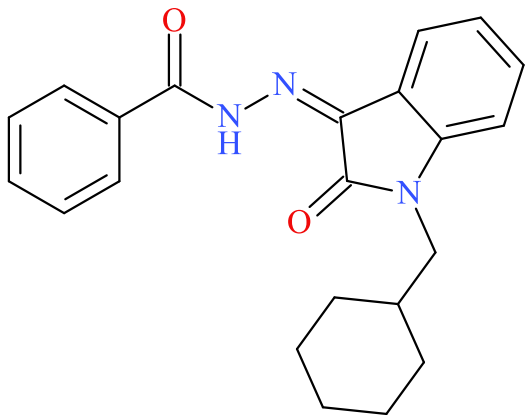
BZO-CHMOXIZID



Sample Type: **Drug Material**

Latest Revision: **November 18, 2021**

Date Received: **November 4, 2021**

Date of Report: **November 18, 2021**

1. GENERAL INFORMATION

IUPAC Name:	N-[(Z)-[1-(cyclohexylmethyl)-2-oxo-indolin-3-ylidene]amino]benzamide
InChI String:	InChI=1S/C22H23N3O2/c26-21(17-11-5-2-6-12-17)24-23-20-18-13-7-8-14-19(18)25(22(20)27)15-16-9-3-1-4-10-16/h2,5-8,11-14,16H,1,3-4,9-10,15H2,(H,24,26)/b23-20-
CFR:	Not Scheduled (11/2021)
CAS#	1048973-67-6
Synonyms:	Cyclohexylmethyl MDA-19, CHM-MDA-19
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; Amanda Mohaupt; Melissa F. Fogarty, MSFS, D-ABFT-FT; and Barry K. Logan, PhD, F-ABFT*

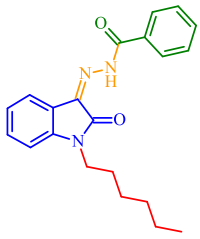
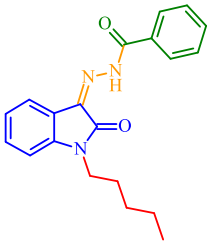
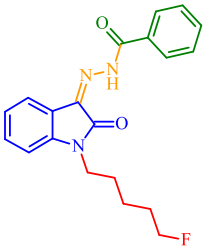
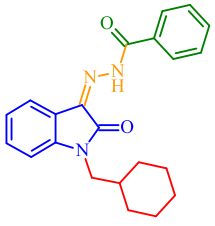
2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{22}H_{23}N_3O_2$	361.4	361	362.1863

3. BRIEF DESCRIPTION

BZO-CHMOXIZID 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. Closely related analogue BZO-HEXOXIZID (MDA 19) was synthesized and studied in the late 2000's by scientists at the University of Texas M. D. Anderson Cancer Center.[1,2,3] BZO-HEXOXIZID is reported to be a potent and selective cannabinoid receptor 2 (CB_2) agonist. Several closely related analogues make up this new generation of synthetic cannabinoids, some of which have been studied and reported.[3,4] Scientists at Cayman Chemical and the CFSRE developed a new naming convention for this subclass, calling these new drugs the "OXIZIDs".[5] OXIZID represents the core/linker region of this new synthetic cannabinoid structure. The OXIZID subclass 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 structural scaffolds.[6] To date, multiple OXIZID analogues have been identified worldwide, most of which are unstudied with pharmacological and human effects undetermined. Currently, no analogues of the OXIZID subclass are scheduled substances in the United States.

