

## 1. SYNONYMS

**CFR:** 4-Bromo-2,5-dimethoxyphenethylamine

**CAS #:** Base: 66142-81  
Hydrochloride: 56281-37-9

**Other Names:** 2C-B  
2-(4-Bromo-2,5-dimethoxyphenyl)-1-aminoethane  
Nexus  
4-Bromo-2,5-dimethoxybenzeneethanamine  
BDMPEA  
♣-Desmethyl DOB  
MFT  
Bromo  
Performax  
Spectrum  
Venus  
Erox  
Cloud Nine  
Cee-Beetje  
Toonies  
2's  
Synergy  
Zenith  
Utopia  
Afterburner Bromo

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1. CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>10</sub> H <sub>14</sub> BrNO <sub>2</sub>	260.13	Not available
Hydrochloride	C <sub>10</sub> H <sub>14</sub> BrNO <sub>2</sub> •HCl	296.59	237-239

## 2.2. SOLUBILITY

Form	A	C	E	H	M	W
Base	N/A	S	S	N/A	S	I
Hydrochloride	SS	S	I	N/A	S	S

A = acetone, C = chloroform, E = ether, H = hexane, M = methanol and W = water, VS = very soluble, FS = freely soluble, S = soluble, PS = sparingly soluble, SS = slightly soluble, VSS = very slightly soluble and I = insoluble, N/A = not available

## 3. SCREENING TECHNIQUES

### 3.1. COLOR TESTS

REAGENT	COLOR PRODUCED
Marquis	green
Mecke	green to yellow (slow) to blue (slow)

### 3.2. GAS CHROMATOGRAPHY

#### *Method SFL4 Screen*

**Instrument:** Gas Chromatograph operated in split mode

**Column:** 100% dimethylpolysiloxane gum  
30 m x 0.25 mm x 0.25 µm film thickness

**Carrier gas:** Hydrogen at 1.3 mL/min

**Makeup gas :** Nitrogen at 40.0 mL/min

**Temperatures:** Injector: 250°C  
Detector: 300°C  
Oven program:  
1) 100°C initial temperature  
2) Ramp to 295°C at 35°C/min  
3) Hold final temperature for 6.43 min

**Injection Parameters:** Split Ratio = 100:1, 1 µL injected

Sample dissolved in water, base extracted with 1-2 M Sodium hydroxide.

COMPOUND	RRT	COMPOUND	RRT
amphetamine	0.507	4-MeOPP	0.966
methamphetamine	0.549	<b>2C-B</b>	<b>1.00 (4.232 min)</b>
nicotinamide	0.677	caffeine	1.010
3,4-MDA	0.765	2C-I	1.069
BZP	0.779	2C-T-2	1.084
TFMPP	0.795	2C-T-7	1.136
3,4-MDMA	0.814	procaine	1.155
benzocaine	0.825	tetracaine	1.284
3,4-MDEA	0.852	quinine	1.681
acetaminophen	0.905		

### 3.3. HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

#### *Method Phen01*

<b>Instrument:</b>	High performance liquid chromatograph equipped with mass spectrometer
<b>Column:</b>	5 µm ODS, 150 mm x 4.6 mm
<b>Detector:</b>	Mass Spectrometer
<b>Flow:</b>	400 µL/min
<b>Injection Volume:</b>	5.0 µL
<b>Buffer:</b>	10 mM ammonium acetate in water
<b>Mobile Phase:</b>	1) Initially, CH <sub>3</sub> OH: buffer 5:95 held for 10 min 2) Gradient to CH <sub>3</sub> OH: buffer 80:20 over 10 min 3) Gradient to CH <sub>3</sub> OH: buffer 5:95 over 10 min

Samples are to be dissolved in buffer solution, sonicated, then filtered with a 0.45-micron filter paper.

COMPOUND	RRT	COMPOUND	RRT
ephedrine/pseudoephedrine	0.786	2C-I	1.031
amphetamine	0.861	2C-T-2	1.036
methamphetamine	0.872	MDMA	1.060
MDEA	0.890	2C-T-7	1.105
<b>2C-B</b>	<b>1.00 (12.88 min)</b>		

#### 4. SEPARATION TECHNIQUES

2C-B can be separated from matrices by solvent extraction using the solubility data found in Section 2.2.

#### 5. QUANTITATIVE PROCEDURES

##### 5.1. GAS CHROMATOGRAPHY

###### *Method 4dimeth1* (SFL-4)

###### *Internal Standard Stock Solution (ISSS):*

1.00 mg/mL tetradecane (C<sub>14</sub>) in methylene chloride.

