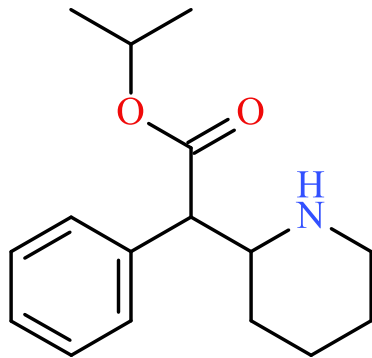


Isopropylphenidate

Sample Type: **Seized Material**



Latest Revision: **October 31, 2019**

Date Received: **August 16, 2019**

Date of Report: **October 31, 2019**

1. GENERAL INFORMATION

IUPAC Name:	Isopropyl 2-phenyl-2-(2-piperidyl)acetate
InChI String:	InChI=1S/C16H23NO2/c1-12(2)19-16(18)15(13-8-4-3-5-9-13)14-10-6-7-11-17-14/h3-5,8-9,12,14-15,17H,6-7,10-11H2,1-2H3
CFR:	Not Scheduled (10/2019)
CAS#	93148-45-9, 1262795-94-7
Synonyms:	Dimethylphenidate, Ritalinic acid isopropyl ester
Source:	Department of Homeland Security
Appearance:	Off-White Solid Material

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 ₁₆ H ₂₃ NO ₂	261.4	261	262.1802

3. BRIEF DESCRIPTION

Isopropylphenidate 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 isopropylphenidate is not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Isopropylphenidate-ID-1171-15-report_final.pdf

<https://www.caymanchem.com/product/19264/>

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: Zebron™ Inferno™ ZB-35HT (15 m x 250 μm x 0.25 μm)

Carrier Gas: Helium (Flow: 1 mL/min)

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

MS Source: 230 °C

MS Quad: 150 °C

Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

Injection Parameters: Injection Type: Splitless

Injection Volume: 1 µL

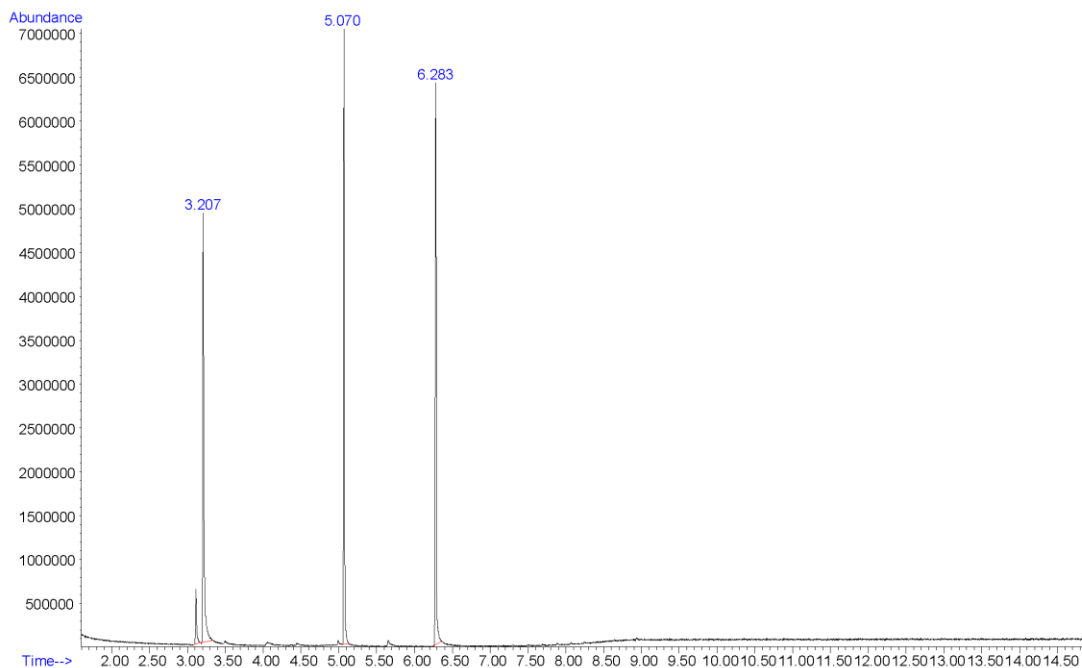
MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 5.070 min

