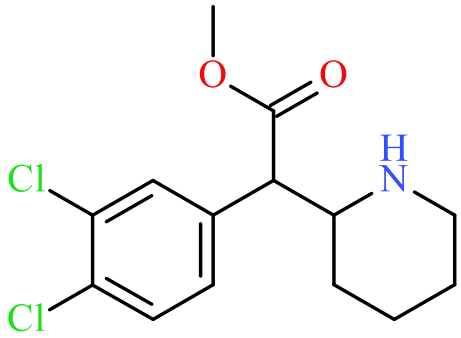
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

# 3,4-Dichloromethylphenidate

Sample Type: **Seized Material**




Latest Revision: **October 31, 2019**

Date Received: **August 16, 2019**

Date of Report: **November 21, 2019**

## 1. GENERAL INFORMATION

| | |
|---|---|
| **IUPAC Name:** | Methyl 2-(3,4-dichlorophenyl)-2-(2-piperidyl)acetate |
| **InChI String:** | InChI=1S/C14H17Cl2NO2/c1-19-14(18)13(12-4-2-3-7-17-12)9-5-6-10(15)11(16)8-9/h5-6,8,12-13,17H,2-4,7H2,1H3 |
| **CFR:** | Not Scheduled (10/2019) |
| **CAS#** | 214149-42-5 |
| **Synonyms:** | 3,4-DCMP, 3,4-CTMP |
| **Source:** | Department of Homeland Security |
| **Appearance:** | Round Brown Tablet |

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF-MS) in comparison to analysis of acquired reference material.*

***Prepared By:** Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT*

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

| Form | Chemical Formula | Molecular Weight | Molecular Ion $[M^+]$ | Exact Mass $[M+H]^+$ |
|---|---|---|---|---|
| Base | $C_{14}H_{17}Cl_2NO_2$ | 302.2 | 301 | 302.0709 |

## 3. BRIEF DESCRIPTION

3,4-Dichloromethylphenidate is classified as a novel stimulant and analogue of methylphenidate (Ritalin). Novel stimulants have been reported to cause effects similar to amphetamine. Novel stimulants have caused adverse events, including deaths, as described in the literature. Structurally similar analogues of methylphenidate include ethylphenidate, 4-fluoromethylphenidate, and 4-fluoroethylphenidate. Methylphenidate is a Schedule II substance in the United States while 3,4-dichloromethylphenidate is not explicitly scheduled.

## 4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/3,4-CTMP-ID-HCl_1100-14A-report_final.pdf

https://www.caymanchem.com/product/18588/

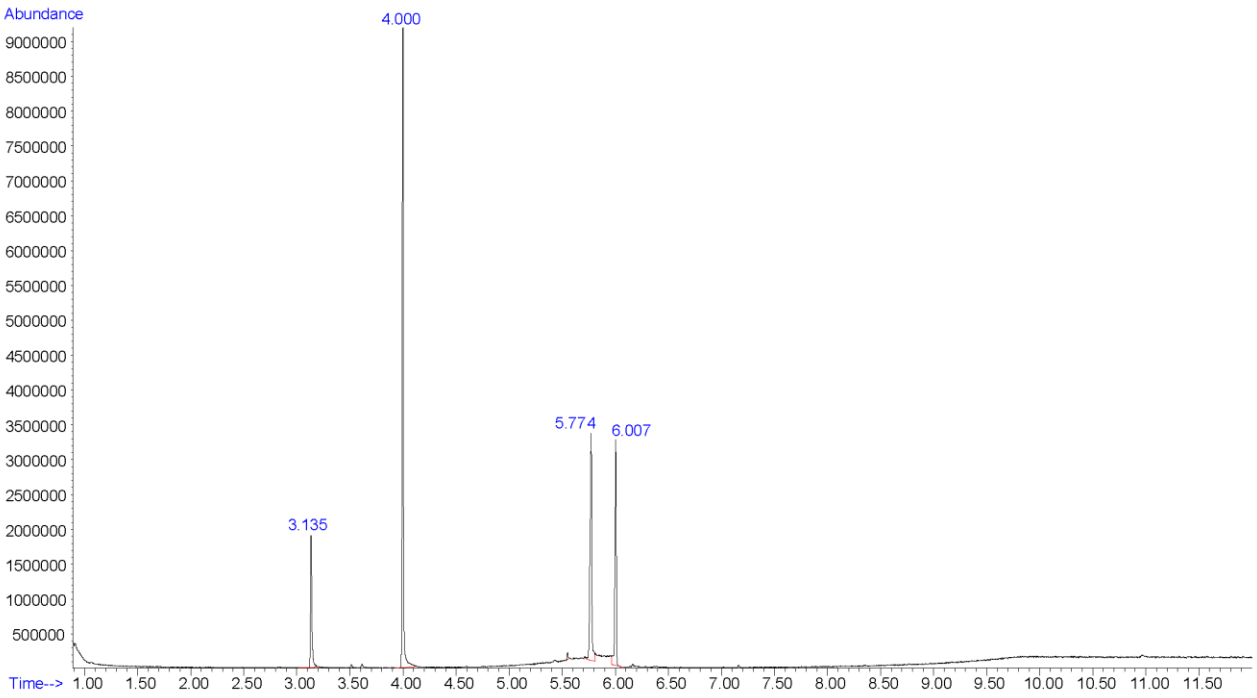
https://db12.designer-drugs.de/db/displayCompound.pl?id=16256#tabs-2

