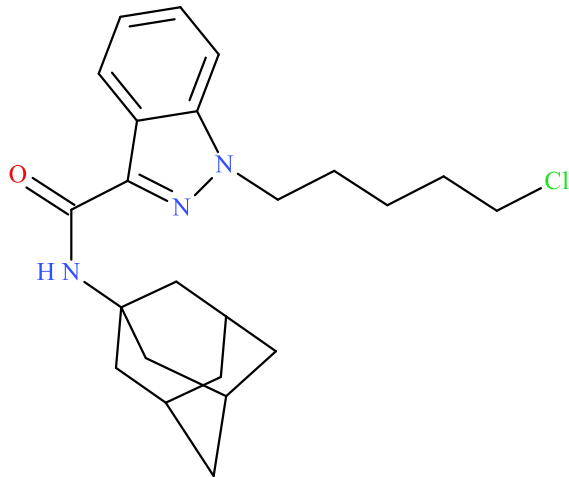


## 5Cl-AKB48 and 5Br-AKB48

Sample Type: **Seized Material**

**5Cl-AKB48**

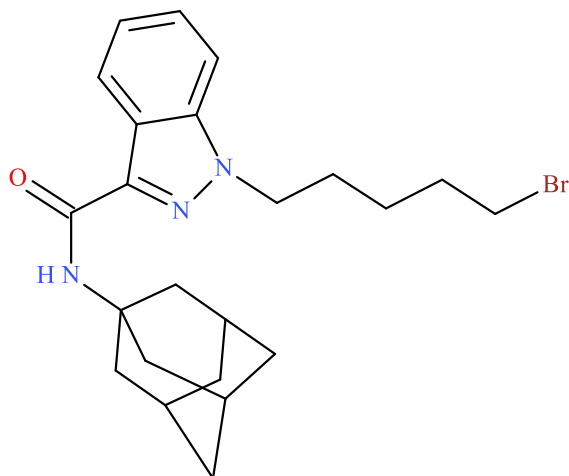


Latest Revision: **May 18<sup>th</sup>, 2018**

Date Received: **February 16<sup>th</sup>, 2018**

Date of Report: **April 10<sup>th</sup>, 2018**

**5Br-AKB48**



**Important Note:** Identification of 5Cl-AKB48 was made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material. Identification of 5Br-AKB48 was made based on evaluation of analytical data only (GC-MS and LC-QTOF), including isotopic distribution and accurate mass formula elucidation, as reference material was not available.

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

## 1. GENERAL INFORMATION

### 1.1 5Cl-AKB48

<b>IUPAC Name:</b>	N-(1-adamantyl)-1-(5-chloropentyl)indazole-3-carboxamide
<b>InChI String:</b>	InChI=1S/C23H30ClN3O/c24-8-4-1-5-9-27-20-7-3-2-6-19(20)21(26-27)22(28)25-23-13-16-10-17(14-23)12-18(11-16)15-23/h2-3,6-7,16-18H,1,4-5,8-15H2,(H,25,28)
<b>CFR:</b>	Not Scheduled (04/2018)
<b>CAS#</b>	Not available
<b>Synonyms:</b>	5-Chloro AKB48, 5Cl-APINACA, 5-Chloro APINACA
<b>Source:</b>	Department of Homeland Security
<b>Appearance:</b>	Brown solid material

### 1.2 5Br-AKB48

<b>IUPAC Name:</b>	N-(1-adamantyl)-1-(5-bromopentyl)indazole-3-carboxamide
<b>InChI String:</b>	InChI=1S/C23H30BrN3O/c24-8-4-1-5-9-27-20-7-3-2-6-19(20)21(26-27)22(28)25-23-13-16-10-17(14-23)12-18(11-16)15-23/h2-3,6-7,16-18H,1,4-5,8-15H2,(H,25,28)
<b>CFR:</b>	Not Scheduled (04/2018)
<b>CAS#</b>	Not available
<b>Synonyms:</b>	5-Bromo AKB48, 5Br-APINACA, 5-Bromo APINACA
<b>Source:</b>	Department of Homeland Security
<b>Appearance:</b>	Brown solid material

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Drug (Form)	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
5Cl-AKB48 (Base)	C <sub>23</sub> H <sub>30</sub> ClN <sub>3</sub> O	399.96	399	400.2150
5Br-AKB48 (Base)	C <sub>23</sub> H <sub>30</sub> BrN <sub>3</sub> O	444.41	443	444.1645

### 3. BRIEF DESCRIPTION

5Cl-AKB48 (5Cl-APINACA) and 5Br-AKB48 (5Br-APINACA) are classified as synthetic cannabinoids. Synthetic cannabinoids have been reported to cause effects similar to delta-9-tetrahydrocannabinol (THC). Synthetic cannabinoids have caused adverse events, including deaths, as described in the literature. Structurally similar compounds include AKB48 (PINACA) and 5F-AKB48 (5F-APINACA). AKB48 and 5F-AKB48 are Schedule I substances in the United States.

