Deschloroetizolam

Sample Type: Seized Material

Latest Revision: February 16, 2021
Date Received: September 24, 2020
Date of Report: February 16, 2021

1. GENERAL INFORMATION

IUPAC Name: 2-ethyl-9-methyl-4-phenyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine

InChI String: InChI=1S/C17H16N4S/c1-3-13-9-14-16(12-7-5-4-6-8-12)18-10-15-20-19-11(2)21(15)17(14)22-13/h4-9H,3,10H2,1-2H3

CFR: Not Scheduled (02/2021)

CAS#: 40054-73-7

Synonyms: Etizolam-2

Source: NMS Labs –Criminalistic Laboratory

Appearance: Rectangular Yellow Tablet “R039”

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.

Prepared By: Alex J. Krotulski, PhD; Sarah A. Shuda, MFSF, F-ABC; Melissa F. Fogarty, MSFS, D-ABFT-FT; Sarah E. Decker, BA; and Barry K. Logan, PhD, F-ABFT
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>C₁₇H₁₆N₄S</td>
<td>308.4</td>
<td>308</td>
<td>309.1168</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

Deschloroetizolam is classified as a novel benzodiazepine. Benzodiazepines are central nervous system depressants. Novel benzodiazepines, typically defined as emergent benzodiazepines not used medicinally, are often pirated from early drug discovery or pharmaceutical studies. Novel benzodiazepines have appeared on illicit drug markets in recent years and have caused adverse events, as described in the literature. Fatalities linked to novel benzodiazepine use have occurred, commonly when used in combination with other depressants (e.g. opioids and alcohol). The synthesis of deschloroetizolam dates back to at least the 1970’s based on previously published literature and patents.¹,²,³ Deschloroetizolam was identified among the illicit drug supply in 2014 by scientists in the United Kingdom.⁴ Deschloroetizolam is structurally similar to etizolam. Neither substance is federally controlled in the United States, however, some states have moved to control etizolam. According to data from NPS Discovery, deschloroetizolam has been identified in at least ten toxicology samples since mid-2020.

4. ADDITIONAL RESOURCES

4. ADDITIONAL RESOURCES (CONTINUED)


https://www.caymanchem.com/product/23107/deschloroetizolam


https://psychonautwiki.org/wiki/Deschloroetizolam

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: 8.60 min
Standard Comparison: Reference material for Deschloroetizolam (Batch: 0589089-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Deschloroetizolam based on retention time (8.64 min) and mass spectral data. (https://www.caymanchem.com/product/23107/deschloroetizolam)

Chromatogram: Deschloroetizolam

Additional peaks present in chromatogram: internal standards (3.18 min and 6.28 min) and flubromazolam (8.69 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Deschloroetizolam
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 extract 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: 7.59 min

Standard Comparison: Reference material for Deschloroetizolam (Batch: 0589089-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Deschloroetizolam based on retention time (7.62 min) and mass spectral data. (https://www.caymanchem.com/product/23107/deschloroetizolam)
Chromatogram: Deschloroetizolam

Additional peaks present in chromatogram: internal standards (4.98 min and 7.31 min) and flubromazolam (7.47 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: Deschloroetizolam
6. FUNDING

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