4-Methylmethylphenidate

**NPS SUBCLASS**
Stimulant

**REPORT DATE**
June 20, 2023

**SAMPLE RECEIVED**
October 31, 2022

**SAMPLE TYPE**
Toxicology

<table>
<thead>
<tr>
<th>Preferred Name</th>
<th>4-Methylmethylphenidate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synonyms</td>
<td>4-MeTMP, 4-Me-TMP, (±)-threo-4-Methylmethylphenidate, (±)-4-MeTMP</td>
</tr>
<tr>
<td>Formal Name</td>
<td>methyl 2-(2-piperidyl)-2-(p-tolyl)acetate</td>
</tr>
<tr>
<td>InChI Key</td>
<td>WJZNCJIOIACDBR-UHFFFAOYSA-N</td>
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<tr>
<td>CAS Number</td>
<td>680996-70-7</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>C_{15}H_{21}NO_{2}</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>247.33</td>
</tr>
<tr>
<td>Molecular Ion [M⁺]</td>
<td>247</td>
</tr>
<tr>
<td>Exact Mass [M+H]⁺</td>
<td>248.1645</td>
</tr>
</tbody>
</table>
4-Methylmethylphenidate

Characterization & Intelligence

The following information was compiled in June 2023 and is subject to change as new research is conducted and as new information becomes available:

Description: 4-Methylmethylphenidate is a novel synthetic stimulant which is structurally similar to methylphenidate and other “phenidate” analogues. In October 2022, 4-methylmethylphenidate was detected by our laboratory for the first time in the United States; however, the drug has emerged in other countries around the world previously.

Sample Source: Office of the Coroner, Lorain County (Ohio, USA).

Sample Appearance: Toxicology specimens – blood, urine, and vitreous fluid.

Pharmacology: Pharmacological studies involving 4-methylmethylphenidate have been published in the literature. Data indicate that 4-methylmethylphenidate is slightly less potent than methylphenidate. Based on structural similarity, 4-methylmethylphenidate is expected to exhibit similar adverse effects to other “phenidate” analogues, including tachycardia, hypertension, irritability, paranoia, and anxiety.

Toxicology: 4-Methylmethylphenidate has been detected in one toxicology case at the CFSRE.

Drug Materials: 4-Methylmethylphenidate has not been identified in drug materials at the CFSRE.

Demographics / Geographics: The toxicology case originated from the state of Ohio.

Legal Status: 4-Methylmethylphenidate is not explicitly scheduled in the United States.

References:

► Cayman Chemical: 4-Methylmethylphenidate
► National Forensic Laboratory (Slovenia): 4-Methylmethylphenidate (referred to as “4- Me-TMP”)  

About: In collaboration with medical examiner and coroner offices, crime laboratories, clinical partners, and other stakeholders, the Center for Forensic Science Research and Education (CFSRE) is documenting first confirmations of NPS through analysis of drug materials and/or toxicology samples. These reports are generated using comprehensive analytical techniques (e.g., GC-MS, LC-QTOF-MS, NMR) and include available information about the new substances identified at the time of reporting, as well as the analytical data generated during testing. Our new drug monographs are intended to assist with the rapid identification of NPS in forensic casework and related disciplines, and should not be used for confirmatory purposes alone.

Analytical Notes: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material.

Acknowledgements: This report was prepared by Alex J. Krotulski, Sara E. Walton, Melissa F. Fogarty, and Barry K. Logan at the Center for Forensic Science Research and Education (CFSRE) at the Fredric Rieders Family Foundation. The authors acknowledge scientists at the CFSRE and NMS Labs for their involvements and contributions. For more information, contact npsdiscovery@cfsre.org or visit www.npsdiscovery.org.

Funding: CFSRE’s NPS Discovery is supported by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 15PNIJ-22-GG-04434-MUMU, “Implementation of NPS Discovery – An Early Warning System for Novel Drug Intelligence, Surveillance, Monitoring, Response, and Forecasting using Drug Materials and Toxicology Populations in the US”). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily represent the official position or policies of the U.S. Department of Justice.

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Gas Chromatography Mass Spectrometry (GC-MS)

**Laboratory:** Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

**Sample Preparation:** Standard diluted in methanol

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

**Methods:** [www.cfsre.org/nps-discovery/monographs](http://www.cfsre.org/nps-discovery/monographs)

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**GC-MS:** Mass Spectrum (EI 70 eV)

![Mass Spectrum Graph](image)
Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (LC-QTOF-MS)

**Laboratory:** Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

**Sample Preparation:** Liquid-liquid extraction

**Instrument:** Sciex X500R LC-QTOF-MS

**Methods:** [www.cfsre.org/nps-discovery/monographs](http://www.cfsre.org/nps-discovery/monographs)

**LC-QTOF-MS:** TOF-MS Precursor Ion Mass Spectrum

**LC-QTOF-MS:** TOF-MS/MS Product Ion Mass Spectrum

**Confirmation Using Drug Standard:** Reference material (Batch: 0661429-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be 4-methylmethylphenidate based on retention time (sample: 5.82 min vs. standard: 5.69 min) and mass spectral data comparisons.