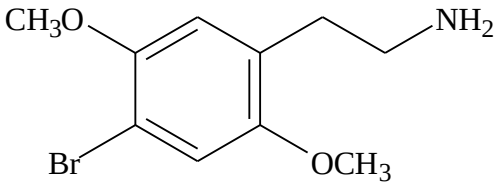
4-BROMO-2,5-DIMETHOXYPHENETHYLAMINE

Latest Revision: August 22, 2005



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
α-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	$C_{10}H_{14}BrNO_2$	260.13	Not available
Hydrochloride	$C_{10}H_{14}BrNO_2$•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	**2C-B**	**1.00 (4.232 min)**
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

Instrument: High performance liquid chromatograph equipped with mass spectrometer

Column: 5 µm ODS, 150 mm x 4.6 mm

Detector: Mass Spectrometer

Flow: 400 µL/min

Injection Volume: 5.0 µL

Buffer: 10 mM ammonium acetate in water

Mobile Phase: 1) Initially, CH_3OH: buffer 5:95 held for 10 min
2) Gradient to CH_3OH: buffer 80:20 over 10 min
3) Gradient to CH_3OH: 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
2C-B	**1.00 (12.88 min)**		

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_{14}) 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: 1µL

Typical Retention Time: 2C-B HCl: 1.80 min
C_{14}: 1.30 min

Linear Range: 0.258 – 3.178 mg/mL

Repeatability: RSD less than 3%

Correlation Coefficient: r^2 greater than 0.998

Accuracy: Error less than 5%

COMPOUND	RRT	COMPOUND	RRT
amphetamine	0.670	**2C-B**	**1.00 (1.804 min)**
methamphetamine	0.679	caffeine	1.023
C_{14}	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 µm polypropylene filter.

Introduce solution via divert valve of the mass spectrometer with a flow rate of 400 µL/minute of HPLC-grade water.

Instrument:	LCQ Advantage MAX in ESI Mode
Sheath Gas (arb):	10
Auxiliary/Sweep Gas (arb):	0
Spray Voltage (kV):	4.50
Spray Current (µA):	0.29
Capillary Temperature (°C):	250.0
Capillary Voltage (V):	13.00
Tube Lens Offset (V):	-25.00
Mass Range:	Normal; 65-550 amu
Scan Mode:	MS or MS^3 (depending on experiment performed)
Scan Type:	Full
Scan Time (microscans):	1
Maximum Injection Time (ms):	1000.0
Source Fragmentation:	Off
For MS^3 experiments	
Parent Masses (m/z):	MS^2: 261.0 MS^3: 244.0
Isolation Width (m/z):	1.0
Normalized Collision Energy (%):	MS^2: 25.0 MS^3: 35.0
Activation Q:	0.250
Activation Time (msec):	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, 13th 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.

