

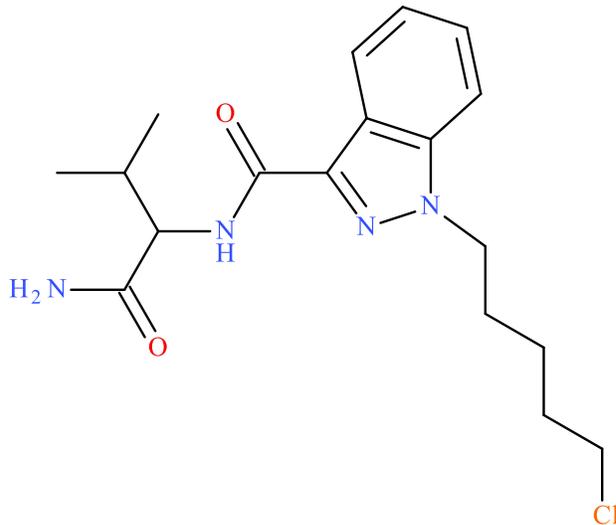
## 5CI-AB-PINACA

Sample Type: **Seized Material**

Latest Revision: **October 5, 2018**

Date Received: **June 6, 2018**

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



### 1. GENERAL INFORMATION

|                      |                                                                                                                                                        |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>IUPAC Name:</b>   | N-(1-carbamoyl-2-methyl-propyl)-1-(5-chloropentyl)indazole-3-carboxamide                                                                               |
| <b>InChI String:</b> | 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) |
| <b>CFR:</b>          | Not Scheduled (10/2018)                                                                                                                                |
| <b>CAS#</b>          | 1801552-02-2                                                                                                                                           |
| <b>Synonyms:</b>     | 5-Chloro AB-PINACA, 5-chloro ABP, 5CI-AMB-PINACA                                                                                                       |
| <b>Source:</b>       | Department of Homeland Security                                                                                                                        |
| <b>Appearance:</b>   | 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.

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## 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>18</sub> H <sub>25</sub> ClN <sub>4</sub> O <sub>2</sub> | 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](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

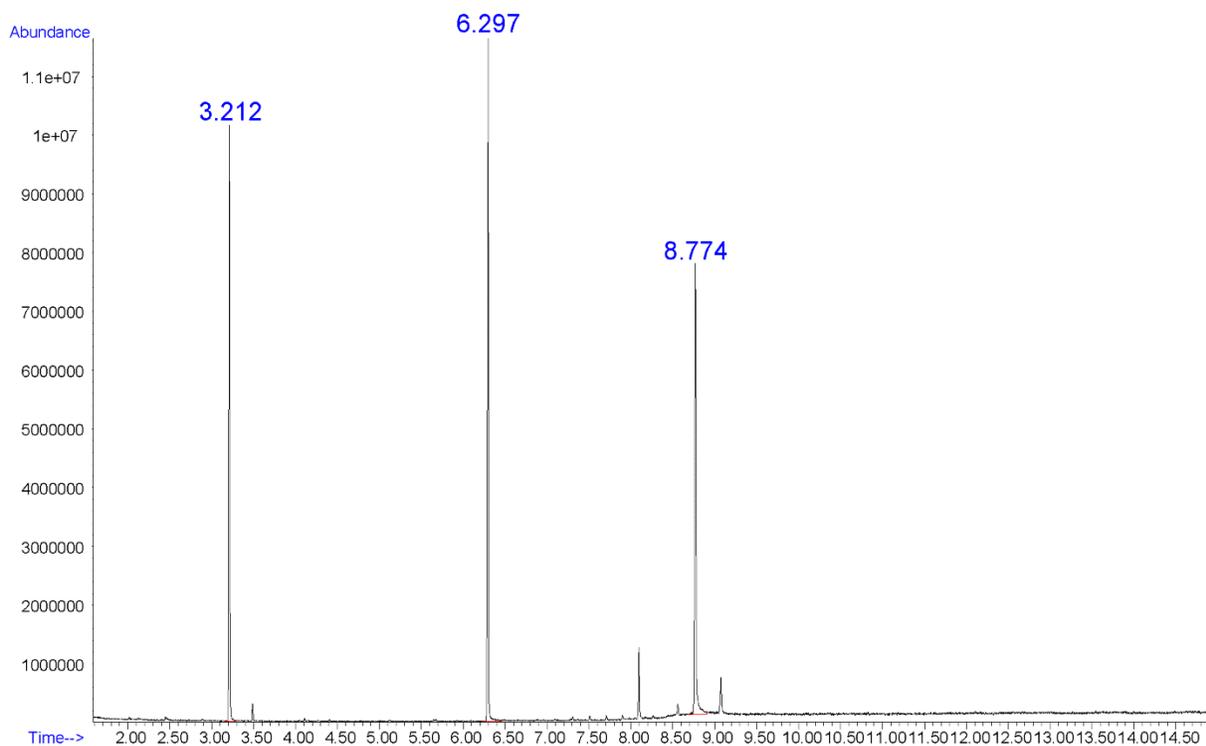
**MS Parameters:** Mass Scan Range: 40-550 m/z

