



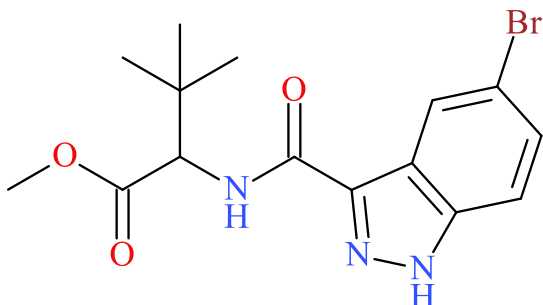
MDMB-5Br-INACA

Sample Type: **Drug Material**

Latest Revision: **May 17, 2022**

Date Received: **March 11, 2022**

Date of Report: **May 17, 2022**



1. GENERAL INFORMATION

IUPAC Name:	Methyl 2-[(5-bromo-1H-indazole-3-carbonyl)amino]-3,3-dimethylbutanoate
InChI String:	InChI=1S/C15H18BrN3O3/c1-15(2,3)12(14(21)22-4)17-13(20)11-9-7-8(16)5-6-10(9)18-19-11/h5-7,12H,1-4H3,(H,17,20)(H,18,19)
CFR:	Not Scheduled (05/2021)
CAS#	Not Available
Synonyms:	5Br-MDMB-INACA, MDMB-5-bromo-INACA
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.

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₁₅ H ₁₈ BrN ₃ O ₃	368.2	367	368.0604

3. BRIEF DESCRIPTION

MDMB-5Br-INACA 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. However, little to no information is currently known about the activity, potency, and/or toxicity of MDMB-5Br-INACA. 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. Currently, MDMB-5Br-INACA is not a scheduled substance in the United States.

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>

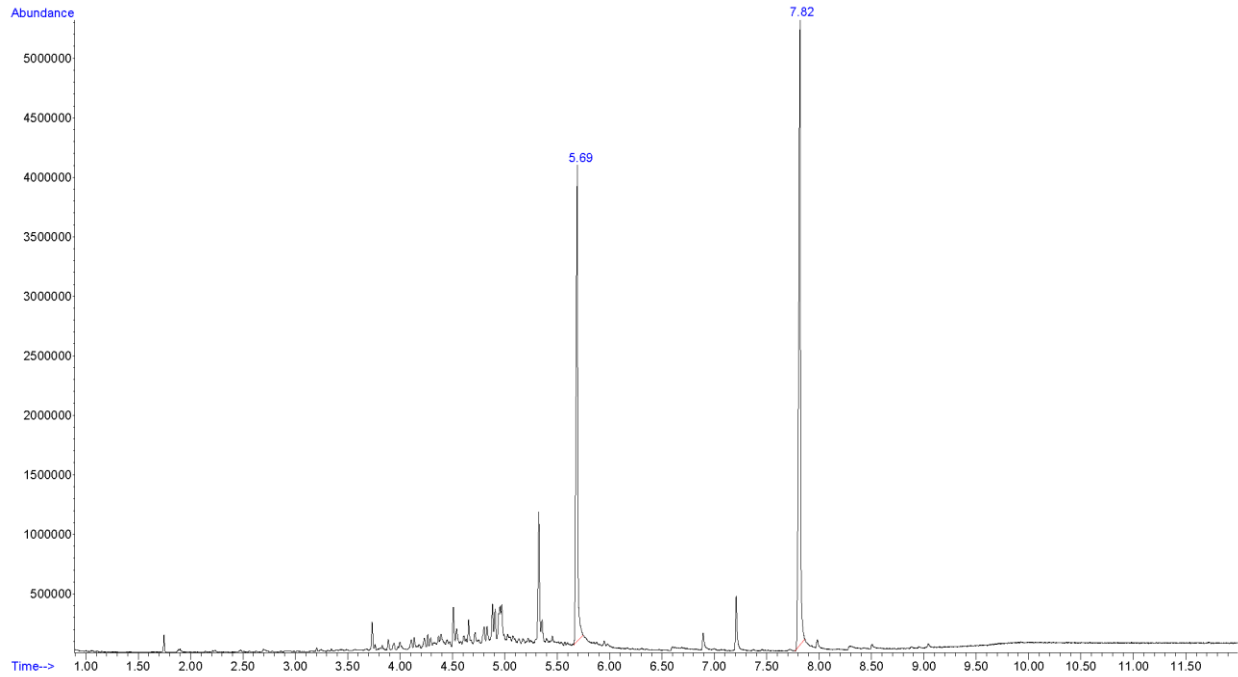
<https://www.caymanchem.com/product/36757/mdmb-5br-inaca>

