

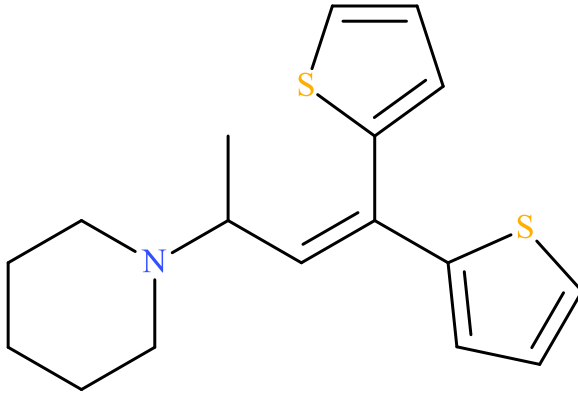
Piperidylthiambutene

Sample Type: **Seized Material**

Latest Revision: **September 18, 2019**

Date Received: **August 16, 2019**

Date of Report: **September 18, 2019**



1. GENERAL INFORMATION

IUPAC Name:	1-[1-methyl-3,3-bis(2-thienyl)allyl]piperidine
InChI String:	InChI=1S/C17H21NS2/c1-14(18-9-3-2-4-10-18)13-15(16-7-5-11-19-16)17-8-6-12-20-17/h5-8,11-14H,2-4,9-10H2,1H3
CFR:	Not Scheduled (09/2019)
CAS#	64037-51-0
Synonyms:	Piperidinohton
Source:	Department of Homeland Security
Appearance:	Tan Solid Material

Important Note: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF) 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 ₁₇ H ₂₁ NS ₂	303.5	303	304.1188

3. BRIEF DESCRIPTION

Piperidylthiambutene is classified as a synthetic opioid. Piperidylthiambutene is structurally distinct from fentanyl, its analogues, and other synthetic opioids previously reported. Piperidylthiambutene is not explicitly a scheduled substance in the United States. Piperidylthiambutene was found to be active with similar activity to morphine when studied in a rat model.¹

4. ADDITIONAL RESOURCES

1. Adamson, D.W.; Green, A.F. (1950). A new series of analgesics. *Nature*. 165 (4186): 122.

<https://www.ncbi.nlm.nih.gov/pubmed/15409854>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Piperidylthiambuten_e-ID-2034-18_report.pdf

<https://www.caymanchem.com/product/26335>

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

Sample Preparation: Acid/Base extraction

Instrument: Agilent 5975 Series GC/MSD System

Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 μm x 0.25 μm)

Carrier Gas: Helium (Flow: 1 mL/min)

Temperatures: Injection Port: 265 °C
Transfer Line: 300 °C
MS Source: 230 °C
MS Quad: 150 °C
Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

