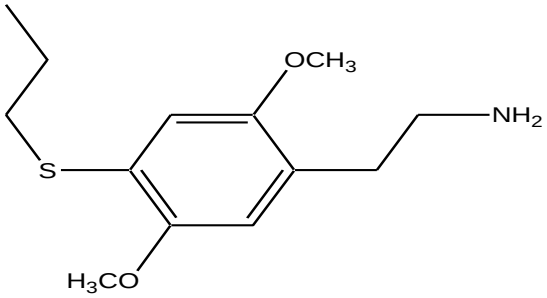
# 2,5-DIMETHOXY-4-*n*-PROPYLTHIOPHENETHYLAMINE

**Latest Revision: August 22, 2005**




## *1. SYNONYMS*

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

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

***Other Names:*** 2,5-Dimethoxy-4-*n*-propylthiophenethylamine
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

| Form | Chemical Formula | Molecular Weight | Melting Point (°C) |
|---|---|---|---|
| Base | $C_{13}H_{21}NO_2S$ | 255.38 | Not available |
| Hydrochloride | $C_{13}H_{21}NO_2S \cdot HCl$ | 291.84 | 195-198 |

### *2.2.* SOLUBILITY

| Form | A | C | E | H | M | W |
|---|---|---|---|---|---|---|
| Base | NA | NA | NA | NA | NA | NA |
| Hydrochloride | PS | S | S | NA | VS | VS |

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

| REAGENT | COLOR PRODUCED |
|---|---|
| Marquis | Pale red |
| Mecke | Orange-Red-Purple |

### *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.

| COMPOUND | RRT | COMPOUND | RRT |
|---|---|---|---|
| amphetamine | 0.446 | 4-MeOPP | 0.850 |
| methamphetamine | 0.483 | 2C-B | 0.880 |
| nicotinamide | 0.596 | caffeine | 0.889 |
| 3,4-MDA | 0.673 | 2C-I | 0.941 |
| TFMPP | 0.700 | 2C-T-2 | 0.954 |
| 3,4-MDMA | 0.717 | **2C-T-7** | **1.000 (4.808 min)** |

| | | | |
|---|---|---|---|
| benzocaine | 0.726 | procaine | 1.017 |
| 3,4-MDEA | 0.750 | tetracaine | 1.130 |
| acetaminophen | 0.797 | quinine | 1.480 |

### *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, and then filtered with a 0.45 µm filter.

| COMPOUND | RRT | COMPOUND | RRT |
|---|---|---|---|
| ephedrine/pseudoephedrine | 0.711 | 2C-I | 0.933 |
| amphetamine | 0.779 | 2C-T-2 | 0.938 |
| methamphetamine | 0.789 | 3,4-MDMA | 0.959 |
| 3,4-MDEA | 0.805 | **2C-T-7** | **1.000 (14.24 min)** |
| 2C-B | 0.904 | | |

### *4. SEPARATION TECHNIQUES*

## *5. QUANTITATIVE PROCEDURES*

### *5.1.* GAS CHROMATOGRAPHY

#### *Method SFL4 4dimeth1*

*Internal Standard Stock Solution:*
1.00 mg/mL tetradecane ($C_{14}$) 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<br>Detector: 275°C<br>Oven program: 220°C isothermal |
| ***Injection Parameters:*** | Split Ratio: 50:1<br>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%

| COMPOUND | RRT | COMPOUND | RRT |
|---|---|---|---|
| amphetamine | 0.505 | 2C-B | 0.754 |
| methamphetamine | 0.512 | caffeine | 0.771 |
| $C_{14}$ | 0.543 | 2C-I | 0.862 |
| 3,4-MDA | 0.575 | 2C-T-2 | 0.886 |
| TFMPP | 0.590 | **2C-T-7** | **1.000 (2.39 min)** |
| 3,4-MDMA | 0.594 | procaine | 1.039 |
| 3,4-MDEA | 0.613 | tetracaine | 1.537 |

