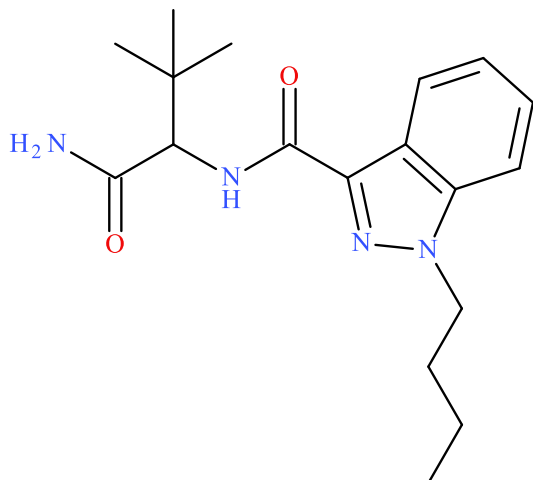


ADB-BINACA

Sample Type: **Seized Material**



Latest Revision: **November 18, 2020**

Date Received: **July 17, 2020**

Date of Report: **November 18, 2020**

1. GENERAL INFORMATION

IUPAC Name:	1-butyl-N-(1-carbamoyl-2,2-dimethyl-propyl)indazole-3-carboxamide
InChI String:	InChI=1S/C18H26N4O2/c1-5-6-11-22-13-10-8-7-9-12(13)14(21-22)17(24)20-15(16(19)23)18(2,3)4/h7-10,15H,5-6,11H2,1-4H3,(H2,19,23)(H,20,24)
CFR:	Not Scheduled (11/2020)
CAS#	Not Available
Synonyms:	ADB-BUTINACA
Source:	NMS Labs – Criminalistic Laboratory
Appearance:	Hand-Rolled Cigarette Containing 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 ₁₈ H ₂₆ N ₄ O ₂	330.4	330	331.2129

3. BRIEF DESCRIPTION

ADB-BINACA 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. ADB-PINACA and MDMB-BINACA are structurally similar synthetic cannabinoids. ADB-BINACA and AB-PINACA are structural isomers, sharing the same formula and parent mass; however, their chemical behavior and mass fragmentation patterns differ allowing for differentiation during analytical testing. ADB-PINACA and AB-PINACA are Schedule I substances in the United States; ADB-BINACA and MDMB-BINACA are not explicitly scheduled.

ADB-BINACA in this report should not be confused with ADB-BENZINACA (which is also referred to as "[ADB-BINACA](#)"; IUPAC Name: N-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-benzyl-1H-indazole-3-carboxamide). ADB-BENZINACA contains a benzyl- moiety as the tail portion of its molecule, while ADB-BINACA containing a butyl- moiety as its tail. The name ADB-BINACA was selected for the drug reported herein for consistency with the naming convention used for drugs associated with previously developed new drug monographs (e.g. 4F-MDMB-BINACA, 4F-MDMB-BICA, 5F-MDMB-PICA, 5F-EDMB-PINACA).

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/ADB-BUTINACA-ID-2082_report.pdf

