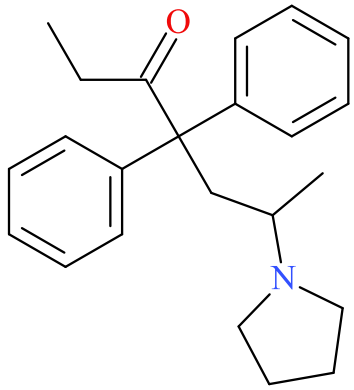
Dipyanone

Sample Type: **Seized Material**



Latest Revision: **March 14, 2022**

Date Received: **November 17, 2021**

Date of Report: **March 14, 2022**

1. GENERAL INFORMATION

IUPAC Name:	4,4-diphenyl-6-pyrrolidin-1-yl-heptan-3-one
InChI String:	InChI=1S/C23H29NO/c1-3-22(25)23(20-12-6-4-7-13-20,21-14-8-5-9-15-21)18-19(2)24-16-10-11-17-24/h4-9,12-15,19H,3,10-11,16-18H2,1-2H3
CFR:	Not Scheduled (03/20212)
CAS#	Not Available
Synonyms:	N-pyrrolidino Methadone
Source:	NMS Labs – Criminalistic Laboratory
Appearance:	White Solid Material

***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.*

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{23}H_{29}NO$	335	335.5	336.2322

3. BRIEF DESCRIPTION

Dipyanone is classified as a novel opioid. Novel opioids have been reported to cause psychoactive effects similar to heroin, fentanyl, and other opioids. Novel opioids have also caused adverse events, including death, as described in the literature. Dipyanone is reported to be slightly less potent that structurally similar opioids methadone and dipipanone.[1] Literature reports involving dipyanone are limited. Dipyanone is not explicitly scheduled in the United States; methadone is a Schedule II drug and dipipanone is a Schedule I drug.

4. ADDITIONAL RESOURCES

1. Ofner P, Walton E (1950). Search for new analgesics. Part IV. Variations in the basic side-chain of amidone. *Journal of the Chemical Society*, 2158-2166. https://pubs.rsc.org/en/content/articlelanding/1950/JR/jr9500002158

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Dipyanone-ID-2955-21_report.pdf

https://www.caymanchem.com/product/33720/dipyanone-(hydrochloride)

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)

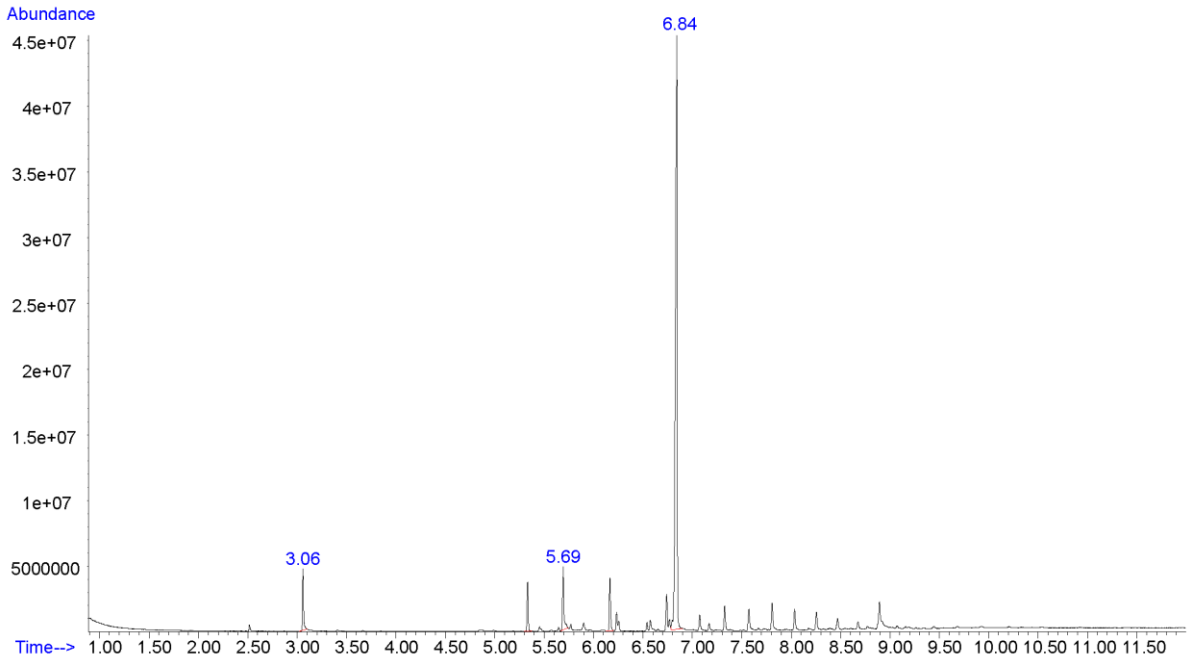
Sample Preparation: Acid/Base extraction (NMS Labs)

