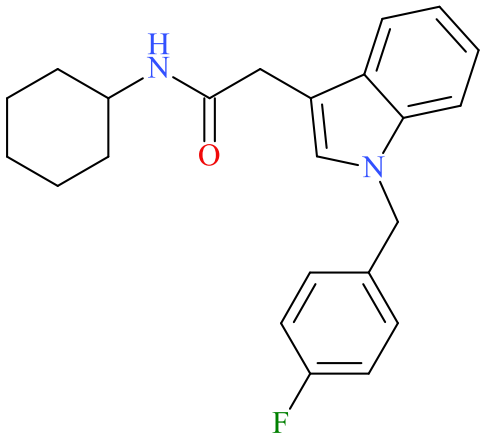
CH-FUBIATA

Sample Type: **Drug Material**



Latest Revision: **June 21, 2022**

Date Received: **May 10, 2022**

Date of Report: **June 21, 2022**

1. GENERAL INFORMATION

IUPAC Name:	N-cyclohexyl-2-[1-[(4-fluorophenyl)methyl]indol-3-yl]acetamide
InChI String:	InChI=1S/C23H25FN2O/c24-19-12-10-17(11-13-19)15-26-16-18(21-8-4-5-9-22(21)26)14-23(27)25-20-6-2-1-3-7-20/h4-5,8-13,16,20H,1-3,6-7,14-15H2,(H,25,27)
CFR:	Not Scheduled (06/2022)
CAS#	922038-77-5
Synonyms:	CH-FUBIACA
Source:	Philadelphia Department of Public Health
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; Jennifer Shinefeld, MS; Melissa F. Fogarty, MSFS, D-ABFT-FT; Joshua DeBord, PhD; and Barry K. Logan, PhD, F-ABFT*

2. CHEMICAL AND PHYSICAL DATA

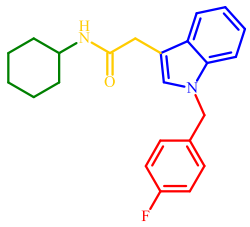
2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{23}H_{25}FN_2O$	364.5	364	365.2024

3. BRIEF DESCRIPTION

CH-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 is currently known about the activity, potency, and/or toxicity of CH-FUBIATA. New synthetic cannabinoids continue to emerge 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 structural scaffolds.[1] Many of these new synthetic cannabinoid analogues are unstudied with pharmacological and human effects undetermined. Structurally similar synthetic cannabinoids include CH-PIATA (reported April 2022) and ADB-FUBIATA (reported November 2021); CH-FUBIATA was identified alongside ADB-FUBIATA in the sample reported. Currently, CH-FUBIATA and related analogues are not scheduled substances in the United States.

