1. SYNONYMS

**CFR:** 2,5-Dimethoxy-4-n-propylthiophenethylamine

**CAS #:**
- Base: Not Available
- Hydrochloride: 207740-26-9

**Other Names:**
- 2,5-Dimethoxy-4-
- 2,5-Dimethoxy-4-n-propylthiophenethylamine
- 2,5-Dimethoxy-4-propylthio-beta-phenethylamine
- 4-n-Propylthio-2,5-dimethoxybenzeneethanamine
- 2C-T-7

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_{13}H_{21}NO_{2}S</td>
<td>255.38</td>
<td>Not available</td>
</tr>
<tr>
<td>Hydrochloride</td>
<td>C_{13}H_{21}NO_{2}S·HCl</td>
<td>291.84</td>
<td>195-198</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>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>Hydrochloride</td>
<td>PS</td>
<td>S</td>
<td>S</td>
<td>NA</td>
<td>VS</td>
<td>VS</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, NA = not available

3. SCREENING TECHNIQUES

3.1. COLOR TESTS
3.2. GAS CHROMATOGRAPHY

Method SFL4 Screen

**Instrument:**
Gas chromatograph operated in split mode with FID

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

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

**Makeup gas:**
FID: 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 injection

Sample dissolved in water and base extracted with 1-5 N sodium hydroxide into an organic solvent.

<table>
<thead>
<tr>
<th>COMPOUND</th>
<th>RRT</th>
<th>COMPOUND</th>
<th>RRT</th>
</tr>
</thead>
<tbody>
<tr>
<td>amphetamine</td>
<td>0.446</td>
<td>4-MeOPP</td>
<td>0.850</td>
</tr>
<tr>
<td>methamphetamine</td>
<td>0.483</td>
<td>2C-B</td>
<td>0.880</td>
</tr>
<tr>
<td>nicotinamide</td>
<td>0.596</td>
<td>caffeine</td>
<td>0.889</td>
</tr>
<tr>
<td>3,4-MDA</td>
<td>0.673</td>
<td>2C-I</td>
<td>0.941</td>
</tr>
<tr>
<td>TFMPP</td>
<td>0.700</td>
<td>2C-T-2</td>
<td>0.954</td>
</tr>
<tr>
<td>3,4-MDMA</td>
<td>0.717</td>
<td>2C-T-7</td>
<td>1.000 (4.808 min)</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, and then filtered with a 0.45 µm filter.

<table>
<thead>
<tr>
<th>COMPOUND</th>
<th>RRT</th>
<th>COMPOUND</th>
<th>RRT</th>
</tr>
</thead>
<tbody>
<tr>
<td>ephedrine/pseudoephedrine</td>
<td>0.711</td>
<td>2C-I</td>
<td>0.933</td>
</tr>
<tr>
<td>amphetamine</td>
<td>0.779</td>
<td>2C-T-2</td>
<td>0.938</td>
</tr>
<tr>
<td>methamphetamine</td>
<td>0.789</td>
<td>3,4-MDMA</td>
<td>0.959</td>
</tr>
<tr>
<td>3,4-MDEA</td>
<td>0.805</td>
<td>2C-T-7</td>
<td>1.000 (14.24 min)</td>
</tr>
<tr>
<td>2C-B</td>
<td>0.904</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

4. SEPARATION TECHNIQUES
5. QUANTITATIVE PROCEDURES

5.1. GAS CHROMATOGRAPHY

Method SFL4 4dimeth1

*Internal Standard Stock Solution:*
1.00 mg/mL tetradecane (C\textsubscript{14}) in methylene chloride.

*Standard Solution Preparation:*
Prepare a standard solution of 2C-T-7·HCl within the linearity range listed below.

*Sample Preparation:*
Accurately weight an amount of sample into a volumetric flask so that the final 2C-T-7 HCl concentration is approximately equivalent to that of the standard solution. Dilute to volume with deionized water. A 2 mL aliquot of the sample is then extracted with 2 mL of 1M-5M sodium hydroxide into 2 mL of the internal standard stock solution.

