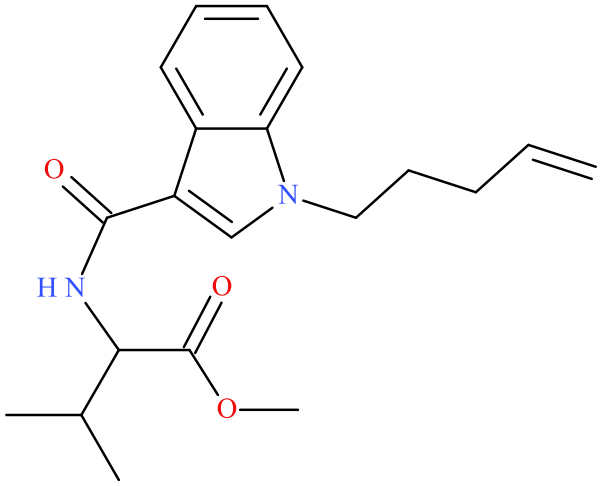
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

MMB-4en-PICA

Sample Type: **Seized Material**



Latest Revision: **October 11, 2019**

Date Received: **August 16, 2019**

Date of Report: **October 11, 2019**

1. GENERAL INFORMATION

IUPAC Name:	Methyl 3-methyl-2-[(1-pent-4-enylindole-3-carbonyl)amino]butanoate
InChI String:	InChI=1S/C20H26N2O3/c1-5-6-9-12-22-13-16(15-10-7-8-11-17(15)22)19(23)21-18(14(2)3)20(24)25-4/h5,7-8,10-11,13-14,18H,1,6,9,12H2,2-4H3,(H,21,23)
CFR:	Not Scheduled (10/2019)
CAS#	Not Available
Synonyms:	MMB022
Source:	Department of Homeland Security
Appearance:	Orange Solid Material

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF) 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	$C_{20}H_{26}N_2O_3$	342.4	342	343.2016

3. BRIEF DESCRIPTION

MMB-4en-PICA 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. MDMB-4en-PINACA, MDMB-4en-PICA, and MDMB-3en-BINACA are structurally similar synthetic cannabinoids. None of the synthetic cannabinoids in this class are explicitly scheduled substances in the United States.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/MMB-022%20(MMB-4en-PICA)-ID-1955-18_report.pdf

https://www.caymanchem.com/product/25906/mmb022

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)

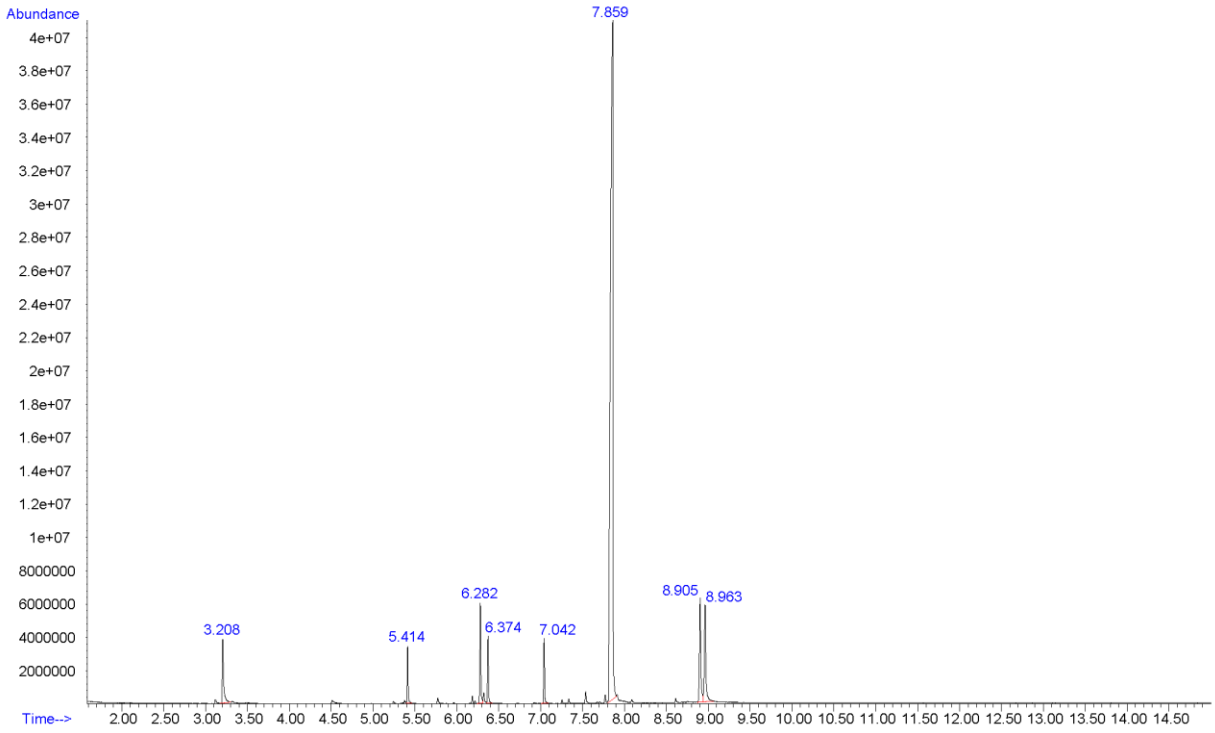
Carrier Gas: Helium (Flow: 1 mL/min)

Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

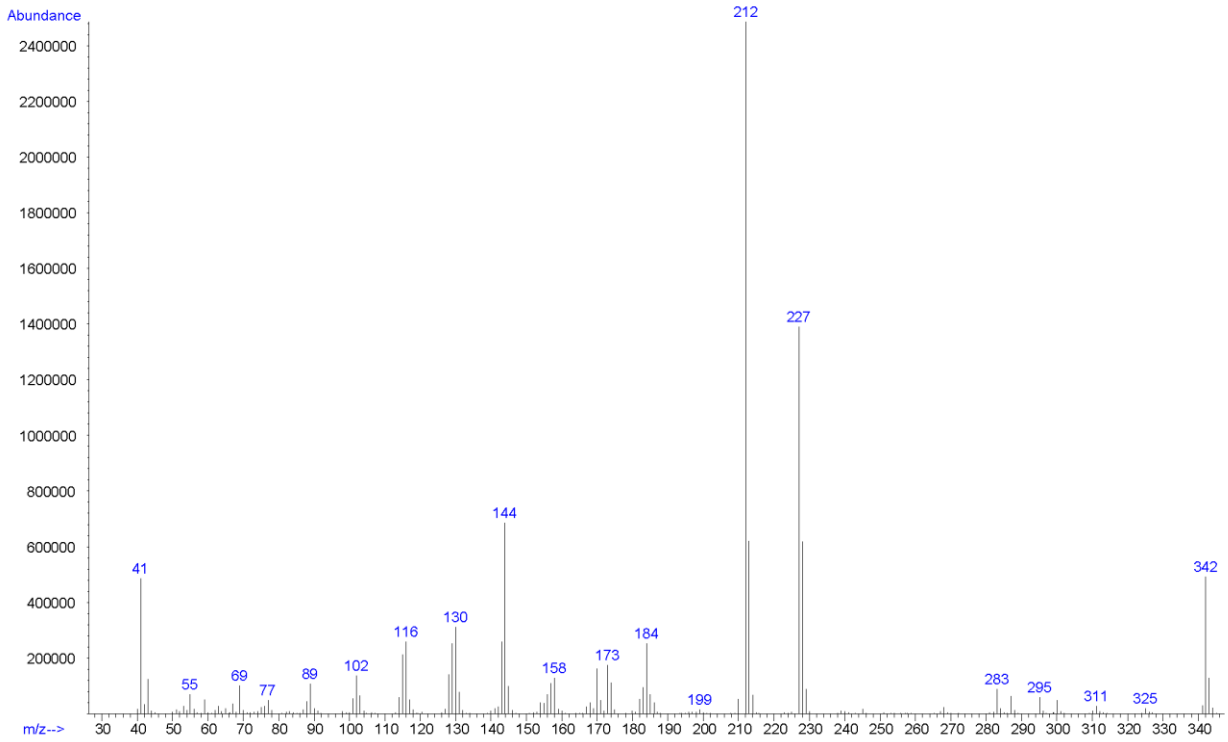
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	7.859 min
Standard Comparison:	Reference material for MMB-4en-PICA (Batch: 0538562-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as MMB-4en-PICA, based on retention time (7.830 min) and mass spectral data. (https://www.caymanchem.com/product/25906/mmb022)