CH-FUBIATA



N-cyclohexyl-2-(1-(4-fluorobenzyl)indol-3-yl)acetamide

Preferred Name: **CH-FUBIATA**

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.3185

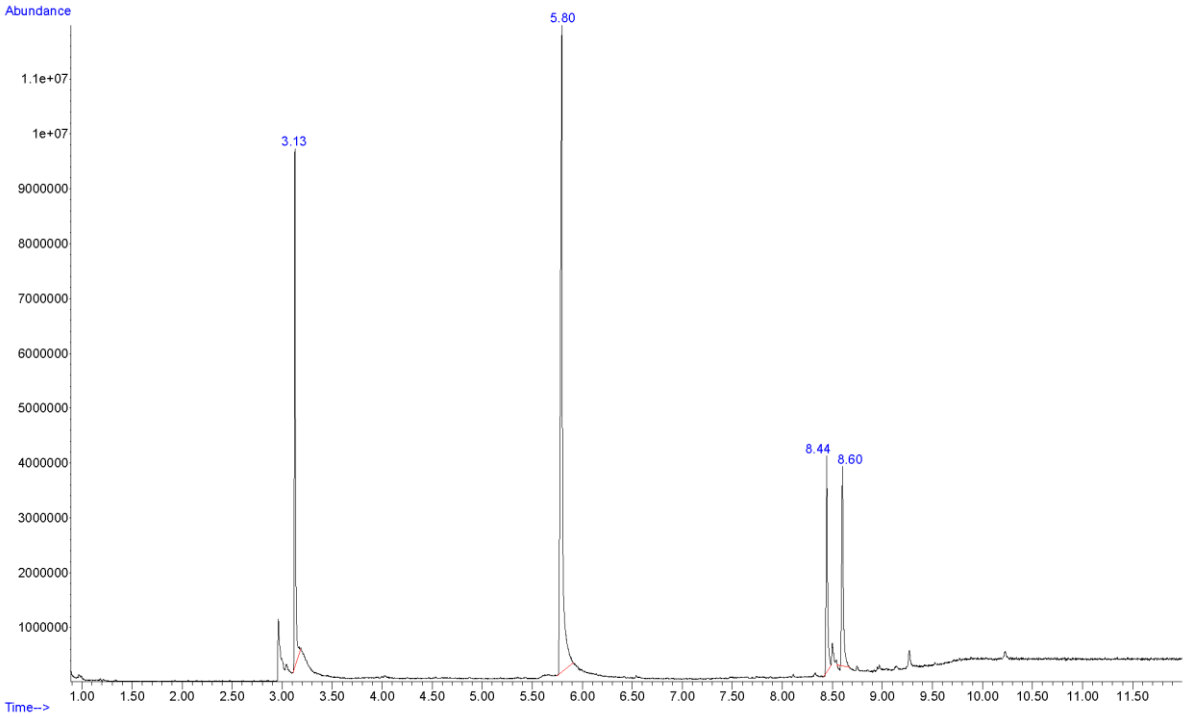
https://www.caymanchem.com/product/37054/ch-fubiata

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

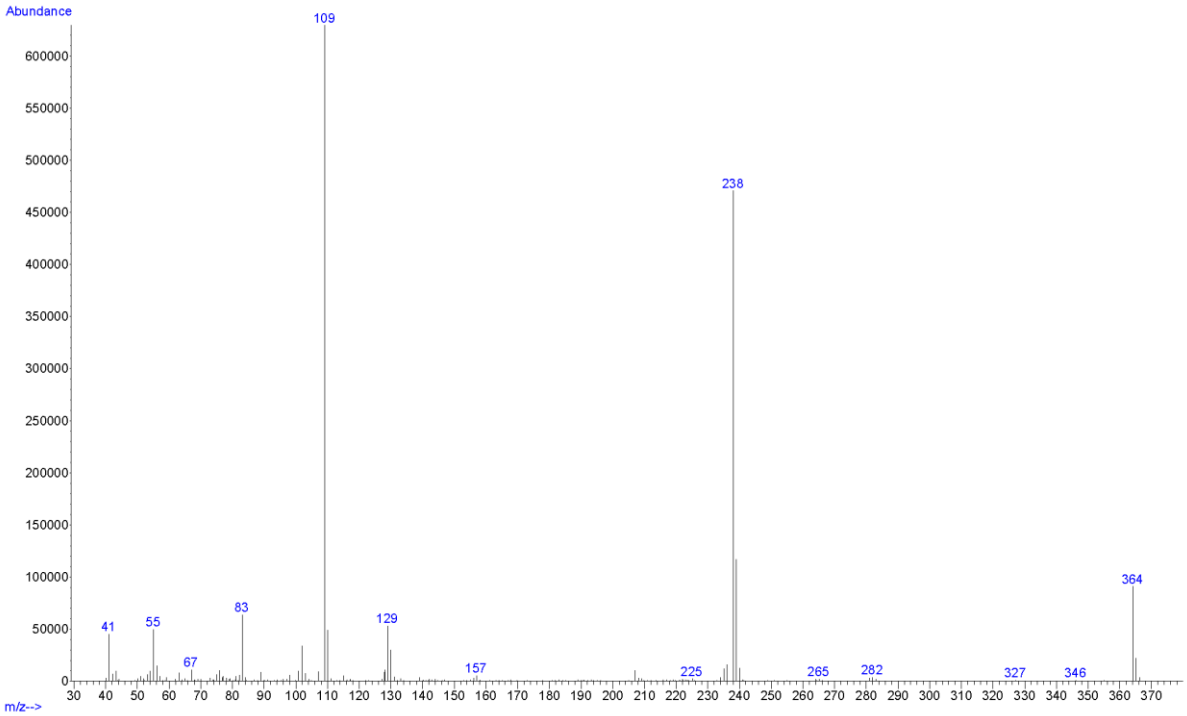
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)
Carrier Gas:	Helium (Flow: 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:	8.44 min
Standard Comparison:	Reference material for CH-FUBIATA (Batch: 0649511-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as CH-FUBIATA based on retention time (8.43 min) and mass spectral data. (https://www.caymanchem.com/product/37054/ch-fubiata)

