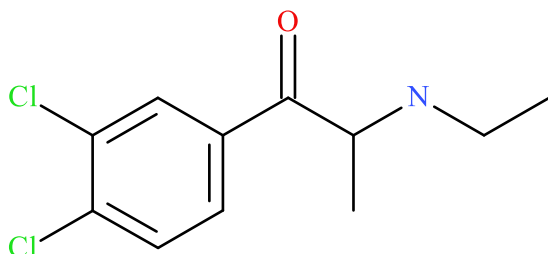


## 3,4-Dichloroethcathinone (DCEC)

Sample Type: **Seized Material**



Latest Revision: **May 18<sup>th</sup>, 2018**

Date Received: **January 25<sup>th</sup>, 2018**

Date of Report: **May 4<sup>th</sup>, 2018**

### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-(3,4-dichlorophenyl)-2-(ethylamino)propan-1-one
<b>InChI String:</b>	InChI=1S/C11H13Cl2NO/c1-3-14-7(2)11(15)8-4-5-9(12)10(13)6-8/h4-7,14H,3H2,1-2H3
<b>CFR:</b>	Not Scheduled (05/2018)
<b>CAS#</b>	Not Available
<b>Synonyms:</b>	3,4-DCEC, DCEC
<b>Source:</b>	Department of Homeland Security
<b>Appearance:</b>	White Solid Material

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>11</sub> H <sub>13</sub> Cl <sub>2</sub> NO	246.1	245	246.0447

**Important Note:** All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

**Prepared By:** Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT

### 3. BRIEF DESCRIPTION

3,4-Dichloroethcathinone (DCEC) is classified as a substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Substituted cathinones have been reported to cause stimulant-like effects, similar to amphetamines, which are structurally related to substituted cathinones. Substituted cathinones have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include cathinone, mephedrone (4-methylmethcathinone), 4-methylethcathinone (4-MEC), ethcathinone (ETH-CAT), and N,N-diethylcathinone. Cathinone, mephedrone, and 4-MEC are all explicitly Schedule I substances in the United States, while ethcathinone is listed as a mephedrone isomer.

### 4. ADDITIONAL RESOURCES

No additional resources available at this time.

### 5. QUALITATIVE DATA

#### 5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

**Testing Performed At:** NMS Labs (Willow Grove, PA)

**Sample Preparation:** Acid/Base extraction

**Instrument:** Agilent 5975 Series GC/MSD System

**Column:** Agilent J&W DB-1 (12 m x 200  $\mu$ m x 0.33  $\mu$ m)

**Carrier Gas:** Helium (Flow: 1.46 mL/min)

**Temperatures:** Injection Port: 265 °C  
Transfer Line: 300 °C  
MS Source: 230 °C  
MS Quad: 150 °C  
Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min

