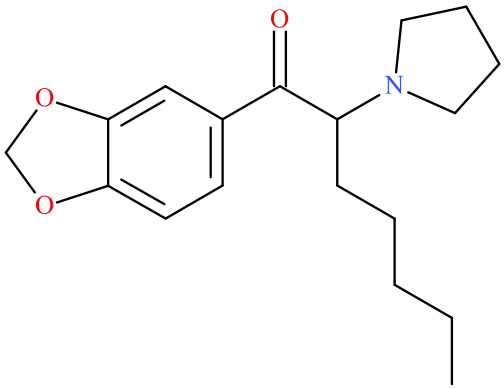
Methylenedioxy-PV8

Sample Type: **Biological Fluid**



Latest Revision: **April 23, 2021**

Date of Report: **April 23, 2021**

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-pyrrolidin-1-yl-heptan-1-one
InChI String:	InChI=1S/C18H25NO3/c1-2-3-4-7-15(19-10-5-6-11-19)18(20)14-8-9-16-17(12-14)22-13-21-16/h8-9,12,15H,2-7,10-11,13H2,1H3
CFR:	Not Scheduled (04/2021)
CAS#	24646-39-7
Synonyms:	MD-PV8, MDPEP, 3,4-Methylenedioxy PV8, MDPV two carbon homolog, Methylenedioxy pyrovalerone two carbon homolog
Source:	NMS Labs – Toxicology Department

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

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{18}H_{25}NO_3$	303.4	303	304.1907

3. SAMPLE HISTORY

Methylenedioxy-PV8 has been identified in two toxicology cases since May 2020 through retrospective data-mining. The geographical and demographical breakdown is below:

Case Type: Postmortem (n=2)

Geographical Location: Minnesota (n=1), South Carolina (n=1)

Biological Sample: Peripheral Blood (n=2)

Date of First Collection: May 2020

Additional NPS Findings: Eutylone (n=1), Etizolam (n=1), Flubromazolam (n=1)

4. BRIEF DESCRIPTION

Methylenedioxy-PV8 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 PV8 (alpha-PHPP) and methylenedioxy-alpha-PHP. Methylenedioxy-PV8 is not explicitly scheduled in the United States; however, PV8 is a Schedule I substance.

5. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/MDPEP-ID-HIFS-013_report.pdf

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/MDPEP-ID-2083-19_report.pdf

https://www.caymanchem.com/product/16358/3%2C4-methylenedioxy-pv8-(hydrochloride)

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

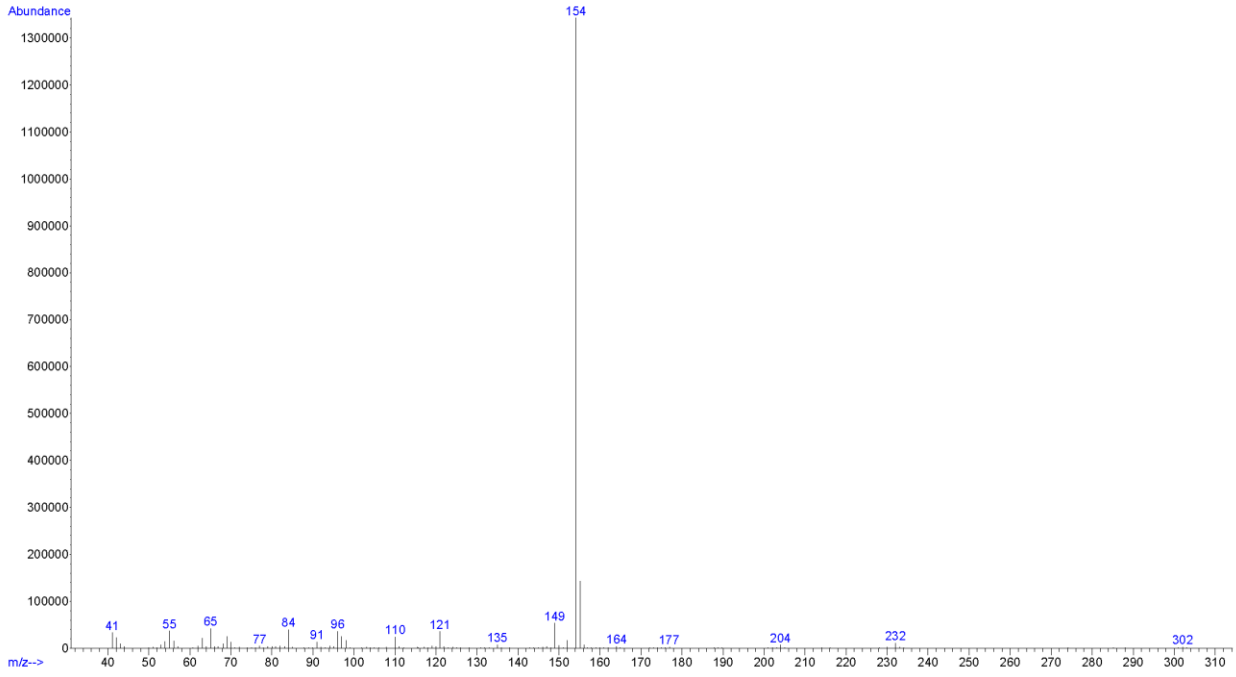
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for 3,4-Methylenedioxy-PV8 (Batch: 0470078-25) was purchased from Cayman Chemical (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/16358/3%2C4-methylenedioxy-pv8-(hydrochloride))

