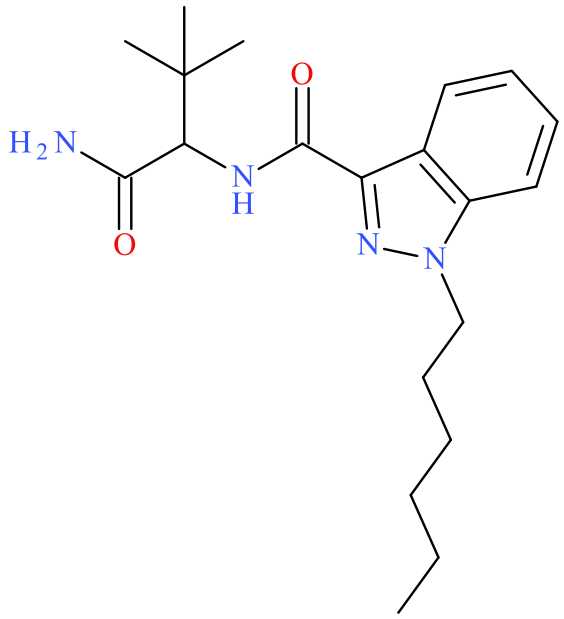
ADB-HEXINACA

Sample Type: **Seized Material**



Latest Revision: **April 29, 2021**

Date Received: **April 12, 2021**

Date of Report: **April 29, 2021**

1. GENERAL INFORMATION

IUPAC Name:	N-(1-carbamoyl-2,2-dimethyl-propyl)-1-hexyl-indazole-3-carboxamide
InChI String:	InChI=1S/C20H30N4O2/c1-5-6-7-10-13-24-15-12-9-8-11-14(15)16(23-24)19(26)22-17(18(21)25)20(2,3)4/h8-9,11-12,17H,5-7,10,13H2,1-4H3,(H2,21,25)(H,22,26)
CFR:	Not Scheduled (04/2021)
CAS#	Not Available
Synonyms:	ADB-HINACA, ADMB-HEXINACA
Source:	Pinellas County Forensic Lab

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

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Appearance: Plant-Like Material (See Image Below)

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{20}H_{30}N_4O_2$	358.5	358	359.2442

3. BRIEF DESCRIPTION

ADB-HEXINACA 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. ADB-PINACA and ADB-BINACA (ADB-BUTINACA) are structurally similar synthetic cannabinoids. ADB-PINACA is a Schedule I substance in the United States; ADB-HEXINACA is not explicitly federally scheduled, although this drug may be controlled under individual state regulations.

4. ADDITIONAL RESOURCES

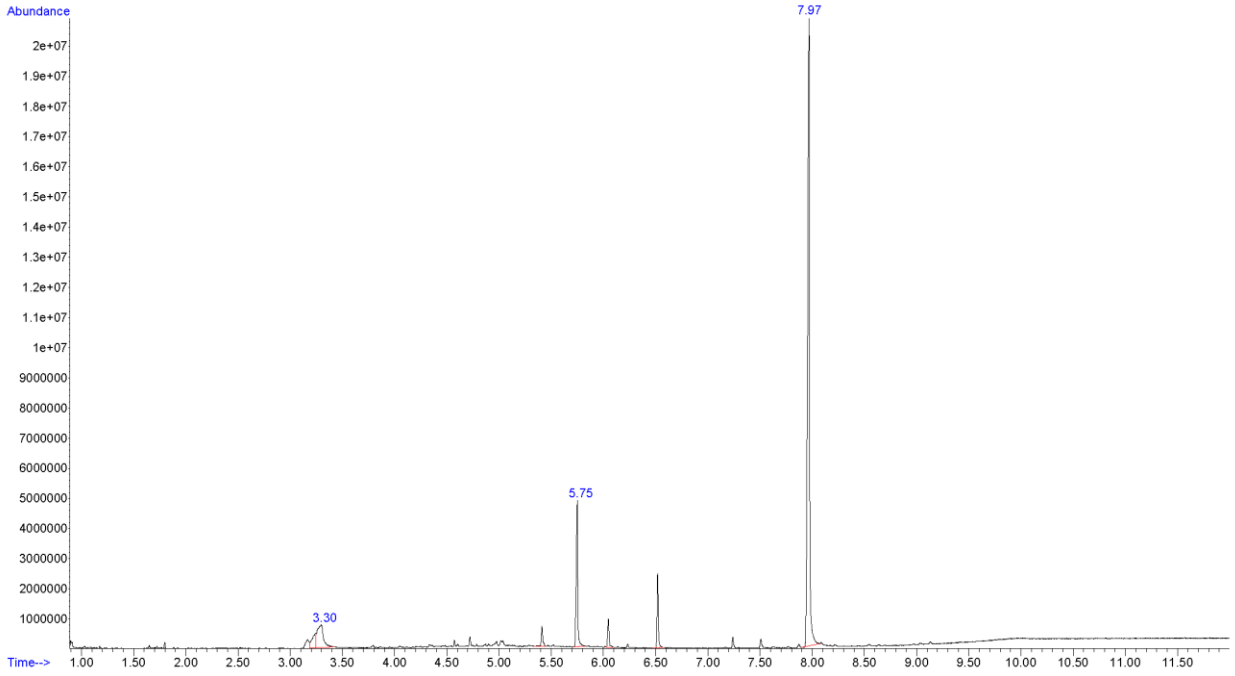
https://www.caymanchem.com/product/33820/adb-hexinaca

