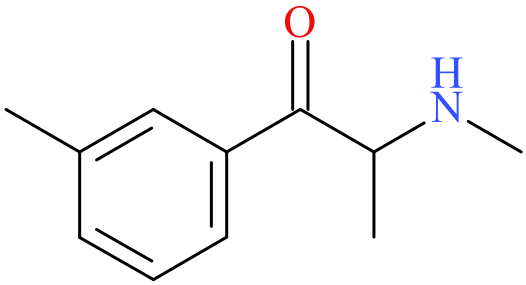
Methylmethcathinone (MMC)

Sample Type: **Toxicology Sample**



Latest Revision: **December 15, 2022**

Date Received: **November 22, 2021**

Date of Report: **December 15, 2022**

1. GENERAL INFORMATION

IUPAC Name:	2-(methylamino)-1-(m-tolyl)propan-1-one
InChI String:	InChI=1S/C11H15NO/c1-8-5-4-6-10(7-8)11(13)9(2)12-3/h4-7,9,12H,1-3H3
CFR:	Schedule I
CAS#	1246815-51-9 (2-MMC), 1246816-62-5 (3-MMC), and 1189726-22-4 (Mephedrone)
Synonyms:	2-MMC, 3-MMC, 4-MMC (Mephedrone), 2-Methyl-N-Methylcathinone, 3-Methyl-N-Methylcathinone, 4-Methyl-N-Methylcathinone
Source:	NMS Labs – Toxicology Department

***Important Note**: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. The "3-methyl" configuration was used for structural purposes. The position of the methyl group was not confirmed during analysis; however, it is believed to be 2- or 3-methyl isomer and not the reemergence of 4-methylmethcathinone (mephedrone).*

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Drug	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Methylmethcathinone	$C_{11}H_{15}NO$	177.2	177	178.1226

3. SAMPLE HISTORY

Methylmethcathinone has been identified in at least two toxicology cases since December 2021. The geographical and demographical breakdown is below:

Case Type: Postmortem (n=2)

Geographical Location: Vancouver (n=1), California (n=1)

Biological Sample: Blood (n=2)

Date of First Collection: November 2021

4. BRIEF DESCRIPTION

Methylmethcathinone is classified as a novel stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause psychoactive effects similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Methylmethcathinone exists in three isomeric forms: 2-methylmethcathinone, 3-methylmethcathinone, and 4-methylmethcathinone (also known as mephedrone). Mephedrone is a Schedule I substance in the United States, while other positional isomers are or may be considered Schedule I due to their structural similarity.

5. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/3-MMC-ID_1048-12A-report_final.pdf

https://www.caymanchem.com/product/11223/2-methylmethcathinone-(hydrochloride)

https://www.caymanchem.com/product/11224/3-methylmethcathinone-(hydrochloride)

https://www.caymanchem.com/product/10801/mephedrone-(hydrochloride)

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

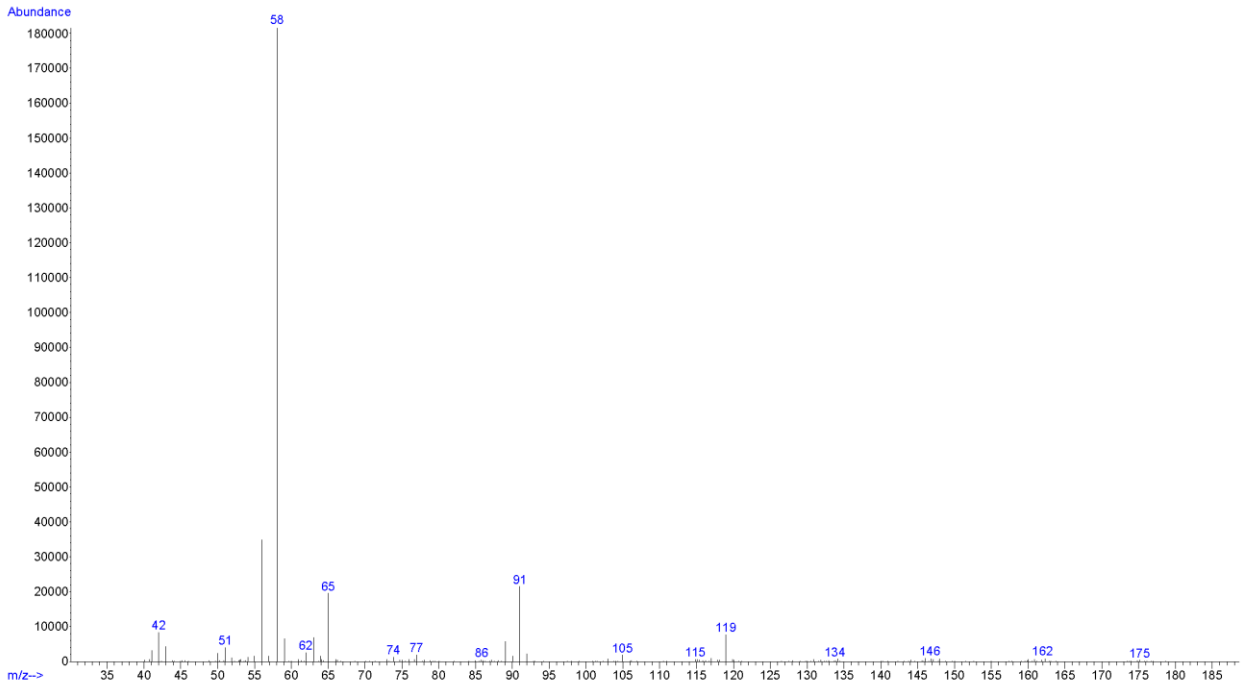
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for 3-methylmethcathinone (Batch: 0614250-1) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/11224/3-methylmethcathinone-(hydrochloride))