### 4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/18166> (5Cl-AKB48)

### 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

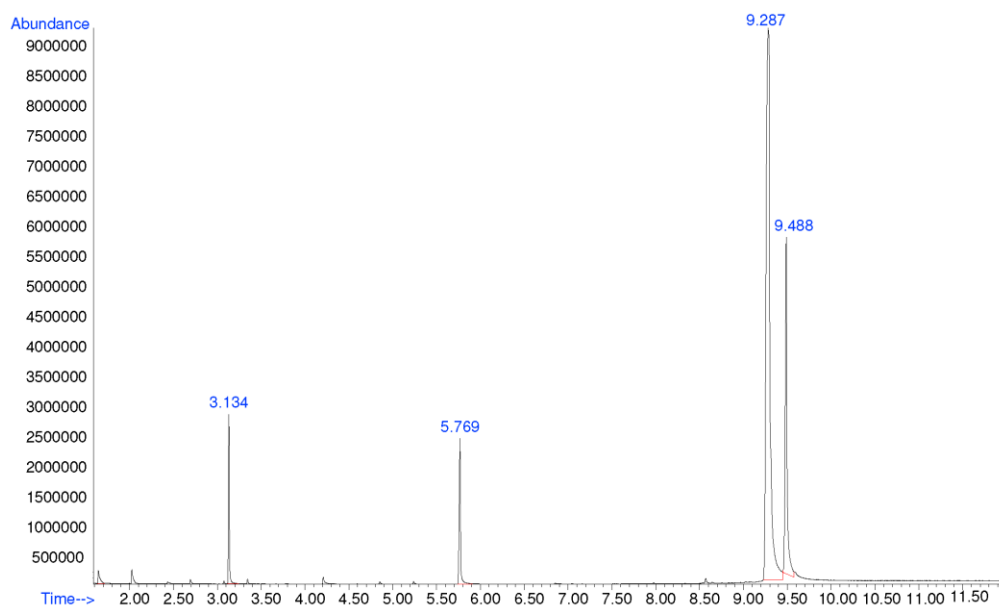
**Retention Time:** *5Cl-AKB48*: 9.287 min

*5Br-AKB48*: 9.488 min

**Standard Comparison:** Reference material for 5Cl-AKB48 (Batch: 0472010-15) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5Cl-AKB48, based on retention time (9.256 min) and mass spectral data.

