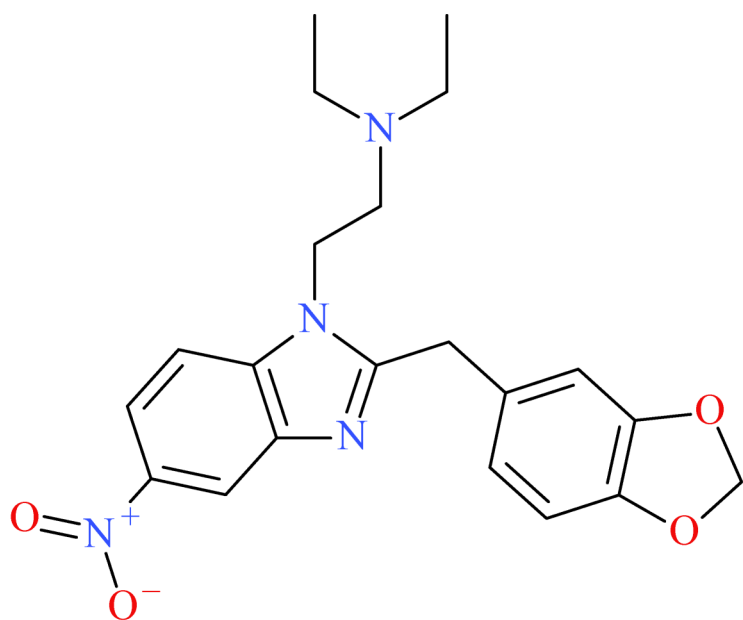




Methylenedioxy nitazene



NPS SUBCLASS	Opioid
REPORT DATE	August 29, 2024
SAMPLE RECEIVED	April 23, 2024
SAMPLE TYPE	Drug Material

Preferred Name	Methylenedioxy nitazene
Synonyms	3',4'-Methylenedioxy nitazene
Formal Name	2-[2-(1,3-benzodioxol-5-ylmethyl)-5-nitro-benzimidazol-1-yl]-N,N-diethyl-ethanamine
InChI Key	RRRJUZFCVIDSM-UHFFFAOYSA-N
CAS Number	N/A
Chemical Formula	C ₂₁ H ₂₄ N ₄ O ₄
Molecular Weight	396.4
Molecular Ion [M ⁺]	396
Exact Mass [M+H] ⁺	397.1870

Characterization & Intelligence

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

Description: Methylenedioxyinitazene is a novel synthetic opioid bearing structural similarity to other nitazene analogues (e.g., etonitazene, isotonitazene) where the ethoxy group is replaced with a 3,4-methylenedioxy ring. Methylenedioxyinitazene was first identified in April 2024 by our laboratory and was confirmed after acquiring standard reference material.

Sample Source: St. Charles County Police Department (O'Fallon, MO)

Sample Appearance: Tan powder

Pharmacology: The activity and potency of methylenedioxyinitazene have not been studied.

Toxicology: Methylenedioxyinitazene has been identified in two toxicology cases to date at the CFSRE.

Drug Materials: Methylenedioxyinitazene has been detected in one drug material to date at the CFSRE.

Demographics / Geographics: Toxicology cases originated from the United Kingdom and the drug material originated from Missouri. Methylenedioxyinitazene was found alongside other nitazene analogues (e.g., *N*-desethyl isotonitazene, *N*-pyrrolidino protonitazene) and traditional opioids (e.g., fentanyl, heroin).

Legal Status: Methylenedioxyinitazene is not explicitly scheduled in the United States.

References:

- ▶ Cayman Chemical: [Methylenedioxyinitazene](#)



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 Sara E. Walton, Rachel Garrett, Max T. Denn, Alexis D. Quinter, Joshua S. DeBord, Barry K. Logan, and Alex J. Krotulski 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: Walton, SE; Garrett, R; Denn, MT; Quinter, AD; DeBord, JS; Logan, BK; Krotulski, AJ. (2024) *Methylenedioxyinitazene* — *NPS Discovery New Drug Monograph*, Center for Forensic Science Research and Education, United States.