**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 program: 220°C isothermal

**Injection Parameters:**
Split Ratio: 50:1
1 µL injection
Typical Retention Time: 2C-T-7·HCl: 2.39 min  
C_{14}: 1.30 min

Linear Range: 0.166 – 4.978 mg/mL

Repeatability: RSD less than 3%

Correlation Coefficient: \( r^2 \) 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>0.505</td>
<td>2C-B</td>
<td>0.754</td>
</tr>
<tr>
<td>methamphetamine</td>
<td>0.512</td>
<td>caffeine</td>
<td>0.771</td>
</tr>
<tr>
<td>C_{14}</td>
<td>0.543</td>
<td>2C-I</td>
<td>0.862</td>
</tr>
<tr>
<td>3,4-MDA</td>
<td>0.575</td>
<td>2C-T-2</td>
<td>0.886</td>
</tr>
<tr>
<td>TFMPP</td>
<td>0.590</td>
<td>2C-T-7</td>
<td>1.000 (2.39 min)</td>
</tr>
<tr>
<td>3,4-MDMA</td>
<td>0.594</td>
<td>procaine</td>
<td>1.039</td>
</tr>
<tr>
<td>3,4-MDEA</td>
<td>0.613</td>
<td>tetracaine</td>
<td>1.537</td>
</tr>
</tbody>
</table>

5.2. NUCLEAR MAGNETIC RESONANCE

Method SFL1 NMR1-2

Reagents: Deuterochloroform (CDCl$_3$) containing TMS (Tetramethysilane) for 0 ppm reference

Internal Standard Stock Solution (ISSS): Commercially available deuterochloroform (CDCl$_3$) containing TMS. Determine TMS concentration by quantitating with a pure reference standard such as dimethylsulfone.

Sample Preparation: Accurately weigh an amount of sample, usually 10-30 mg, into a centrifuge tube and add 1 mL of CDCl$_3$ that does not contain TMS. Vortex for several seconds. If insolubles are present, sonicate 15 min. Add 1.0 mL ISSS, mix and filter if necessary. Place in NMR sample tube.
**Instrument:** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

**Parameters:**
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse width: lesser of 10 µs or 90°
- Delay between pulses: 45 s
- Number of scans (NT): multiple of 4
- Number of steady state scans: 0
- Linearity throughout spectrum: oversampling of 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

**Total Run Time per Sample:**
- 6 min (NT = 4)
- 14 min (NT = 16)

**Uniformity within spectral width:** 0.3% RSD (-0.6 to 11.4 ppm)

**Linear Range:** 0.6 - 60 mg/mL

**Repeatability:** less than 4%

**Correlation Coefficient:** 1.000

**Accuracy:** less than 3%

**Signals used for quantitation (position in ppm with number of protons):**
- 6.8 (2)
- 3.2 (2)
- 3.0 (2)
- 1.0 (3)

**Method SFL1 NMR1-5**

**Reagents:**
deuterochloroform (CDCl$_3$) containing TMS (tetramethylsilane) for 0 ppm reference and deuteromethanol (CD$_3$OD) to aid solubility

**Internal Standard Stock Solution (ISSS):**
Commercially available deuterochloroform (CDCl$_3$) containing TMS. Determine TMS concentration by quantitating with a pure reference standard such as dimethylsulfone.

**Sample Preparation:**
Accurately weigh an amount of sample, usually 10-30 mg, into a centrifuge tube and add 2 mL of ISSS and 1 mL of CD$_3$OD, not containing TMS. Vortex for several seconds. If insolubles are present, sonicate 15 minutes. Filter if necessary. Place in NMR sample tube.

