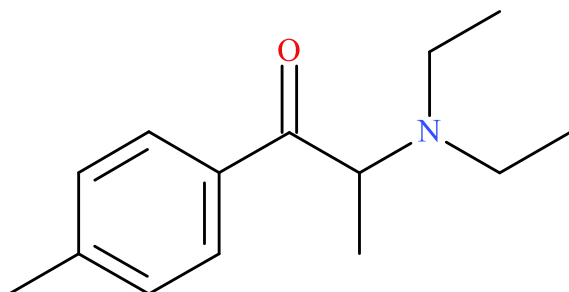


4-Methyldiethcathinone (4-MDEC)

Sample Type: **Seized Material**



Latest Revision: **May 18th, 2018**

Date Received: **December 12th, 2017**

Date of Report: **February 27th, 2018**

1. GENERAL INFORMATION

IUPAC Name:	2-(diethylamino)-1-(4-methylphenyl)propan-1-one
InChI String:	InChI=1S/C14H21NO/c1-5-15(6-2)12(4)14(16)13-9-7-11(3)8-10-13/h7-10,12H,5-6H2,1-4H3
CFR:	Not Scheduled (02/2018)
CAS#	676316-90-8
Synonyms:	N,N,-diethyl-4-methylcathinone; N,N-DEMC; 4-MEC ET, MDEC
Source:	Department of Homeland Security
Appearance:	Off-white solid material

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₁₄ H ₂₁ NO	219.3	219	220.1696

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

4-Methyldiethcathinone 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

<https://www.chemspider.com/Chemical-Structure.28593991.html>

https://comptox.epa.gov/dashboard/dsstoxdb/results?exact=1&mass=0&search=655742&single_component=0

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4-MDEC-ID-1858-17_report.pdf

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:	Zebtron™ Inferno™ ZB-35HT (15 m x 250 μm x 0.25 μm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C

Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

Injection Parameters: Injection Type: Splitless

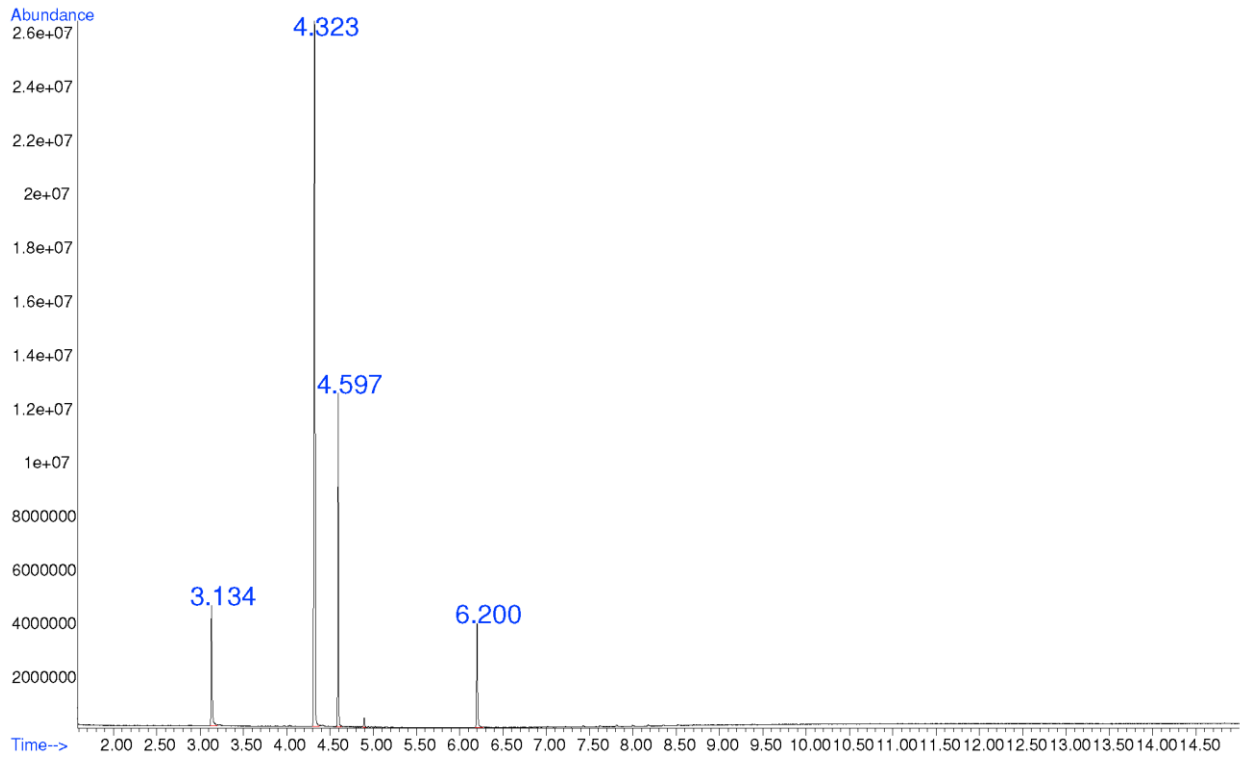
Injection Volume: 1 µL

