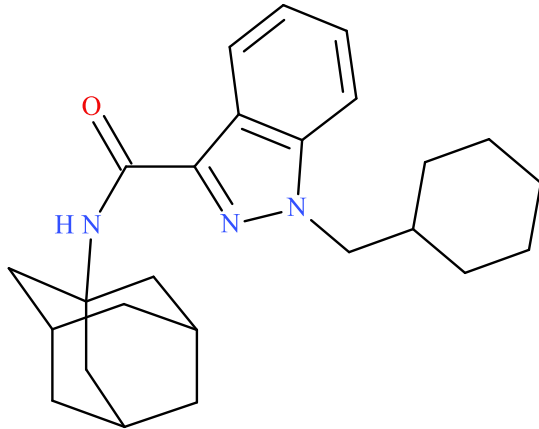


## Adamantyl-CHMINACA

Sample Type: **Seized Material**



Latest Revision: **May 18<sup>th</sup>, 2018**

Date Received: **January 26<sup>th</sup>, 2018**

Date of Report: **March 20<sup>th</sup>, 2018**

### 1. GENERAL INFORMATION

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

**InChI String:** InChI=1S/C25H33N3O/c29-24(26-25-13-18-10-19(14-25)12-20(11-18)15-25)23-21-8-4-5-9-22(21)28(27-23)16-17-6-2-1-3-7-17/h4-5,8-9,17-20H,1-3,6-7,10-16H2,(H,26,29)

**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

Form	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>25</sub> H <sub>33</sub> N <sub>3</sub> O	391.6	391	392.2696

**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)

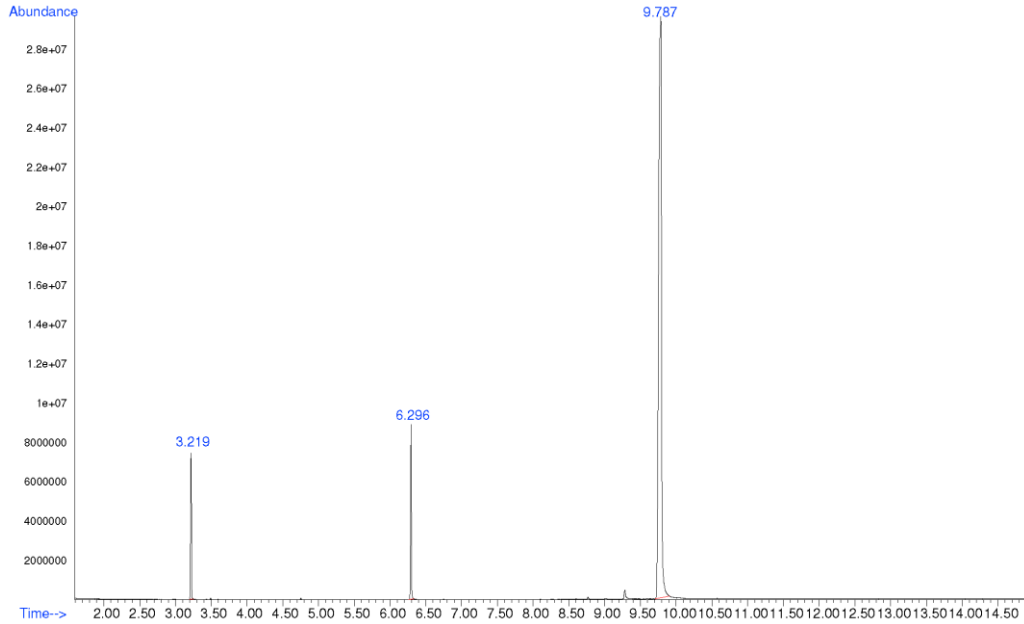
**Temperatures:** Injection Port: 265 °C  
Transfer Line: 300 °C  
MS Source: 230 °C  
MS Quad: 150 °C  
Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

