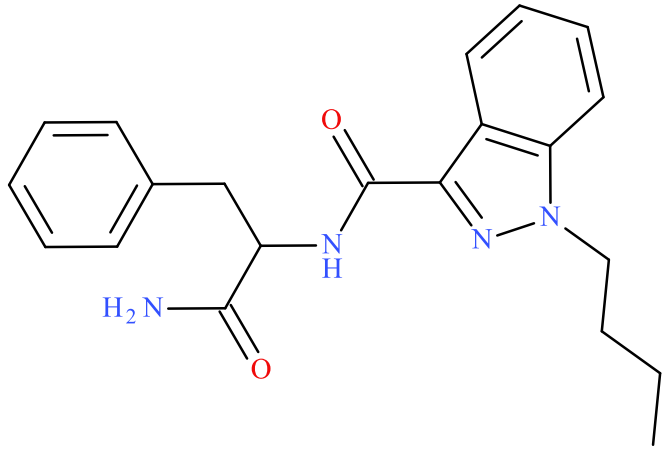
The Center for Forensic Science Research and Education
At the Fredric Rieders Family Foundation
2300 Stratford Ave
Willow Grove, PA 19090

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

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{21}H_{24}N_4O_2$	364.44	364	365.1972

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)

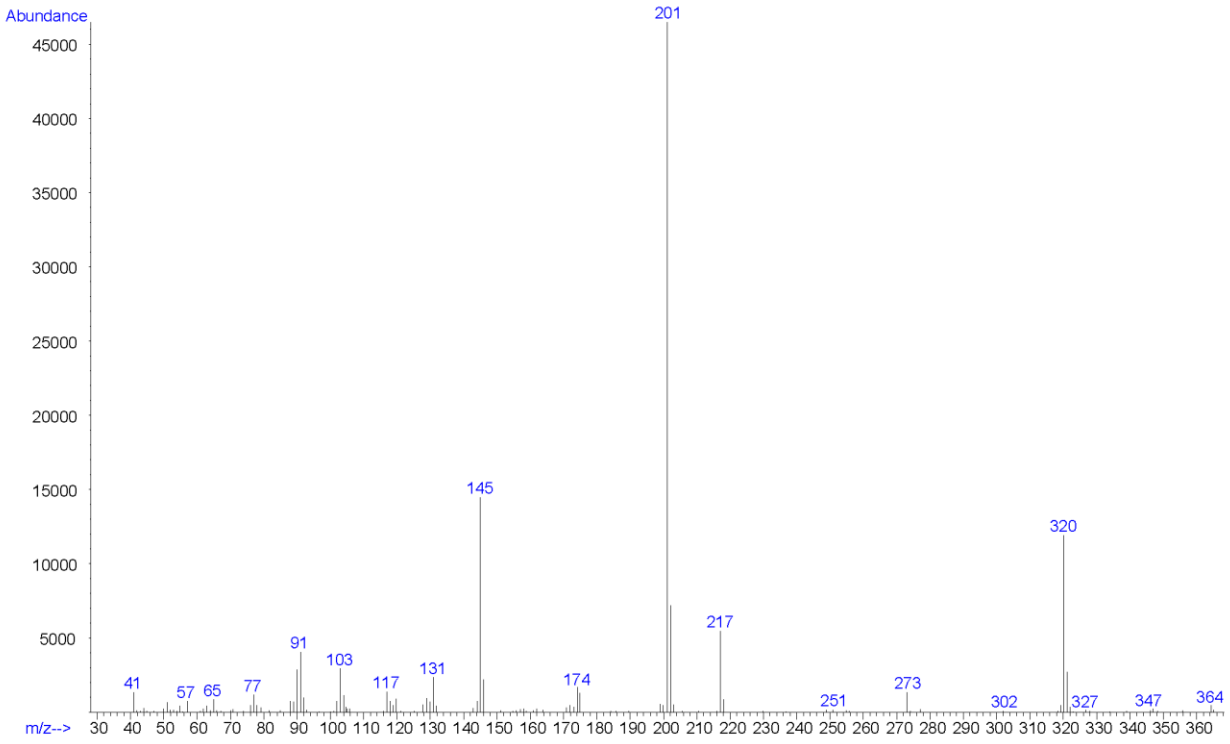
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