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

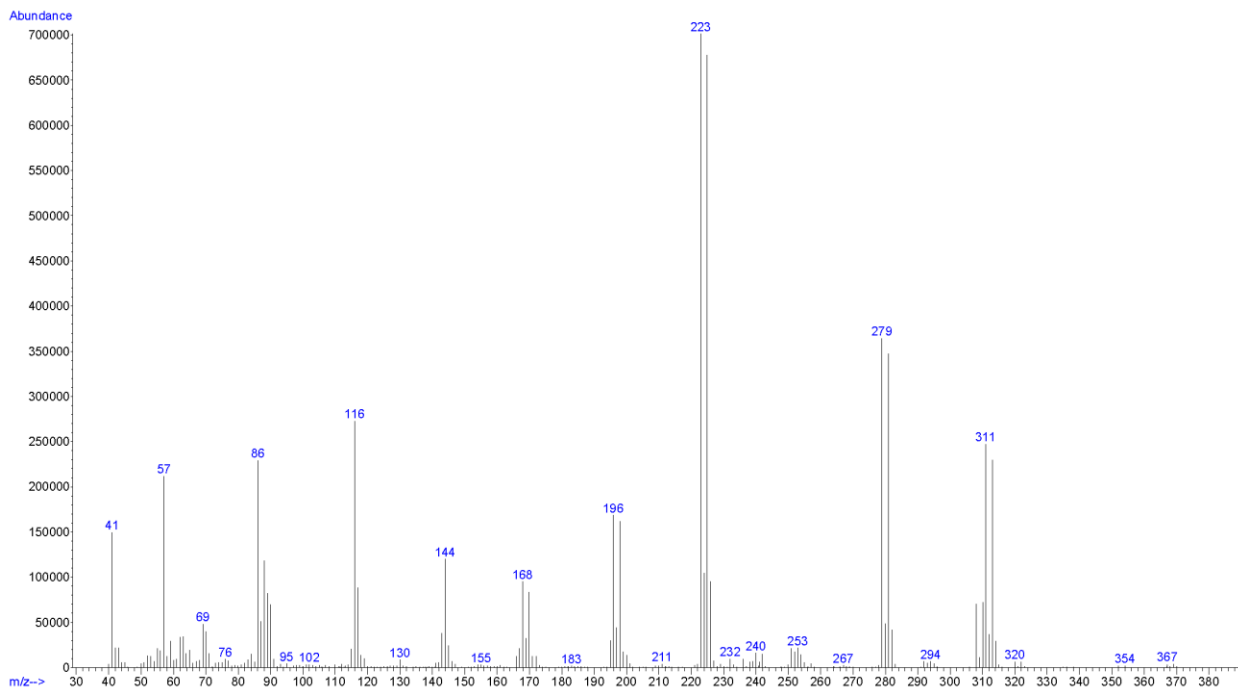
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency)
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 μ m x 0.33 μ m)
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 μ L
MS Parameters:	Mass Scan Range: 40-550 m/z Threshold: 250
Retention Time:	7.82 min
Standard Comparison:	Reference material for MDMA-5Br-INACA (Batch: 0643322-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as MDMA-5Br-INACA based on retention time (7.80 min) and mass spectral data. https://www.caymanchem.com/product/36757/mdmb-5br-inaca

Chromatogram: MDMB-5Br-INACA



Additional peaks in chromatogram: internal standard (5.69 min)

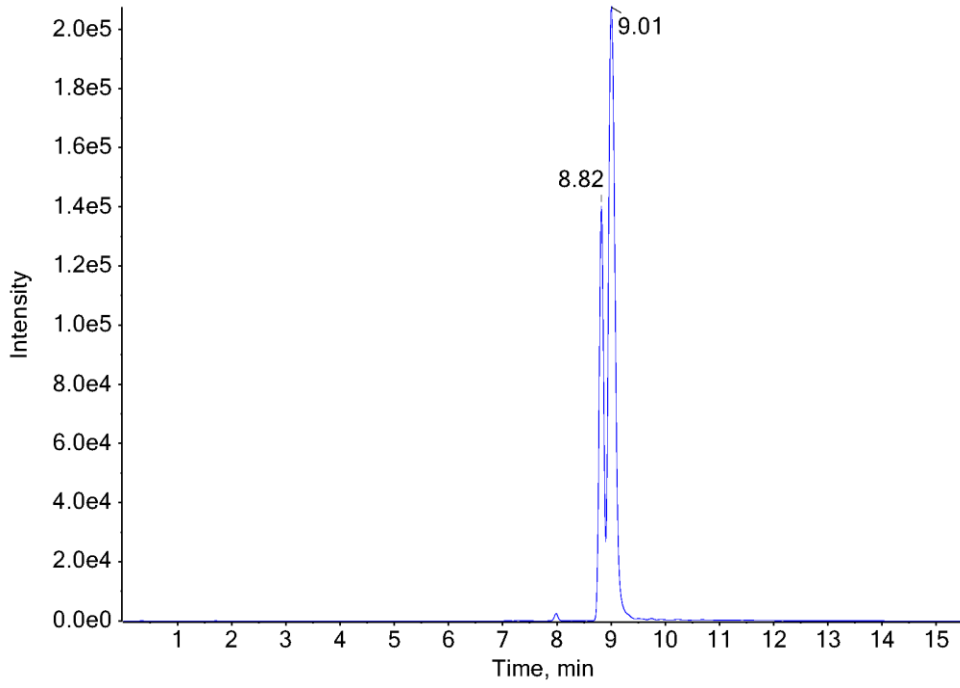
EI (70 eV) Mass Spectrum: MDMB-5Br-INACA



