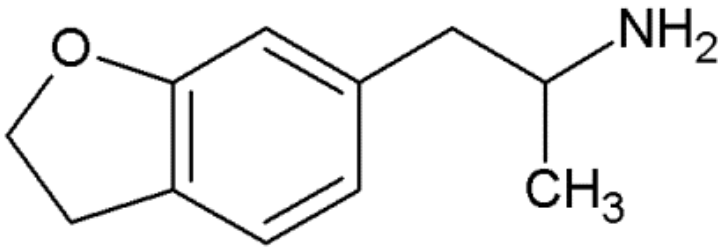
6-(2-Aminopropyl)-2,3-dihydrobenzofuran

Latest Revision: December 10, 2012



1. GENERAL INFORMATION

IUPAC Name: 1-(2,3-Dihydro-1-benzofuran-6-yl)propan-2-amine

CFR: Not Scheduled (12/2012)

CAS #: 152623-93-3

Synonyms: 6-APDB; 4-Desoxy-MDA; EMA-3

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max}: Not Determined

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	$C_{11}H_{15}NO \cdot HCl$	213	243.4

3. ADDITIONAL RESOURCES

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

Wikipedia

4. QUALITATIVE DATA

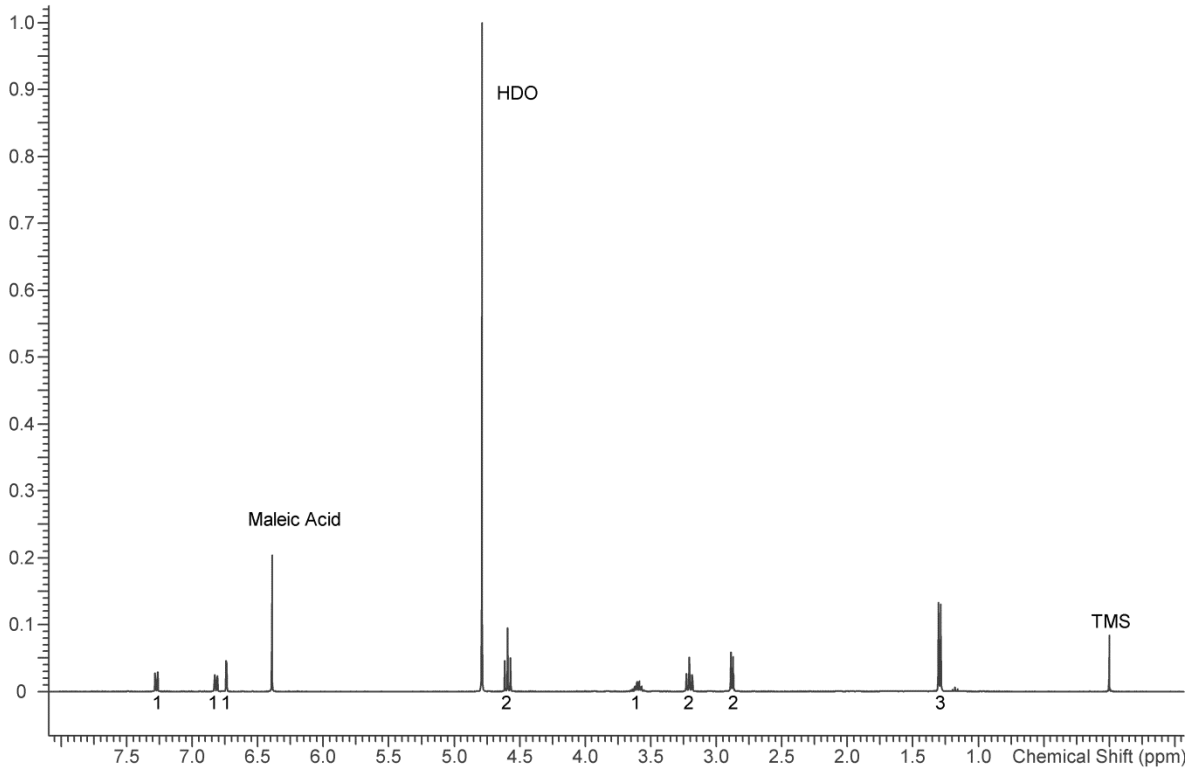
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

