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

<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>C₂₀H₃₀N₄O₂</td>
<td>358.5</td>
<td>358</td>
<td>359.2442</td>
</tr>
</tbody>
</table>

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

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: Collision 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](https://www.caymanchem.com/product/33820/adb-hexinaca))

**Chromatogram: ADB-HEXINACA**

![Chromatogram](image)

*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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