**Injection Parameters:** Injection Type: Splitless  
Injection Volume: 1 µL

**MS Parameters:** Mass Scan Range: 40-550 m/z  
Threshold: 250

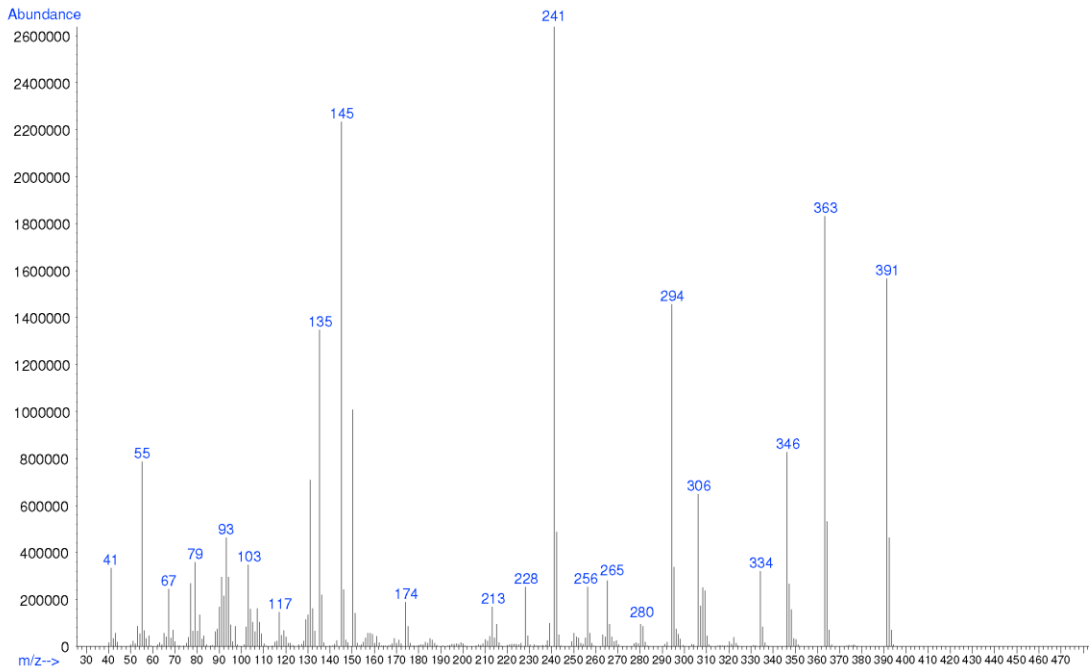
**Retention Time:** 9.787 min

## Chromatogram: Adamantyl-CHMINACA

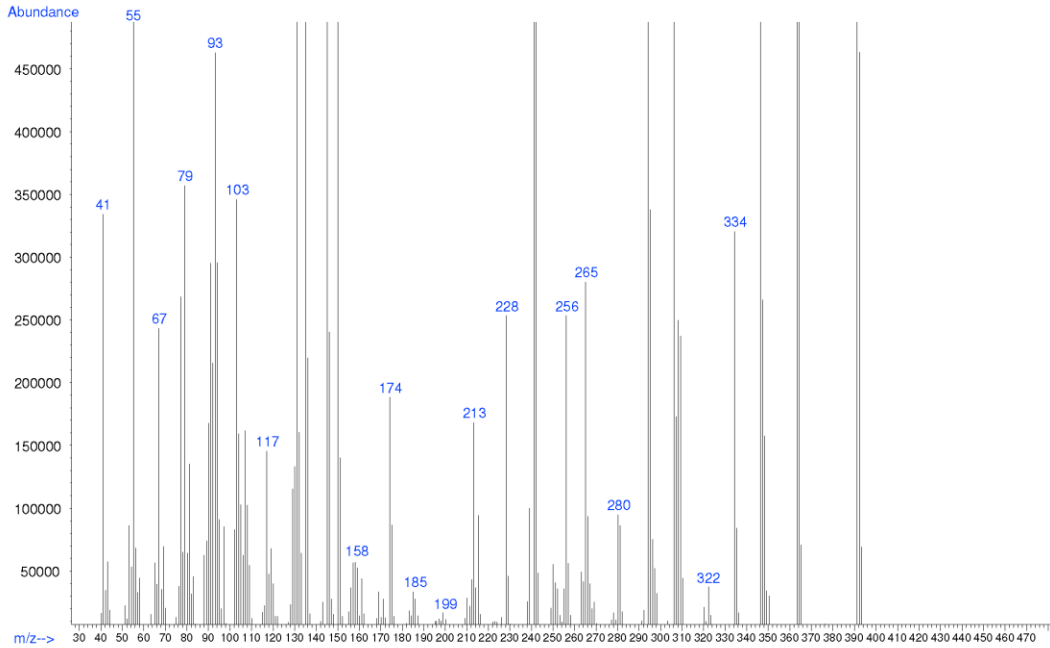


*Additional peaks present in chromatogram: internal standard 1 (3.219 min) and internal standard 2 (6.296 min)*

