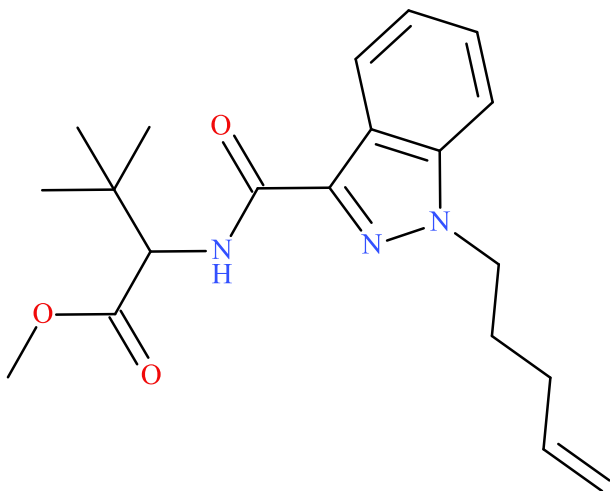


## MDMB-4en-PINACA

Sample Type: **Biological Fluid**

Latest Revision: **September 12, 2019**

Date of Report: **September 12, 2019**



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	Methyl 3,3-dimethyl-2-[(1-pent-4-enylindazole-3-carbonyl)amino]butanoate
<b>InChI String:</b>	InChI=1S/C20H27N3O3/c1-6-7-10-13-23-15-12-9-8-11-14(15)16(22-23)18(24)21-17(19(25)26-5)20(2,3)4/h6,8-9,11-12,17H,1,7,10,13H2,2-5H3,(H,21,24)
<b>CFR:</b>	Not Scheduled (09/2019)
<b>CAS#</b>	Not Available
<b>Synonyms:</b>	MDMB-PENINACA, MDMB-PINACA N1-pentyl-4-en isomer, 5-CL-ADB-A
<b>Source:</b>	NMS Labs – Toxicology Department

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

**Prepared By:** Alex J. Krotulski, MSFS, Amanda L.A. Mohr, 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 <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>20</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>	357.5	357	358.2125

### 3. BRIEF DESCRIPTION

MDMB-4en-PINACA is classified as a synthetic cannabinoid. Synthetic cannabinoids have been reported to cause psychoactive effects similar to delta-9-tetrahydrocannabinol (THC). Synthetic cannabinoids have caused adverse events, including deaths, as described in the literature. 5F-MDMB-PINACA (5F-ADB) is a structurally similar synthetic cannabinoid and scheduled substance in the United States; MDMB-4en-PINACA is not explicitly scheduled.

### 4. SAMPLE HISTORY

MDMB-4en-PINACA has been identified in two cases since the end of July 2019. The geographical and demographical breakdown is below:

**Geographical Location:** Indiana (n=2)  
**Case Type:** Postmortem Investigation (n=2)  
**Biological Sample:** Blood (n=2)  
**Date of First Collection:** July 21, 2019  
**Date of First Receipt:** July 23, 2019  
**Additional Cannabinoids:** 5F-MDMB-PICA (n=1)

### 5. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/26097/mdmb-4en-pinaca>

[https://www.policija.si/apps/nfl\\_response\\_web/0\\_Analytical\\_Reports\\_final/MDMB-4en-PINACA%20\(MDMB-PINACA%20N1-pentyl-4-en%20isomer\)-ID-1951-18%20\\_report.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/MDMB-4en-PINACA%20(MDMB-PINACA%20N1-pentyl-4-en%20isomer)-ID-1951-18%20_report.pdf)

