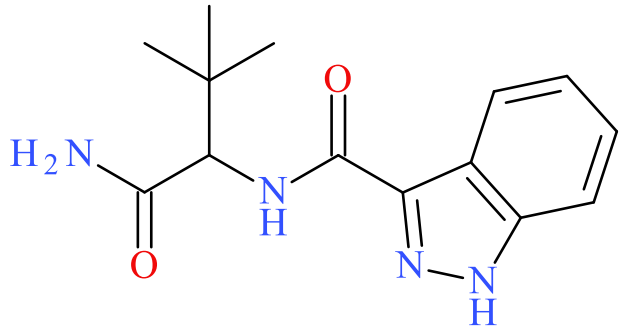
ADB-INACA

Sample Type: **Drug Material**



Latest Revision: **December 14, 2022**

Date Received: **November 3, 2022**

Date of Report: **December 14, 2022**

1. GENERAL INFORMATION

IUPAC Name:	N-(1-carbamoyl-2,2-dimethyl-propyl)-1H-indazole-3-carboxamide
InChI String:	InChI=1S/C14H18N4O2/c1-14(2,3)11(12(15)19)16-13(20)10-8-6-4-5-7-9(8)17-18-10/h4-7,11H,1-3H3,(H2,15,19)(H,16,20)(H,17,18)
CFR:	Not Scheduled (12/2022)
CAS#	1887742-42-8
Synonyms:	None Available
Source:	NMS Labs – Criminalistic Laboratory
Appearance:	White Solid Material on White Paper

***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	$C_{14}H_{18}N_4O_2$	274.3	274	275.1503

3. BRIEF DESCRIPTION

ADB-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-INACA. It is suspected that ADB-INACA is a precursor, specifically to other synthetic cannabinoids like ADB-BINACA (ADB-BUTINACA), and therefore 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. Many of these new synthetic cannabinoid analogues are unstudied with pharmacological and human effects undetermined. Currently, ADB-INACA is not a scheduled substance in the United States.

4. ADDITIONAL RESOURCES

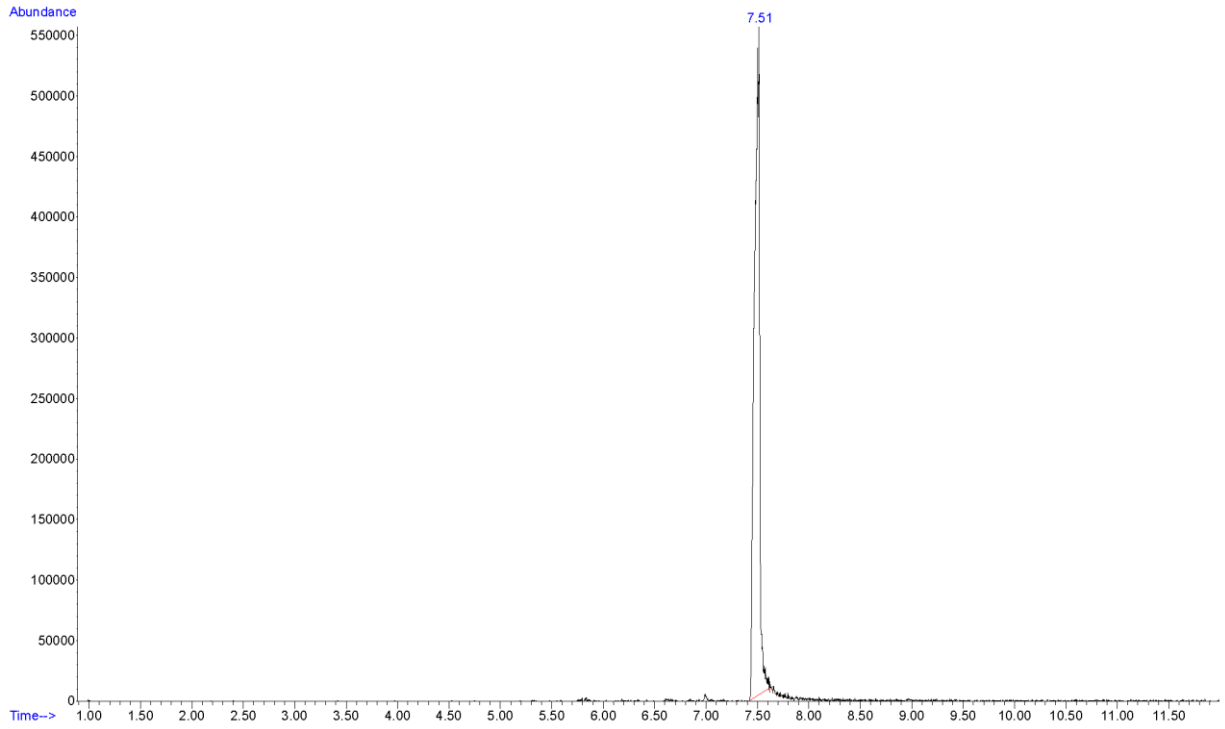
https://www.caymanchem.com/product/37729/adb-inaca

