**Trimethoxyamphetamine**

Sample Type: Drug Material

Latest Revision: **December 30, 2022**

Date Received: **November 3, 2022**

Date of Report: **December 30, 2022**

1. GENERAL INFORMATION

IUPAC Name: 1-(2,4,5-trimethoxyphenyl)propan-2-amine

InChI String: InChI=1S/C12H19NO3/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-8H,5,13H2,1-4H3

CFR: Schedule I (3,4,5-Trimethoxyamphetamine)

CAS#: 5688-80-2 (3,4,5-Trimethoxyamphetamine)

Synonyms: Mescalamphetamine (3,4,5-TMA), 2,3,4-Trimethoxyamphetamine, 2,4,5-Trimethoxyamphetamine, 2,4,6-Trimethoxyamphetamine, 2,3,5-Trimethoxyamphetamine, 2,3,6-Trimethoxyamphetamine, TMA-2, TMA-3, TMA-4, TMA-5, TMA-6, TMA

Source: New York City Department of Health and Mental Hygiene's Drug Checking Initiative

Appearance: Round Green Tablet →

*Important Note:* All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF-MS) in comparison to analysis of acquired reference material. The data suggest the sample contains the “2,4,5-trimethoxy” configuration; however, the exact positioning of the methoxy groups were not confirmed by NMR analysis.

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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>Trimethoxyamphetamine</td>
<td>C₁₂H₁₉NO₃</td>
<td>225.3</td>
<td>225</td>
<td>226.1438</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

Trimethoxyamphetamine 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. Trimethoxyamphetamine exists in many isomeric forms, including 3,4,5-trimethoxyamphetamine (also known as mescalamphetamine). 3,4,5-Trimethoxyamphetamine is a Schedule I substance in the United States, while other positional isomers may be considered Schedule I due to their structural similarity.

4. ADDITIONAL RESOURCES

https://en.wikipedia.org/wiki/Trimethoxyamphetamine

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/2,3,4-TMA-ID-2069_19_report.pdf

https://www.caymanchem.com/product/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride)

https://www.caymanchem.com/product/13887/3%2C4%2C5-trimethoxyamphetamine-(hydrochloride)
5. QUALITATIVE DATA

5.1 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: Dilution in methanol

Instrument: Agilent 5975 Series GC/MSD System

Column: Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)

Carrier Gas: Helium (Flow: 1.46 mL/min)

Temperatures: Injection Port: 265 °C, Transfer Line: 300 °C

MS Source: 230 °C, MS Quad: 150 °C,

Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min

Injection Parameters: Injection Type: Splitless, Injection Volume: 1 µL

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

Threshold: 250

Retention Time: 4.69 min

Standard Comparison: Reference material for 2,4,5-Trimethoxyamphetamine (Batch: 0609858-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Trimethoxyamphetamine based on retention time (4.70 min) and mass spectral data. (https://www.caymanchem.com/product/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride))
Chromatogram: Trimethoxyamphetamine

Additonal peaks in chromatogram: internal standard (3.12 min), suspected formyl artifact of trimethoxyamphetamine in MeOH (4.65 min), not controlled substances (4.95 min and 5.02 min), and internal standard (5.76 min)

EI (70 eV) Mass Spectrum: Trimethoxyamphetamine
5.1 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: 4.37 min

Standard Comparison: Reference material for 2,4,5-Trimethoxyamphetamine (Batch: 0609858-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Trimethoxyamphetamine based on retention time (4.24 min) and mass spectral data. (https://www.caymanchem.com/product/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride))
Chromatogram: Trimethoxyamphetamine

Additional peaks in chromatogram: internal standards (4.96 and 7.28 mins)

TOF MS Spectra: Trimethoxyamphetamine
6. FUNDING

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