Instrument: Agilent 5975 Series GC/MSD System

Column: Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)

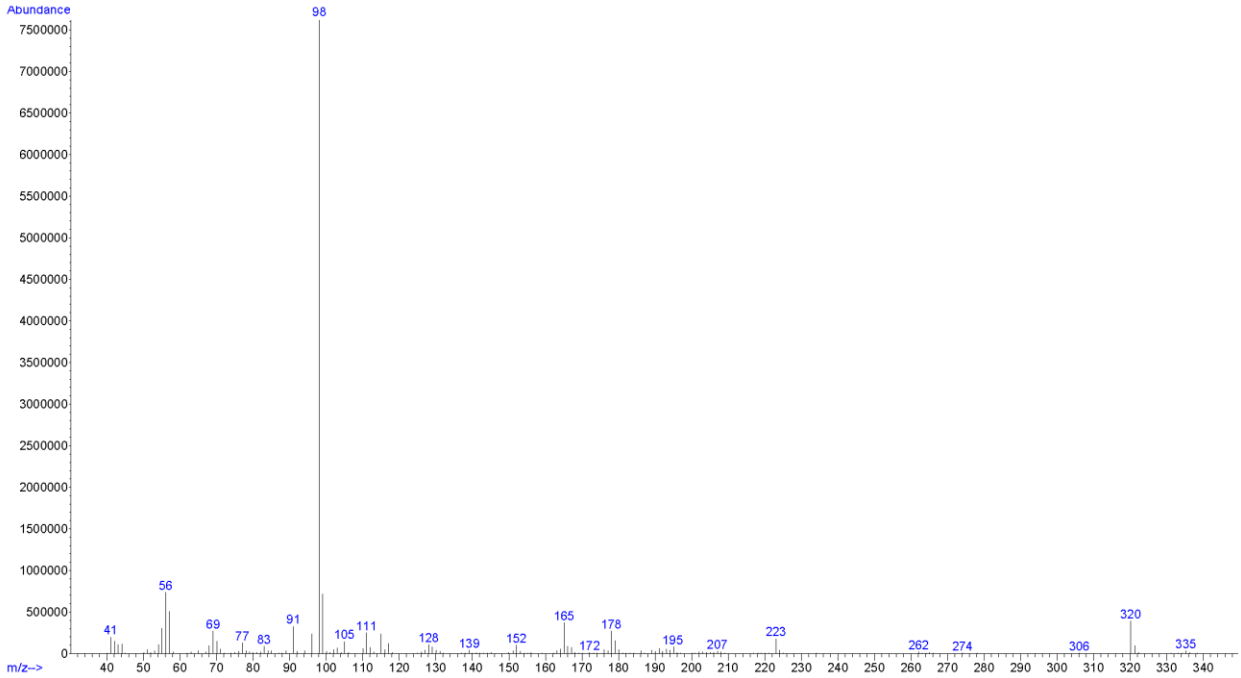
Carrier Gas:	Helium (Flow: 1.46 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	6.84 min
Standard Comparison:	Reference material for Dipyanone (Batch: 0626300-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Dipyanone based on retention time (6.83 min) and mass spectral data. (https://www.caymanchem.com/product/33720/dipyanone-(hydrochloride))

