

## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-(4-bromo-2,5-dimethoxyphenyl)propan-2-amine
<b>CFR:</b>	Schedule I
<b>CAS #:</b>	29705-96-2 (HCl)
<b>Synonyms:</b>	DOB; 2,5-dimethoxy-4-bromoamphetamine; dimethoxybromoamphetamine; brolamphetamine; bromo-DMA
<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>	Not Determined

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>11</sub> H <sub>16</sub> BrNO <sub>2</sub>	274	Not Determined
HCl	C <sub>11</sub> H <sub>16</sub> BrNO <sub>2</sub> · HCl	310	204.7

### 3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

### 4. QUALITATIVE DATA

#### 4.1 NUCLEAR MAGNETIC RESONANCE

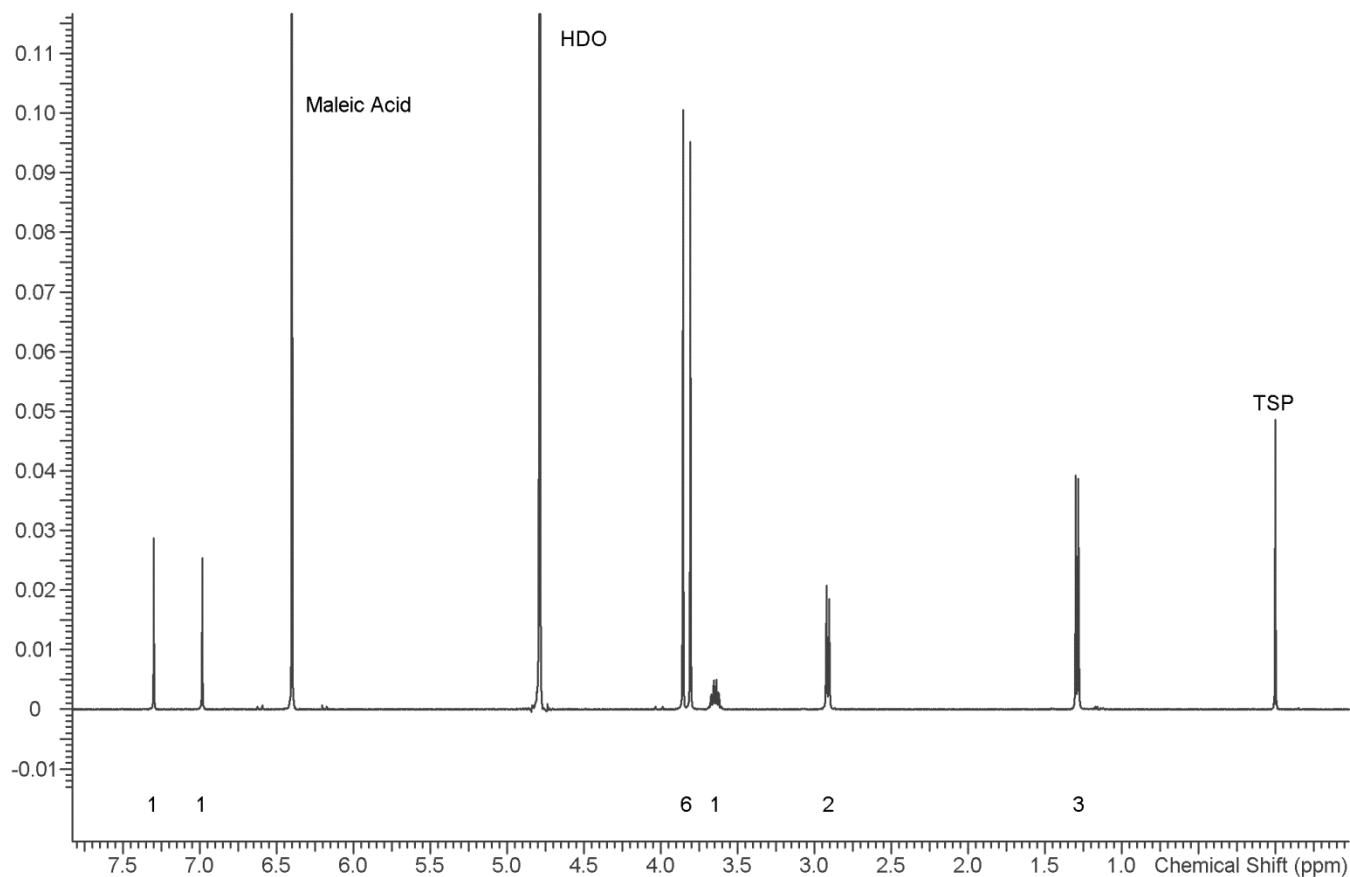
##### *Method NMR D<sub>2</sub>O*

*Sample Preparation:* Dilute analyte to ~5 mg/mL in D<sub>2</sub>O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

