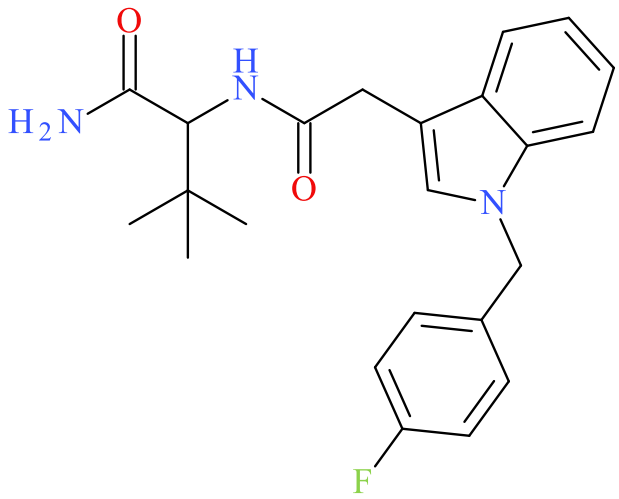
ADB-FUBIATA



Sample Type: **Drug Material**

Latest Revision: **November 17, 2021**

Date Received: **October 8, 2021**

Date of Report: **November 17, 2021**

1. GENERAL INFORMATION

IUPAC Name:	2-[[2-[1-[(4-fluorophenyl)methyl]indol-3-yl]acetyl]amino]-3,3-dimethyl-butanamide
InChI String:	InChI=1S/C23H26FN3O2/c1-23(2,3)21(22(25)29)26-20(28)12-16-14-27(19-7-5-4-6-18(16)19)13-15-8-10-17(24)11-9-15/h4-11,14,21H,12-13H2,1-3H3,(H2,25,29)(H,26,28)
CFR:	Not Scheduled (11/2021)
CAS#	Not Available
Synonyms:	AD-18, FUB-ACADB
Source:	Indianapolis-Marion County Forensic Services Agency
Appearance:	Plant-Like Material

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF-MS) in comparison to analysis of acquired reference material.*

***Prepared By:** Alex J. Krotulski, PhD; Ryan Farrell; Kaitlin Schilde; Robert M. Schelkun, MS; Donna M. Iula, PhD; Melissa F. Fogarty, MSFS, D-ABFT-FT; and Barry K. Logan, PhD, F-ABFT*

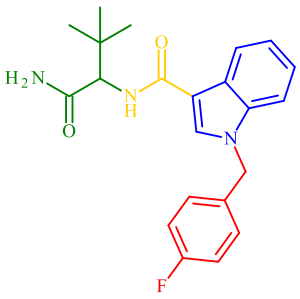
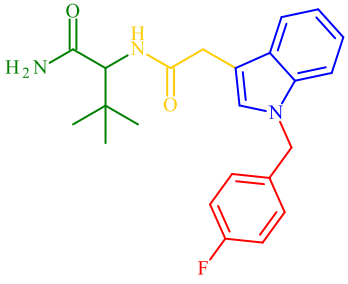
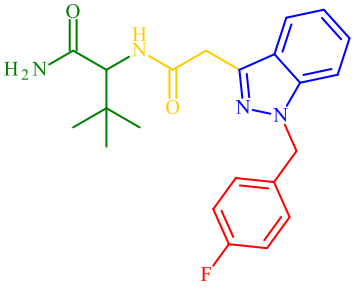
2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M^+]	Exact Mass [$M+H]^+$
Base	$C_{23}H_{26}FN_3O_2$	395.5	395	396.2082

3. BRIEF DESCRIPTION

ADB-FUBIATA 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. Little to no information regarding ADB-FUBIATA is currently available, specifically regarding activity and potency. Scientists at Cayman Chemical and the CFSRE developed a new naming convention for this drug and related analogues, using "ATA" to represent the acetamide linker compared to prior "CA" used for a carboxamide linker (see below). Several new synthetic cannabinoids have recently emerged among the recreation drug supply internationally, seemingly as replacements after a synthetic cannabinoid class-wide ban implemented by China in July 2021 which included most traditional indole and indazole carboxamide structural scaffolds.[1] Other new synthetic cannabinoids to emerge recently include "OXIZID" analogues, most of which are unstudied with undetermined pharmacological and human effects, and like ADB-FUBIATA are not included under the class-wide ban announced by China.[1,2] Currently, ADB-FUBIATA is not a scheduled substance in the United States.

