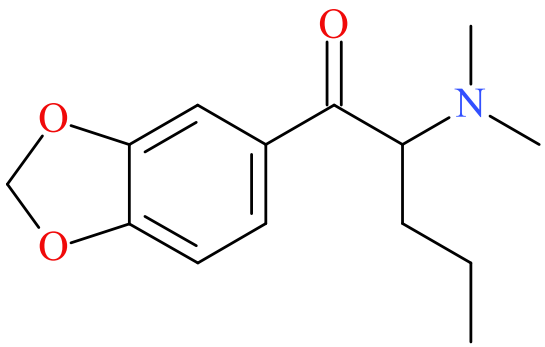
N,*N*-Dimethylpentylone

Sample Type: **Toxicology Sample**



Latest Revision: **December 17, 2021**

Date Received: **November 1, 2021**

Date of Report: **December 17, 2021**

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)pentan-1-one
InChI String:	InChI=1S/C14H19NO3/c1-4-5-11(15(2)3)14(16)10-6-7-12-13(8-10)18-9-17-12/h6-8,11H,4-5,9H2,1-3H3
CFR:	Not Scheduled (12/2021)
CAS#	17763-13-2
Synonyms:	Dipentylone, Dimethylpentylone, bk-DMBDP, *beta*-keto-DMBDP, beta-keto-Dimethylbenzodioxolylpentanamine, bk-dimethyl-K
Source:	NMS Labs – Toxicology Department

***Important Note**: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material.*

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

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Drug	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
N,*N*-Dimethylpentylone	$C_{14}H_{19}NO_3$	249.3	249	250.1438

3. BRIEF DESCRIPTION

N,*N*-Dimethylpentylone 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 compounds include *N*-ethyl pentylone, pentylone, and eutylone. *N*-Ethyl pentylone and pentylone are Schedule I substances in the United States, while eutylone can be considered an isomer of pentylone. *N*,*N*-Dimethylpentylone is not explicitly scheduled in the United States; however, this drug may be considered a scheduled substance being an isomer of *N*-ethyl pentylone. Since *N*,*N*-dimethylpentylone is a structural isomer of *N*-ethyl pentylone (and other beta-keto methylenedioxyamphetamines), analytical methods will require increased specificity for accurate identification and distinction. Preliminary data show that pentylone may be a major metabolite of *N*,*N*-dimethylpentylone – laboratories detecting pentylone, or commonly encountering novel stimulants, should consider adding *N*,*N*-dimethylpentylone to their scope of analytical testing as soon as possible.

4. ADDITIONAL RESOURCES

Koppe, H.; Ludwig, G.; and Zeile, K. Aryl-alpha-Aminoketone Derivatives. CH Boehringer Sohn AG and Co KG, Boehringer Ingelheim GmbH, Assignee. Patent GB1085135A. 08 Apr. 1964. https://patents.google.com/patent/GB1085135A/ru

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Dipentylone-ID-HIFS-005_report.pdf

https://www.caymanchem.com/product/9001933/n%2Cn-dimethylpentylone-(hydrochloride)

N-Ethyl Pentylone: https://www.deadiversion.usdoj.gov/drug_chem_info/n-ethylpentylone.pdf