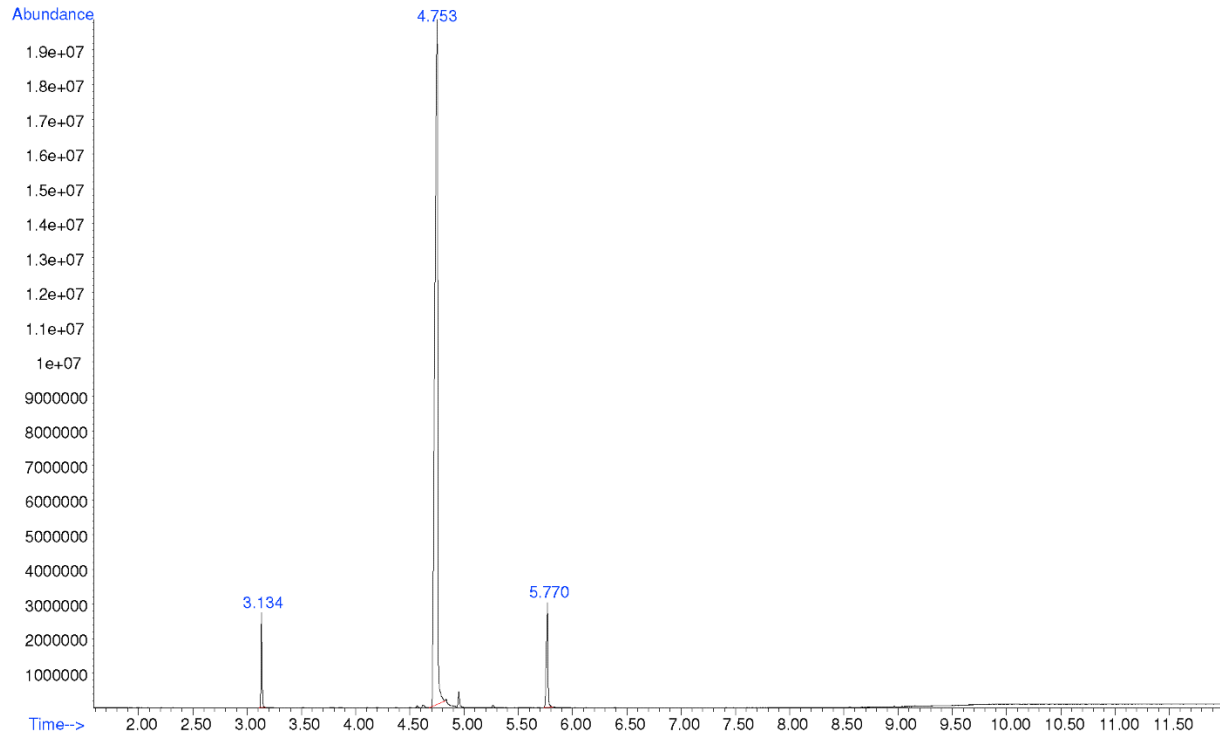
**Injection Parameters:** Injection Type: Splitless  
Injection Volume: 1  $\mu$ L

