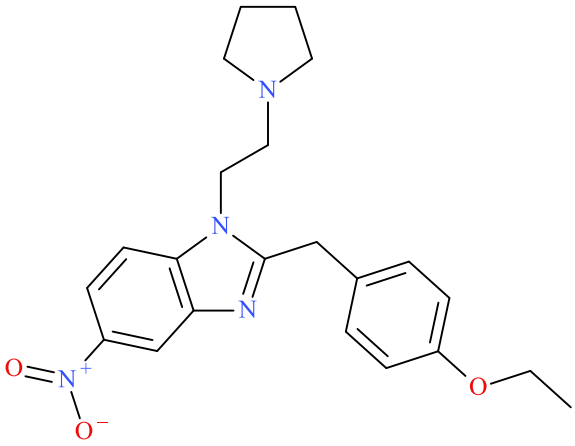
N-Pyrrolidino Etonitazene

Sample Type: **Biological Fluid**



Latest Revision: **May 13, 2021**

Date of Report: **May 13, 2021**

1. GENERAL INFORMATION

IUPAC Name: 2-[(4-ethoxyphenyl)methyl]-5-nitro-1-(2-pyrrolidin-1-ylethyl)benzimidazole

InChI String: InChI=1S/C22H26N4O3/c1-2-29-19-8-5-17(6-9-19)15-22-23-20-16-18(26(27)28)7-10-21(20)25(22)14-13-24-11-3-4-12-24/h5-10,16H,2-4,11-15H2,1H3

CFR: Not Scheduled (05/2021)

CAS# Not Available

Synonyms: Etonitazepyne

Source: NMS Labs – Toxicology Department

***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 [$M+H]^+$
N-Pyrrolidino Etonitazene	$C_{22}H_{26}N_4O_3$	394.5	394	395.2078

3. SAMPLE HISTORY

N-Pyrrolidino Etonitazene has been identified in one case in May 2021. The geographical and demographical breakdown is below:

Geographical Location: West Virginia (n=1)

Biological Sample: Blood (n=1)

Date of First Receipt: March 2021

Other Notable Findings: Flualprazolam (n=1), Fentanyl (n=1), Methamphetamine (n=1)

4. BRIEF DESCRIPTION

N-Pyrrolidino Etonitazene 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 etonitazene, metonitazene, and isotonitazene. Etonitazene and its analogue 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fentanyl.[2,3] Recent *in vitro* data suggest that *N*-pyrrolidino etonitazene is similar in potency to etonitazene (unpublished data from M. Vandeputte and C. Stove). *N*-Pyrrolidino Etonitazene is not explicitly scheduled in the United States; however, etonitazene and isotonitazene 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/article/10.1007/BF02161116

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

3. Vandeputte, MM; Van Uytfanghe, K; Layle, NK; St. Germaine, DM; Iula, DM; Stove , CP. Synthesis, Chemical Characterization, and μ-Opioid Receptor Activity Assessment of the Emerging Group of "Nitazene" 2-Benzylbenzimidazole Synthetic Opioids. *ACS Chem. Neurosci*. 2021. https://pubs.acs.org/doi/10.1021/acschemneuro.1c00064

https://www.caymanchem.com/product/33169/n-pyrrolidino-etonitazene

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 *N*-pyrrolidino etonitazene (Batch: 0607145-2) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/33169/n-pyrrolidino-etonitazene)

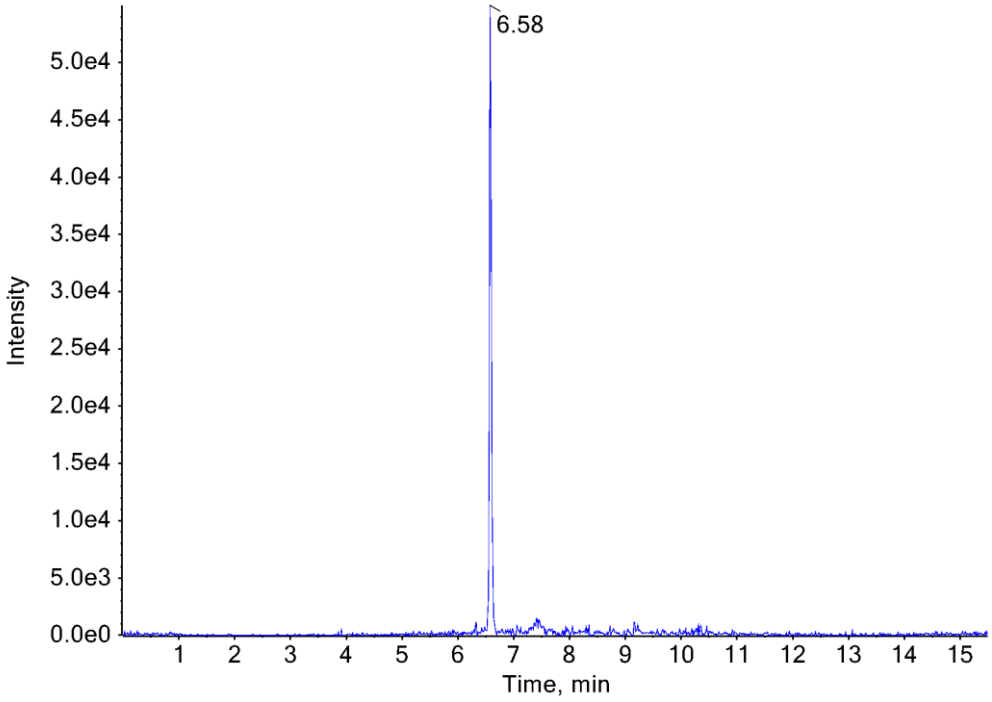
EI (70 eV) Mass Spectrum: *N*-Pyrrolidino Etonitazene (Standard)