BZO-HEXOXIZID	BZO-POXIZID	5F-BZO-POXIZID	BZO-CHMOXIZID
			
(*Z*)-*N'*-(1-**HEX**yl-2-**OX**o**I**ndolin-3-ylidene)**B**en**ZO**hydra**ZID**e	(*Z*)-*N'*-(1-**P**entyl-2-**OX**o**I**ndolin-3-ylidene)**B**en**ZO**hydra**ZID**e	(*Z*)-*N'*-(1-(**5-F**luoro**P**entyl-2-**OX**o**I**ndolin-3-ylidene) **B**en**ZO**hydra**ZID**e	(*Z*)-*N'*-(1-(**C**yclo**H**exyl**M**ethyl)-2-**OX**o**I**ndolin-3-ylidene) **B**en**ZO**hydra**ZID**e
Name: **BZO-HEXOXIZID**	*Name:* **BZO-POXIZID**	*Name:* **5F-BZO-POXIZID**	*Name:* **BZO-CHMOXIZID**
Synonyms: **MDA-19, MDA19, MDA 19**	*Synonyms:* **5C-MDA-19, MDA-19 pentyl analogue**	*Synonyms:* **5F-MDA-19, MDA-19 5-fluoropentyl analogue**	*Synonyms:* **CHM-MDA-19, Cyclohexylmethyl MDA-19**

4. ADDITIONAL RESOURCES

1. Attala MN, Daiz P. (2009) Patent WO2009012227A1. Hydrazone Modulators of Cannabinoid Receptors. https://patents.google.com/patent/US20180200225A1/en

2. Xu JJ, Diaz P, Astruc-Diaz F, Craig S, Munoz E, Naguib M. (2010) Pharmacological characterization of a novel cannabinoid ligand, MDA19, for treatment of neuropathic pain. *Anesthesia and Analgesia*. 111, 99–109. https://pubmed.ncbi.nlm.nih.gov/20522703/

3. Diaz P, Xu J, Astruc-Diaz F, Pan H, Brown DL, Naguib M. (2008) Design and Synthesis of a Novel Series of N-Alkyl Isatin Acylhydrazone Derivatives that Act as Selective Cannabinoid Receptor 2 Agonist for the Treatment of Neuropathic Pain. *J. Med. Chem.* 2008, 51, 4932–4947. https://pubs.acs.org/doi/10.1021/jm8002203

4. Diaz P, Phatak SS, Xu J, Astruc-Diaz F, Cavasotto CN, and Naguib M. (2009) 6-Methoxy-N-alkyl Isatin Acylhydrazone Derivatives as a Novel Series of Potent Selective Cannabinoid Receptor 2 Inverse Agonists: Design, Synthesis, and Binding Mode Prediction. *J. Med. Chem*. 52, 433–444. https://pubs.acs.org/doi/10.1021/jm801353p

5. 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/

6. 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

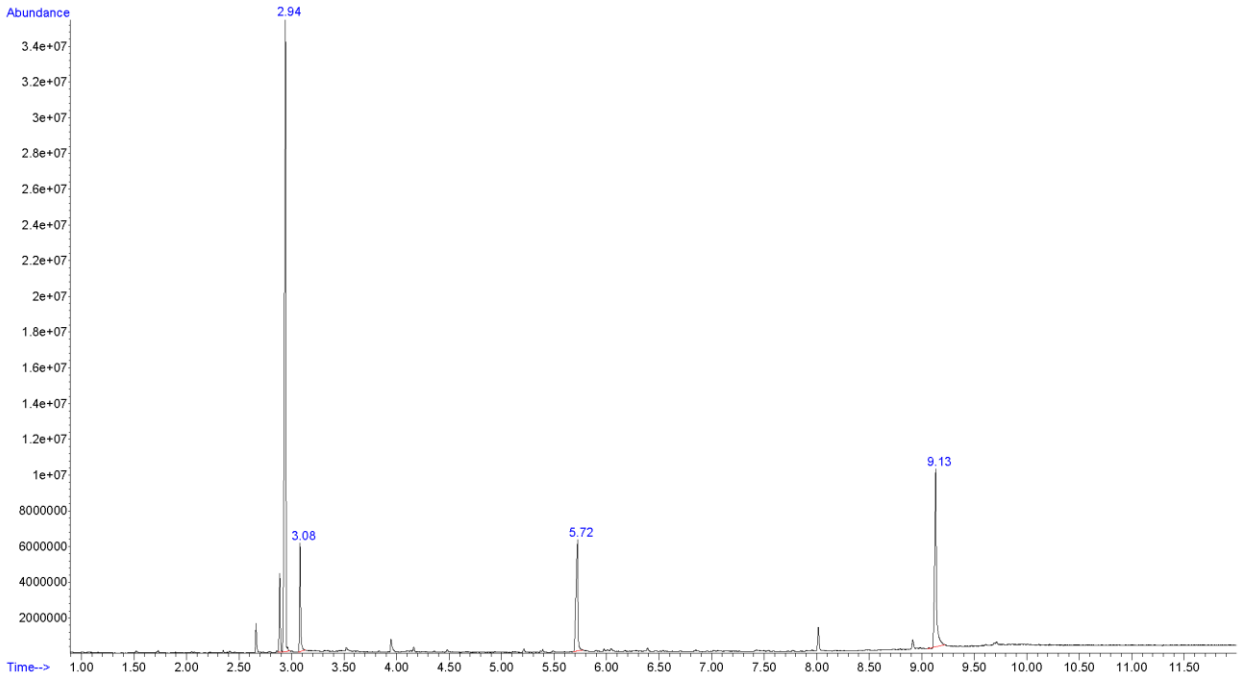
https://www.caymanchem.com/product/34956/bzo-chmoxizid