###### *Standard Solution Preparation:*

Accurately weigh and prepare a standard solution 2C-B HCl in deionized water within the linearity ranges listed below. Extract a 2 mL aliquot of the standard solution with 2 mL of 1M Sodium hydroxide into 2 mL of ISSS.

###### *Sample Preparation:*

Accurately weigh an amount of sample into an appropriately sized volumetric flask so that the final concentration of 2C-B HCl is approximately equivalent to that of the standard solution. Dilute to volume with deionized water. Extract a 2 mL aliquot of the standard solution with 2 mL of 1M Sodium hydroxide into 2 mL of ISSS.

###### *Instrument:*

Gas Chromatograph operated in split mode with FID

###### *Column:*

100% dimethylpolysiloxane gum,  
30 m x 0.25 mm x 0.25 µm film thickness

###### *Carrier gas:*

Hydrogen at 1.2 mL/min

###### *Make-Up gas:*

Nitrogen at 30 mL/min

###### *Temperatures:*

Injector: 265°C  
Detector: 275°C  
Oven Temperature: 220°C isothermal

**Injection Parameters:** Split Ratio: 50:1  
Injection Volume: 1 $\mu$ L

**Typical Retention Time:** 2C-B HCl: 1.80 min  
C<sub>14</sub>: 1.30 min

**Linear Range:** 0.258 – 3.178 mg/mL

**Repeatability:** RSD less than 3%

**Correlation Coefficient:** r<sup>2</sup> greater than 0.998

**Accuracy:** Error less than 5%

COMPOUND	RRT	COMPOUND	RRT
amphetamine	0.670	<b>2C-B</b>	<b>1.00 (1.804 min)</b>
methamphetamine	0.679	caffeine	1.023
C <sub>14</sub>	0.7211	2-C-I	1.144
3,4-MDA	0.763	2C-T-2	1.175
TFMPP	0.783	2C-T-7	1.327
3,4-MDMA	0.788	procaine	1.379
3,4-MDEA	0.813	tetracaine	2.040

## 6. QUALITATIVE DATA

### 6.1. ULTRAVIOLET SPECTROPHOTOMETRY

SOLVENT	MAXIMUM ABSORBANCE (NM)
Aqueous Acid	293

### 6.2. LIQUID CHROMATOGRAPHY/MASS SPECTROMETRY

#### Method Phen01

##### Sample Preparation:

Dilute analyte in an appropriate volume of HPLC-grade water and pass through 0.45  $\mu$ m polypropylene filter.

Introduce solution via divert valve of the mass spectrometer with a flow rate of 400  $\mu\text{L}/\text{minute}$  of HPLC-grade water.

<b><i>Instrument:</i></b>	LCQ Advantage MAX in ESI Mode	
<b><i>Sheath Gas (arb):</i></b>	10	
<b><i>Auxiliary/Sweep Gas (arb):</i></b>	0	
<b><i>Spray Voltage (kV):</i></b>	4.50	
<b><i>Spray Current (<math>\mu\text{A}</math>):</i></b>	0.29	
<b><i>Capillary Temperature (<math>^{\circ}\text{C}</math>):</i></b>	250.0	
<b><i>Capillary Voltage (V):</i></b>	13.00	
<b><i>Tube Lens Offset (V):</i></b>	-25.00	
<b><i>Mass Range:</i></b>	Normal; 65-550 amu	
<b><i>Scan Mode:</i></b>	MS or $\text{MS}^3$ (depending on experiment performed)	
<b><i>Scan Type:</i></b>	Full	
<b><i>Scan Time (microscans):</i></b>	1	
<b><i>Maximum Injection Time (ms):</i></b>	1000.0	
<b><i>Source Fragmentation:</i></b>	Off	
<b><i>For <math>\text{MS}^3</math> experiments</i></b>		
<b><i>Parent Masses (m/z):</i></b>	$\text{MS}^2$ : 261.0	$\text{MS}^3$ : 244.0
<b><i>Isolation Width (m/z):</i></b>	1.0	
<b><i>Normalized Collision Energy (%):</i></b>	$\text{MS}^2$ : 25.0	$\text{MS}^3$ : 35.0
<b><i>Activation Q:</i></b>	0.250	
<b><i>Activation Time (msec):</i></b>	30.0	

See spectra on the following pages for [Mass Spectrometry](#), [Nuclear Magnetic Resonance Spectroscopy](#), and [Infrared Spectroscopy](#).