## EI (70 eV) Mass Spectrum: Adamantyl-CHMINACA



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



### 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

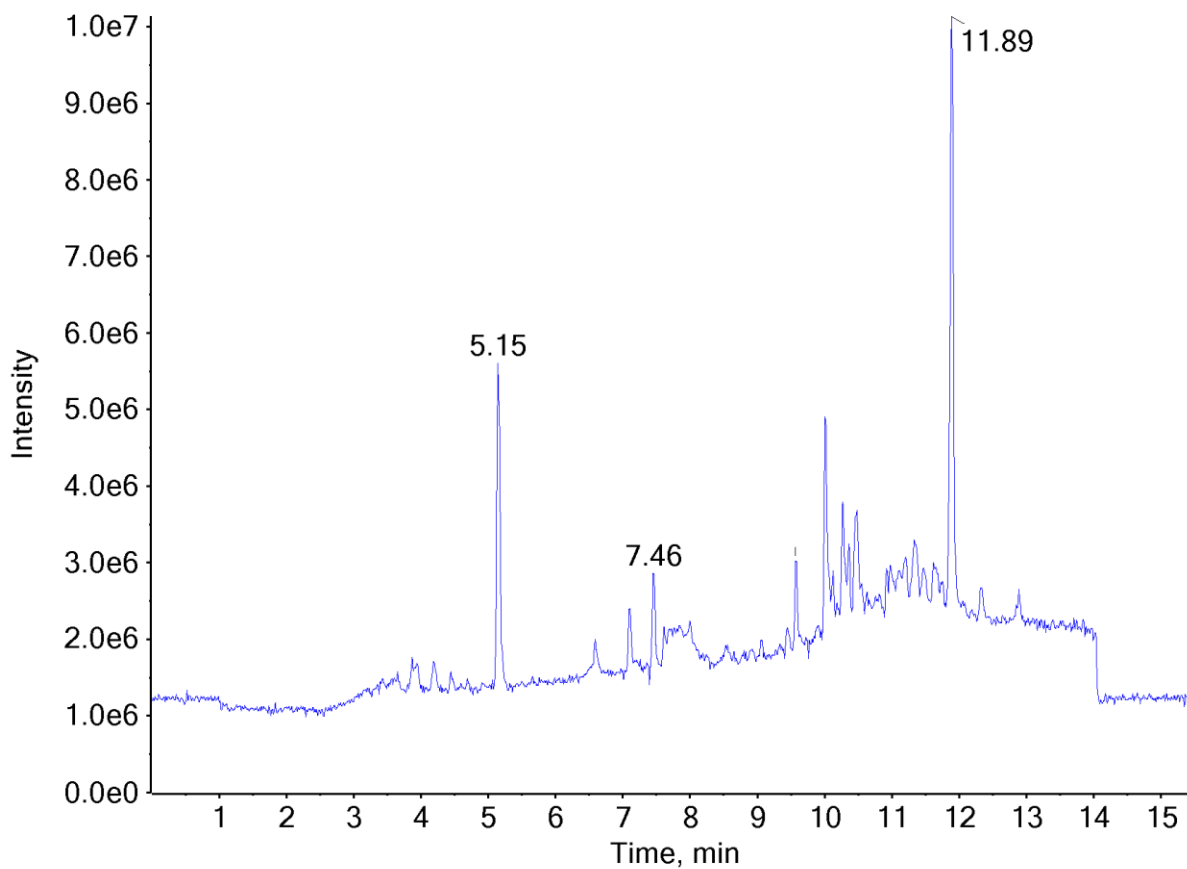
**Temperatures:** Autosampler: 15 °C

Column Oven: 30 °C

Source Heater: 600 °C

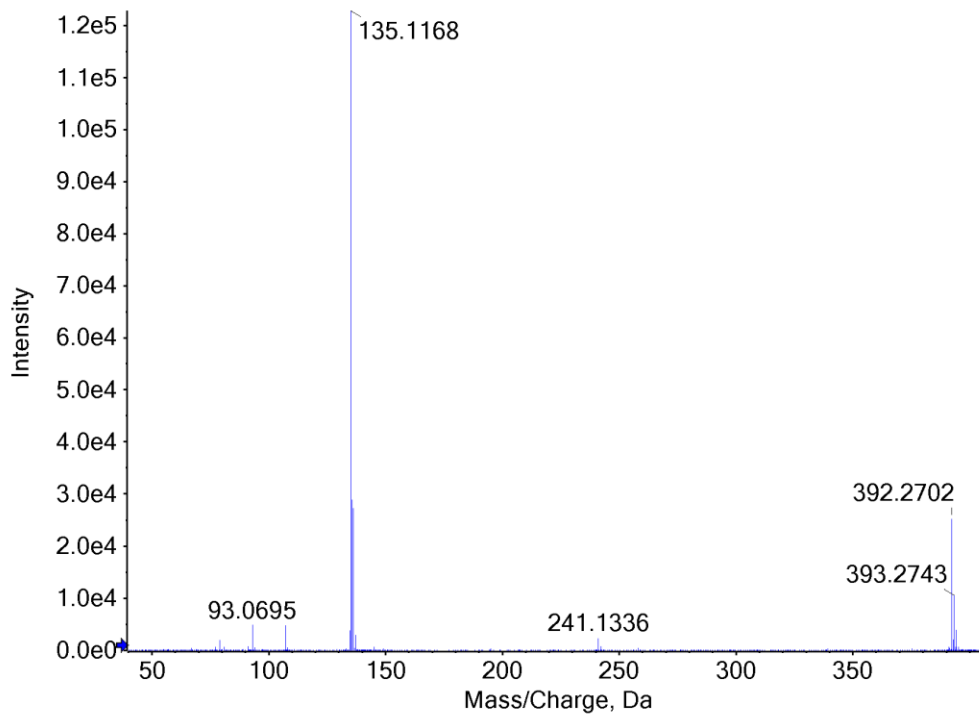
