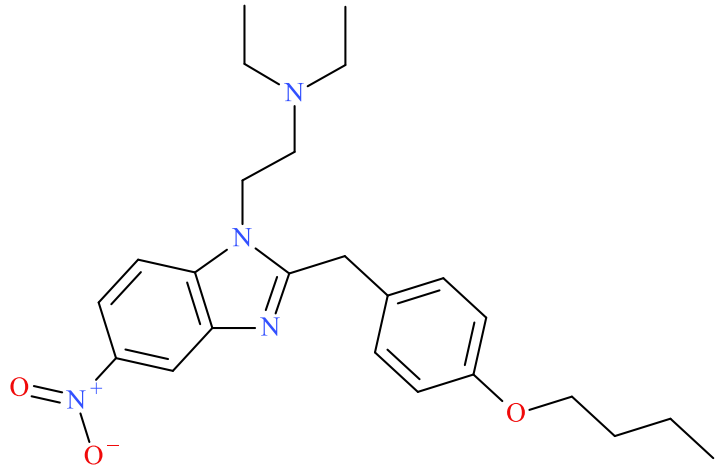
Butonitazene

Sample Type: **Biological Fluid**



Latest Revision: **January 15, 2021**

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

1. GENERAL INFORMATION

IUPAC Name: 2-[2-[(4-butoxyphenyl)methyl]-5-nitro-benzimidazol-1-yl]-N,N-diethyl-ethanamine

InChI String: InChI=1S/C24H32N4O3/c1-4-7-16-31-21-11-8-19(9-12-21)17-24-25-22-18-20(28(29)30)10-13-23(22)27(24)15-14-26(5-2)6-3/h8-13,18H,4-7,14-17H2,1-3H3

CFR: Not Scheduled (01/2021)

CAS# 95810-54-1

Synonyms: Butoxynitazene

Source: Summit County Medical Examiner's Office

***Important Notes**: 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 DATA

Analyte	Chemical Formula	Molecular Weight	Molecular Ion [M^+]	Exact Mass [$M+H]^+$
Butonitazene	$C_{24}H_{32}N_4O_3$	424.5	424	425.2547

3. SAMPLE HISTORY

Butonitazene has been identified in one case since January 2021. The geographical and demographical breakdown is below:

Geographical Location: Ohio (n=1)

Biological Sample: Blood, serum, and urine (n=1)

Date of First Receipt: January 6, 2021

Other Notable Findings: Metonitazene (n=1), *N*-Ethyl Pentedrone (n=1)

4. BRIEF DESCRIPTION

Butonitazene is classified as a novel opioid of the benzimidazole sub-class and is structurally dissimilar from fentanyl. 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. Structurally similar compounds include isotonitazene, etonitazene, and metonitazene. These synthetic opioids were first synthesized and reported in the literature in the 1950s.[1] Data suggest that this group of analogues can have potency similar to or greater than fentanyl.[2] Etonitazene is reported to be the most potent followed by isotonitazene and metonitazene. Butonitazene is not explicitly scheduled in the United States; however, isotonitazene and etonitazene are Schedule I substances.

5. ADDITIONAL RESOURCES

1. Hunger, A; Kebrle, J; Rossi, A; Hoffmann, K. (1957) Synthesis of analgesically active benzimidazole derivatives with basic substitutions. *Experientia*, **13**, 400-401. https://link-springer-com.proxyiub.uits.iu.edu/article/10.1007/BF02161116

2. Hoffmann, K; Hunger, A; Rossi, A. (3 May 1960). "Patent US2935514A – Benzimidazoles." https://patents.google.com/patent/US2935514A/en