### *5.2.* NUCLEAR MAGNETIC RESONANCE

***Method SFL1 NMR1-2***

*Reagents:*
Deuterochloroform ($CDCl_3$) containing TMS (Tetramethylsilane) 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<br>Pulse width: lesser of 10 µs or 90°<br>Delay between pulses: 45 s<br>Number of scans (NT): multiple of 4<br>Number of steady state scans: 0<br>Linearity throughout spectrum: oversampling of 4 or more<br>Shimming: automatic gradient shimming of Z1-4 shims<br>Phasing, Drift Correction: automatic or manual |
| ***Total Run Time per Sample:*** | 6 min (NT = 4)<br>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)<br>3.2 (2)<br>3.0 (2)<br>1.0 (3) |

***Method SFL1 NMR1-5***

*Reagents:*
deuterochloroform ($CDCl_3$) containing TMS (tetramethylsilane) for 0 ppm reference and deuteromethanol ($CD_3OD$) 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 $CD_3OD$, 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<br>Pulse width: lesser of 10 µs or 90°<br>Delay between pulses: 45 s<br>Number of scans (NT): multiple of 4<br>Number of steady state scans: 0<br>Linearity throughout spectrum: oversampling of 4 or more<br>Shimming: automatic gradient shimming of Z1-4 shims<br>Phasing, Drift Correction: automatic or manual |
| ***Total Run Time per Sample:*** | 6 min. (NT = 4)<br>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)<br>6.8s(1)<br>3.85s(3)<br>3.8s(3)<br>3.2t(2)<br>3.0t(2)<br>2.8dd(2)<br>1.6sextet(2)<br>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, 35ºC |
| ***Detector:*** | UV, 254,310 nm |
| ***Flow:*** | 1.0 mL/min |
| ***Injection Volume:*** | 5.0 µL |
| ***Buffer:*** | 4000 mL water<br>22.5 mL phosphoric acid<br>22.5 mL triethanolamine<br>Check pH; adjust as necessary to between 2.2 and 2.3 with phosphoric acid or triethanolamine<br>Filter the buffer. |
| ***Mobile Phase:*** | Buffer: Methanol<br>10% MeOH for 12 min<br>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

| SOLVENT | MAXIMUM ABSORBANCE (NM) |
|---|---|
| Water | 251, 303<br>(0.08 mg/mL) |

### *6.2.* LIQUID CROMATOGRAPHY/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 $MS^3$<br>(depending on experiment being performed) |
| ***Mass Range:*** | Normal; MS: 50-550 amu; $MS^3$: 60 – 550 amu |
| ***Scan Type:*** | Full |
| ***Scan Time (microscans):*** | 1 |
| ***Maximum Injection Time (ms):*** | 1000.0 |
| ***Source Fragmentation:*** | Off |
| ***For $MS^3$:*** | |
| ***Parent Masses (m/z):*** | $MS^2$: 256.0<br>$MS^3$: 239.1 |
| ***Isolation Width (m/z):*** | 1.0 |
| ***Normalized Collision Energy (%):*** | $MS^2$: 25.0<br>$MS^3$: 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*

Analytical Standard Certificate of Quality, Alltech-Applied Science Labs.