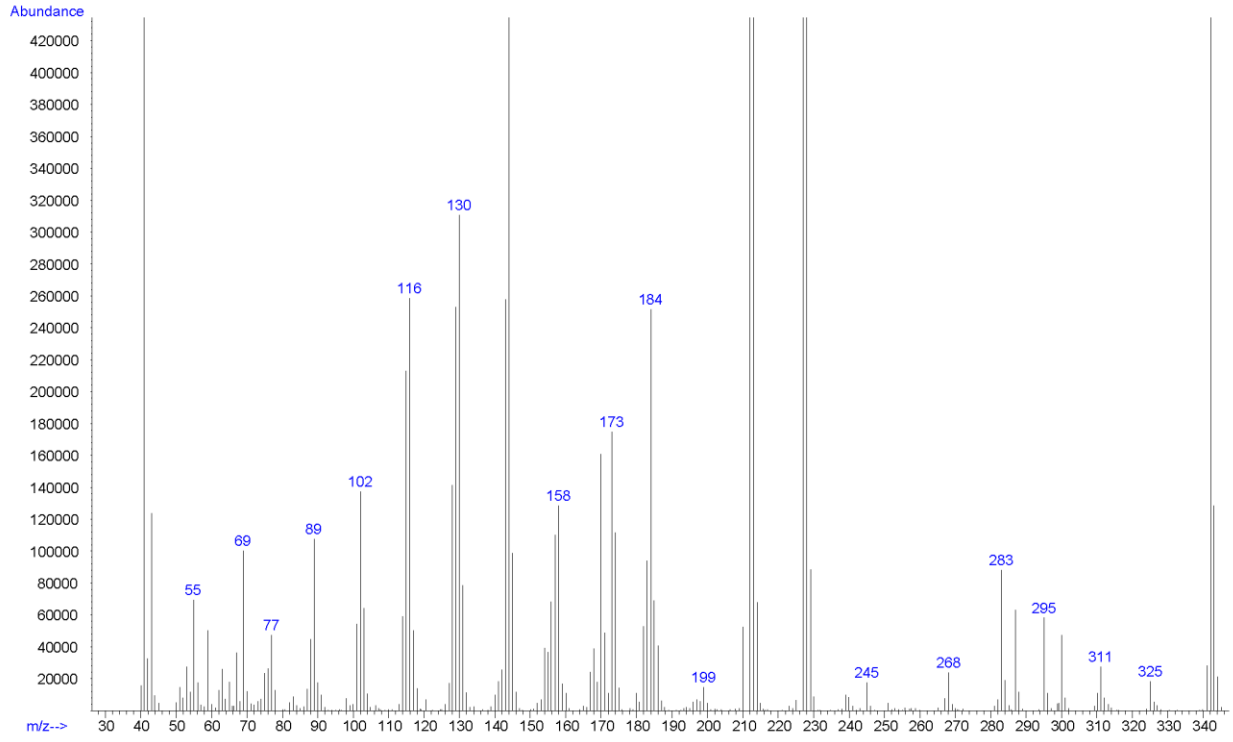
Chromatogram: MMB-4en-PICA



Additional peaks present in chromatogram: internal standards (3.208 min and 6.282 min) and not controlled substances (5.414 min, 6.374 min, 7.042 min, 8.905 min, 8.963 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): MMB-4en-PICA