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

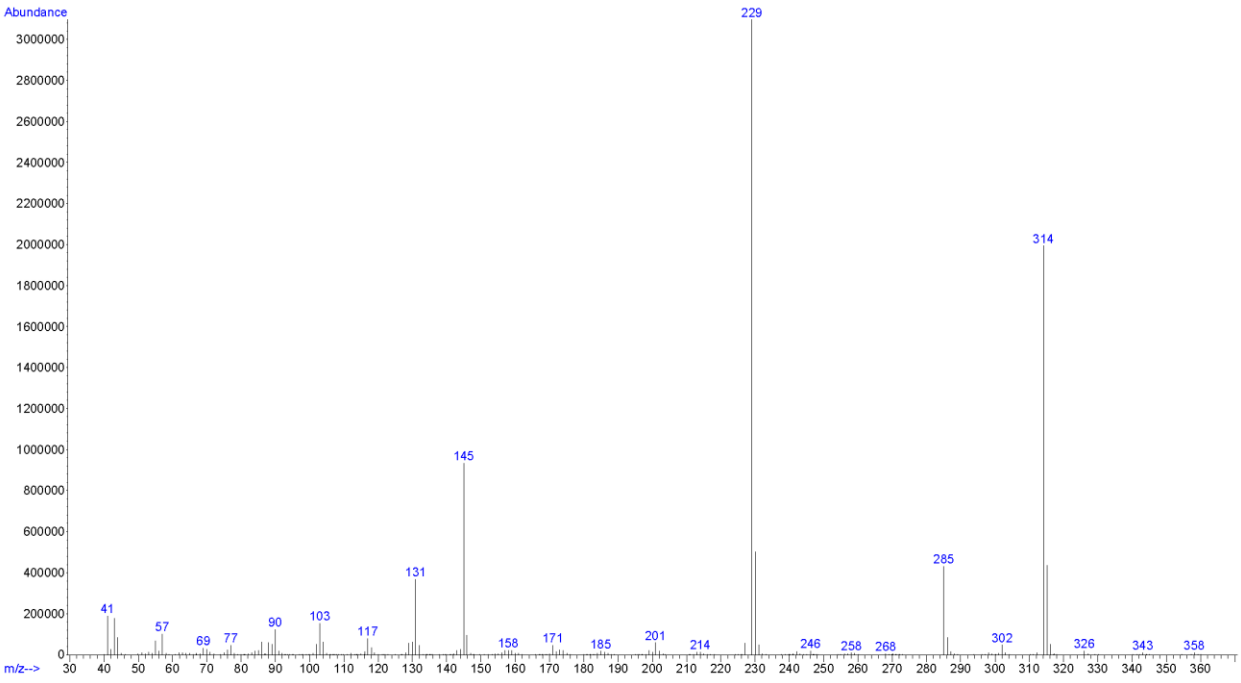
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)
Carrier Gas:	Helium (Flow: 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:	7.97 min
Standard Comparison:	Reference material for ADB-HEXINACA (Batch: 0611894-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-HEXINACA based on retention time (7.96 min) and mass spectral data. (https://www.caymanchem.com/product/33820/adb-hexinaca)