## **7. REFERENCES**

Budavari, S., *The Merck Index, 13<sup>th</sup> Edition*, Merck and Co., Inc., 2001, p. 323.

Clark, C.C., "IR Spectrum of 4-Bromo-2,5-Dimethoxyphenethylamine HCl," *Microgram*, Vol. XII, No. 12, p. 240.

Galichet, L., *Clarke's Analysis of Drugs and Poisons, 3rd Edition*, The Pharmaceutical Press, 2004.  
*National Drug Intelligence Center*, "2C-B (Nexus) Reappears on the Club Drug Scene," Information Bulletin, May 2001.

Noggle, F.T., DeRuiter, J., and Clark, C. R., "Analytical Profiles of 4-Bromo-2,5-Dimethoxyphenethylamine ("Nexus") and Related Precursor Chemicals," *Microgram*, Vol. XXVII, No. 10, October 1994, pp. 343-355.

Samuels, M.S., "4-Bromo-2,5-Dimethoxyphenethylamine," *Microgram*, Vol. XII, No. 1, pp. 4-11.

*Federal Register*, Vol. 59, No. 4, Jan. 6, 1994, pp. 671-673.

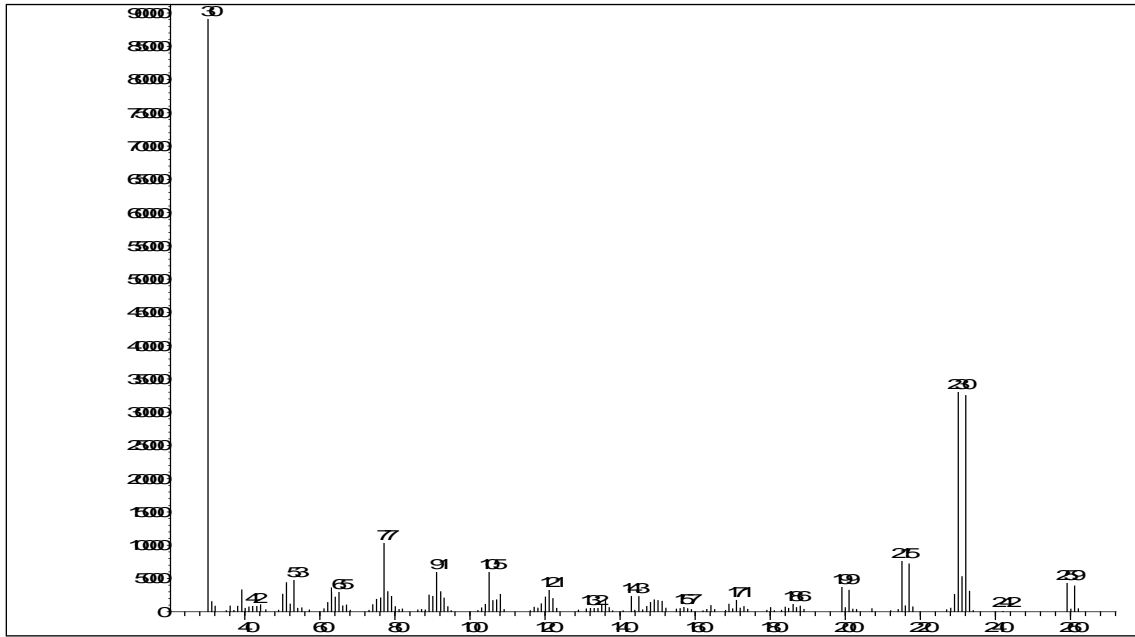
## **8. ADDITIONAL RESOURCES**

[Forendex](#)