Threshold: 250

**Retention Time:** 8.774 min

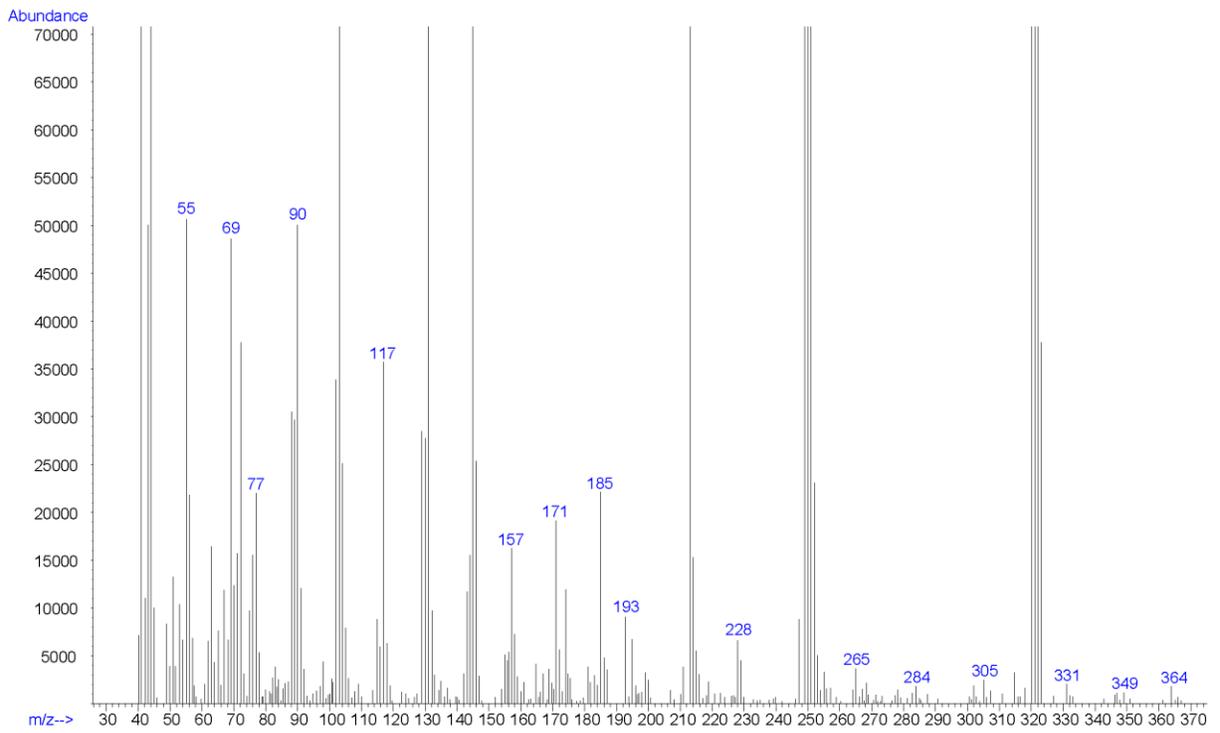
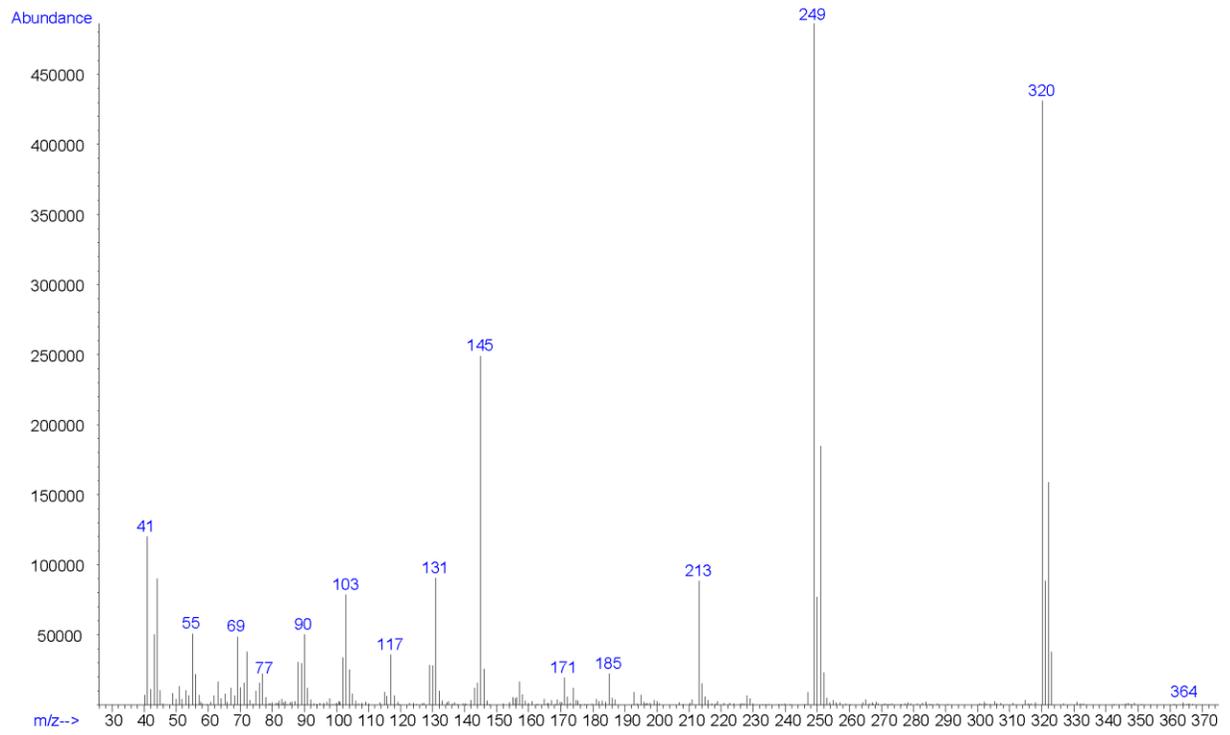
**Standard Comparison:** Reference material for 5Cl-AB-PINACA (Batch: 0515642-11) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5Cl-AB-PINACA, based on retention time (8.745 min) and mass spectral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