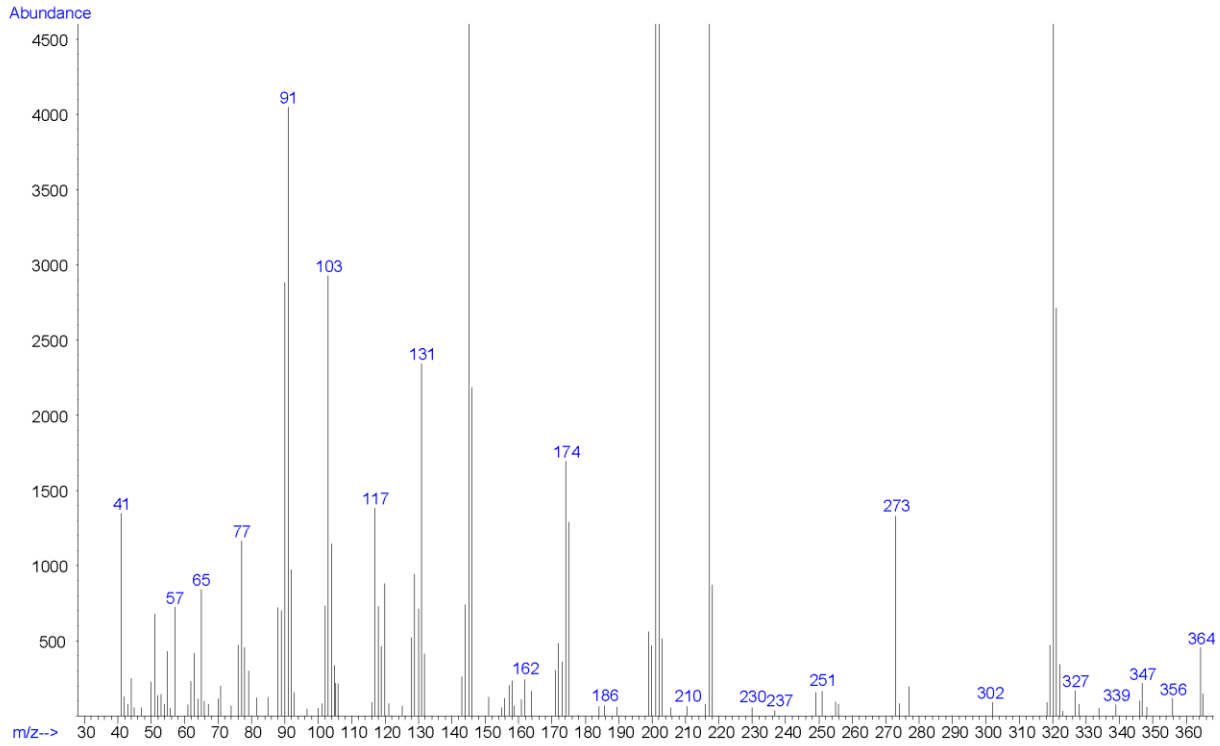
Instrument: Agilent 5975 Series GC/MSD System

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)



EI (70 eV) Mass Spectrum 10x: APP-BINACA (Standard)