Chromatogram: Dipyanone

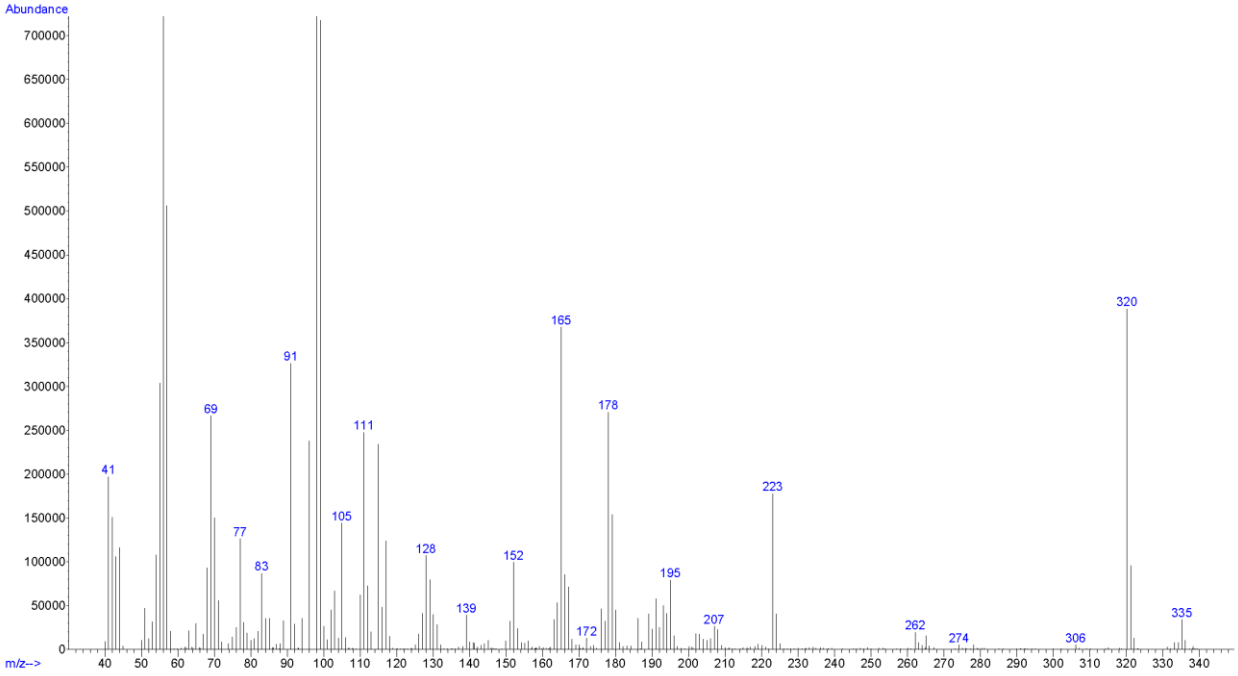


Additional peaks present in chromatogram: internal standards (3.06 min and 5.69 min)

EI (70 eV) Mass Spectrum: Dipyanone



EI (70 eV) Mass Spectrum 10x: Dipyanone

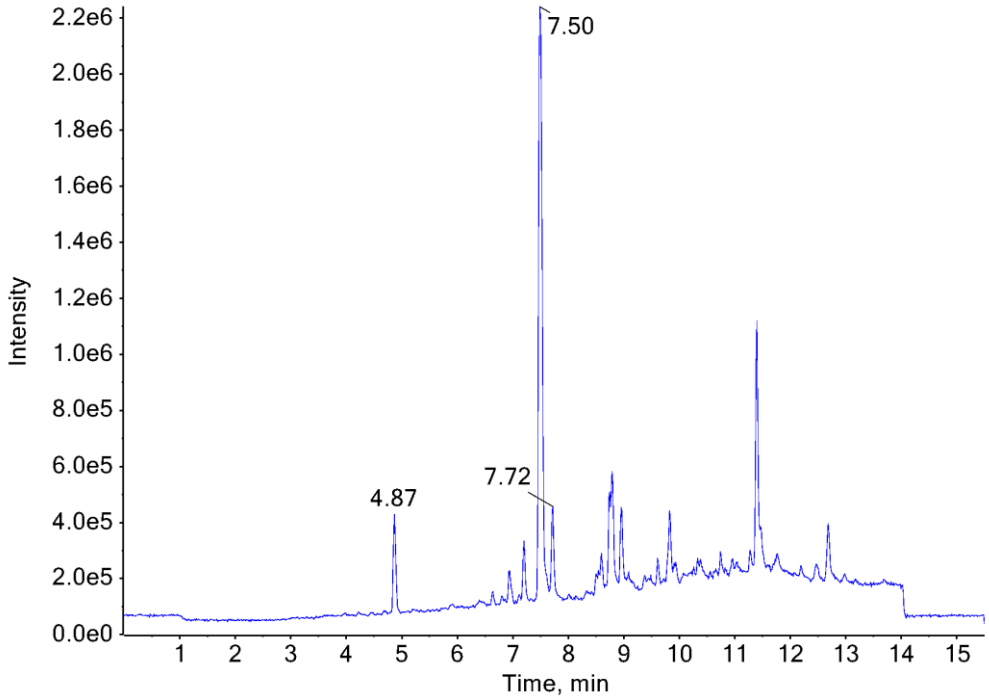


5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
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

