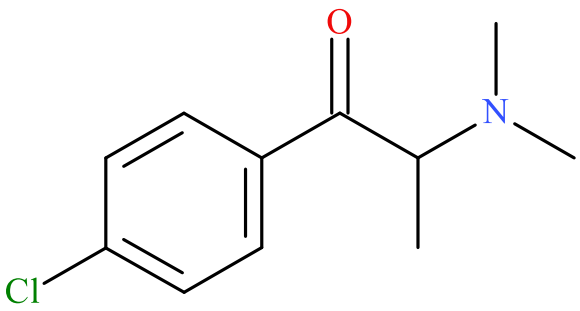
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

4-CDMC



Sample Type: **Seized Material**

Latest Revision: **October 30, 2018**

Date Received: **August 17, 2018**

Date of Report: **October 30, 2018**

1. GENERAL INFORMATION

IUPAC Name: 1-(4-chlorophenyl)-2-(dimethylamino)propan-1-one

InChI String: InChI=1S/C11H14ClNO/c1-8(13(2)3)11(14)9-4-6-10(12)7-5-9/h4-8H,1-3H3

CFR: Not Scheduled (10/2018)

CAS# Not Available

Synonyms: 4-CDC, 4-Chloro-*N*,*N*-Dimethylcathinone, 4-chloro-*N*,*N*-DMC

Source: Department of Homeland Security

Appearance: 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	$C_{11}H_{14}ClNO$	211.7	211	212.0837

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material.*

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

3. BRIEF DESCRIPTION

4-CDMC (4-chloro-*N*,*N*-dimethylcathinone) 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, methcathinone, mephedrone, dimethylcathinone, and 4-fluoromethcathinone (4-FMC). Cathinone, methcathinone, mephedrone, and 4-FMC are all explicitly Schedule I substances in the United States.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/24432

