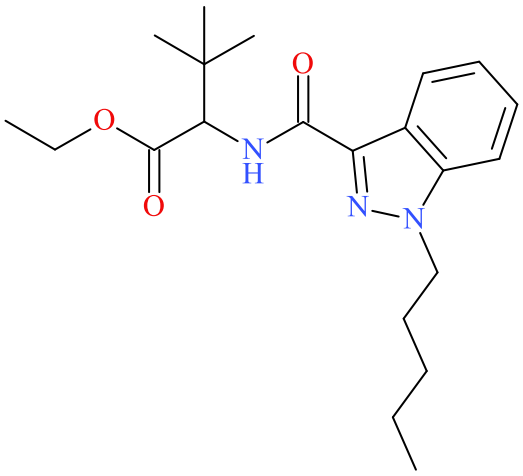
EDMB-PINACA

Sample Type: **Drug Material**



Latest Revision: **December 20, 2021**

Date Received: **September 20, 2021**

Date of Report: **December 20, 2021**

1. GENERAL INFORMATION

IUPAC Name:	Ethyl 3,3-dimethyl-2-[(1-pentylindazole-3-carbonyl)amino]butanoate
InChI String:	InChI=1S/C21H31N3O3/c1-6-8-11-14-24-16-13-10-9-12-15(16)17(23-24)19(25)22-18(21(3,4)5)20(26)27-7-2/h9-10,12-13,18H,6-8,11,14H2,1-5H3,(H,22,25)
CFR:	Not Scheduled (12/2021)
CAS#	Not Available
Synonyms:	None Available
Source:	Virginia Department of Forensic Science

***Important Note**: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. The "2-napthyl" configuration was used for structural purposes; however, position of the naphthyl group was not confirmed during analysis.*

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Drug	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
EDMB-PINACA	$C_{21}H_{31}N_3O_3$	373.5	373	374.2438

3. BRIEF DESCRIPTION

EDMB-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-EDMB-PINACA and 5F-MDMB-PINACA (5F-ADB) are structurally similar synthetic cannabinoids. 5F-EDMB-PINACA was first reported by NPS Discovery in April 2018, while 5F-MDMB-PINACA was the most prevalent synthetic cannabinoid in 2018. 5F-EDMB-PINACA and 5F-MDMB-PINACA are Schedule I substances in the United States. EDMB-PINACA is not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/EDMB-PINACA-ID-2994-21_report.pdf

https://www.caymanchem.com/product/33663/edmb-pinaca

5. QUALITATIVE DATA

5.1 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)

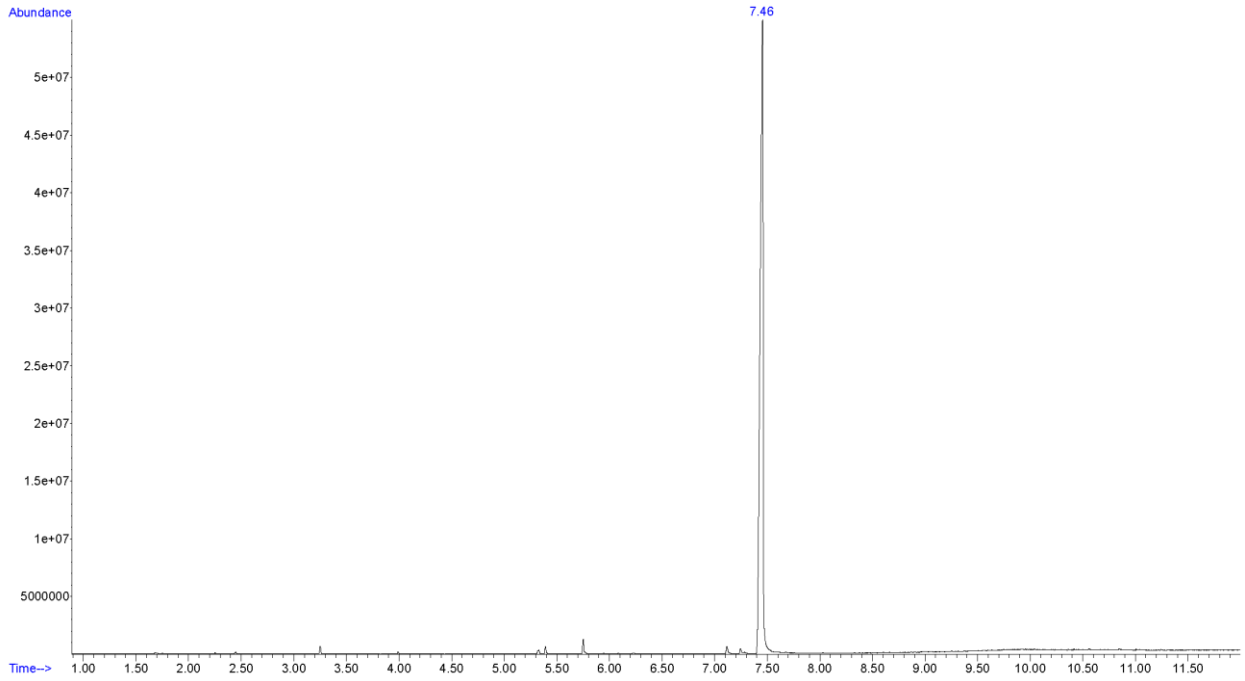
Sample Preparation: Dilution in methanol

