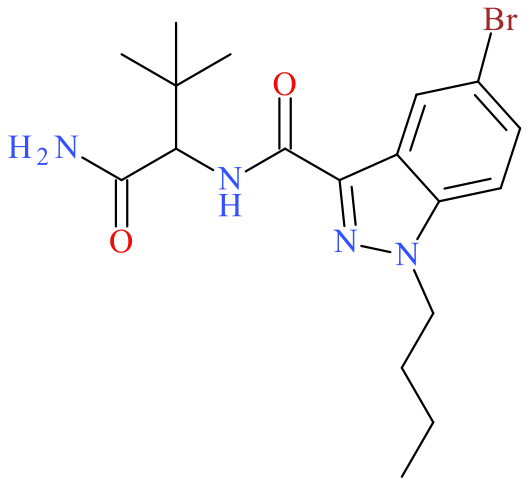
ADB-5'Br-BINACA



Sample Type: **Drug Material**

Latest Revision: **May 26, 2022**

Date Received: **May 10, 2022**

Date of Report: **May 26, 2022**

1. GENERAL INFORMATION

IUPAC Name:	5-bromo-1-butyl-N-(1-carbamoyl-2,2-dimethyl-propyl)indazole-3-carboxamide
InChI String:	InChI=1S/C18H25BrN4O2/c1-5-6-9-23-13-8-7-11(19)10-12(13)14(22-23)17(25)21-15(16(20)24)18(2,3)4/h7-8,10,15H,5-6,9H2,1-4H3,(H2,20,24)(H,21,25)
CFR:	Not Scheduled (05/2021)
CAS#	Not Available
Synonyms:	ADB-5'Br-BUTINACA, ADB-BUT-5Br-INACA, 5Br-ADB-BUTINACA *(sold online)*
Source:	Philadelphia Department of Public Health
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

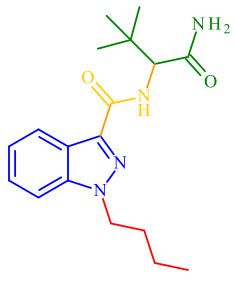
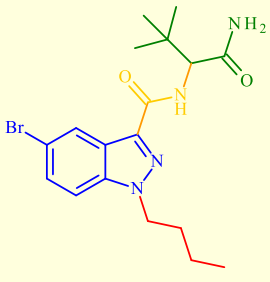
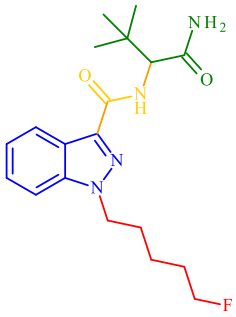
2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M$^+$]	Exact Mass [M+H]$^+$
Base	$C_{18}H_{25}BrN_4O_2$	409.3	408	409.1234

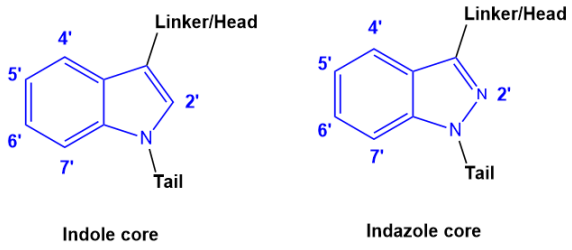
3. BRIEF DESCRIPTION

ADB-5'Br-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. Little to no information is currently known about the activity, potency, and/or toxicity of ADB-5'Br-BINACA. 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-5'Br-BINACA is not a scheduled substance in the United States.

Scientists at Cayman Chemical and the CFSRE developed a revised naming convention for new synthetic cannabinoids containing core substituents (e.g., 5-bromo indazole). To avoid confusion with tail substituents, the location of the core substituent(s) will be denoted by a prime (') designation and will be placed in the middle of the name. Below is an illustration explaining how this revised naming convention will be applied.