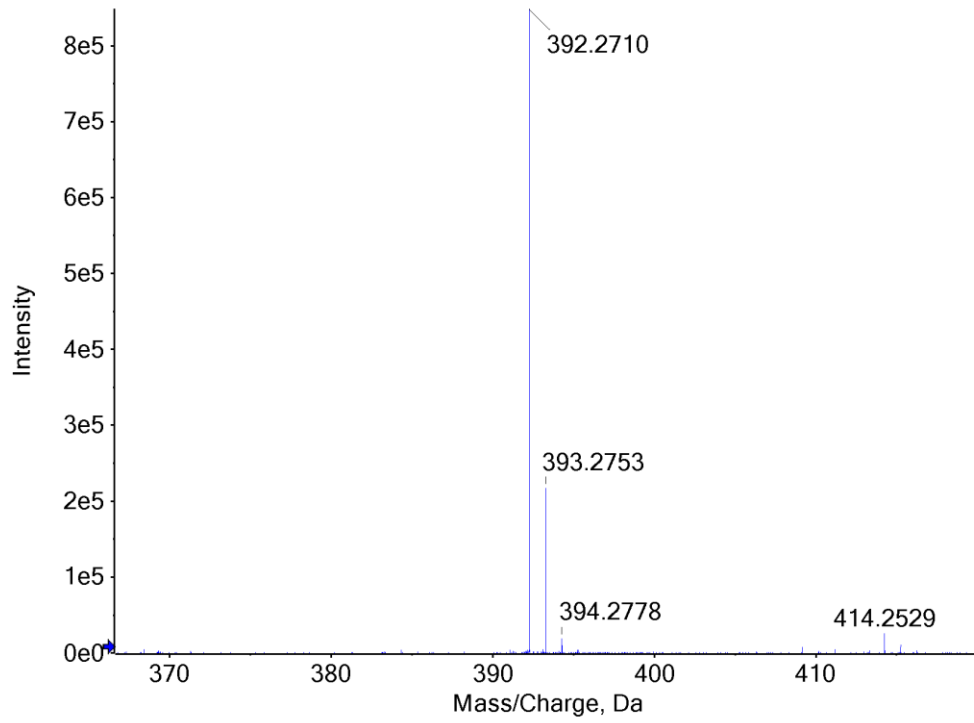
**Injection Parameters:** Injection Volume: 10  $\mu$ L  
**QTOF Parameters:** TOF MS Scan Range: 100-510 Da  
Precursor Isolation: SWATH® acquisition (27 windows)  
Fragmentation: Collision Energy Spread (35 $\pm$ 15 eV)  
MS/MS Scan Range: 50-510 Da  
**Retention Time:** 11.89 min