5. QUALITATIVE DATA

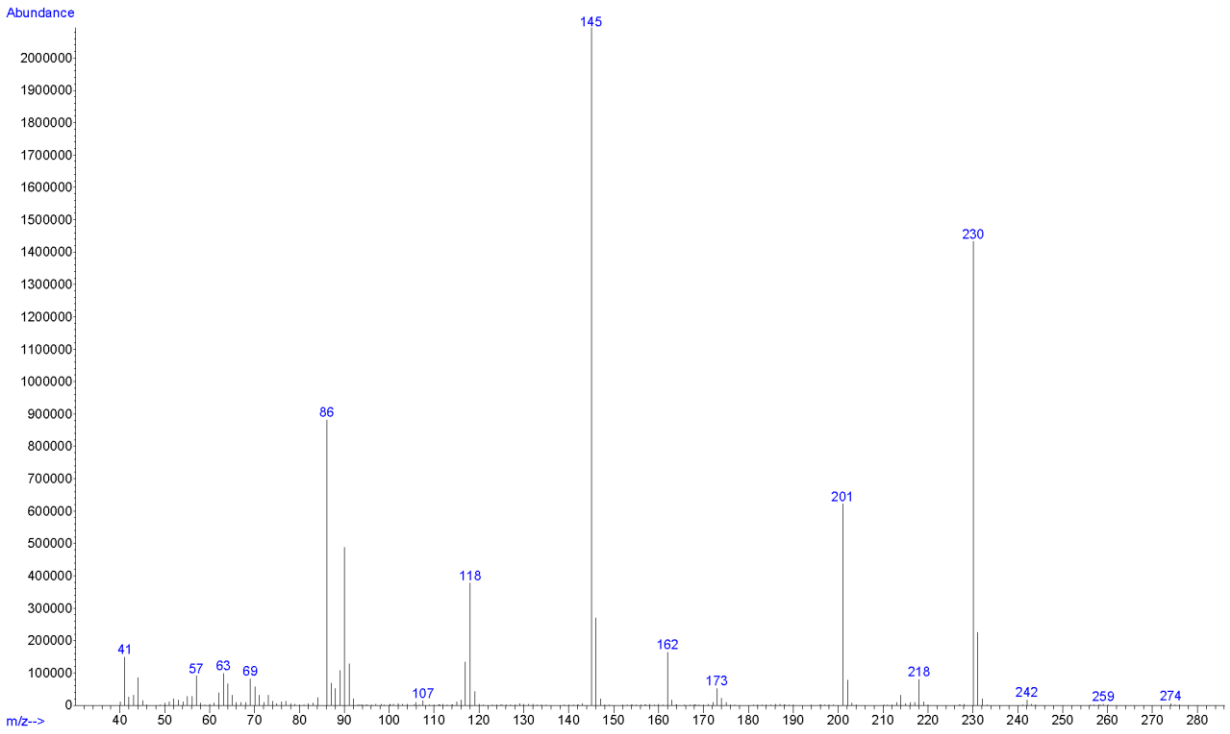
5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Acid/Base Extraction (NMS Labs)
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:	7.51 min
Standard Comparison:	Reference material for ADB-INACA (Batch: 0661443-1) 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-INACA based on retention time (7.50 min) and mass spectral data. (https://www.caymanchem.com/product/37729/adb-inaca)