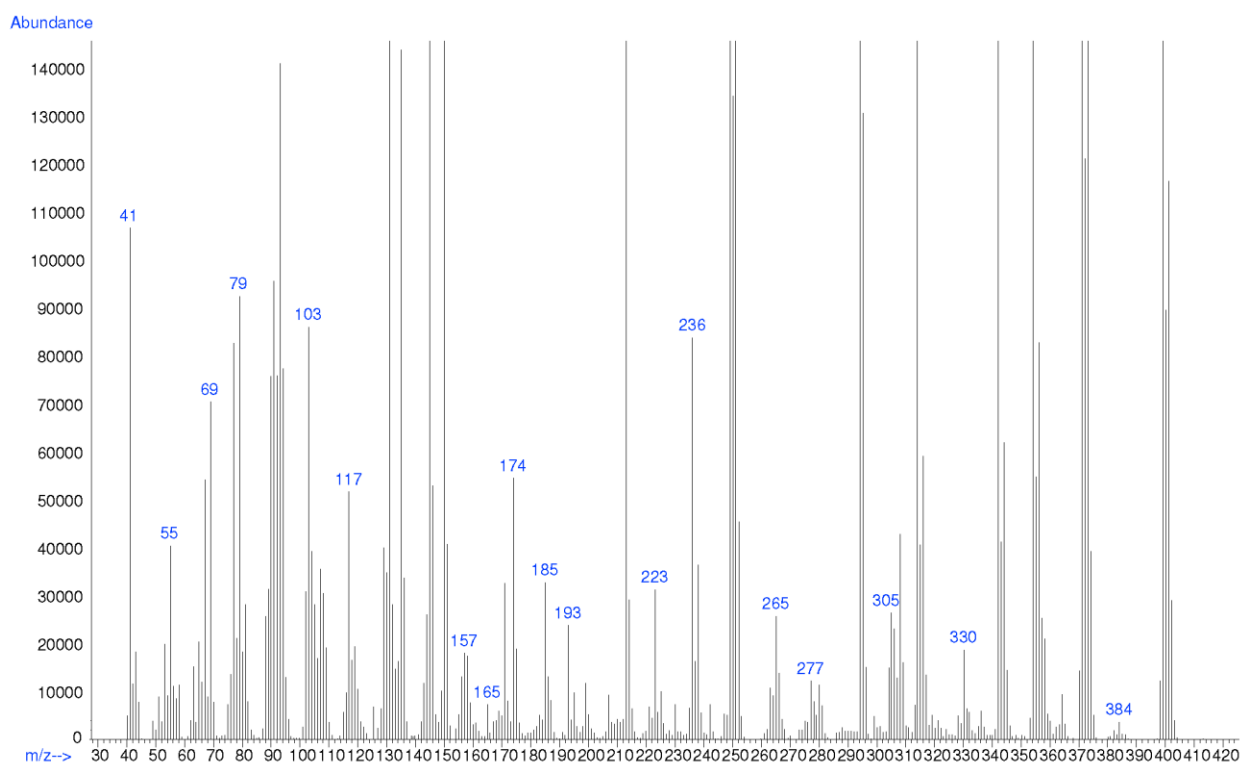
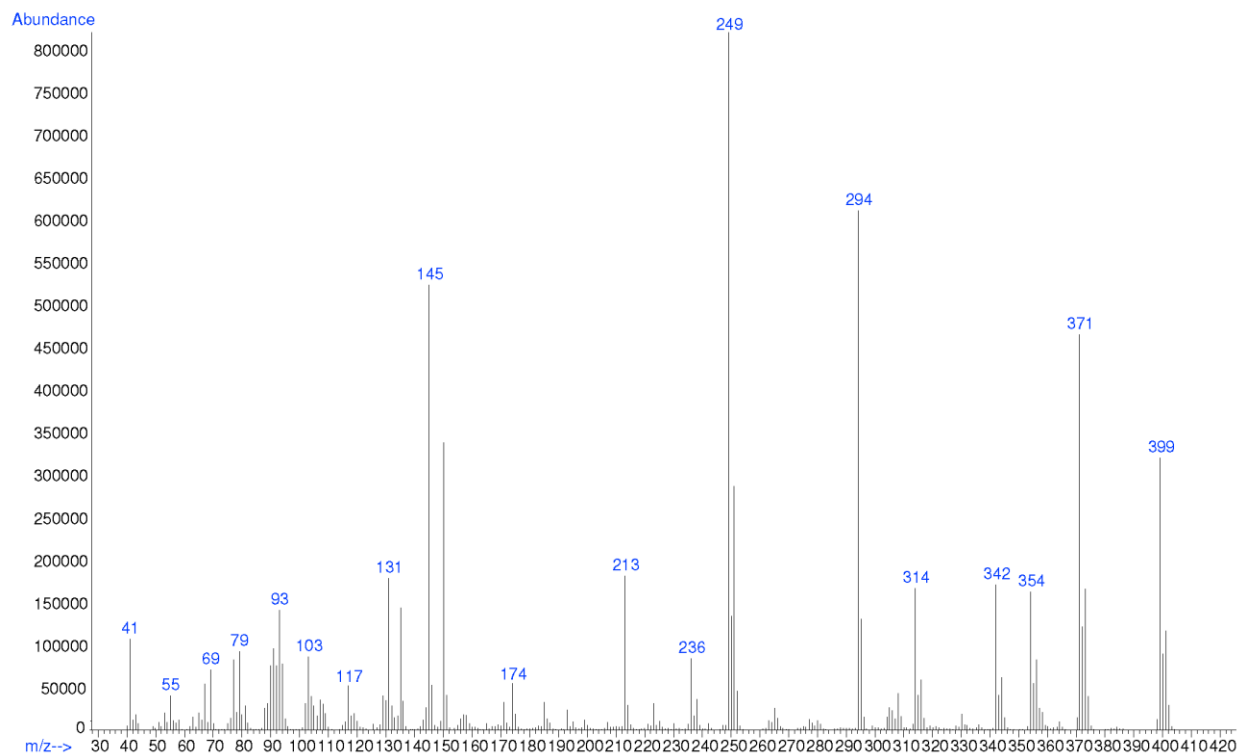
<https://www.caymanchem.com/product/18166>

