



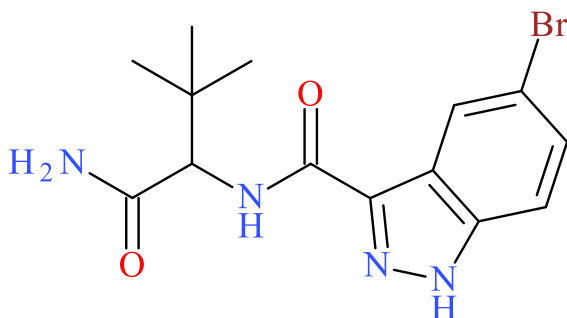
ADB-5Br-INACA

Sample Type: **Drug Material**

Latest Revision: **May 17, 2022**

Date Received: **November 4, 2021**

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



1. GENERAL INFORMATION

IUPAC Name: 5-bromo-N-(1-carbamoyl-2,2-dimethyl-propyl)-1H-indazole-3-carboxamide

InChI String: InChI=1S/C14H17BrN4O2/c1-14(2,3)11(12(16)20)17-13(21)10-8-6-7(15)4-5-9(8)18-19-10/h4-6,11H,1-3H3,(H2,16,20)(H,17,21)(H,18,19)

CFR: Not Scheduled (05/2021)

CAS# Not Available

Synonyms: 5Br-ADB-INACA, ADB-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.

Prepared By: Alex J. Krotulski, PhD; Ryan Farrell; Zackery Roberson, PhD; Melissa F. Fogarty, MSFS, D-ABFT-FT; Sara E. Walton, MS; 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 ₁₄ H ₁₇ BrN ₄ O ₂	353.2	352	353.0608

3. BRIEF DESCRIPTION

ADB-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. Little information is currently known about the activity, potency, and/or toxicity of ADB-5Br-INACA. However, recent *in vitro* studies have shown ADB-5Br-INACA to exhibit cannabinoid (CB) receptor activity (unpublished data by Deventer MH et al.; Ghent University), but overall potency is expected to be low. 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, ADB-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>

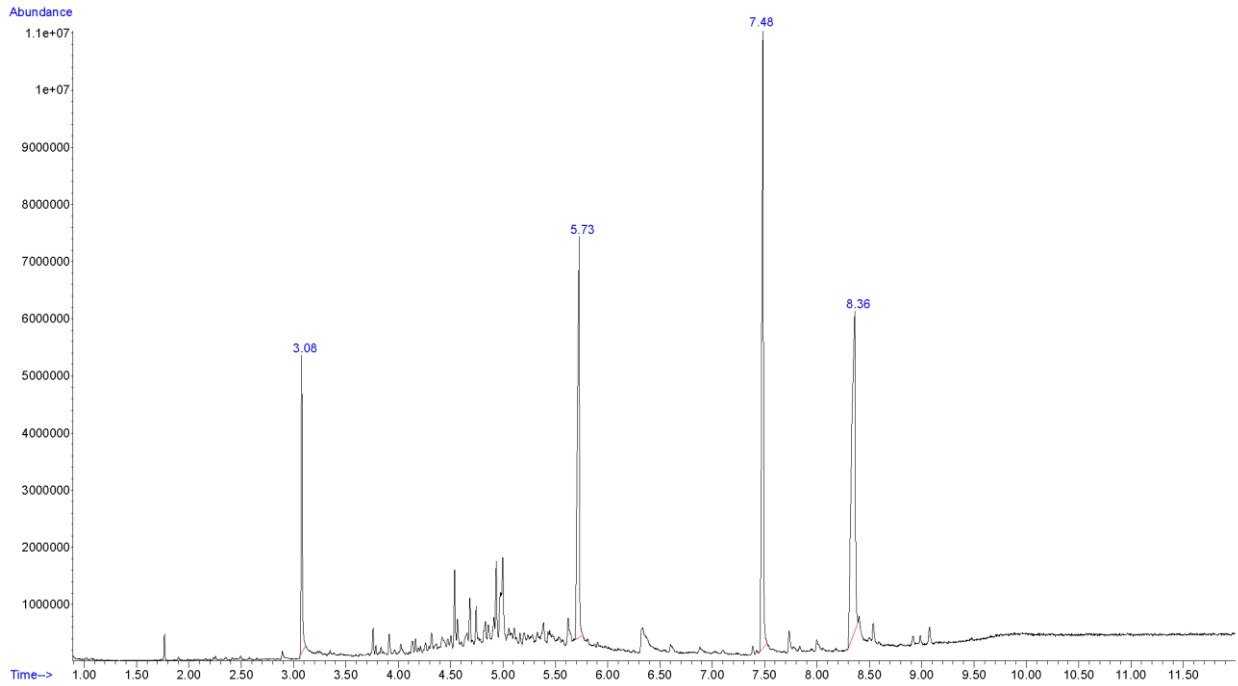
<https://www.caymanchem.com/product/36263/adb-5br-inaca>