## 6. QUALITATIVE DATA

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

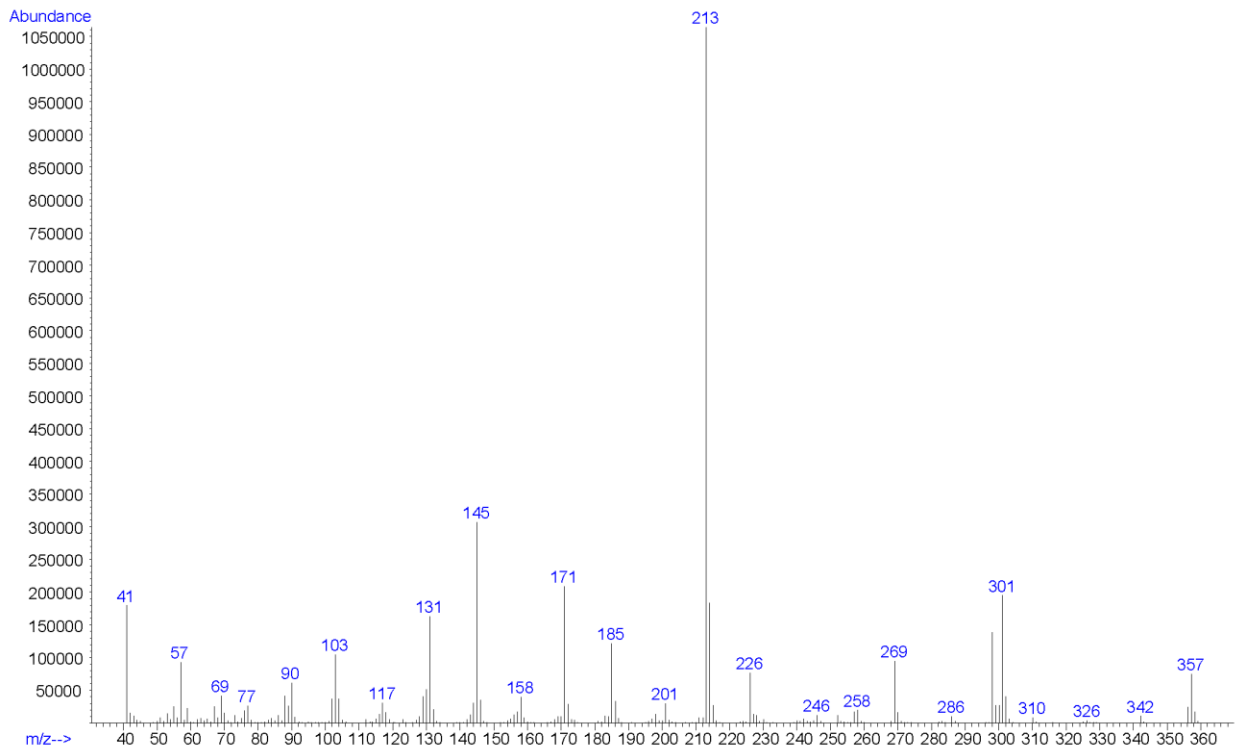
**Testing Performed At:** The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

**Sample Preparation:** Standard diluted in methanol

**Instrument:** Agilent 5975 Series GC/MSD System

**Standard:** Reference material for MDMB-4en-PINACA (Batch: 0540771-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). (<https://www.caymanchem.com/product/26097/mdmb-4en-pinaca>)

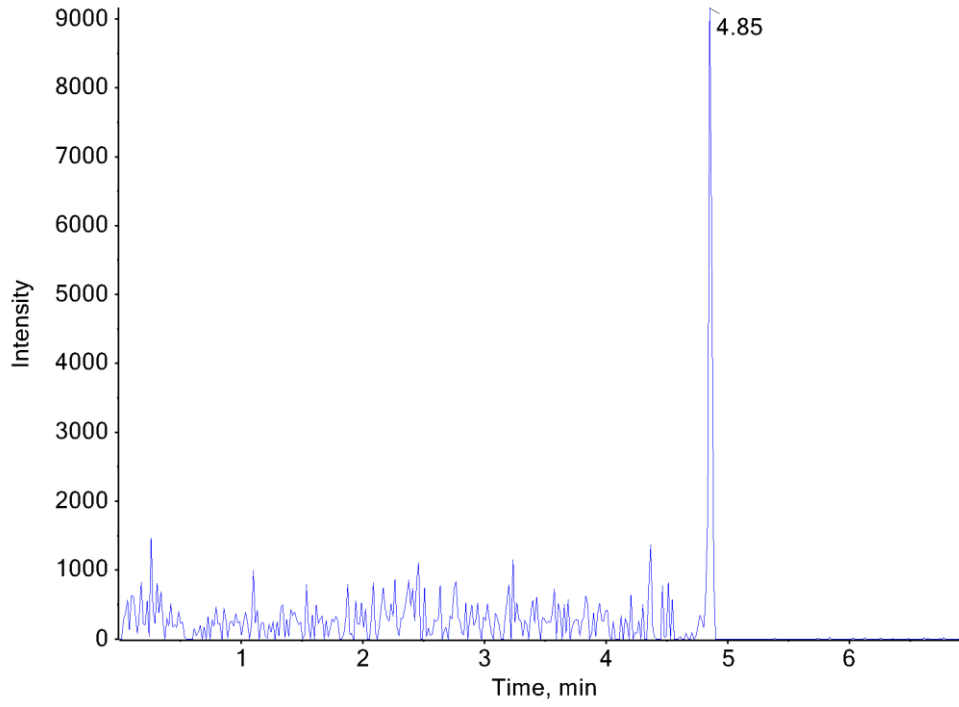
#### EI (70 eV) Mass Spectrum: MDMB-4en-PINACA (Standard)



