

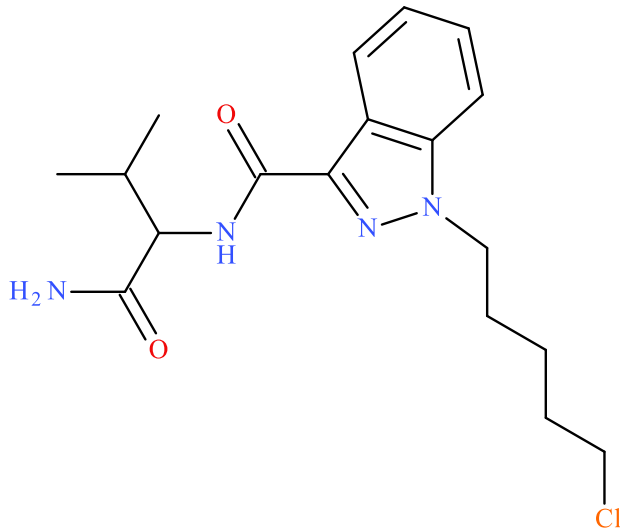
5CI-AB-PINACA

Sample Type: **Seized Material**

Latest Revision: **October 5, 2018**

Date Received: **June 6, 2018**

Date of Report: **October 5, 2018**



1. GENERAL INFORMATION

IUPAC Name:	N-(1-carbamoyl-2-methyl-propyl)-1-(5-chloropentyl)indazole-3-carboxamide
InChI String:	InChI=1S/C18H25ClN4O2/c1-12(2)15(17(20)24)21-18(25)16-13-8-4-5-9-14(13)23(22-16)11-7-3-6-10-19/h4-5,8-9,12,15H,3,6-7,10-11H2,1-2H3,(H2,20,24)(H,21,25)
CFR:	Not Scheduled (10/2018)
CAS#	1801552-02-2
Synonyms:	5-Chloro AB-PINACA, 5-chloro ABP, 5CI-AMB-PINACA
Source:	Department of Homeland Security
Appearance:	Off-White 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.

Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT

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 ClN ₄ O ₂	364.9	364	365.1739

3. BRIEF DESCRIPTION

5Cl-AB-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-AB-PINACA and AB-PINACA are structurally similar synthetic cannabinoids. 5F-AB-PINACA and AB-PINACA are Schedule I substances in the United States.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/9001857>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5Cl-AB-PINACA-ID-1815-17_report.pdf