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

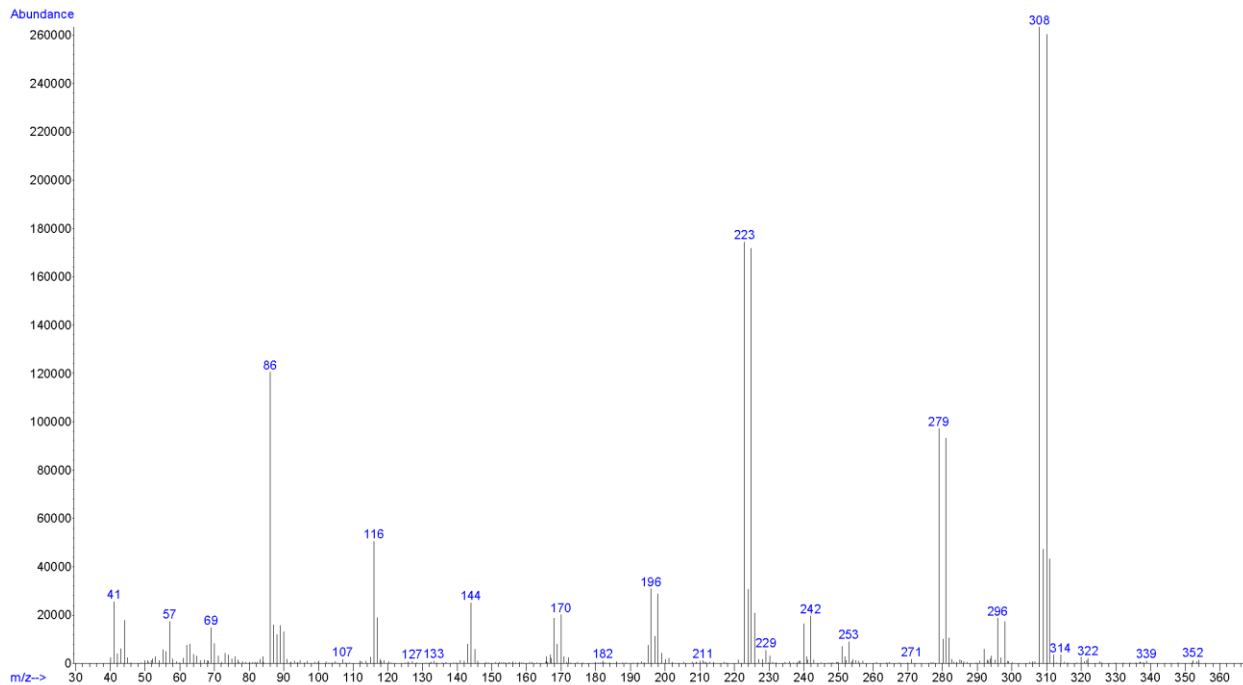
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency)
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (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:	8.36 min
Standard Comparison:	Reference material for ADB-5Br-INACA (Batch: 0638474-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-5Br-INACA based on retention time (8.32 min) and mass spectral data. https://www.caymanchem.com/product/36263/adb-5br-inaca