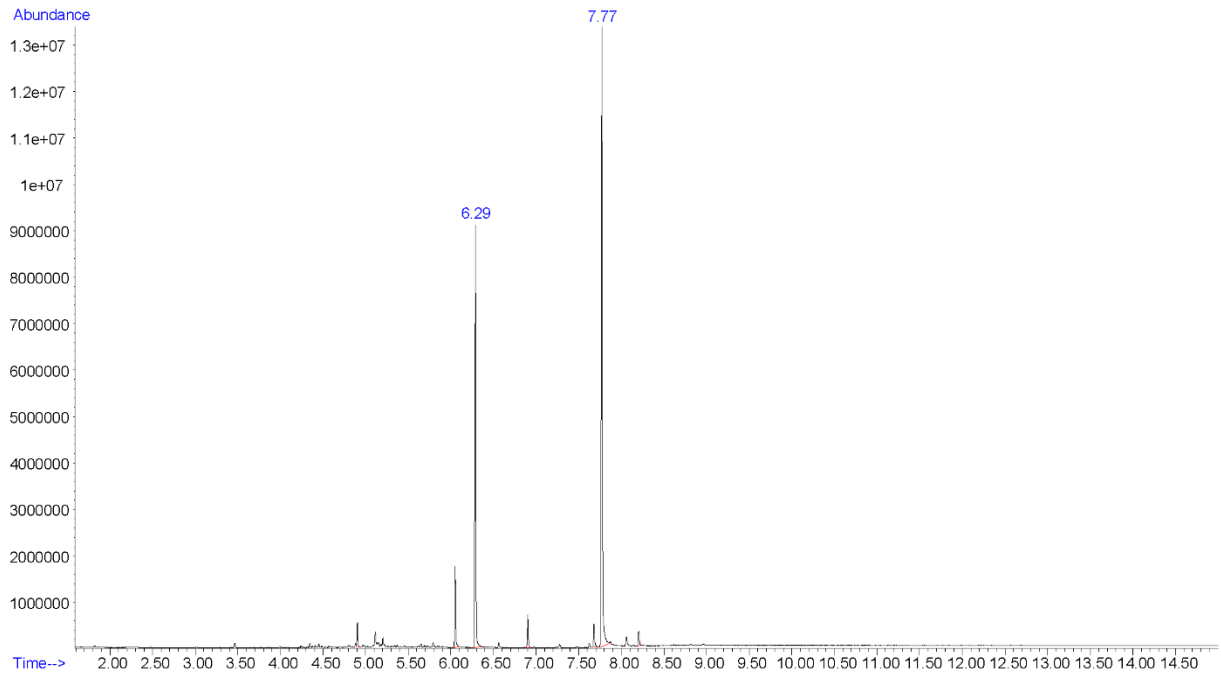
<https://www.caymanchem.com/product/29350/adb-butinaca>

