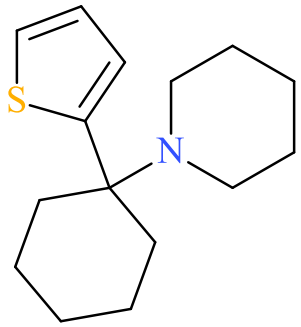
Tenocyclidine

Sample Type: **Toxicology Sample**



Latest Revision: **December 15, 2021**

Date Received: **June 30, 2021**

Date of Report: **December 15, 2021**

1. GENERAL INFORMATION

IUPAC Name:	1-[1-(2-thienyl)cyclohexyl]piperidine
InChI String:	InChI=1S/C15H23NS/c1-3-9-15(10-4-1,14-8-7-13-17-14)16-11-5-2-6-12-16/h7-8,13H,1-6,9-12H2
CFR:	Schedule I (U.S.)
CAS#	1867-65-8
Synonyms:	TCP
Source:	ACMT's Toxicology Investigators Consortium (ToxIC)

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

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Drug	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Tenocyclidine	$C_{15}H_{23}NS$	249.4	249	250.1624

3. SAMPLE HISTORY

To date, tenocyclidine was identified in nine clinical cases since June 2021. The geographical and demographical breakdown is below:

Geographical Location: New York (n=9)

Biological Sample: Plasma (n=9)

Date of First Receipt: June 2021

Other Notable Findings: PCP (n=8), Methadone (n=6), Fentanyl (n=2)

4. BRIEF DESCRIPTION

Tenocyclidine (TCP) is classified as a hallucinogen bearing structural and pharmacological similarity to phencyclidine (PCP). Novel hallucinogens have been reported to cause effects similar to phencyclidine and ketamine, and have caused adverse events, including death, as described in the literature. Tenocyclidine was first synthesized and reported in the literature in the 1950s.[1] Tenocyclidne is reported to be more potent than phencyclidine, with higher affinity for the *N*-methyl-D-aspartate (NMDA) receptor.[2] Tenocyclidine and phencyclidine are explicitly Schedule I drugs in the United States.

5. ADDITIONAL RESOURCES

1. Parcell, RF. (19 September 1957). “Patent US2921076 – Heterocyclic compounds and methods for producing the same.” https://patents.google.com/patent/US2921076

2. Stirling, JM; Cross, AJ; Green, AR. (1989). "The binding of [3H]thienyl cyclohexylpiperidine ([3H]TCP) to the NMDA-phencyclidine receptor complex". *Neuropharmacology*. **28** (1): 1–7. https://www.sciencedirect.com/science/article/abs/pii/0028390889900592?via%3Dihub

https://www.caymanchem.com/product/17014/tenocyclidine-(hydrochloride)

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

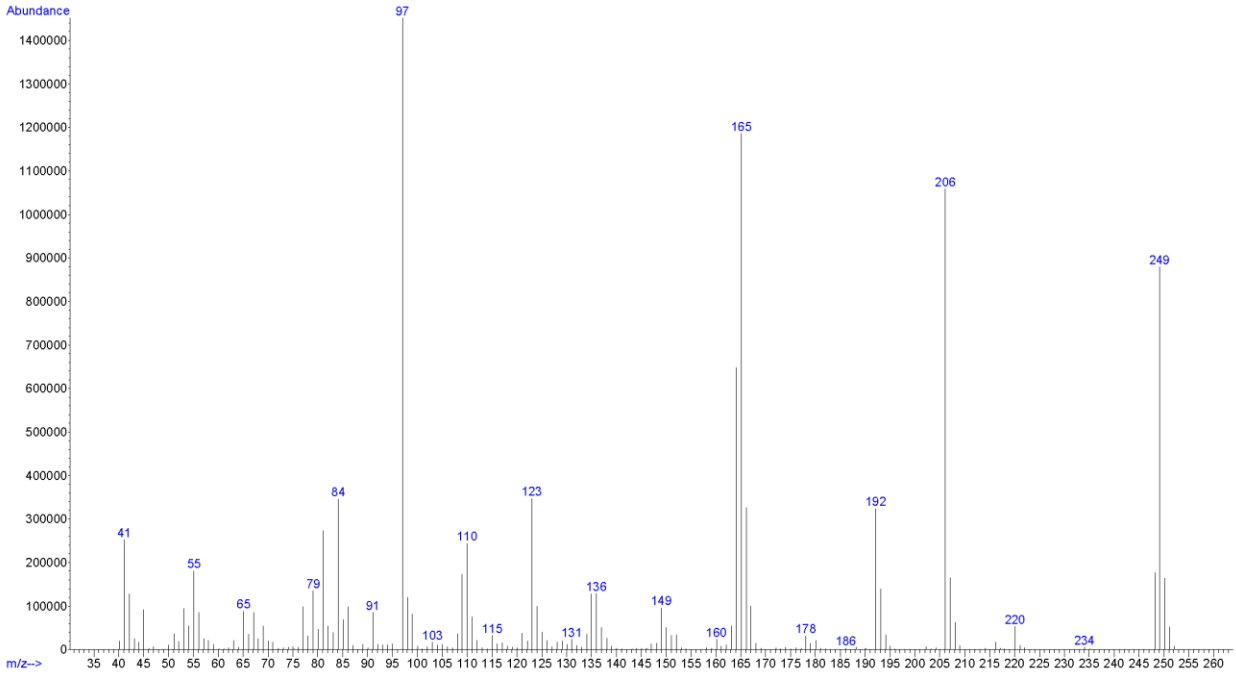
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for Tenocyclidine (Batch: 0526785-14) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/17014/tenocyclidine-(hydrochloride))

