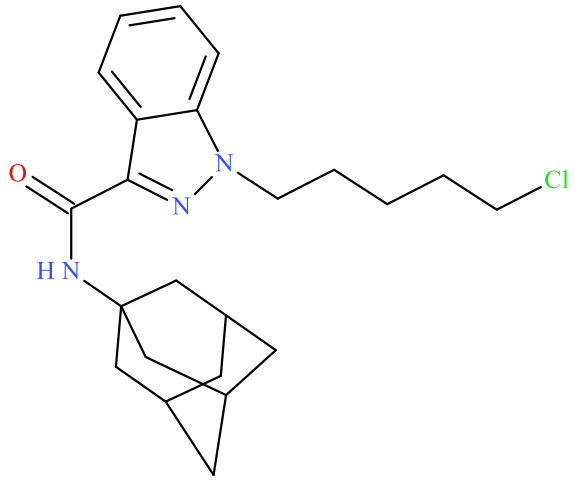
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

5Cl-AKB48 and 5Br-AKB48

Sample Type: **Seized Material**

5Cl-AKB48

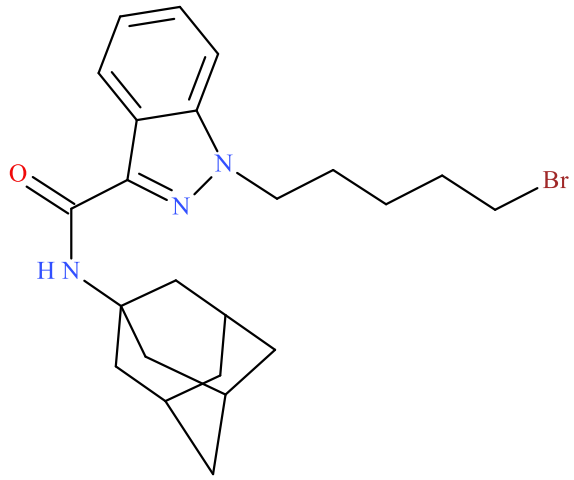


Latest Revision: **May 18th, 2018**

Date Received: **February 16th, 2018**

Date of Report: **April 10th, 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

IUPAC Name:	N-(1-adamantyl)-1-(5-chloropentyl)indazole-3-carboxamide
InChI String:	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)
CFR:	Not Scheduled (04/2018)
CAS#	Not available
Synonyms:	5-Chloro AKB48, 5Cl-APINACA, 5-Chloro APINACA
Source:	Department of Homeland Security
Appearance:	Brown solid material

1.2 5Br-AKB48

IUPAC Name:	N-(1-adamantyl)-1-(5-bromopentyl)indazole-3-carboxamide
InChI String:	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)
CFR:	Not Scheduled (04/2018)
CAS#	Not available
Synonyms:	5-Bromo AKB48, 5Br-APINACA, 5-Bromo APINACA
Source:	Department of Homeland Security
Appearance:	Brown solid material

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Drug (Form)	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
5Cl-AKB48 (Base)	$C_{23}H_{30}ClN_3O$	399.96	399	400.2150
5Br-AKB48 (Base)	$C_{23}H_{30}BrN_3O$	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