**MS Parameters:** Mass Scan Range: 40-550 m/z

Threshold: 250

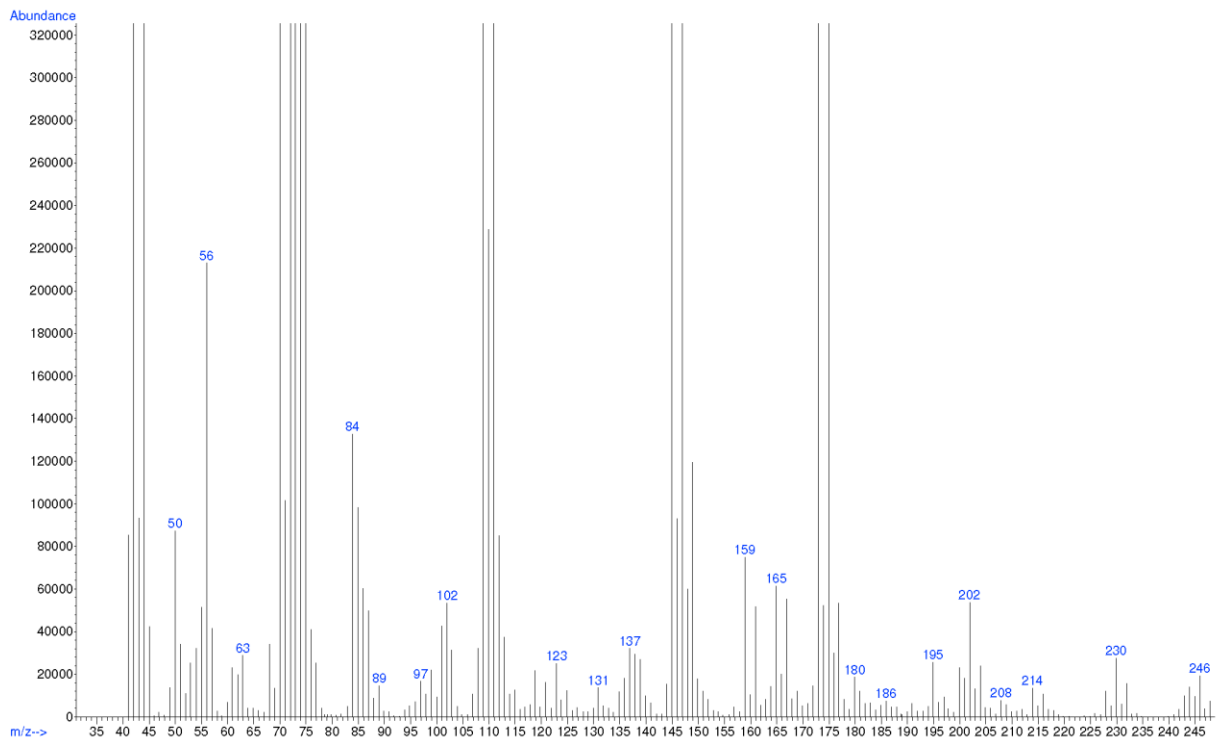
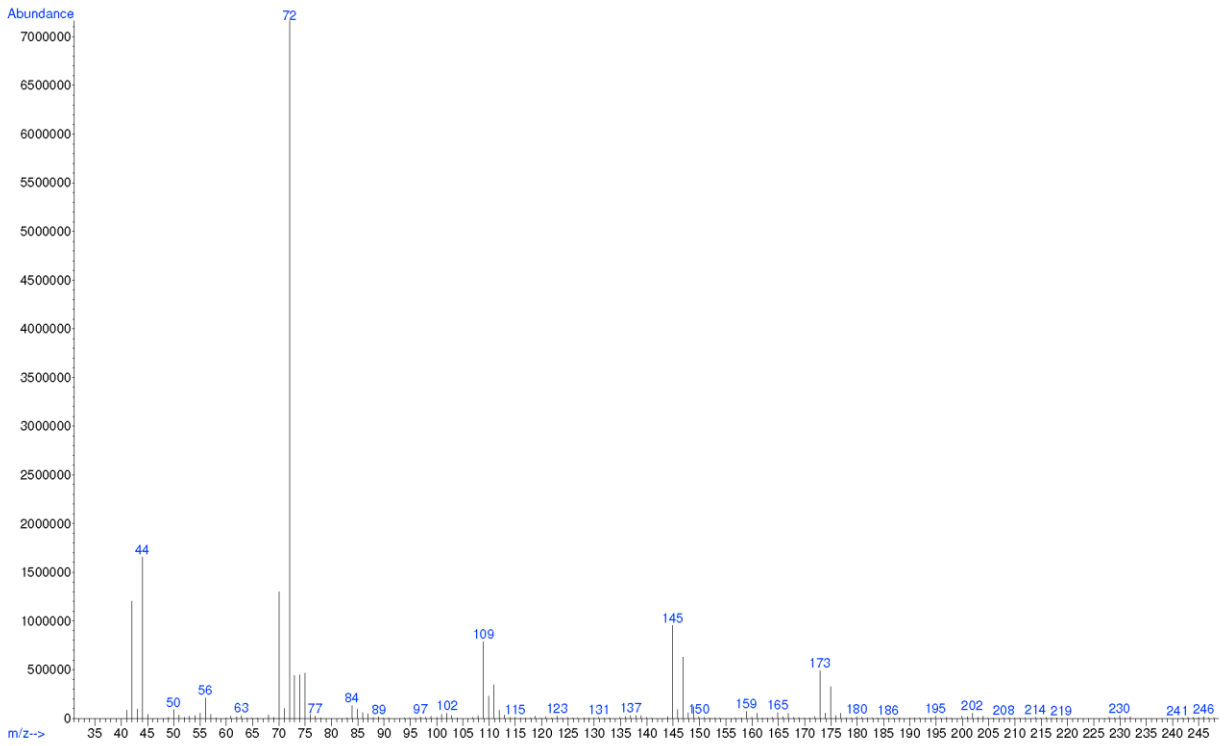
**Retention Time:** 4.753 min

**Chromatogram: 3,4-Dichloroethcathinone**



*Additional peaks present in chromatogram: internal standard 1 (3.134 min),  
internal standard 2 (5.770 min)*

