ADB-4en-PINACA

Sample Type: Seized Material

Latest Revision: March 4, 2021
Date Received: January 8, 2021
Date of Report: March 4, 2021

1. GENERAL INFORMATION

IUPAC Name: N-(1-carbamoyl-2,2-dimethyl-propyl)-1-pent-4-enyl-indazole-3-carboxamide

InChI String: InChI=1S/C19H26N4O2/c1-5-6-9-12-23-14-11-8-7-10-13(14)15(22-23)18(25)21-16(17(20)24)19(2,3)4/h5,7-8,10-11,16H,1,6,9,12H2,2-4H3,(H2,20,24)(H,21,25)

CFR: Not Scheduled (03/2021)

CAS#: Not Available

Synonyms: ADMB-4en-PINACA, ADB-PENINACA

Source: NMS Labs – Criminalistic Laboratory

Appearance: Plant-Like Material

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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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>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C_{19}H_{26}N_{4}O_{2}</td>
<td>342.4</td>
<td>342</td>
<td>343.2129</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

ADB-4en-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. MDMB-4en-PINACA and ADB-PINACA are structurally similar synthetic cannabinoids. ADB-PINACA is a Schedule I substance in the United States; ADB-4en-PINACA and MDMB-4en-PINACA are not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/33205/adb-4en-pinaca

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: 7.99 min

Standard Comparison: Reference material for ADB-4en-PINACA (Batch: 0606857-1) 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-4en-PINACA based on retention time (7.96 min) and mass spectral data. ([https://www.caymanchem.com/product/33205/adb-4en-pinaca](https://www.caymanchem.com/product/33205/adb-4en-pinaca))

Chromatogram: ADB-4en-PINACA

Additional peaks present in chromatogram: internal standard (6.29 min) and 4F-ABINACA (8.80 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): ADB-4en-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 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: 8.99 min

Standard Comparison: Reference material for ADB-4en-PINACA (Batch: 0606857-1) 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-4en-PINACA based on retention time (8.99 min) and mass spectral data. (https://www.caymanchem.com/product/33205/adb-4en-pinaca)
Chromatogram: ADB-4en-PINACA

Additional peaks present in chromatogram: internal standard (7.28 min) and 4F-ABINACA (10.48 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: ADB-4en-PINACA
6. FUNDING

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