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

Threshold: 250

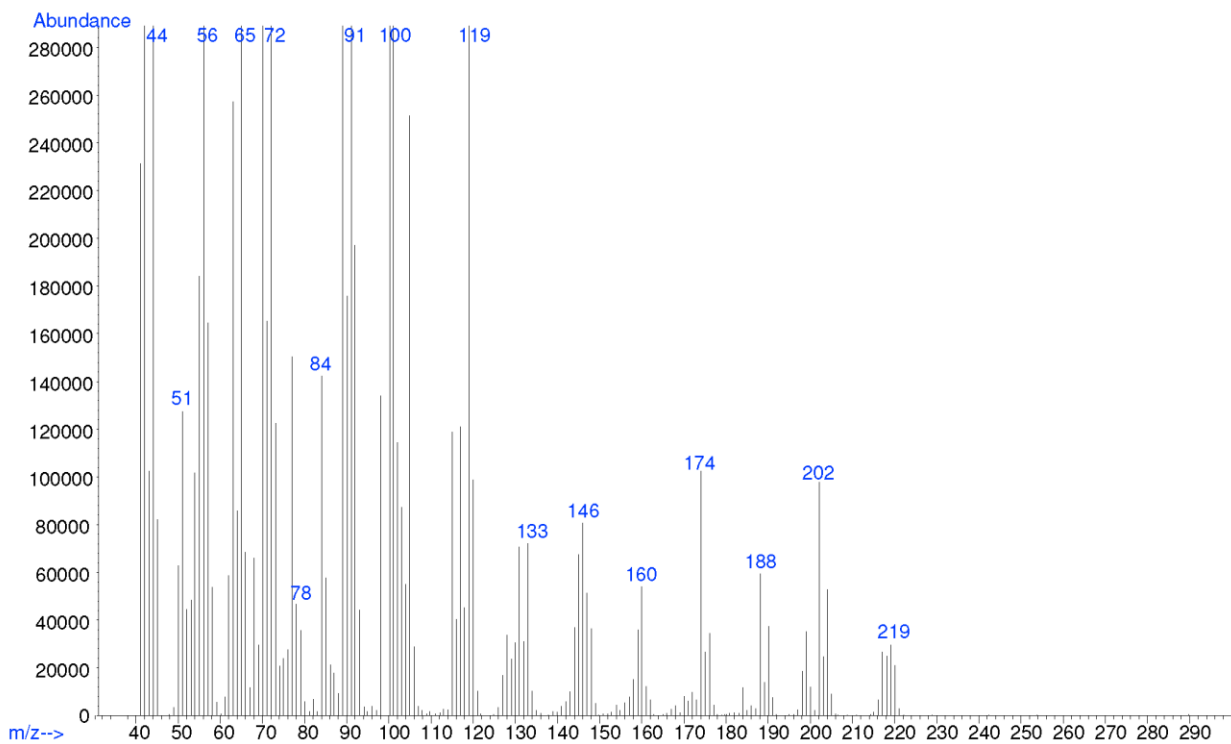
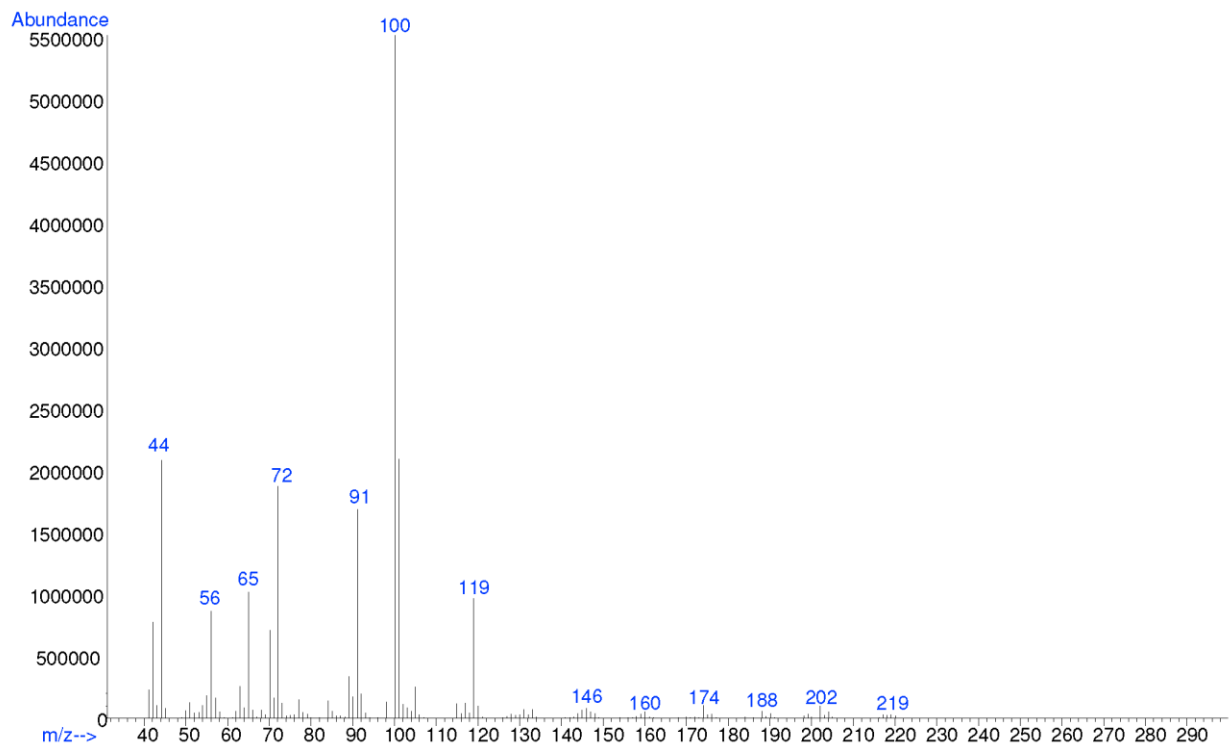
Retention Time: 4.323 min

