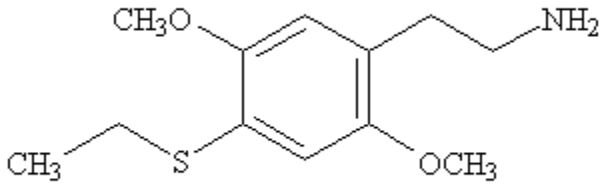
2,5-DIMETHOXY-4-ETHYLTHIOPHENYLAMINE

Latest Revision: August 22, 2005



1. SYNONYMS

CFR: Not Available

CAS #: Base: Not Available
Hydrochloride: 207740-24-7

Other Names: 4-Ethylthio-2,5-dimethoxyphenethylamine
4-Ethylthio-2,5-dimethoxybenzeneethanamine
2C-T-2

2. CHEMICAL AND PHYSICAL DATA

2.1. CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{12}H_{19}NO_2S$	241.35	Not available
Hydrochloride	$C_{12}H_{19}NO_2S \cdot HCl$	277.81	204-207

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 orange
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: 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 injection

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

COMPOUND	RRT	COMPOUND	RRT
amphetamine	0.468	4-MeOPP	0.891
methamphetamine	0.506	2C-B	0.923
nicotinamide	0.625	caffeine	0.932
3,4-MDA	0.706	2C-I	0.986

BZP	0.719	**2C-T-2**	**1.000 (4.587 min)**
TFMPP	0.733	2C-T-7	1.048
3,4-MDMA	0.751	procaine	1.065
benzocaine	0.761	tetracaine	1.185
3,4-MDEA	0.786	quinine	1.551
acetaminophen	0.835		

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	0.759	2C-I	0.996
amphetamine	0.831	**2C-T-2**	**1.000 (13.35 min)**
methamphetamine	0.841	3,4-MDMA	1.022
3,4-MDEA	0.858	2C-T-7	1.067
2C-B	0.965		

4. SEPARATION TECHNIQUES

2C-T-2 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 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-2·HCl within the linearity range listed below.

Sample Preparation:
Accurately weigh an amount of sample into a volumetric flask so that the final 2C-T-2·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 1 M-5 M sodium hydroxide into 2 mL of 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-2·HCl: 2.12 min C_{14}: 1.30 min
Linear Range:	0.252 - 4.032 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	0.570	2C-B	0.851
methamphetamine	0.578	caffeine	0.871
C_{14}	0.613	2C-I	0.973
3,4-MDA	0.649	**2C-T-2**	**1.000 (2.12 min)**
TFMPP	0.666	2C-T-7	1.129
3,4-MDMA	0.671	procaine	1.173
3,4-MDEA	0.692	tetracaine	1.735

6. QUALITATIVE DATA

6.1. ULTRAVIOLET SPECTROPHOTOMETRY

SOLVENT	MAXIMUM ABSORBANCE (NM)
Water	251, 302 (0.1 mg/mL)

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/min 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 (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: 242.0 MS^3: 225.1
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 FTIR ATR, Vapor Phase IR, GC Mass Spectrometry, Mass Spectrometry (MS^1), Mass Spectrometry (MS^3), and Nuclear Magnetic Resonance.

