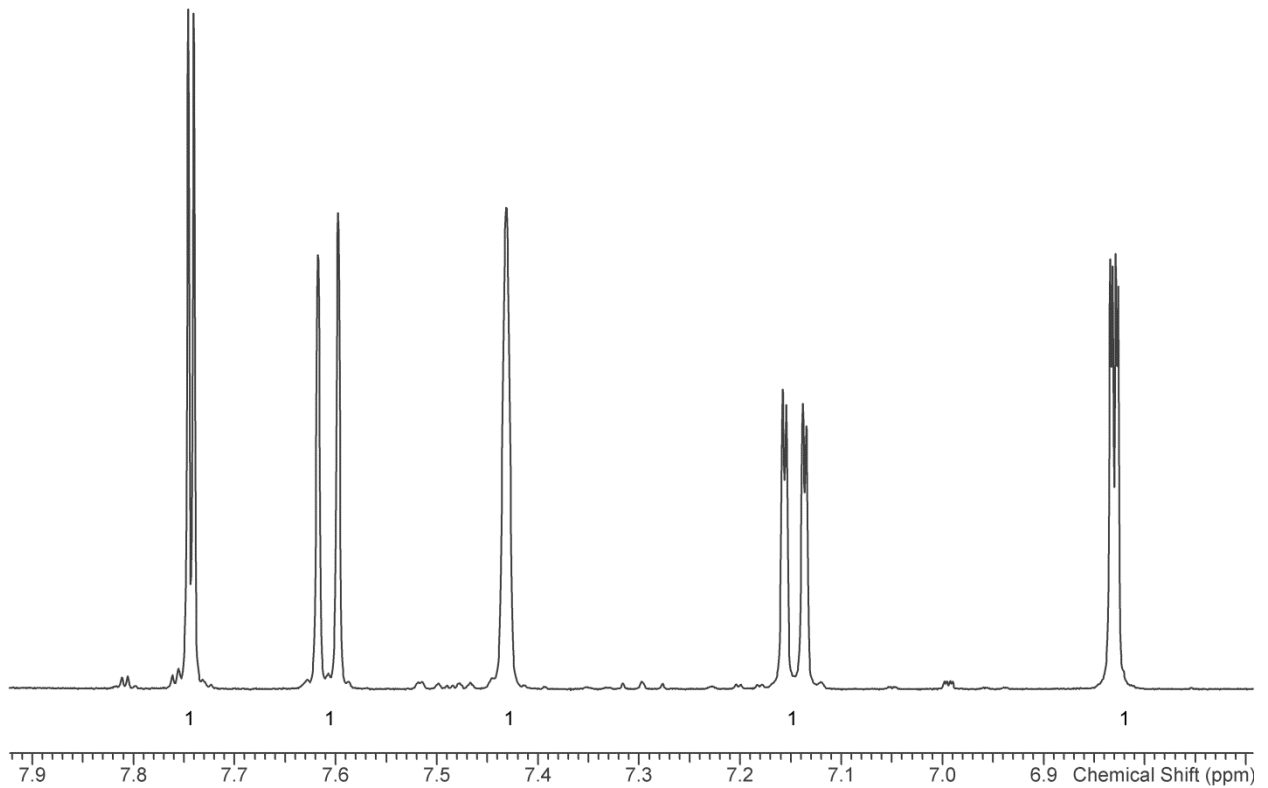
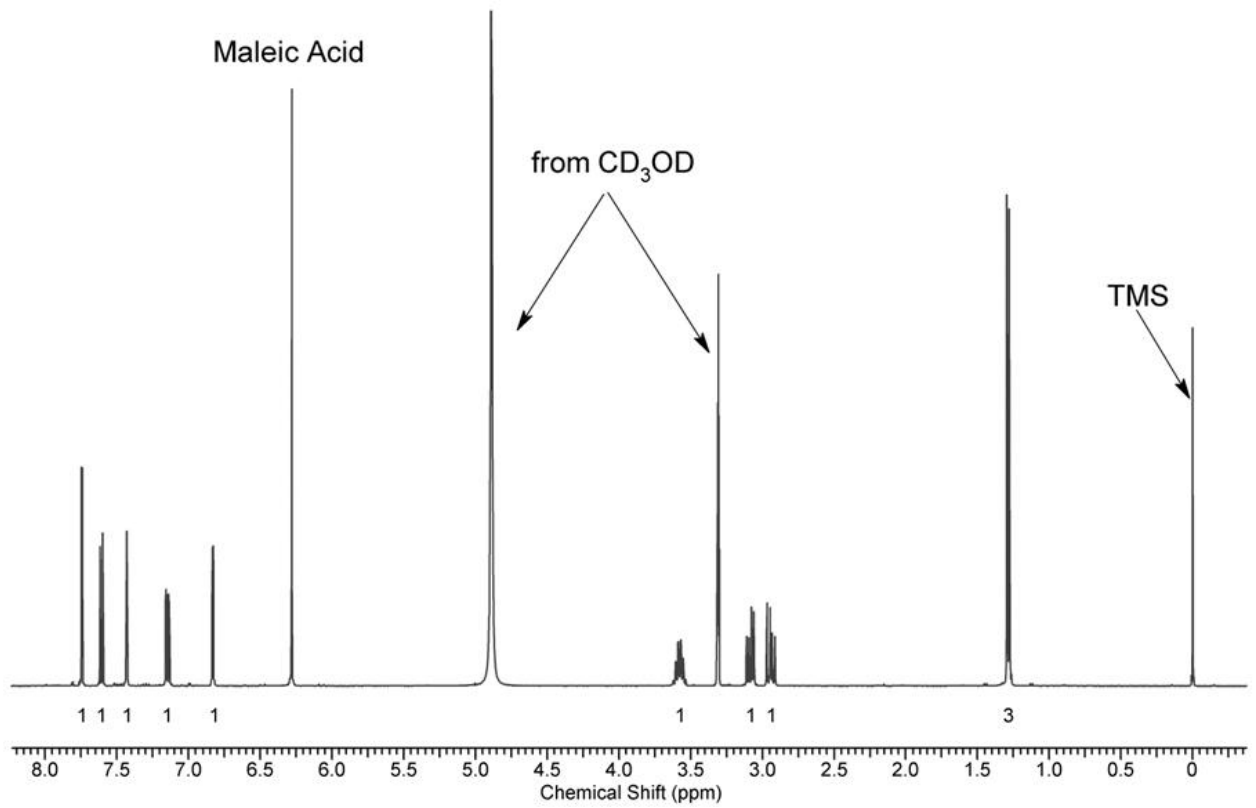
##### *Method NMR CD<sub>3</sub>OD*