ADB-BINACA	**ADB-5'Br-BINACA**	**5F-ADB-PINACA**
		
N-(1-**A**mino-3,3-**D**imethyl-1-oxo**B**utan-2-yl)-1-**B**utyl-**IN**d**A**zole-3-**C**arbox**A**mide	*N*-(1-**A**mino-3,3-**D**imethyl-1-oxo**B**utan-2-yl)-1-**B**utyl-**5**-**Br**omo-**IN**d**A**zole-3-**C**arbox**A**mide	*N*-(1-**A**mino-3,3-**D**imethyl-1-oxo**B**utan-2-yl)-1-**5**-**F**luoro**P**entyl-**IN**d**A**zole-3-**C**arbox**A**mide
Name: **ADB-BINACA**	*Name:* **ADB-5'Br-BINACA**	*Name:* **5F-ADB-PINACA**
Synonyms: **ADB-BUTINACA**	*Synonyms:* **ADB-5'Br-BUTINACA**	*Synonyms:* **N/A**

Core Substituent Numbering Designation for Use in Future Naming Conventions



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.3185

2. Alex J. Krotulski, Ryan Farrell, Zackery Roberson, Melissa F. Fogarty, Sara E. Walton, Barry K. Logan. (2022) New Drug Monograph: ADB-5Br-INACA. Center for Forensic Science Research and Education, United States of America. https://www.npsdiscovery.org/wp-content/uploads/2022/05/ADB-5Br-INACA_051722_CFSRE-Chemistry_Report.pdf

https://www.caymanchem.com/product/36770/adb-5'br-butinaca

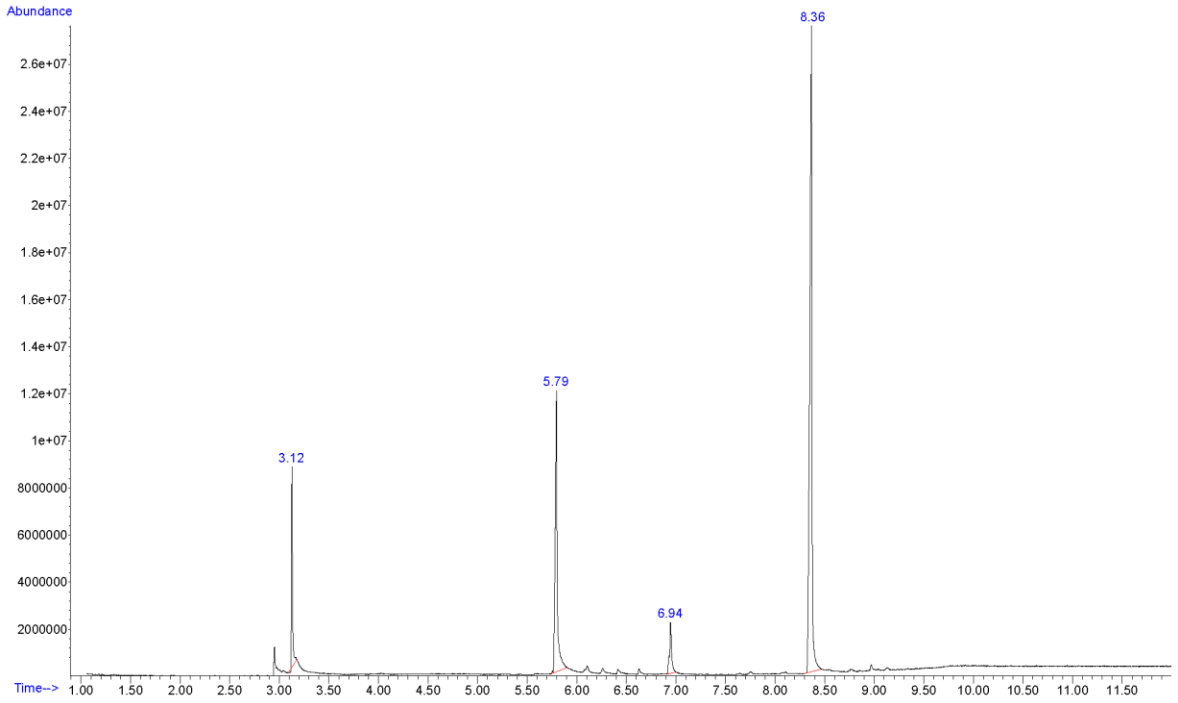
5. QUALITATIVE DATA

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
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