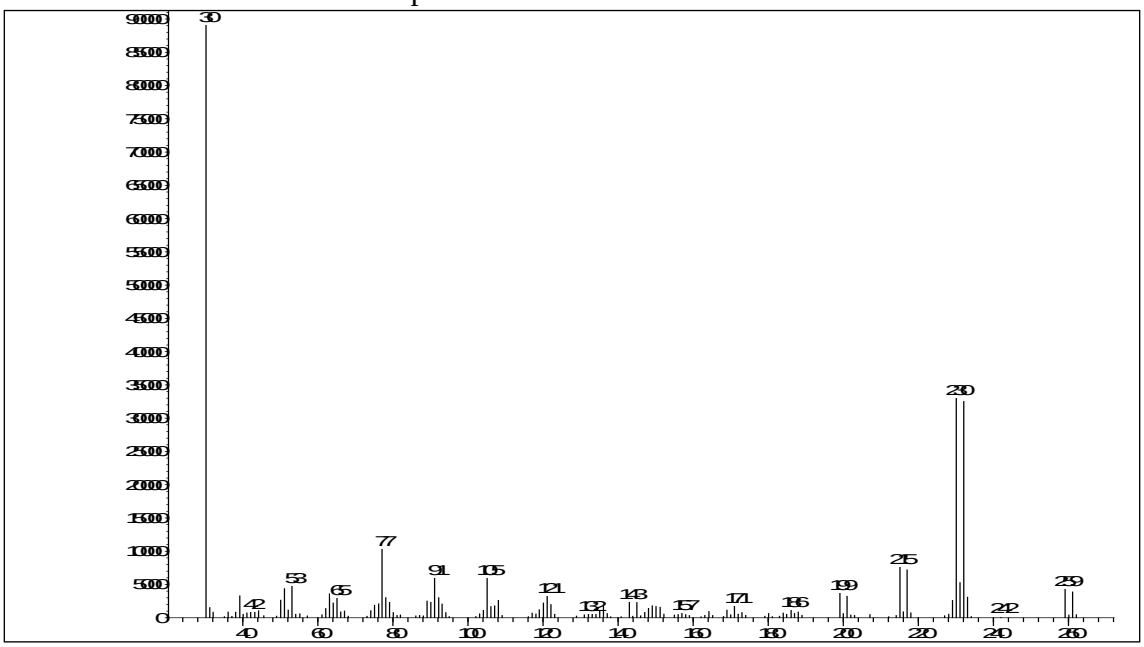
Federal Register, Vol. 59, No. 4, Jan. 6, 1994, pp. 671-673.