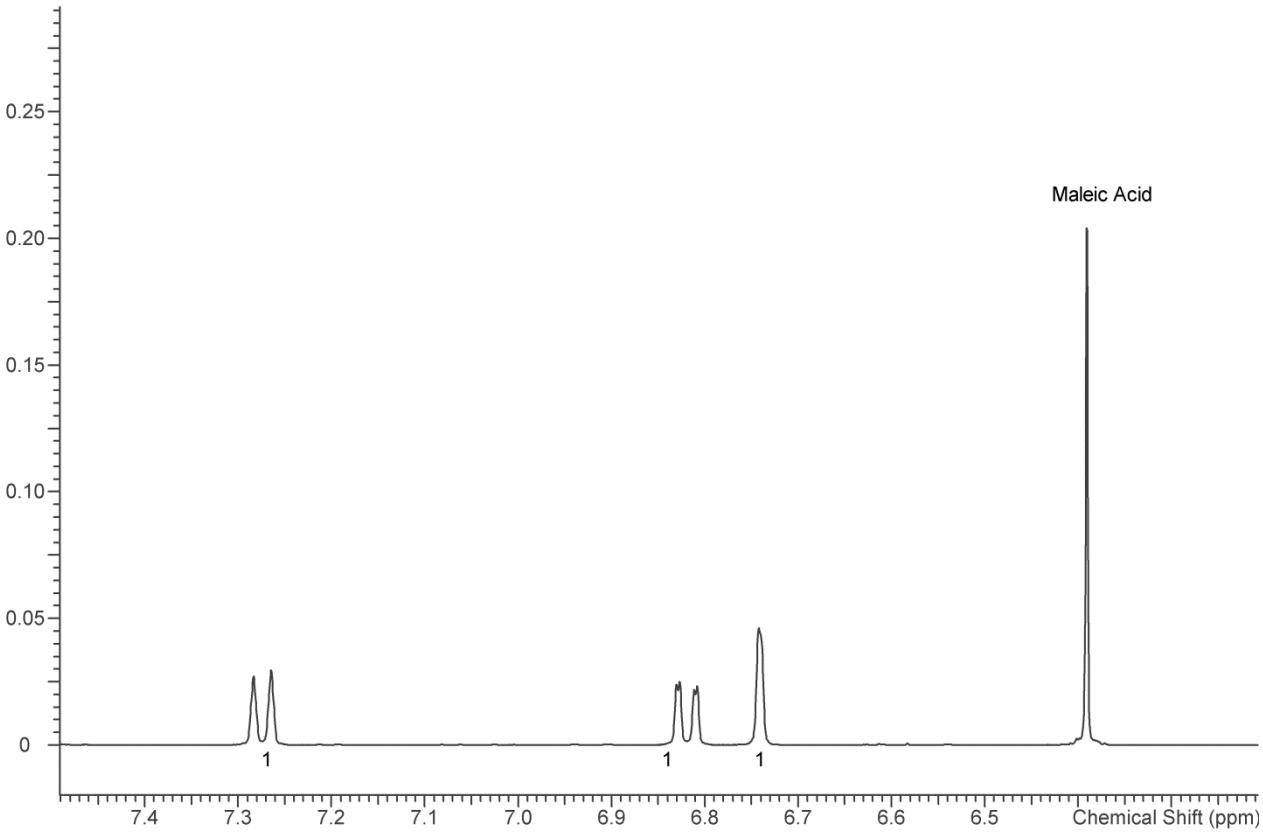
Sample Preparation: Dilute analyte to ~10 mg/mL in D_2O containing TMS for 0 ppm reference and maleic acid as quantitative ISTD.