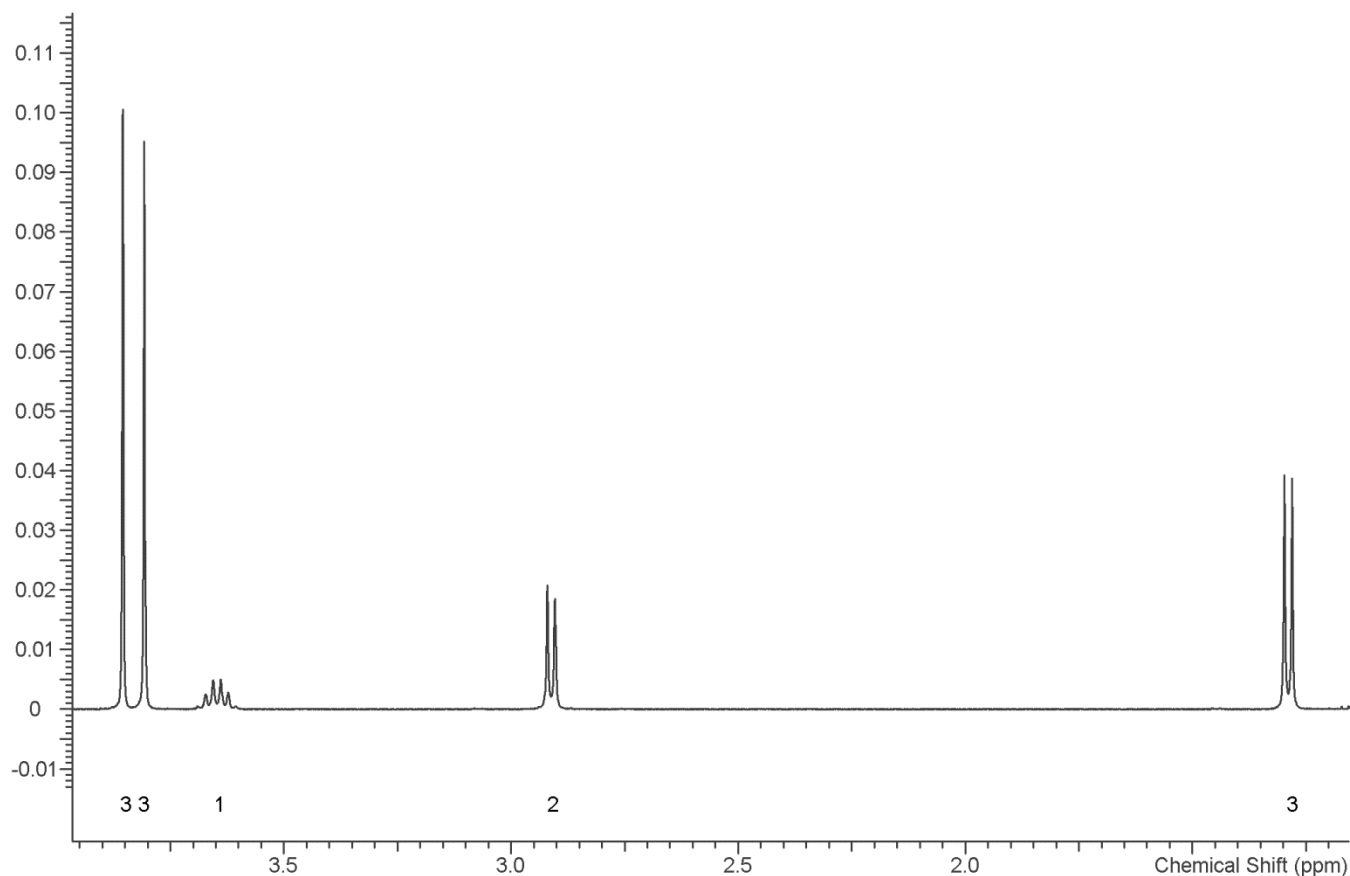
**Instrument:** 400 MHz NMR spectrometer

