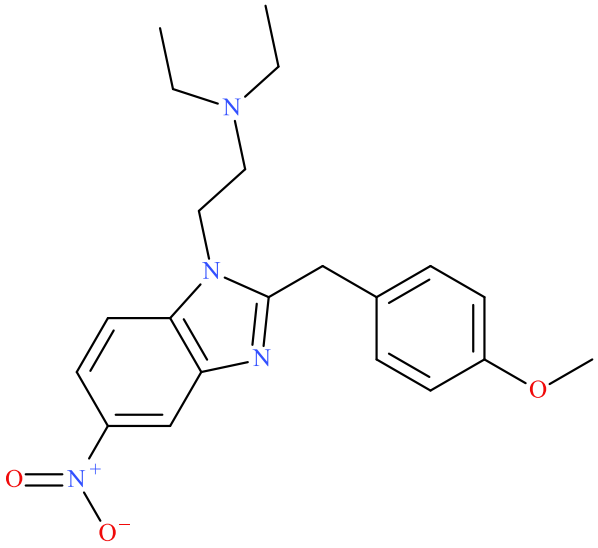
Metonitazene

Sample Type: **Seized Material**



Latest Revision: **July 30, 2020**

Date Received: **July 7, 2020**

Date of Report: **July 30, 2020**

1. GENERAL INFORMATION

IUPAC Name:	N,N-diethyl-2-[2-[(4-methoxyphenyl)methyl]-5-nitro-benzimidazol-1-yl]ethanamine
InChI String:	InChI=1S/C21H26N4O3/c1-4-23(5-2)12-13-24-20-11-8-17(25(26)27)15-19(20)22-21(24)14-16-6-9-18(28-3)10-7-16/h6-11,15H,4-5,12-14H2,1-3H3
CFR:	Not Scheduled (07/2020)
CAS#	14680-51-4
Synonyms:	None Available
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	$C_{21}H_{26}N_4O_3$	382.5	382	383.2078

3. BRIEF DESCRIPTION

Metonitazene is classified as a novel opioid but is dissimilar from fentanyl and U-series analogues. Novel opioids have been reported to cause psychoactive effects similar to heroin, fentanyl, and other opioids. Novel opioids have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds to metonitazene include etonitazene, isotonitazene, and clonitazene. These synthetic opioids were first synthesized and reported in the literature in the 1950s.[1] Data suggests that this group of analogues have potency similar to or greater than fentanyl.[2] Etonitazene is reported to be the most potent followed by isotonitazene and metonitazene. Metonitazene is not explicitly a scheduled substance in the United States; however, etonitazene and clonitazene are Schedule I substances and isotonitazene was recently temporarily placed into Schedule I. Isotonitazene was previously confirmed by NPS Discovery in November 2019, followed by proliferation in the United States initiating from the midwestern region[3,4] Tentative identification of metonitazene was previously reported in March 2019 out of Canada (Alberta) from testing of drug paraphernalia also containing isotonitazene.

4. 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://pubmed.ncbi.nlm.nih.gov/13473817/

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

3. Krotulski, AJ; Logan, BK. (2019). New Drug Monograph: Isotonitazene. *NPS Discovery*.

4. Krotulski, AJ; Papsun, DM; Kacinko, SL; Logan, BK. (2020) Isotonitazene Quantitation and Metabolite Discovery in Authentic Forensic Casework. *Journal of Analytical Toxicology*. [Epub ahead of print]. https://doi.org/10.1093/jat/bkaa016