8. ADDITIONAL RESOURCES

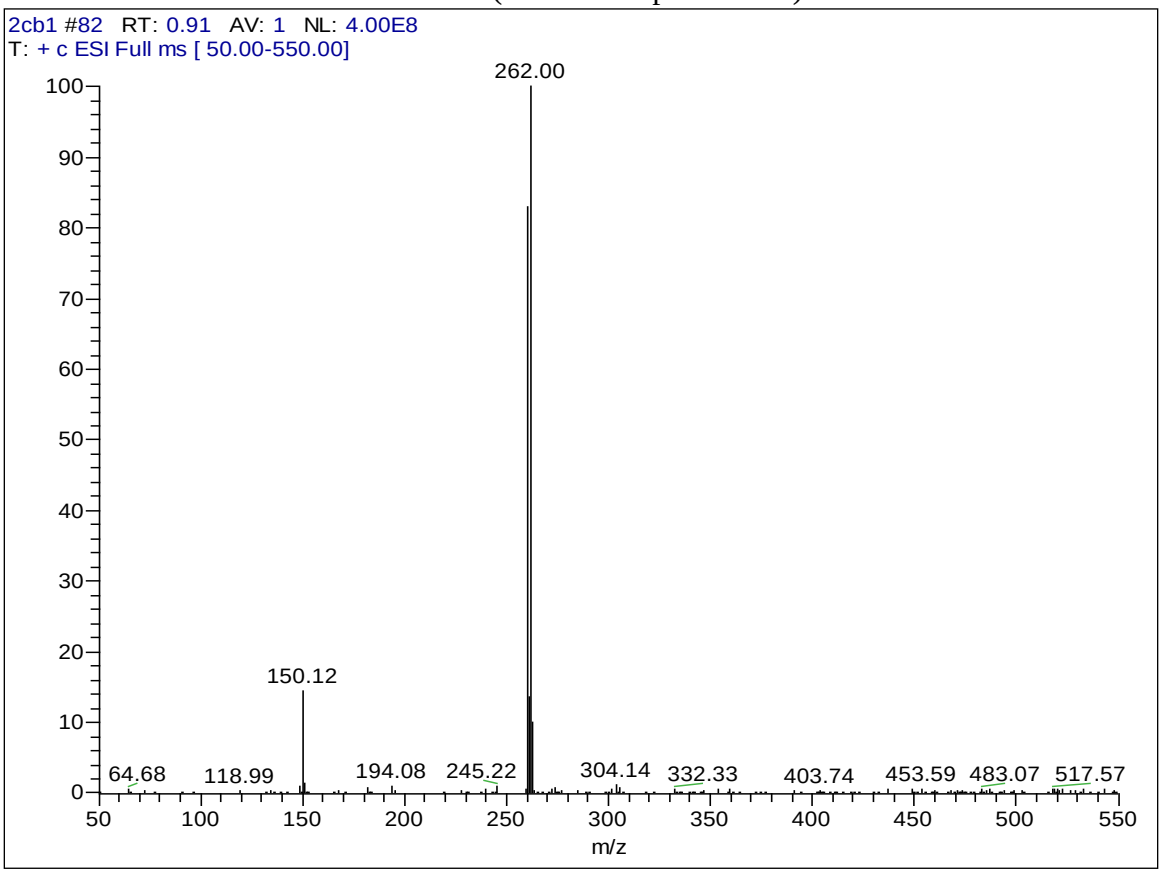
Forendex

Wikipedia

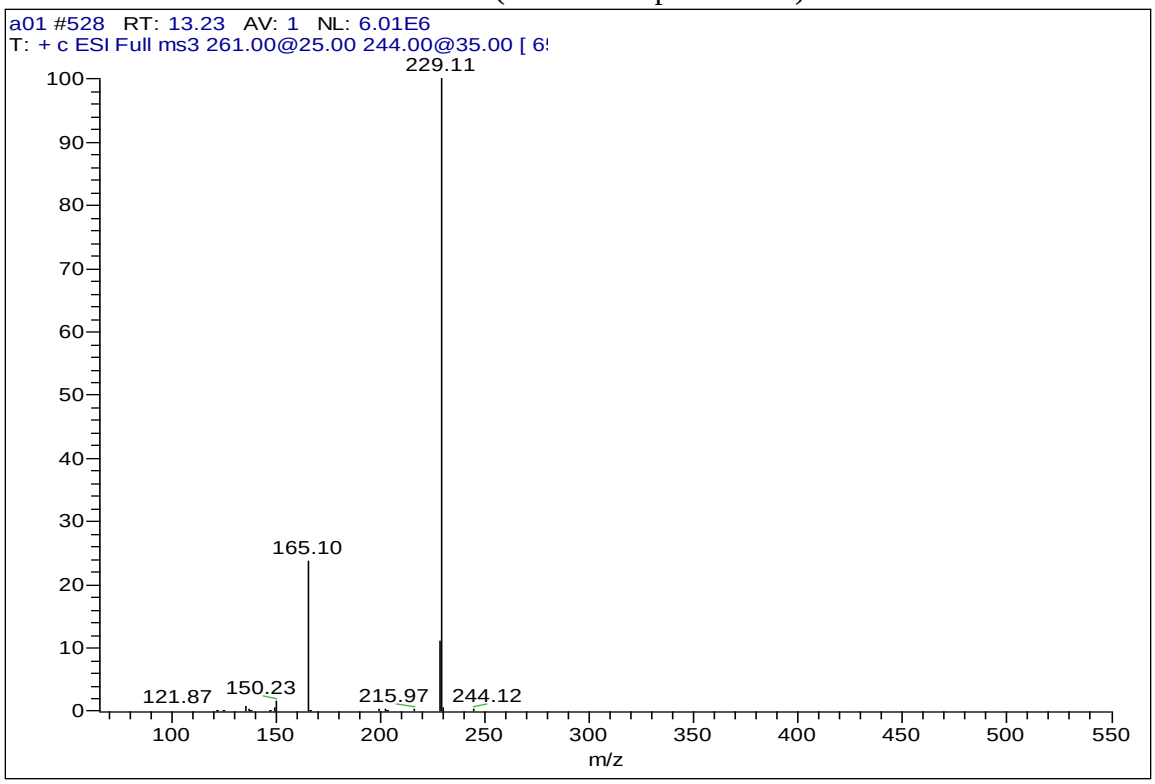