Chromatogram: CH-FUBIATA



Additional peaks in chromatogram: internal standards (3.13 and 5.80 mins) & ADB-FUBIATA (8.60 min)

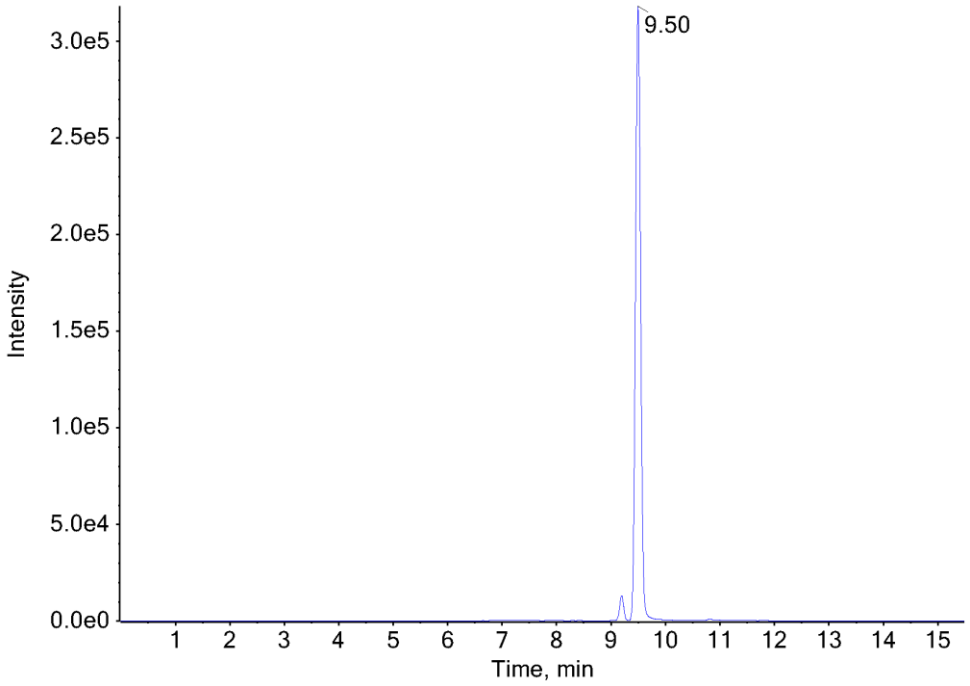
EI (70 eV) Mass Spectrum: CH-FUBIATA



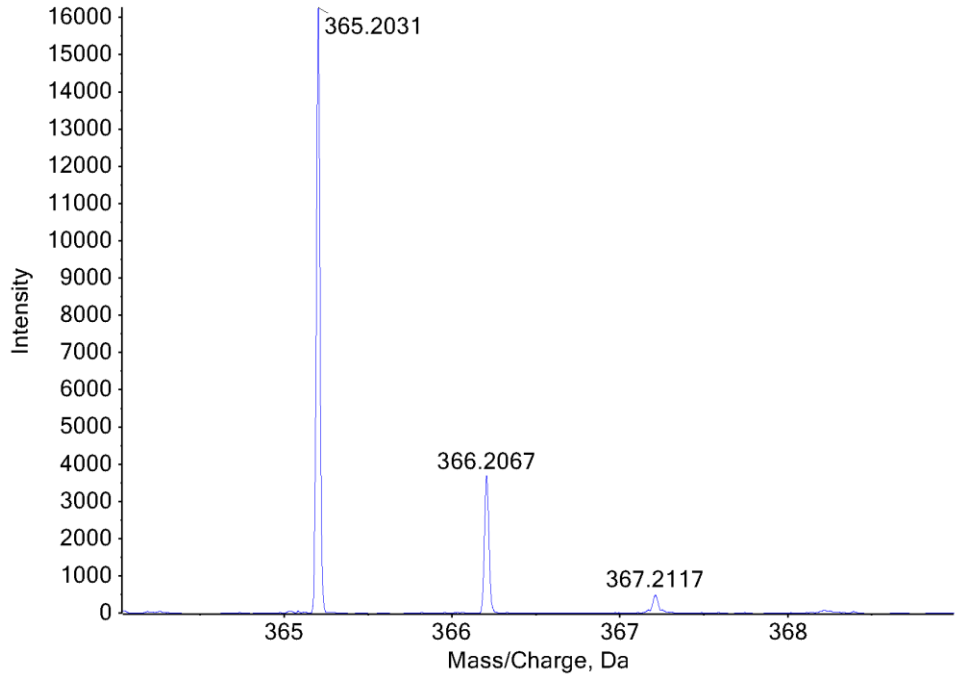
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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 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:	9.50 min