Chromatogram: ADB-HEXINACA

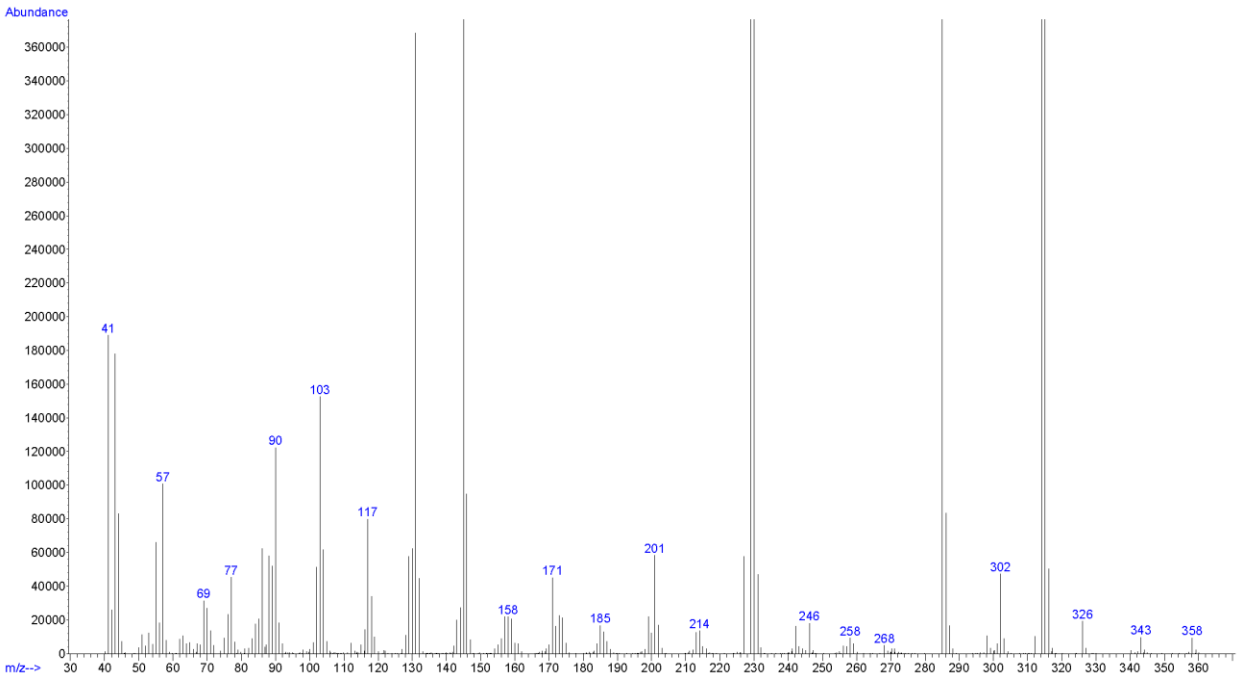


Additional peaks present in chromatogram: internal standards (3.30 min and 5.75 min)