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

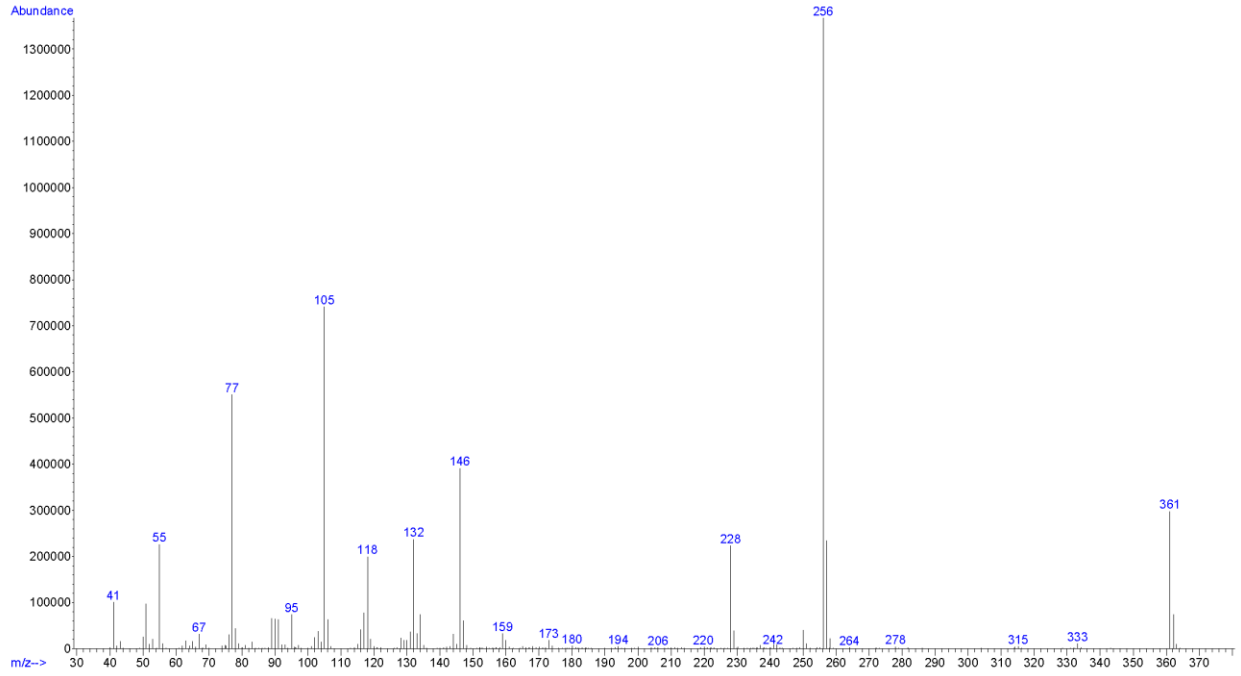
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency)
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (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:	9.13 min
Standard Comparison:	Reference material for BZO-CHMOXIZID (Batch: 0628347-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as BZO-CHMOXIZID based on retention time (9.12 min) and mass spectral data. (https://www.caymanchem.com/product/34956/bzo-chmoxizid)