ADB-FUBICA	**ADB-FUBIATA**	**ADB-FUBINAATA**
		
N-(1-**A**mino-3,3-**D**imethyl-1-oxo**B**utan-2-yl)-1-(4-**F**l**U**oro**B**enzyl)-1H-**I**ndole-3-**C**arbox**A**mide*	*N*-(1-**A**mino-3,3-**D**imethyl-1-oxo**B**utan-2-yl)-1-(4-**F**l**U**oro**B**enzyl)-1H-**I**ndole-3-**A**ce**TA**mide*	*N*-(1-**A**mino-3,3-**D**imethyl-1-oxo**B**utan-2-yl)-1-(4-**F**l**U**oro**B**enzyl)-1H- **IN**d**A**zole-3-**A**ce**TA**mide*

**This represents the chemical name of the drug, not the IUPAC name.*

4. ADDITIONAL RESOURCES

1. Cui-Mei Liu, Zhen-Dong Hua, Wei Jia, Tao Li. (2021) Identification of AD-18, 5F-MDA-19, and pentyl MDA-19 in seized materials after the class-wide ban of synthetic cannabinoids in China. *Drug Test Anal*. https://doi.org/10.1002/dta.31858

2. Robert M. Schelkun, Alex J. Krotulski, Donna M. Iula, and Barry K. Logan. (2021) New Systematic Naming for Synthetic Cannabinoid "MDA-19" and Its Related Analogues: BZO-HEXOXIZID, 5F-BZO-POXIZID, and BZO-POXIZID. *Center for Forensic Science Research and Education*. https://www.npsdiscovery.org/new-systematic-naming-for-synthetic-cannabinoid-mda-19-and-its-related-analogues-bzo-hexoxizid-5f-bzo-poxizid-and-bzo-poxizid/

https://www.caymanchem.com/product/35059/adb-fubiata

5. QUALITATIVE DATA

5.1 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:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency)
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)
Carrier Gas:	Helium (Flow: 1.46 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL

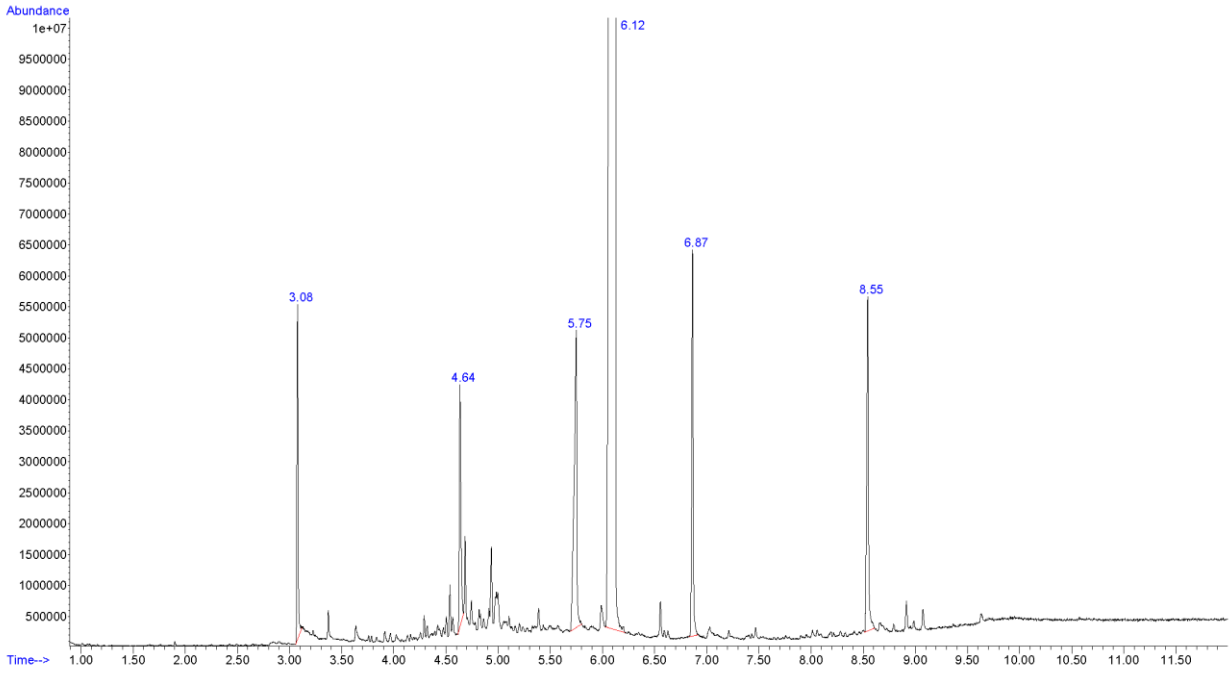
MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 8.55 min

