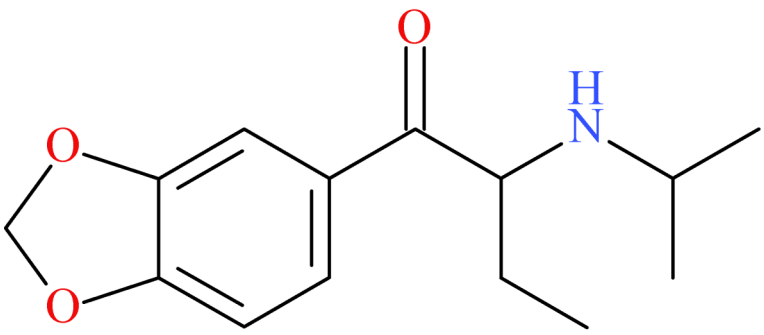
N-Isopropyl Butylone



NPS SUBCLASS
Stimulant
REPORT DATE
September 4, 2024
SAMPLE RECEIVED
August 14, 2024
SAMPLE TYPE
Drug Material

Preferred Name	*N*-Isopropyl Butylone
Synonyms	3,4-Methylenedioxy-α-Isopropylaminobutiophenone, NiPB, Isopropylbutylone
Formal Name	1-(1,3-benzodioxol-5-yl)-2-(isopropylamino)butan-1-one
InChI Key	YLUWYCAYKBCHRS-UHFFFAOYSA-N
CAS Number	17762-92-4
Chemical Formula	$C_{14}H_{19}NO_3$
Molecular Weight	249.3
Molecular Ion [M⁺]	249
Exact Mass [M+H]⁺	250.1438

Characterization & Intelligence

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

Description: *N*-Isopropyl butylone is a novel synthetic stimulant and substituted cathinone bearing structural similarity to other beta-keto methylenedioxyamphetamines (noted by the suffix "-ylone"). *N*-Isopropyl butylone is one of many structural isomers with the chemical formula $C_{14}H_{19}NO_3$ (e.g., *N*-ethyl pentylone, *N,N*-dimethylpentylone, *N*-propyl butylone). *N*-Isopropyl butylone was first identified in August 2024 in our laboratory. Confirmation was achieved using a specialized chromatographic method with analysis of standard reference materials for *N*-Isopropyl butylone and its isomers.

Sample Source: NMS Labs – Forensic Chemistry (Willow Grove, PA)

Sample Appearance: Off-white crystalline material

Pharmacology: The activity and potency of *N*-isopropyl butylone are unknown. Based on the structural similarity to other substituted cathinones (e.g., *N*-ethyl pentylone, eutylone), *N*-isopropyl butylone is hypothesized to be a potent inhibitor for the reuptake of dopamine and serotonin.[1]

Toxicology: Toxicology cases that screened positive for *N*-Isopropyl butylone (or an isomer) are currently pending confirmatory analysis at the CFSRE.

Drug Materials: *N*-Isopropyl butylone has been detected in one drug material to date at the CFSRE.

Demographics / Geographics: The drug material positive for *N*-isopropyl butylone originated from the state of Georgia. *N*-Isopropyl butylone was identified alongside methamphetamine.

Legal Status: *N*-Isopropyl butylone is not explicitly scheduled in the United States. *N*-Isopropyl butylone may be considered a positional isomer of *N*-ethyl pentylone, a Schedule I drug (21 CFR 1308).

References:

- Cayman Chemical: *N*-Isopropyl Butylone
- [1]Nadal-Gratacos *et al.* (2021) Structure-activity relationship of novel second generation synthetic cathinones...

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, LC-QTOF-MS, and LC-QQQ-MS) in comparison to analysis of acquired reference material.

Acknowledgements: This report was prepared by Sara E. Walton, Nicole Lattanzio, Kyle Brown, Branden Brunner, Melanie Liston, Donna M. Papsun, 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 and staff 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.