EI Mass Spectrum: 2C-B Lot # 3TDM-20-02



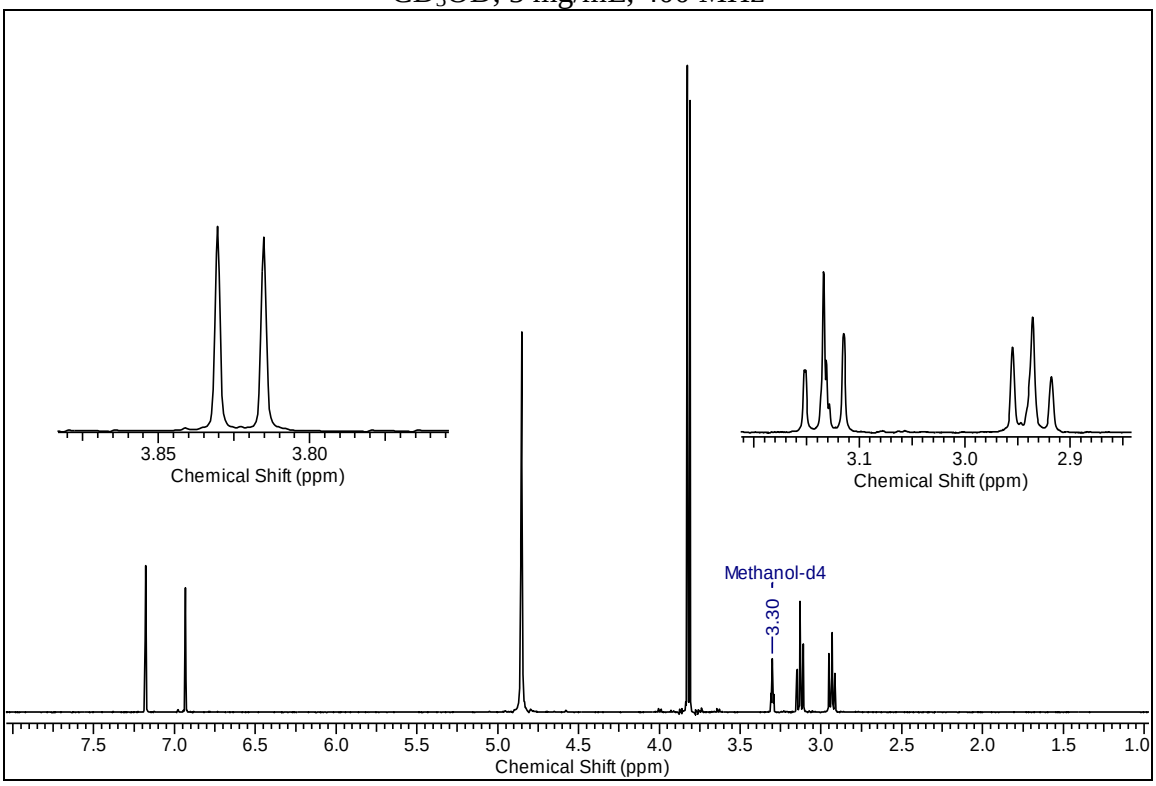
API – ESI Mass Spectrum: 2C-B Lot # 3TDM-20-02
MS mode (see text for parameters)