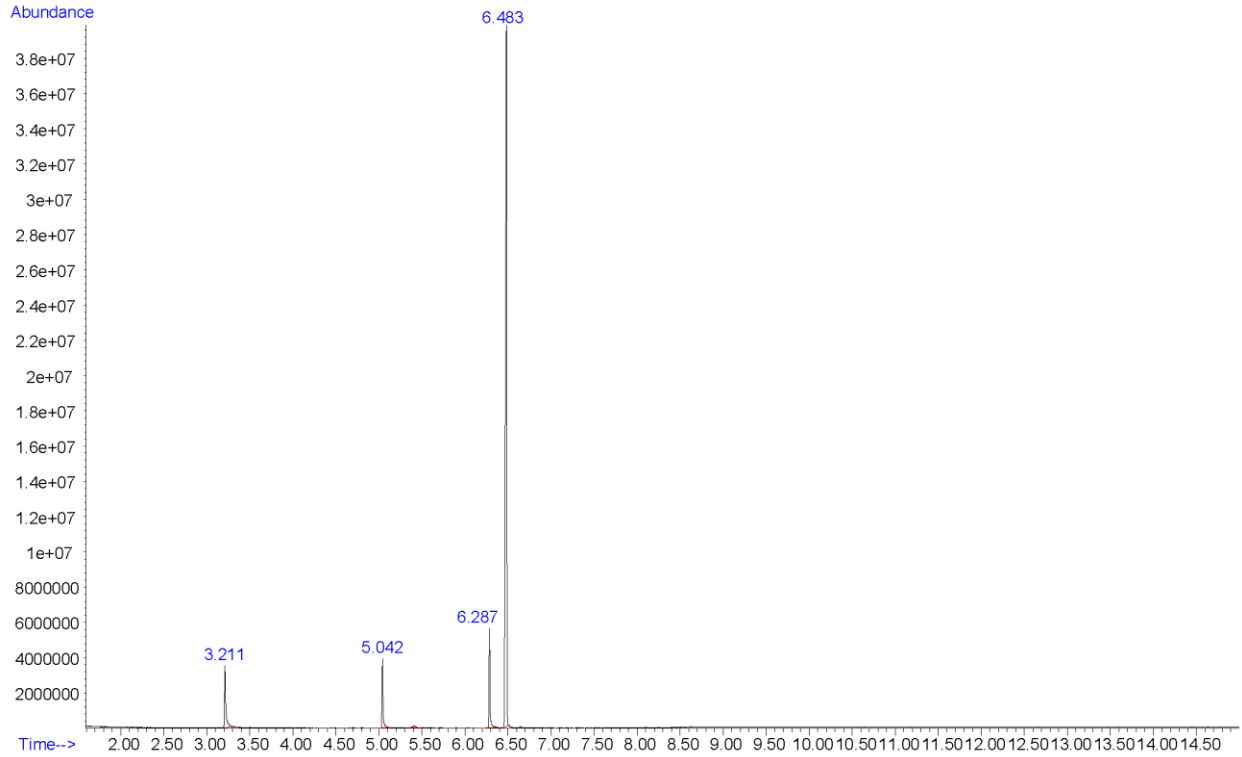
Injection Parameters: Injection Type: Splitless
Injection Volume: 1 µL