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4-CDC-ID-1908-18_report.pdf

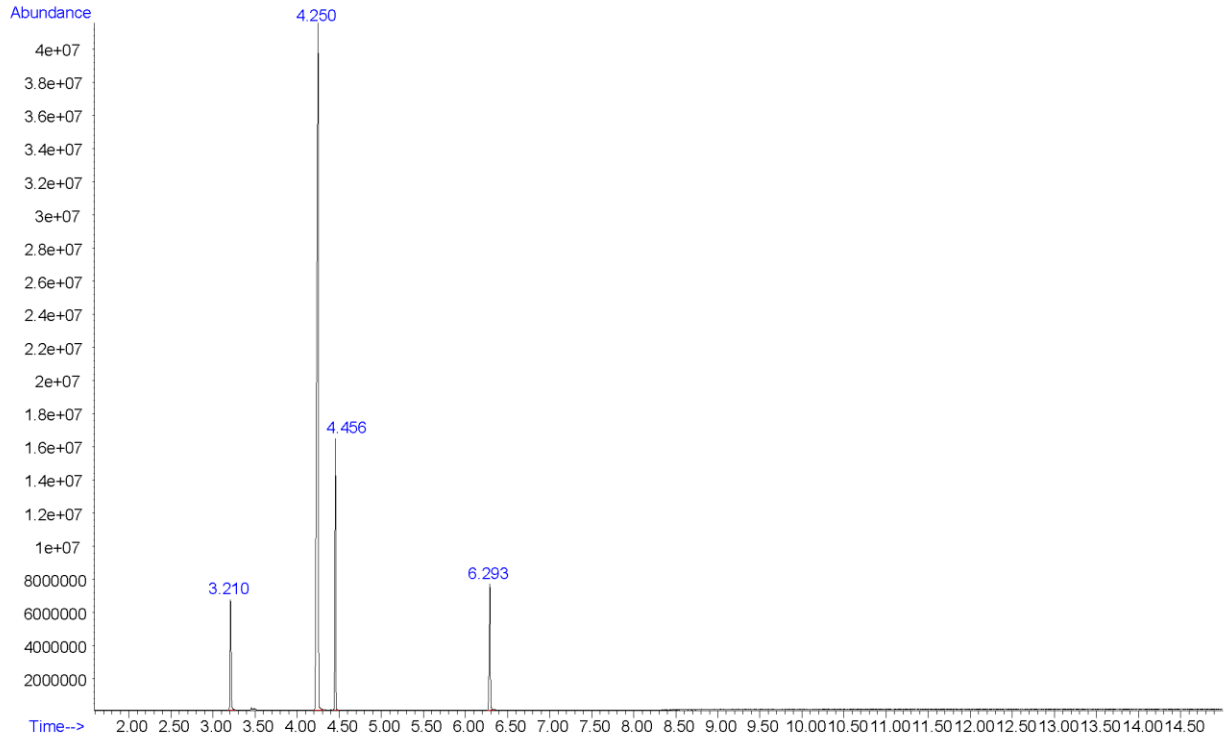
5. QUALITATIVE DATA

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:	Zebron™ 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

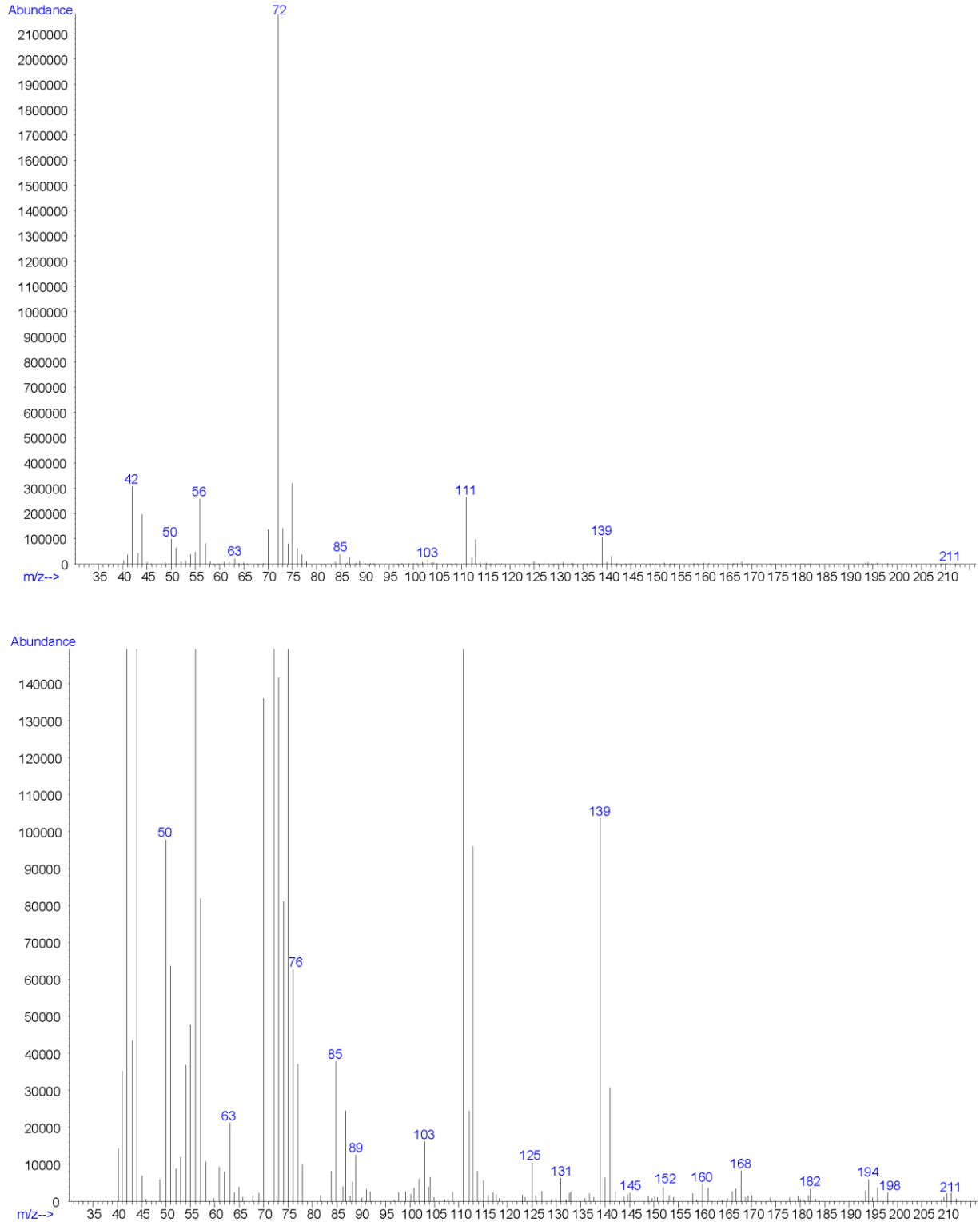
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	4.250 min
Standard Comparison:	Reference material for 4-CDMC (Batch: 0523448-11) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4-CDMC, based on retention time (4.220 min) and mass spectral data. (https://www.caymanchem.com/product/24432)