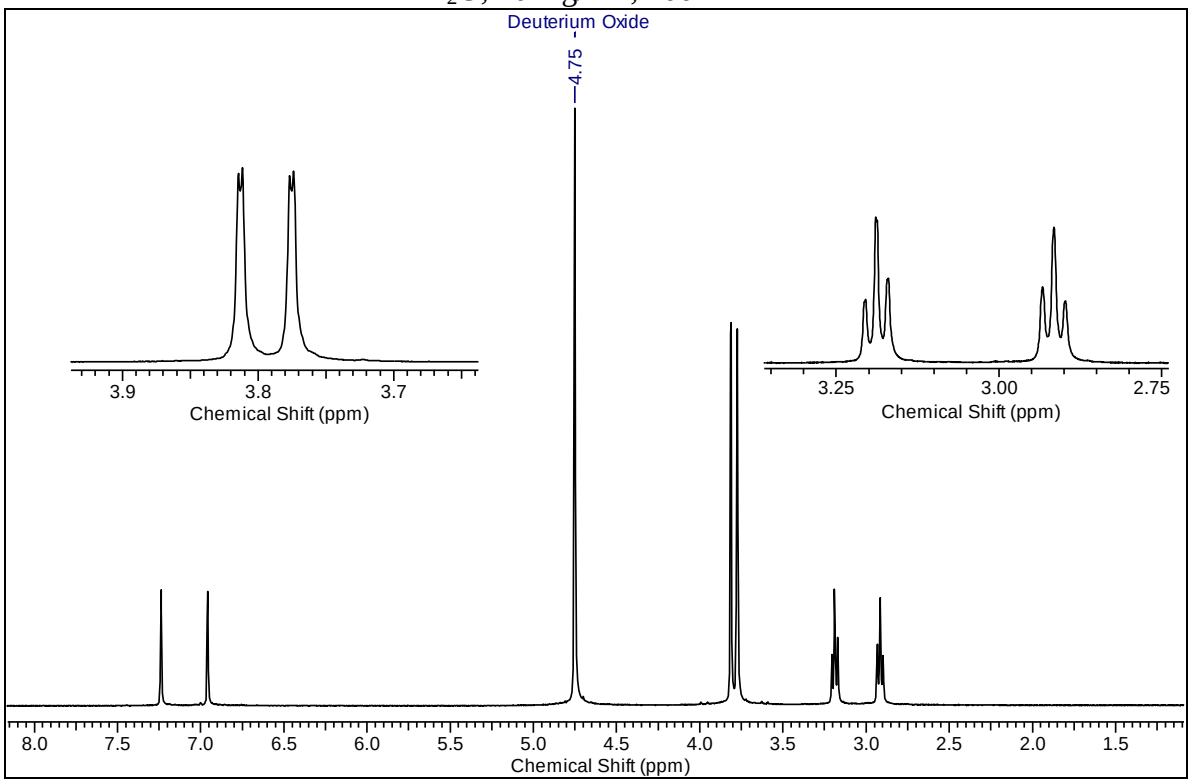
API – ESI Mass Spectrum: 2C-B Lot # 3TDM-20-02
MS^3 mode (see text for parameters)



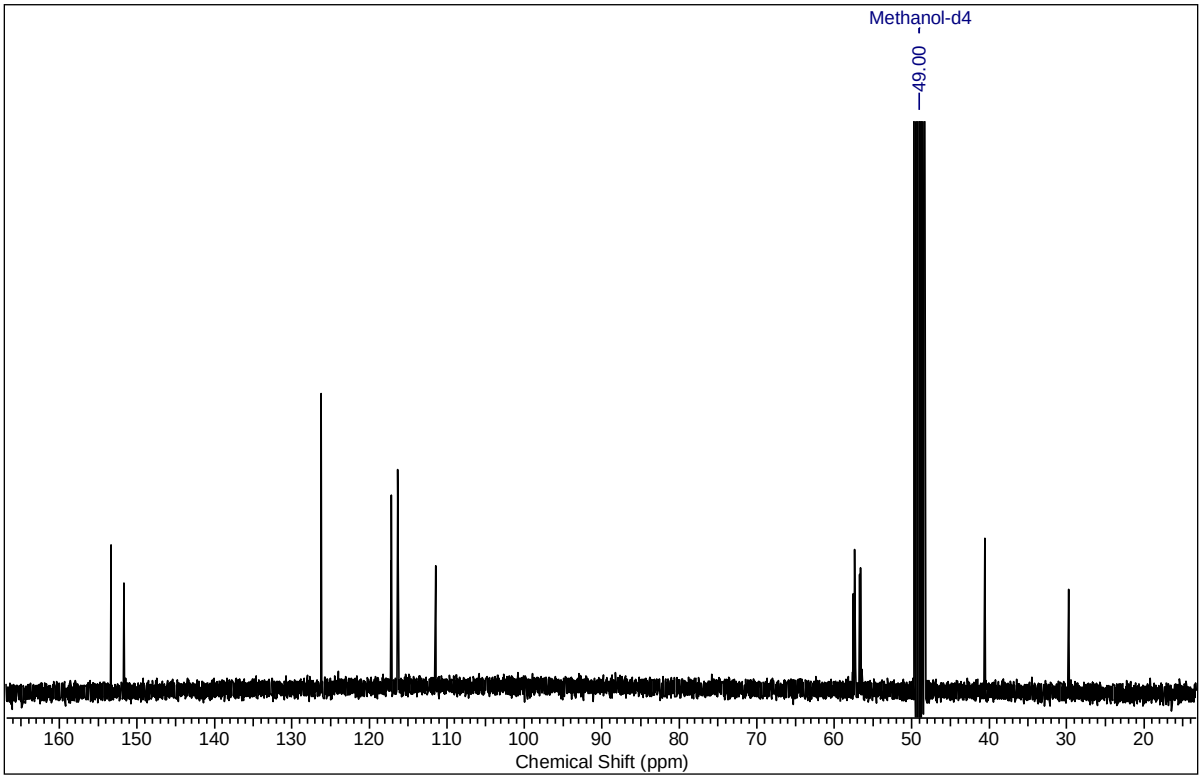
^1H NMR: 2C-B HCl Lot # 3TDM-20-02
CD_3OD, 5 mg/mL, 400 MHz



