1. GENERAL INFORMATION

IUPAC Name: 6-(4-chlorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine

InChI String: InChI=1S/C17H13ClN4/c1-11-20-21-16-10-19-17(12-6-8-13(18)9-7-12)14-4-2-3-5-15(14)22(11)16/h2-9H,10H2,1H3

CFR: Not Scheduled (12/2022)

CAS#: 92262-72-1

Synonyms: 4'-Chloro Deschloroalprazolam

Source: NMS Labs – Toxicology Department

Important Note: All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material.

Prepared By: Alex J. Krotulski, PhD; Kayla N. Ellefsen, PhD; Sara E. Walton, MS; Melissa F. Fogarty, MSFS, D-ABFT-FT; Donna M. Papsun, MS, D-ABFT; and Barry K. Logan, PhD, F-ABFT
2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Drug</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>4′Cl-Deschloroalprazolam</td>
<td>C₁₇H₁₃ClN₄</td>
<td>308.8</td>
<td>308</td>
<td>309.0902</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

4′Cl-Deschloroalprazolam 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). 4′Cl-Deschloroalprazolam was identified in Australia in pills collected in December 2021.¹ 4′Cl-Deschloroalprazolam is structurally similar to alprazolam. 4′Cl-Deschloroalprazolam is not federally controlled in the United States; however, alprazolam is a Schedule IV drug.

Analytical Note: Although 4′Cl-deschloroalprazolam and alprazolam are isomers, the two can be distinguished by mass spectral data by identifying unique fragment ions of each drug (e.g., alprazolam = 165.0214 Da vs. 4′Cl-deschloroalprazolam = 131.0604 Da).

4. ADDITIONAL RESOURCES


https://www.caymanchem.com/product/36057/4′-chloro-deschloroalprazolam
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: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for 4'Cl-deschloroalprazolam (Batch: 0634946-2) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). (https://www.caymanchem.com/product/36057/4'-chloro-deschloroalprazolam)

EI (70 eV) Mass Spectrum: 4'Cl-Deschloroalprazolam (Standard)
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: 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: 7.43 min

Standard Comparison: Reference material for 4’Cl-deschloroalprazolam (Batch: 0634946-2) 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 4’Cl-deschloroalprazolam, based on retention time (7.43 min) and mass spectral data. (https://www.caymanchem.com/product/36057/4'-chloro-deschloroalprazolam)
Extracted Ion Chromatogram: 4'Cl-Deschloroalprazolam

TOF MS Spectra: 4'Cl-Deschloroalprazolam
MS/MS Spectra: 4’Cl-Deschloralprazolam

6. FUNDING

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