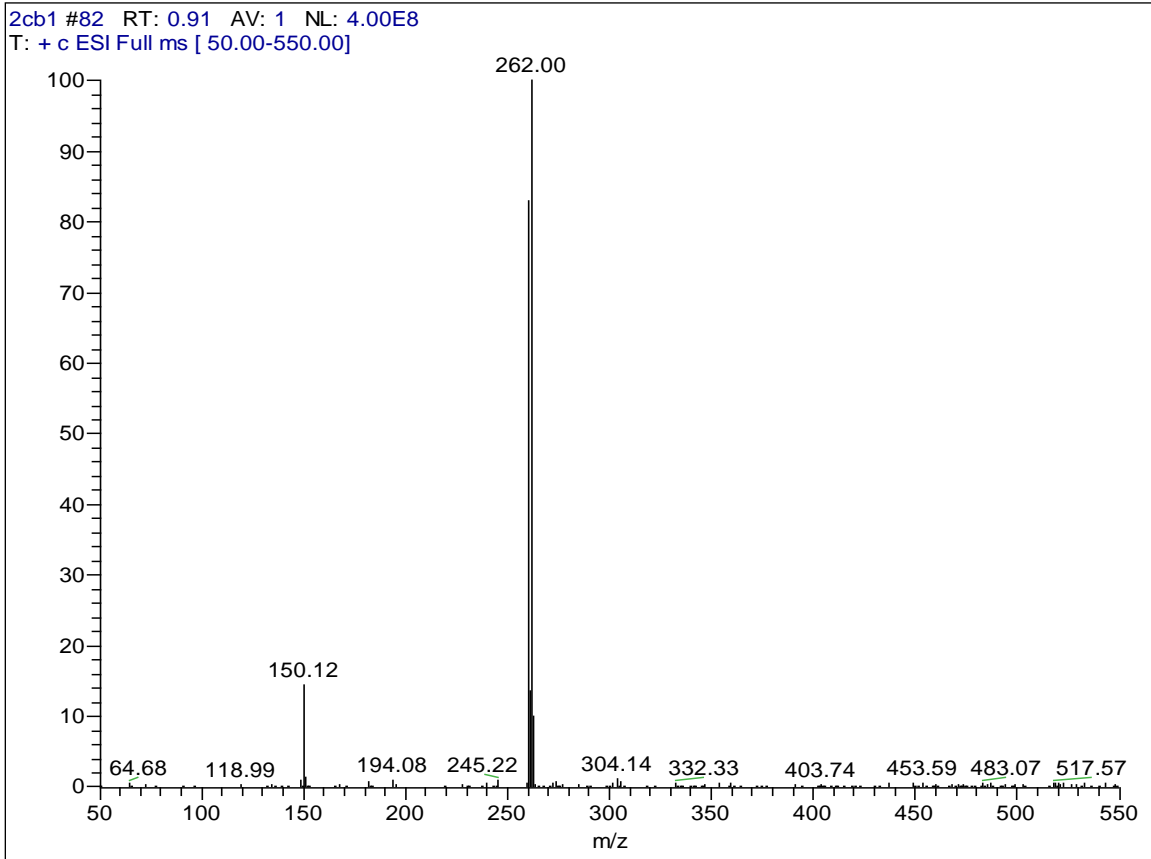
[Wikipedia](#)

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EI Mass Spectrum: 2C-B Lot # 3TDM-20-02