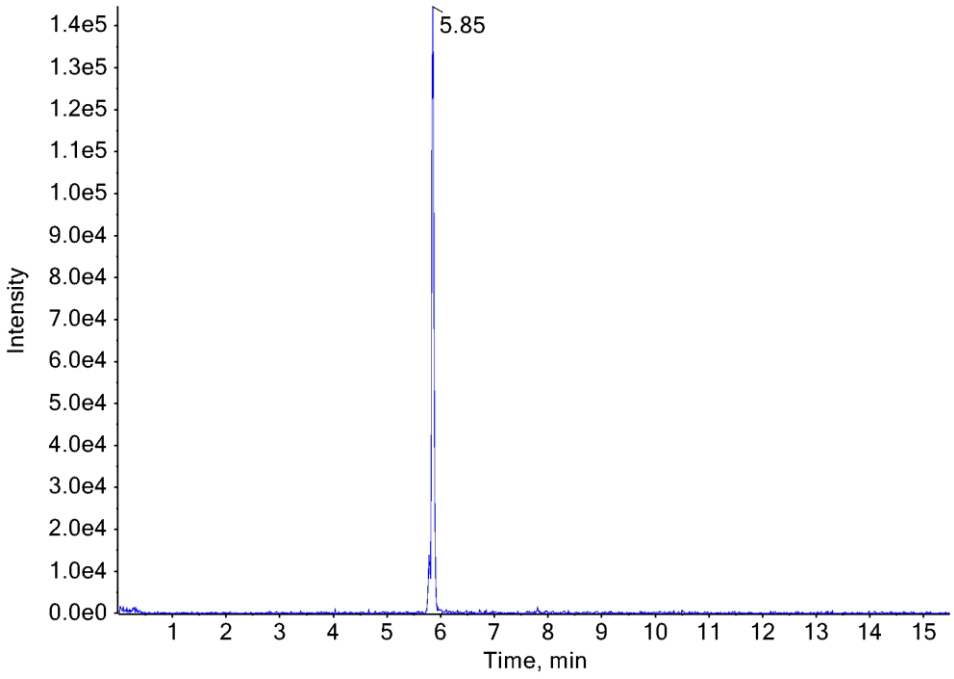
EI (70 eV) Mass Spectrum: Tenocyclidine (Standard)