### Chromatogram: *5Cl-AKB48* and *5Br-AKB48*

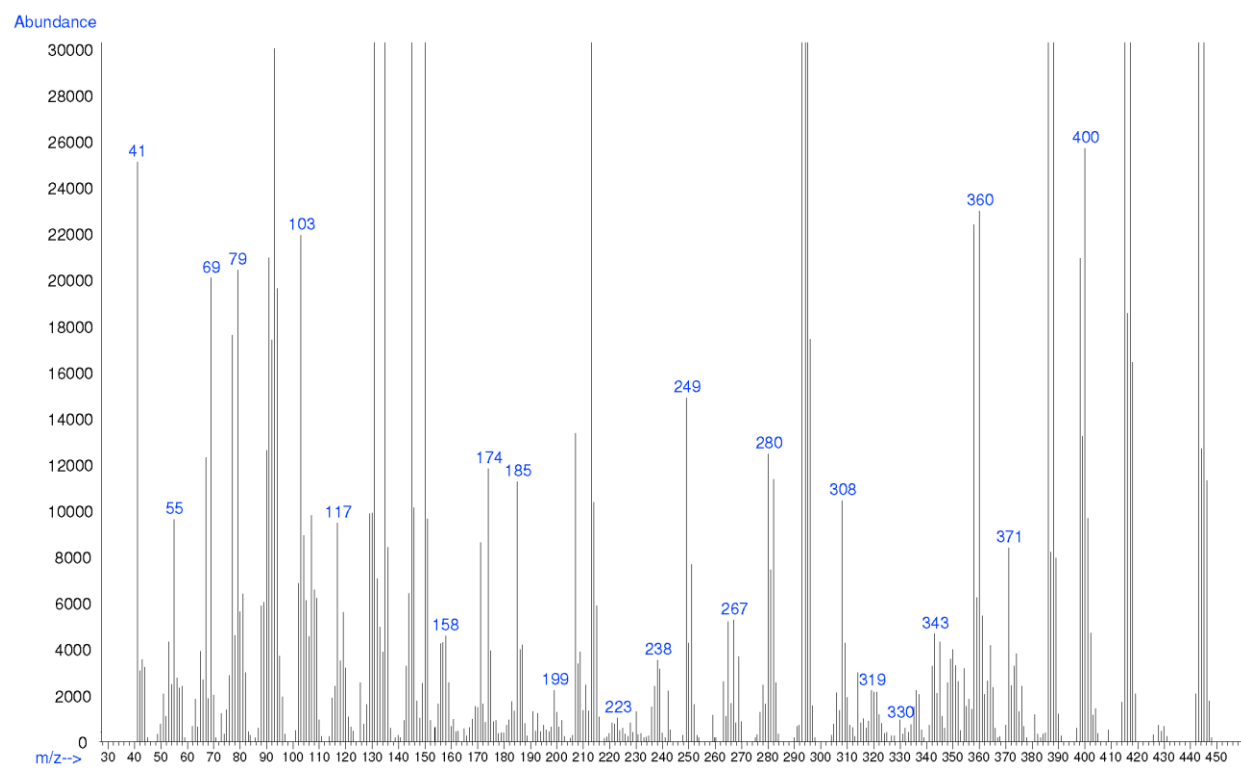
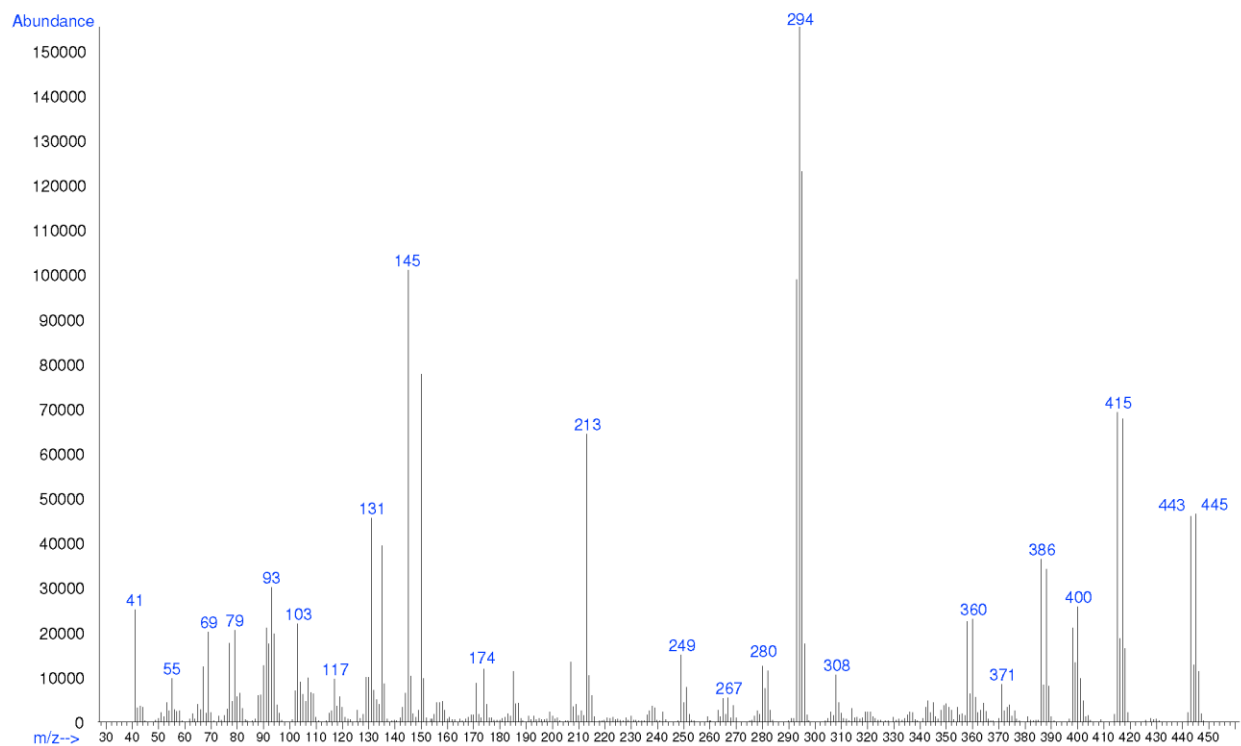


