APP-BINACA

Sample Type: Biological Fluid

Latest Revision: March 6, 2019
Date of Report: March 6, 2019

1. GENERAL INFORMATION

IUPAC Name: N-(2-amino-1-benzyl-2-oxo-ethyl)-1-butyl-indazole-3-carboxamide

InChI String: InChI=1S/C21H24N4O2/c1-2-3-13-25-18-12-8-7-11-16(18)19(24-25)21(27)23-17(20(22)26)14-15-9-5-4-6-10-15/h4-12,17H,2-3,13-14H2,1H3,(H2,22,26)(H,23,27)

CFR: Not Scheduled (03/2019)

CAS#: Not Available

Synonyms: APP-BUTINACA

Source: NMS Labs – Toxicology Department

Important Note: All identifications were made based on evaluation of analytical data (LC-QTOF) in comparison to analysis of acquired reference material.

Prepared By: Alex J. Krotulski, MSFS, Amanda L.A. Mohr, MSFS, D-ABFT-FT, 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>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₂₁H₂₄N₄O₂</td>
<td>364.44</td>
<td>364</td>
<td>365.1972</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

APP-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. APP-PICA, PX1 (5F-APP-PICA), and PX2 (5F-APP-PINACA) are structurally similar synthetic cannabinoids. APP-BINACA, APP-PICA, PX1, and PX2 are not scheduled substances in the United States.

4. SAMPLE HISTORY

APP-BINACA has been identified in two cases since the beginning of February 2019. The geographical and demographical breakdown is below:

Geographical Location: Indiana (n=2)
Case Type: Post-Mortem Investigation (n=2)
Biological Sample: Blood (n=2)
Date of First Collection: February 5th, 2019
Date of First Receipt: February 6th, 2019
Additional Cannabinoids: 4F-MDMB-BINACA (n=2)

5. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/26905
6. QUALITATIVE DATA

6.1 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: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for APP-BINACA (Batch: 0552311-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/26905)

EI (70 eV) Mass Spectrum: APP-BINACA (Standard)
6.2 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:** No additional preparation - direct analysis of sample extract

**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) with 0.1% formic acid

Flow rate: 0.5 mL/min

**Gradient:** Initial: 95A:5B; 5A:95B over 4 min, hold 2 min; 95A:5B at 7 min
Temperatures:
- Autosampler: 15 °C
- Column Oven: 30 °C
- Source Heater: 600 °C

Injection Parameters:
- Injection Volume: 20 µL

QTOF Parameters:
- TOF MS Scan Range: 100-550 Da
- Precursor Isolation: SWATH® acquisition (10-25 Da)
- Fragmentation: Collison Energy Spread (35±15 eV)
- MS/MS Scan Range: 50-550 Da

Retention Time:
- 4.25 min

Standard Comparison:
Reference material for APP-BINACA (Batch: 0552311-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as APP-BINACA, based on retention time (4.38 min) and mass spectral data. (https://www.caymanchem.com/product/26905)

Extracted Ion Chromatogram: APP-BINACA (Blood Extract)
TOF MS (Top) and MS/MS (Bottom) Spectra: APP-BINACA (Blood Extract)
7. FUNDING

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