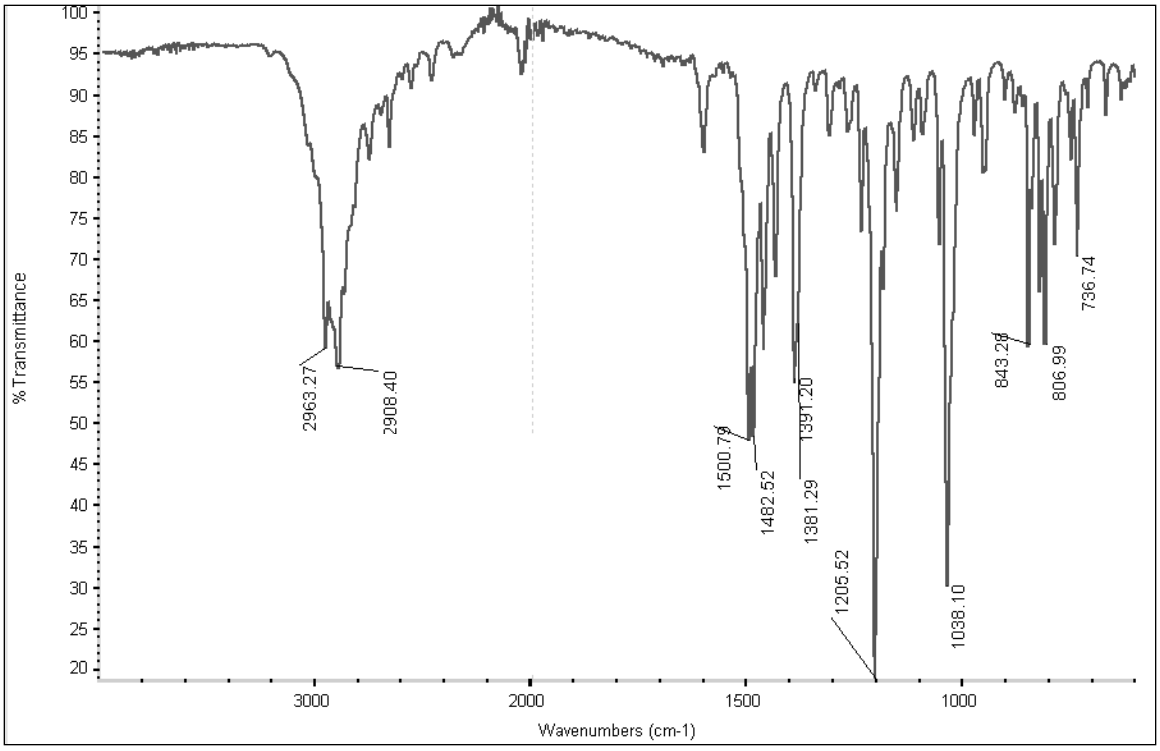
Zimmerman, M.M., "The identification of 2,5-dimethoxy-4-(n)-propylthiophenethylamine (2C-T-7)," *Microgram*, Vol. XXXIV, No. 7, July 2001, pp. 169-173.