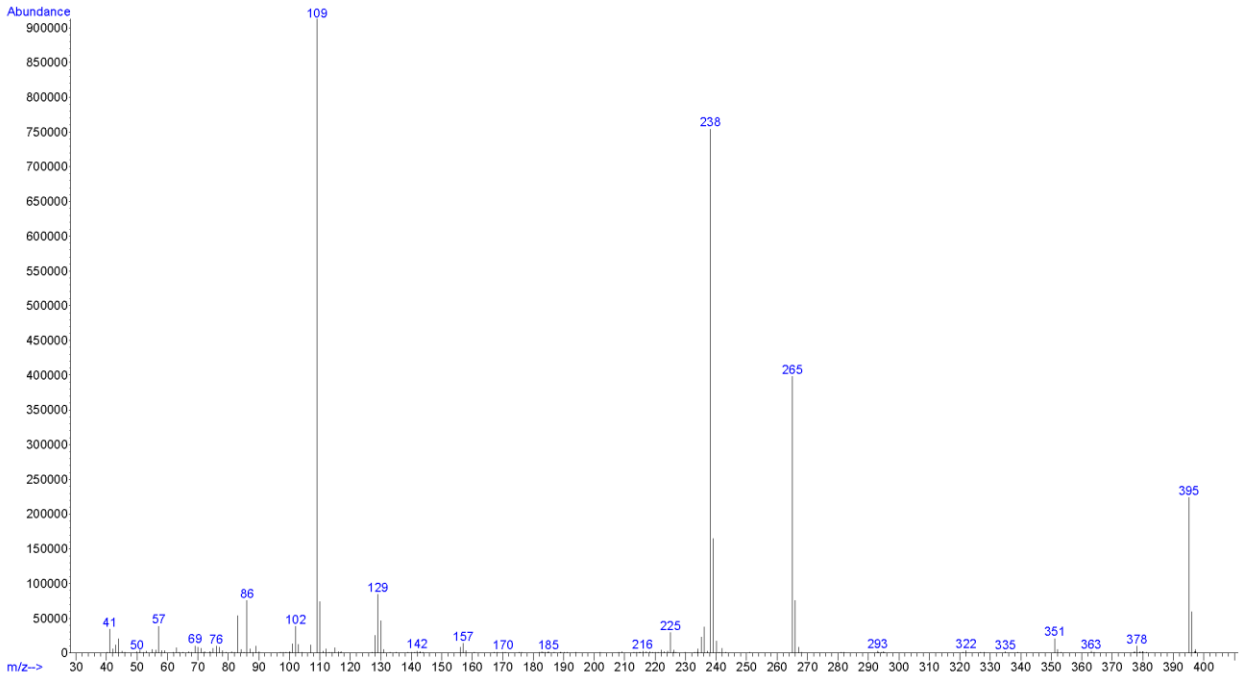
Standard Comparison: Reference material for ADB-FUBIATA (Batch: 0628021-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-FUBIATA based on retention time (8.54 min) and mass spectral data. (https://www.caymanchem.com/product/35059/adb-fubiata)