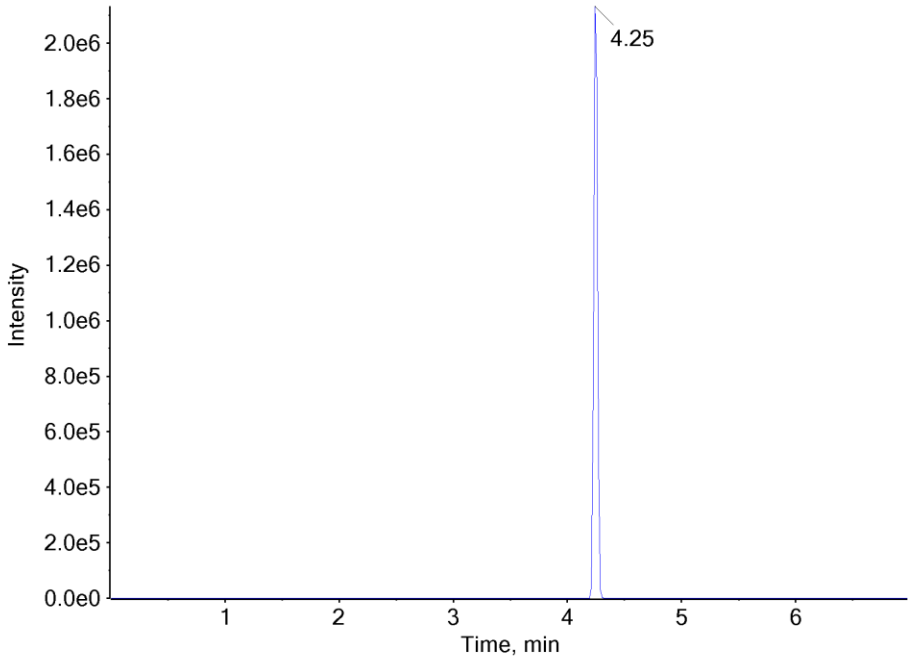


6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

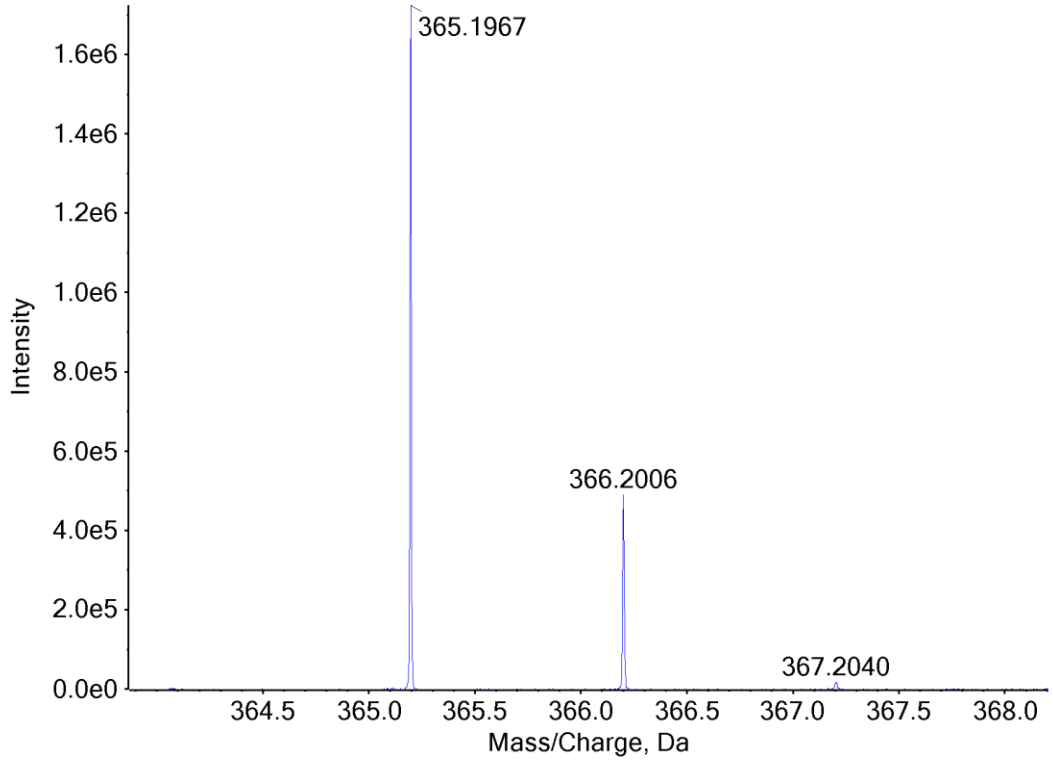
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	No additional preparation - direct analysis of sample extract
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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

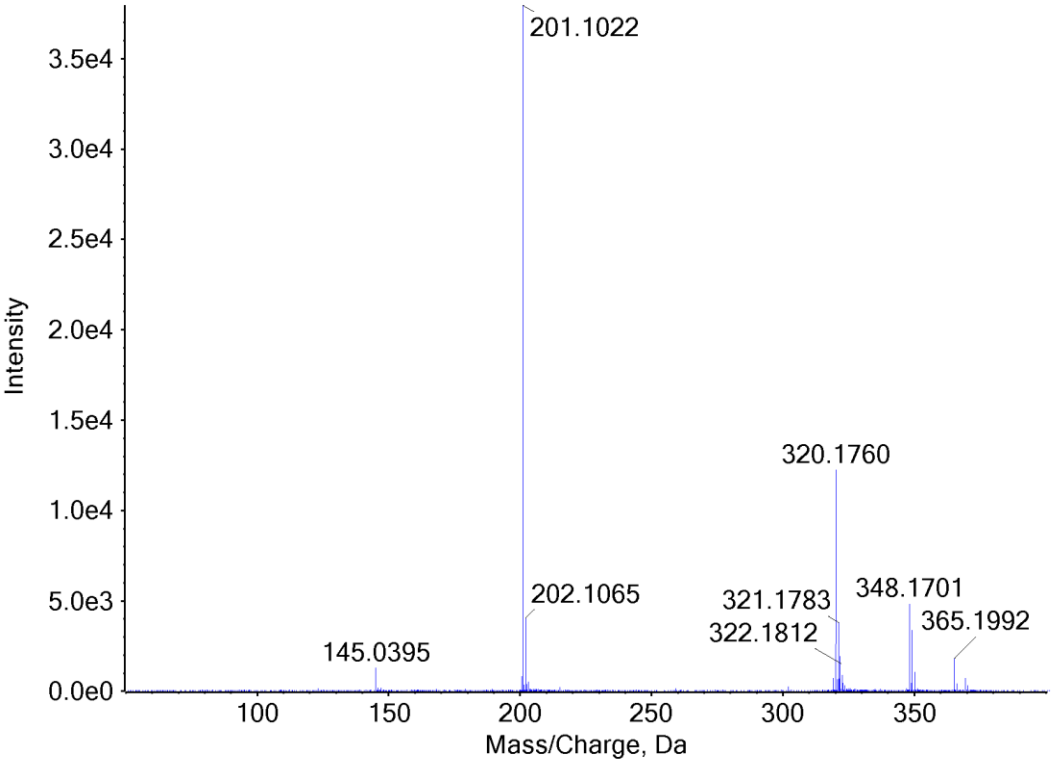
Temperatures:	Autosampler: 15 °C
	Column Oven: 30 °C
	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 20 µL
QTOF Parameters:	TOF MS Scan Range: 100-550 Da
	Precursor Isolation: SWATH® acquisition (10-25 Da)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-550 Da
Retention 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

This project was supported by Award Number 2017-R2-CX-0021, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect those of the Department of Justice.