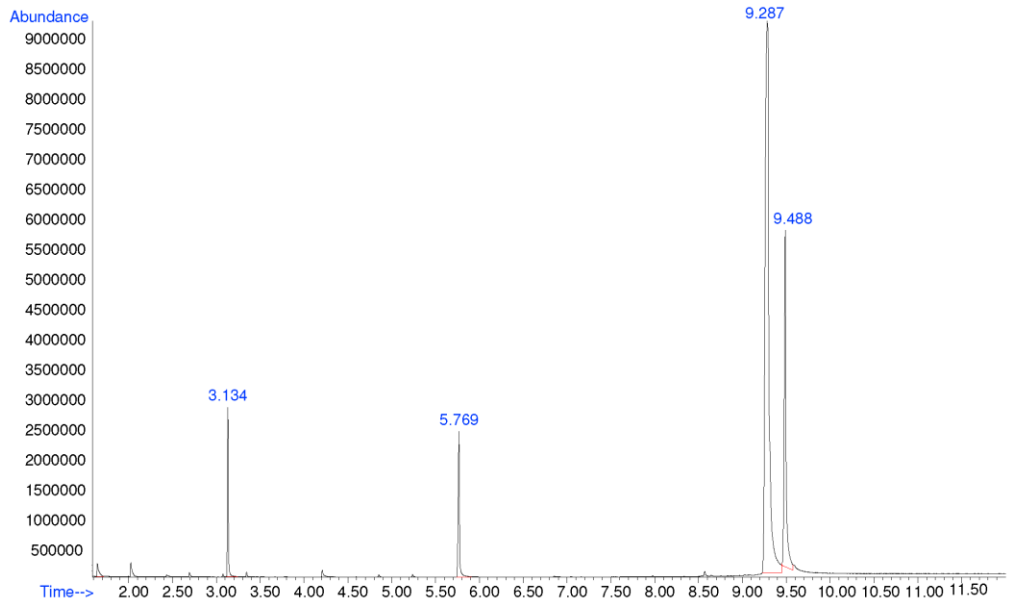
Threshold: 250

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

5Br-AKB48: 9.488 min

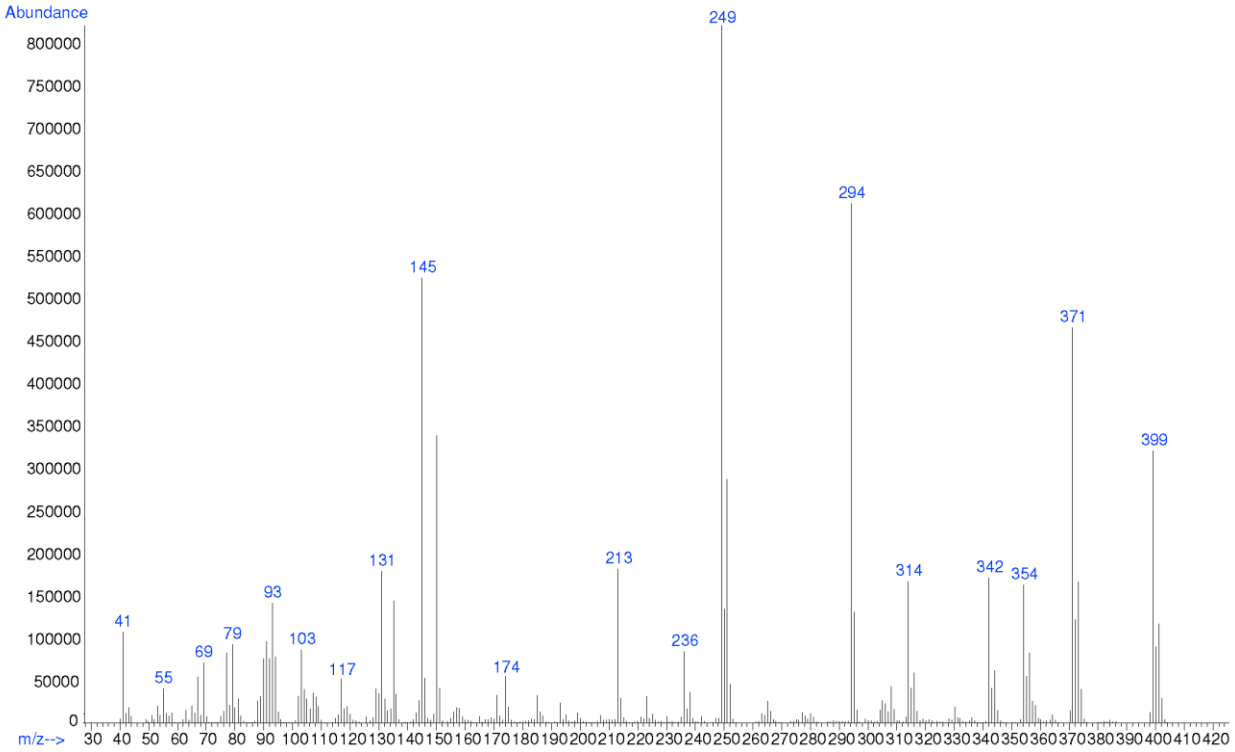
Standard Comparison: Reference material for 5Cl-AKB48 (Batch: 0472010-15) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5Cl-AKB48, based on retention time (9.256 min) and mass spectral data. (https://www.caymanchem.com/product/18166)