Instrument: Agilent 5975 Series GC/MSD System

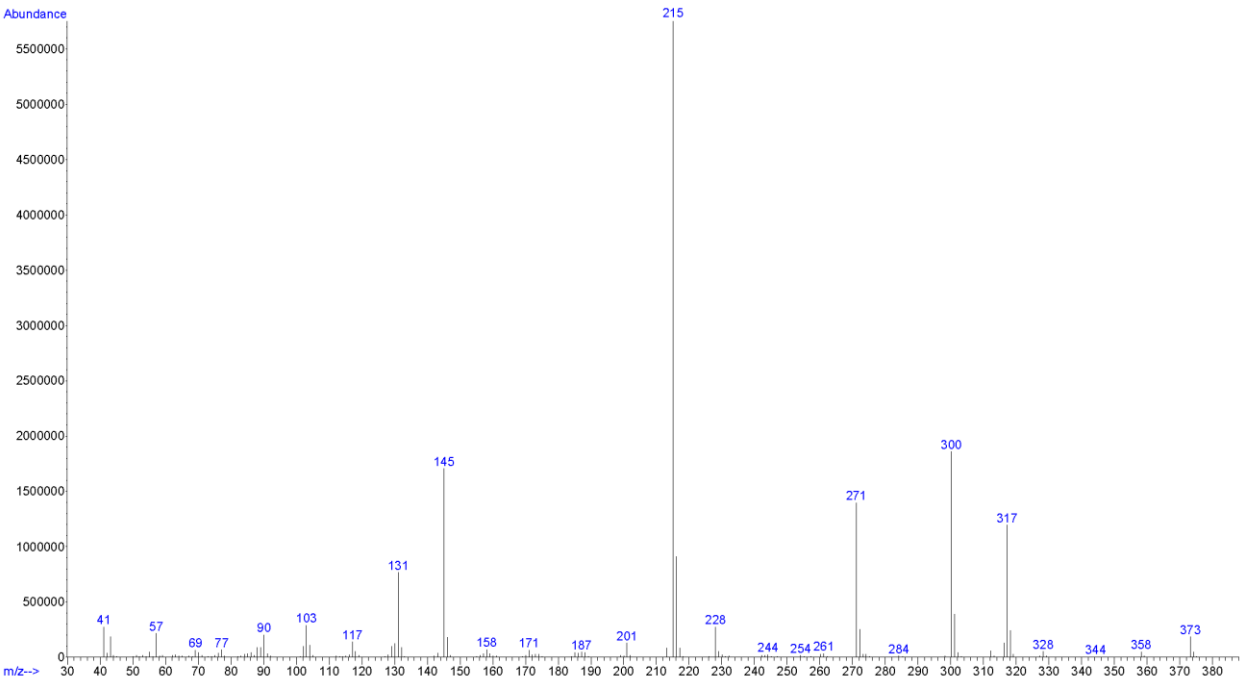
Column: Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)

