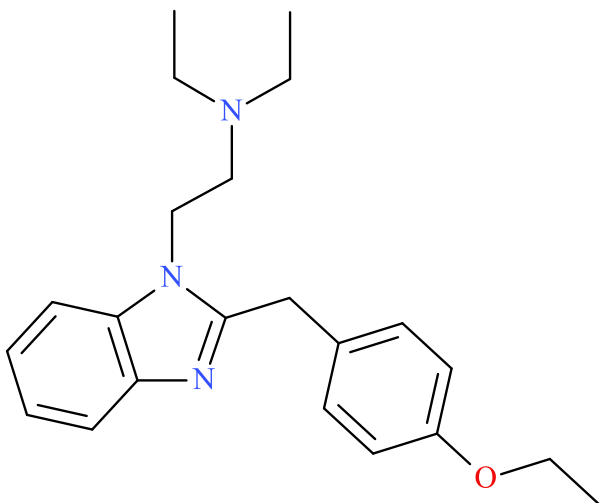


## Etodesnitazene

Sample Type: **Biological Fluid**

Latest Revision: **February 23, 2021**

Date of Report: **February 23, 2021**



### 1. GENERAL INFORMATION

**IUPAC Name:** 2-[2-[(4-ethoxyphenyl)methyl]benzimidazol-1-yl]-N,N-diethylethanamine

**InChI String:** InChI=1S/C22H29N3O/c1-4-24(5-2)15-16-25-21-10-8-7-9-20(21)23-22(25)17-18-11-13-19(14-12-18)26-6-3/h7-14H,4-6,15-17H2,1-3H3

**CFR:** Not Scheduled (02/2021)

**CAS#** Not available

**Synonyms:** Etazene, Desnitroetonitazene, Etazen, Etazone

**Source:** Oregon State Police Forensic Laboratory

**Important Notes:** All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. This drug was also confirmed via LC-MS/MS.

**Prepared By:** Janet Schultz, PhD; Sailee Raje; Sara Short, MS, D-ABFT-FT; Michele Stauffenberg, MD; Alex J. Krotulski, PhD; Melissa F. Fogarty, MSFS, D-ABFT-FT; and Barry K. Logan, PhD, F-ABFT

## 2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Etodesnitazene	C <sub>22</sub> H <sub>29</sub> N <sub>3</sub> O	351.5	351	352.2383

## 3. SAMPLE HISTORY

Etodesnitazene has been identified in one case since December 2020. The geographical and demographical breakdown is below:

- Geographical Location:** Oregon (n=1)
- Biological Sample:** Subclavian Blood (n=1)
- Date of First Receipt:** December 2020
- Other Notable Findings:** Etizolam, Methamphetamine, Mitragynine

## 4. BRIEF DESCRIPTION

Etodesnitazene 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; however, these substances contain a nitro moiety attached to the benzimidazole core. Etonitazene and its analogue synthetic opioids were first synthesized and reported in the literature in the 1950s.<sup>1</sup> Data suggest that this group of nitro-containing analogues can have potency similar to or greater than fentanyl.<sup>2</sup> Recent in vitro data suggest that etodesnitazene is less potent than fentanyl.<sup>3</sup> Etodesnitazene is not explicitly scheduled in the United States; however, etonitazene and isotonitazene are Schedule I substances.