## 5. QUALITATIVE DATA

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

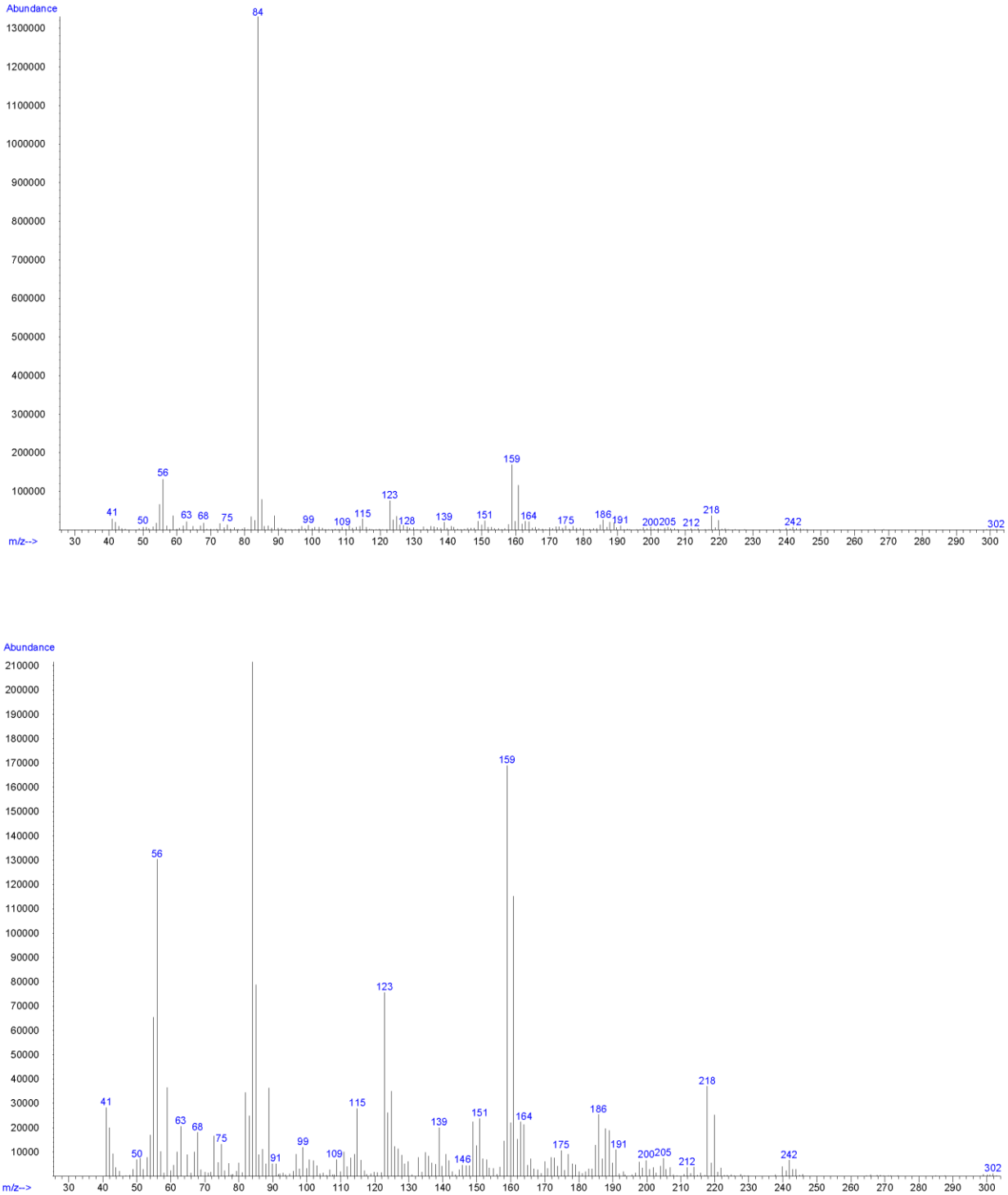
| | |
|---|---|
| **Testing Performed At:** | NMS Labs (Willow Grove, PA) |
| **Sample Preparation:** | Acid/Base extraction |
| **Instrument:** | Agilent 5975 Series GC/MSD System |
| **Column:** | Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm) |
| **Carrier Gas:** | Helium (Flow: 1.46 mL/min) |
| **Temperatures:** | 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:** | 6.007 min |
| **Standard Comparison:** | Reference material for (±)-threo-3,4-Dichloromethylphenidate (Batch: 0475221-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 3,4-Dichloromethylphenidate based on retention time (6.001 min) and mass spectral data. (https://www.caymanchem.com/product/18588/) |