https://www.caymanchem.com/product/30278/butonitazene

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

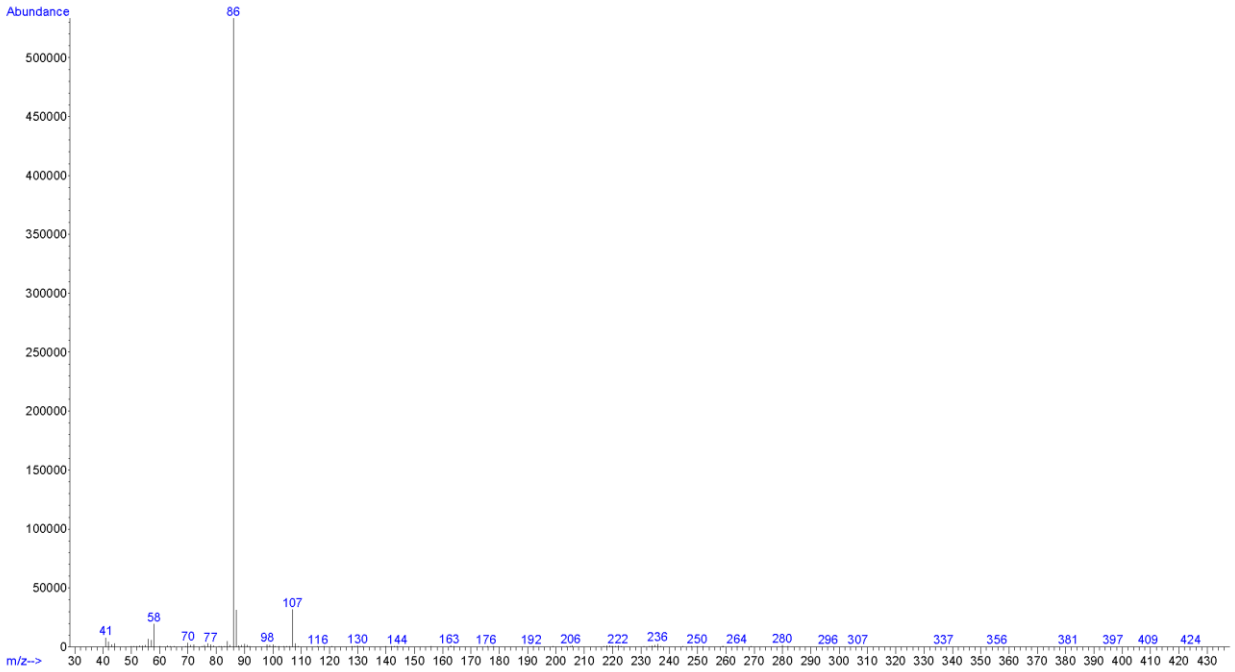
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for Butonitazene (Batch: 0601698-1) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/30278/butonitazene)

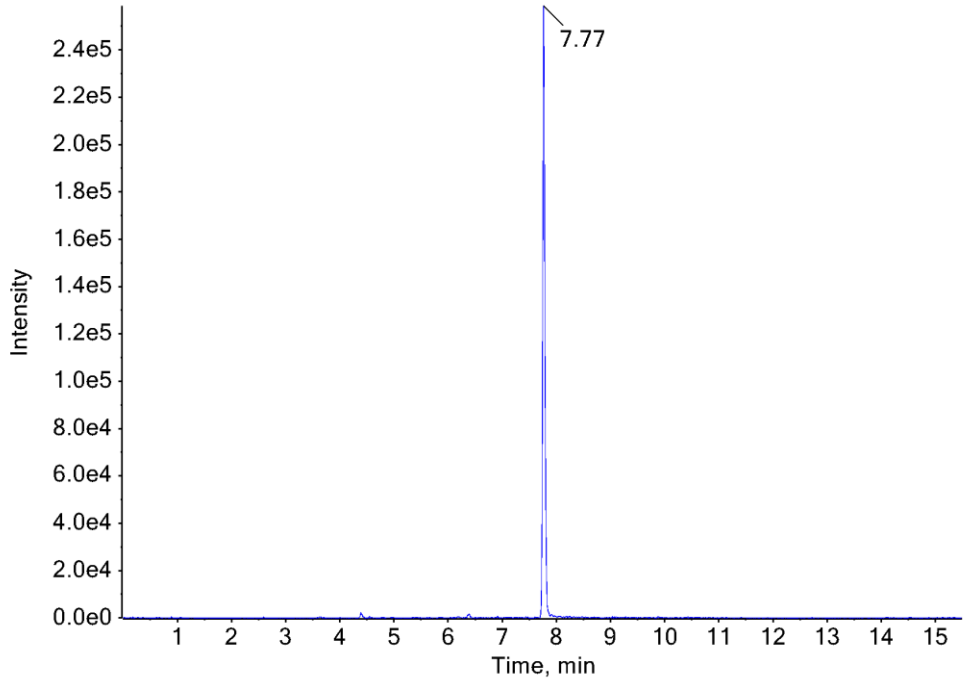
EI (70 eV) Mass Spectrum: Butonitazene (Standard)