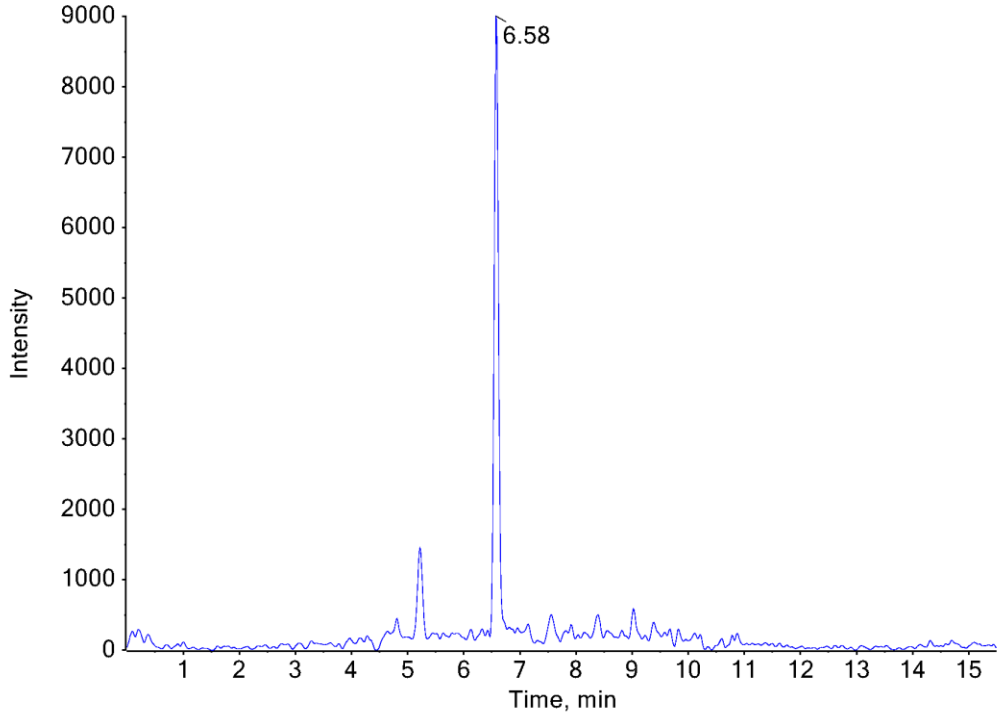
EI (70 eV) Mass Spectrum: Methylenedioxy-PV8