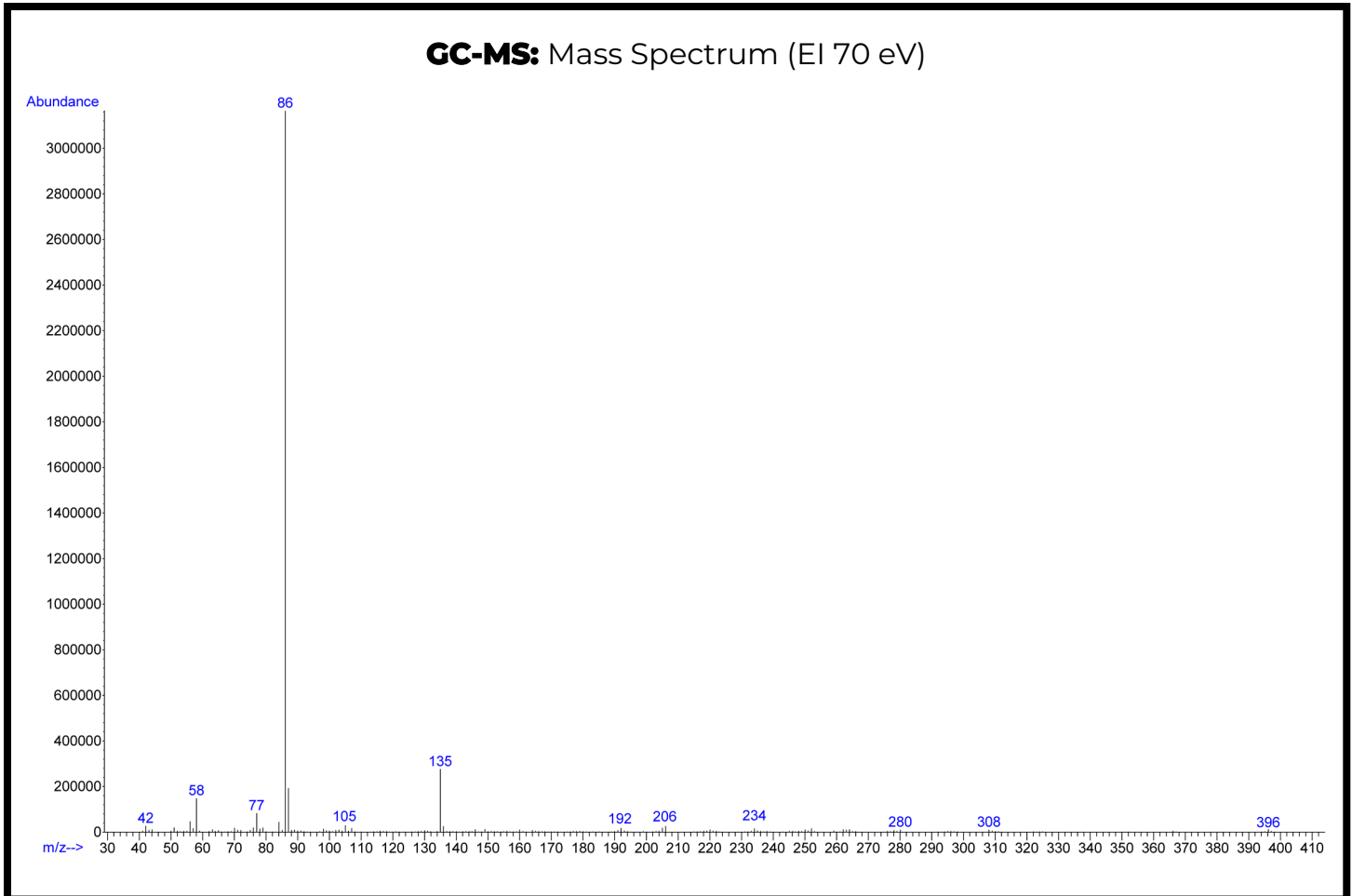
Gas Chromatography Mass Spectrometry (GC-MS)

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

Instrument: Agilent 5975 Series GC/MSD

Methods: [GC-MS Method Details](#) & [Monographs](#)

Sample Preparation: Dilution in methanol



Confirmation Using Drug Standard: Reference material (Batch: 0698653-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be methylenedioxyvitazene based on retention time (sample: 9.31 min vs. standard: 9.32 min) and mass spectral data comparisons.