Chromatogram: ADB-FUBIATA



Additional peaks in chromatogram: internal standard (3.08 min), not a controlled substance (4.64 min), internal standard (5.75 min), not a controlled substance (6.12 min), and not a controlled substance (6.87 min)

EI (70 eV) Mass Spectrum: ADB-FUBIATA

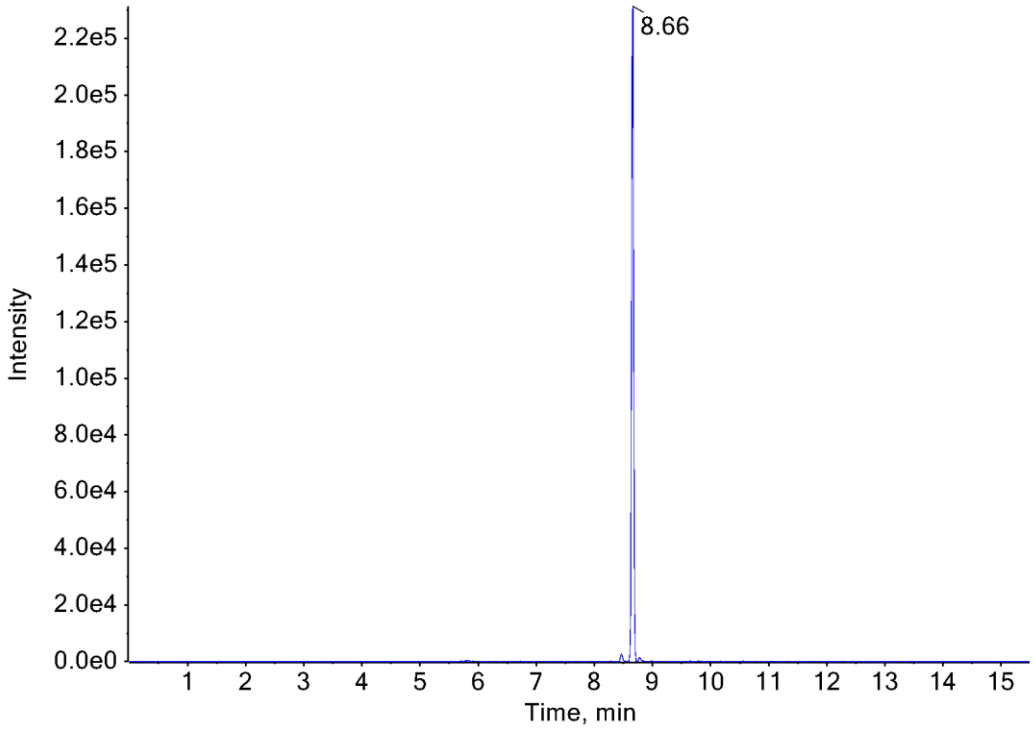


5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

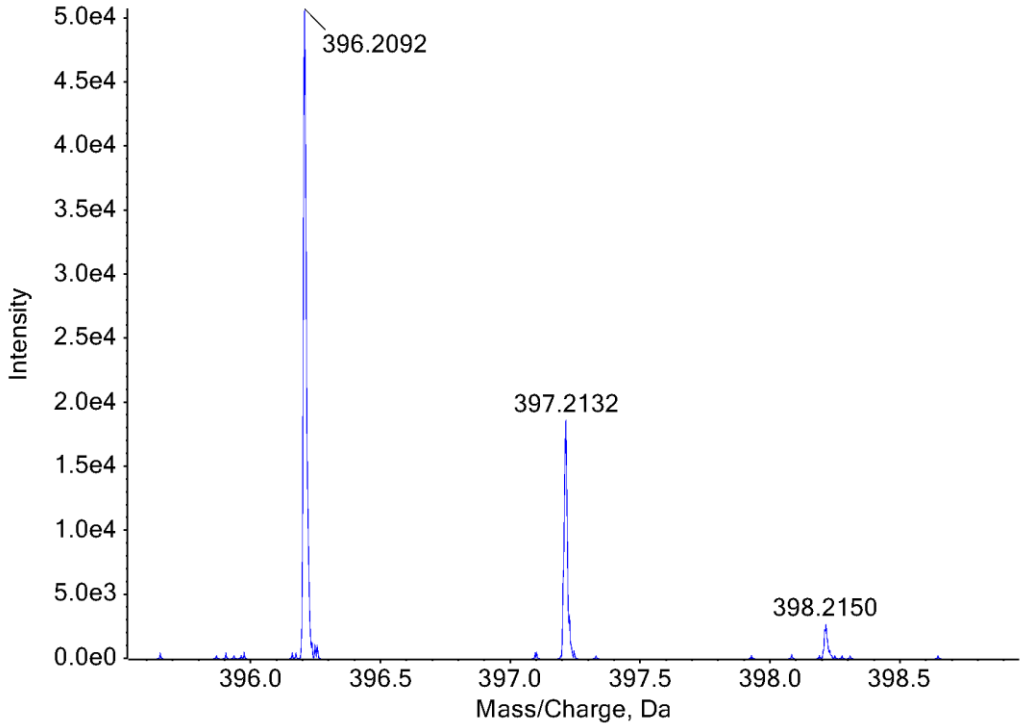
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency) followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)