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

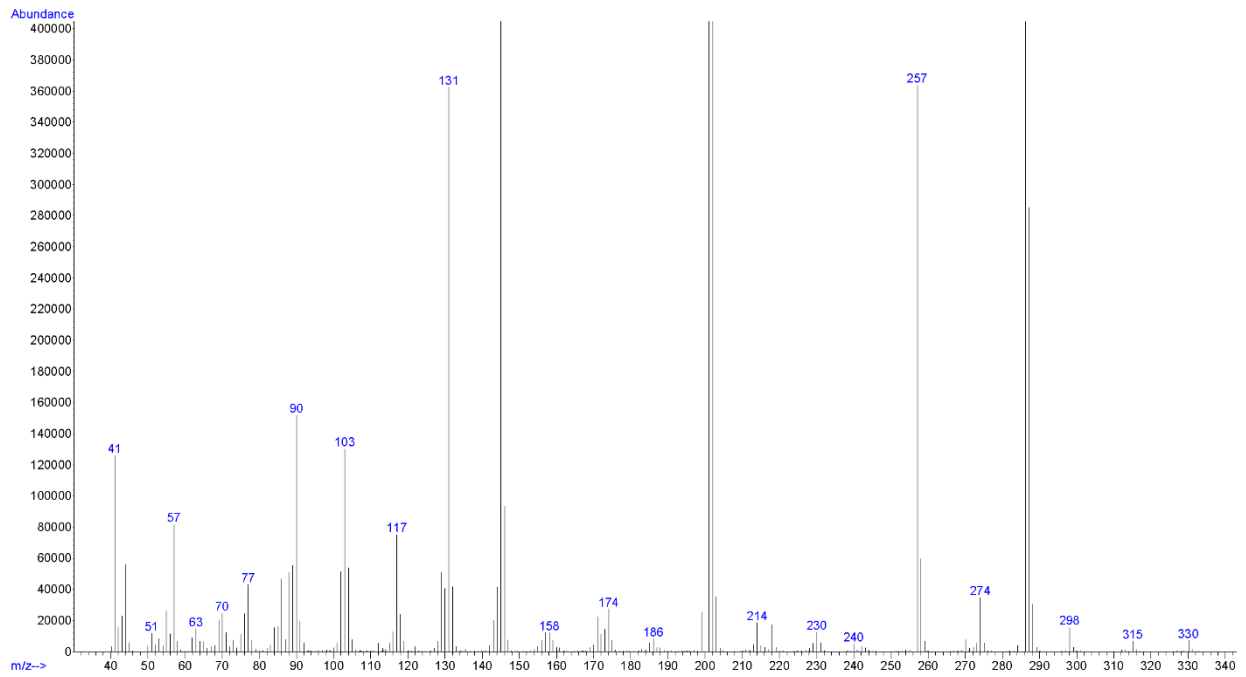
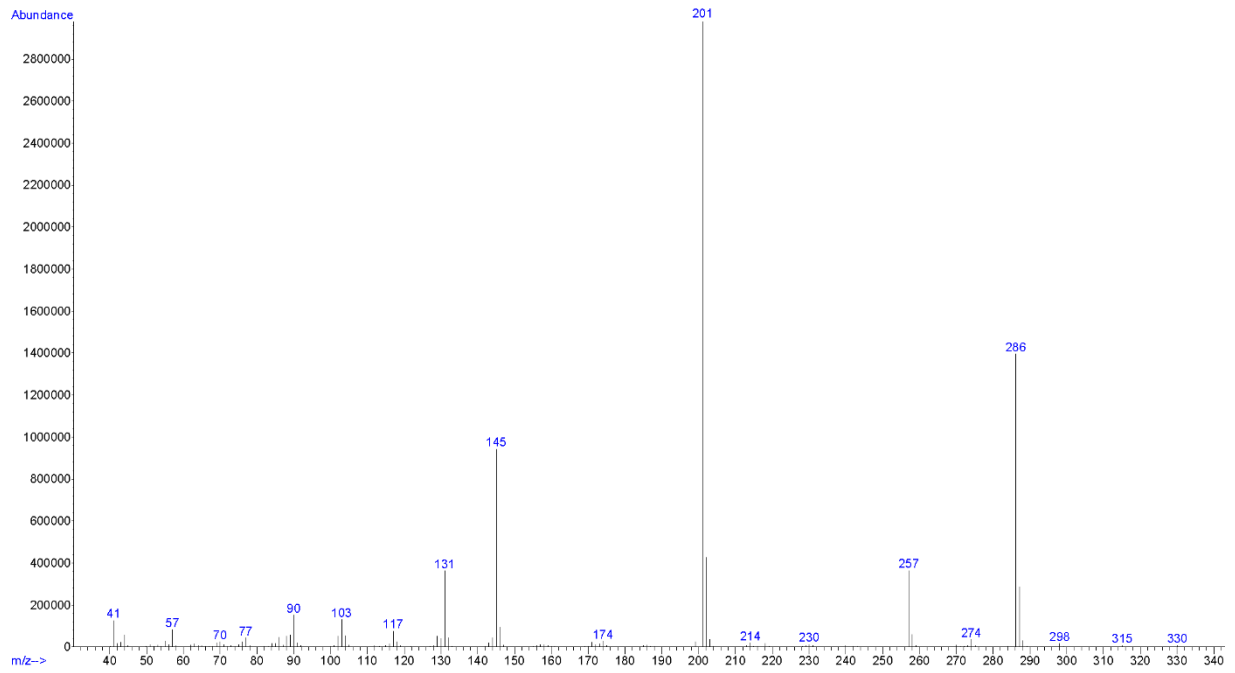
Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebtron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C Transfer Line: 300 °C MS Source: 230 °C MS Quad: 150 °C Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z Threshold: 250
Retention Time:	7.77 min
Standard Comparison:	Reference material for ADB-BINACA (Batch: 0576506-5) 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-BINACA based on retention time (7.76 min) and mass spectral data. (https://www.caymanchem.com/product/29350/adb-butinaca)