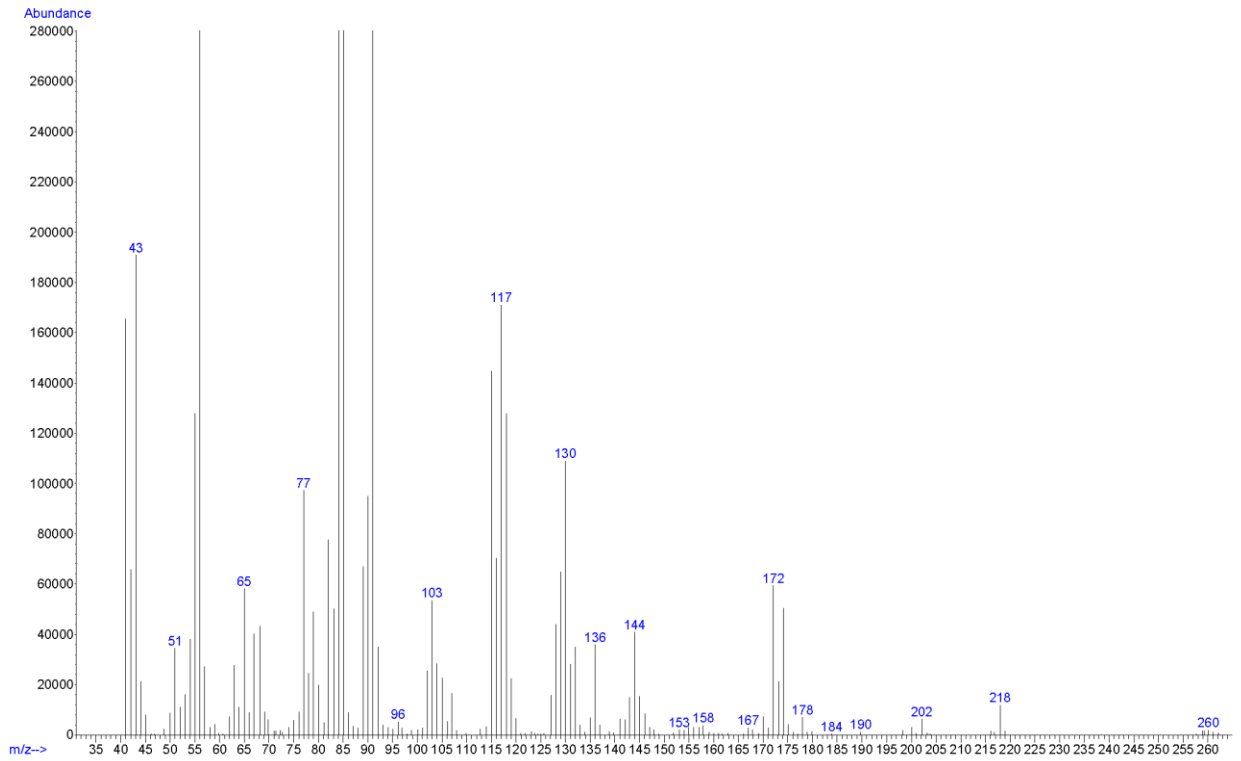
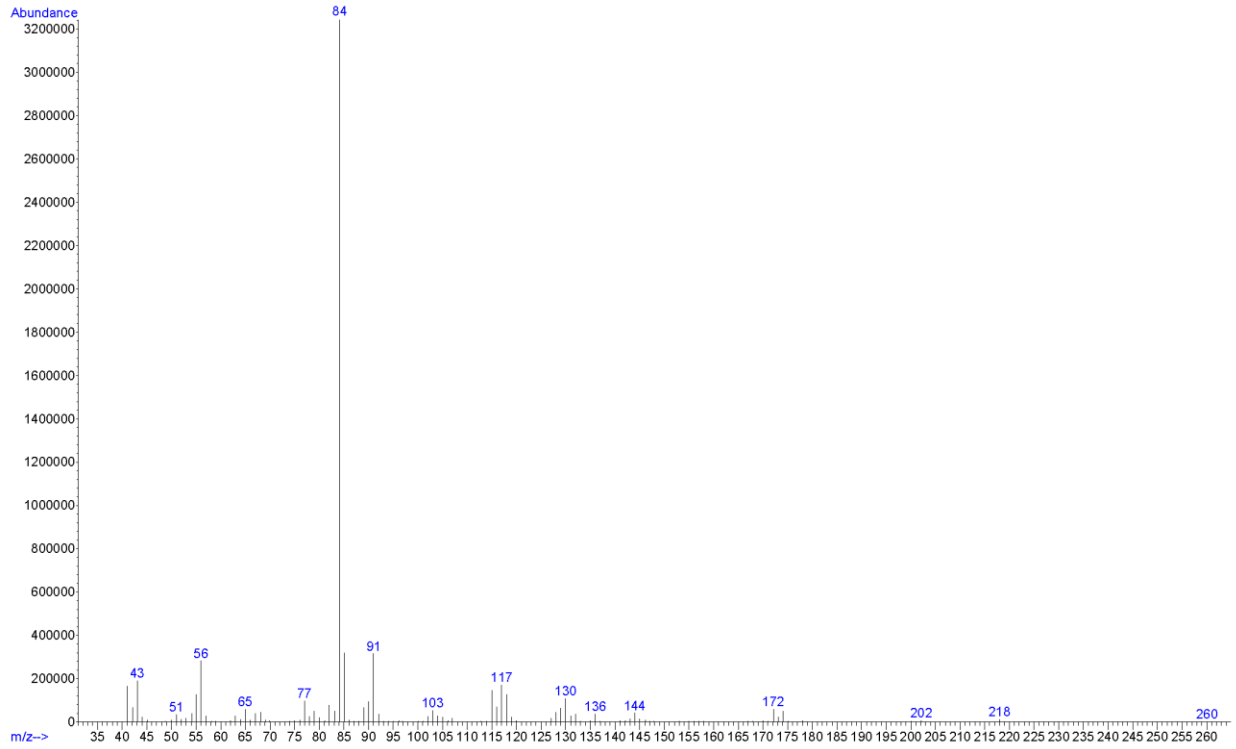
Standard Comparison: Reference material for (±)-threo-Isopropylphenidate (Batch: 0479222-19) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Isopropylphenidate based on retention time (5.081 min) and mass spectral data.
[\(https://www.caymanchem.com/product/19264/\)](https://www.caymanchem.com/product/19264/)