## *8. ADDITIONAL RESOURCES*

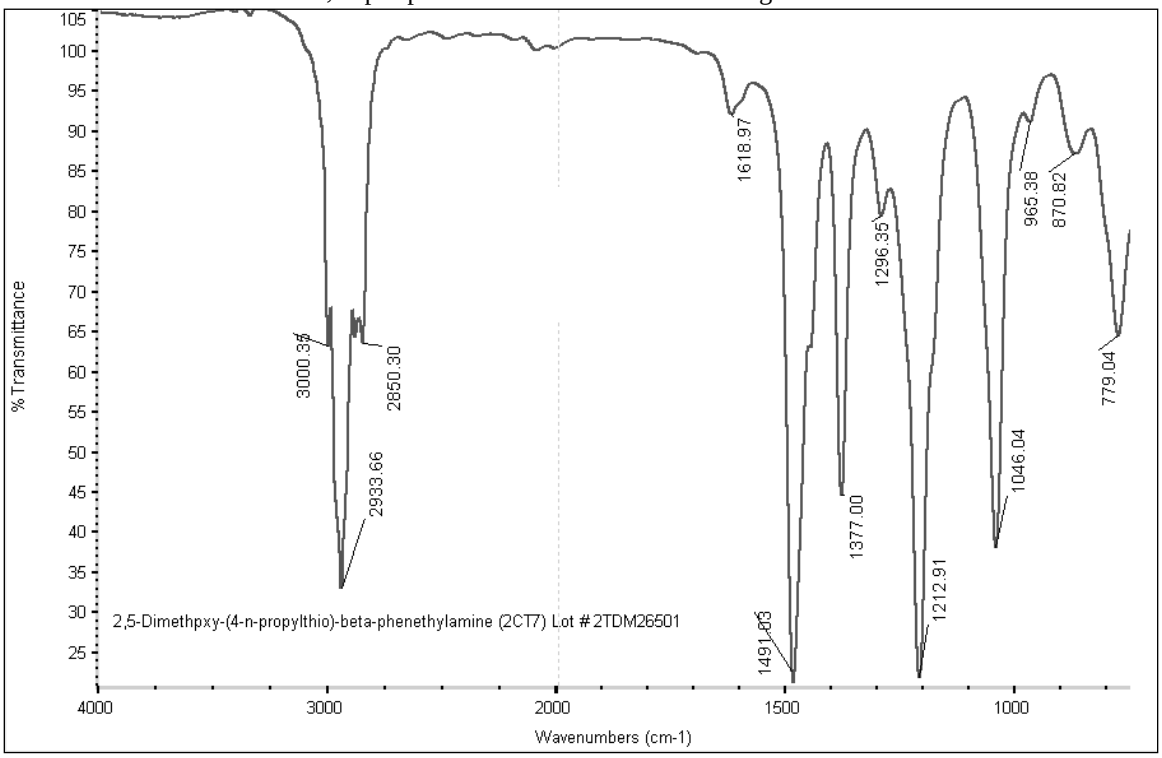
Forendex

Wikipedia

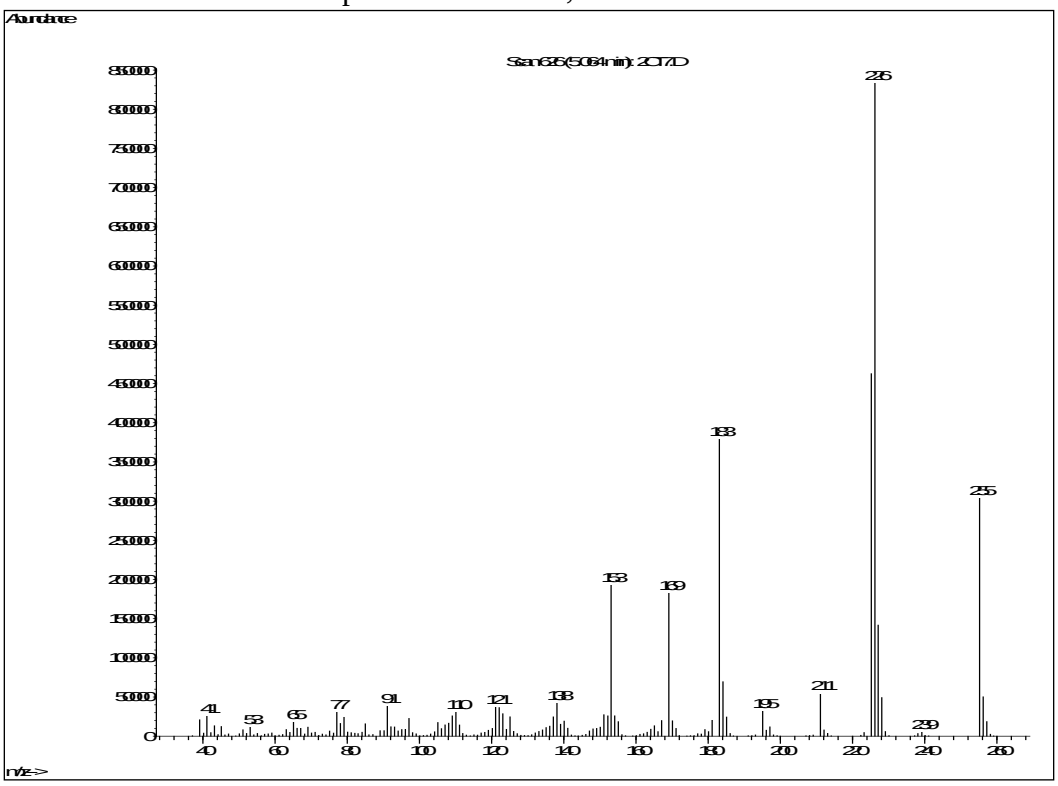
FTIR, (Diamond ATR, 3 Bounce): 2C-T-7 HCL, Lot # 2TDM-265-01
32 scans, 4cm $^{-1}$ resolution