**Parameters:** Spectral width: at least containing -3 ppm through 13 ppm  
Pulse angle: 90°  
Delay between pulses: 45 seconds

1H NMR: DOB HCl Lot 274.1B1.1; D<sub>2</sub>O; 400MHz



1H NMR: DOB HCl Lot 274.1B1.1; D<sub>2</sub>O; 400MHz



## 4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte to 4 mg/mL base extracted in CHCl<sub>3</sub>.

**Instrument:** Agilent 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:

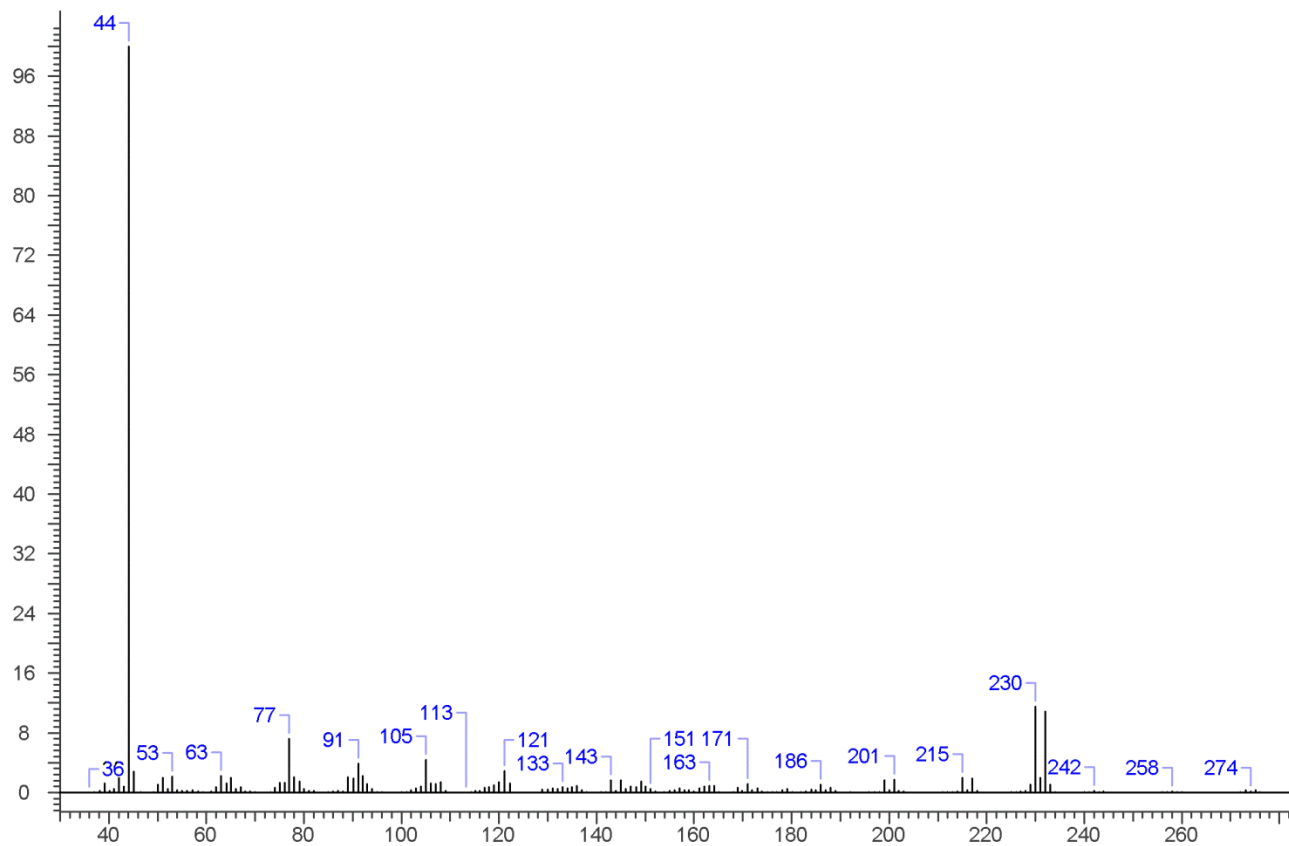
- 1) 100°C initial temperature for 1.0 min
- 2) Ramp to 300°C at 12°C/min
- 3) Hold final temperature for 9.0 min

