Adamantyl-CHMINACA

Sample Type: Seized Material

Latest Revision: May 18th, 2018

Date Received: January 26th, 2018

Date of Report: March 20th, 2018

1. GENERAL INFORMATION

IUPAC Name: N-(1-adamantyl)-1-(cyclohexylmethyl)indazole-3-carboxamide


CFR: Not Scheduled (03/2018)

CAS#: Not Available

Synonyms: SGT-37, ACHMINACA

Source: Department of Homeland Security

Appearance: Off-White Solid Material

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_{25}H_{33}N_{3}O</td>
<td>391.6</td>
<td>391</td>
<td>392.2696</td>
</tr>
</tbody>
</table>

Important Note: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT
3. BRIEF DESCRIPTION

Adamantyl-CHMINACA (ACHMINACA) 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. Structurally similar compounds include APINACA (AKB48) and 5F-APINACA (5F-AKB48). APINACA and 5F-APINACA are Schedule I substances in the United States.

4. ADDITIONAL RESOURCES

No additional resources available at this time.

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: 9.787 min
Chromatogram: Adamantyl-CHMINACA

Additional peaks present in chromatogram: internal standard 1 (3.219 min) and internal standard 2 (6.296 min)

EI (70 eV) Mass Spectrum: Adamantyl-CHMINACA
EI (70 eV) Mass Spectrum (10x): Adamantyl-CHMINACA

![Mass Spectrogram](image)

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: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 11.89 min

Chromatogram: Adamantyl-CHMINACA

Additional peaks present in chromatogram: internal standard 1 (5.15 min) and internal standard 2 (7.46 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: Adamantyl-CHMINACA
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in CDCl₃

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters:

- Pulse Sequence: Proton
- Solvent: CDCl₃
- Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D
- Delay between pulses: 1st delay, d1 = 1.000

^1H NMR: Adamantyl-CHMINACA
### 6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
<th>Revision</th>
</tr>
</thead>
<tbody>
<tr>
<td>05/18/2018</td>
<td>Added “Sample Type: Seized Material” to Page 1.</td>
</tr>
<tr>
<td>05/18/2018</td>
<td>Added “Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT” to Page 1 footer.</td>
</tr>
</tbody>
</table>