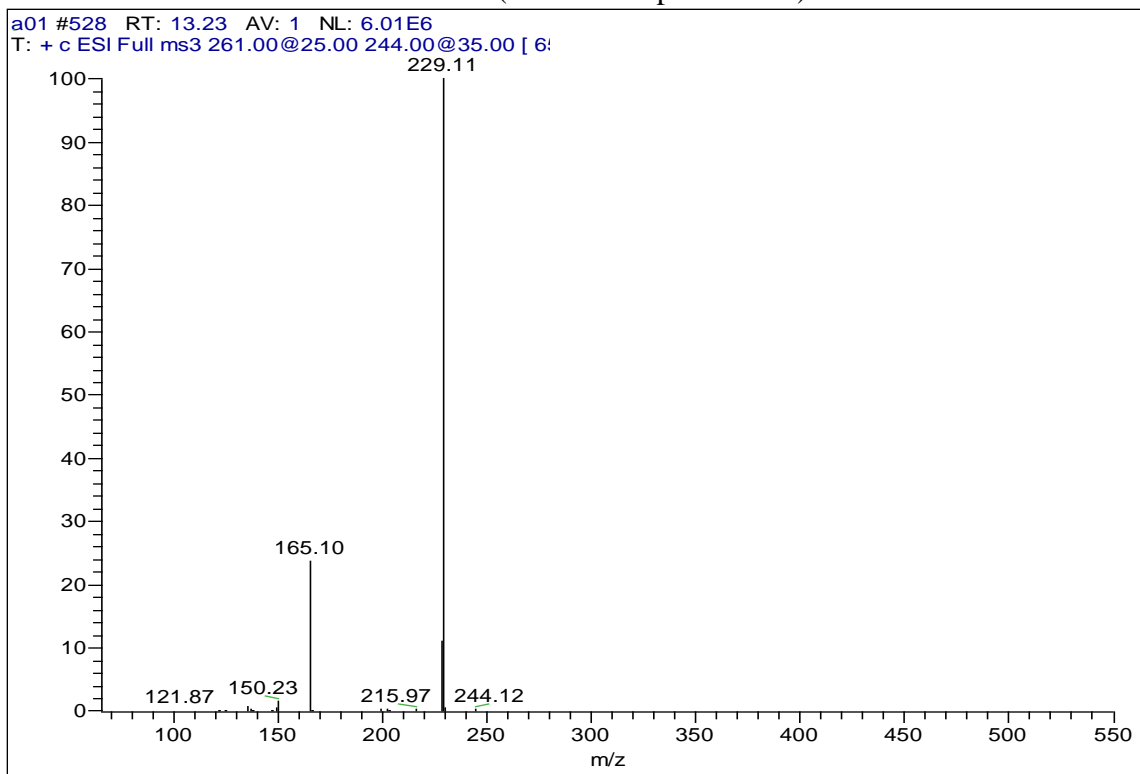


API – ESI Mass Spectrum: 2C-B Lot # 3TDM-20-02  
MS mode (see text for parameters)