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

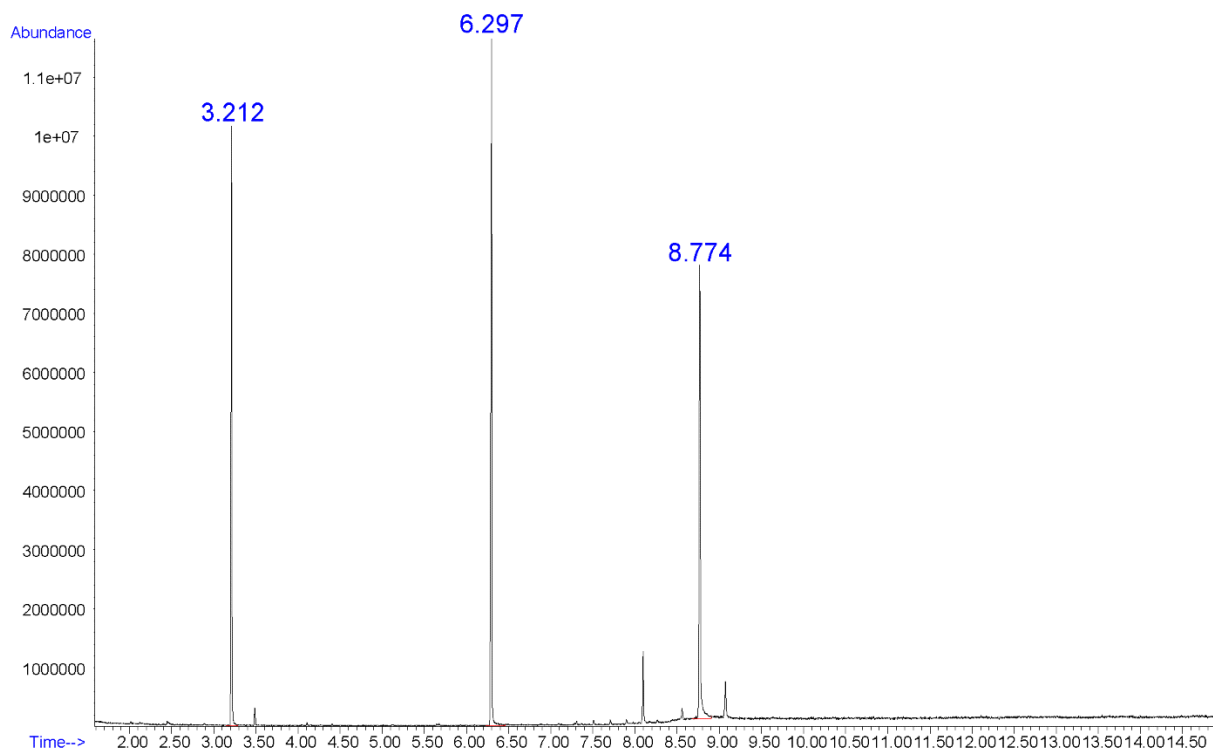
MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 8.774 min

