ADB-INACA

**Sample Type:** Drug Material

**IUPAC Name:** N-(1-carbamoyl-2,2-dimethyl-propyl)-1H-indazole-3-carboxamide

**InChI String:** InChI=1S/C14H18N4O2/c1-14(2,3)11(12(15)19)16-13(20)10-8-6-4-5-7-9(8)17-18-10/h4-7,11H,1-/3H3,(H2,15,19)(H,16,20)(H,17,18)

**CFR:** Not Scheduled (12/2022)

**CAS#** 1887742-42-8

**Synonyms:** None Available

**Source:** NMS Labs – Criminalistic Laboratory

**Appearance:** White Solid Material on White Paper

**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_{14}H_{18}N_{4}O_{2}</td>
<td>274.3</td>
<td>274</td>
<td>275.1503</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

ADB-INACA 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. Little information is currently known about the activity, potency, and/or toxicity of ADB-INACA. It is suspected that ADB-INACA is a precursor, specifically to other synthetic cannabinoids like ADB-BINACA (ADB-BUTINACA), and therefore overall potency is expected to be low. New synthetic cannabinoids continue to emerge among the recreation drug supply internationally, seemingly as replacements after a synthetic cannabinoid class-wide ban implemented by China in July 2021 which included most traditional indole and indazole structural scaffolds. Many of these new synthetic cannabinoid analogues are unstudied with pharmacological and human effects undetermined. Currently, ADB-INACA is not a scheduled substance in the United States.

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: Acid/Base Extraction (NMS Labs)

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: 7.51 min

Standard Comparison: Reference material for ADB-INACA (Batch: 0661443-1) 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-INACA based on retention time (7.50 min) and mass spectral data.

Extracted Ion Chromatogram: ADB-INACA

EI (70 eV) Mass Spectrum: ADB-INACA
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: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 6.58 min

Standard Comparison: Reference material for ADB-INACA (Batch: 0661443-1) 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-INACA based on retention time (6.45 min) and mass spectral data. (https://www.caymanchem.com/product/37729/adb-inaca)
Chromatogram: ADB-INACA

Additional peaks present in chromatogram: internal standards (4.99 min and 7.30 min)

TOF MS Spectrum: ADB-INACA
6. FUNDING

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