NPS Discovery — New Drug Monograph







4CI-MDMB-BINACA

NPS SUBCLASS
Cannabinoid
REPORT DATE
December 16, 2024
SAMPLE RECEIVED
September 13, 2024
SAMPLE TYPE
Drug Material

Preferred Name	4CI-MDMB-BINACA
Synonyms	4CI-MDMB-BUTINACA, 4-Chloro MDMB-BINACA, 4-Chloro MDMB-BUTINACA
Formal Name	methyl 2-[[1-(4-chlorobutyl)indazole-3-carbonyl]amino]-3,3-dimethyl-butanoate
InChl Key	CZOQQMLVUUBCLA-UHFFFAOYSA-N
CAS Number	N/A
Chemical Formula	C ₁₉ H ₂₆ CIN ₃ O ₃
Molecular Weight	379.9
Molecular Ion [M ⁺]	379
Exact Mass [M+H]*	380.1735

Characterization & Intelligence

The following information was compiled in December 2024 and is subject to change as new research is conducted and as new information becomes available:

Description: 4CI-MDMB-BINACA is a novel synthetic cannabinoid bearing structural similarity to 4F-MDMB-BINACA, MDMB-BINACA, and other synthetic cannabinoids. 4CI-MDMB-BINACA was first detected in September 2024 by our laboratory and was confirmed in November 2024 after acquisition of standard reference material.

Sample Source: Center of Forensic & Digital Science Abu Dhabi Judicial Department

Sample Appearance: Bottle containing transparent liquid

Pharmacology: No information is available at this time for 4Cl-MDMB-BINACA; however, based on structural similarity to other indazole synthetic cannabinoids (i.e., 4F-MDMB-BINACA), 4Cl-MDMB-BINACA is assumed to be a potent CB₁ receptor agonist.¹

Toxicology: 4CI-MDMB-BINACA has not been identified in toxicology cases to date at the CFSRE.

Drug Materials: 4CI-MDMB-BINACA has been detected in one drug material to date at the CFSRE.

Demographics / Geographics: The drug material positive for 4CI-MDMB-BINACA originated from Abu Dhabi and was identified alongside other synthetic cannabinoids (e.g., MDMB-BINACA, MDMB-INACA).

Legal Status: 4CI-MDMB-BINACA is not currently a scheduled drug in the United States.

References:

- ► Cayman Chemical: <u>4CI-MDMB-BUTINACA</u>
- ► ¹Tokarcyzk et al. (2022) Fatal intoxication with new synthetic cannabinoids 5F-MDMB-PICA...

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. The Abu Dhabi Judicial Department was responsible for the preliminary identification and the CFSRE was responsible for the confirmation, including the procuring of the standard reference material.

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Gas Chromatography Mass Spectrometry (GC-MS)

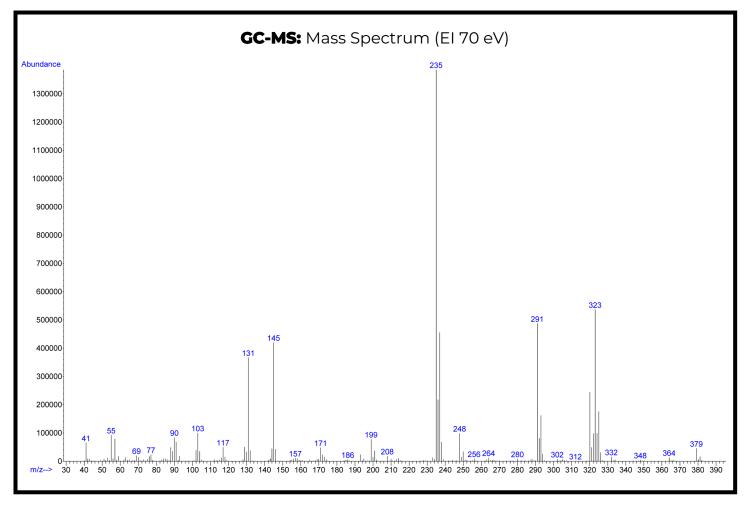
Laboratory: Center for Forensic Science Research and

Education (CFSRE, Horsham, PA, USA)

Sample Preparation: Dilution in methanol

Instrument: Agilent 5975 Series GC/MSD

Methods: GC-MS Method Details & Monographs



Confirmation Using Drug Standard: Reference material (Batch: 0722830-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be 4CI-MDMB-BINACA based on retention time (sample: 7.78 min vs. standard: 7.74 min) and mass spectral data comparisons.

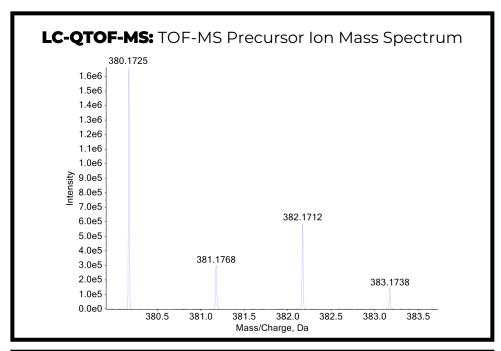
Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (LC-QTOF-MS)

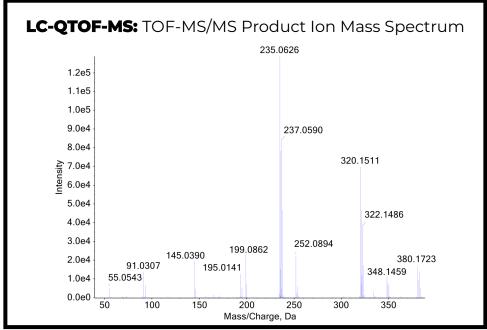
Laboratory: Center for Forensic Science Research and Education (CFSRE, Horsham, PA, USA)

Instrument: Sciex 5600+ LC-QTOF-MS

Sample Preparation: Dilution in mobile phase

Methods: LC-QTOF-MS Method Details & Monographs





Confirmation Using Drug Standard: Reference material (Batch: 0722830-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be 4CI-MDMB-BINACA based on retention time (sample: 9.50 min vs. standard: 9.62 min) and mass spectral data comparisons.