Carrier Gas:	Helium (Flow: 1.46 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	7.46 min
Standard Comparison:	Reference material for EDMB-PINACA (Batch: 0612469-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as EDMB-PINACA based on retention time (7.41 min) and mass spectral data. (https://www.caymanchem.com/product/33663/edmb-pinaca)

Chromatogram: EDMB-PINACA



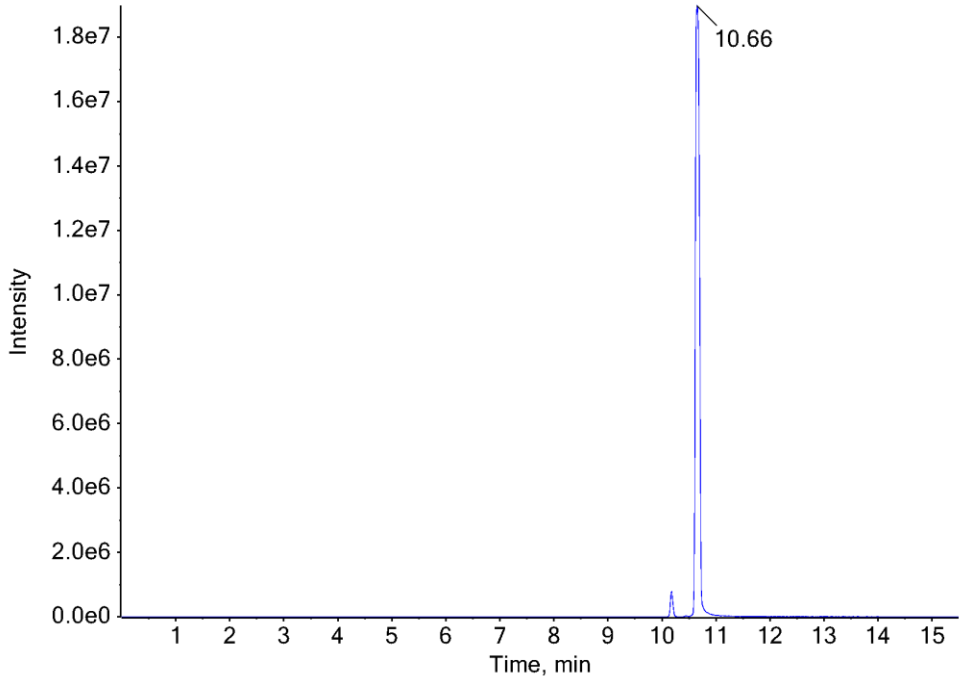
EI (70 eV) Mass Spectrum: EDMB-PINACA



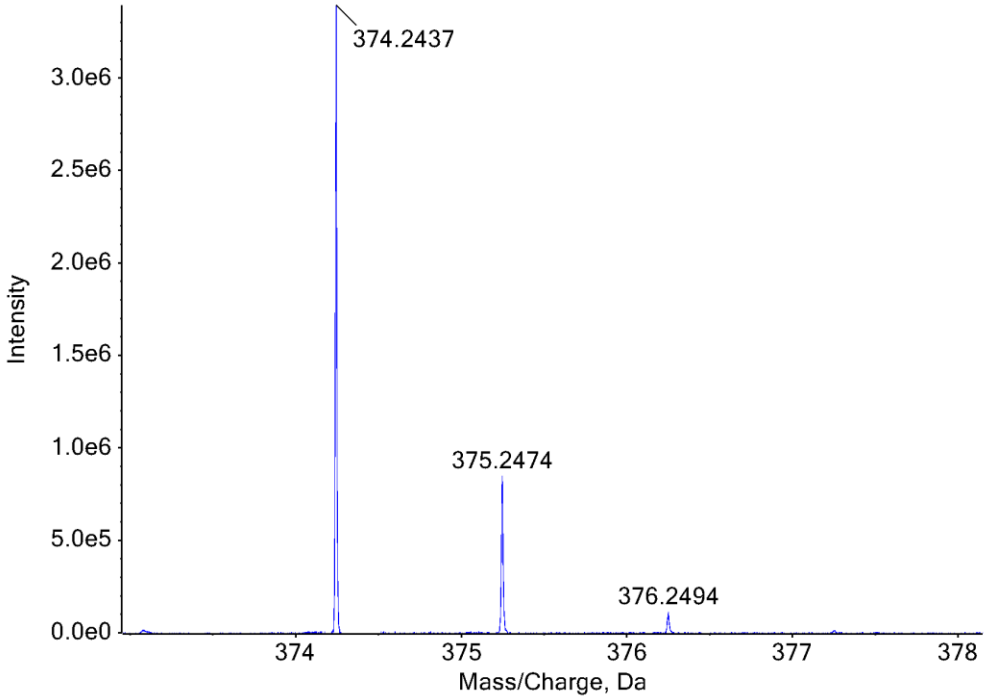