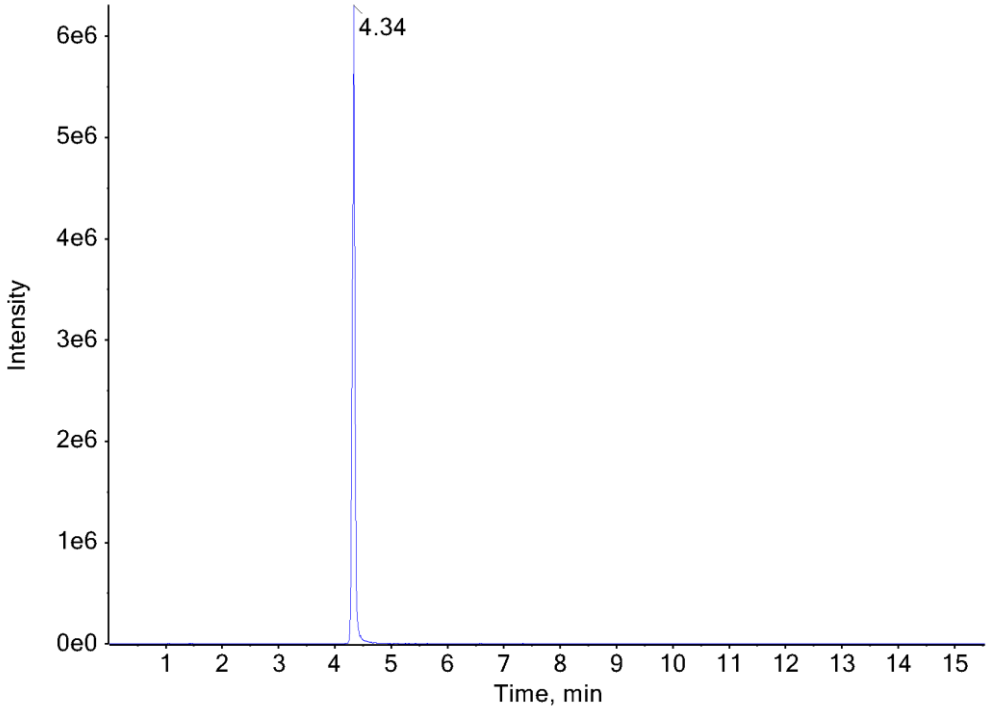
EI (70 eV) Mass Spectrum: 3-Methylmethcathinone (Standard)