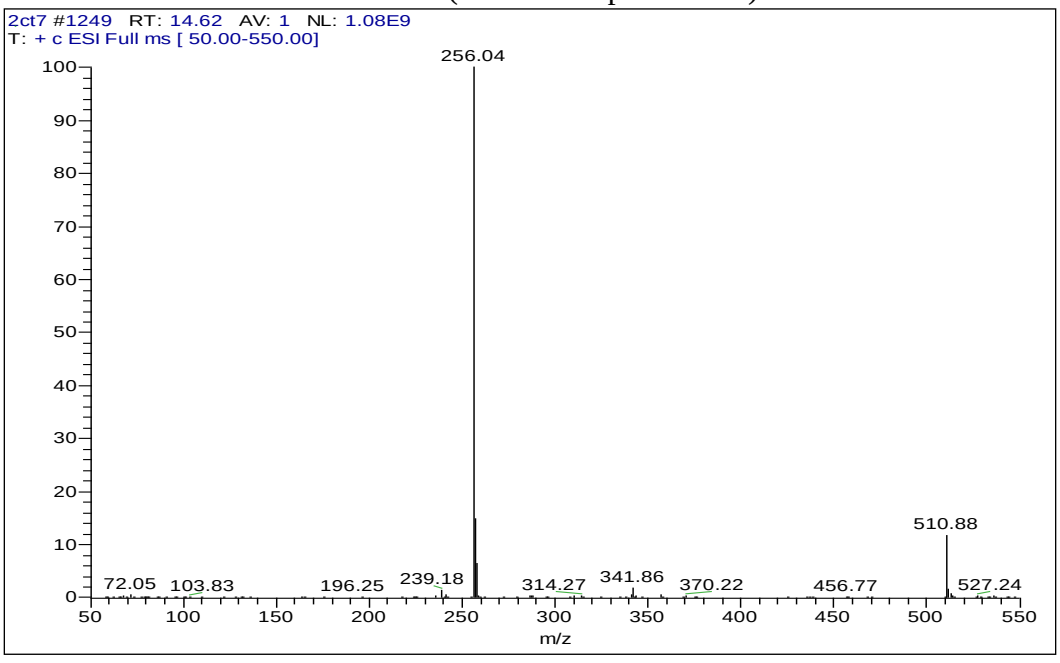

IR(Vapor Phase): 2C-T-7, Lot # 2TDM-265-01
280°C, 8 cm$^{-1}$ resolution
Under the above conditions, vapor phase IR cannot be used to distinguish between 2C-T-2 and 2C-T-7