Chromatogram: Isopropylphenidate



Additional peaks present in chromatogram: internal standards (3.207 min and 6.283 min)

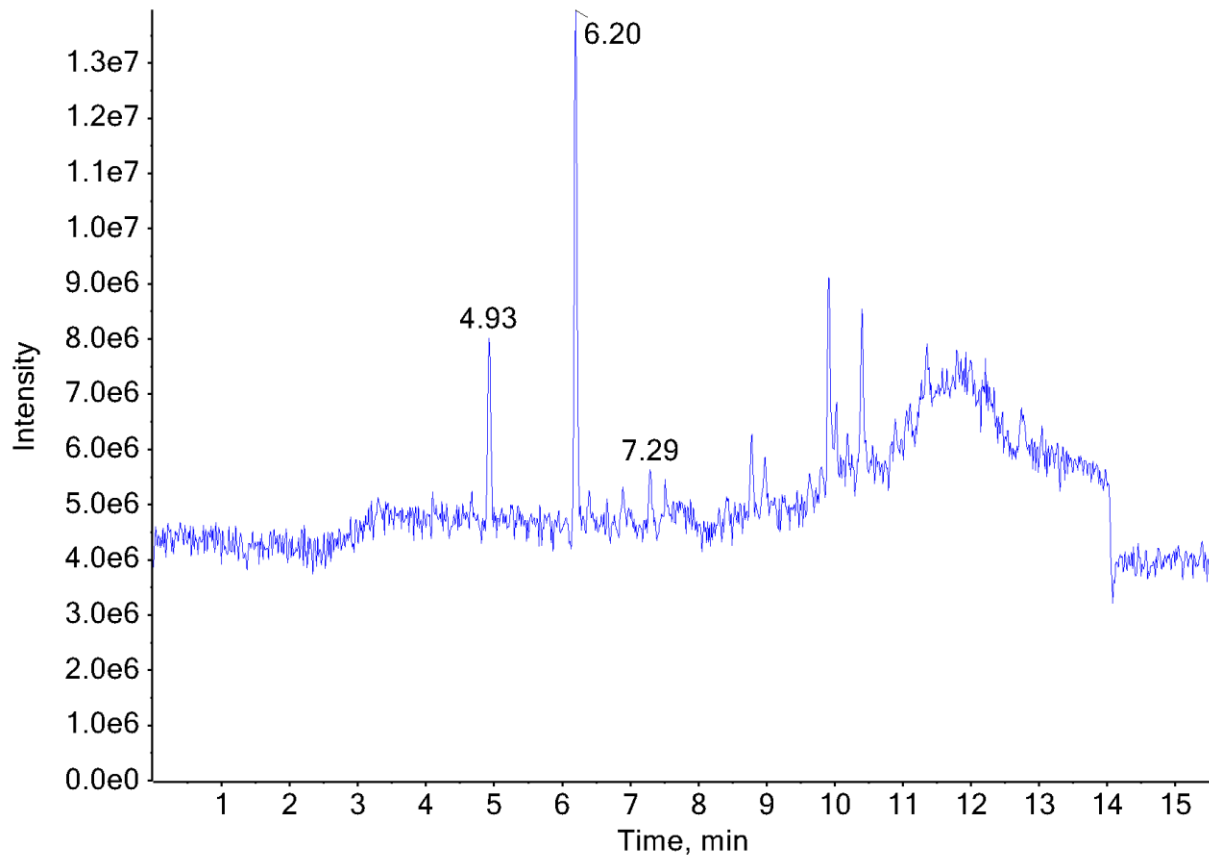
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Isopropylphenidate



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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	6.20 min
Standard Comparison:	Reference material for (±)-threo-Isopropylphenidate (Batch: 0479222-19) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Isopropylphenidate based on retention time (6.22 min) and mass spectral data. (https://www.caymanchem.com/product/19264/)

Chromatogram: Isopropylphenidate



Additional peaks present in chromatogram: internal standards (4.93 min and 7.29 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Isopropylphenidate

