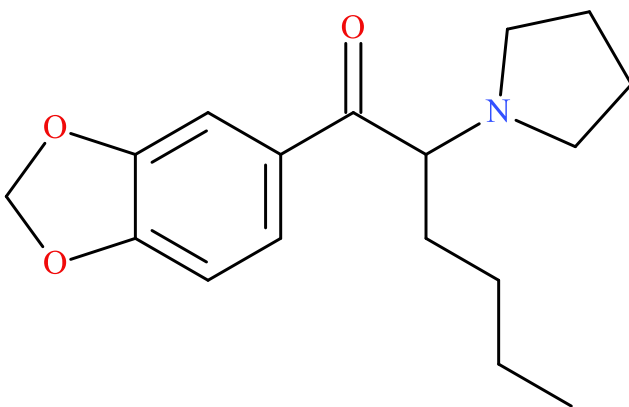


3,4-Methylenedioxy-alpha-PHP (MDPHP)

Sample Type: **Biological Fluid**



Latest Revision: **September 4, 2018**

Date of Report: **September 4, 2018**

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-pyrrolidin-1-yl-hexan-1-one
InChI String:	InChI=1S/C17H23NO3/c1-2-3-6-14(18-9-4-5-10-18)17(19)13-7-8-15-16(11-13)21-12-20-15/h7-8,11,14H,2-6,9-10,12H2,1H3
CFR:	Not Scheduled (09/2018)
CAS#	24622-61-5
Synonyms:	MDPHP; 3,4-Methylenedioxy-alpha-Pyrrolidinohexanophenone; 3,4-MD-alpha-PHP; 3,4-MDPHP
Source:	NMS Labs – Toxicology Department

2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Exact Mass [M+H] ⁺
3,4-Methylenedioxy-alpha-PHP	C ₁₇ H ₂₃ NO ₃	289.37	290.1751

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

Report Prepared By: Alex J. Krotulski, MSFS, and Barry K. Logan, PhD, F-ABFT

3. SAMPLE HISTORY

3,4-Methylenedioxy-alpha-PHP has been identified in one case since August 2018. The geographical and demographic breakdown is below:

Geographical Location:	Northern Indiana
Biological Sample:	Cardiac Blood
Date of First Collection:	August 5, 2018
Date of First Receipt:	August 7, 2018
Additional NPS:	Cyclopropylfentanyl, Methoxyacetylfentanyl, 4-ANPP

4. BRIEF DESCRIPTION

3,4-Methylenedioxy-alpha-PHP 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 stimulant-like effects, similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include alpha-PVP, alpha-PBP, and alpha-PHP. Alpha-PVP and alpha-PBP are all Schedule I substances in the United States, while alpha-PHP is not scheduled in the United States.

5. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/16361>

<http://www.chemspider.com/Chemical-Structure.34450909.html?rid=e2a0ee0f-697c-4c8b-9975-00344241de5f>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/MDPHP-ID-HCl-1245-15-report_final.pdf

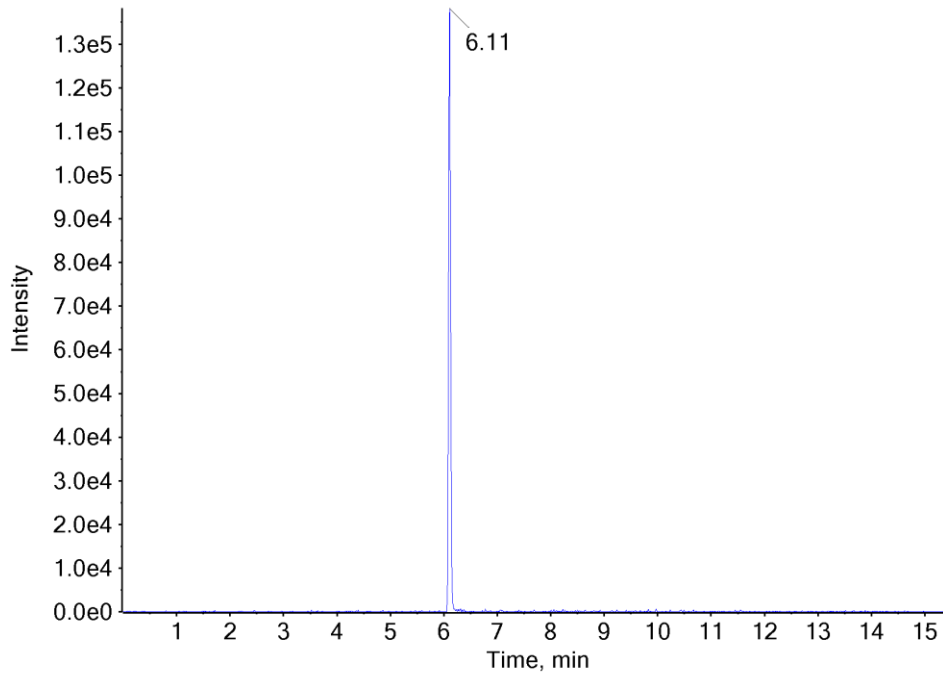
<http://www.emcdda.europa.eu/system/files/publications/1018/TDAN15001ENN.pdf>