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Gas Chromatography Mass Spectrometry (GC-MS)

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

Sample Preparation: Acid/base extraction

Instrument: Agilent 5975 Series GC/MSD

Methods: GC-MS Method Details & Monographs

GC-MS: Mass Spectrum (EI 70 eV)

Confirmation Using Drug Standard: *Reference material (Batch: 0634229-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be N-isopropyl butylone based on retention time (sample: 5.13 min vs. standard: 5.14 min) and mass spectral data comparisons.*

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

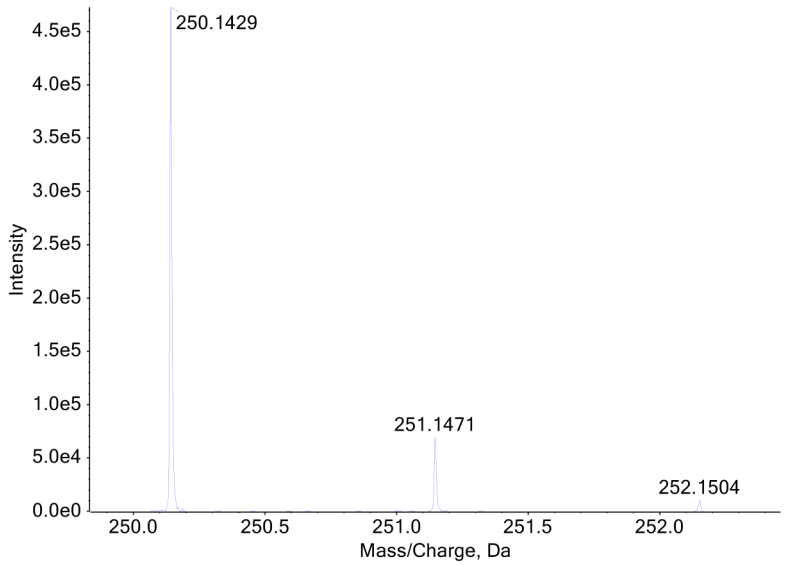
Laboratory: Center for Forensic Science Research and Education (CFSRE, Horsham, PA, USA)

Sample Preparation: Dilution in mobile phase

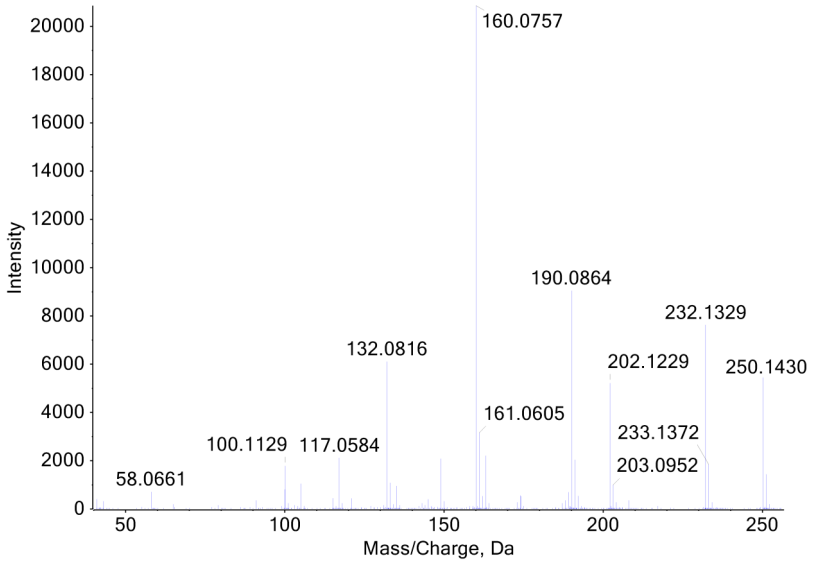
Instrument: Sciex X500R LC-QTOF-MS

Methods: LC-QTOF-MS Method Details & Monographs

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: 0634229-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be N-isopropyl butylone based on retention time (sample: 4.93 min vs. standard: 4.86 min) and mass spectral data comparisons.*