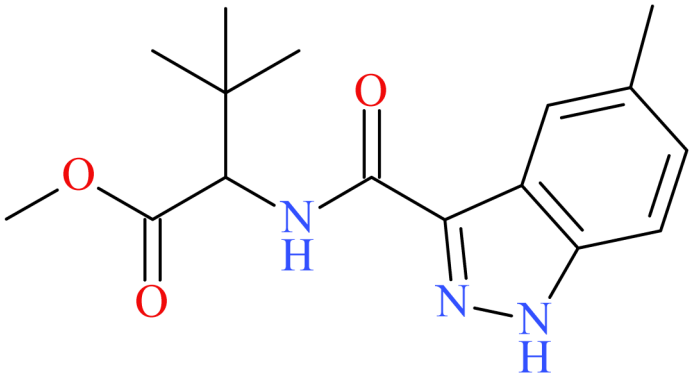
MDMB-5Me-INACA



NPS SUBCLASS
Synthetic Cannabinoid
REPORT DATE
November 21, 2023
SAMPLE RECEIVED
August 25, 2023
SAMPLE TYPE
Drug Material

Preferred Name	MDMB-5Me-INACA
Synonyms	5Me-MDMB-INACA, MDMB-5-methyl INACA
Formal Name	methyl 3,3-dimethyl-2-[(5-methyl-1H-indazole-3-carbonyl)amino]butanoate
InChI Key	OBEPVZFBSIMMHX-UHFFFAOYSA-N
CAS Number	Not Available
Chemical Formula	$C_{16}H_{21}N_3O_3$
Molecular Weight	303.36
Molecular Ion [M⁺]	303
Exact Mass [M+H]⁺	304.1656

Characterization & Intelligence

The following information was compiled in November 2023 and is subject to change as new research is conducted and as new information becomes available:

Description: MDMB-5Me-INACA is a synthetic cannabinoid precursor that could be used to produce structurally related synthetic cannabinoid final products. Synthetic cannabinoid precursors (e.g., MDMB-INACA, ADB-INACA, MDMB-5'Br-INACA) began appearing after the implementation of a national class-wide synthetic cannabinoid scheduling action imposed by China in July 2021.

Sample Source: NMS Labs – Drug Chemistry

Sample Appearance: Paper containing no visible residue

Pharmacology: The activity and potency of MDMB-5Me-INACA are unknown; however, based on structurally similar synthetic cannabinoid precursors, MDMB-5Me-INACA is expected to be inactive or have low potency.

Toxicology: MDMB-5Me-INACA has not been detected in toxicology cases at the CFSRE.

Drug Materials: MDMB-5Me-INACA has been detected in one drug material at the CFSRE.

Demographics / Geographics: The drug material originated from the state of New York.

Legal Status: MDMB-5Me-INACA is not explicitly scheduled in the United States.

References:

- Cayman Chemical: MDMB-5Me-INACA

About: In collaboration with medical examiner and coroner offices, crime laboratories, clinical partners, and other stakeholders, the Center for Forensic Science Research and Education (CFSRE) is documenting first confirmations of NPS through analysis of drug materials and/or toxicology samples. These reports are generated using comprehensive analytical techniques (e.g., GC-MS, LC-QTOF-MS, NMR) and include available information about the new substances identified at the time of reporting, as well as the analytical data generated during testing. Our new drug monographs are intended to assist with the rapid identification of NPS in forensic casework and related disciplines, and should not be used for confirmatory purposes alone.

Analytical Notes: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF-MS) in comparison to analysis of acquired reference material.

Acknowledgements: This report was prepared by Alex J. Krotulski, Nicole Lattanzio, Bridget McGinty, Sara E. Walton, Melissa F. Fogarty, and Barry K. Logan at the Center for Forensic Science Research and Education (CFSRE) at the Fredric Rieders Family Foundation. The authors acknowledge scientists at the CFSRE and NMS Labs for their involvements and contributions. For more information, contact npsdiscovery@cfsre.org or visit www.npsdiscovery.org.

Funding: CFSRE's NPS Discovery is supported by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 15PNIJ-22-GG-04434-MUMU, "Implementation of NPS Discovery – An Early Warning System for Novel Drug Intelligence, Surveillance, Monitoring, Response, and Forecasting using Drug Materials and Toxicology Populations in the US"). 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.