6. QUALITATIVE DATA

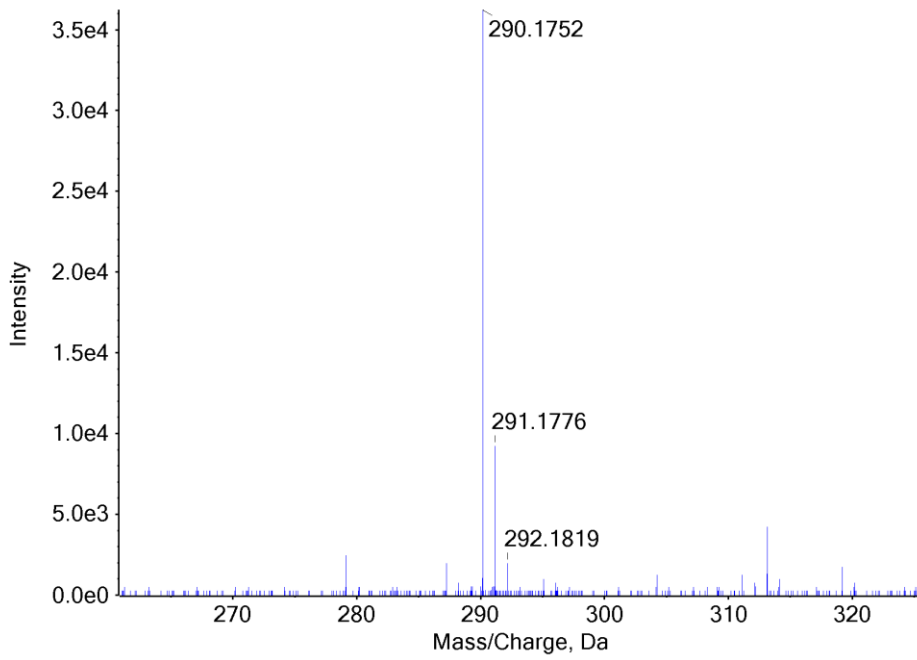
6.1 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	No additional preparation - direct analysis of sample extract
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:	6.11 min
Standard Comparison:	Reference material for 3,4-Methylenedioxy-alpha-PHP (Batch: 0464802-27) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as 3,4-Methylenedioxy-alpha-PHP, based on retention time (6.01 min) and mass spectral data. (https://www.caymanchem.com/product/16361)

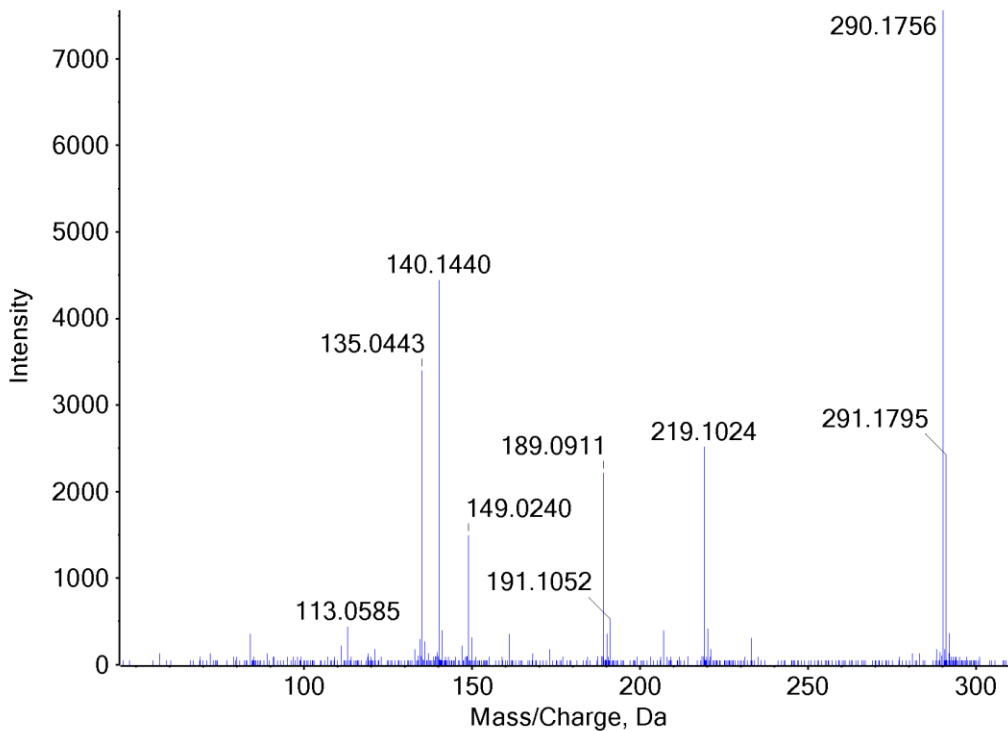
Extracted Ion Chromatogram: 3,4-Methylenedioxy-alpha-PHP



TOF MS Spectrum: 3,4-Methylenedioxy-alpha-PHP



MS/MS Spectrum: 3,4-Methylenedioxy-alpha-PHP



7. FUNDING

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