7. REFERENCES

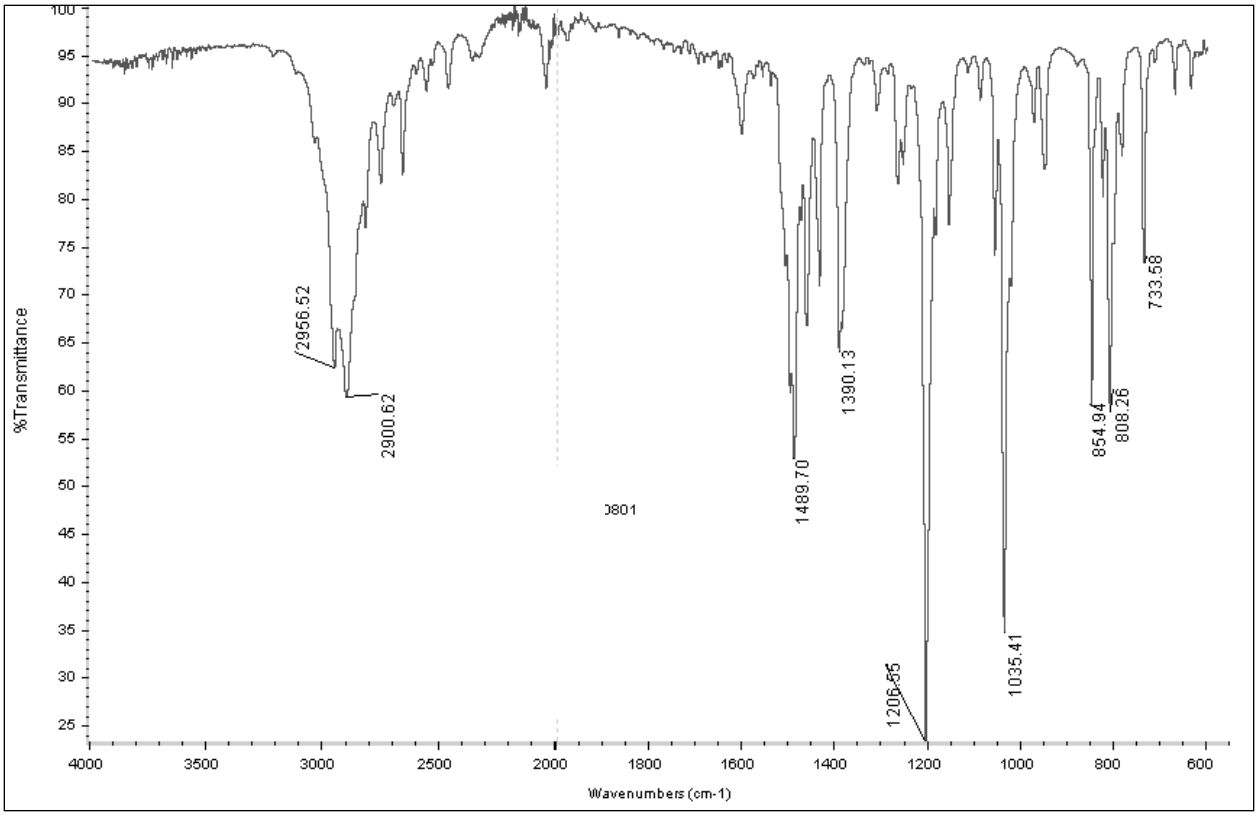
Analytical Standard Certificate of Quality, Alltech-Applied Science Labs.

Poortman, A.J., "The Synthesis of 2,5-Dimethoxy-4-ethylthiophenethylamine (2C-T-2). A Case Report," *Journal of the Clandestine Laboratory Investigating Chemists Association*, Vol. 9, No. 4, October 1999, pp. 17-20.