Chromatogram: ADB-5Br-INACA



Additional peaks in chromatogram: internal standards (3.08 and 5.73 mins) and ADB-BINACA (also known as ADB-BUTINACA, 7.48 mins)

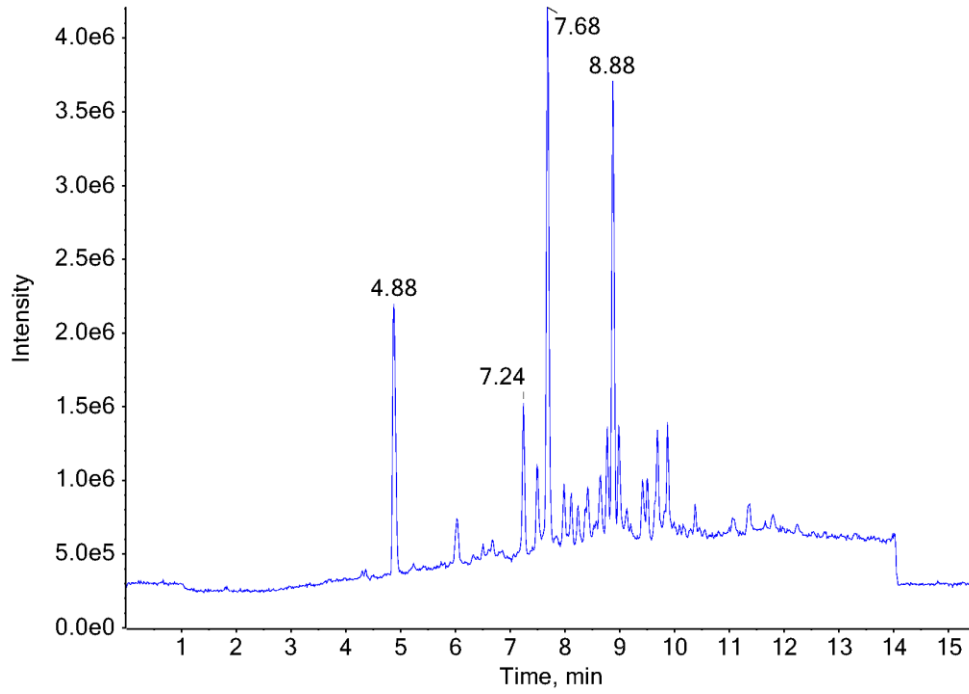
EI (70 eV) Mass Spectrum: ADB-5Br-INACA



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

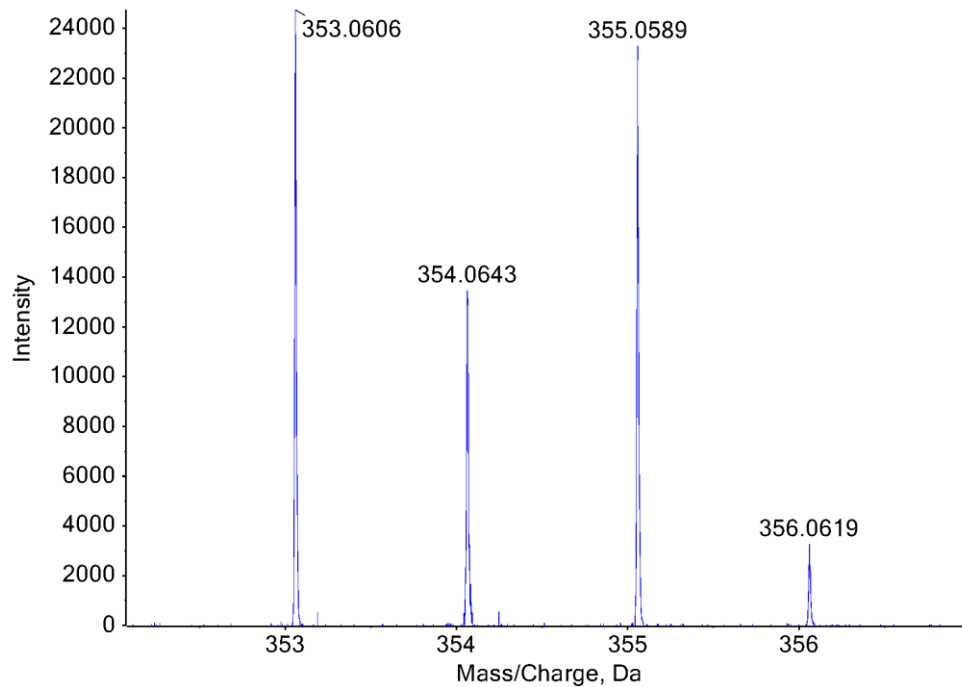
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Indianapolis-Marion County Forensic Services Agency) followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)
Instrument:	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:	7.68 min
Standard Comparison:	Reference material for ADB-5Br-INACA (Batch: 0638474-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-5Br-INACA based on retention time (7.71 min) and mass spectral data. (https://www.caymanchem.com/product/36263/adb-5br-inaca)