MS Parameters: Mass Scan Range: 40-550 m/z
Threshold: 250

Retention Time: 6.483 min

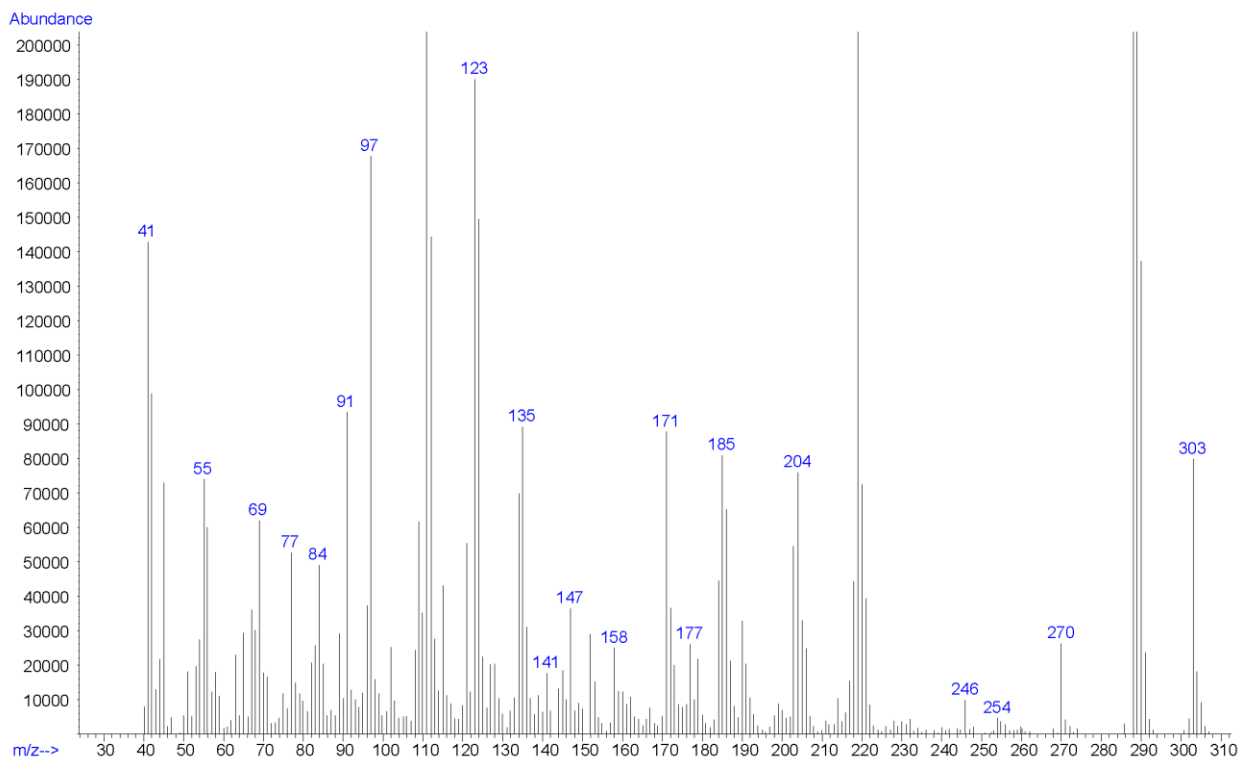
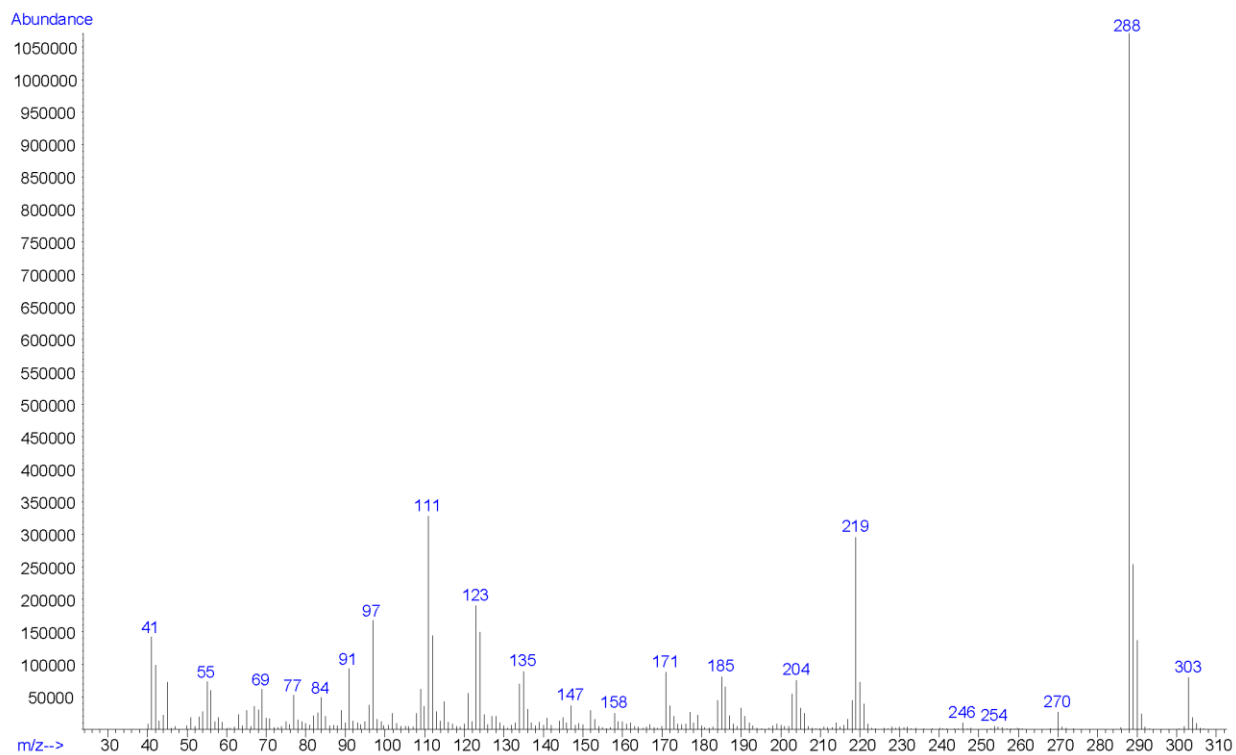
Standard Comparison: Reference material for Piperidylthiambutene (Batch: 0545005-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Piperidylthiambutene, based on retention time (6.468 min) and mass spectral data.
(<https://www.caymanchem.com/product/26335>)

