**N-Desethyl Isotonitazene**

Sample Type: **Drug Material**

Latest Revision: **December 19, 2022**

Date Received: **November 22, 2022**

Date of Report: **December 19, 2022**

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1. **GENERAL INFORMATION**

- **IUPAC Name:** N-ethyl-2-[2-[(4-isopropoxyphenyl)methyl]-5-nitro-benzimidazol-1-yl]ethanamine

- **InChI String:** InChI=1S/C21H26N4O3/c1-4-22-11-12-24-20-10-7-17(25(26)27)14-19(20)23-21(24)13-16-5-8-18(9-6-16)28-15(2)3/h5-10,14-15,22H,4,11-13H2,1-3H3

- **CFR:** Not Scheduled (12/2022)

- **CAS#:** 2732926-24-6

- **Synonyms:** Desethyl Isotonitazene, “Des-Iso”

- **Source:** Pinellas County Forensic Lab

- **Appearance:** Round Blue Pill

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*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

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₂₁H₂₆N₄O₃</td>
<td>382.5</td>
<td>382</td>
<td>383.2078</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

*N*-Desethyl Isotonitazene is classified as a novel opioid of the 2-benzyl 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. *N*-Desethyl Isotonitazene is a known metabolite of isotonitazene¹; however, it is now being manufactured and distributed as a parent drug on its own, which has been observed through sales on online gray market sites and demonstrated through the detection of this drug without isotonitazene in drug materials. Etonitazene and its analogue synthetic opioids were first synthesized and reported in the literature in the 1950s.² Data suggest that this group of analogues can have potency similar to or greater than fentanyl.³⁴ *In vitro* data shows that *N*-desethyl isotonitazene is similar in potency to etonitazene, and approximately 20 times more potent than fentanyl.⁴ Structurally similar drugs include isotonitazene and other nitazene analogues. *N*-Desethyl Isotonitazene is not explicitly scheduled in the United States; however, etonitazene, isotonitazene, and other nitazene analogues are designated as Schedule I substances.

4. ADDITIONAL RESOURCES


5. QUALITATIVE DATA

5.1 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: Dilution in methanol

Instrument: Agilent 5975 Series GC/MSD System

Column: Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)

Carrier Gas: Helium (Flow: 1.46 mL/min)

Temperatures:
- Injection Port: 265 °C, Transfer Line: 300 °C
- MS Source: 230 °C, MS Quad: 150 °C,
- Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min

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

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

Retention Time: 9.06 min

Standard Comparison: Reference material for N-desethyl isotonitazene (Batch: 0588587-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as N-desethyl isotonitazene based on retention time (9.05 min) and mass spectral data. (https://www.caymanchem.com/product/30216/n-desethyl-isotonitazene-(hydrochloride))
Chromatogram: N-Desethyl Isotonitazene

Additional peaks in chromatogram: not a controlled substance (2.48 mins) and internal standards (3.13 and 5.77 mins)

EI (70 eV) Mass Spectrum: N-Desethyl Isotonitazene
5.2 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: Dilution in methanol followed by 1:100 dilution of GC-MS sample in mobile phase (CFSRE)

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: 6.81 min

Standard Comparison: Reference material for N-desethyl isotonitazene (Batch: 0588587-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as N-desethyl isotonitazene based on retention time (6.84 min) and mass spectral data. (https://www.caymanchem.com/product/30216/n-desethyl-isotonitazene-(hydrochloride))
Chromatogram: N-Desethyl Isotonitazene

Additional peaks in chromatogram: internal standards (4.93 and 7.25 mins)
TOF MS Spectra: N-Desethyl Isotonitazene

TOF MS/MS Spectra: N-Desethyl Isotonitazene
5.3 GAS CHROMATOGRAPHY INFRARED SPECTROSCOPY (GC-IR)

Testing Performed At: Pinellas County Forensic Lab (Largo, FL)

Sample Preparation: Dilution in methylene chloride

Instrument: Agilent 7890B GC ASAP IRD3

Temperatures: Injector 250 °C, Lightpipe 250 °C, Transfer Lines 275 °C

Oven Program: 80 °C for 1.2 min, 30 °C/min to 320 °C for 4.0 min

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

IR Spectrum: N-Desethyl Isotonitazene
6. FUNDING

NPS Discovery at the CFSRE is supported in part by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 2020-DQ-BX-0007, “Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS)”). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily represent the official position or policies of the U.S. Department of Justice.