## 5. ADDITIONAL RESOURCES

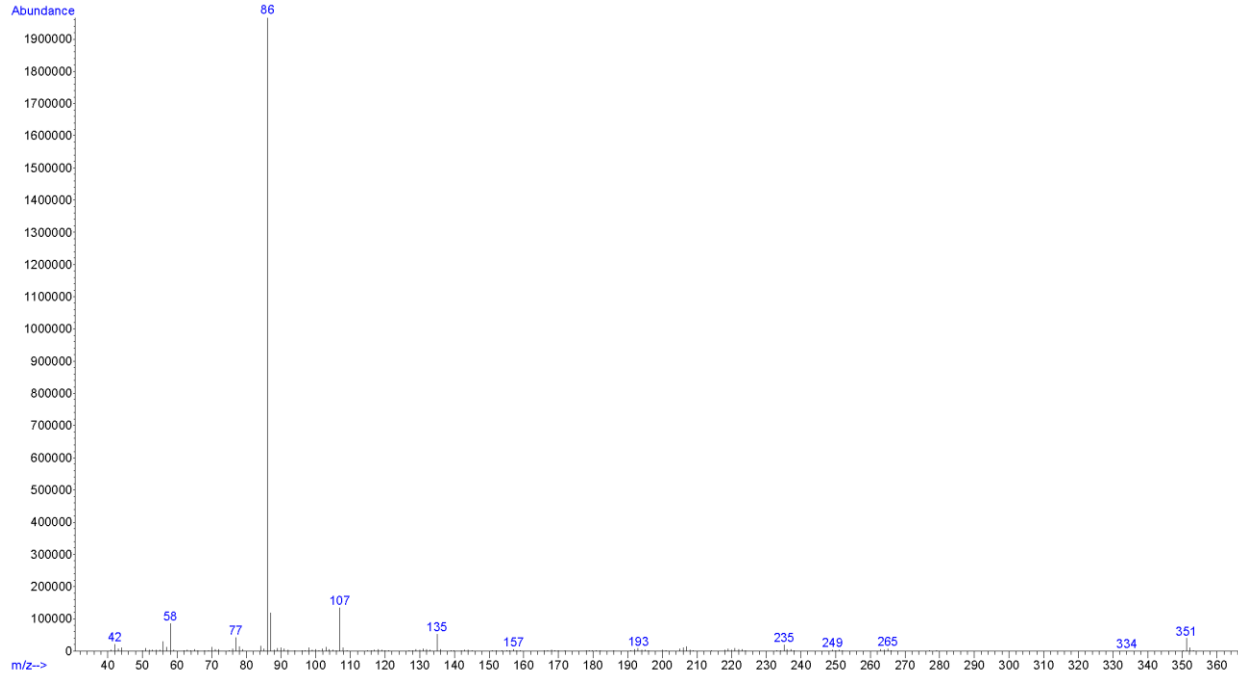
1. Hunger, A; Kebrle, J; Rossi, A; Hoffmann, K. (1957) Synthesis of analgesically active benzimidazole derivatives with basic substitutions. *Experientia*, **13**, 400-401.  
<https://link.springer.com/article/10.1007/BF02161116>
2. Hoffmann, K; Hunger, A; Rossi, A. (3 May 1960). "Patent US2935514A – Benzimidazoles."  
<https://patents.google.com/patent/US2935514A/en>
3. Marthe Vandeputte, Katleen Van Uytfanghe, Nathan Layle, et al. Synthesis, chemical characterization, and  $\mu$ -opioid receptor activity assessment of the emerging group of nitazene new synthetic opioids. Authorea. November 12, 2020.  
<https://www.authorea.com/users/375382/articles/492636-synthesis-chemical-characterization-and-%C2%B5-opioid-receptor-activity-assessment-of-the-emerging-group-of-nitazene-new-synthetic-opioids>  
[https://www.caymanchem.com/product/29916/etodesnitazene-\(citrate\)](https://www.caymanchem.com/product/29916/etodesnitazene-(citrate))

## 6. QUALITATIVE DATA

### 6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	Standard diluted in methanol
<b>Instrument:</b>	Agilent 5975 Series GC/MSD System
<b>Standard:</b>	Reference material for Etodesnitazene (Batch: 0591547-14) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). <a href="https://www.caymanchem.com/product/29916/etodesnitazene-(citrate)">https://www.caymanchem.com/product/29916/etodesnitazene-(citrate)</a>

## EI (70 eV) Mass Spectrum: Etodesnitazene (Standard)



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

**Testing Performed At:** Oregon State Police Forensic Laboratory (Clackamas, OR)

**Sample Preparation:** Supported Liquid Extraction (SLE+, Biotage)

**Instrument:** Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

**Column:** Phenomenex® Kinetex Biphenyl (50 mm x 2.1 mm, 2.6 µm)

**Mobile Phase:**  
A: 0.05% Formic Acid, 5 mM Ammonium Formate  
B: 0.05% Formic Acid in Methanol/acetonitrile (50:50)  
Flow rate: 0.4 mL/min