**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 CDCl<sub>3</sub>

**Instrument:** 300 MHz INOVA VARIAN Spectrometer

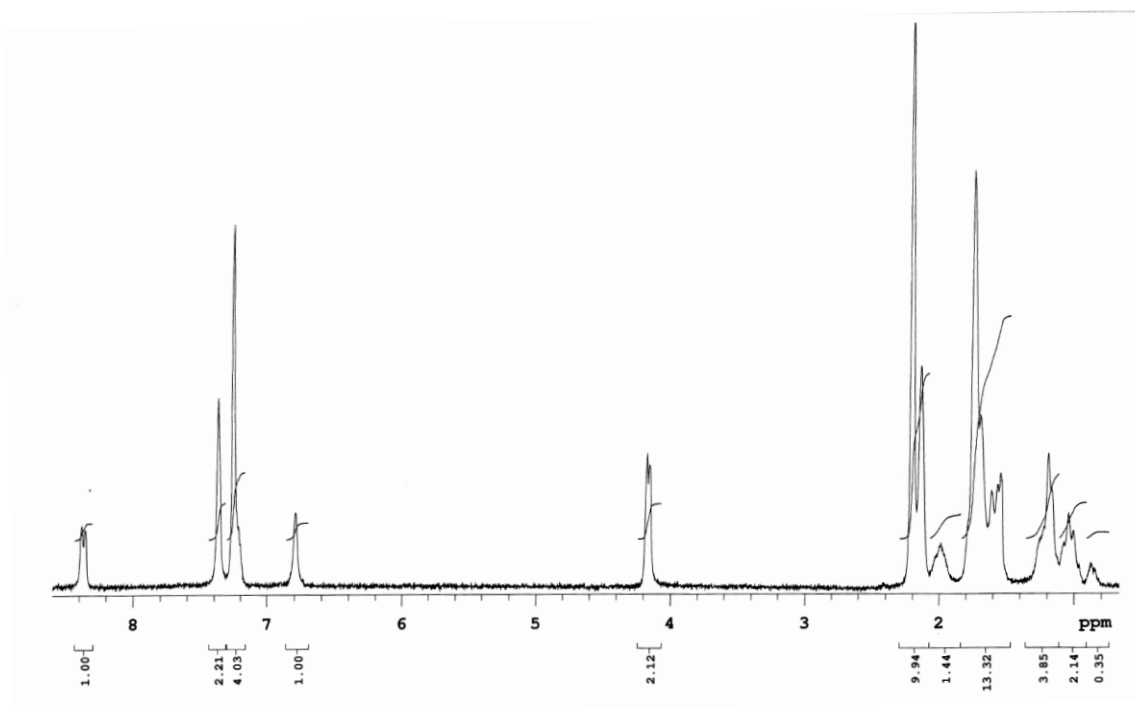
**Parameters:** Pulse Sequence: Proton

Solvent: CDCl<sub>3</sub>

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

#### **<sup>1</sup>H NMR: Adamantyl-CHMINACA**



## 6. REVISION HISTORY

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