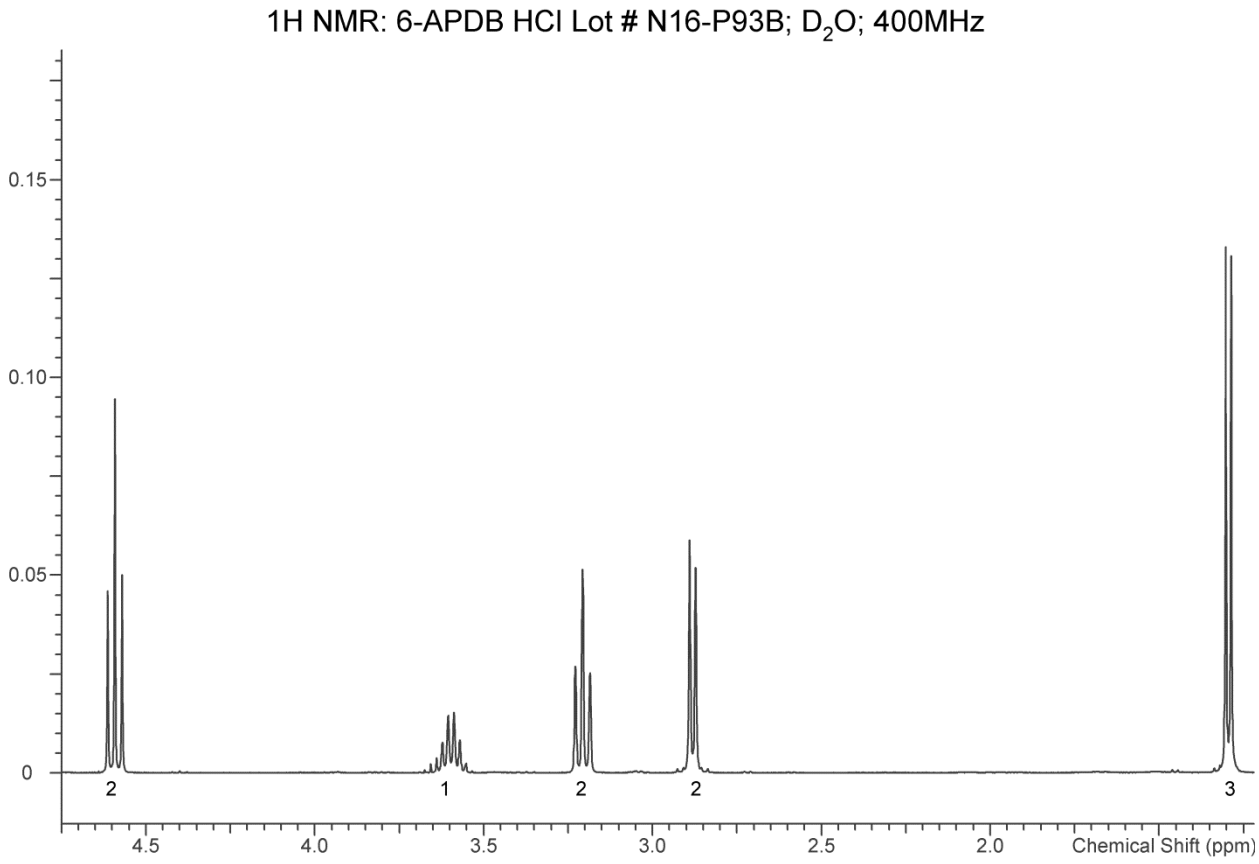
Instrument:	Varian Mercury 400 MHz NMR spectrometer with proton detection probe
Parameters:	Spectral width: at least containing -3 ppm through 13 ppm (Portion of spectra chosen to best display all signal peaks) Pulse angle: 90° Delay between pulses: 45 seconds Number of scans (NT): 8 Number of steady state scans: 0 Oversampling: 4 or more Shimming: automatic gradient shimming of Z1-4 shims Phasing, Drift Correction: automatic or manual