Peaks present in chromatogram: internal standard 1 (3.134 min), internal standard 2 (5.769 min), *5Cl-AKB48* (9.287 min), and *5Br-AKB48* (9.488 min)

# EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5Cl-AKB48



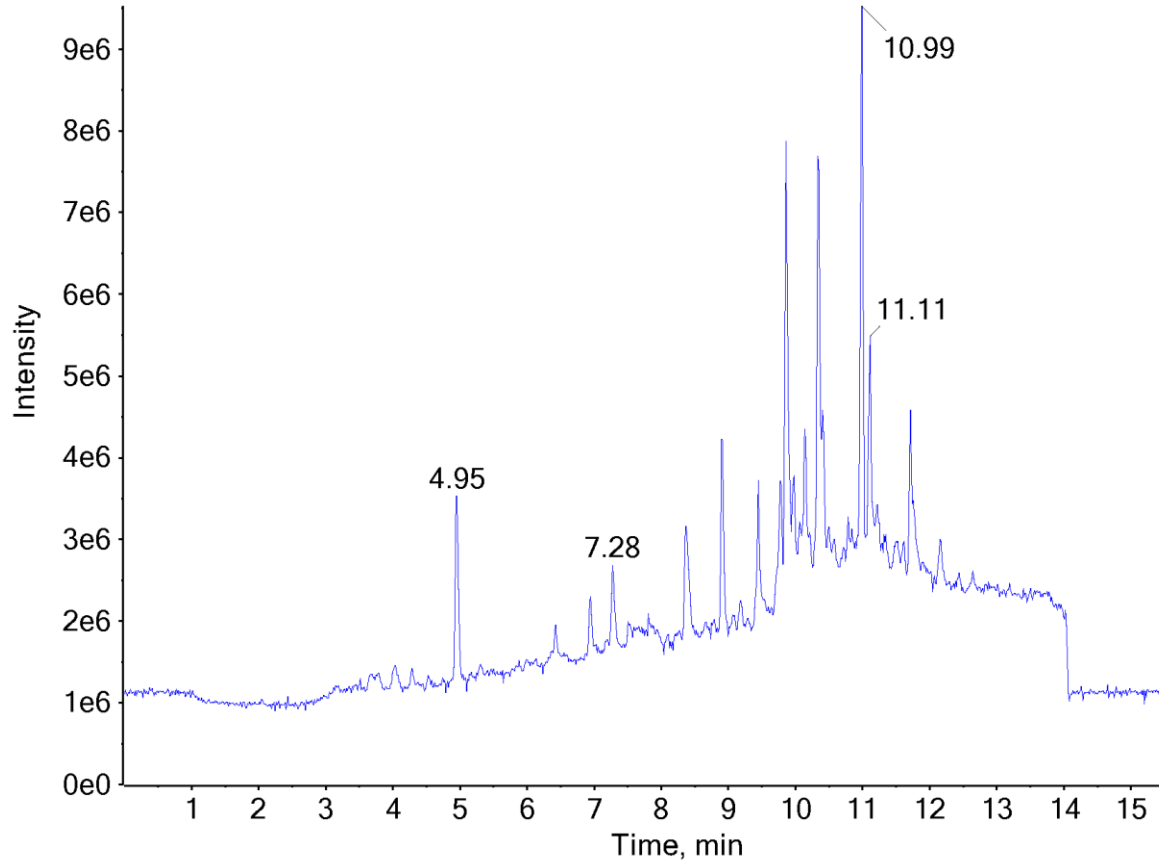
### EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5Br-AKB48



## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	1:100 dilution of acid/base extraction in mobile phase
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	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
<b>Retention Time:</b>	<i>5Cl-AKB48</i> : 10.99 min <i>5Br-AKB48</i> : 11.11 min
<b>Standard Comparison:</b>	Reference material for <i>5Cl-AKB48</i> (Batch: 0520119) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as <i>5Cl-AKB48</i> , based on retention time (10.997 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/18166">https://www.caymanchem.com/product/18166</a> )