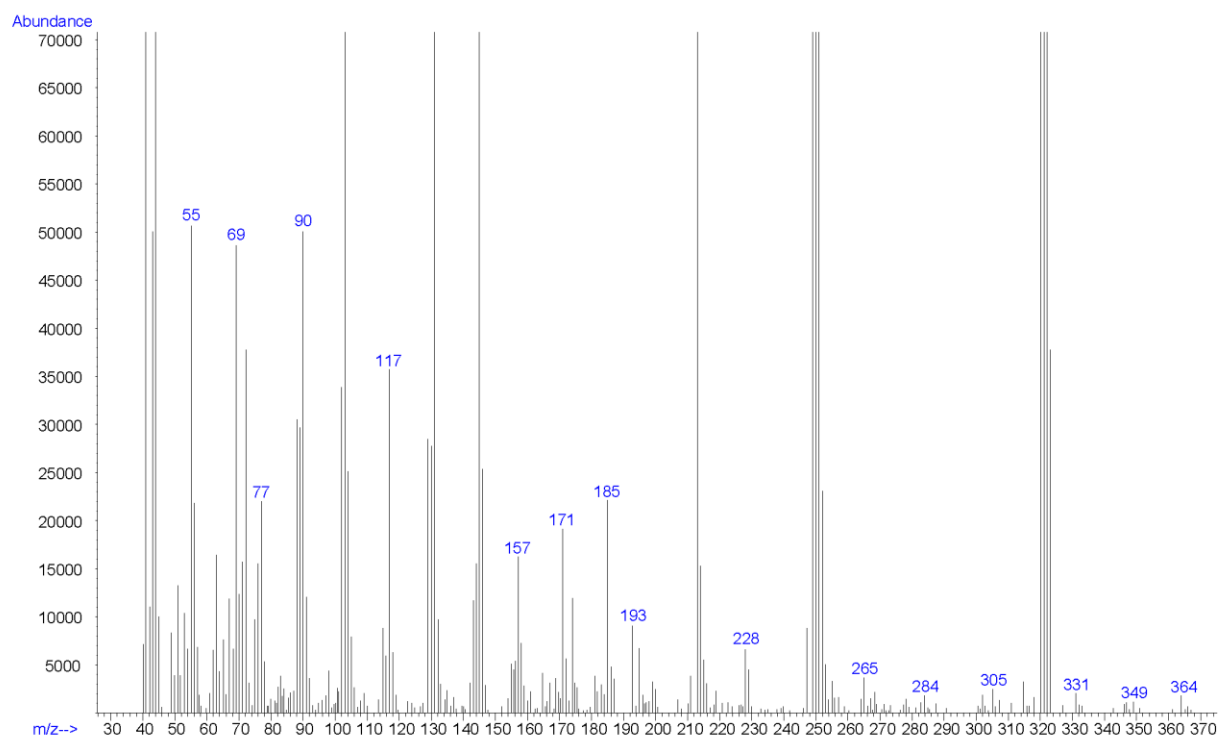
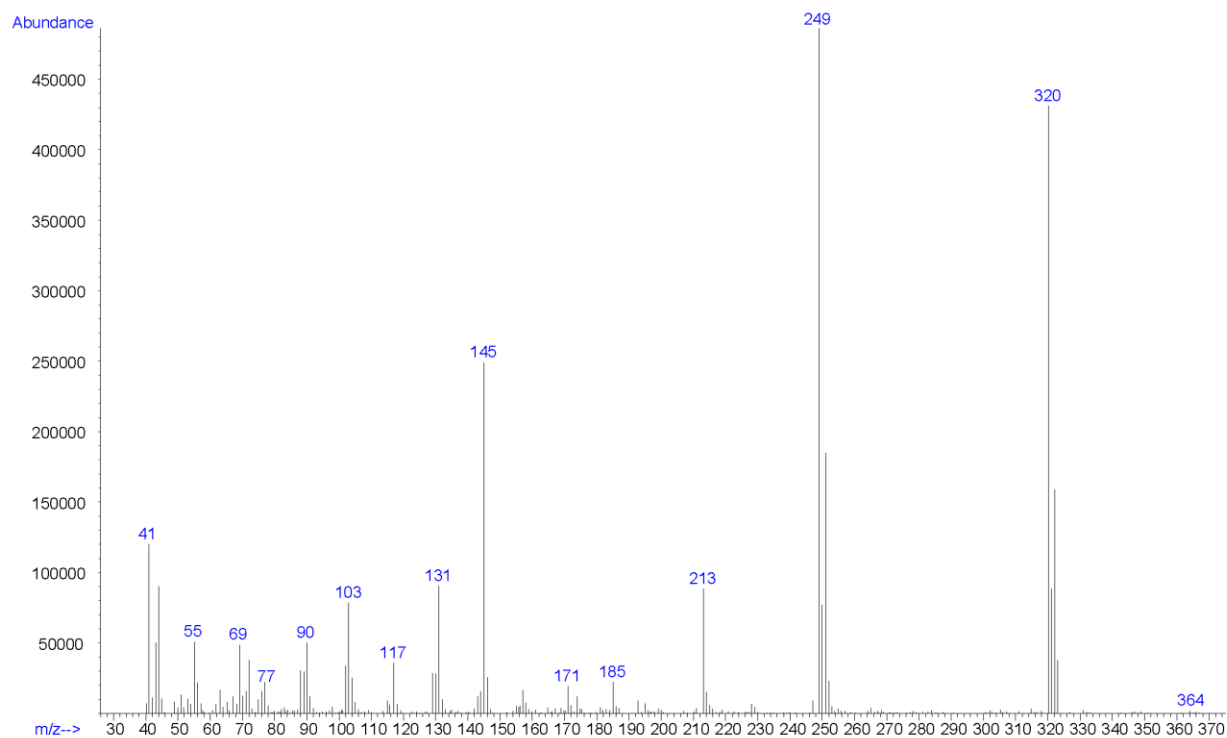
Standard Comparison: Reference material for 5Cl-AB-PINACA (Batch: 0515642-11) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5Cl-AB-PINACA, based on retention time (8.745 min) and mass spectral data.
(<https://www.caymanchem.com/product/9001857>)

Chromatogram: 5Cl-AB-PINACA



Additional peaks present in chromatogram: internal standards (3.212 and 6.297 min)