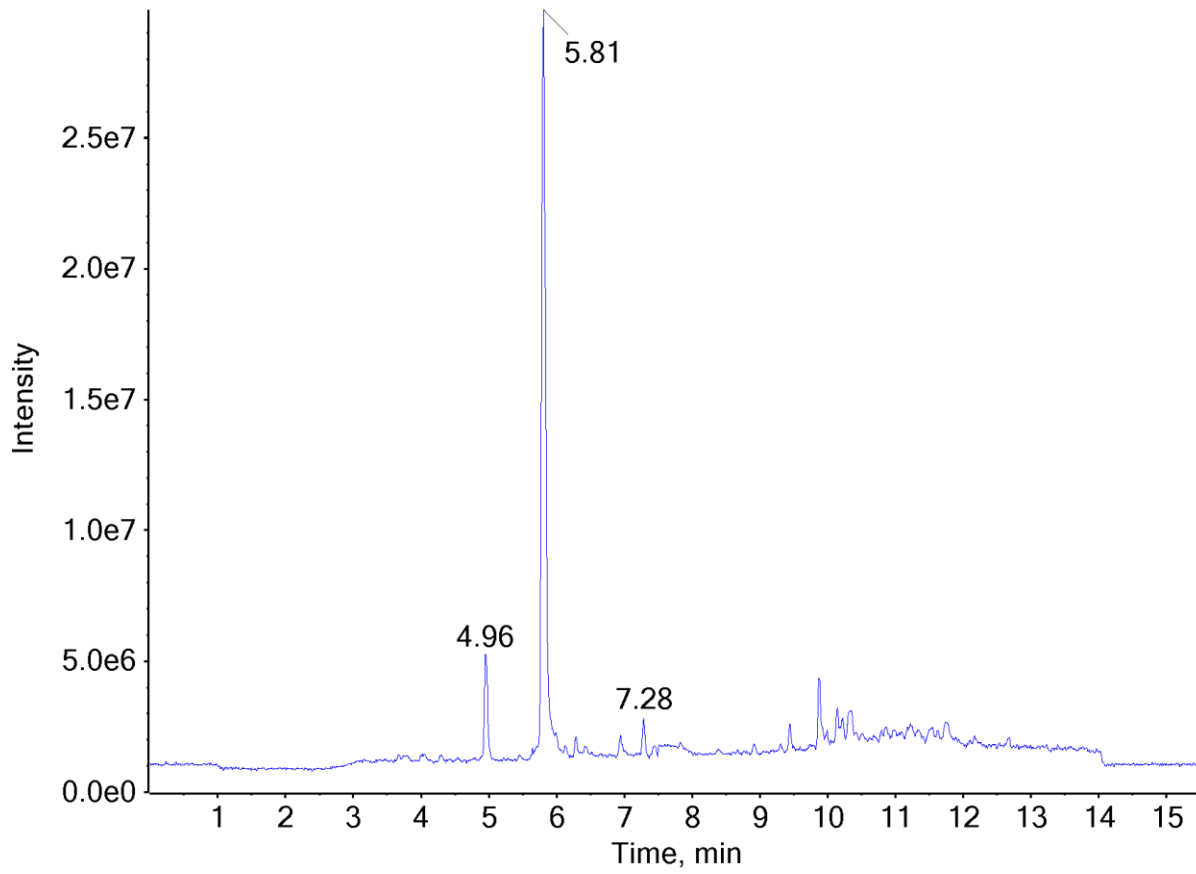
# EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 3,4-Dichloroethcathinone



## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

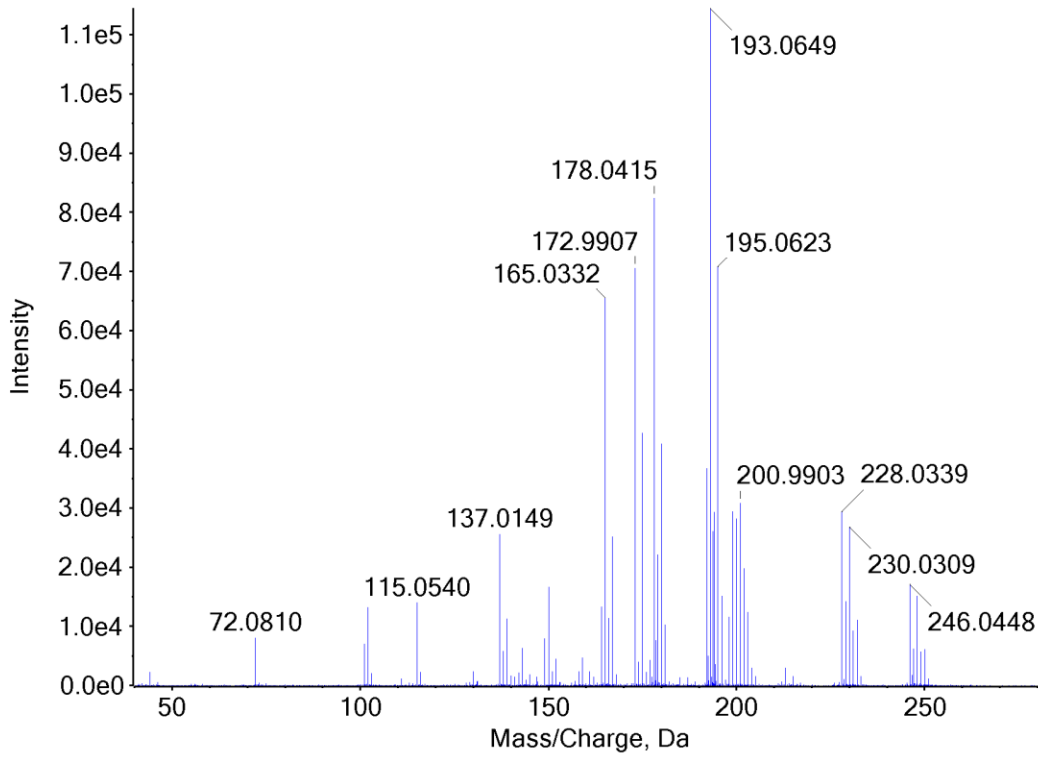
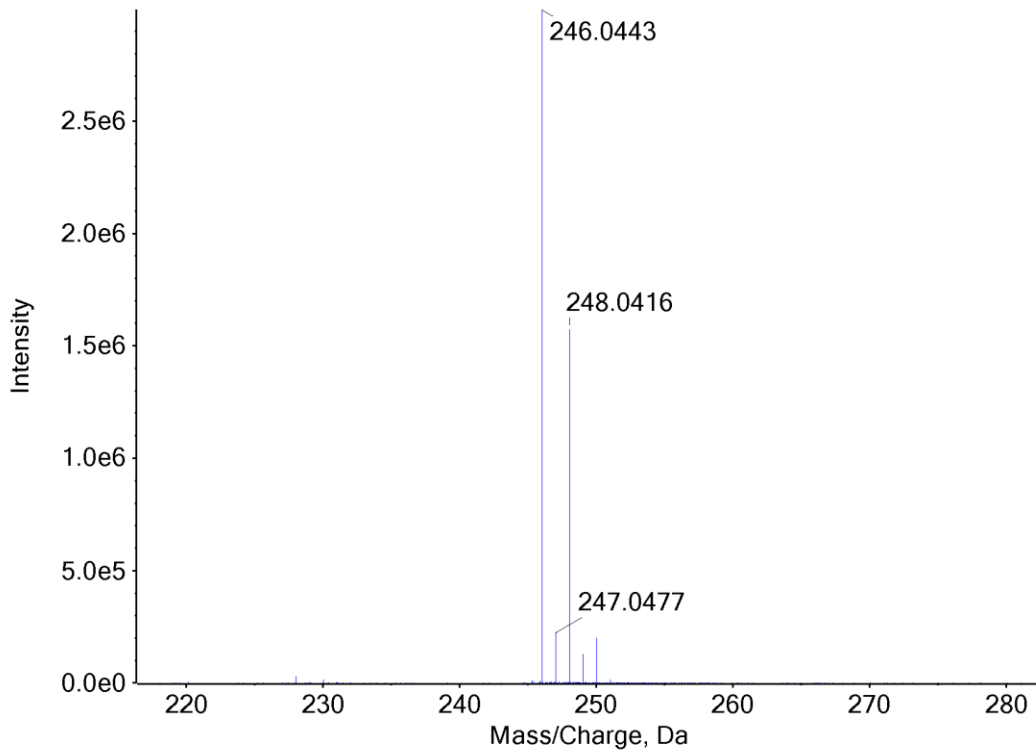
<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	1:100 dilution of acid/base extraction in mobile phase
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	TOF MS Scan Range: 100-510 Da Precursor Isolation: SWATH® acquisition (27 windows) Fragmentation: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
<b>Retention Time:</b>	5.81 min