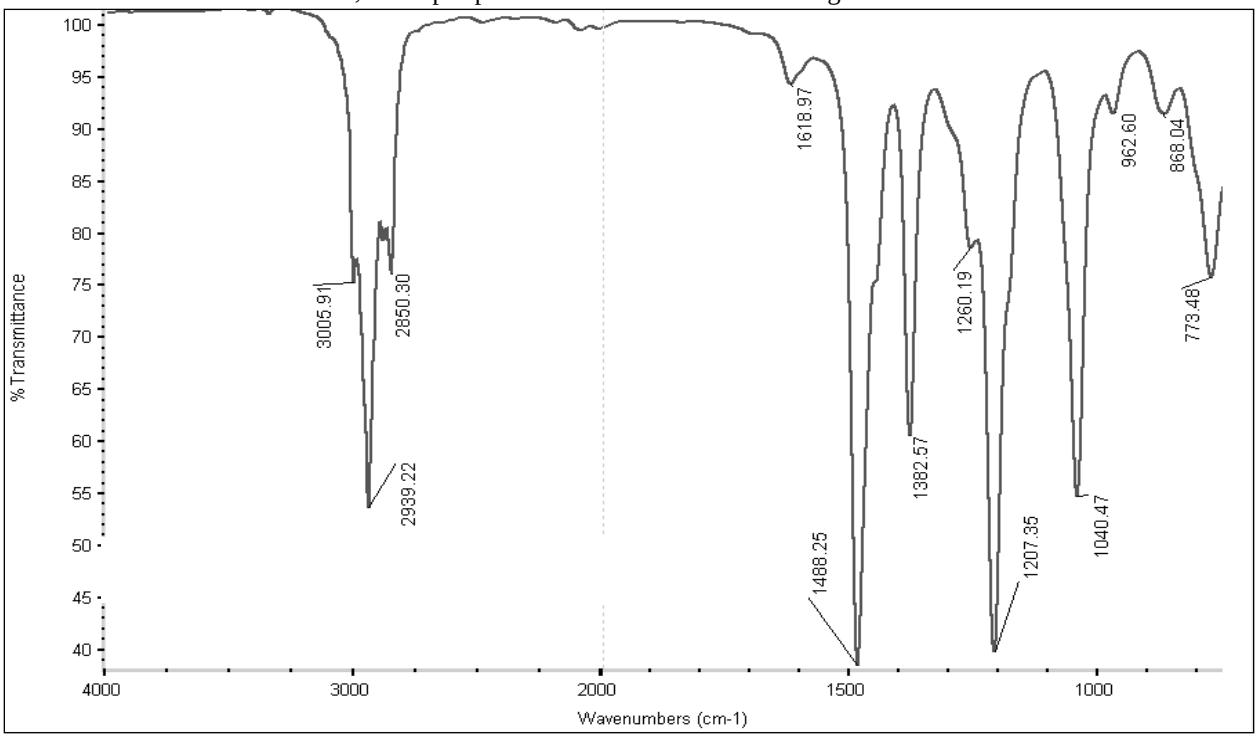
8. ADDITIONAL RESOURCES

Wikipedia

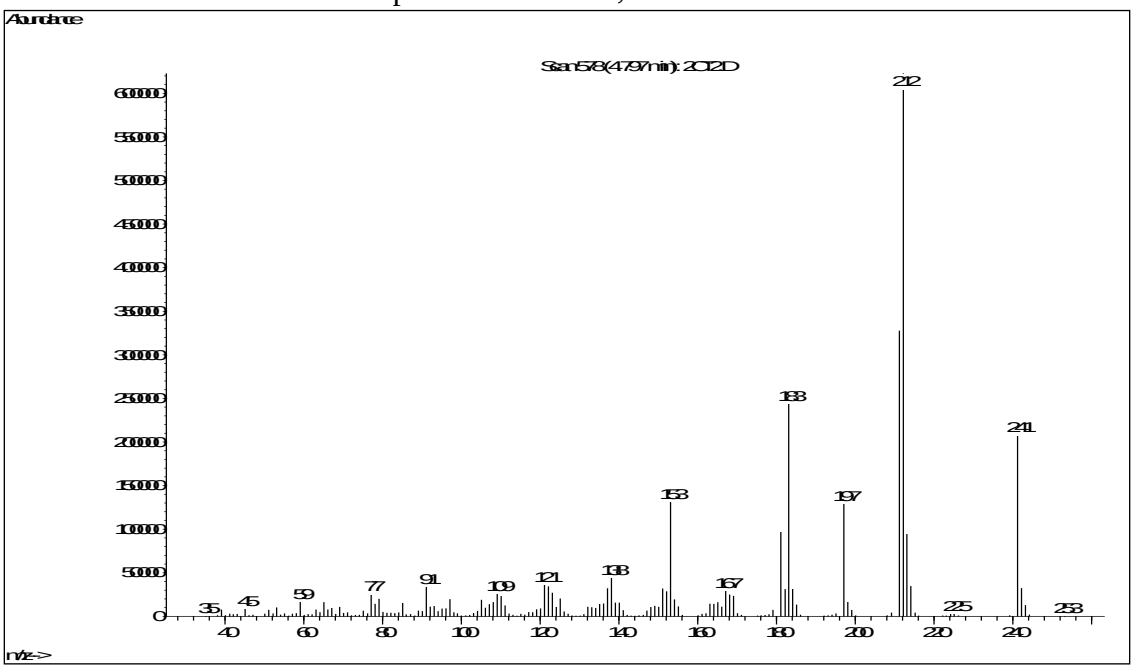
FTIR (Diamond ATR, 3 Bounce): 2C-T-2 HCl, Lot # DAK-08-01
32 scans, 4 cm^{-1} resolution