Suggested Citation: Krotulski, AJ; Lattanzio, N; McGinty, B; Walton, SE; Fogarty, MF; Logan, BK. (2023) *MDMB-5Me-INACA — NPS Discovery New Drug Monograph*, Center for Forensic Science Research and Education, United States.

Gas Chromatography Mass Spectrometry (GC-MS)

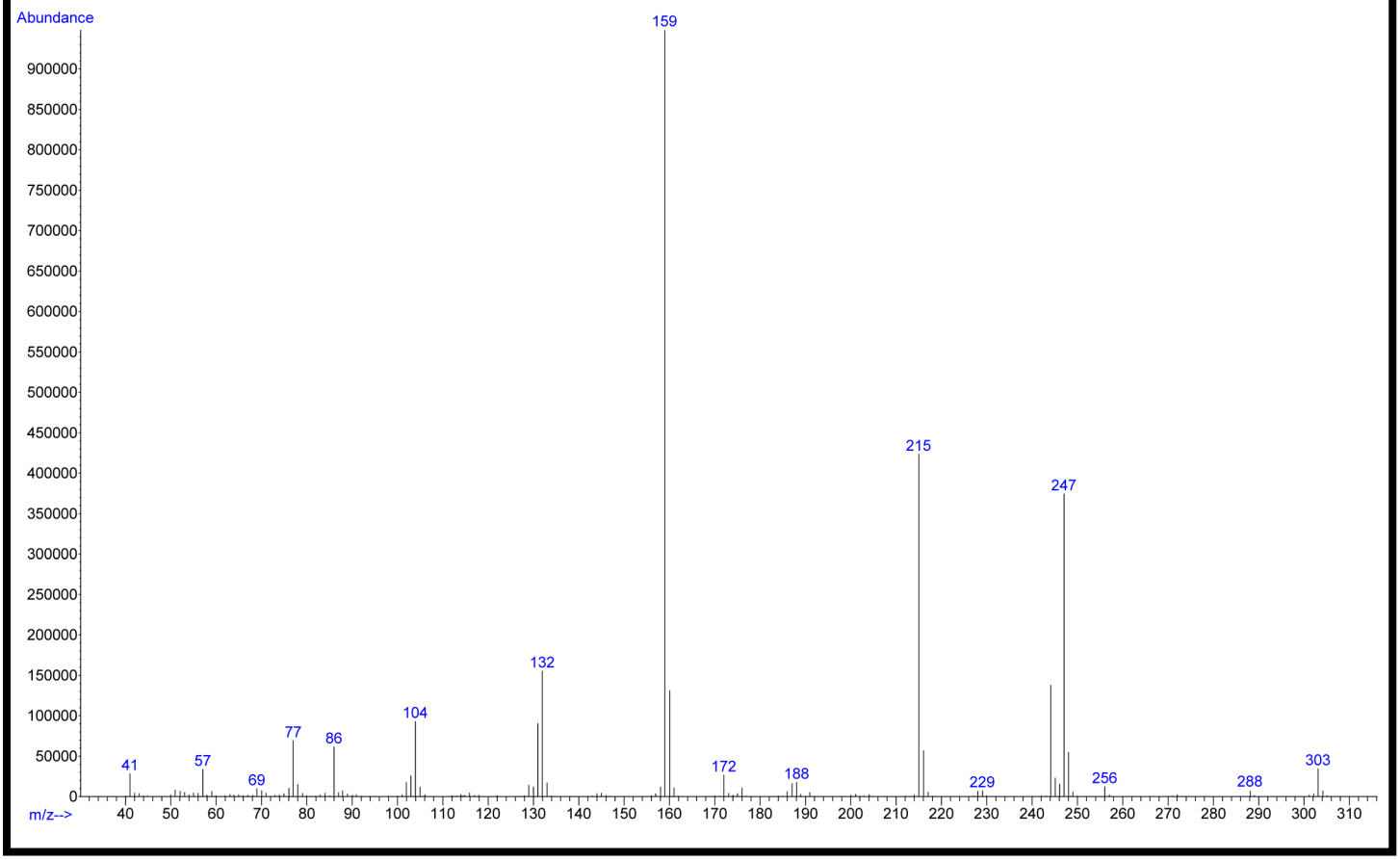
Laboratory: Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