**Chromatogram: 3,4-Dichloroethcathinone**



*Additional peaks present in chromatogram: internal standard 1 (4.96 min),  
internal standard 2 (7.28 min)*

**TOF MS (Top) and MS/MS (Bottom) Spectra: 3,4-Dichloroethcathinone**



### 5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

**Testing Performed At:** IteraMed™ (Doylestown, PA)

**Sample Preparation:** Dilute powder in DMSO

**Instrument:** 300 MHz INOVA VARIAN Spectrometer

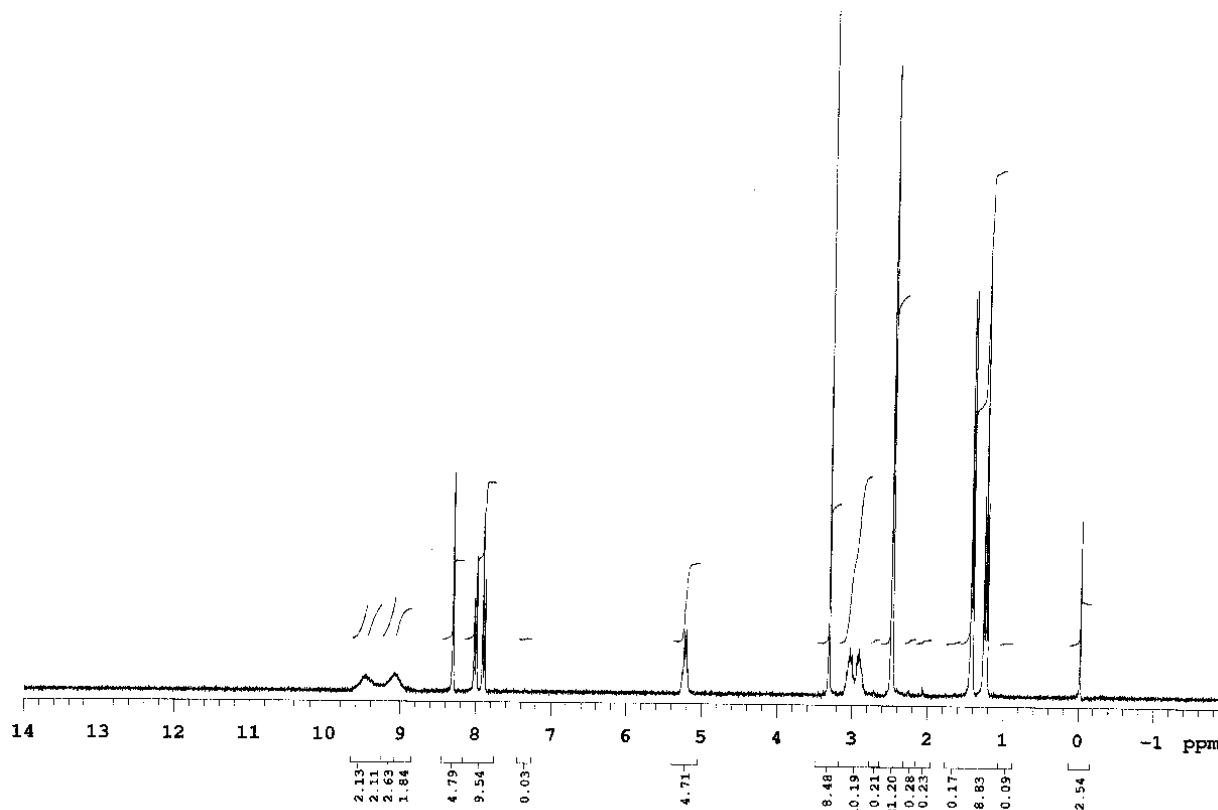