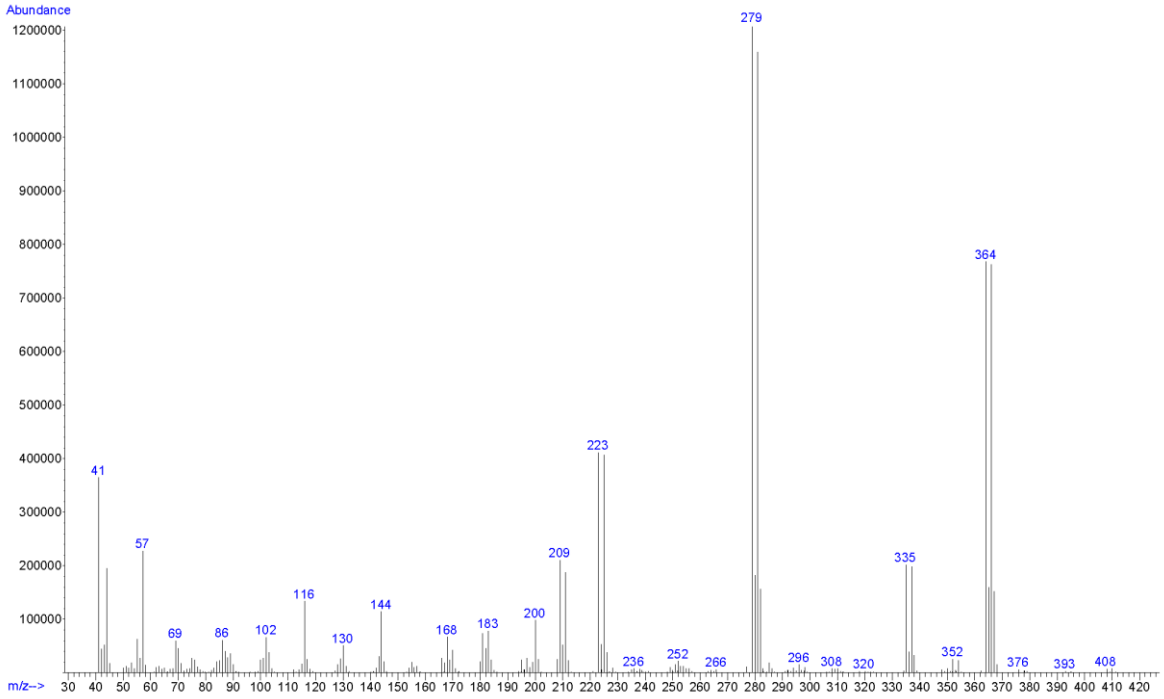
	MS Quad: 150 °C
	Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	8.36 min
Standard Comparison:	Reference material for ADB-5'Br-BINACA (Batch: 0644026-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-5'Br-BINACA based on retention time (8.33 min) and mass spectral data. (https://www.caymanchem.com/product/36770/adb-5'br-butinaca)