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

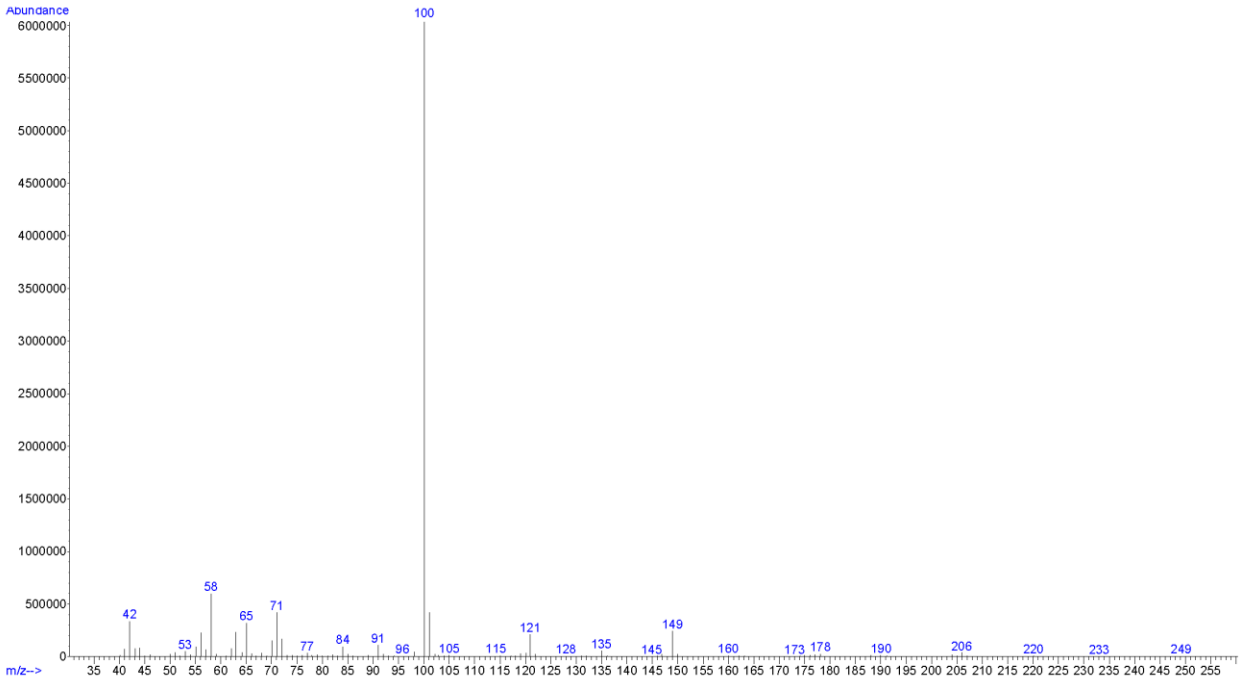
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for *N*,*N*-Dimethylpentylone (Batch: 0489680-18) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/9001933/n%2Cn-dimethylpentylone-(hydrochloride))

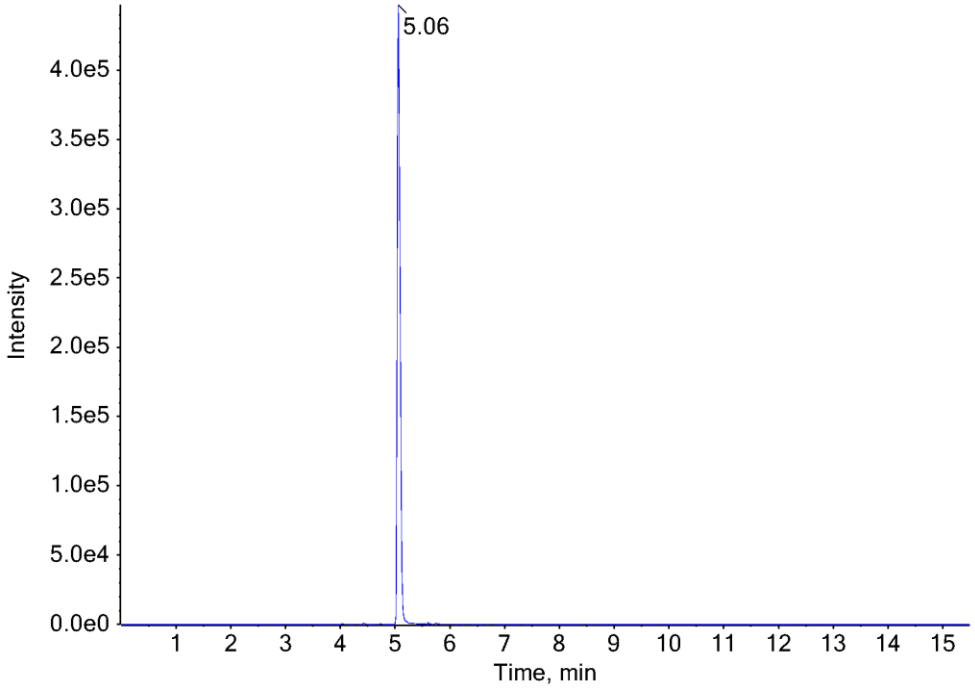
EI (70 eV) Mass Spectrum: *N*,*N*-Dimethylpentylone (Standard)