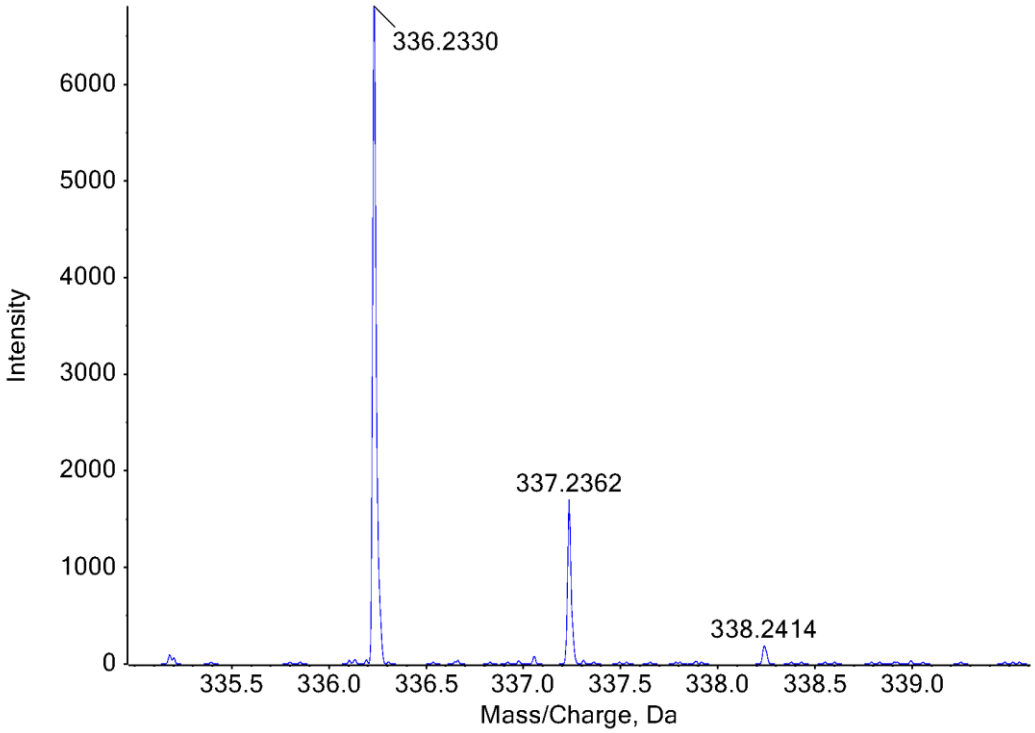
	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 10 µL
QTOF Parameters:	TOF MS Scan Range: 100-510 Da
	Precursor Isolation: SWATH® acquisition (27 windows)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	7.50 min
Standard Comparison:	Reference material for Dipyanone (Batch: 0626300-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Dipyanone based on retention time (7.60 min) and mass spectral data. (https://www.caymanchem.com/product/33720/dipyanone-(hydrochloride))

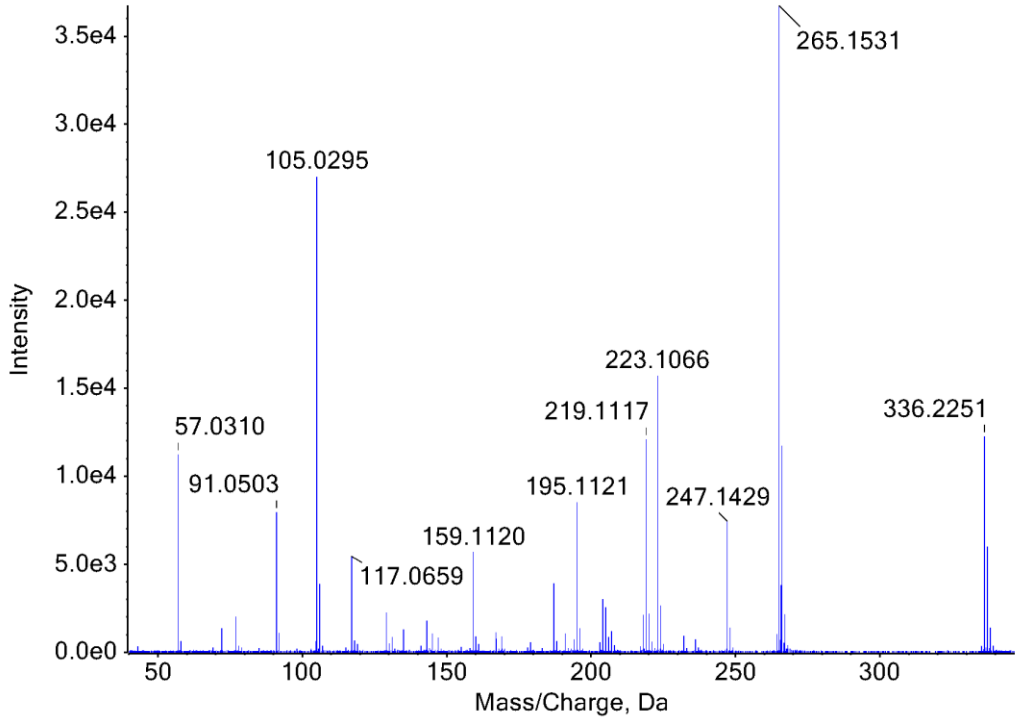
Chromatogram: Dipyanone



Additional peaks present in chromatogram: internal standards (4.87 min and 7.72 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Dipyanone





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.