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
- β-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

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C_{10}H_{14}BrNO_{2}</td>
<td>260.13</td>
<td>Not available</td>
</tr>
<tr>
<td>Hydrochloride</td>
<td>C_{10}H_{14}BrNO_{2}\cdot HCl</td>
<td>296.59</td>
<td>237-239</td>
</tr>
</tbody>
</table>
2.2. SOLUBILITY

<table>
<thead>
<tr>
<th>Form</th>
<th>A</th>
<th>C</th>
<th>E</th>
<th>H</th>
<th>M</th>
<th>W</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>N/A</td>
<td>S</td>
<td>S</td>
<td>N/A</td>
<td>S</td>
<td>I</td>
</tr>
<tr>
<td>Hydrochloride</td>
<td>SS</td>
<td>S</td>
<td>I</td>
<td>N/A</td>
<td>S</td>
<td>S</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>REAGENT</th>
<th>COLOR PRODUCED</th>
</tr>
</thead>
<tbody>
<tr>
<td>Marquis</td>
<td>green</td>
</tr>
<tr>
<td>Mecke</td>
<td>green to yellow (slow) to blue (slow)</td>
</tr>
</tbody>
</table>

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.

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

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, CH₃OH: buffer 5:95 held for 10 min
2) Gradient to CH₃OH: buffer 80:20 over 10 min
3) Gradient to CH₃OH: buffer 5:95 over 10 min

Samples are to be dissolved in buffer solution, sonicated, then filtered with a 0.45-micron filter paper.
<table>
<thead>
<tr>
<th>COMPOUND</th>
<th>RRT</th>
<th>COMPOUND</th>
<th>RRT</th>
</tr>
</thead>
<tbody>
<tr>
<td>ephedrine/pseudoephedrine</td>
<td>0.786</td>
<td>2C-I</td>
<td>1.031</td>
</tr>
<tr>
<td>amphetamine</td>
<td>0.861</td>
<td>2C-T-2</td>
<td>1.036</td>
</tr>
<tr>
<td>methamphetamine</td>
<td>0.872</td>
<td>MDMA</td>
<td>1.060</td>
</tr>
<tr>
<td>MDEA</td>
<td>0.890</td>
<td>2C-T-7</td>
<td>1.105</td>
</tr>
<tr>
<td>2C-B</td>
<td>1.00 (12.88 min)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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 (C₁₄) 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
C₁₄: 1.30 min

Linear Range:
0.258 – 3.178 mg/mL

Repeatability:
RSD less than 3%

Correlation Coefficient:
r² greater than 0.998

Accuracy:
Error less than 5%

<table>
<thead>
<tr>
<th>COMPOUND</th>
<th>RRT</th>
<th>COMPOUND</th>
<th>RRT</th>
</tr>
</thead>
<tbody>
<tr>
<td>amphetamine</td>
<td>0.670</td>
<td>2C-B</td>
<td>1.00 (1.804 min)</td>
</tr>
<tr>
<td>methamphetamine</td>
<td>0.679</td>
<td>caffeine</td>
<td>1.023</td>
</tr>
<tr>
<td>C₁₄</td>
<td>0.7211</td>
<td>2-C-I</td>
<td>1.144</td>
</tr>
<tr>
<td>3,4-MDA</td>
<td>0.763</td>
<td>2C-T-2</td>
<td>1.175</td>
</tr>
<tr>
<td>TFMPP</td>
<td>0.783</td>
<td>2C-T-7</td>
<td>1.327</td>
</tr>
<tr>
<td>3,4-MDMA</td>
<td>0.788</td>
<td>procaine</td>
<td>1.379</td>
</tr>
<tr>
<td>3,4-MDEA</td>
<td>0.813</td>
<td>tetracaine</td>
<td>2.040</td>
</tr>
</tbody>
</table>

6. QUALITATIVE DATA

6.1. ULTRAVIOLET SPECTROPHOTOMETRY

<table>
<thead>
<tr>
<th>SOLVENT</th>
<th>MAXIMUM ABSORBANCE (NM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aqueous Acid</td>
<td>293</td>
</tr>
</tbody>
</table>

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 MS³ (depending on experiment performed)

**Scan Type:**
Full

**Scan Time (microscans):**
1

**Maximum Injection Time (ms):**
1000.0

**Source Fragmentation:**
Off

**For MS³ experiments**

**Parent Masses (m/z):**
MS²: 261.0  MS³: 244.0

**Isolation Width (m/z):**
1.0

**Normalized Collision Energy (%):**
MS²: 25.0  MS³: 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


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
MS² mode (see text for parameters)

¹H NMR: 2C-B HCl Lot # 3TDM-20-02
CD₃OD, 5 mg/mL, 400 MHz
\(^1\)H NMR: 2C-B HCl Lot #3 TDM-20-02
D\(_2\)O, 10 mg/mL, 400 MHz

\(^{13}\)C NMR: 2C-B HCl Lot #3 TDM-20-02
CD\(_3\)OD, 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