**Parameters:** Pulse Sequence: Proton

Solvent: DMSO

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

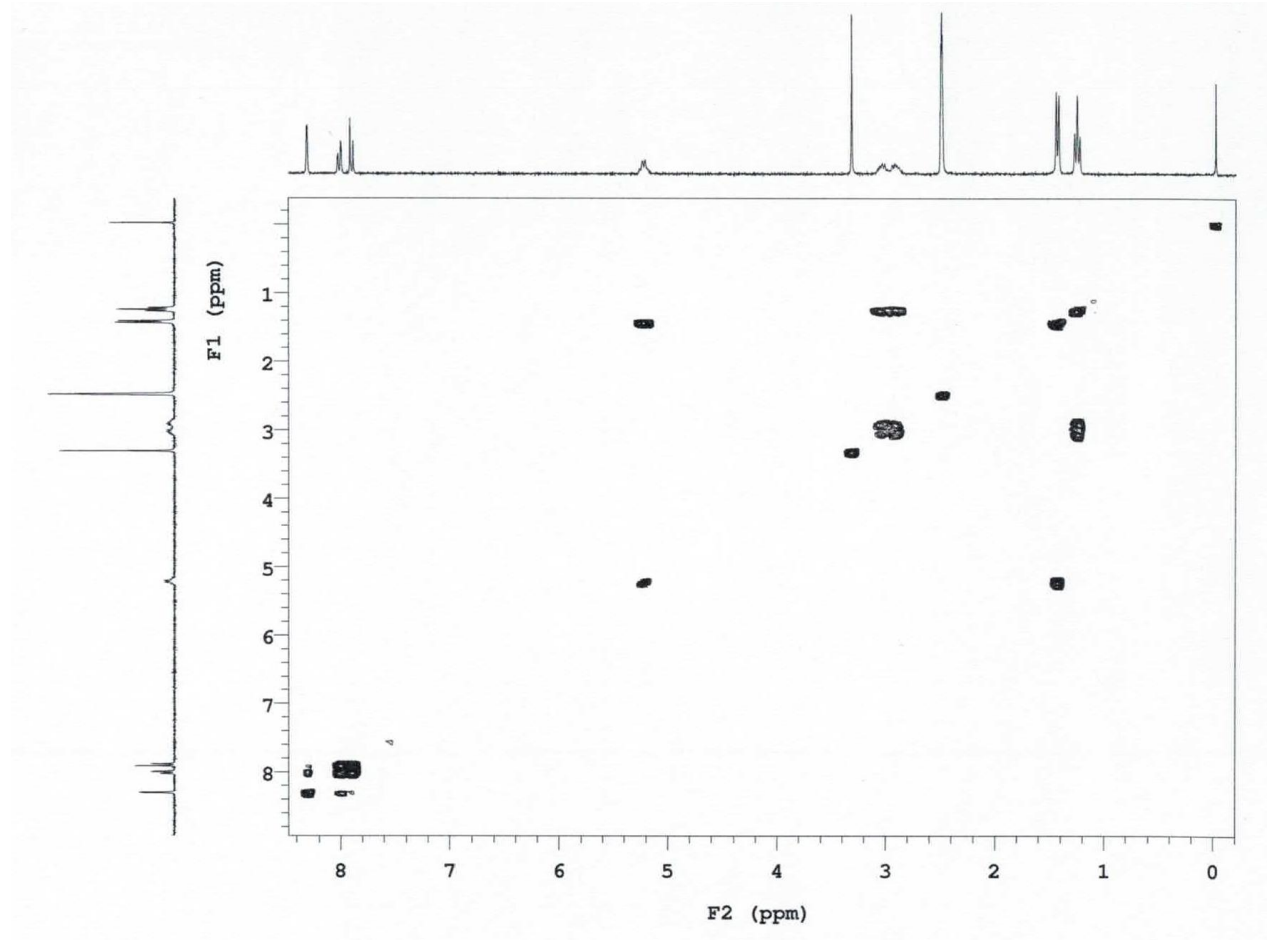
Delay between pulses: 1st delay, d1 = 1.000

#### <sup>1</sup>H NMR: 3,4-Dichloroethcathinone





**gCOSY NMR: 3,4-Dichloroethcathinone**



**6. REVISION HISTORY**

<u>Date</u>	<u>Revision</u>
05/18/2018	Added "Sample Type: Seized Material" to Page 1.
05/18/2018	Added "Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT" to Page 1 footer.