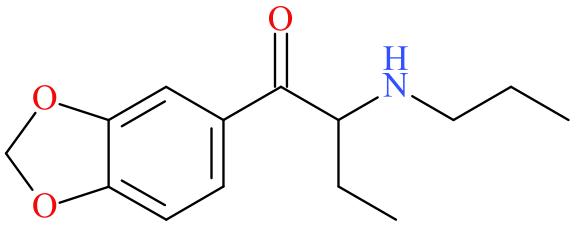
N-Propyl Butylone

Sample Type: **Drug Material**



Latest Revision: **July 21, 2022**

Date Received: **February 17, 2022**

Date of Report: **July 21, 2022**

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-(propylamino)butan-1-one
InChI String:	InChI=1S/C14H19NO3/c1-3-7-15-11(4-2)14(16)10-5-6-12-13(8-10)18-9-17-12/h5-6,8,11,15H,3-4,7,9H2,1-2H3
CFR:	Not Scheduled (07/2022)
CAS#	17762-91-3
Synonyms:	Putylone, bk-PBDB, Propylbutylone, 3,4-Methylenedioxy-α-Propylaminobutiophenone
Source:	Miami Dade Police Department
Appearance:	White Powder

***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.*

***Prepared By:** Alex J. Krotulski, PhD; Vanquilla Shellman Francis, PhD; Melissa F. Fogarty, MSFS, D-ABFT-FT; Sara E. Walton, MS; and Barry K. Logan, PhD, F-ABFT*

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{14}H_{19}NO_3$	249.3	249	250.1438

3. BRIEF DESCRIPTION

N-Propyl butylone is classified as a novel stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause psychoactive effects similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar drugs include butylone and eutylone (also known as *N*-ethyl butylone), among other *beta*-keto methylenedioxyamphetamine (or "-ylones"). Butylone is a Schedule I substance in the United States; *N*-propyl butylone is not explicitly scheduled. *N*-Propyl butylone was first reported in Europe (Czech Republic) in July 2013; however, there is no evidence that the drug had previously proliferated or emerged with regularity in the United States. *N*-Propyl butylone is a structural isomer of *N*,*N*-dimethylpentylone, *N*-ethyl pentylone and others, requiring increased specificity during analysis. In addition to the drug material reported herein, to date, *N*-propyl butylone has been identified in at least four toxicology samples alongside *N*,*N*-dimethylpentylone (requiring chromatographic resolution for quantitation).

4. ADDITIONAL RESOURCES

EMCDDA–Europol 2013 Annual Report on the implementation of Council Decision 2005/387/JHA