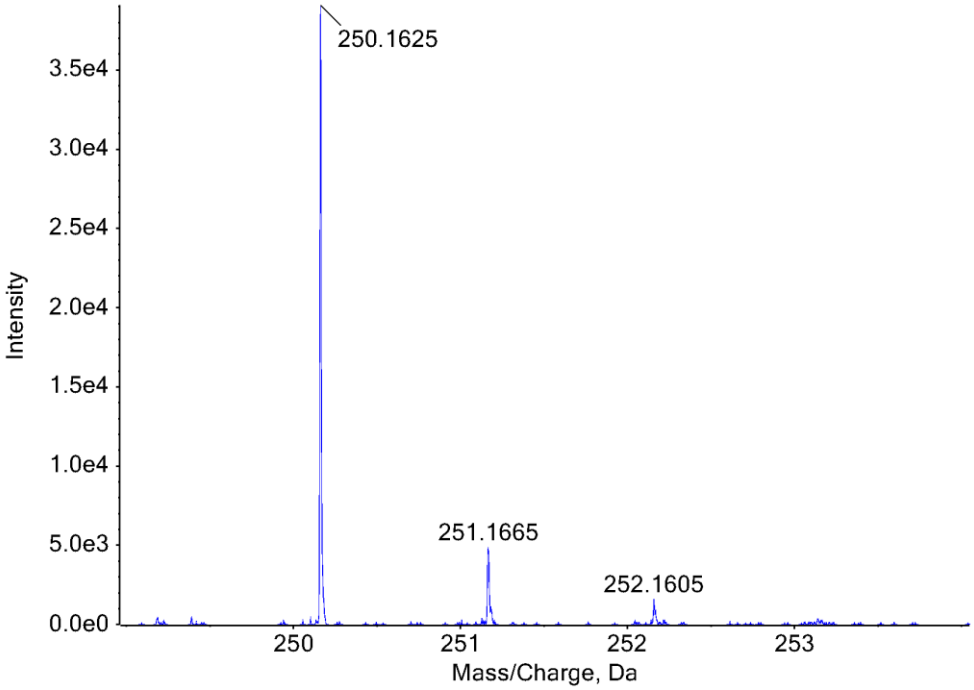
6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

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:	5.85 min
Standard Comparison:	Reference material for Tenocyclidine (Batch: 0526785-14) 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 Tenocyclidine, based on retention time (5.75 min) and mass spectral data. (https://www.caymanchem.com/product/17014/tenocyclidine-(hydrochloride))

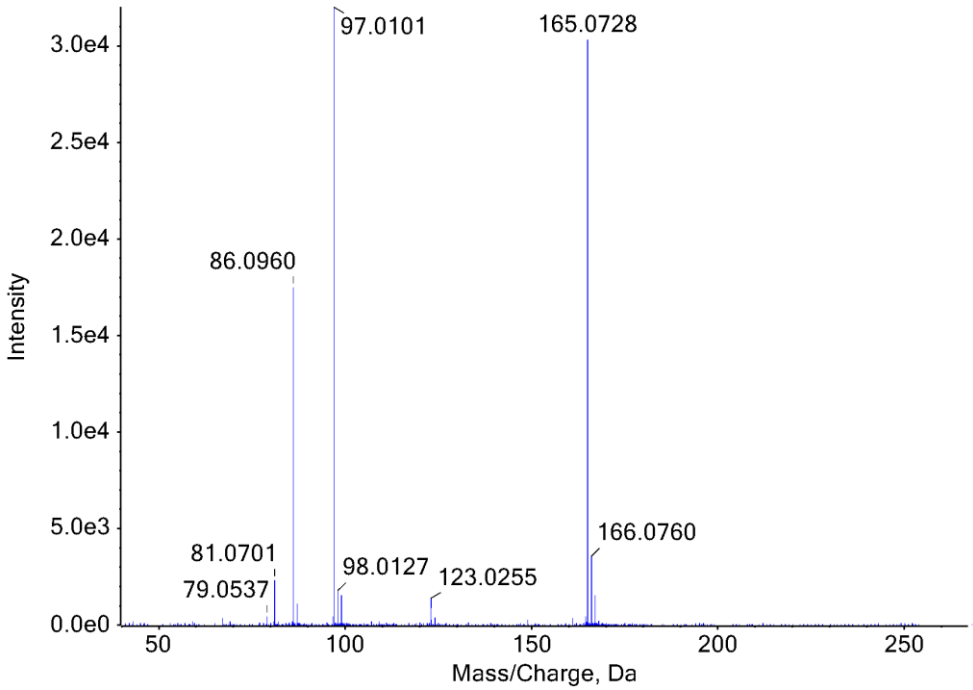
Extracted Ion Chromatogram: Tenocyclidine



TOF MS Spectra: Tenocyclidine



MS/MS Spectra: Tenocyclidine



7. FUNDING

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