Standard Comparison:	Reference material for CH-FUBIATA (Batch: 0649511-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as CH-FUBIATA based on retention time (9.51 min) and mass spectral data. (https://www.caymanchem.com/product/37054/ch-fubiata)

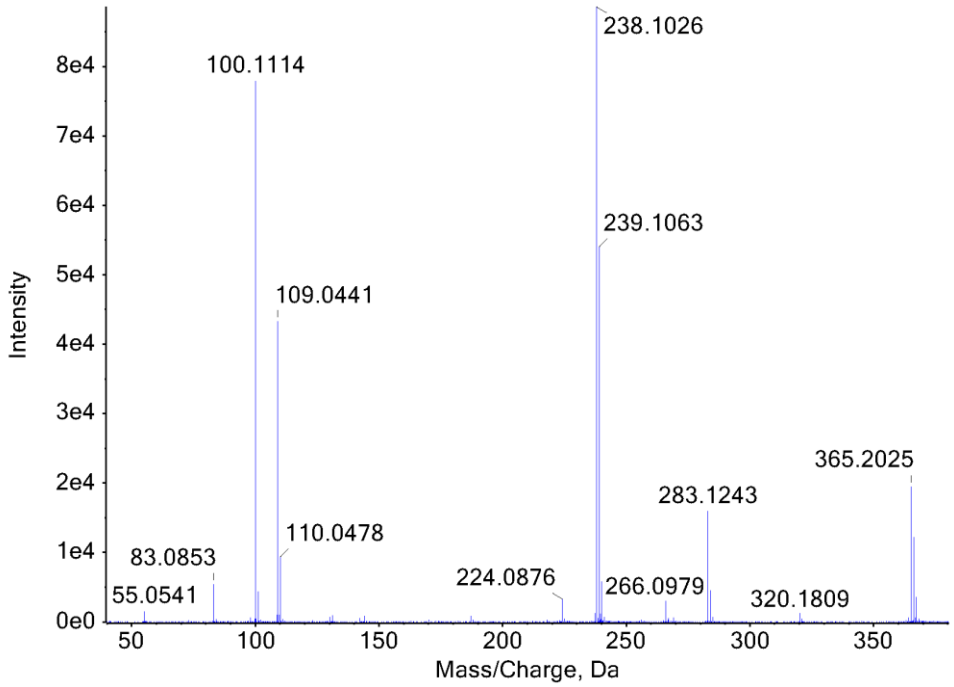
Extracted Ion Chromatogram: CH-FUBIATA



TOF MS Spectra: CH-FUBIATA



TOF MS/MS Spectra: CH-FUBIATA



6. FUNDING

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