Chromatogram: ADB-5'Br-BINACA

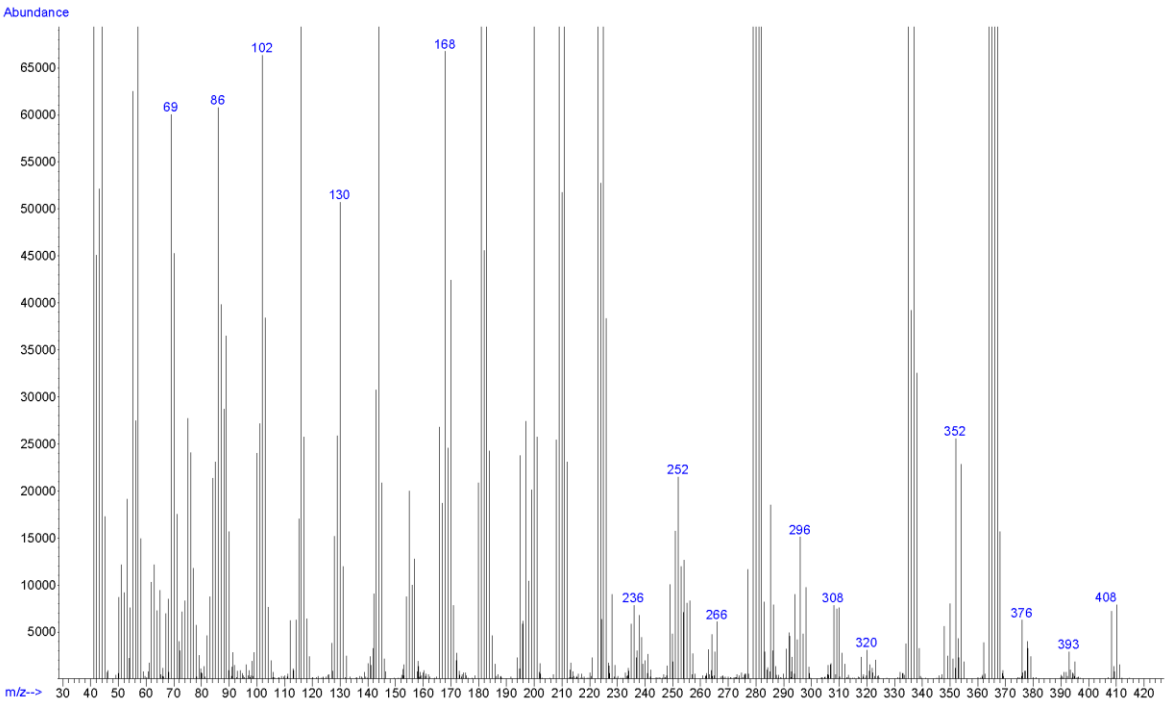


Additional peaks in chromatogram: internal standards (3.12 and 5.79 mins), unknown brominated analyte (6.94 min)

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



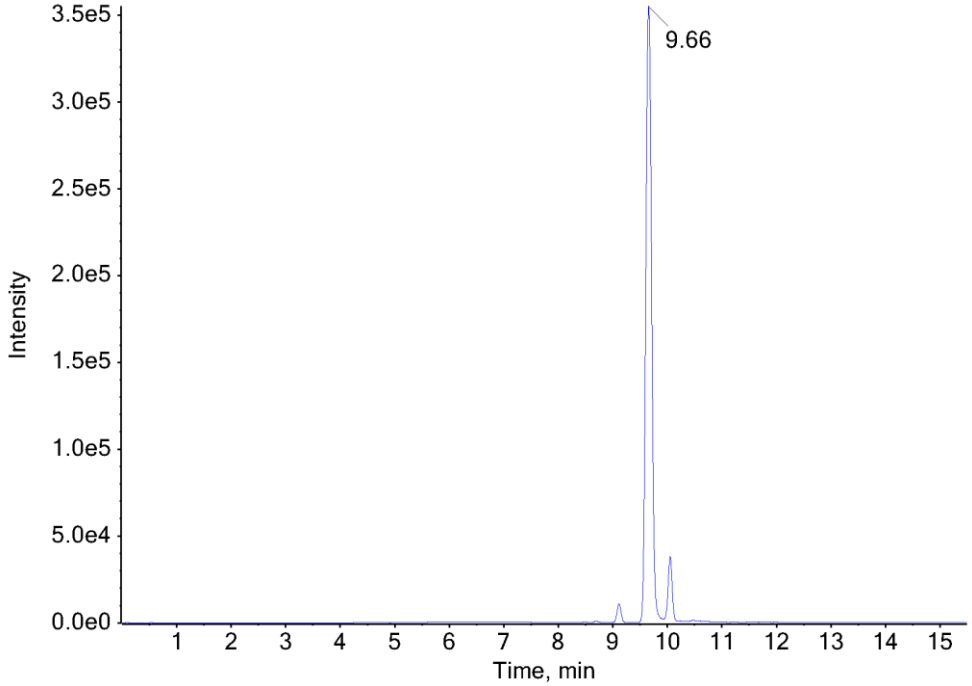
EI (70 eV) Mass Spectrum (10x Zoom): ADB-5'Br-BINACA