2022 Q2 NPS Stimulants and Hallucinogens Trend Report

https://www.caymanchem.com/product/30892

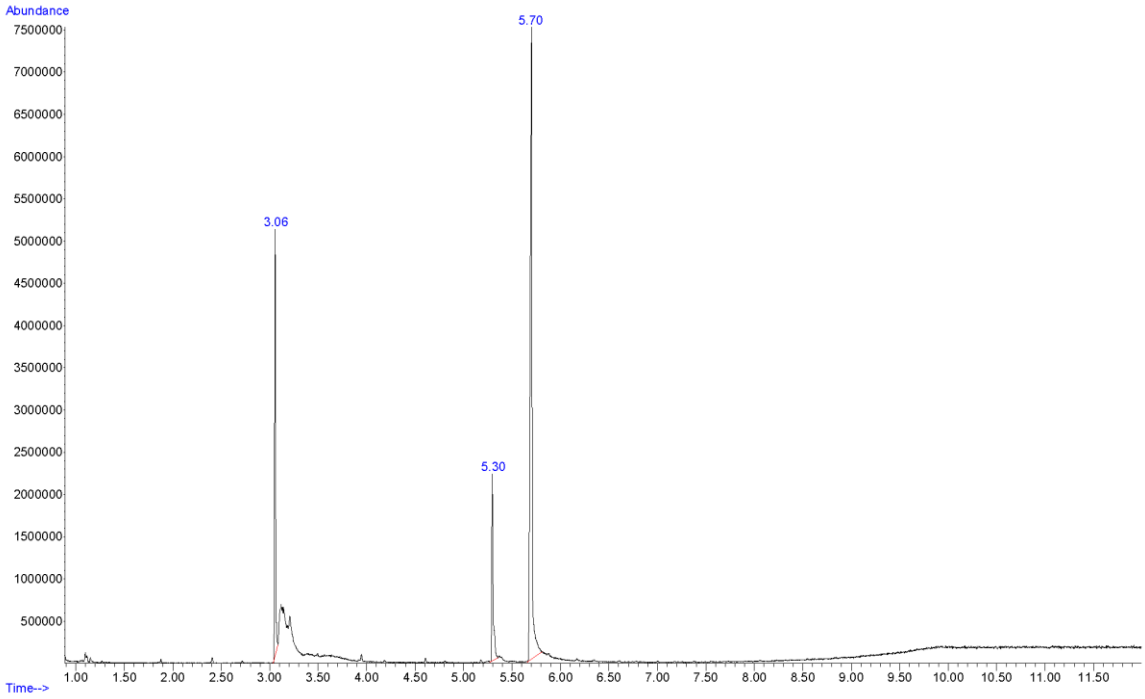
https://drugs.ncats.io/substance/46BQ874756

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

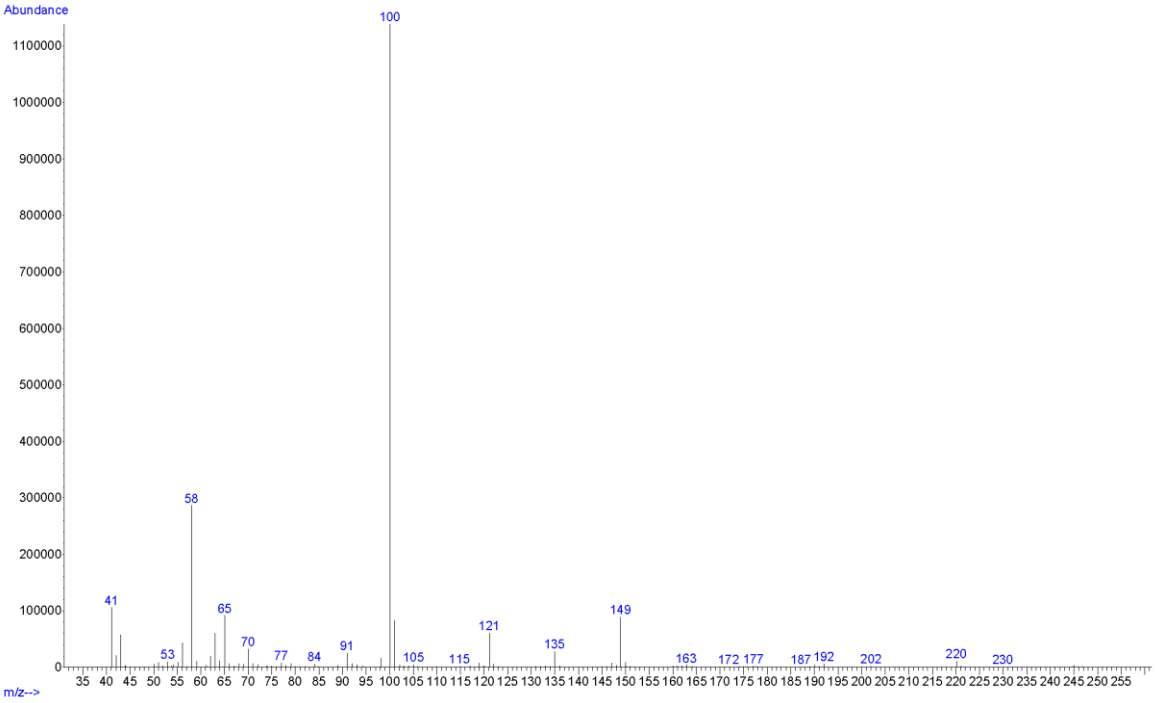
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Dilution in methanol (Miami Dade Police Department)
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 µm x 0.33 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:	5.30 min
Standard Comparison:	Reference material for *N*-Propyl Butylone (Batch: 0634227-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *N*-Propyl Butylone based on retention time (5.31 min) and mass spectral data. (https://www.caymanchem.com/product/30892)