EI (70 eV) Mass Spectrum: ADB-HEXINACA



EI (70 eV) Mass Spectrum 10x: ADB-HEXINACA

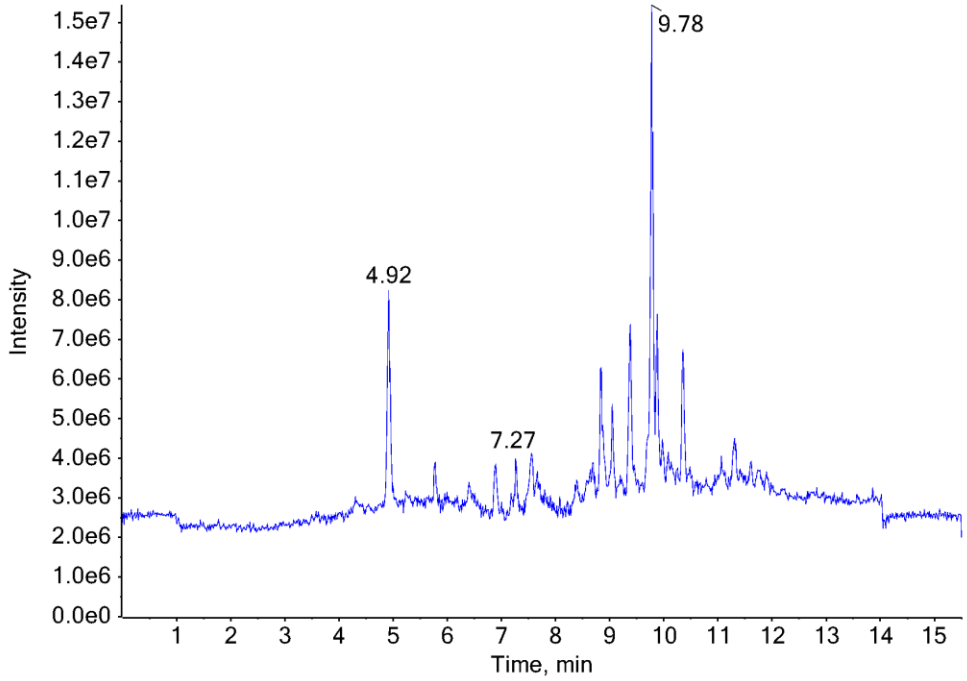


5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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 GC-MS sample 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

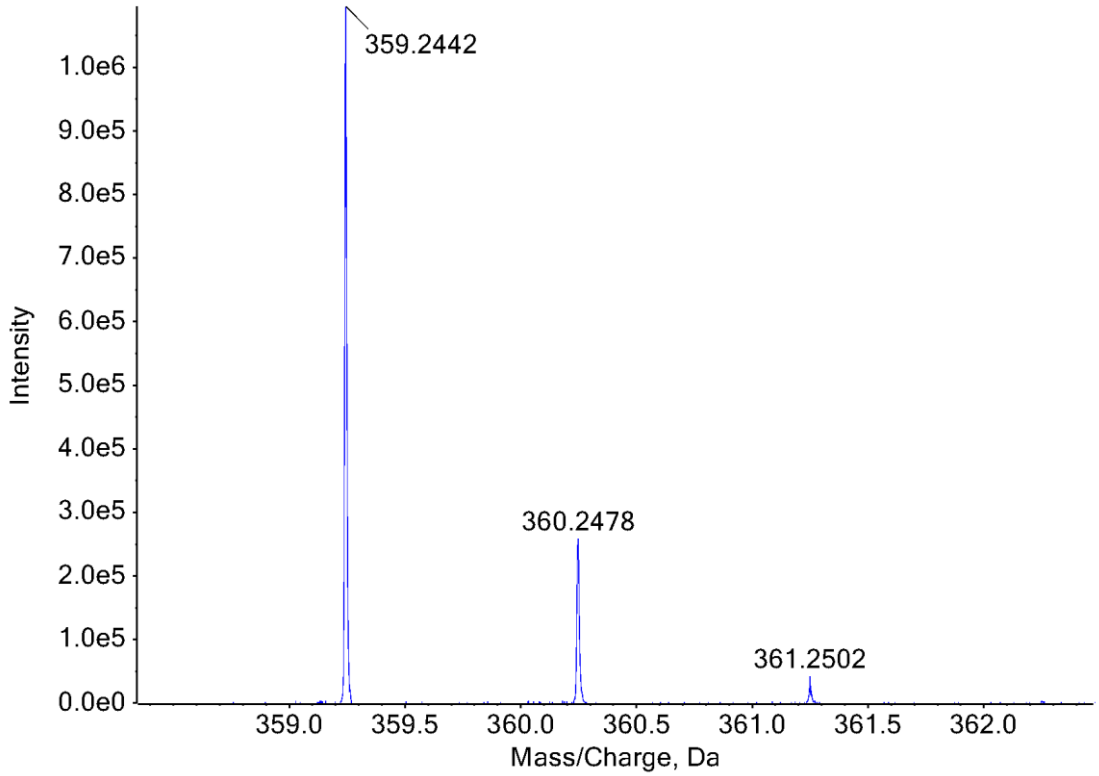
	Column Oven: 30 °C
	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 10 µL
QTOF Parameters:	TOF MS Scan Range: 100-510 Da
	Precursor Isolation: SWATH® acquisition (27 windows)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	9.78 min
Standard Comparison:	Reference material for ADB-HEXINACA (Batch: 0611894-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-HEXINACA based on retention time (9.78 min) and mass spectral data. (https://www.caymanchem.com/product/33820/adb-hexinaca)