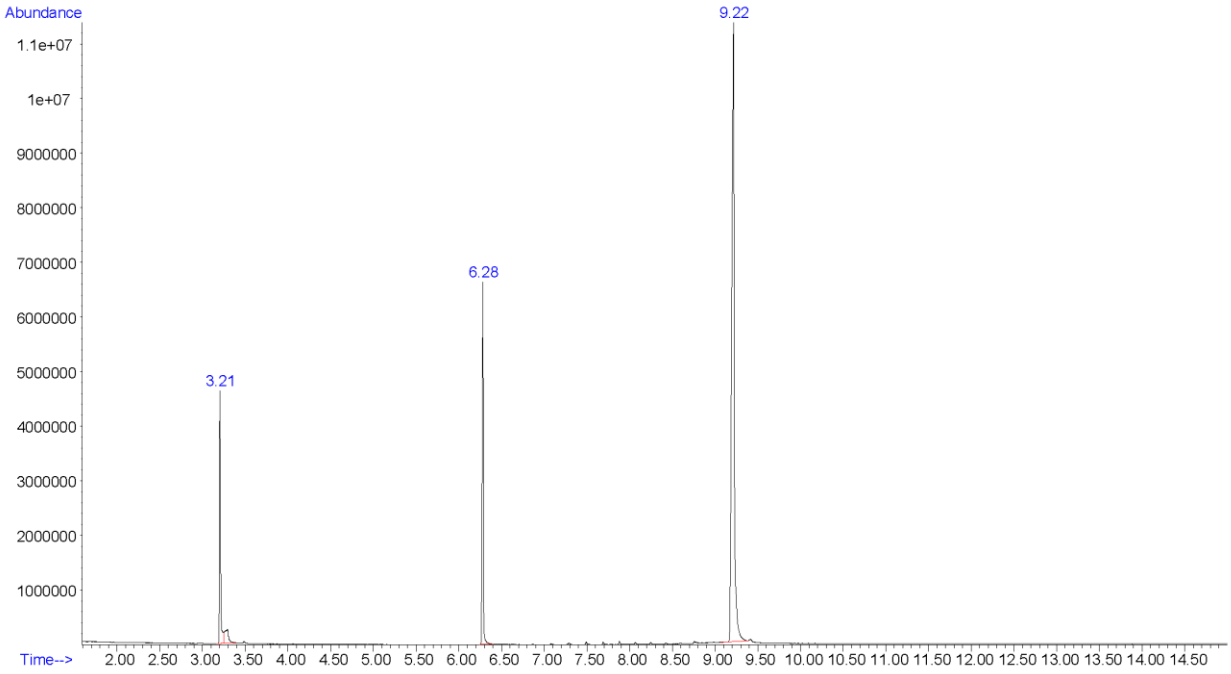
https://www.caymanchem.com/product/26398/metonitazene

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

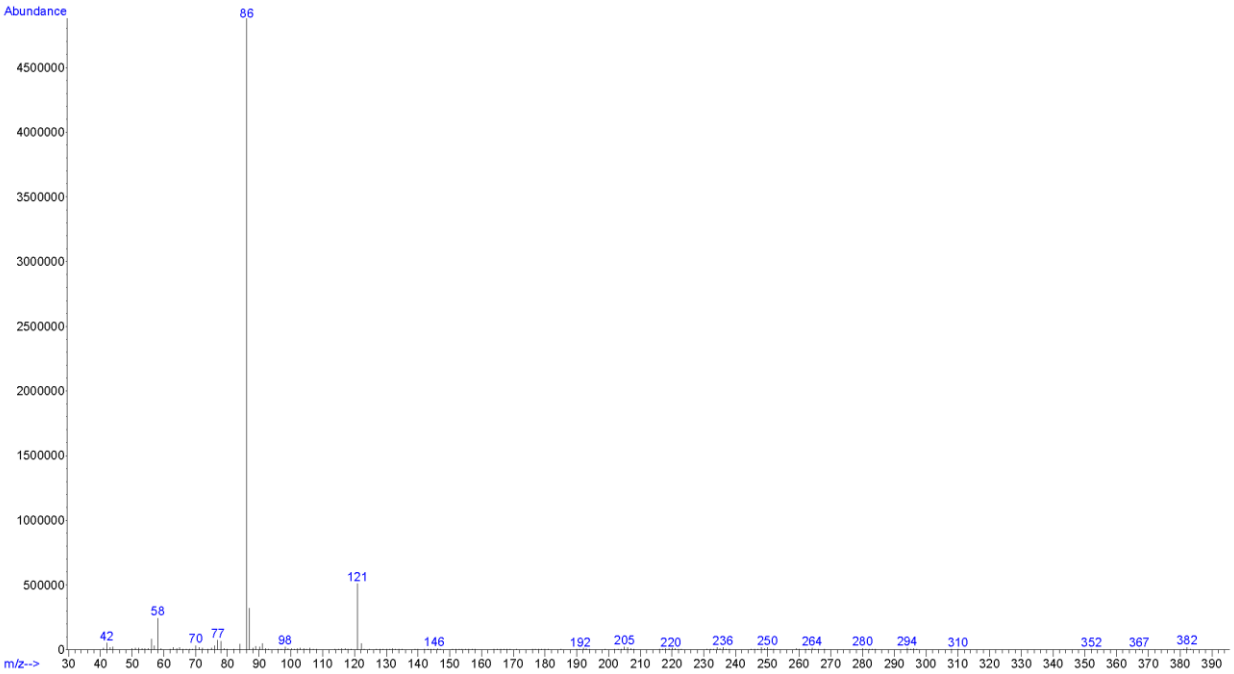
Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 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:	9.22 min
Standard Comparison:	Reference material for Metonitazene (Batch: 0575805-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Metonitazene based on retention time (9.20 min) and mass spectral data. (https://www.caymanchem.com/product/26398/metonitazene)