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

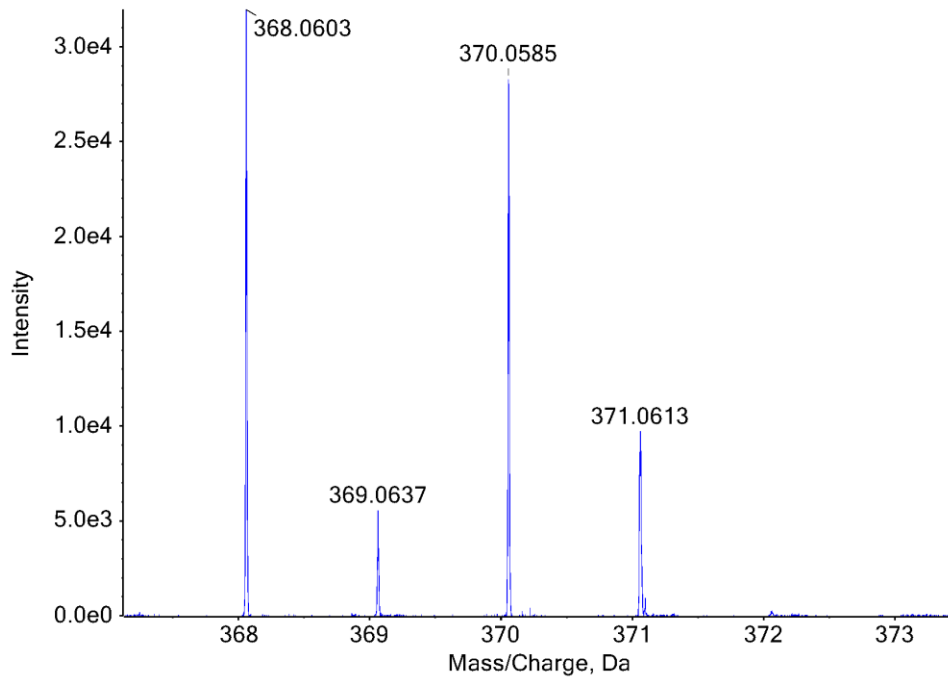
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency) followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)
Instrument:	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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	9.01 min
Standard Comparison:	Reference material for MDMA-5Br-INACA (Batch: 0643322-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as MDMA-5Br-INACA based on retention time (9.06 min) and mass spectral data. https://www.caymanchem.com/product/36757/mdmb-5br-inaca

Extracted Ion Chromatogram: MDMA-5Br-INACA

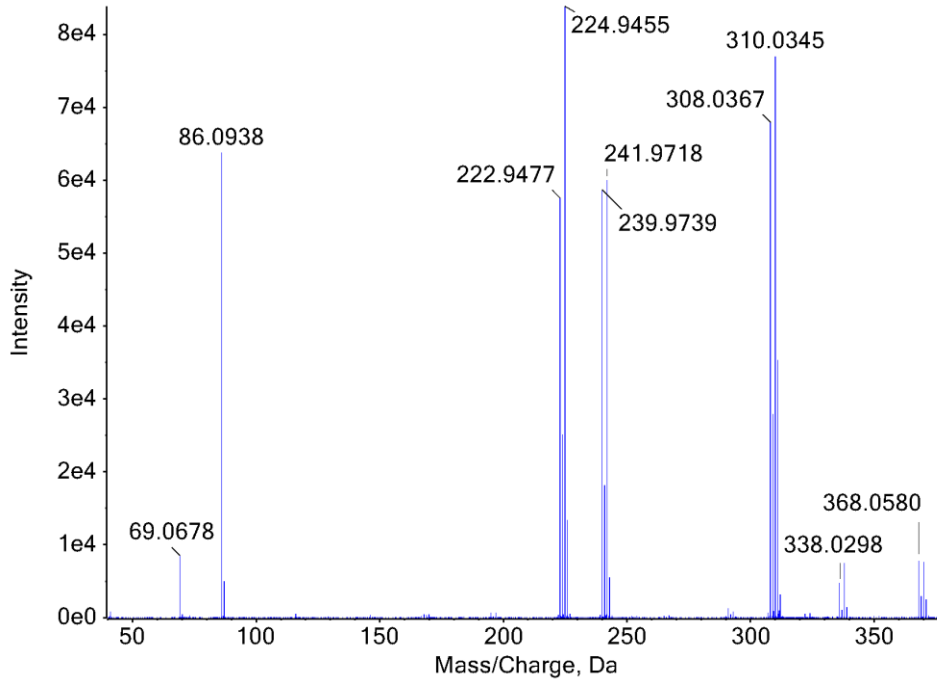


[peak at 8.82 mins has identical MS data to MDMA-5Br-INACA, 9.01 min]

TOF MS Spectra: MDMA-5Br-INACA



TOF MS/MS Spectra: MDMB-5Br-INACA



6. FUNDING

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