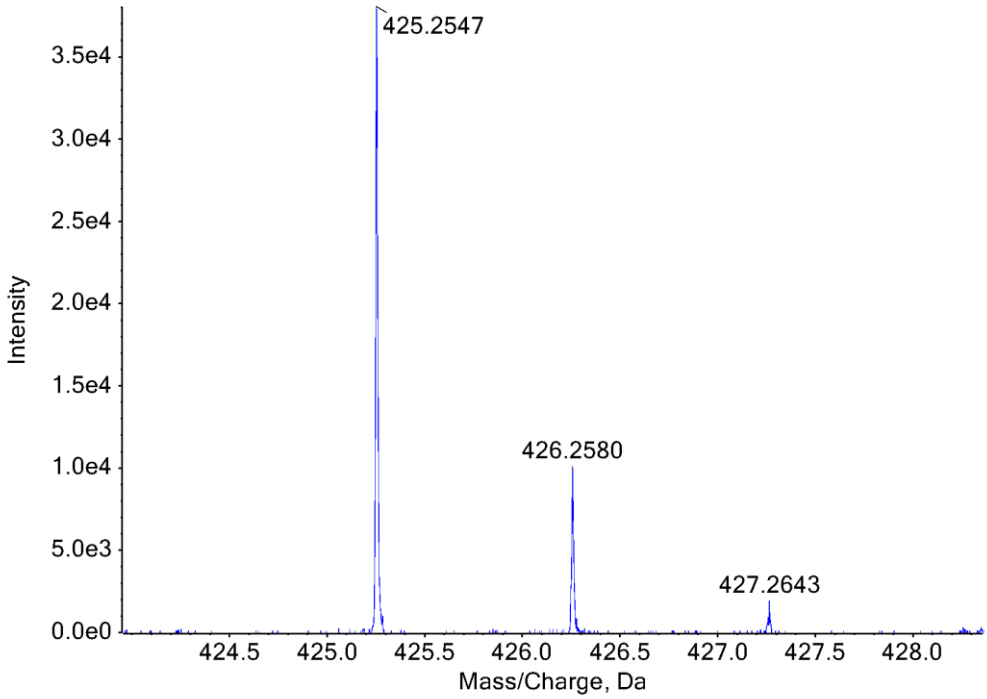
6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	No additional preparation - direct analysis of sample extract
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:	7.77 min
Standard Comparison:	Reference material for Butonitazene (Batch: 0601698-1) 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 Butonitazene, based on retention time (7.73 min) and mass spectral data. (https://www.caymanchem.com/product/30278/butonitazene)

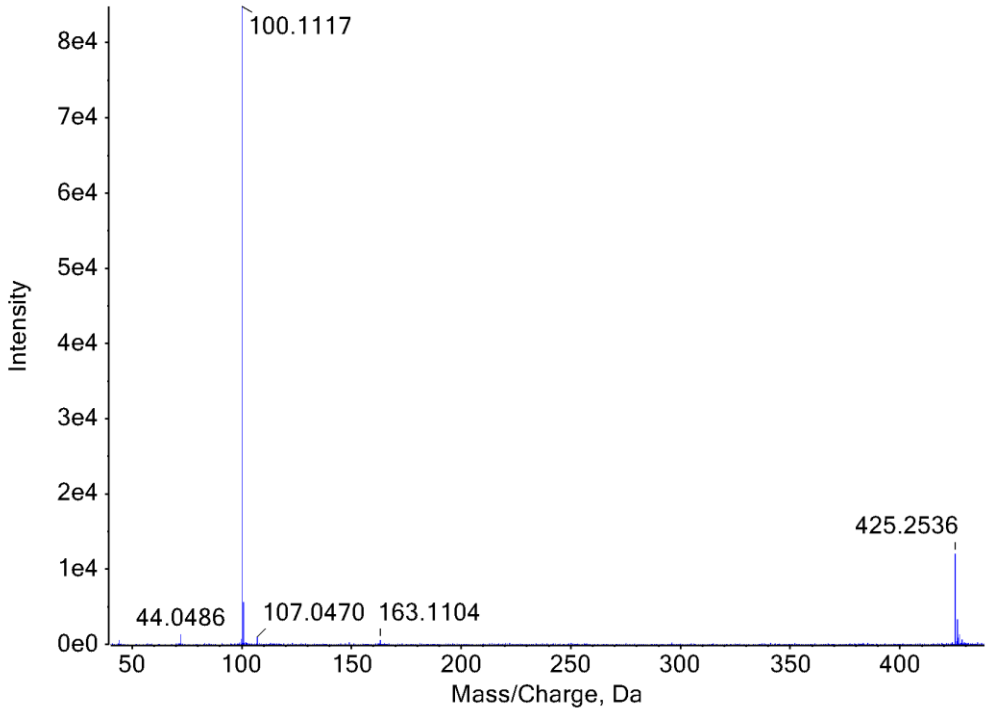
Extracted Ion Chromatogram: Butonitazene (Biological Sample)



TOF MS Spectrum: Butonitazene (Biological Sample)



MS/MS Spectrum: Butonitazene (Biological Sample)



7. FUNDING

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