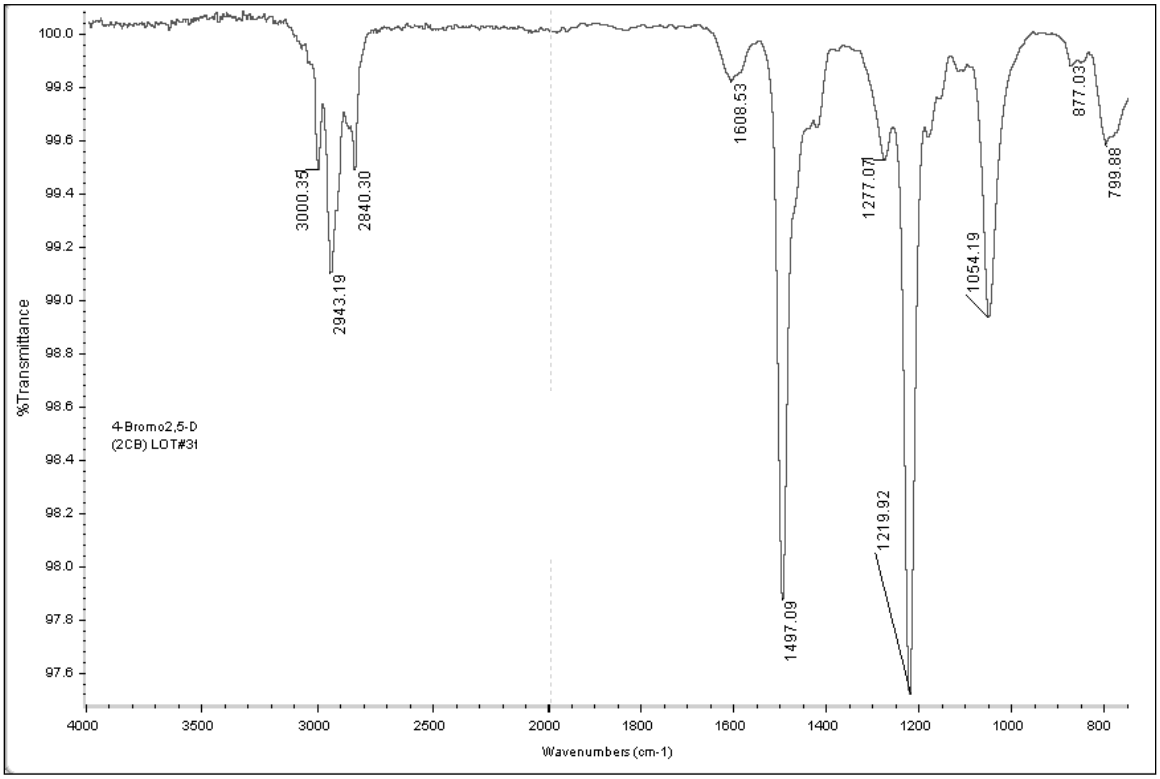
^{1}H NMR: 2C-B HCl Lot #3 TDM-20-02
D_2O, 10 mg/mL, 400 MHz