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

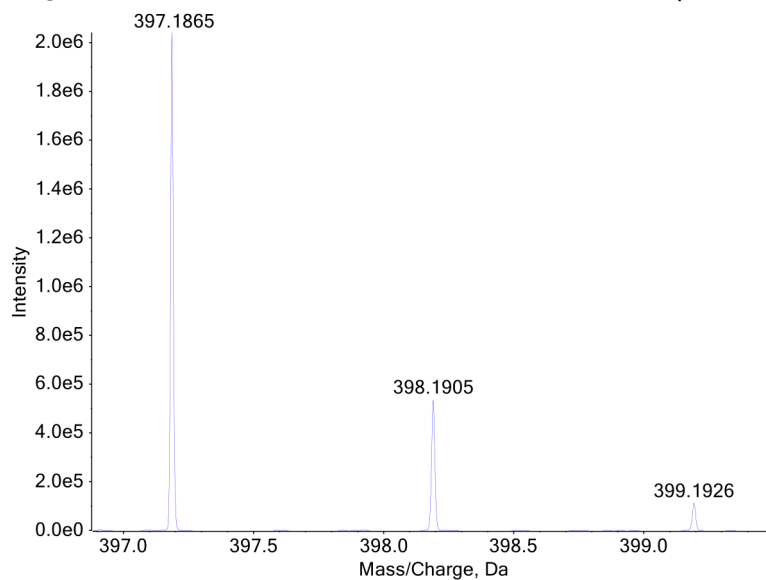
Laboratory: Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

Instrument: Sciex 5600+ LC-QTOF-MS

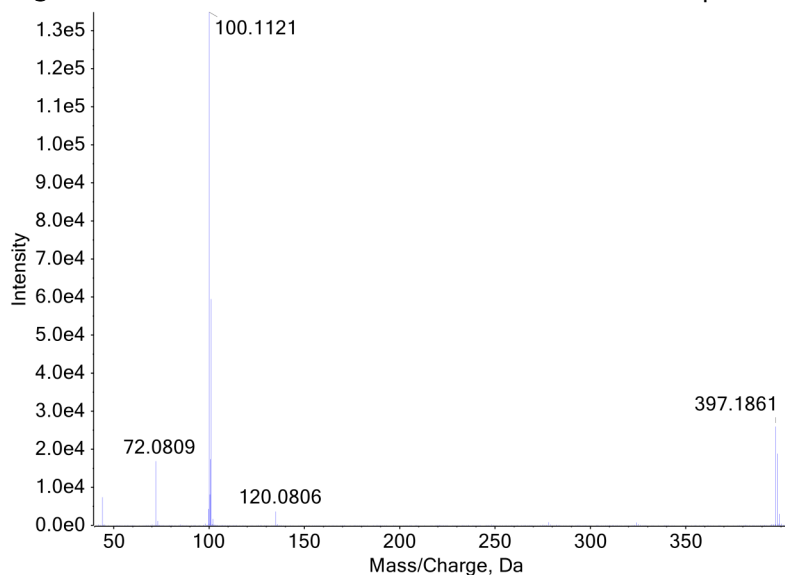
Methods: [LC-QTOF-MS Method Details](#) & [Monographs](#)

Sample Preparation: Dilution in mobile phase

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: 0698653-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be methylenedioxyvitazene based on retention time (sample: 5.91 min vs. standard: 5.94 min) and mass spectral data comparisons.