1H NMR: 6-APDB HCl Lot # N16-P93B; D_2O; 400MHz



1H NMR: 6-APDB HCl Lot # N16-P93B; D_2O; 400MHz



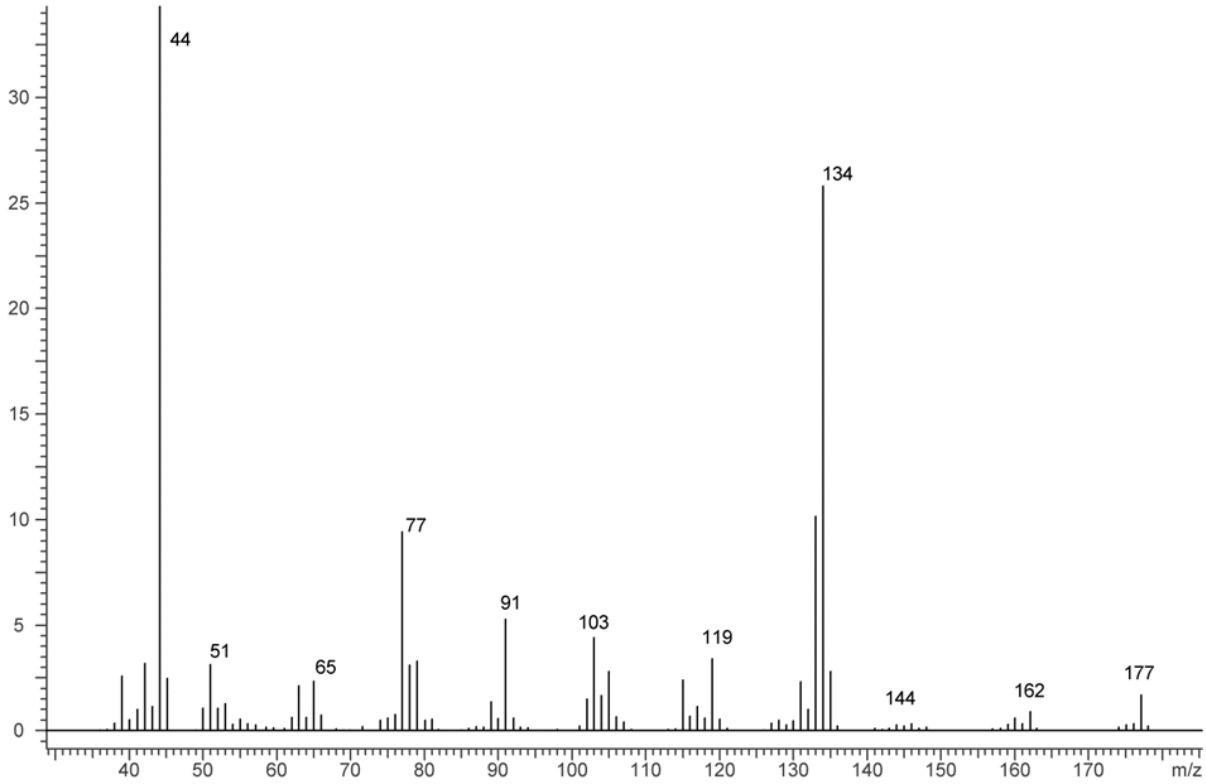


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in 0.5N NaOH/$CHCl_3$.

Instrument:	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: 34-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention time:	8.402 min

EI Mass Spectrum: 6-APDB HCl, Lot # N16-P93B

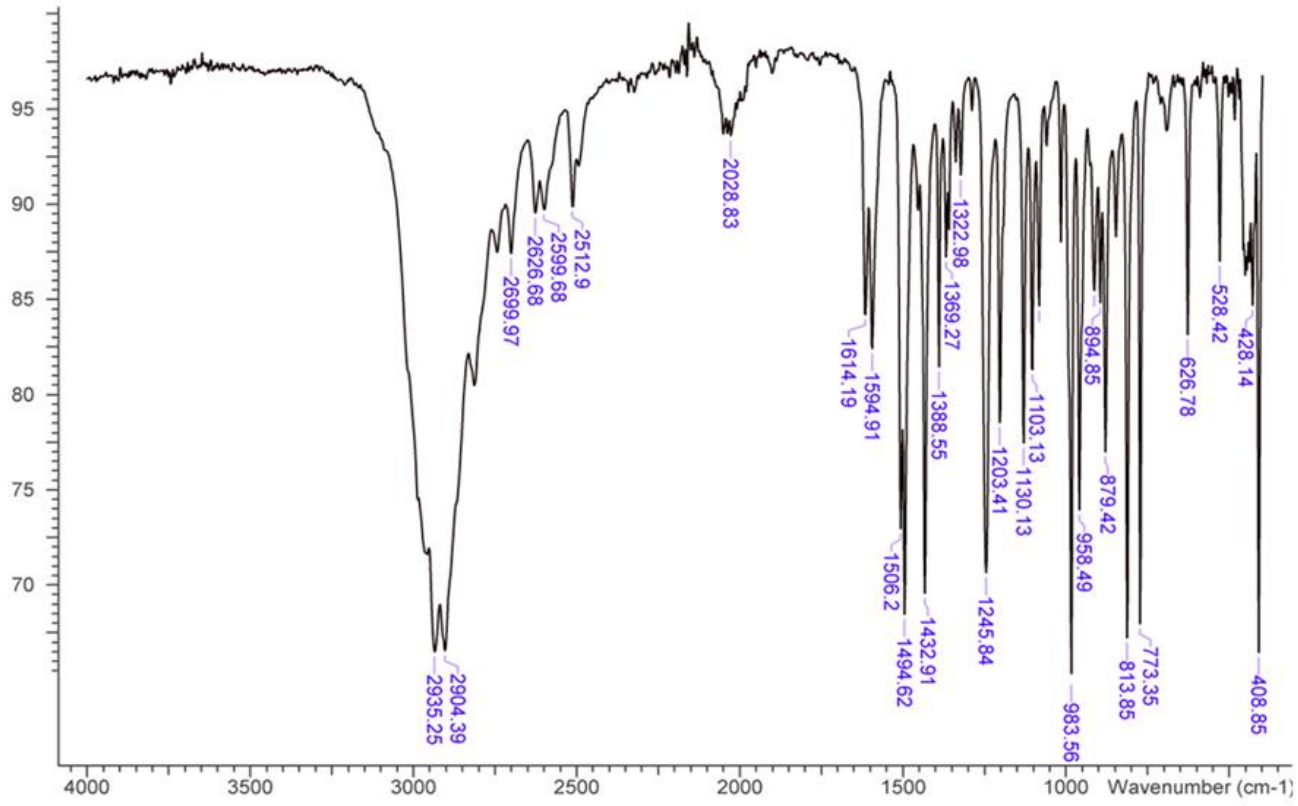


4.3 INFRARED SPECTROSCOPY (FTIR)

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 ATR (Diamond, 3 Bounce): 6-APDB HCl, Lot # N16-P93B



FTIR (Diamond ATR, 3 Bounce): 6-APDB HCl Lot # N16-P93B