GC Chromatogram: 4-Methyldiethcathinone (4-MDEC)



Additional peaks present in chromatogram: internal standard 1 (3.134 min), probable breakdown (4.597 min), internal standard 2 (6.200 min)

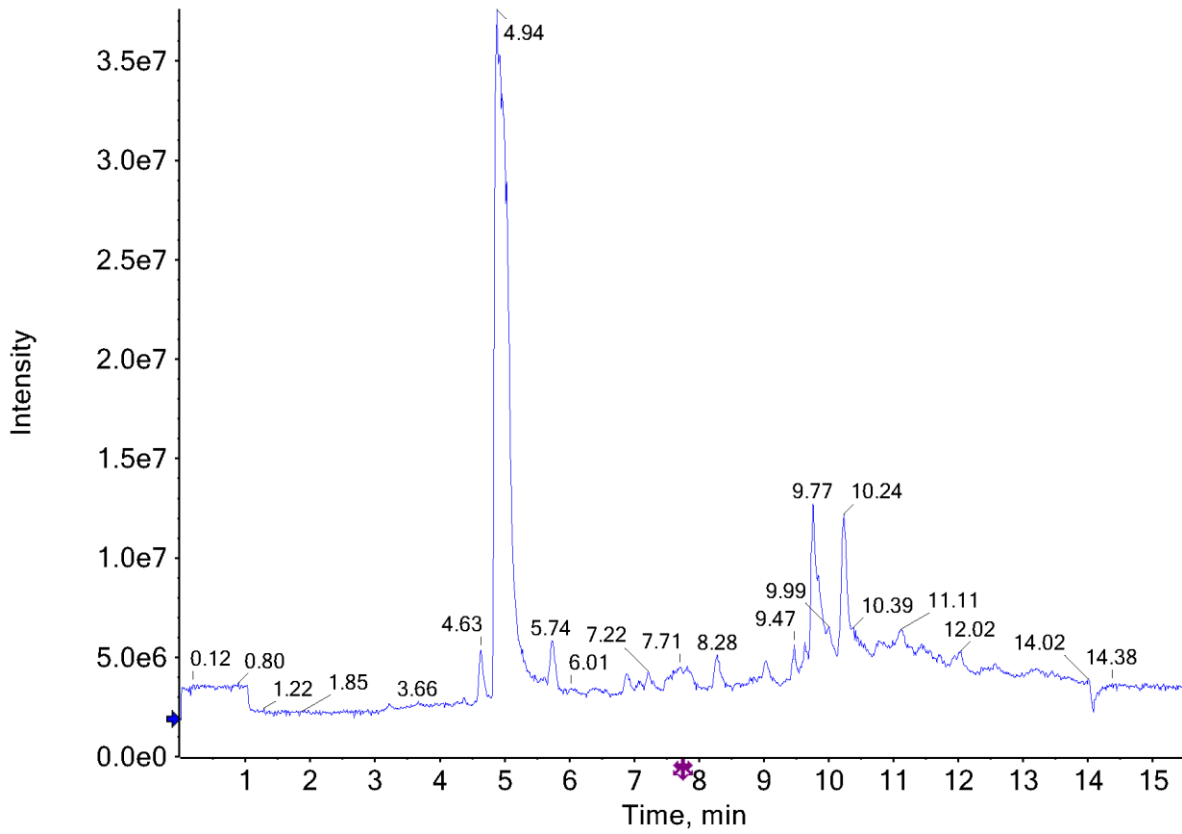
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4-Methyldiethcathinone (4-MDEC)



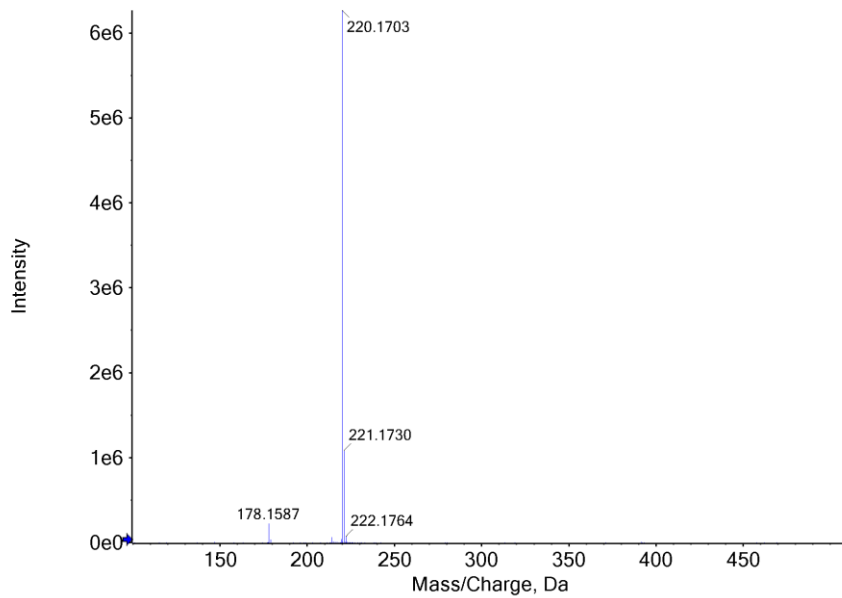
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

