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, 5Cl-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

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]⁺</th>
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</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₁₈H₂₅ClN₄O₂</td>
<td>364.9</td>
<td>364</td>
<td>365.1739</td>
</tr>
</tbody>
</table>

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-tetrahyrocannabinol (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](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: Collison 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