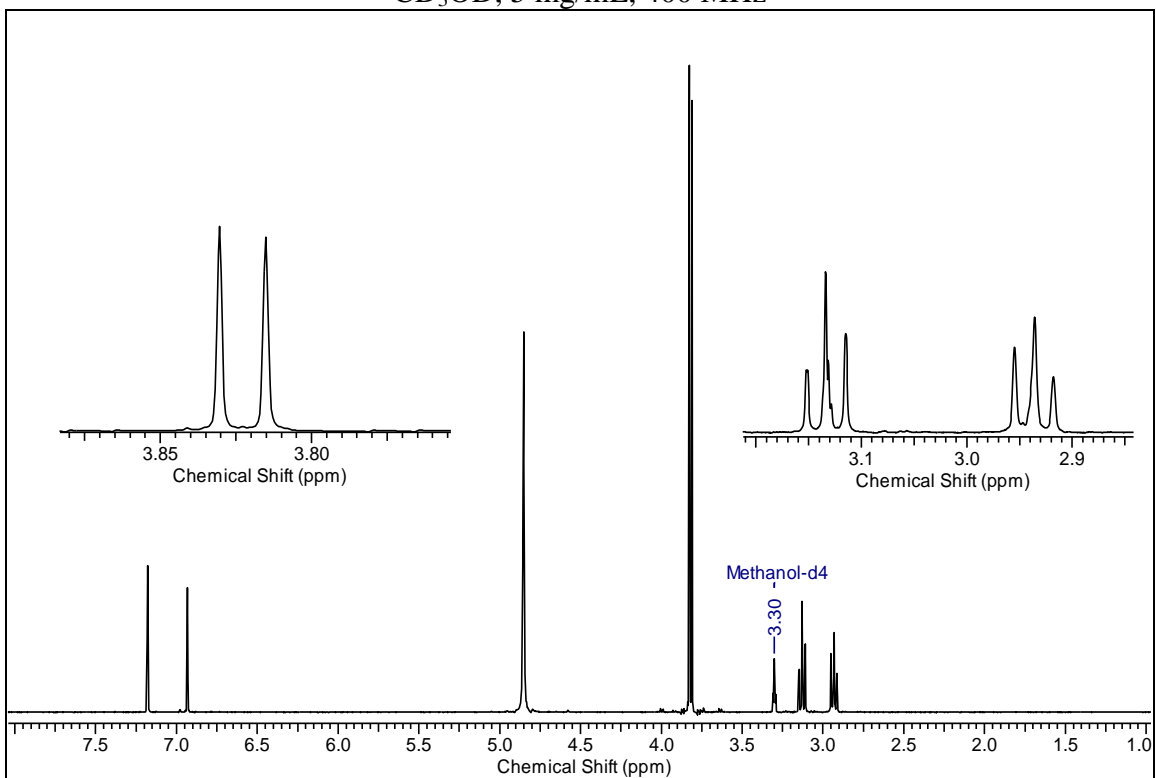




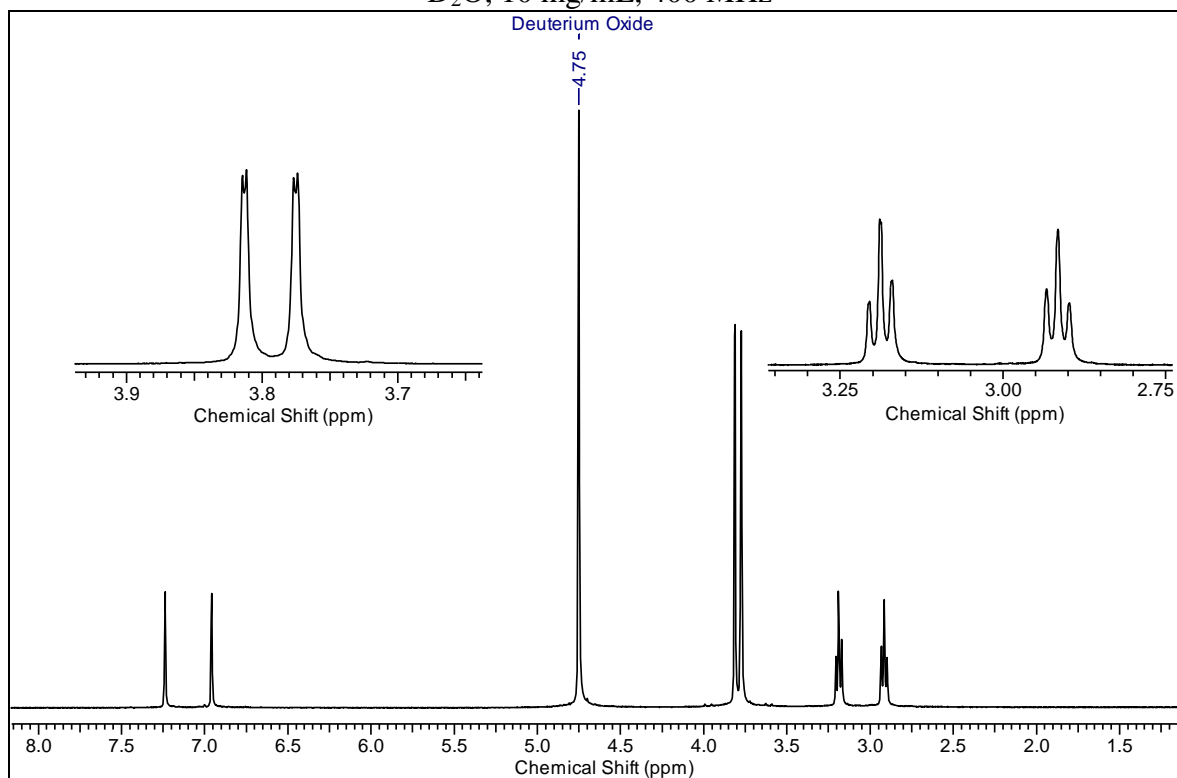
API – ESI Mass Spectrum: 2C-B Lot # 3TDM-20-02  
MS<sup>3</sup> mode (see text for parameters)