**Instrument:** Varian Mercury 400 MHz NMR spectrometer with proton detection probe
**Parameters:**
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse width: lesser of 10 µs or 90°
- Delay between pulses: 45 s
- Number of scans (NT): multiple of 4
- Number of steady state scans: 0
- Linearity throughout spectrum: oversampling of 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

**Total Run Time per Sample:**
- 6 min. (NT = 4)
- 14 min. (NT = 16)

**Uniformity within spectral width:**
- 0.3% RSD (-0.6 to 11.4 ppm)

**Linear Range:**
- 0.6 - 60 mg/mL

**Repeatability:**
- less than 4%

**Correlation Coefficient:**
- 1.000

**Accuracy:**
- less than 3%

**Signals used for quantitation (position in ppm with number of protons):**
- 6.9s(1)
- 6.8s(1)
- 3.85s(3)
- 3.8s(3)
- 3.2t(2)
- 3.0t(2)
- 2.8dd(2)
- 1.6sextet(2)
- 1.0t(3)

### 5.3. HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

**Method SFL1 LC1-51**

**Standard Solution Preparation:**
Prepare a standard solution of 2C-T-7 at approximately 350 µg/mL using methanol. Store solution in freezer covered with foil.

**Sample Preparation:**
Accurately weigh an amount of sample into an appropriate volumetric or Erlenmeyer flask and dilute so that the final 2C-T-7 concentration is approximately that of the standard solution.

**Instrument:**
HP 1100 (or comparable) liquid chromatograph equipped with a diode array detector
**Column:**
5 µm Phenomenex Luna, 250 mm x 3.2 mm, 35°C

**Detector:**
UV, 254,310 nm

**Flow:**
1.0 mL/min

**Injection Volume:**
5.0 µL

**Buffer:**
4000 mL water
22.5 mL phosphoric acid
22.5 mL triethanolamine
Check pH; adjust as necessary to between 2.2 and 2.3 with phosphoric acid or triethanolamine
Filter the buffer.

**Mobile Phase:**
Buffer: Methanol
10% MeOH for 12 min
20% MeOH for 8 min

**Linear Range:**
3.5 - 7062 µg/mL

**Repeatability:**
RSD less than 0.5%

**Correlation Coefficient:**
0.9999

**Accuracy:**
less than 5%

**6. QUALITATIVE DATA**

**6.1. ULTRAVIOLET SPECTROPHOTOMETRY**

<table>
<thead>
<tr>
<th>SOLVENT</th>
<th>MAXIMUM ABSORBANCE (NM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>251, 303 (0.08 mg/mL)</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 0.45µm 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

Scan Mode: MS or MS³ (depending on experiment being performed)

Mass Range: Normal; MS: 50-550 amu; MS³: 60 – 550 amu

Scan Type: Full

Scan Time (microscans): 1

Maximum Injection Time (ms): 1000.0

Source Fragmentation: Off

For MS³:
Parent Masses (m/z): MS²: 256.0
MS³: 239.1

Isolation Width (m/z): 1.0

Normalized Collision Energy (%): MS²: 25.0
MS³: 40.0
Activation Q: 0.250

Activation Time (msec): 30.0

See spectra on the following pages for, FTIR ATR, Vapor Phase IR, GC Mass Spectrometry, Mass Spectrometry (MS$^1$), Mass Spectrometry (MS$^3$), and Nuclear Magnetic Resonance.

7. REFERENCES


8. ADDITIONAL RESOURCES

Forendex

Wikipedia
Under the above conditions, vapor phase IR cannot be used to distinguish between 2C-T-2 and 2C-T-7.
EI Mass Spectrum: 2C-T-7, Lot # 2TDM-265-01

API – ESI Mass Spectrum: 2C-T-7, Lot # 2TDM-265-01

MS\(^1\) mode (see text for parameters)
API – ESI Mass Spectrum: 2C-T-7, Lot # 2TDM-265-01
MS³ mode (see text for parameters)

¹H NMR: 2C-T-7, Lot # 2TDM-265-01
Deuterium Oxide, 400MHz
$^{13}$C NMR: 2C-T-7, Lot # 2TDM-265-01
CD$_3$OD, 100.6 MHz

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