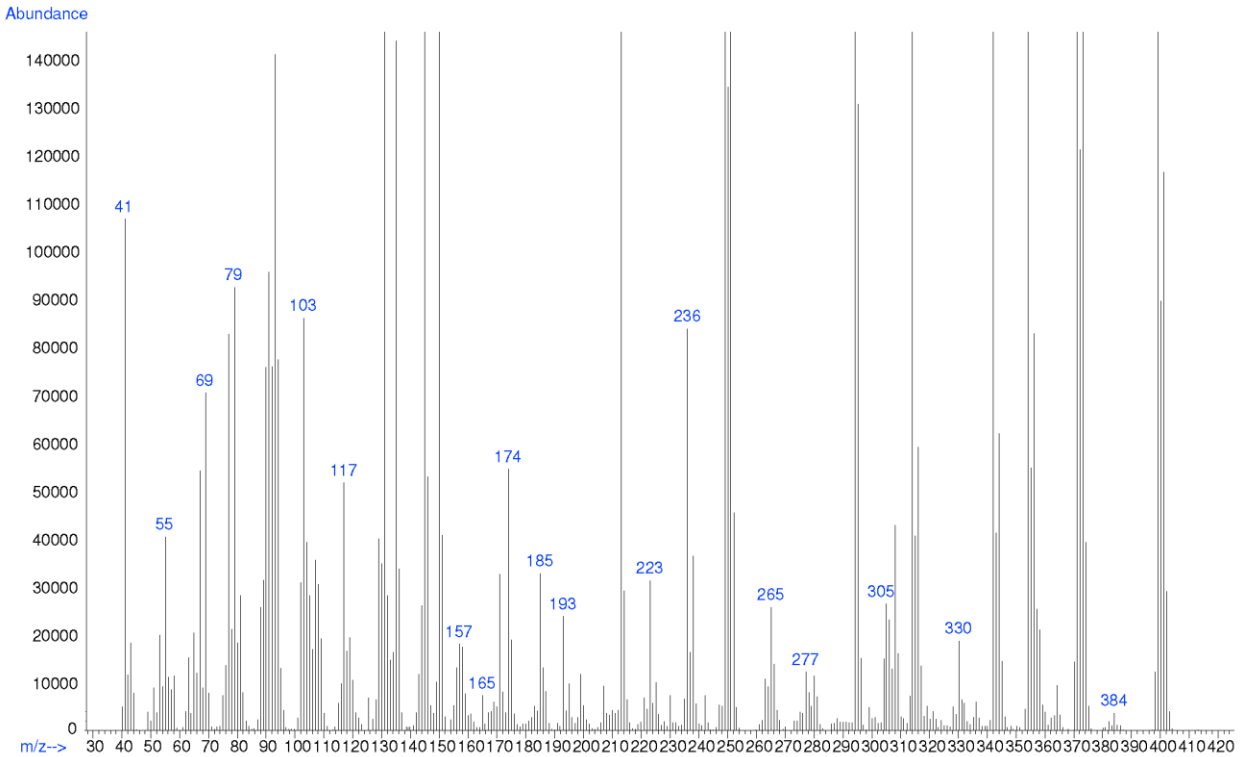
Chromatogram: *5Cl-AKB48 and 5Br-AKB48*



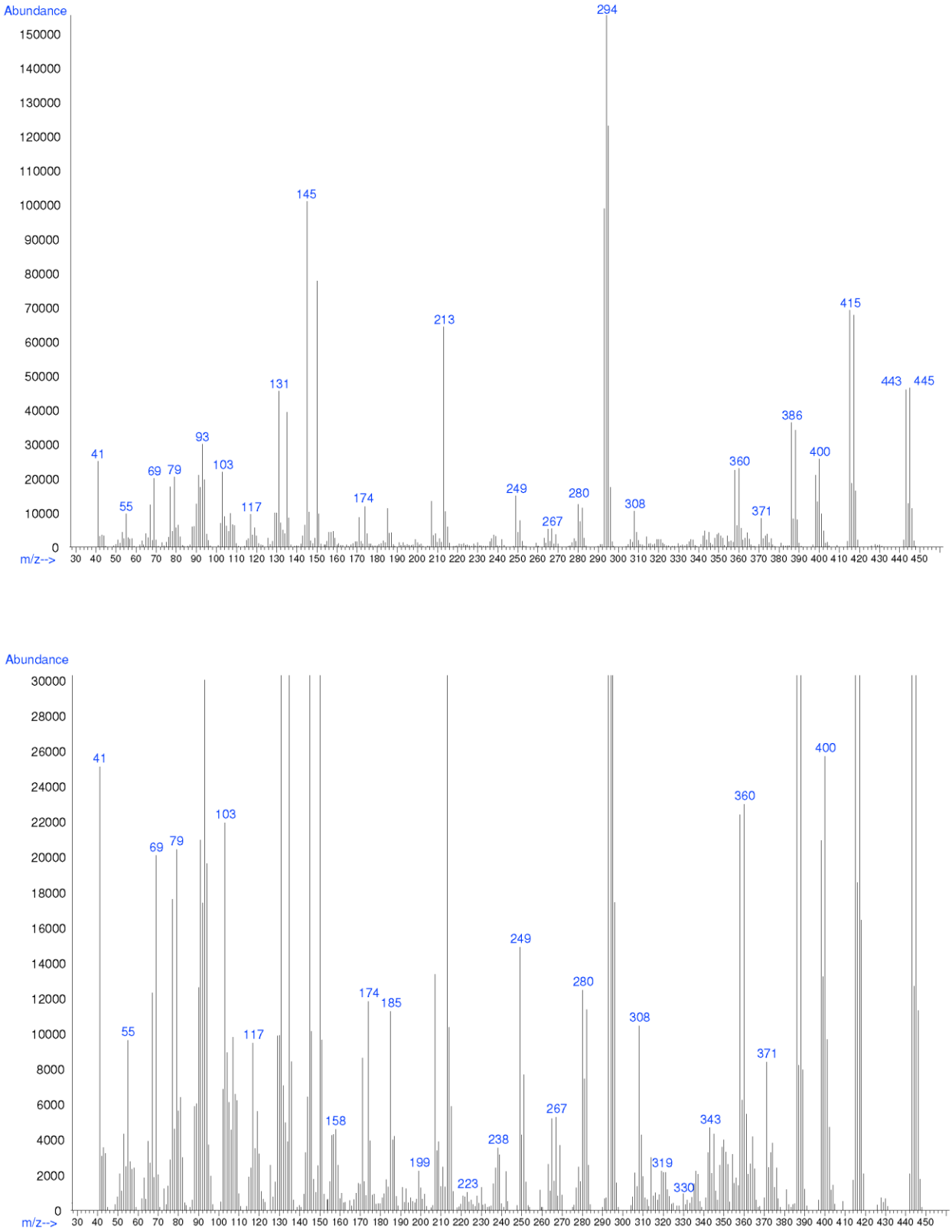
Peaks present in chromatogram: internal standard 1 (3.134 min), internal standard 2 (5.769 min), 5Cl-AKB48 (9.287 min), and 5Br-AKB48 (9.488 min)