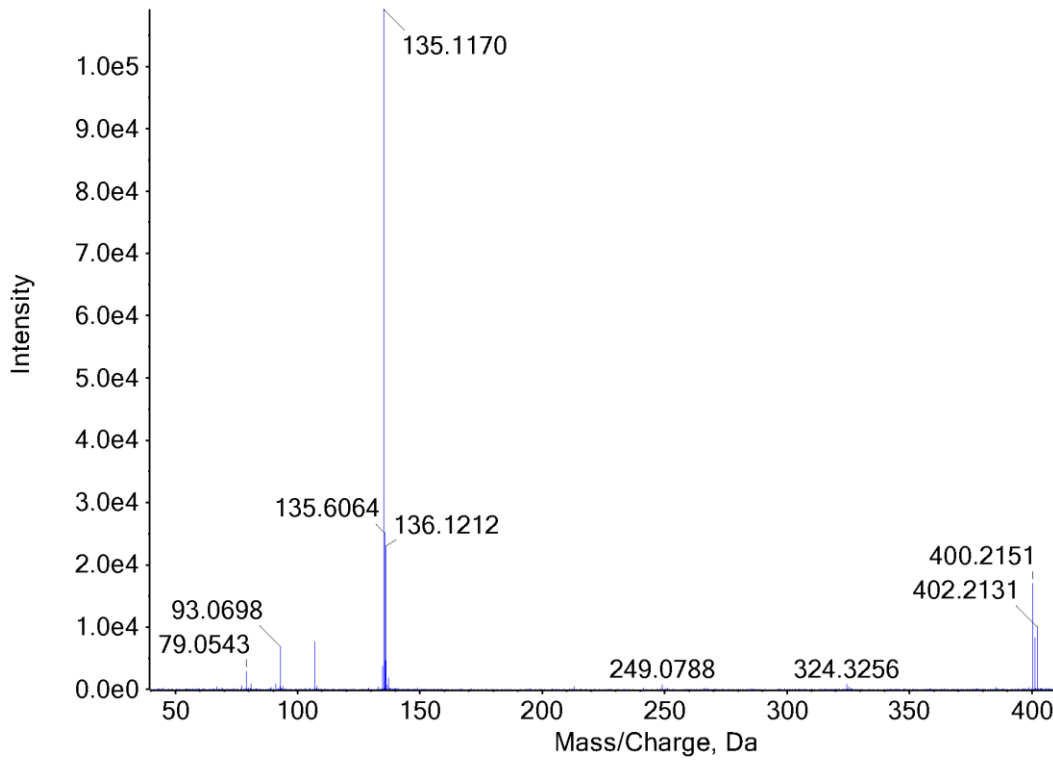
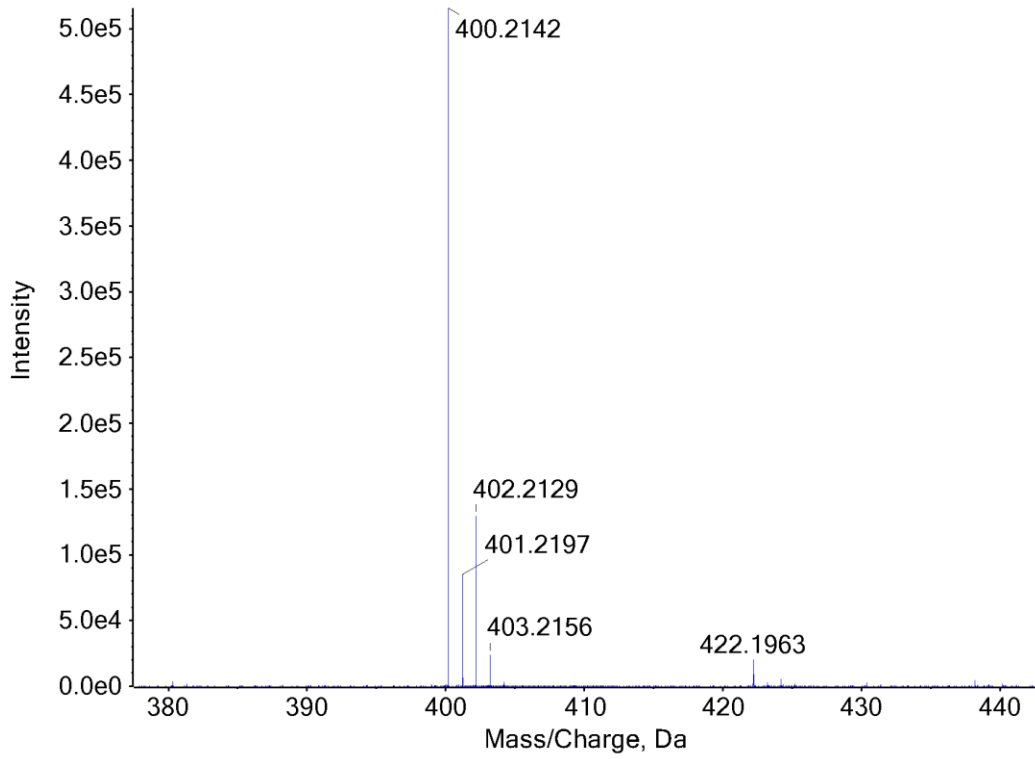
**Chromatogram: 5Cl-AKB48 and 5Br-AKB48**