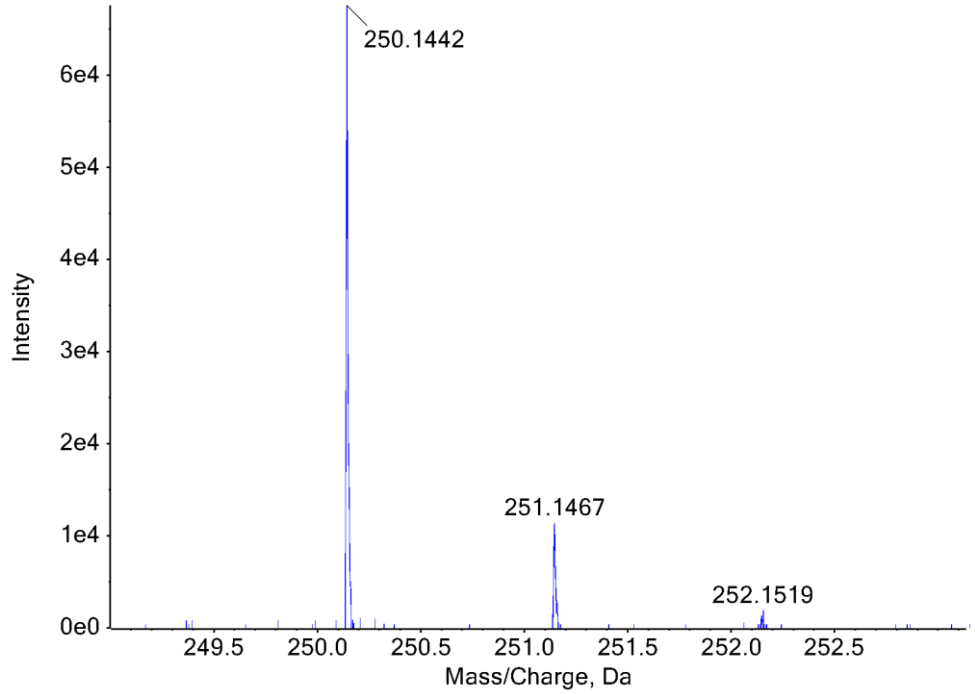
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Liquid-liquid extraction (LLE)
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:	5.06 min
Standard Comparison:	Reference material for *N*,*N*-Dimethylpentylone (Batch: 0489680-18) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as *N*,*N*-dimethylpentylone, based on retention time (5.13 min) and mass spectral data. (https://www.caymanchem.com/product/9001933/n%2Cn-dimethylpentylone-(hydrochloride))

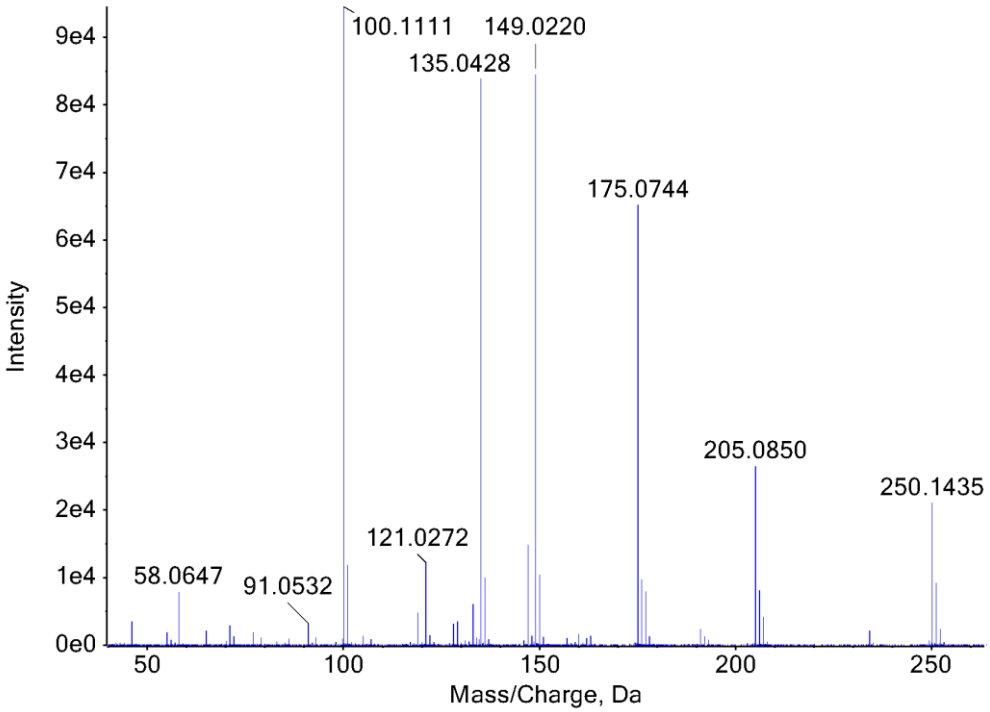
Extracted Ion Chromatogram: *N,N*-Dimethylpentylone



TOF MS Spectra: *N,N*-Dimethylpentylone



MS/MS Spectra: *N,N*-Dimethylpentylone



6. FUNDING

NPS Discovery 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 DOJ.