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





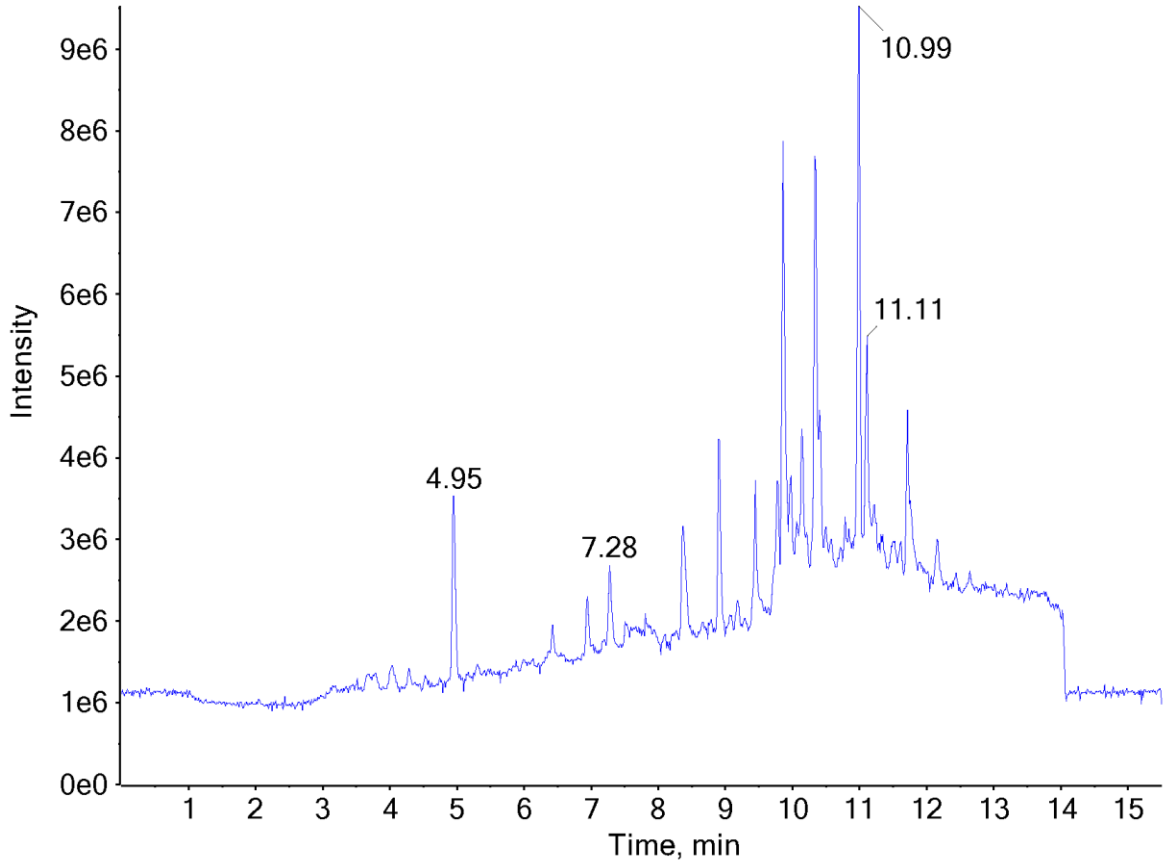
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *5Br-AKB48*



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

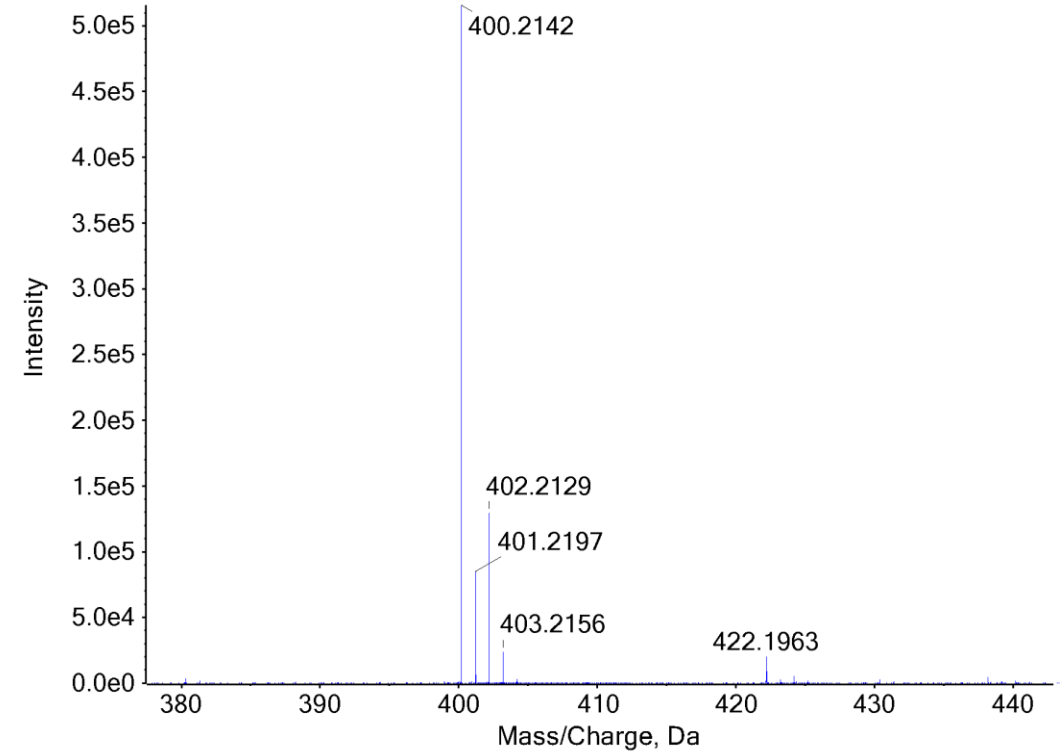
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	*5Cl-AKB48:* 10.99 min
	5Br-AKB48: 11.11 min
Standard Comparison:	Reference material for 5Cl-AKB48 (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 5Cl-AKB48, based on retention time (10.997 min) and mass spectral data. (https://www.caymanchem.com/product/18166)