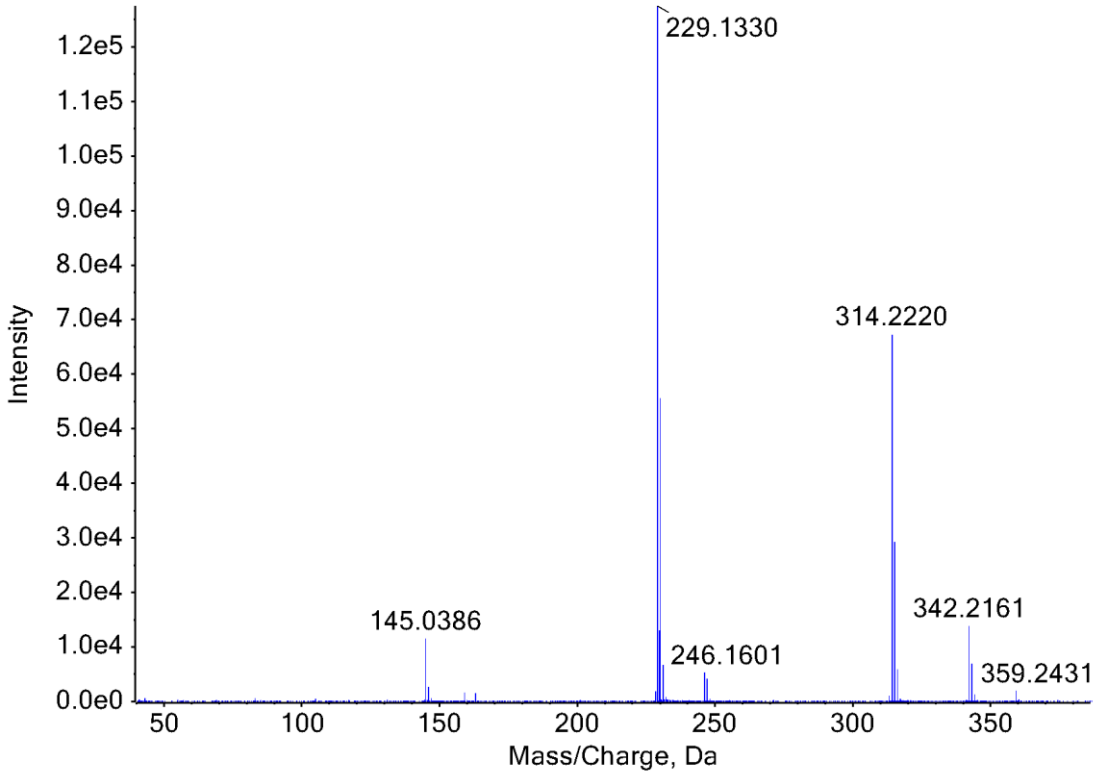
Chromatogram: ADB-HEXINACA



Additional peaks present in chromatogram: internal standards (4.92 min and 7.27 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: ADB-HEXINACA





6. FUNDING

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