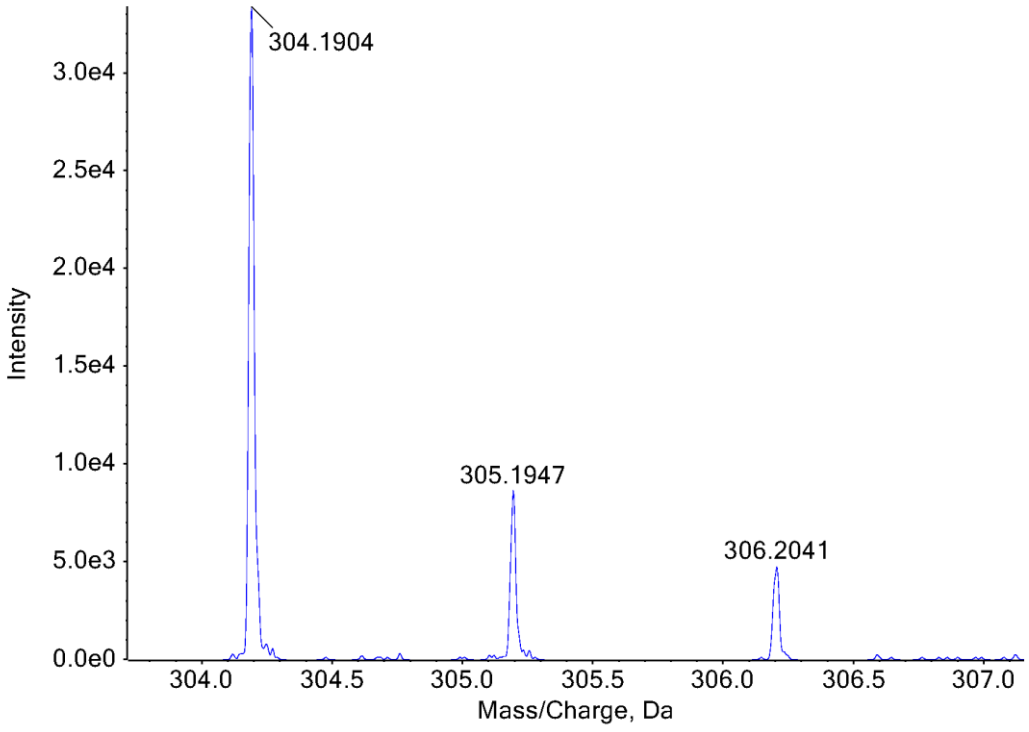
6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	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: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	6.58 min
Standard Comparison:	Reference material for 3,4-Methylenedioxy-PV8 (Batch: 0470078-25) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Methylenedioxy-PV8, based on retention time (6.61 min) and mass spectral data. (https://www.caymanchem.com/product/16358/3%2C4-methylenedioxy-pv8-(hydrochloride))

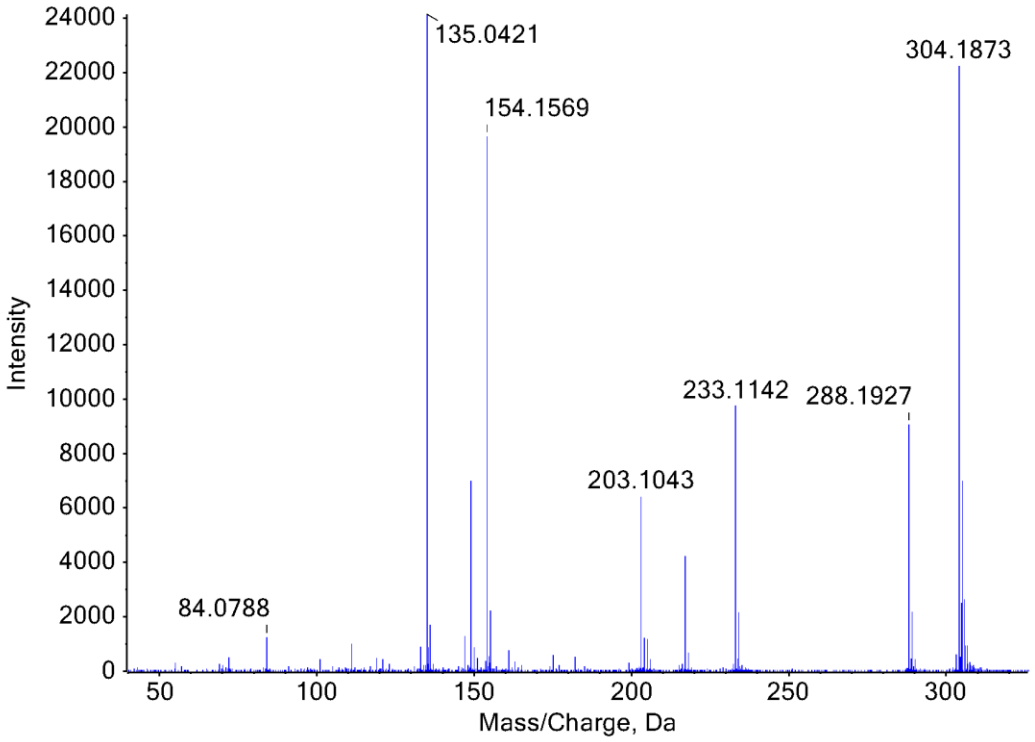
Extracted Ion Chromatogram (XIC): Methylenedioxy-PV8



TOF MS Spectrum: Methylenedioxy-PV8



TOF MS/MS Spectrum: Methylenedioxy-PV8



7. FUNDING

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