Chromatogram: BZO-CHMOXIZID



Additional peaks in chromatogram: not a controlled substance (2.94 min) and internal standards (3.08 and 5.72 mins)

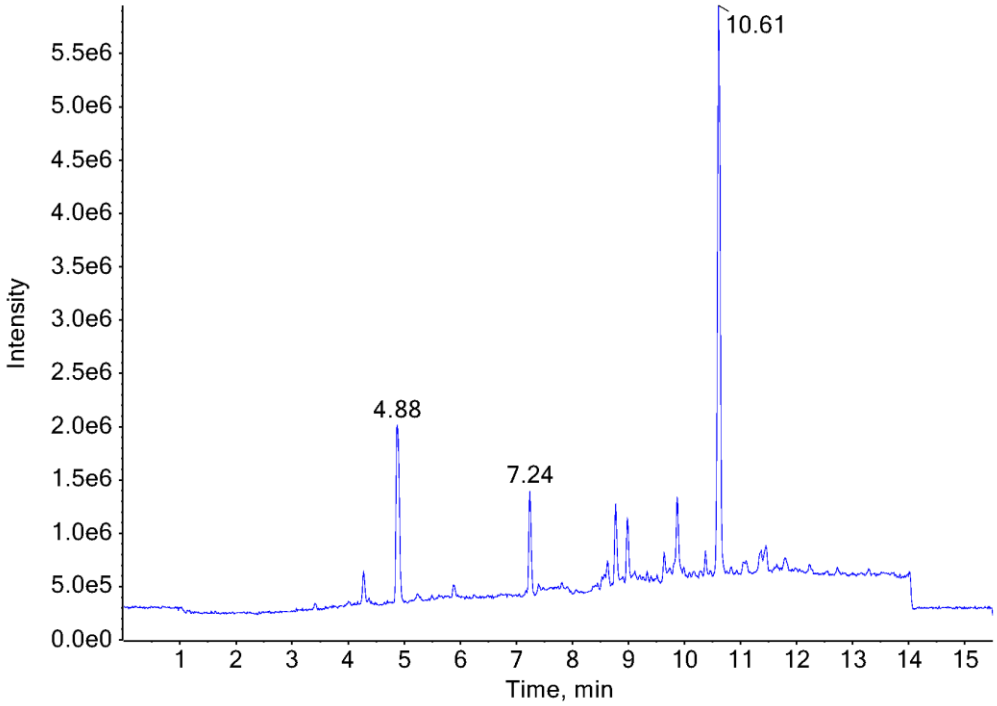
EI (70 eV) Mass Spectrum: BZO-CHMOXIZID



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

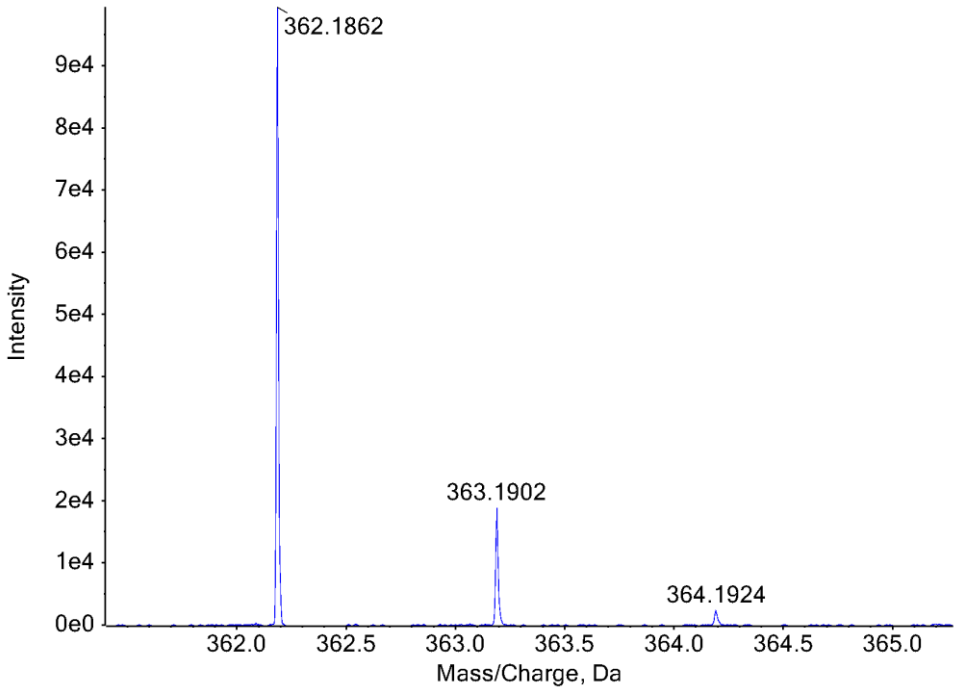
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency) followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)
Instrument:	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:	10.61 min