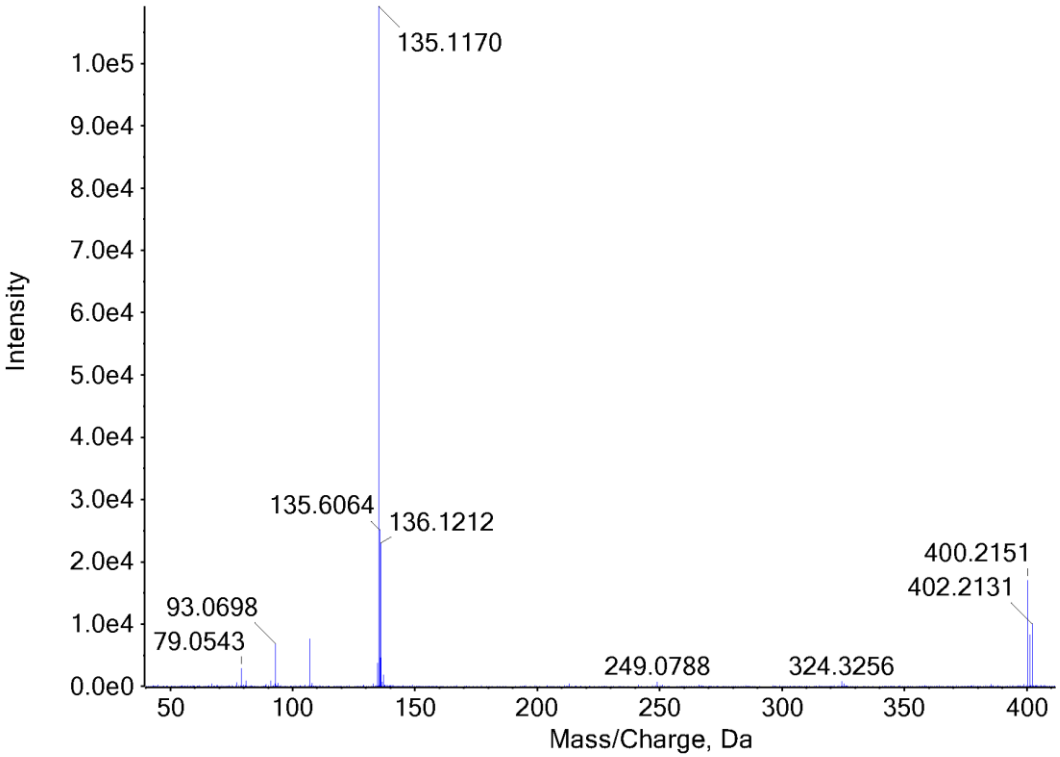
Chromatogram: *5Cl-AKB48 and 5Br-AKB48*



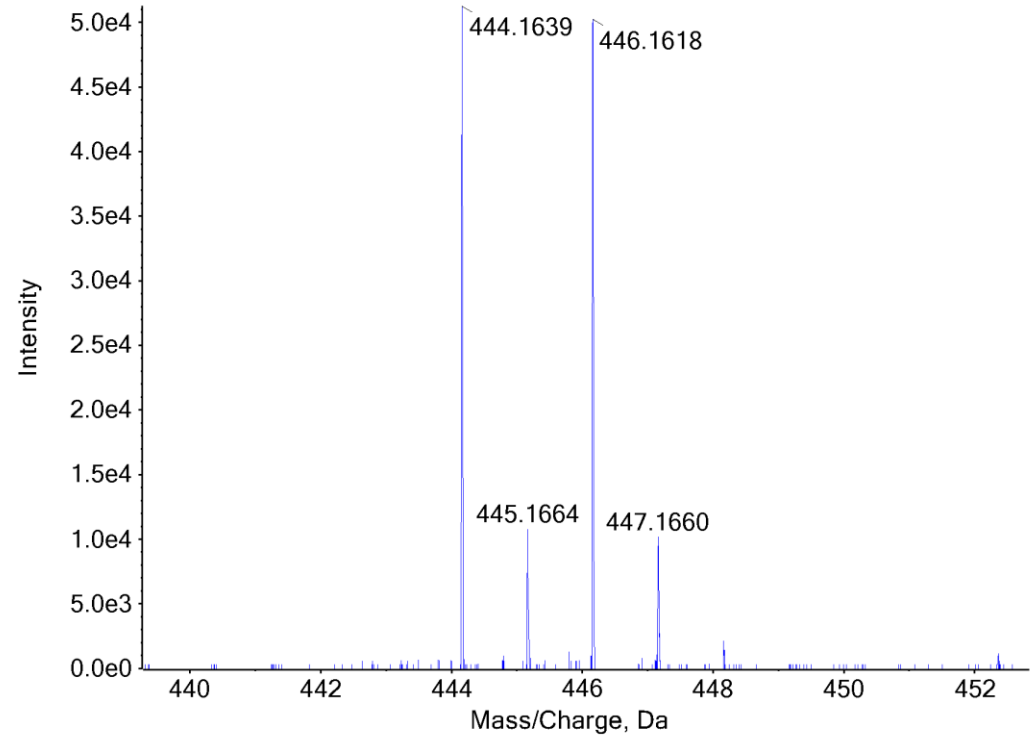
Peaks present in chromatogram: internal standard 1 (4.95 min), internal standard 2 (7.28 min), 5Cl-AKB48 (10.99 min), and 5Br-AKB48 (11.11 min)