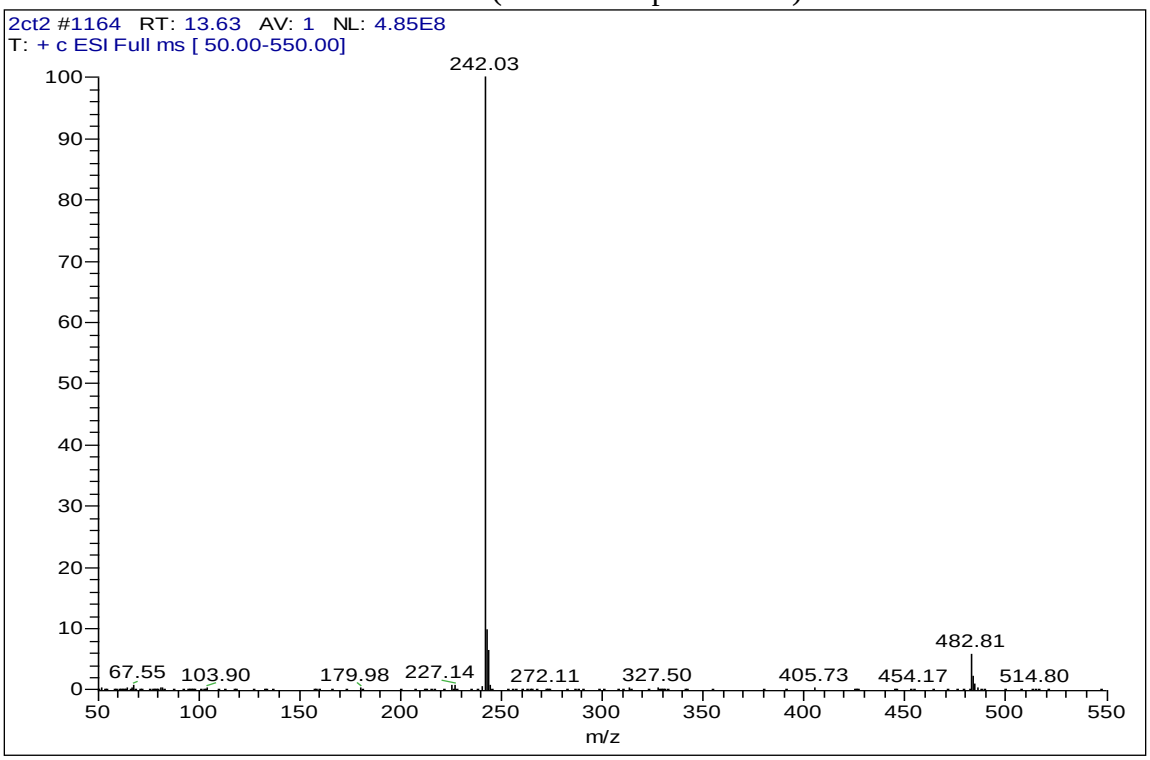
IR (Vapor Phase): 2C-T-2 Lot # DAK- 08-01
280˚C, 8 cm^{-1} resolution
Under the above conditions, the vapor phase IR cannot be used to distinguish between 2C-T-2 and 2C-T-7



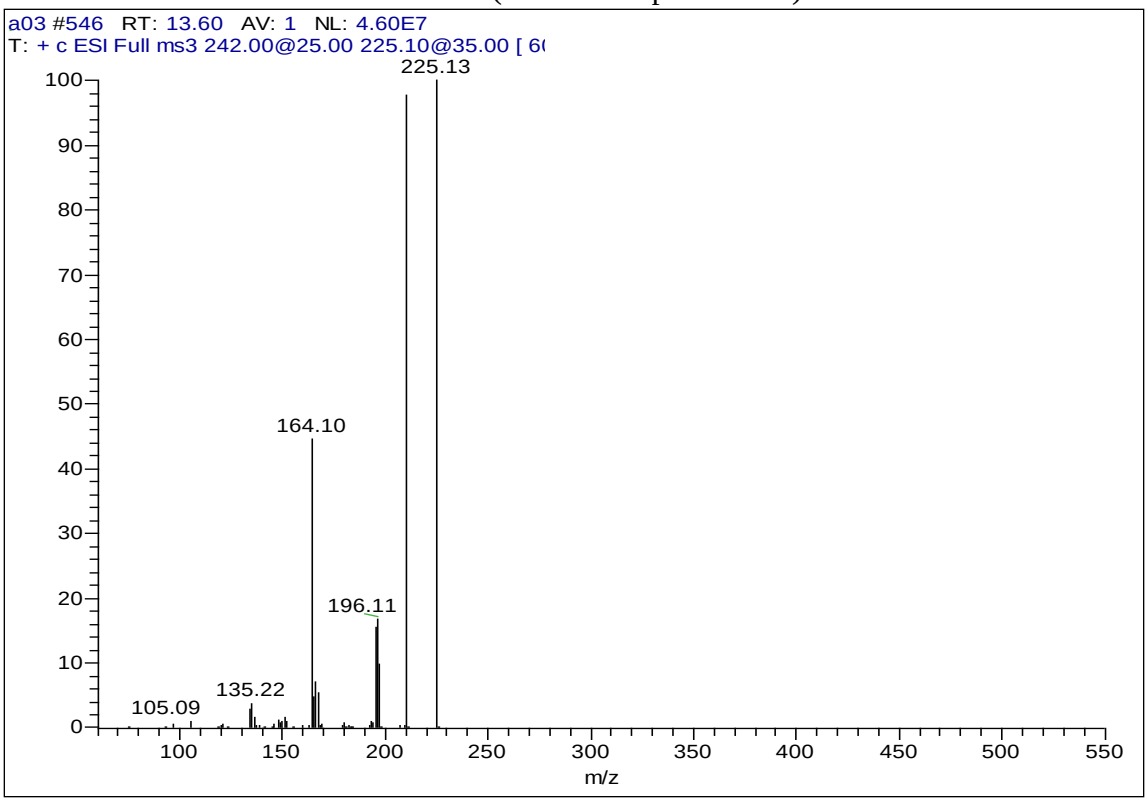
EI Mass Spectrum: 2C-T-2, Lot # DAK -08-01