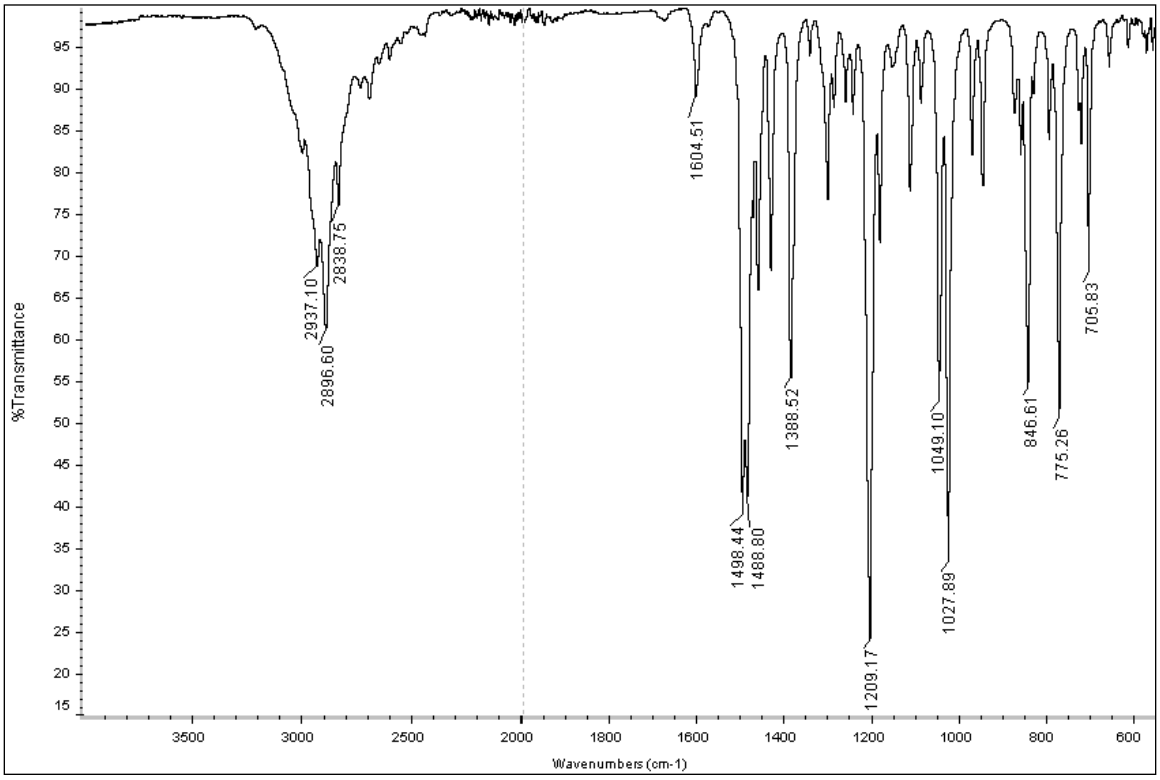
^{13}C NMR: 2C-B HCl Lot #3TDM-20-02
CD_3OD, 30 mg/mL, 100.6 MHz



IR: (Vapor Phase) 2C-B* Lot #3TDM-20-02
280°C, 8 cm^{-1} resolution



FTIR (Diamond ATR, 3 bounce): 2C-B HCl Lot # 3TDM-20-02
32 scans, 4 cm^{-1} 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