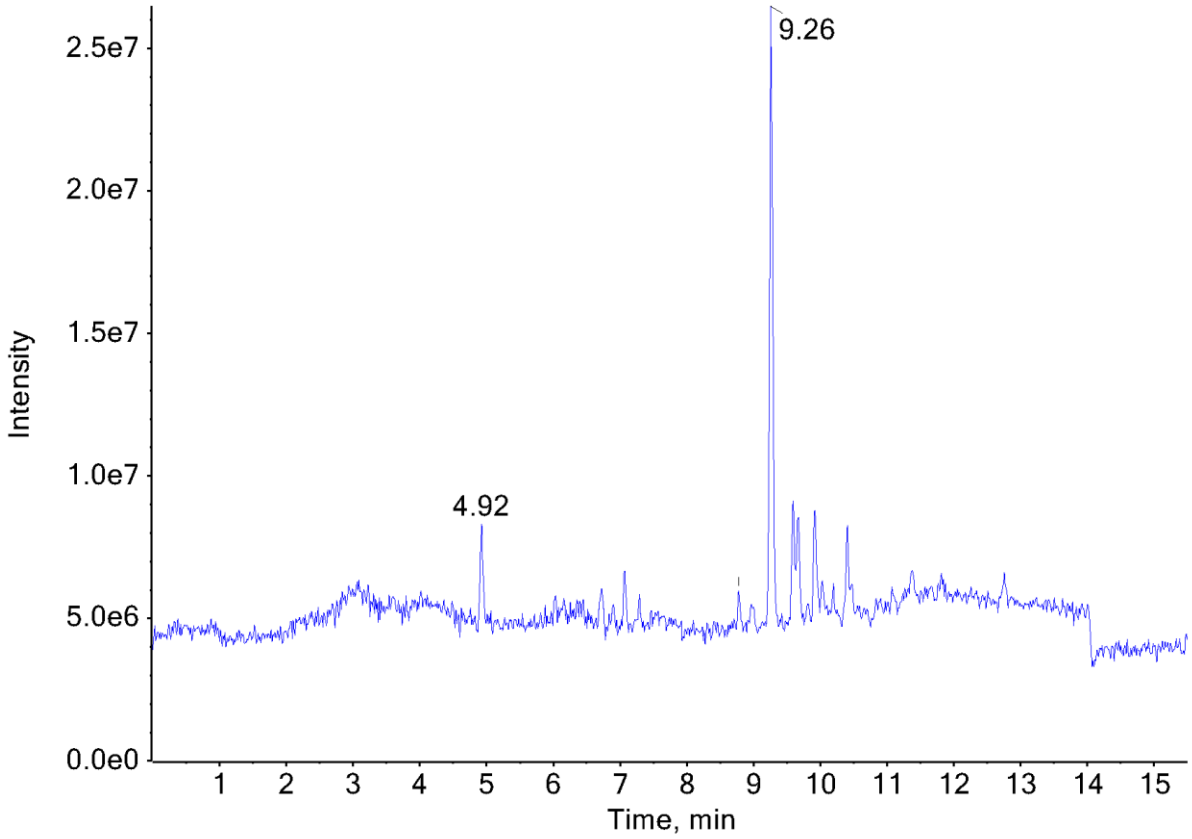




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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 extraction 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:	9.26 min
Standard Comparison:	Reference material for MMB-4en-PICA (Batch: 0538562-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as MMB-4en-PICA, based on retention time (9.25 min) and mass spectral data. (https://www.caymanchem.com/product/25906/mmb022)

Chromatogram: MMB-4en-PICA



Additional peak present in chromatogram: internal standard (4.92 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: MMB-4en-PICA