ADB-BINACA

Sample Type: Seized Material

Latest Revision: November 18, 2020
Date Received: July 17, 2020
Date of Report: November 18, 2020

1. GENERAL INFORMATION

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

InChI String: InChI=1S/C18H26N4O2/c1-5-6-11-22-13-10-8-7-9-12(13)14(21-22)17(24)20-15(16(19)23)18(2,3)4/h7-10,15H,5-6,11H2,1-4H3,(H2,19,23)(H,20,24)

CFR: Not Scheduled (11/2020)

CAS#: Not Available

Synonyms: ADB-BUTINACA

Source: NMS Labs – Criminalistic Laboratory

Appearance: Hand-Rolled Cigarette Containing 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>C₁₈H₂₆N₄O₂</td>
<td>330.4</td>
<td>330</td>
<td>331.2129</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

ADB-BINACA 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 MDMB-BINACA are structurally similar synthetic cannabinoids. ADB-BINACA and AB-PINACA are structural isomers, sharing the same formula and parent mass; however, their chemical behavior and mass fragmentation patterns differ allowing for differentiation during analytical testing. ADB-PINACA and AB-PINACA are Schedule I substances in the United States; ADB-BINACA and MDMB-BINACA are not explicitly scheduled.

ADB-BINACA in this report should not be confused with ADB-BENZINACA (which is also referred to as “ADB-BINACA”; IUPAC Name: N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-benzyl-1H-indazole-3-carboxamide). ADB-BENZINACA contains a benzyl- moiety as the tail portion of its molecule, while ADB-BINACA containing a butyl- moiety as its tail. The name ADB-BINACA was selected for the drug reported herein for consistency with the naming convention used for drugs associated with previously developed new drug monographs (e.g. 4F-MDMB-BINACA, 4F-MDMB-BICA, 5F-MDMB-PICA, 5F-EDMB-PINACA).

4. ADDITIONAL RESOURCES


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: 7.77 min

Standard Comparison: Reference material for ADB-BINACA (Batch: 0576506-5) 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-BINACA based on retention time (7.76 min) and mass spectral data. (https://www.caymanchem.com/product/29350/adb-butinaca)
Chromatogram: ADB-BINACA

Additional peak present in chromatogram: internal standard (6.29 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): ADB-BINACA
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:** 8.89 min

**Standard Comparison:** Reference material for ADB-BINACA (Batch: 0576506-5) 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-BINACA based on retention time (8.94 min) and mass spectral data. ([https://www.caymanchem.com/product/29350/adb-butinaca](https://www.caymanchem.com/product/29350/adb-butinaca))
Extracted Ion Chromatogram: ADB-BINACA
TOF MS (Top) and MS/MS (Bottom) Spectra: ADB-BINACA