## Chromatogram: 3,4-Dichloromethylphenidate




*Additional peaks present in chromatogram: internal standards (3.135 min), breakdown product (4.000), internal standard (6.282 min)*

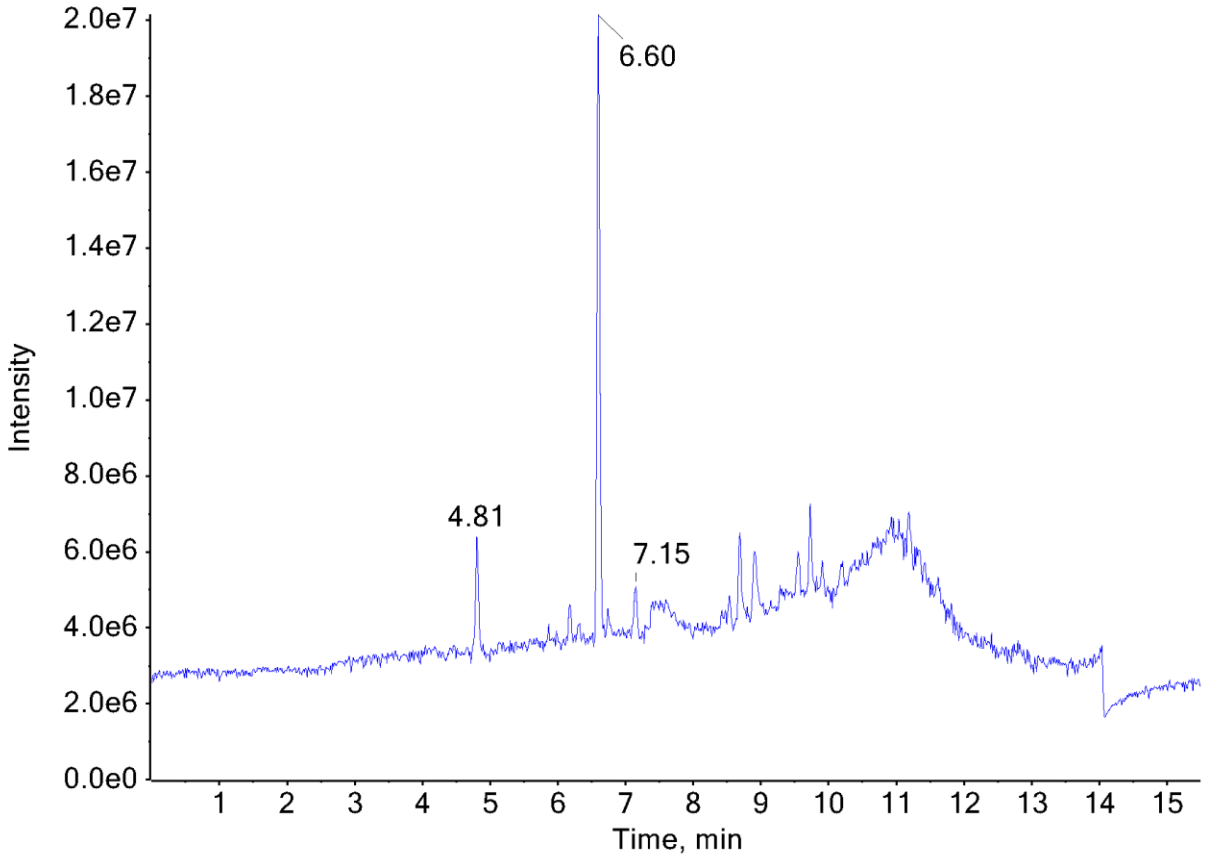
## EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 3,4-Dichloromethylphenidate