Chromatogram: ADB-BINACA



Additional peak present in chromatogram: internal standard (6.29 min)

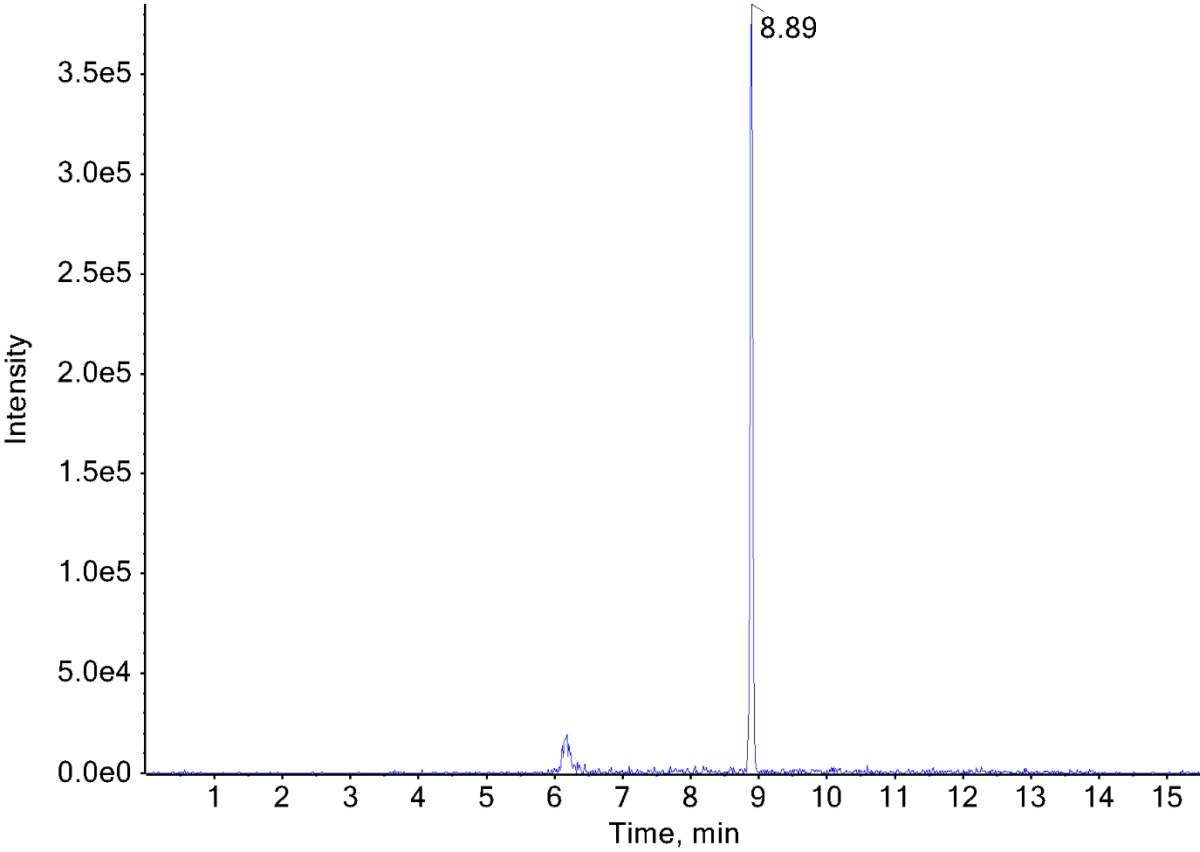
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): ADB-BINACA



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 extraction 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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	8.89 min
Standard Comparison:	Reference material for ADB-BINACA (Batch: 0576506-5) 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-BINACA based on retention time (8.94 min) and mass spectral data. (https://www.caymanchem.com/product/29350/adb-butinaca)

Extracted Ion Chromatogram: ADB-BINACA



TOF MS (Top) and MS/MS (Bottom) Spectra: ADB-BINACA

