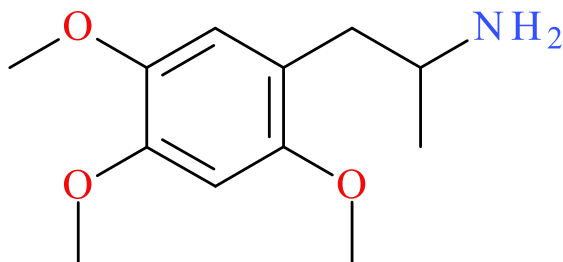


## Trimethoxyamphetamine

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

Drug	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Trimethoxyamphetamine	C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub>	225.3	225	226.1438

### 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.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/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride))

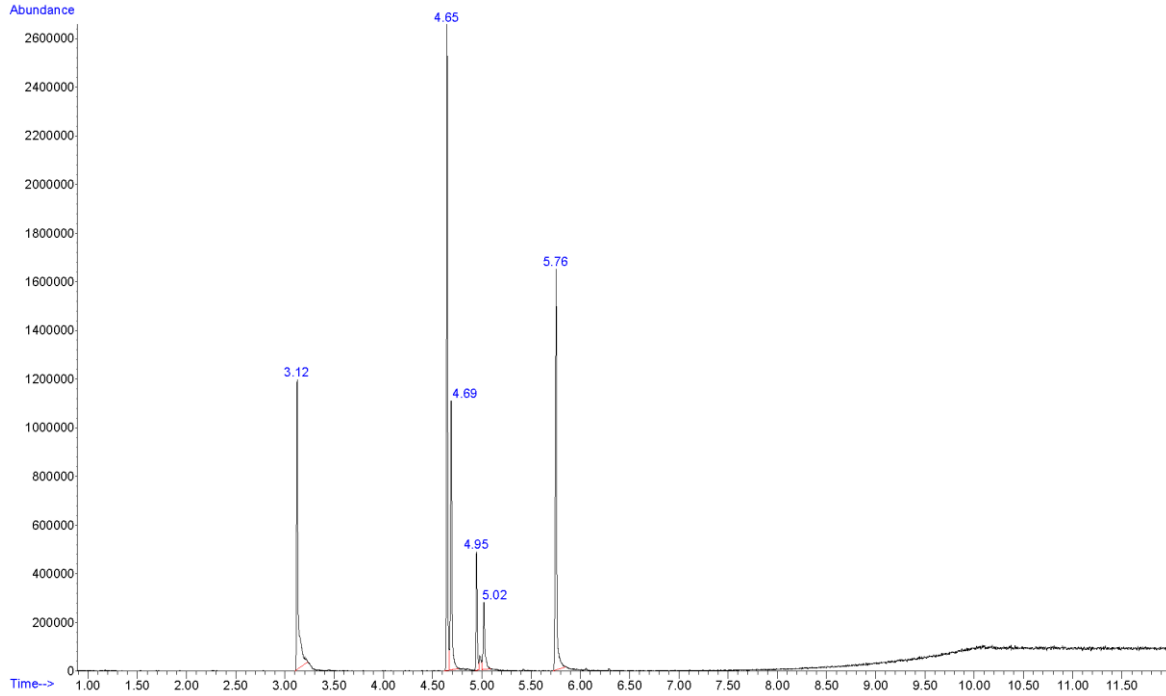
[https://www.caymanchem.com/product/13887/3%2C4%2C5-trimethoxyamphetamine-\(hydrochloride\)](https://www.caymanchem.com/product/13887/3%2C4%2C5-trimethoxyamphetamine-(hydrochloride))