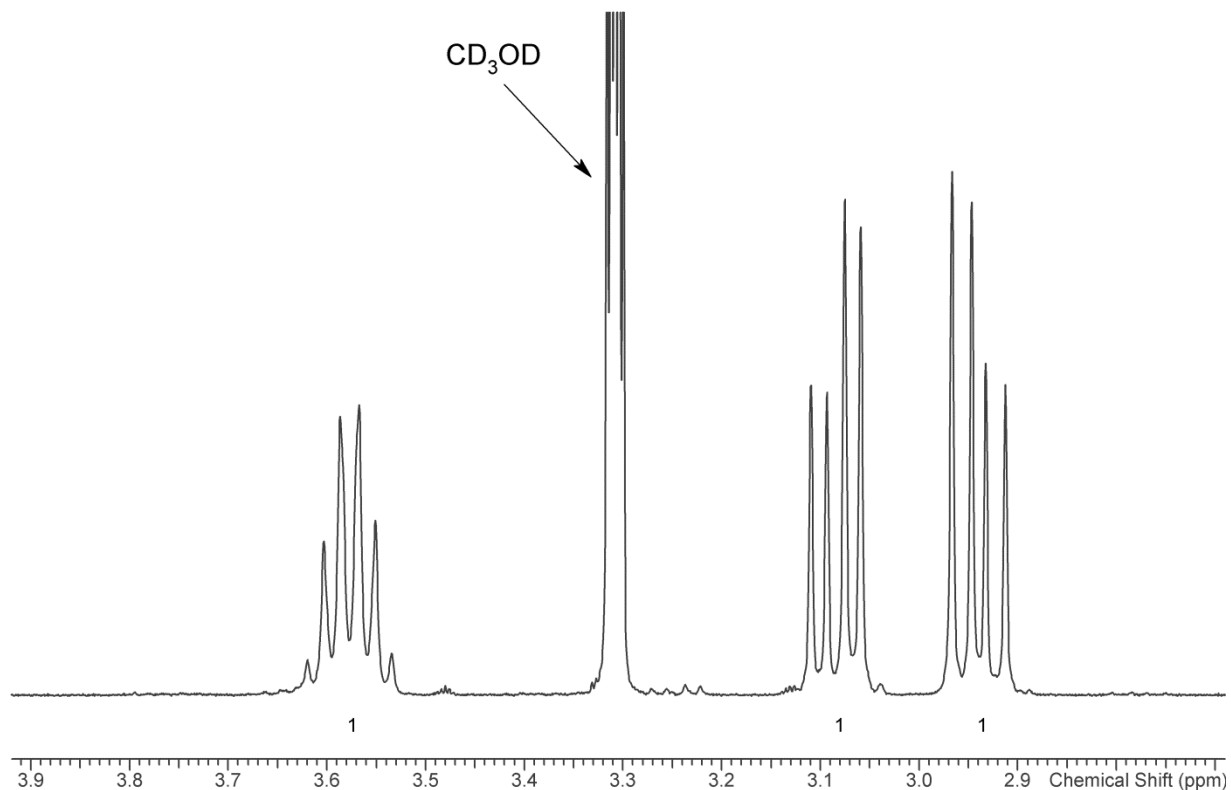
*Sample Preparation:* Dilute analyte to ~10 mg/mL in deuterated methanol (CD<sub>3</sub>OD) containing TMS for 0 ppm reference and maleic acid as an internal standard.