Extracted Ion Chromatogram: ADB-INACA



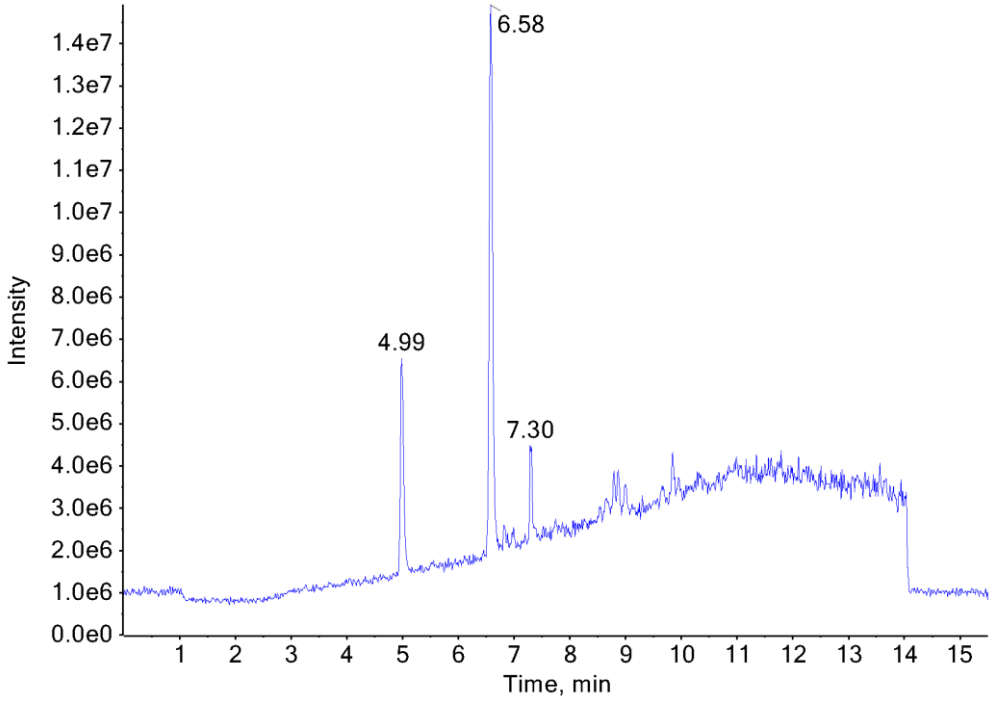
EI (70 eV) Mass Spectrum: ADB-INACA



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

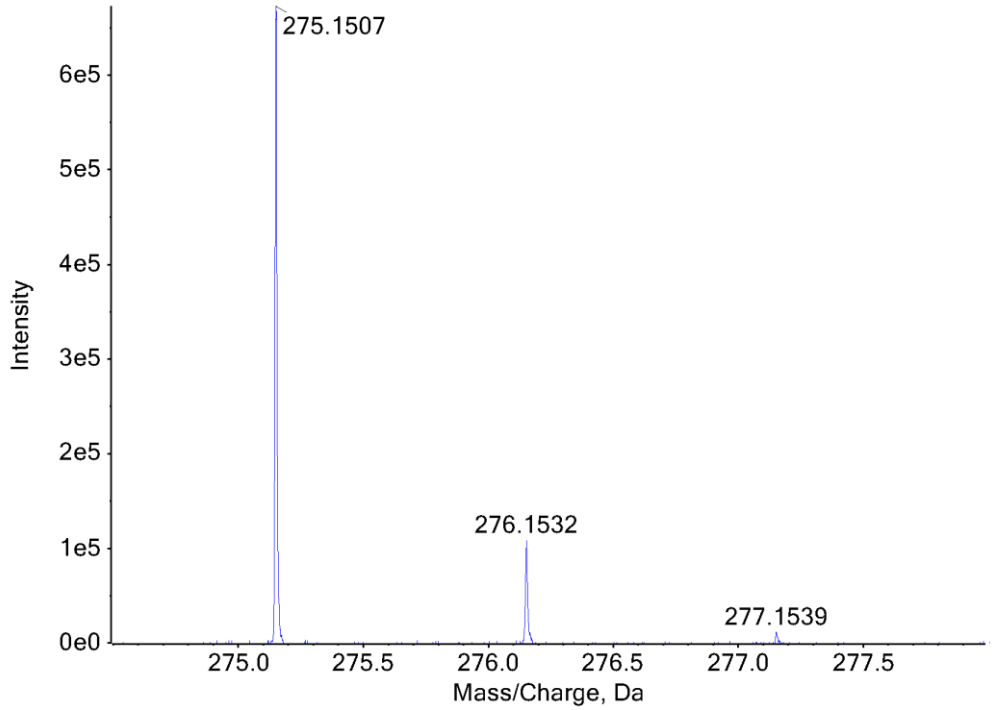
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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:	6.58 min
Standard Comparison:	Reference material for ADB-INACA (Batch: 0661443-1) 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-INACA based on