Sample Preparation: Acid/base extraction

Instrument: Agilent 5975 Series GC/MSD

Methods: www.cfsre.org/nps-discovery/monographs
GC-MS Method Details

GC-MS: Mass Spectrum (EI 70 eV)



Confirmation Using Drug Standard: *Reference material (Batch: 0688513-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be MDMB-5Me-INACA based on retention time (sample: 7.267 min vs. standard: 7.267 min) and mass spectral data comparisons.*

Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (LC-QTOF-MS)

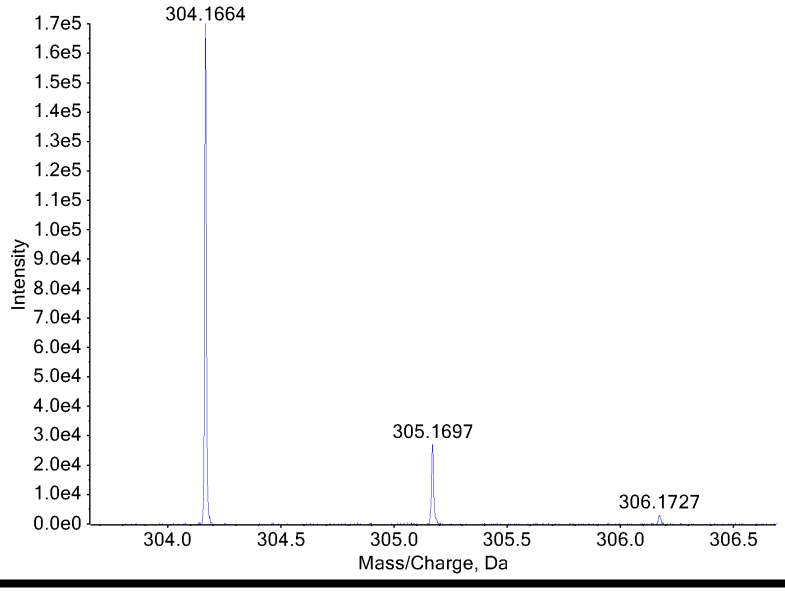
Laboratory: Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

Sample Preparation: Acid/base extraction

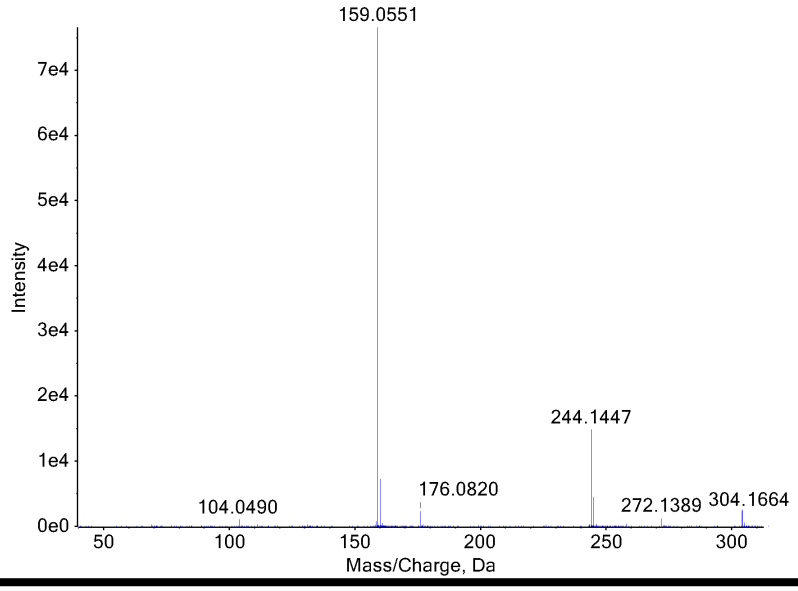
Instrument: Sciex TripleTOF® 5600+ LC-QTOF-MS

Methods: www.cfsre.org/nps-discovery/monographs
LC-QTOF-MS Method Details

LC-QTOF-MS: TOF-MS Precursor Ion Mass Spectrum



LC-QTOF-MS: TOF-MS/MS Product Ion Mass Spectrum



Confirmation Using Drug Standard: *Reference material (Batch: 0688513-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be MDMB-5Me-INACA based on retention time (sample: 8.55 min vs. standard: 8.54 min) and mass spectral data comparisons.*