Standard Comparison:	Reference material for BZO-CHMOXIZID (Batch: 0628347-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as BZO-CHMOXIZID based on retention time (10.62 min) and mass spectral data. (https://www.caymanchem.com/product/34956/bzo-chmoxizid)

Chromatogram: BZO-CHMOXIZID

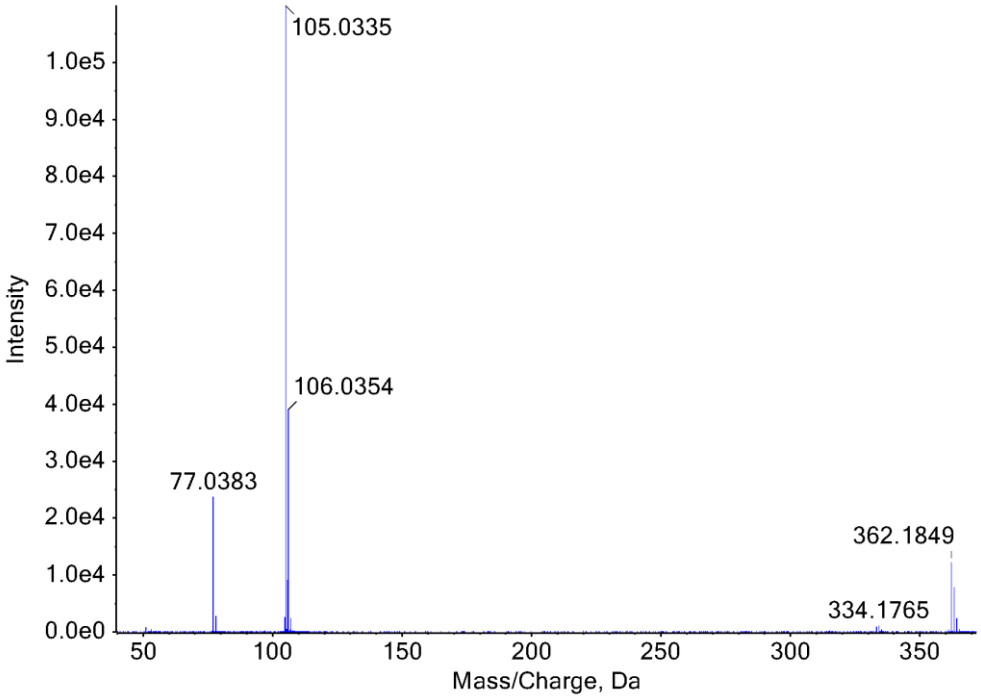


Additional peaks in chromatogram: internal standards (4.88 and 7.24 mins)

TOF MS Spectra: BZO-CHMOXIZID



TOF MS/MS Spectra: BZO-CHMOXIZID



6. FUNDING

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