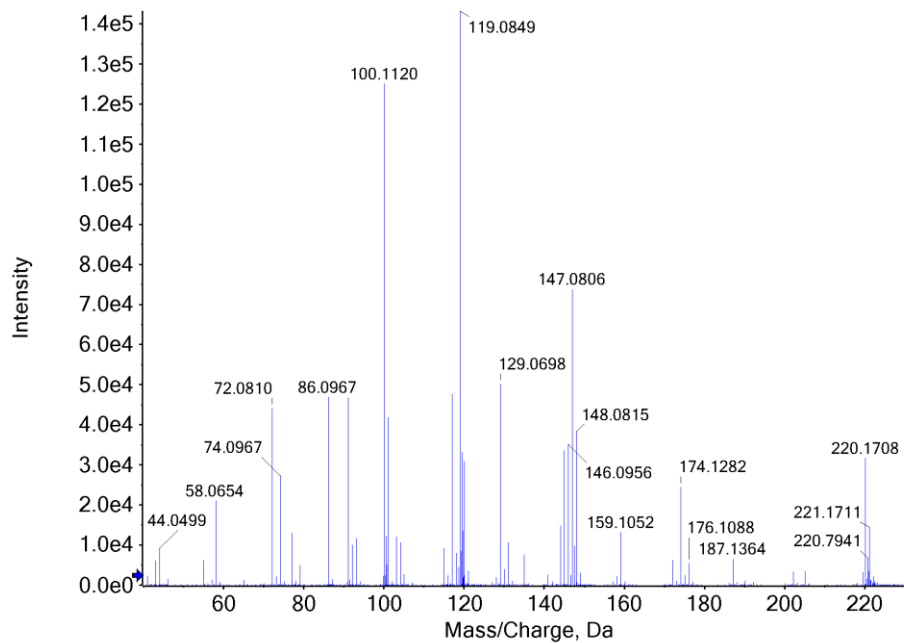
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:10 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
Mobile Phase:	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
Gradient:	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
Temperatures:	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
Injection Parameters:	Injection Volume: 10 µL
QTOF Parameters:	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
Retention Time:	4.94 min

LC Chromatogram: 4-Methyldiethcathinone (4-MDEC)



TOF MS (Top) and MS/MS (Bottom) Spectra: 4-Methyldiethcathinone (4-MDEC)