**Injection Parameters:** Split Ratio = 20:1, 1 μL injected

**MS Parameters:**  
Mass scan range: 30-550 amu  
Threshold: 100  
Tune file: stune.u  
Acquisition mode: scan

**Retention Time:** 10.672 minutes

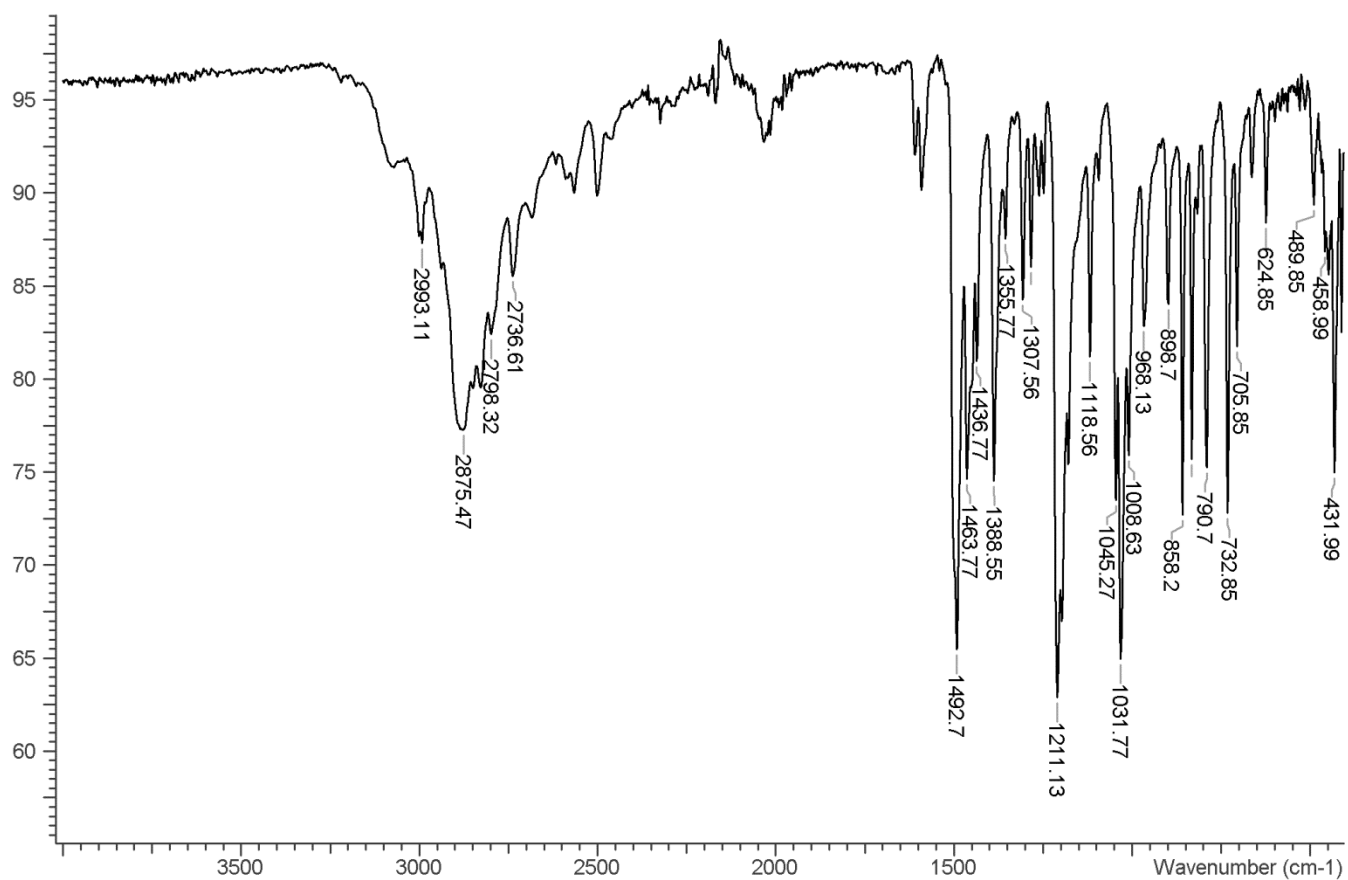
## EI Mass Spectrum: DOB HCl Lot 274.1B1.1



### 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:  $4\text{cm}^{-1}$   
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): DOB HCl Lot 274.1B1.1



FTIR ATR (Diamond, 3 Bounce): DOB HCl Lot 274.1B1.1