## 5. QUALITATIVE DATA

### 5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

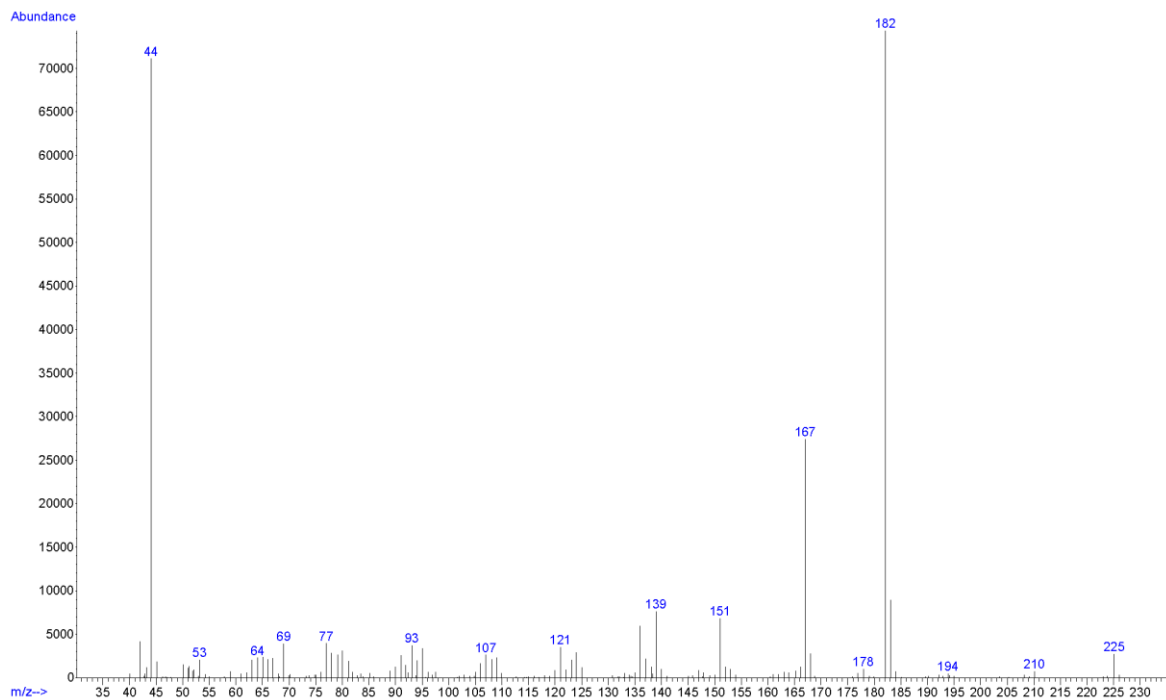
<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	Dilution in methanol
<b>Instrument:</b>	Agilent 5975 Series GC/MSD System
<b>Column:</b>	Agilent J&W DB-1 (12 m x 200 $\mu$ m x 0.33 $\mu$ m)
<b>Carrier Gas:</b>	Helium (Flow: 1.46 mL/min)
<b>Temperatures:</b>	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
<b>Injection Parameters:</b>	Injection Type: Splitless, Injection Volume: 1 $\mu$ L
<b>MS Parameters:</b>	Mass Scan Range: 40-550 m/z Threshold: 250
<b>Retention Time:</b>	4.69 min
<b>Standard Comparison:</b>	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. <a href="https://www.caymanchem.com/product/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride))">https://www.caymanchem.com/product/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride))</a>

## Chromatogram: Trimethoxyamphetamine



*Additional 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)*

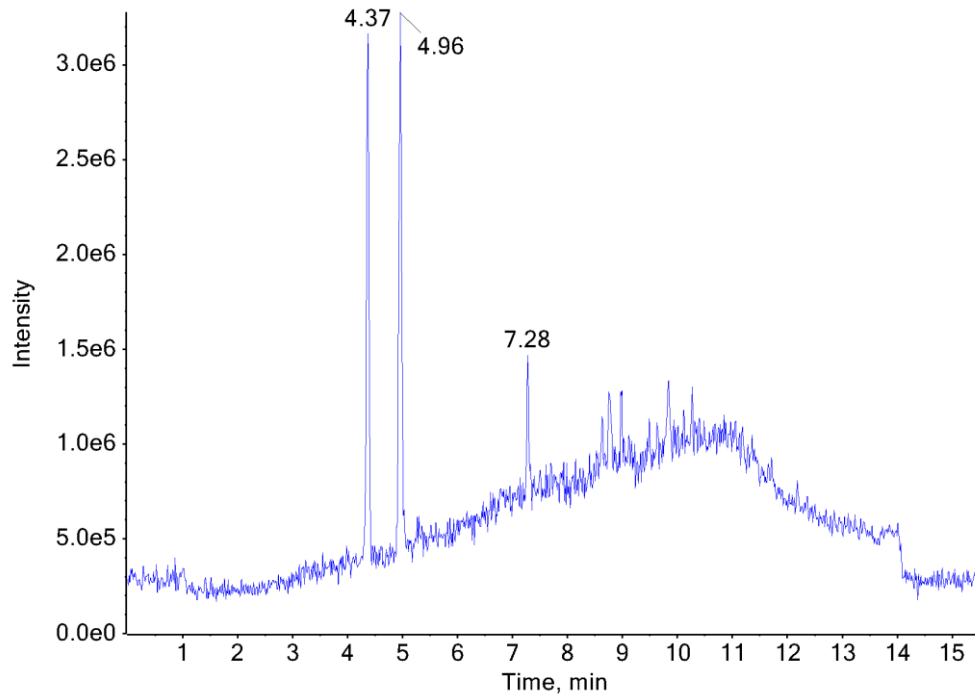
## EI (70 eV) Mass Spectrum: Trimethoxyamphetamine