***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: 6-APB HCl Lot # N17-P51C CD<sub>3</sub>OD, 400MHz





## 4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte to ~1 mg/mL in CHCl<sub>3</sub>: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

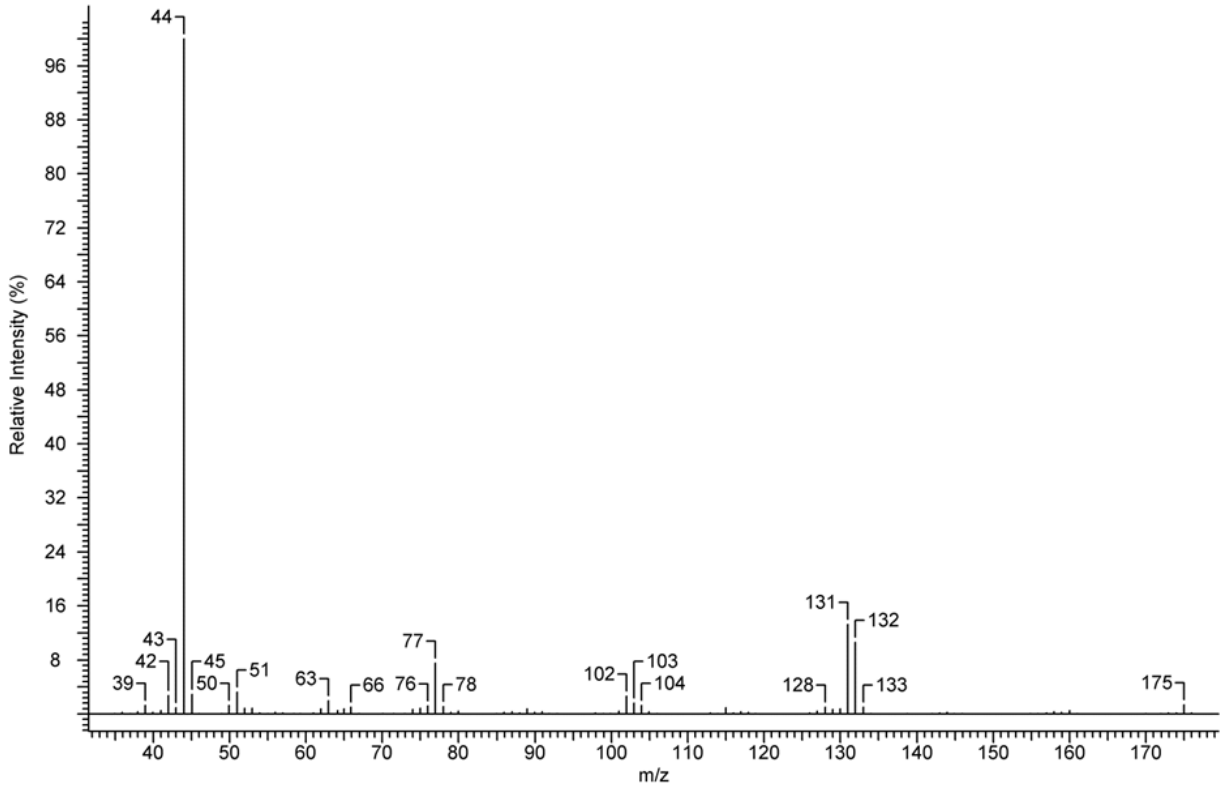
***Temperatures:*** Injector: 280°C  
MSD transfer line: 280°C  
MS Source: 230°C  
MS Quad: 150°C  
Oven program:  
1) 100°C initial temperature for 1.0 min  
2) Ramp to 300°C at 12°C/min  
3) Hold final temperature for 9.0 min

***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:*** 7.531 min

EI Mass Spectrum: 6-APB HCl, Lot # N17-P51C



**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): 6-APB HCl Lot # N17-P58A