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

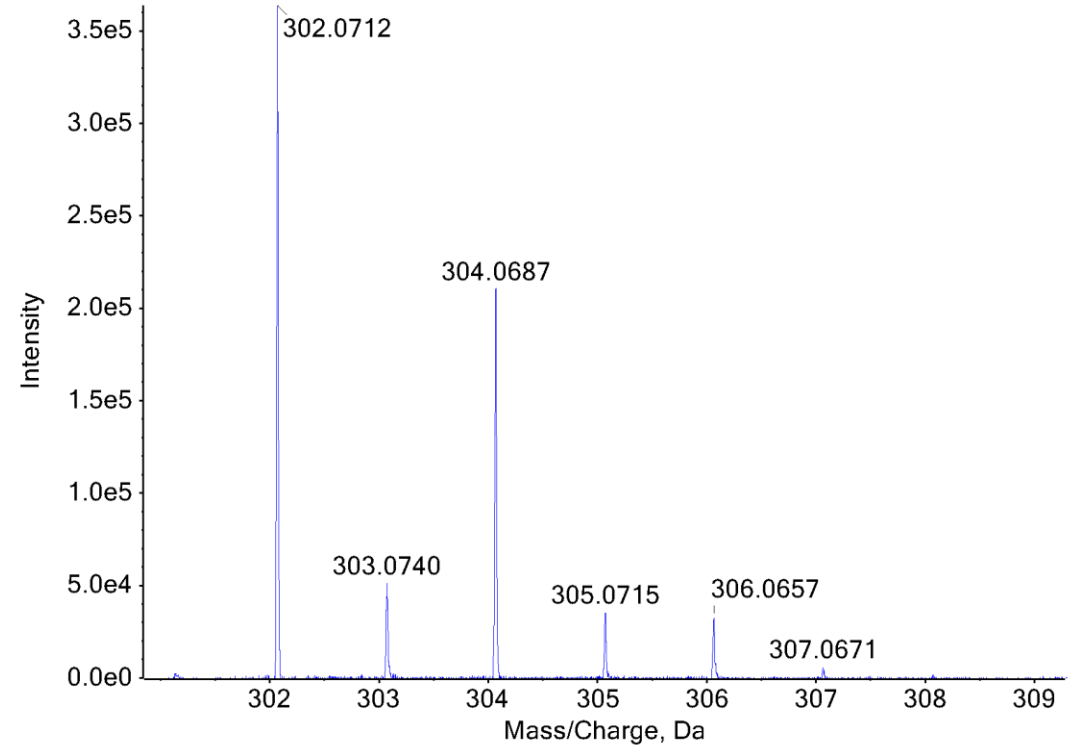
| | |
|---|---|
| **Testing Performed At:** | The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA) |
| **Sample Preparation:** | 1:100 dilution of acid/base extract in mobile phase |
| **Instrument:** | Sciex TripleTOF® 5600+, Shimadzu Nexera 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:** | 6.60 min |
| **Standard Comparison:** | Reference material for (±)-threo-3,4-Dichloromethylphenidate (Batch: 0475221-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 3,4-Dichloromethylphenidate based on retention time (6.69 min) and mass spectral data. (https://www.caymanchem.com/product/18588/) |