### Chromatogram: 5Cl-AB-PINACA



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

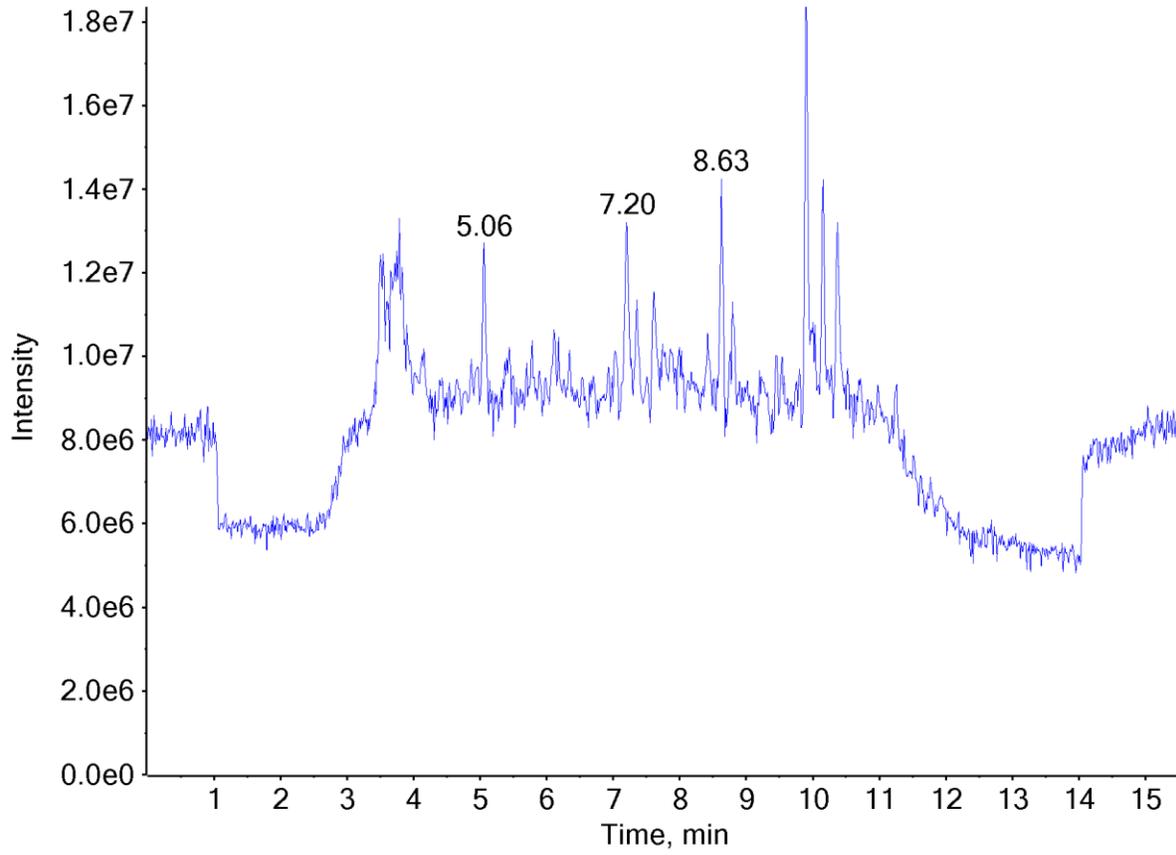
# EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5Cl-AB-PINACA



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

|                              |                                                                                                                                                                                                                                                                                                                                                                                                    |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <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>   | 1:100 dilution of acid/base extraction in mobile phase                                                                                                                                                                                                                                                                                                                                             |
| <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)<br>B: Methanol/acetonitrile (50:50)<br>Flow rate: 0.4 mL/min                                                                                                                                                                                                                                                                                                   |
| <b>Gradient:</b>             | Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min                                                                                                                                                                                                                                                                                                                                            |
| <b>Temperatures:</b>         | Autosampler: 15 °C<br>Column Oven: 30 °C<br>Source Heater: 600 °C                                                                                                                                                                                                                                                                                                                                  |
| <b>Injection Parameters:</b> | Injection Volume: 10 µL                                                                                                                                                                                                                                                                                                                                                                            |
| <b>QTOF Parameters:</b>      | TOF MS Scan Range: 100-510 Da<br>Precursor Isolation: SWATH® acquisition (27 windows)<br>Fragmentation: Collision Energy Spread (35±15 eV)<br>MS/MS Scan Range: 50-510 Da                                                                                                                                                                                                                          |
| <b>Retention Time:</b>       | 8.63 min                                                                                                                                                                                                                                                                                                                                                                                           |
| <b>Standard Comparison:</b>  | Reference material for 5CI-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 5CI-AB-PINACA, based on retention time (8.58 min) and mass spectral data.<br>( <a href="https://www.caymanchem.com/product/9001857">https://www.caymanchem.com/product/9001857</a> ) |

**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**