Chromatogram: *N*-Propyl Butylone



Additional peaks in chromatogram: internal standards (3.06 and 5.70 mins)

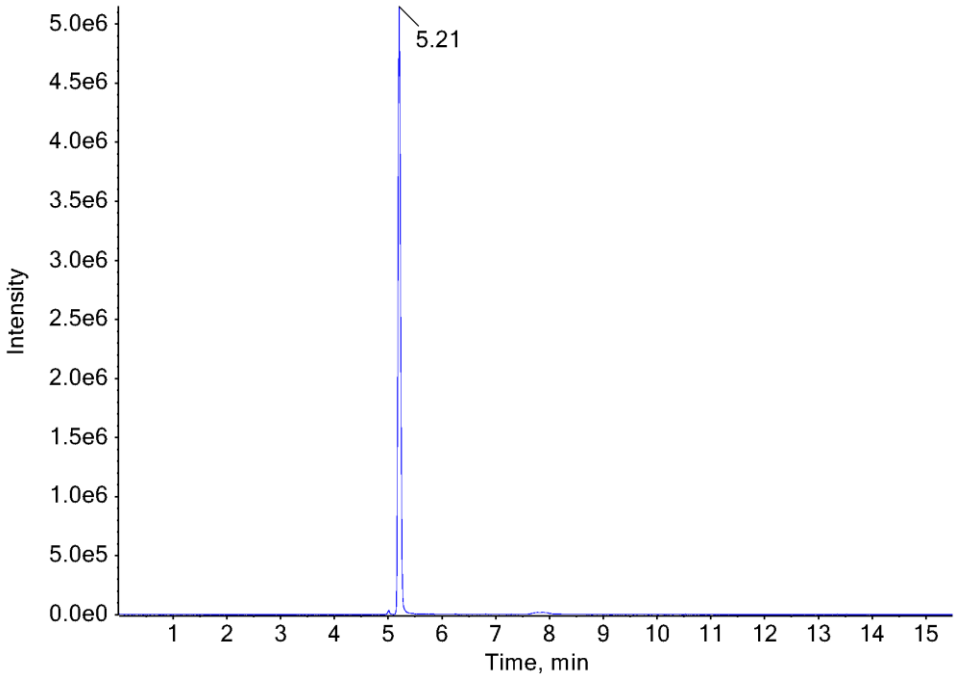
EI (70 eV) Mass Spectrum: *N*-Propyl Butylone