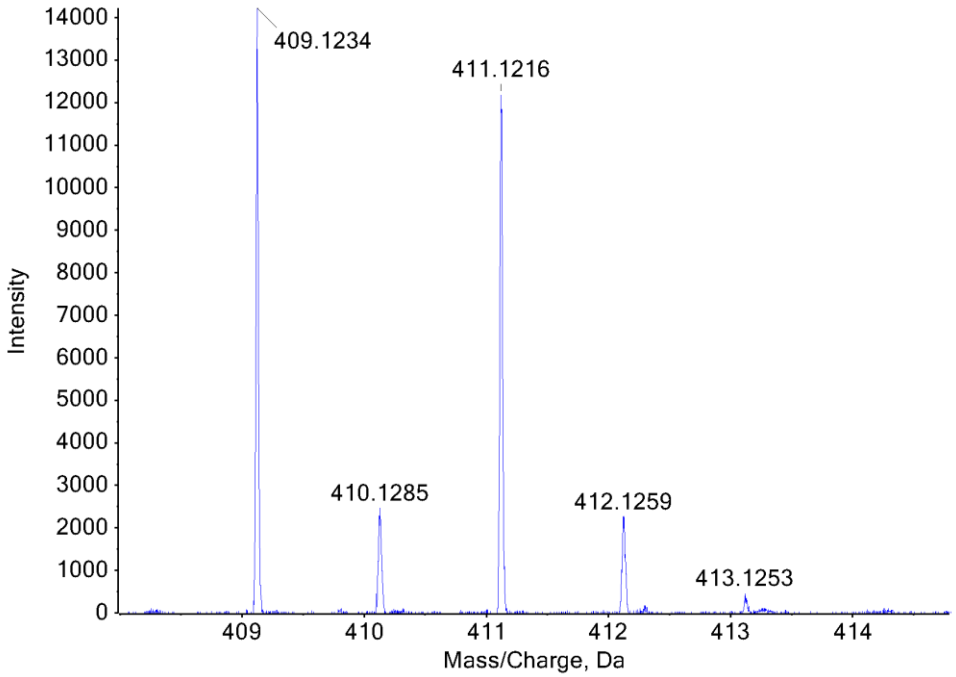
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol 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:	9.66 min
Standard Comparison:	Reference material for ADB-5'Br-BINACA (Batch: 0644026-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as ADB-5'Br-BINACA based on retention time (9.70 min) and mass spectral data. (https://www.caymanchem.com/product/36770/adb-5'br-butinaca)

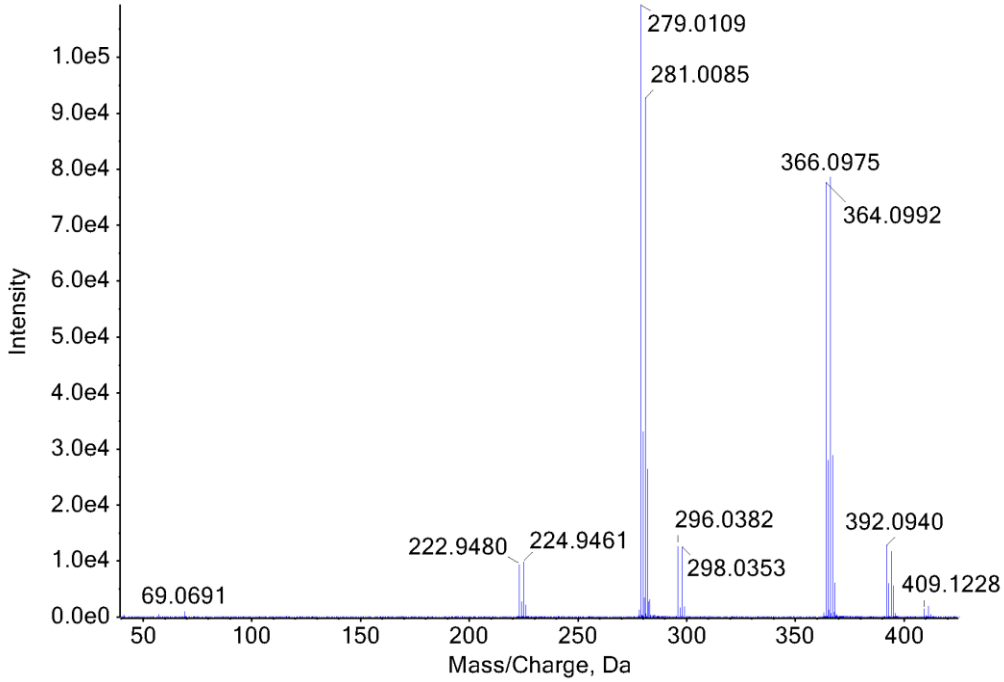
Extracted Ion Chromatogram: ADB-5'Br-BINACA



TOF MS Spectra: ADB-5'Br-BINACA



TOF MS/MS Spectra: ADB-5'Br-BINACA



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.