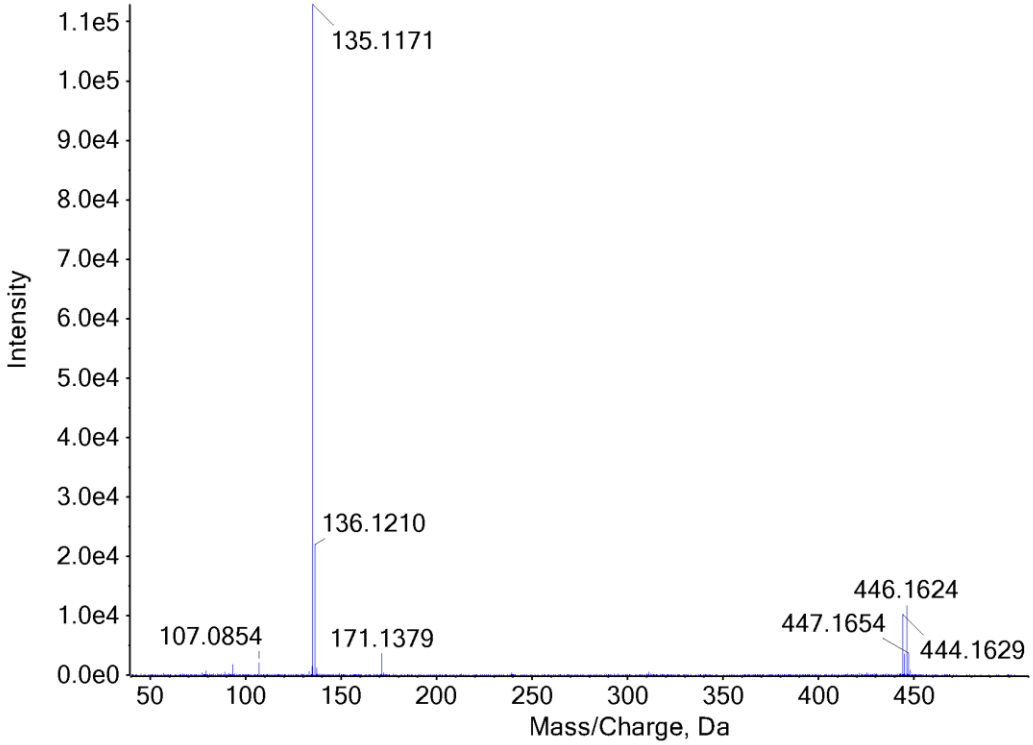
TOF MS (Top) and MS/MS (Bottom) Spectra: *5Cl-AKB48*





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





6. REVISION HISTORY

Date	Revision
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.