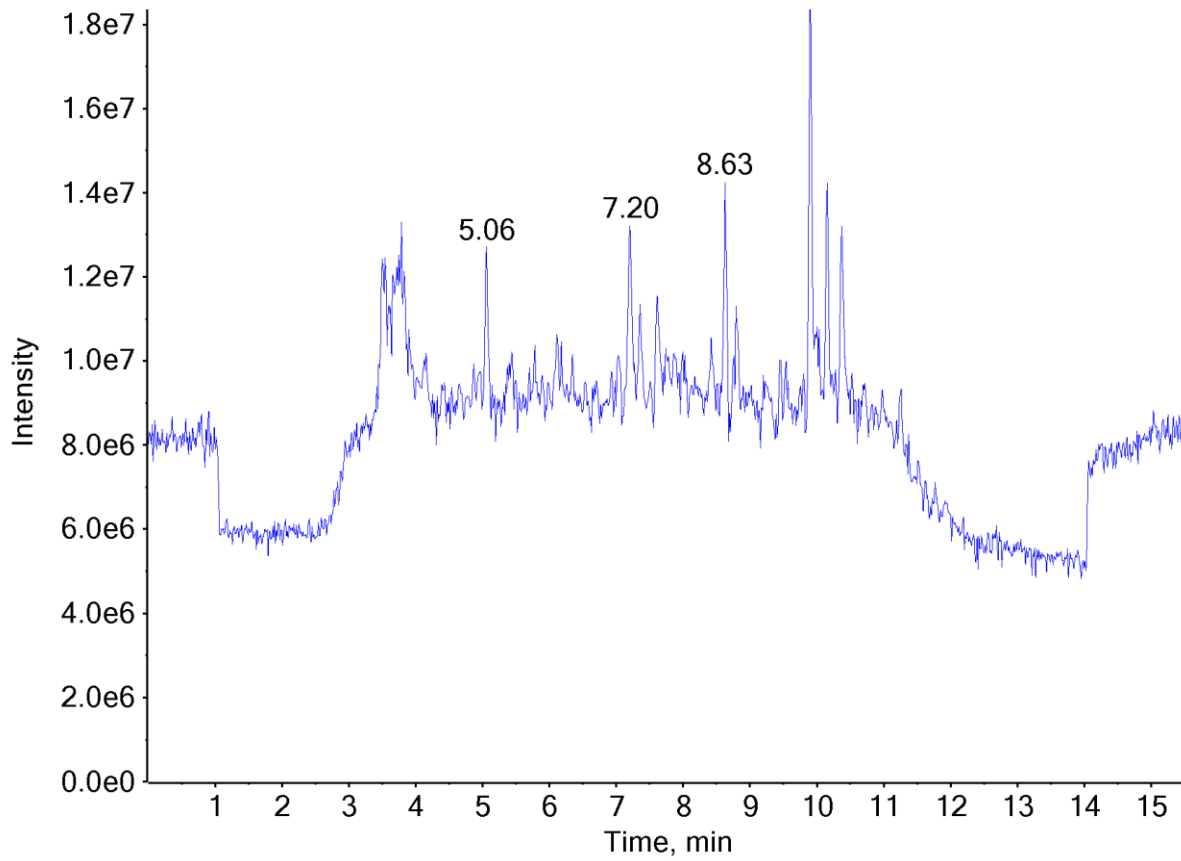
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5Cl-AB-PINACA



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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	8.63 min
Standard Comparison:	Reference material for 5Cl-AB-PINACA (Batch: 0520119) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5Cl-AB-PINACA, based on retention time (8.58 min) and mass spectral data. (https://www.caymanchem.com/product/9001857)

Chromatogram: 5Cl-AB-PINACA



*Additional peaks present in chromatogram: internal standards (5.06 min),
not a controlled substance (7.20 min)*

TOF MS (Top) and MS/MS (Bottom) Spectra: 5Cl-AB-PINACA