**Gradient:** Initial: 98A:2B; 0A:100B over 9 min; 2A:98B at 14.5 min

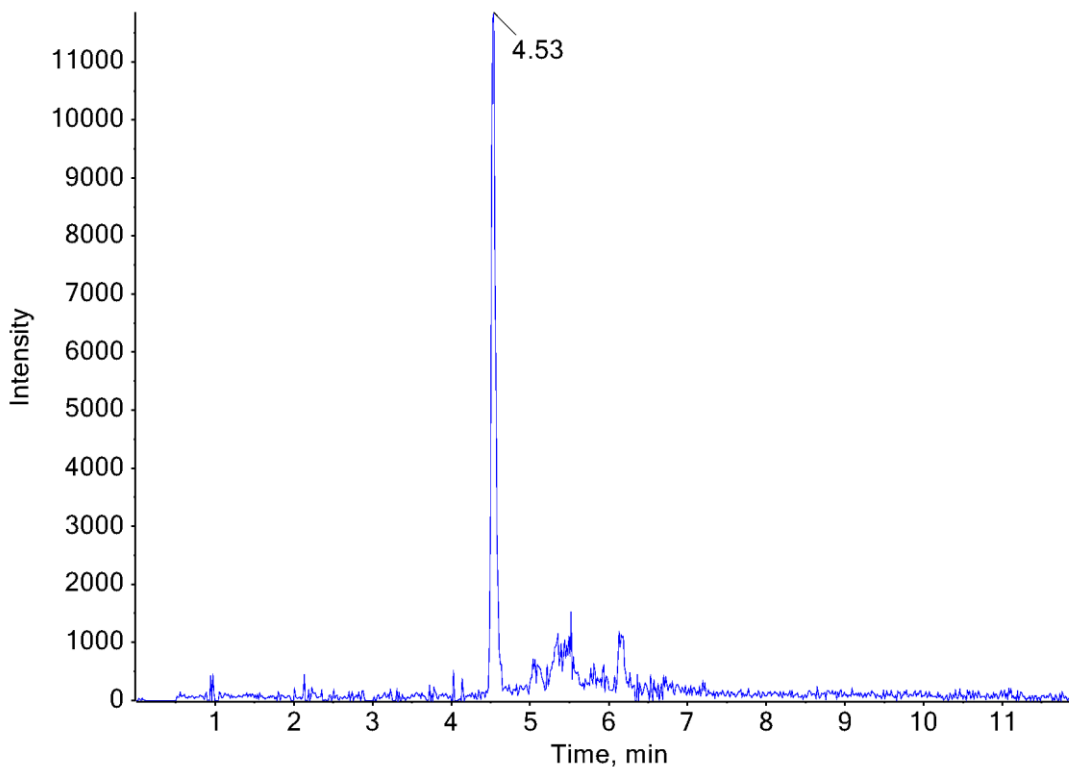
**Temperatures:**  
Autosampler: 10 °C  
Column Oven: 30 °C  
Source Heater: 600 °C

**Injection Parameters:** Injection Volume: 10  $\mu$ L  
**QTOF Parameters:** TOF MS Scan Range: 50-800 Da  
Precursor Isolation: SWATH® acquisition (Variable window)  
Fragmentation: Collision Energy Spread (35 $\pm$ 15 eV)  
MS/MS Scan Range: 35-800 Da