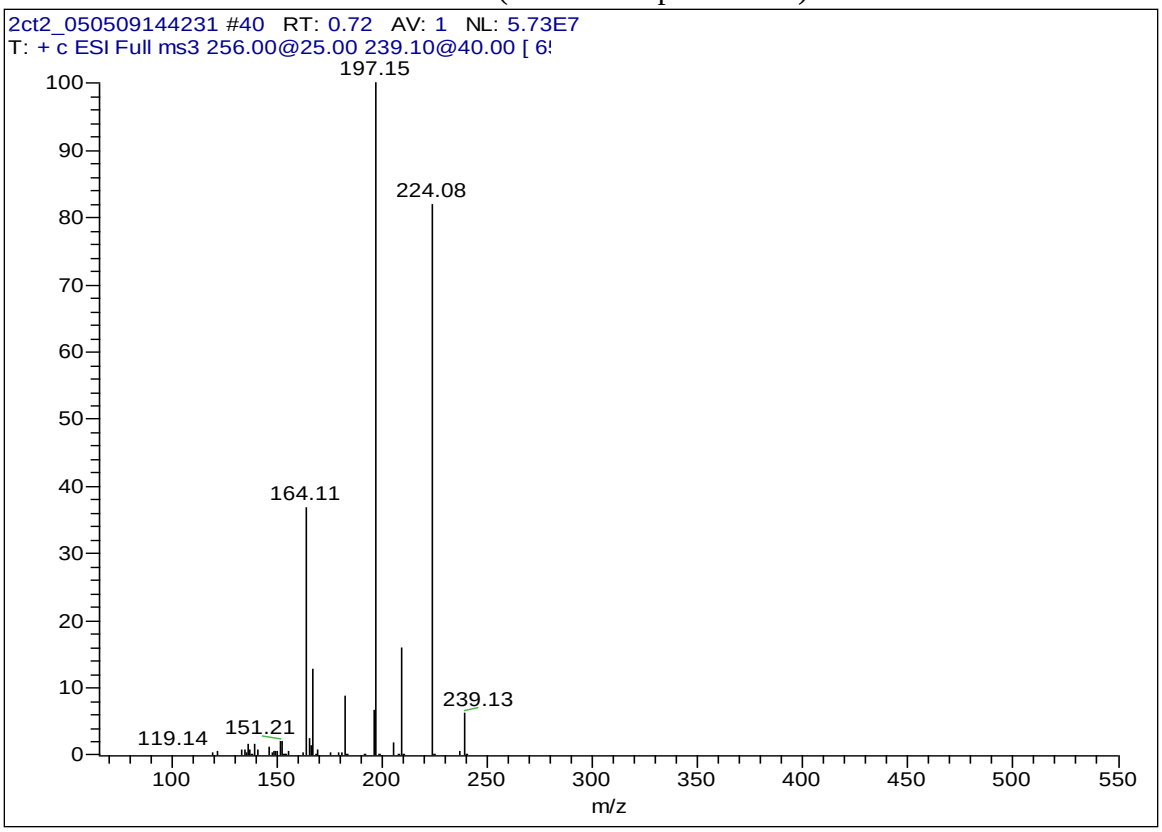
EI Mass Spectrum:  2C-T-7, Lot # 2TDM-265-01