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

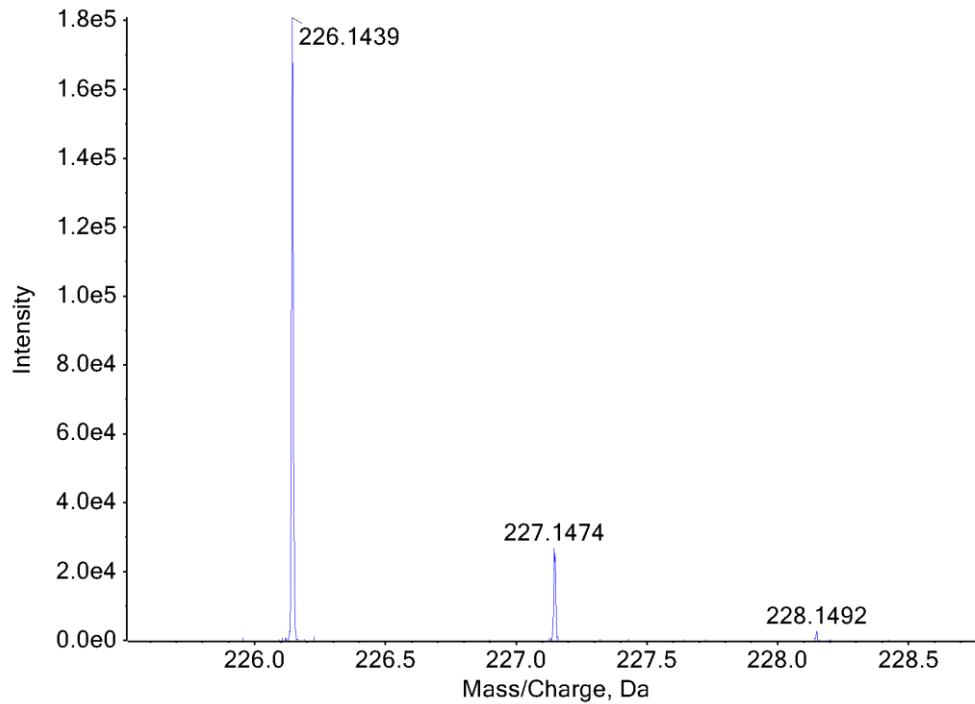
<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	Liquid-liquid extraction (LLE)
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	TOF MS Scan Range: 100-510 Da Precursor Isolation: SWATH® acquisition (27 windows) Fragmentation: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
<b>Retention Time:</b>	4.37 min
<b>Standard Comparison:</b>	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. <a href="https://www.caymanchem.com/product/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride)">https://www.caymanchem.com/product/33715/2%2C4%2C5-trimethoxyamphetamine-(hydrochloride)</a>

### Chromatogram: Trimethoxyamphetamine

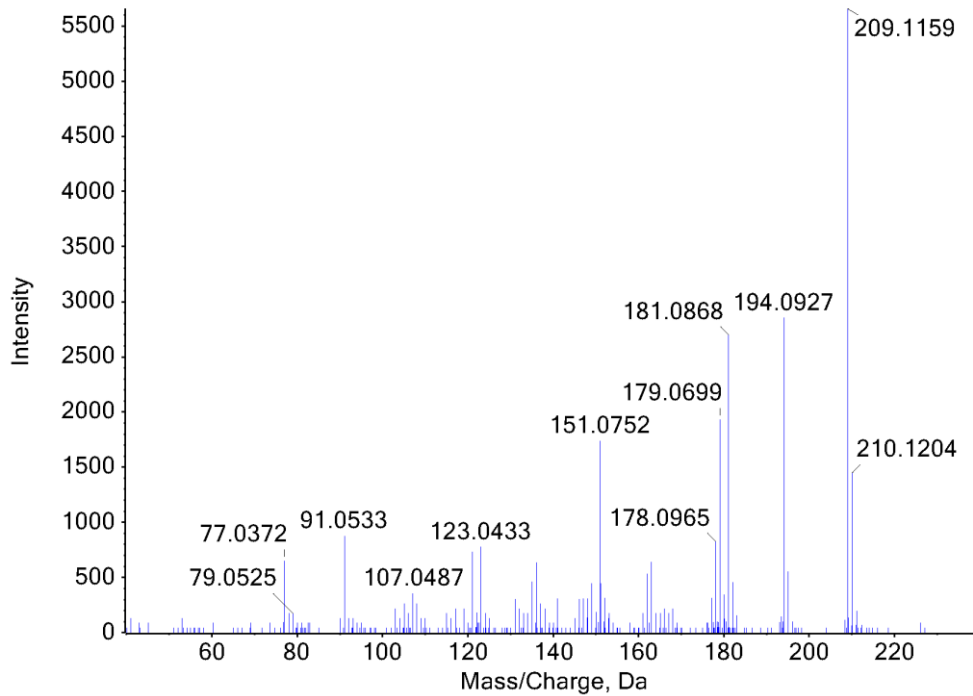


*Additional peaks in chromatogram: internal standards (4.96 and 7.28 mins)*

### TOF MS Spectra: Trimethoxyamphetamine



## MS/MS Spectra: Trimethoxyamphetamine



## 6. FUNDING

NPS Discovery at the CFSRE is supported in part by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 2020-DQ-BX-0007, “Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS)”). 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.