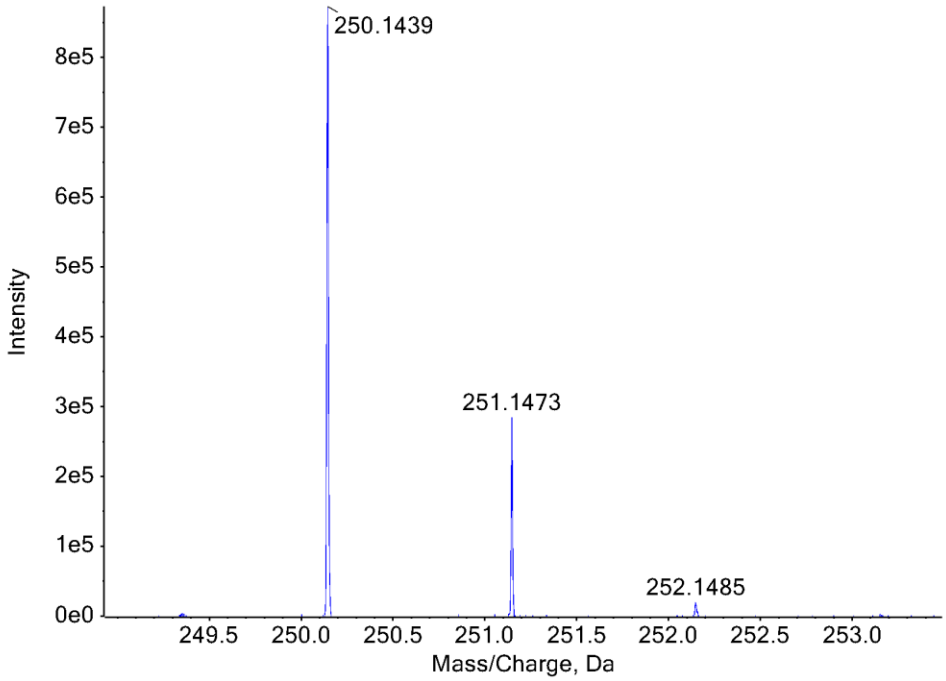
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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 (Miami Dade Police Department) 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:	5.21 min
Standard Comparison:	Reference material for *N*-Propyl Butylone (Batch: 0634227-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *N*-Propyl Butylone based on retention time (5.11 min) and mass spectral data. (https://www.caymanchem.com/product/30892)

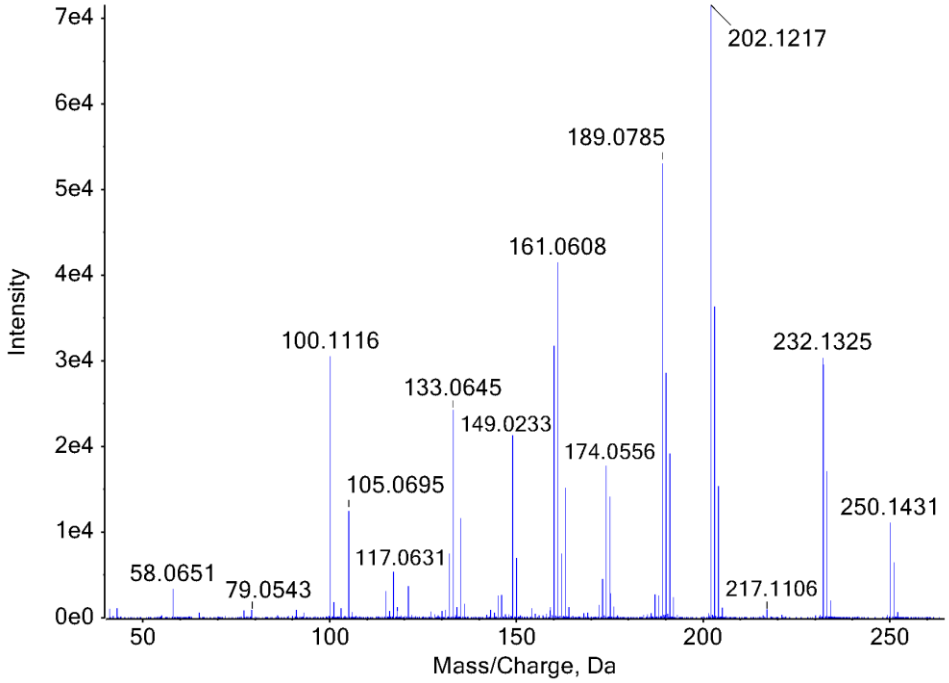
Extracted Ion Chromatogram: *N*-Propyl Butylone



TOF MS Spectra: *N*-Propyl Butylone



TOF MS/MS Spectra: *N*-Propyl Butylone



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.