retention time (6.45 min) and mass spectral data. (https://www.caymanchem.com/product/37729/adb-inaca)

Chromatogram: ADB-INACA

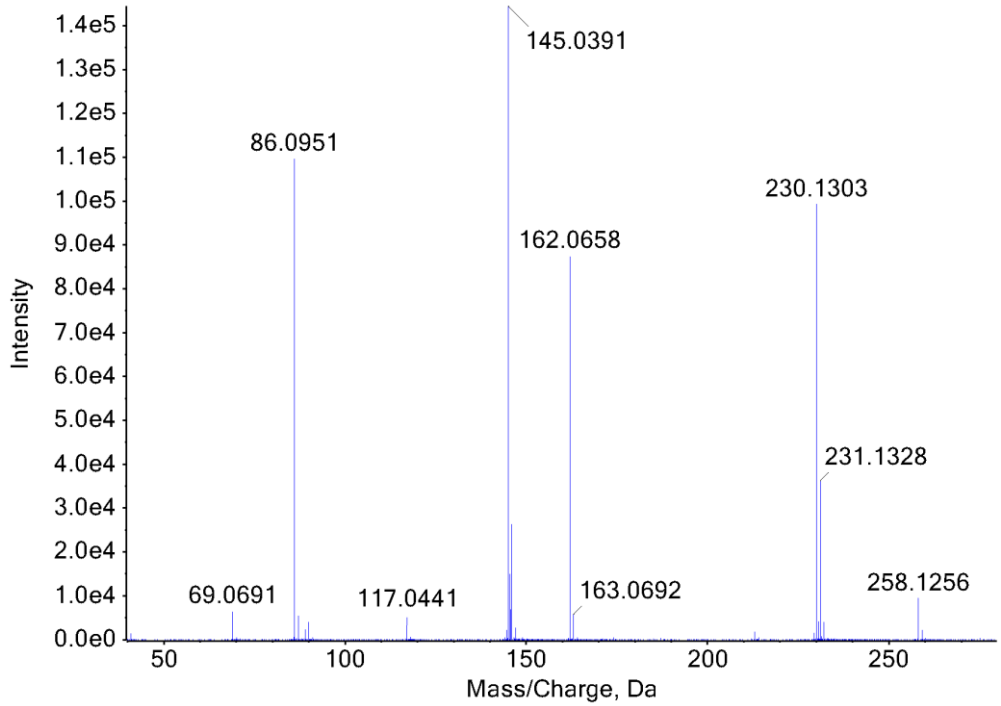


Additional peaks present in chromatogram: internal standards (4.99 min and 7.30 min)

TOF MS Spectrum: ADB-INACA



MS/MS Spectrum: ADB-INACA



6. FUNDING

NPS Discovery at the 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 represent the official position or policies of the U.S. Department of Justice.