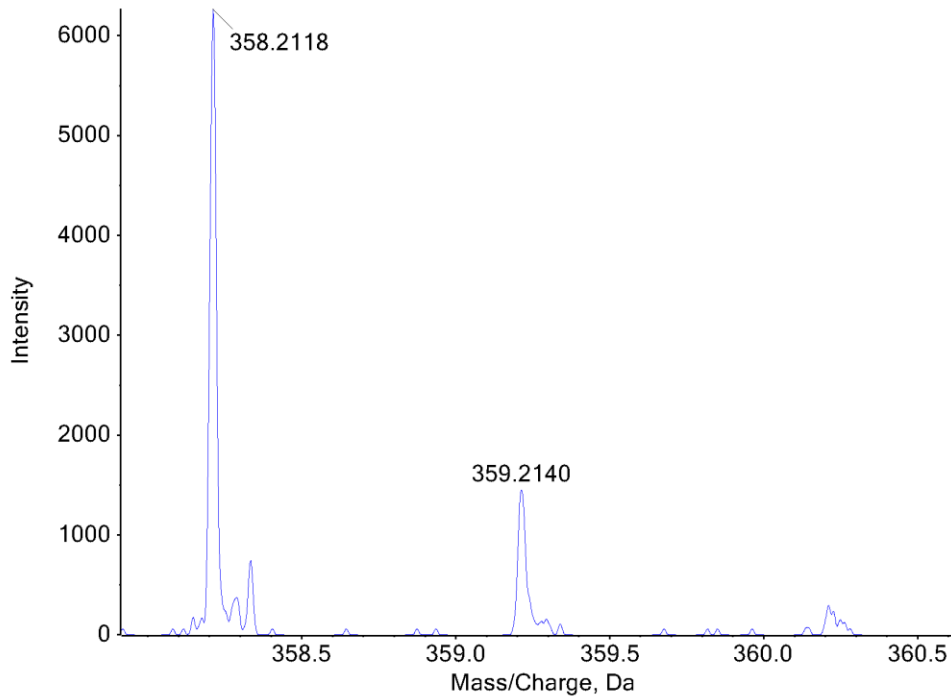
## 6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

<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>	No additional preparation - direct analysis of sample extract
<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) with 0.1% formic acid Flow rate: 0.5 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 4 min, hold 2 min; 95A:5B at 7 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 20 µL
<b>QTOF Parameters:</b>	TOF MS Scan Range: 100-550 Da Precursor Isolation: SWATH® acquisition (10-25 Da) Fragmentation: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-550 Da
<b>Retention Time:</b>	4.85 min
<b>Standard Comparison:</b>	Reference material for MDMA-4en-PINACA (Batch: 0540771-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as MDMA-4en-PINACA, based on retention time (4.90 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/26097/mdmb-4en-pinaca">https://www.caymanchem.com/product/26097/mdmb-4en-pinaca</a> )

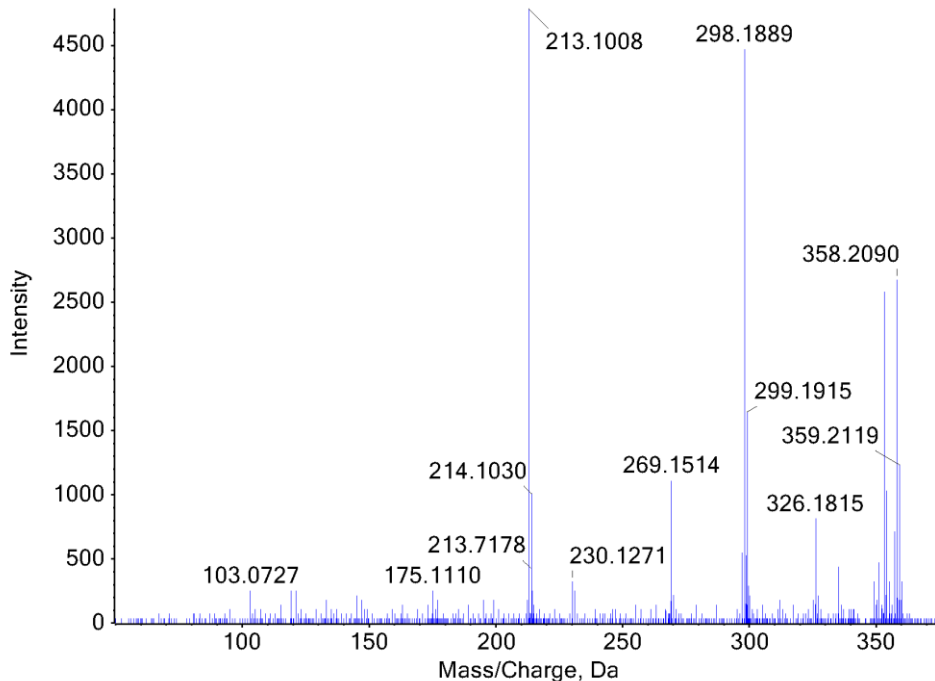
**Extracted Ion Chromatogram: MDMB-4en-PINACA (Blood Extract)**



**TOF MS Spectrum: MDMB-4en-PINACA (Blood Extract)**



### MS/MS Spectrum: MDMB-4en-PINACA (Blood Extract)



## 7. FUNDING

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