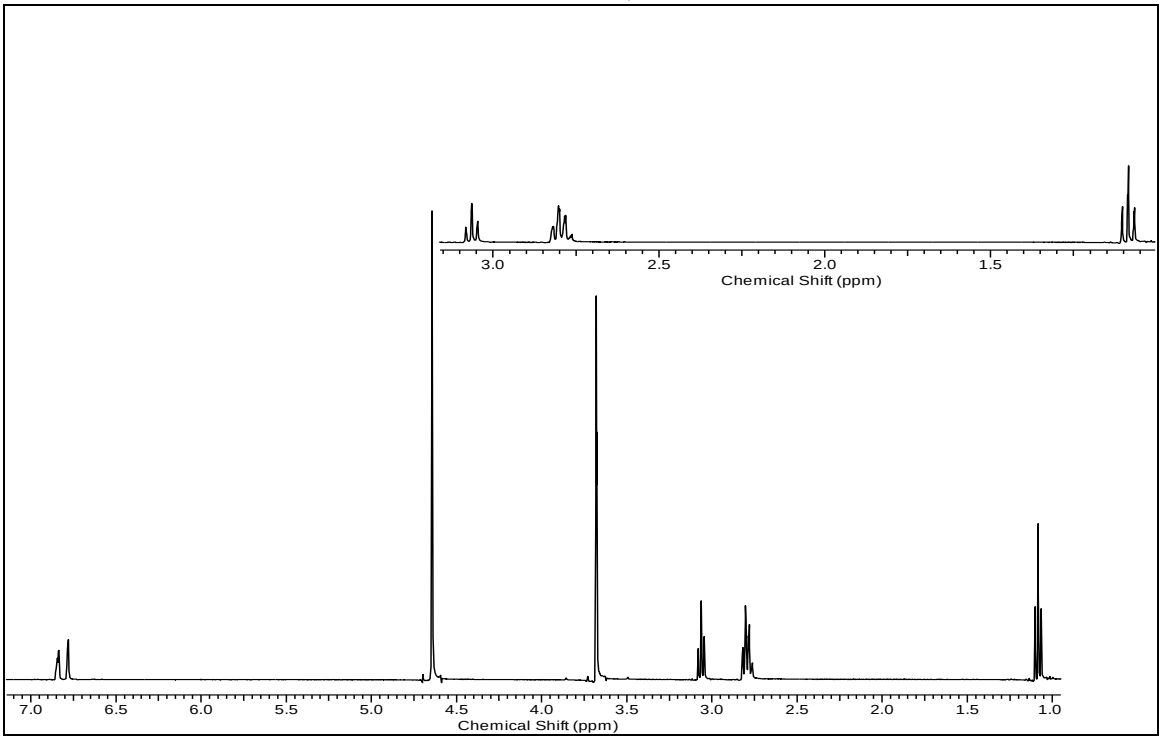
API – ESI Mass Spectrum: 2C-T-2, Lot # DAK-08-01
MS^1 mode (see text for parameters)



API – ESI Mass Spectrum: 2C-T-2, Lot # DAK-08-01
MS^3 mode (see text for parameters)



^1H NMR: 2C-T-2, Lot # DAK 08-01
Deuterium Oxide, 400MHz



^{13}C NMR: 2-CT-2, Lot # 2DAK-08-01
Deuterium Oxide, 100.6 MHz