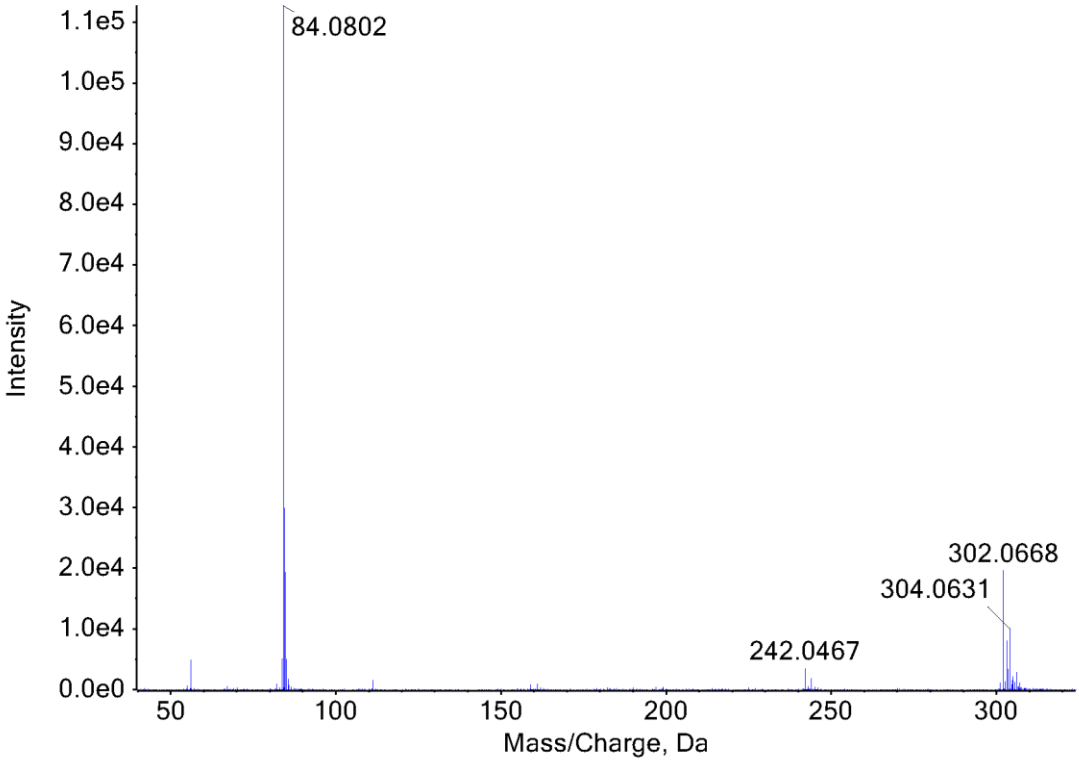
**Chromatogram: 3,4-Dichloromethylphenidate**




*Additional peaks present in chromatogram: internal standards (4.81 min and 7.15 min)*

**TOF MS (Top) and MS/MS (Bottom) Spectra: 3,4-Dichloromethylphenidate**



## 6. REVISION HISTORY

| Date | Revision |
| --- | --- |
| 11/21/2019 | GC-MS data (chromatography and mass spectrum) were revised due to the discovery of breakdown |