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of methanol 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: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	10.66 min
Standard Comparison:	Reference material for EDMB-PINACA (Batch: 0612469-3) 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 EDMB-PINACA, based on retention time (10.73 min) and mass spectral data. (https://www.caymanchem.com/product/33663/edmb-pinaca)

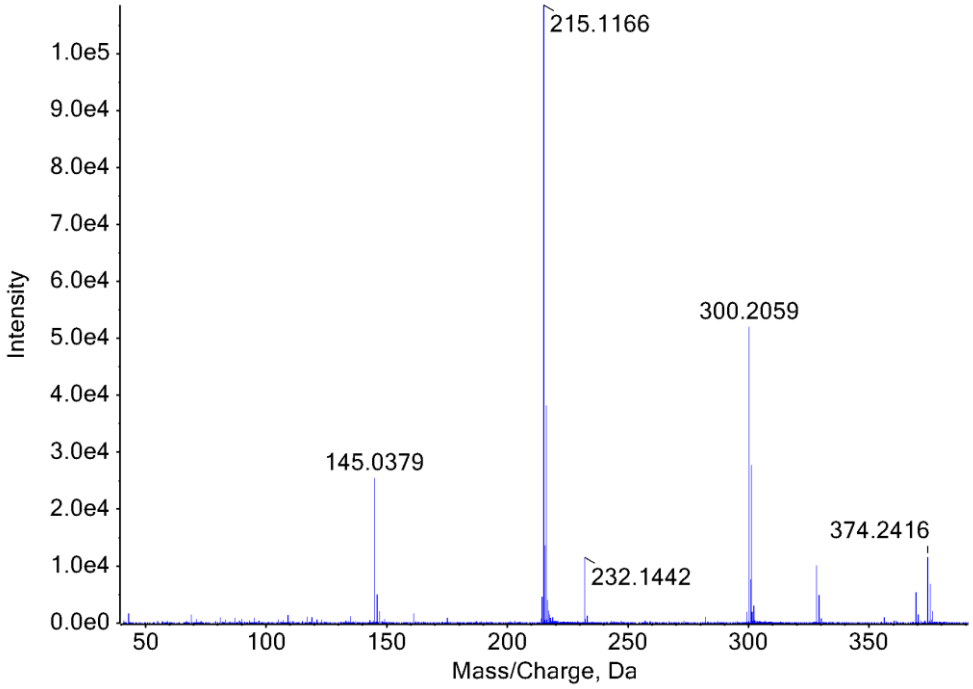
Extracted Ion Chromatogram: EDMB-PINACA



TOF MS Spectra: EDMB-PINACA



MS/MS Spectra: EDMB-PINACA



6. FUNDING

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