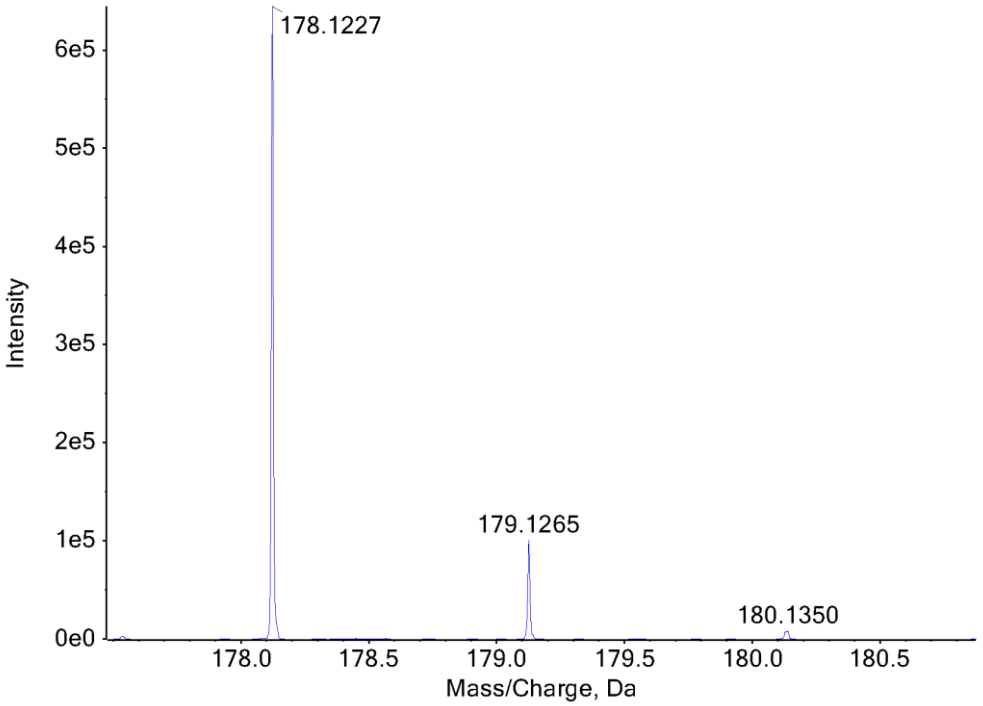
6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Liquid-liquid extraction (LLE)
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:	4.34 min
Standard Comparison:	Reference material for 3-methylmethcathinone (Batch: 0614250-1) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as 3-methylmethcathinone, based on retention time (4.38 min) and mass spectral data. (https://www.caymanchem.com/product/11224/3-methylmethcathinone-(hydrochloride))

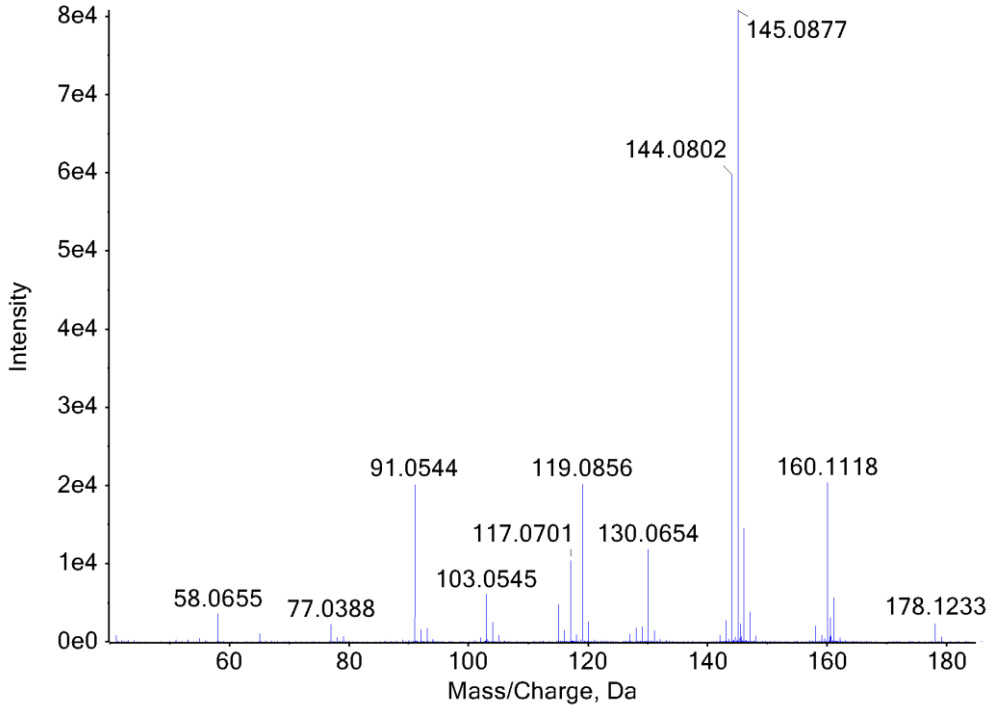
Extracted Ion Chromatogram: Methylmethcathinone



TOF MS Spectra: Methylmethcathinone



MS/MS Spectra: Methylmethcathinone



7. FUNDING

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