5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in CDCl₃

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

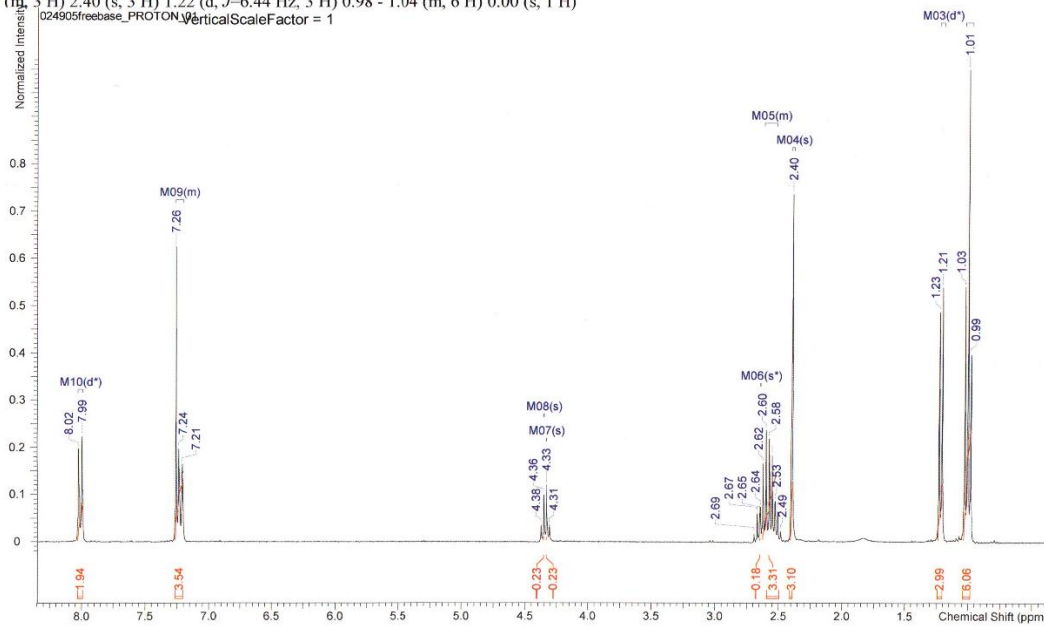
Solvent: CDCl₃

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

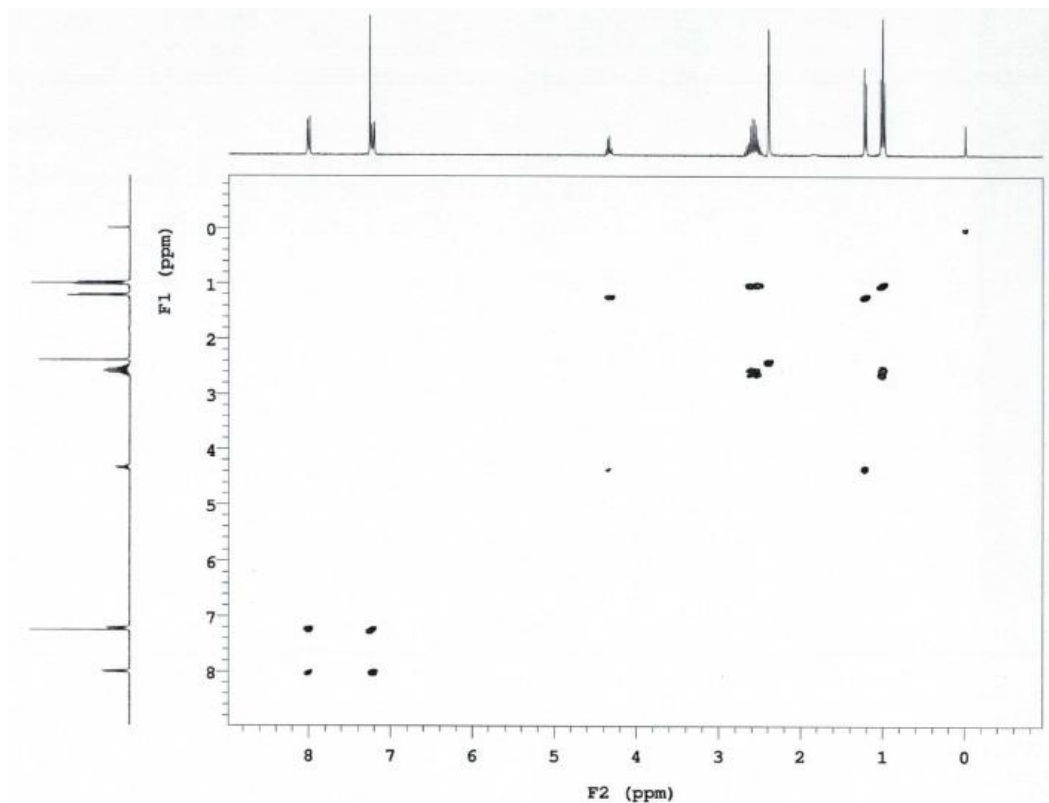
Delay between pulses: 1st delay, d1 = 1.000

¹H NMR: 4-Methyldiethcathinone (4-MDEC)

¹H NMR (300 MHz, CHLOROFORM-*d*) δ ppm 8.01 (d, *J*=8.20 Hz, 2 H) 7.20 - 7.26 (m, 4 H) 4.36 (s, 1 H) 4.33 (s, 1 H) 2.64 (s, 1 H) 2.53 - 2.63 (m, 3 H) 2.40 (s, 3 H) 1.22 (d, *J*=6.44 Hz, 3 H) 0.98 - 1.04 (m, 6 H) 0.00 (s, 1 H)



gCOSY: 4-Methyldiethcathinone (4-MDEC)



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.