Chromatogram: ADB-5Br-INACA

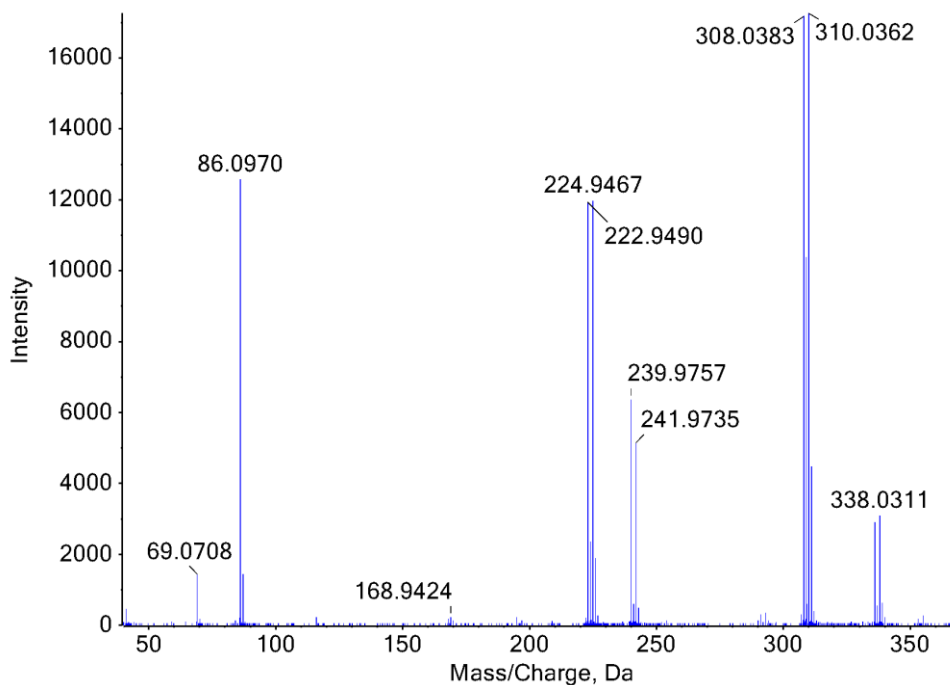


Additional peaks in chromatogram: internal standards (4.88 and 7.24 mins) and ADB-BINACA (also known as ADB-BUTINACA, 8.88 mins)

TOF MS Spectra: ADB-5Br-INACA



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



6. FUNDING

NPS Discovery at the Center for Forensic Science Research and Education (CFSRE) is supported in part by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 2020-DQ-BX-0007, “Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS)”). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect those of the Department of Justice.