Chromatogram: 4-CDMC



Additional peaks present in chromatogram: internal standard (3.210 min), not a controlled substance (4.456 min), internal standard (6.293 min)

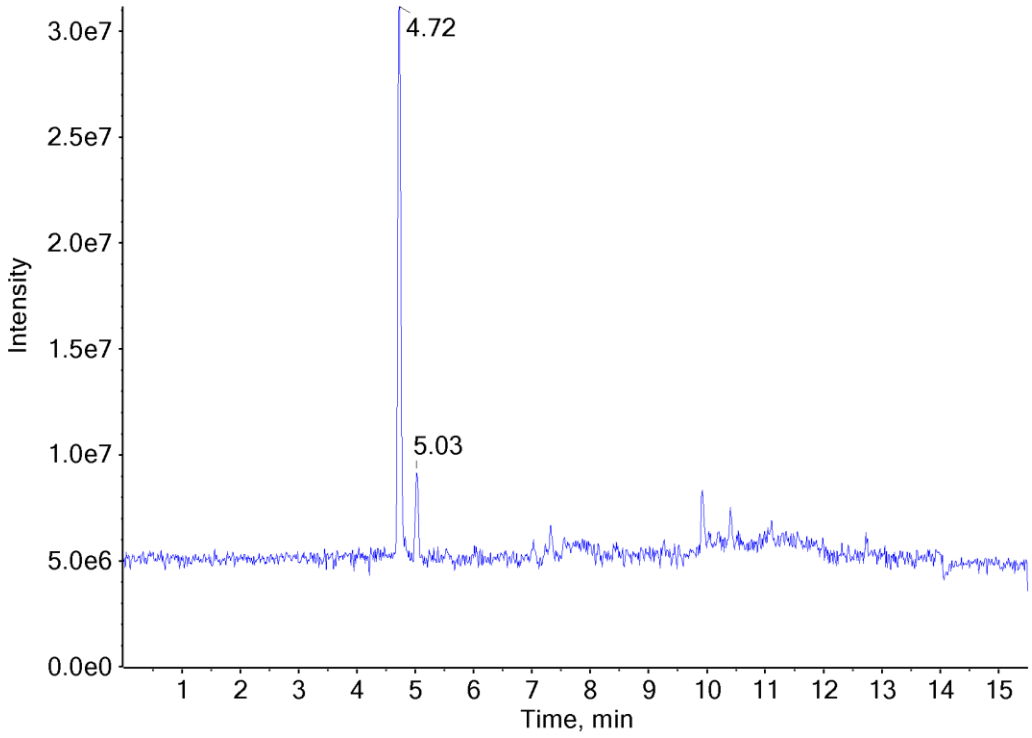
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4-CDMC



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:	1:100 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: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	4.72 min
Standard Comparison:	Reference material for 4-CDMC (Batch: 0523448-11) was purchased from Cayman Chemical (Ann Arbon, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4-CDMC, based on retention time (4.59 min) and mass spectral data. (https://www.caymanchem.com/product/24432)

Chromatogram: 4-CDMC



Additional peaks present in chromatogram: internal standard (5.03 min)

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