Chromatogram: Piperidylthiambutene



Additional peaks present in chromatogram: internal standard (3.211 min), not a controlled substance (5.042 mins) and internal standard (6.287 min)

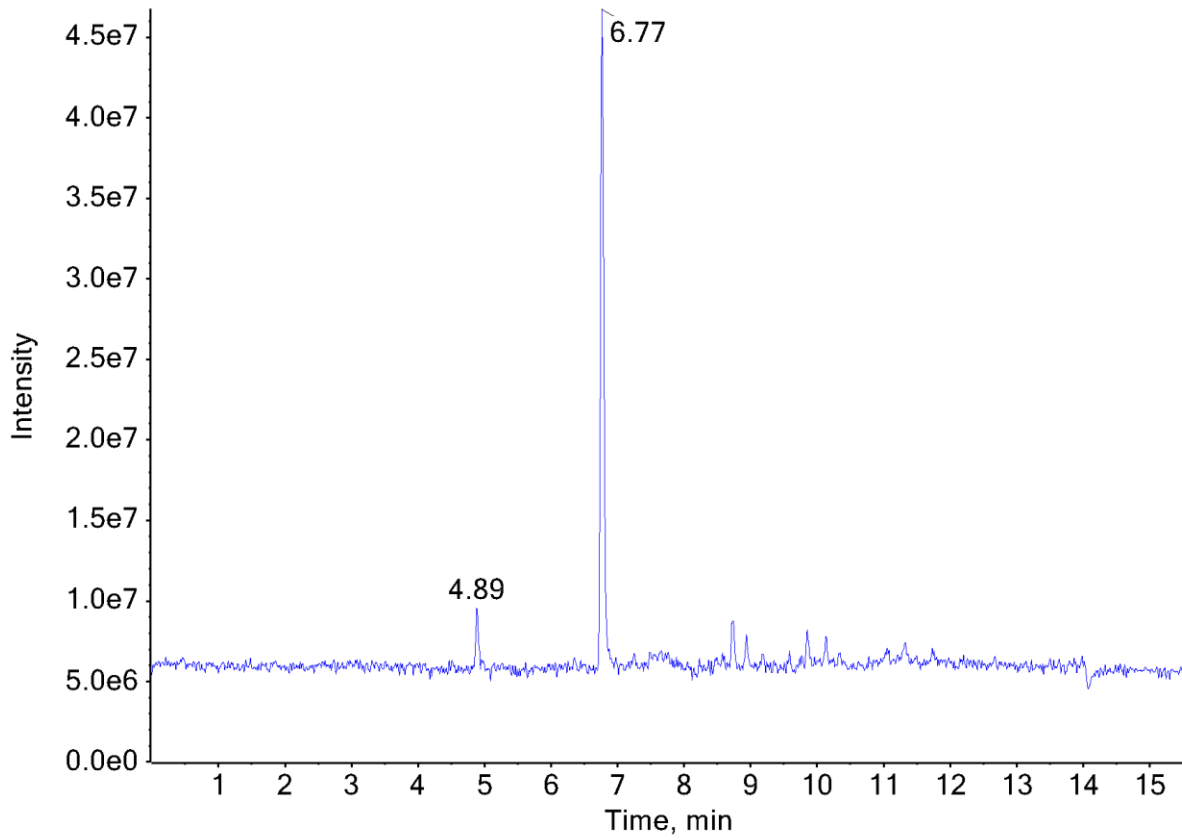
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Piperidylthiambutene



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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	6.77 min
Standard Comparison:	Reference material for Piperidylthiambutene (Batch: 0545005-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Piperidylthiambutene, based on retention time (6.78 min) and mass spectral data. (https://www.caymanchem.com/product/26335)

Chromatogram: Piperidylthiambutene



Additional peaks present in chromatogram: internal standards (4.89 min)

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