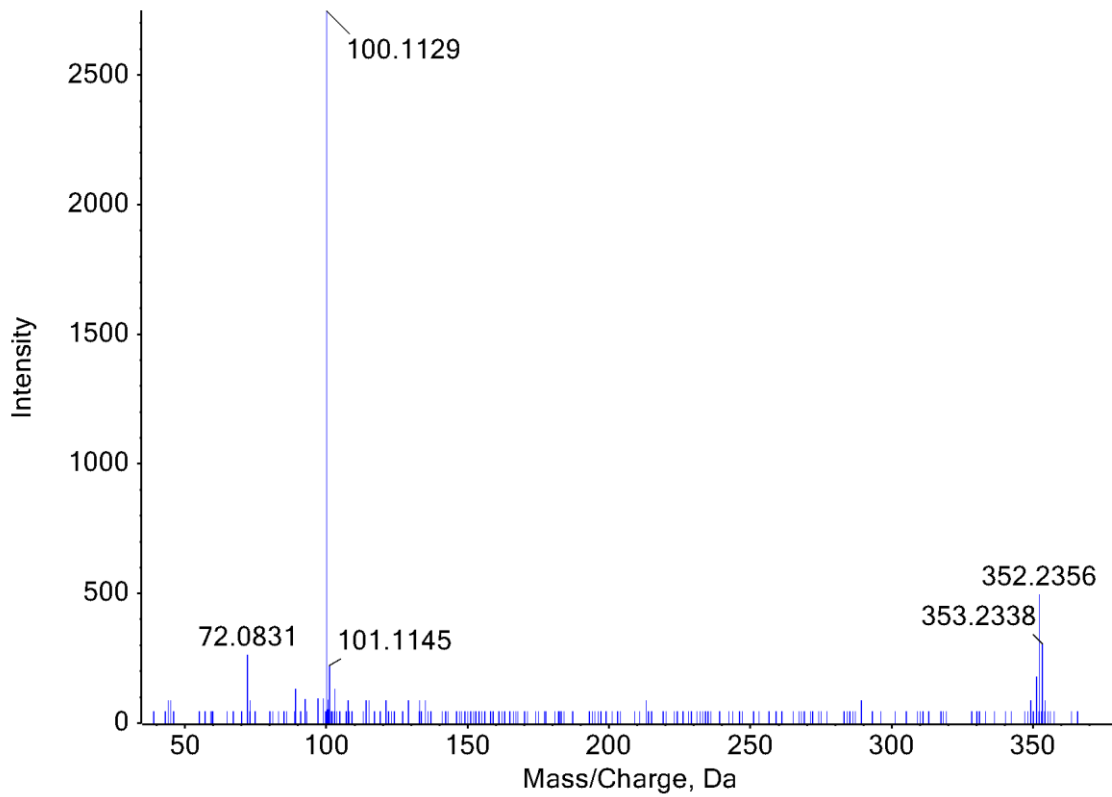
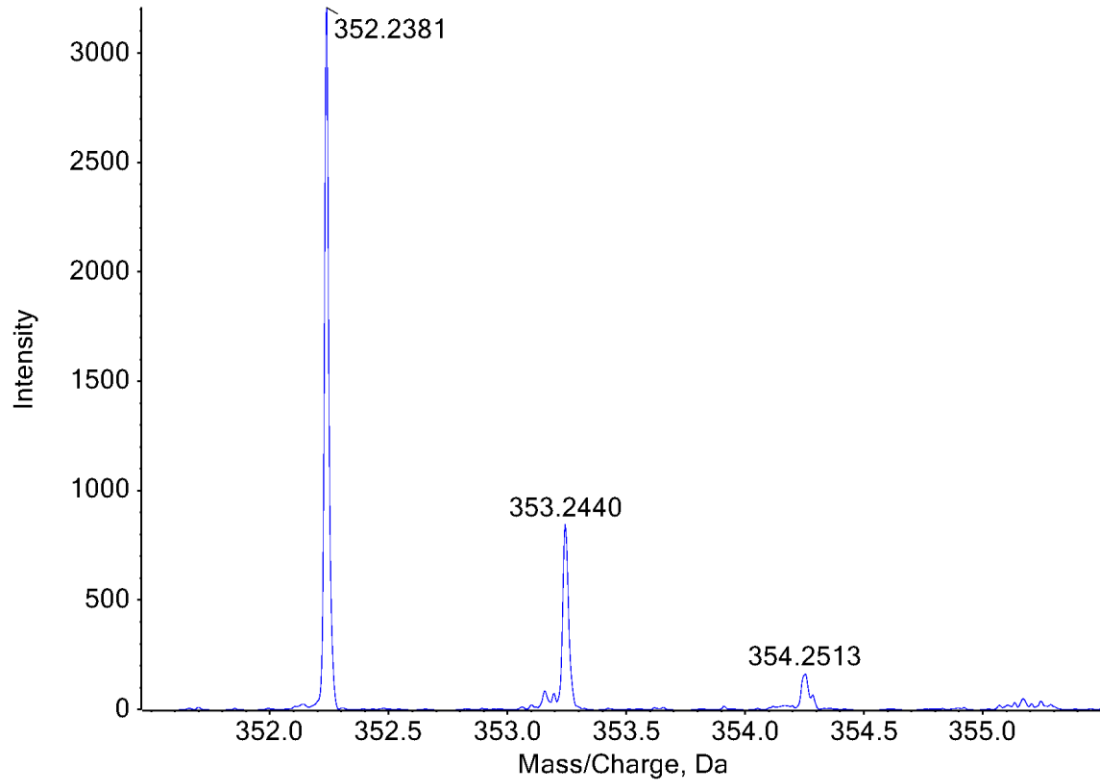
**Retention Time:** 4.53 min

**Standard Comparison:** Reference material for Etodesnitazene (Batch: 0591547-14) 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 Etodesnitazene, based on retention time (4.53 min) and mass spectral data.  
<https://www.caymanchem.com/product/29916/etodesnitazene-citrate>

**Extracted Ion Chromatogram: Etodesnitazene (Biological Sample)**



**TOF MS (Top) and MS/MS (Bottom) Spectra: Etodesnitazene (Biological Sample)**



## **7. FUNDING**

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