Instrument:	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:	8.66 min
Standard Comparison:	Reference material for ADB-FUBIATA (Batch: 0628021-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-FUBIATA based on retention time (8.66 min) and mass spectral data. (https://www.caymanchem.com/product/35059/adb-fubiata)

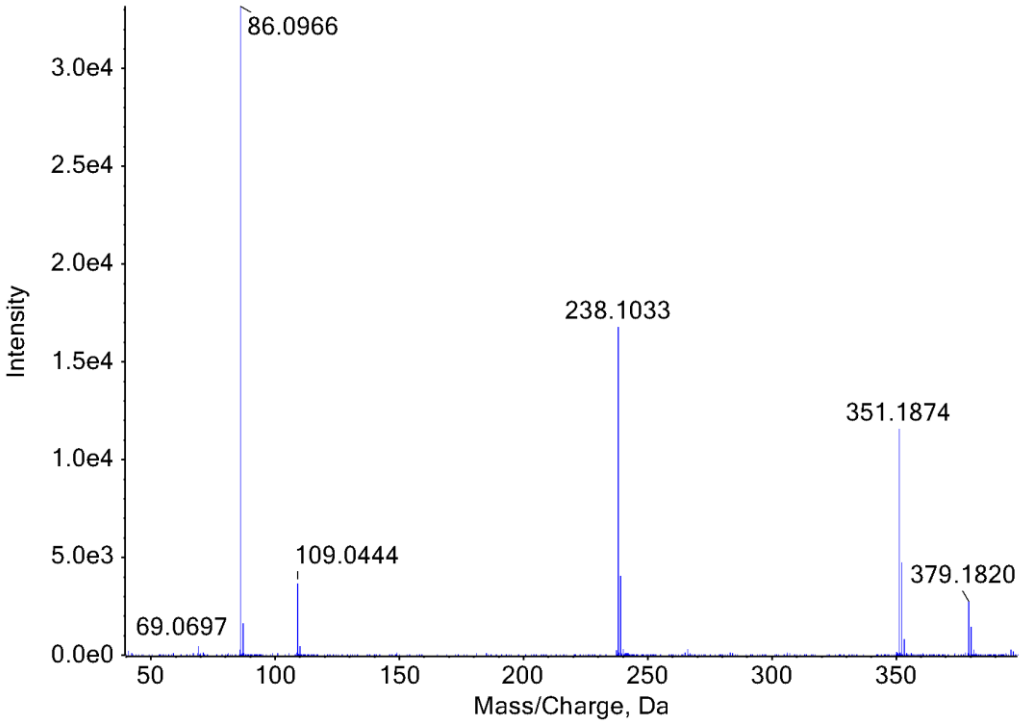
Extracted Ion Chromatogram: ADB-FUBIATA



TOF MS Spectra: ADB-FUBIATA



TOF MS/MS Spectra: ADB-FUBIATA



6. FUNDING

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