Chromatogram: Metonitazene



Additional peaks present in chromatogram: internal standards (3.21 and 6.28 min)

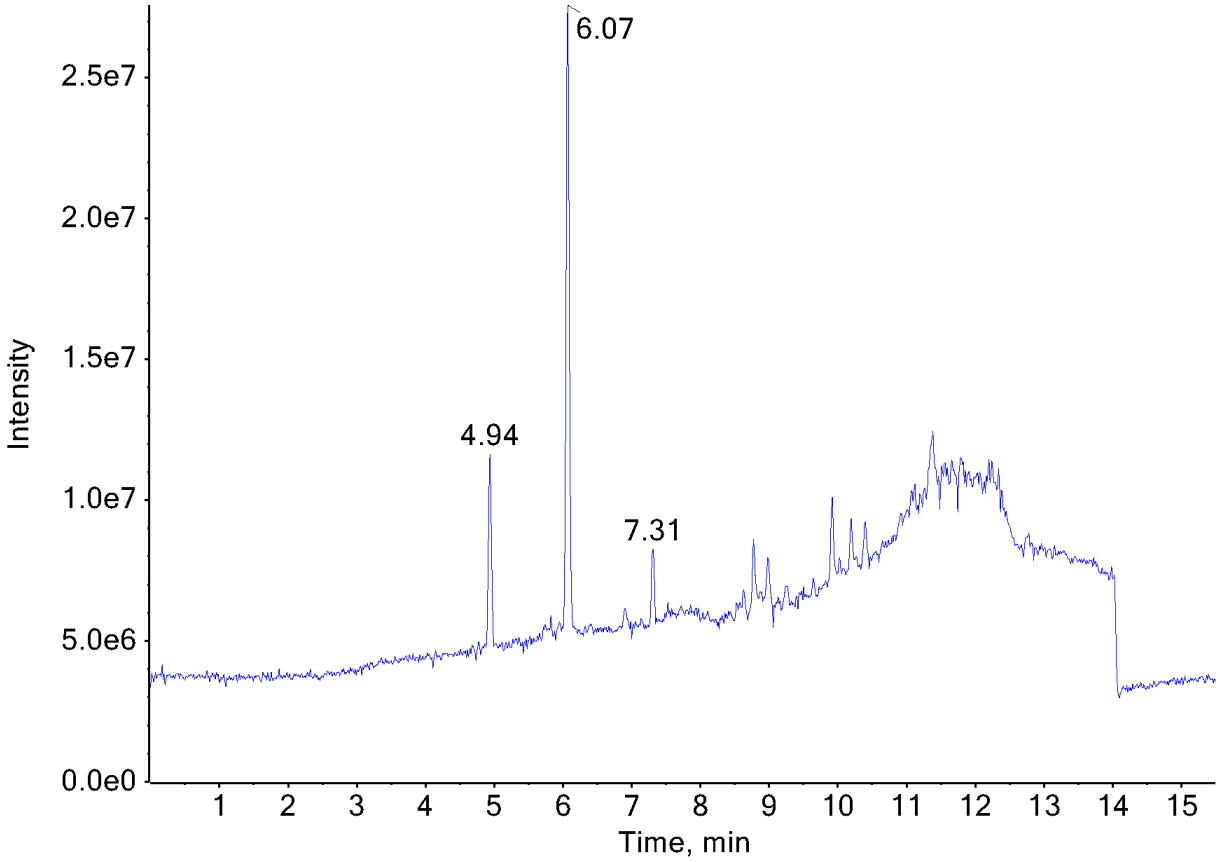
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Metonitazene



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 extraction 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:	6.07 min
Standard Comparison:	Reference material for Metonitazene (Batch: 0575805-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Metonitazene based on retention time (6.09 min) and mass spectral data. (https://www.caymanchem.com/product/26398/metonitazene)

Chromatogram: Metonitazene



Additional peaks present in chromatogram: internal standards (4.94 and 7.31 min)

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