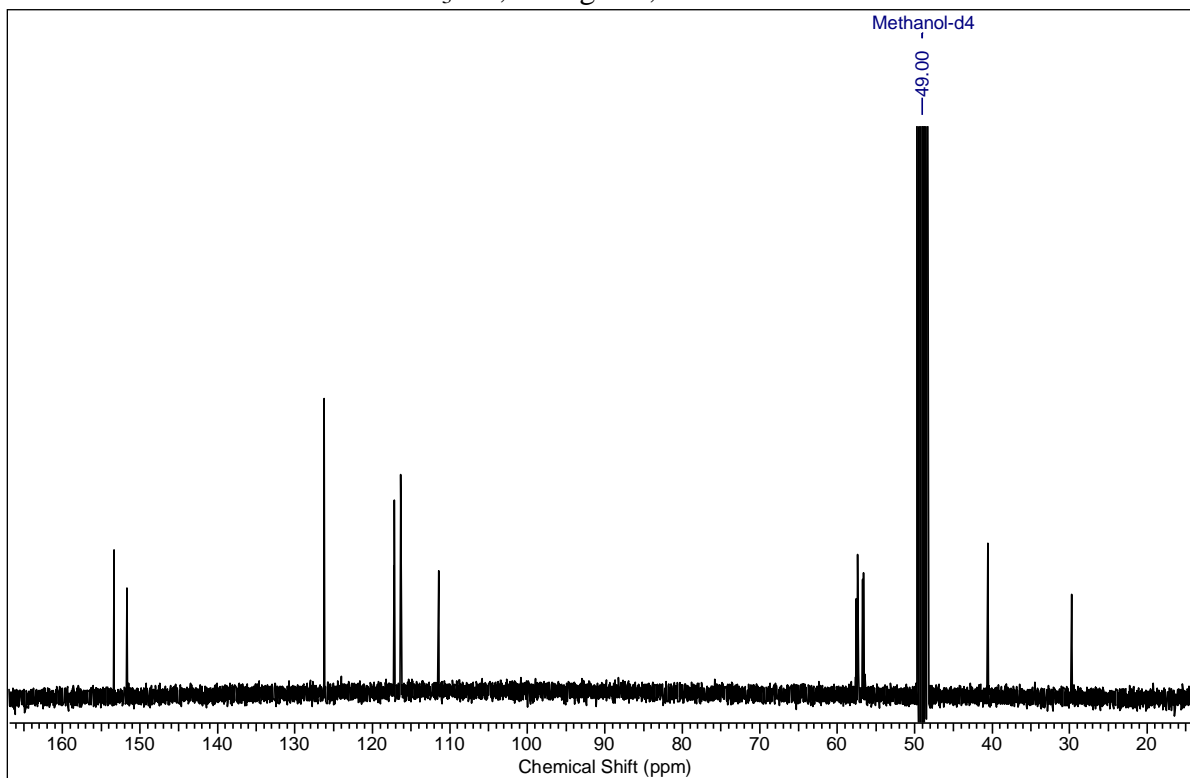
<sup>1</sup>H NMR: 2C-B HCl Lot # 3TDM-20-02  
CD<sub>3</sub>OD, 5 mg/mL, 400 MHz



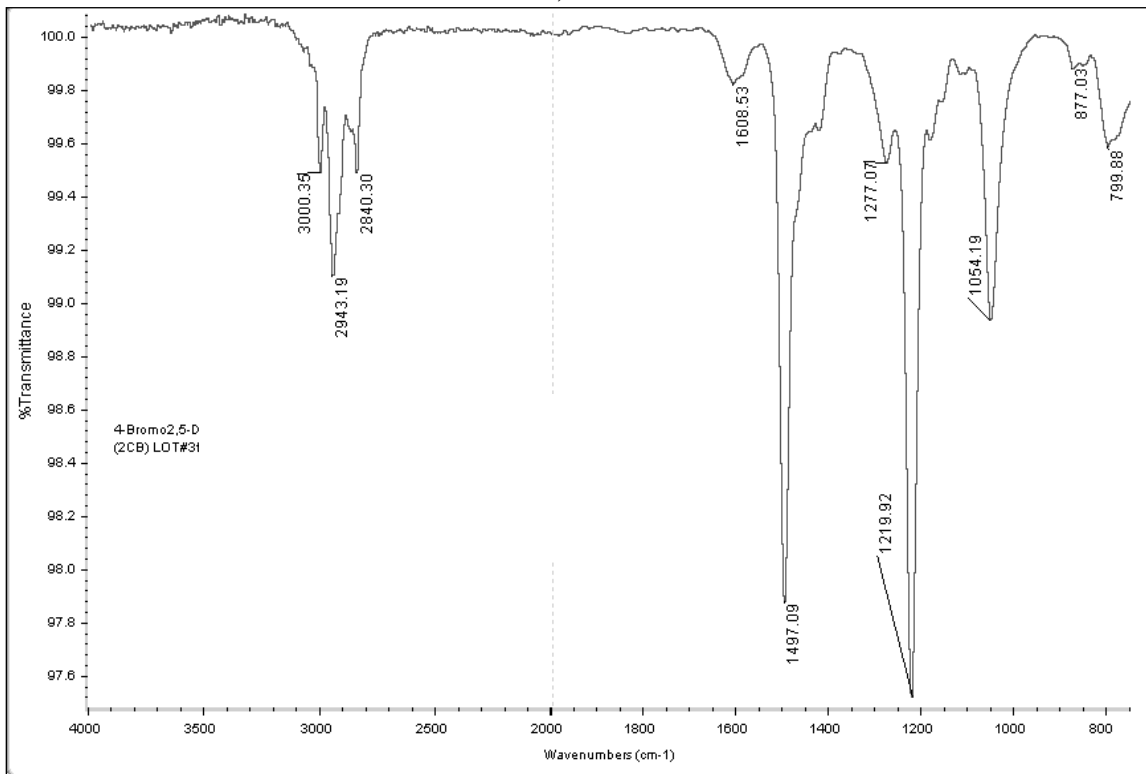
$^1\text{H}$  NMR: 2C-B HCl Lot #3 TDM-20-02  
 $\text{D}_2\text{O}$ , 10 mg/mL, 400 MHz