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

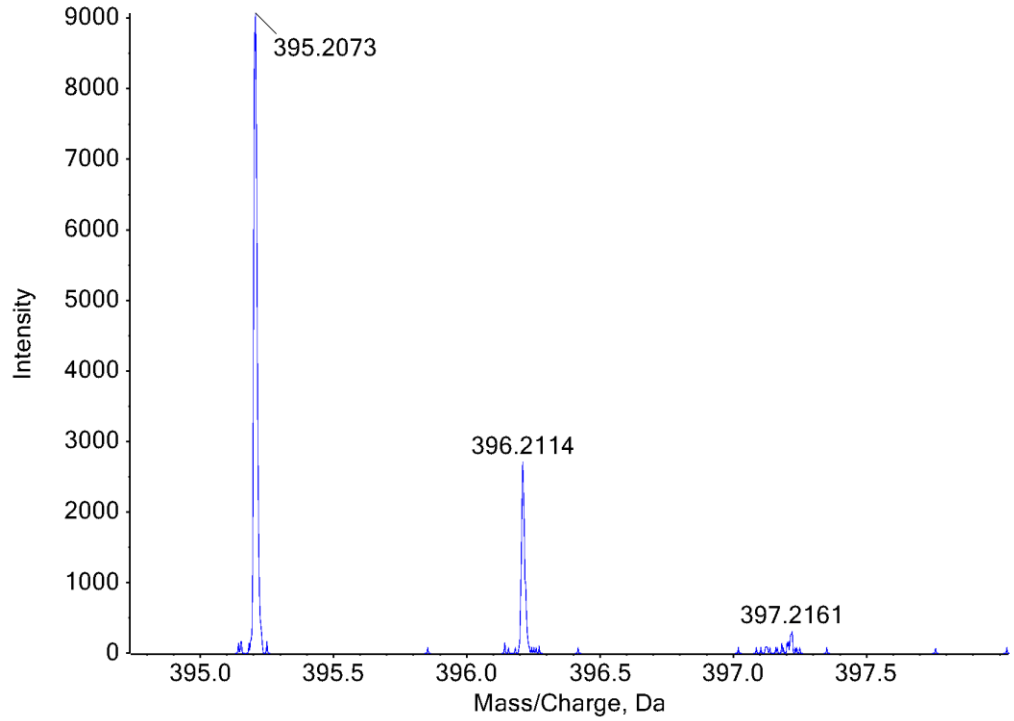
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Liquid-liquid extraction (LLE)
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 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:	6.58 min
Standard Comparison:	Reference material for *N*-pyrrolidino etonitazene (Batch: 0607145-2) 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*-pyrrolidino etonitazene, based on retention time (6.48 min) and mass spectral data. (https://www.caymanchem.com/product/33169/n-pyrrolidino-etonitazene)

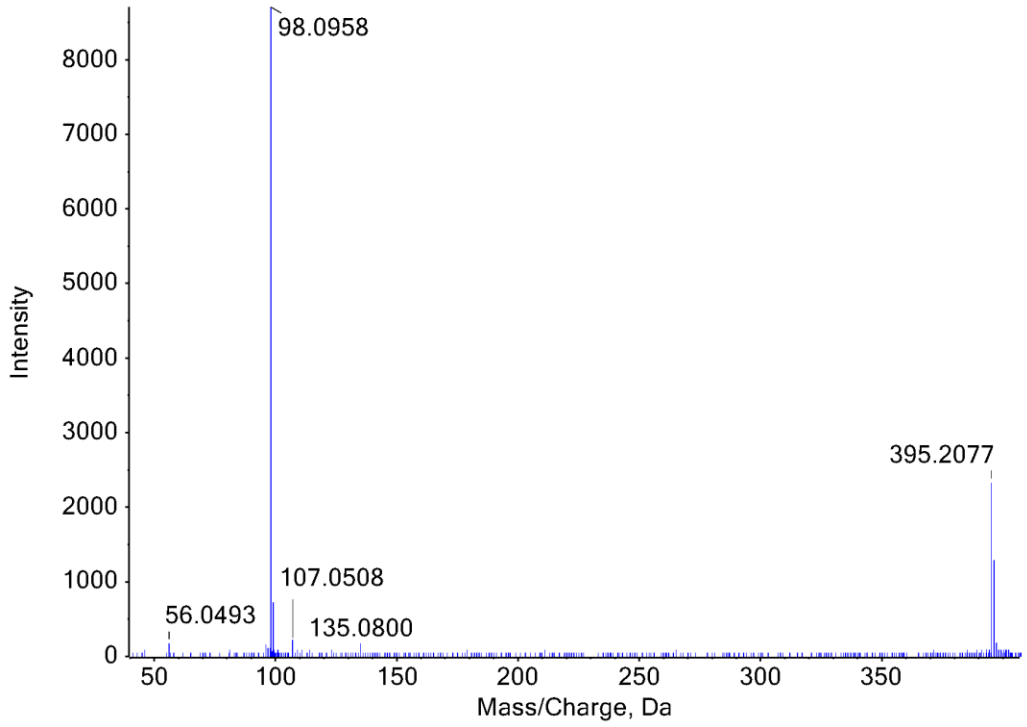
Extracted Ion Chromatogram: *N*-Pyrrolidino Etonitazene (Biological Sample)



TOF MS Spectra: *N*-Pyrrolidino Etonitazene (Biological Sample)



MS/MS Spectra: *N*-Pyrrolidino Etonitazene (Biological Sample)



7. FUNDING

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