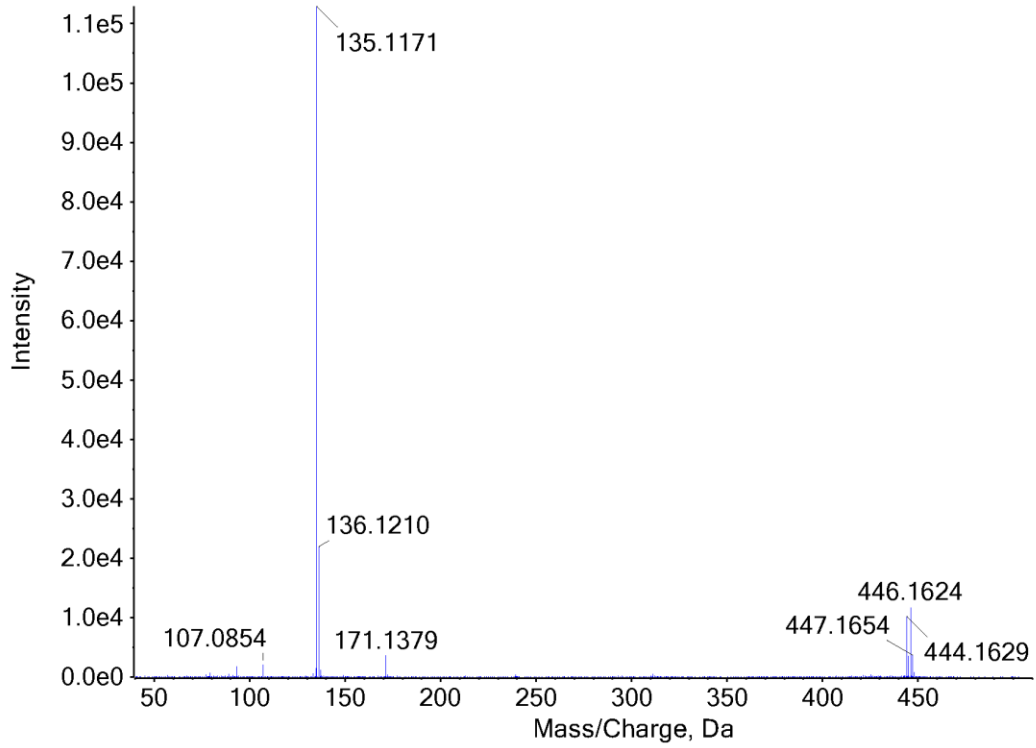
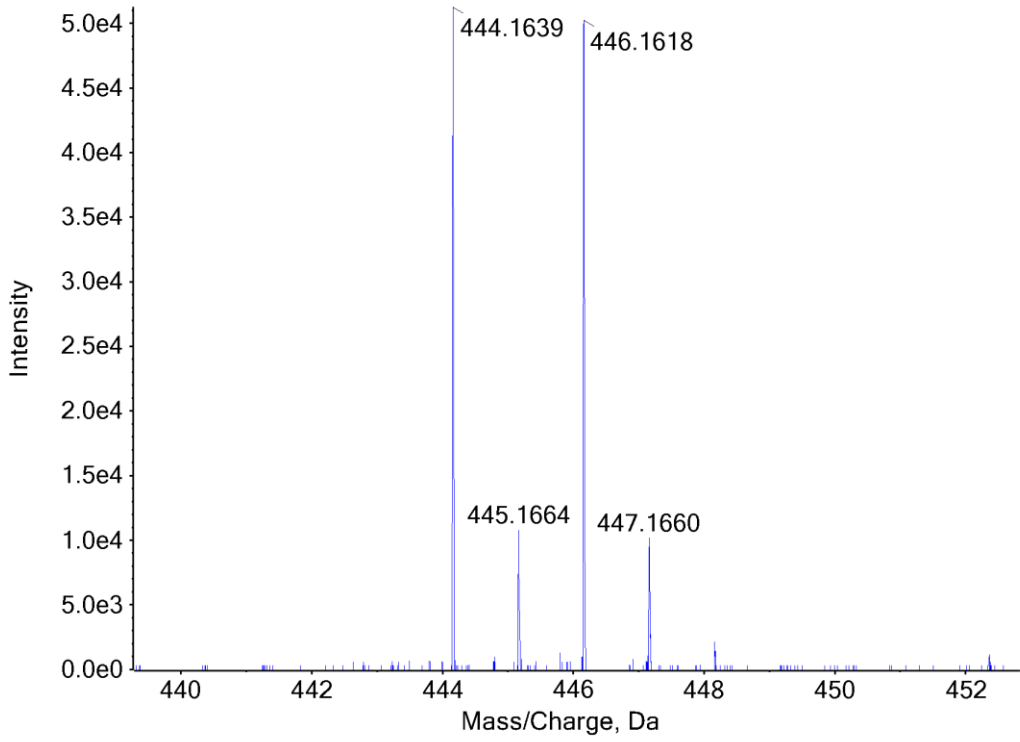
*Peaks present in chromatogram: internal standard 1 (4.95 min), internal standard 2 (7.28 min), 5Cl-AKB48 (10.99 min), and 5Br-AKB48 (11.11 min)*



**TOF MS (Top) and MS/MS (Bottom) Spectra: 5Cl-AKB48**



**TOF MS (Top) and MS/MS (Bottom) Spectra: 5Br-AKB48**



## **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.