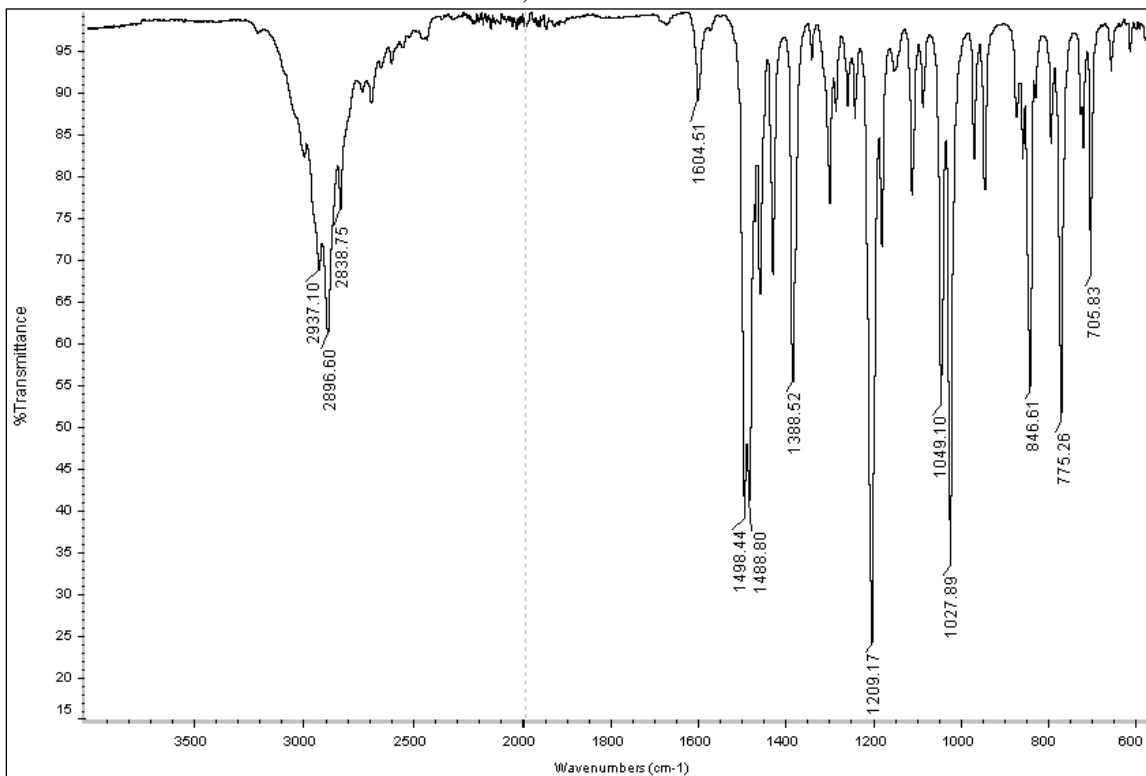
$^{13}\text{C}$  NMR: 2C-B HCl Lot #3 TDM-20-02  
 $\text{CD}_3\text{OD}$ , 30 mg/mL, 100.6 MHz



IR: (Vapor Phase) 2C-B\* Lot #3TDM-20-02  
280°C, 8 cm<sup>-1</sup> resolution



FTIR (Diamond ATR, 3 bounce): 2C-B HCl Lot # 3TDM-20-02  
32 scans, 4 cm<sup>-1</sup> resolution



\*Note: cannot be used to distinguish from 2C-I using above parameters

Abbreviations used:

BZP = 1-benzylpiperazine

2C-B = 4-bromo-2,5-dimethoxyphenethylamine

2C-T-2 = 2,5-dimethoxy-4-ethylthiophenethylamine

2C-T-7 = 2,5-dimethoxy-(4-N-propylthio)-beta-phenethylamine

2C-I = 4-iodo-2,5-dimethoxy-beta-phenethylamine

4-MeOPP = 1-(4-methoxyphenyl)piperazine

TFMPP = trifluoromethylphenylpiperazine

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