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).

Prepared By: Alex J. Krotulski, PhD; Sara E. Walton, MS; Melissa F. Fogarty, MSFS, D-ABFT-FT; Donna M. Papsun, MS, D-ABFT-FT; and Barry K. Logan, PhD, F-ABFT
2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Drug</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methylmethcathinone</td>
<td>C₁₁H₁₅NO</td>
<td>177.2</td>
<td>177</td>
<td>178.1226</td>
</tr>
</tbody>
</table>

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.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

![Extracted Ion Chromatogram: Methylmethcathinone](image)

TOF MS Spectra: Methylmethcathinone

![TOF MS Spectra: Methylmethcathinone](image)
7. FUNDING

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