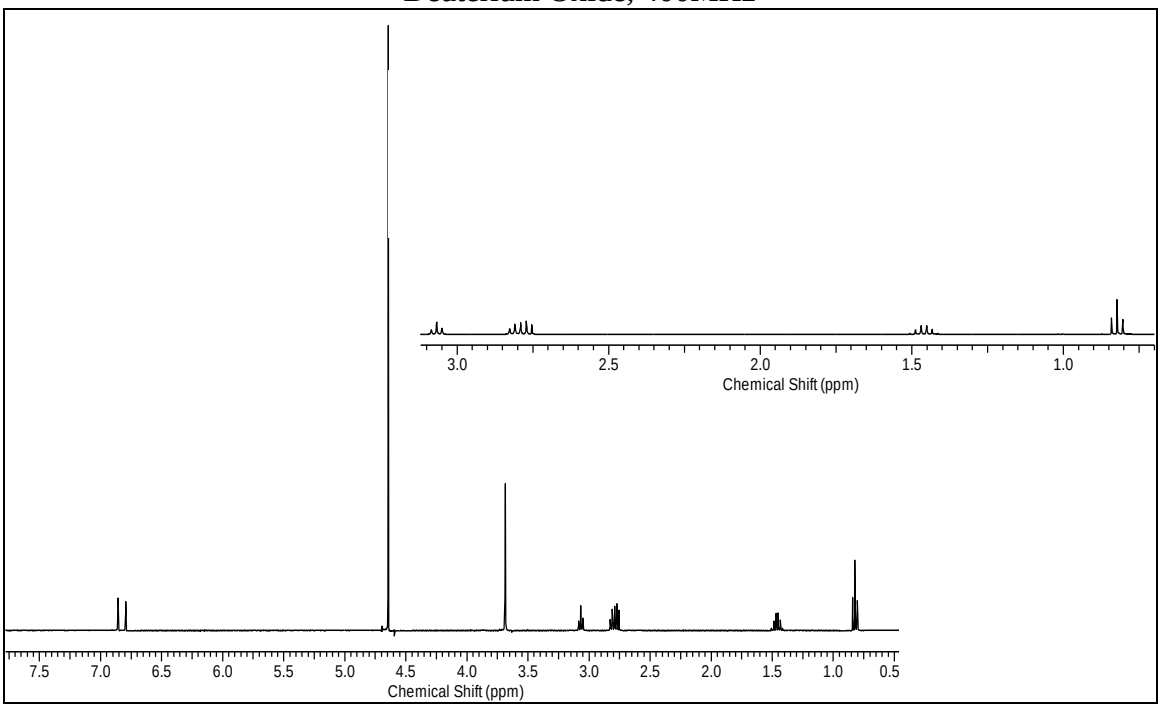

API – ESI Mass Spectrum:  2C-T-7, Lot # 2TDM-265-01
$MS^1$ mode (see text for parameters)



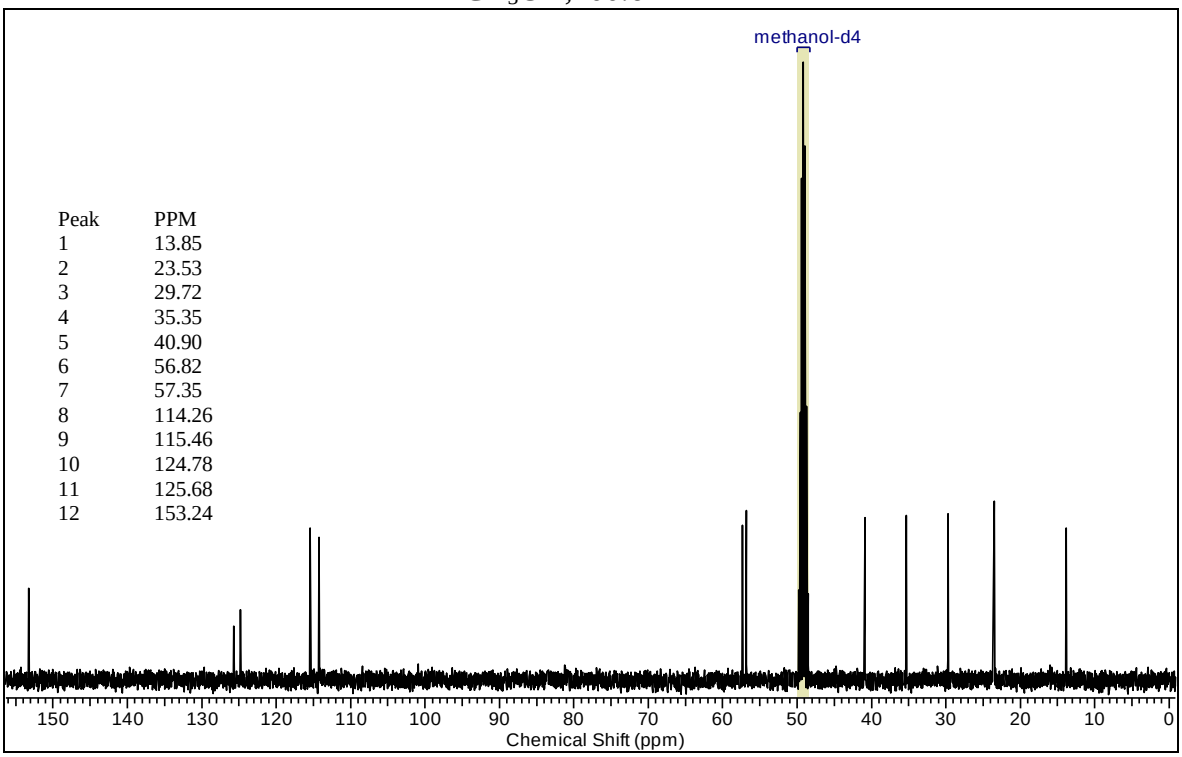
API – ESI Mass Spectrum: 2C-T-7, Lot # 2TDM-265-01
$MS^3$ mode (see text for parameters)




$^1H$ NMR: 2C-T-7, Lot # 2TDM-265-01
Deuterium Oxide, 400MHz



$^{13}$C NMR:  2C-T-7, Lot # 2TDM-265-01
$CD_3OD$,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