

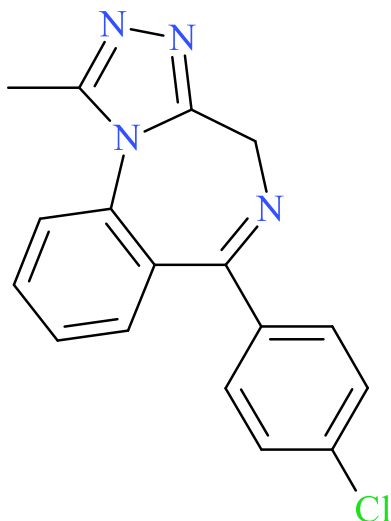
## 4'-Cl-Deschloroalprazolam

Sample Type: **Toxicology Sample**

Latest Revision: **December 7, 2022**

Date Received: **November 10, 2022**

Date of Report: **December 7, 2022**



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	6-(4-chlorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine
<b>InChI String:</b>	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
<b>CFR:</b>	Not Scheduled (12/2022)
<b>CAS#</b>	92262-72-1
<b>Synonyms:</b>	4'-Chloro Deschloroalprazolam
<b>Source:</b>	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.

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## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Drug	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
4'Cl-Deschloroalprazolam	C <sub>17</sub> H <sub>13</sub> ClN <sub>4</sub>	308.8	308	309.0902

### 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.<sup>1</sup> 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

Trigg S, Wells JM, McGann J, Bock S, Holman A, Harrison SM, Goh CY, Moggach SA, Brown DH. (2022) The alprazolam analogue 4'-chloro deschloroalprazolam identified in seized capsules. *Drug Testing and Analysis*.

<https://analyticalsciencejournals.onlinelibrary.wiley.com/doi/10.1002/dta.3325>

<https://www.caymanchem.com/product/36057/4'-chloro-deschloroalprazolam>

## 5. QUALITATIVE DATA

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

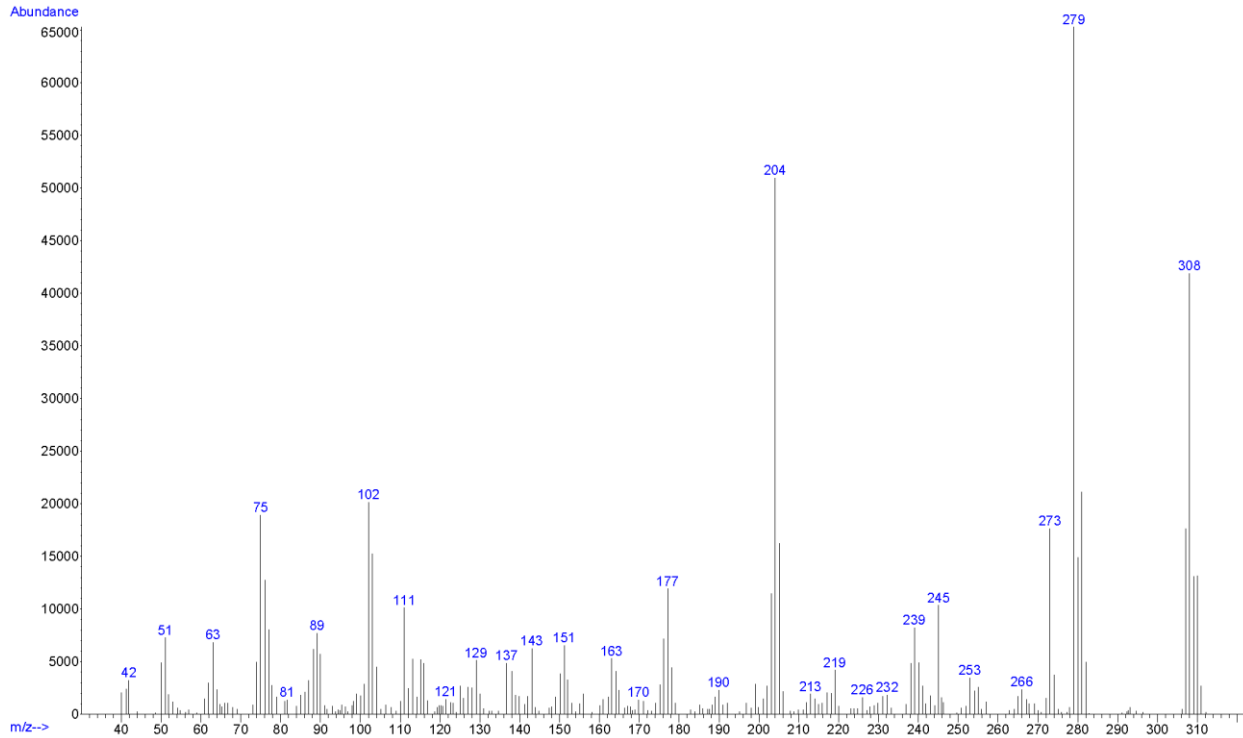
**Testing Performed At:** The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

**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>)

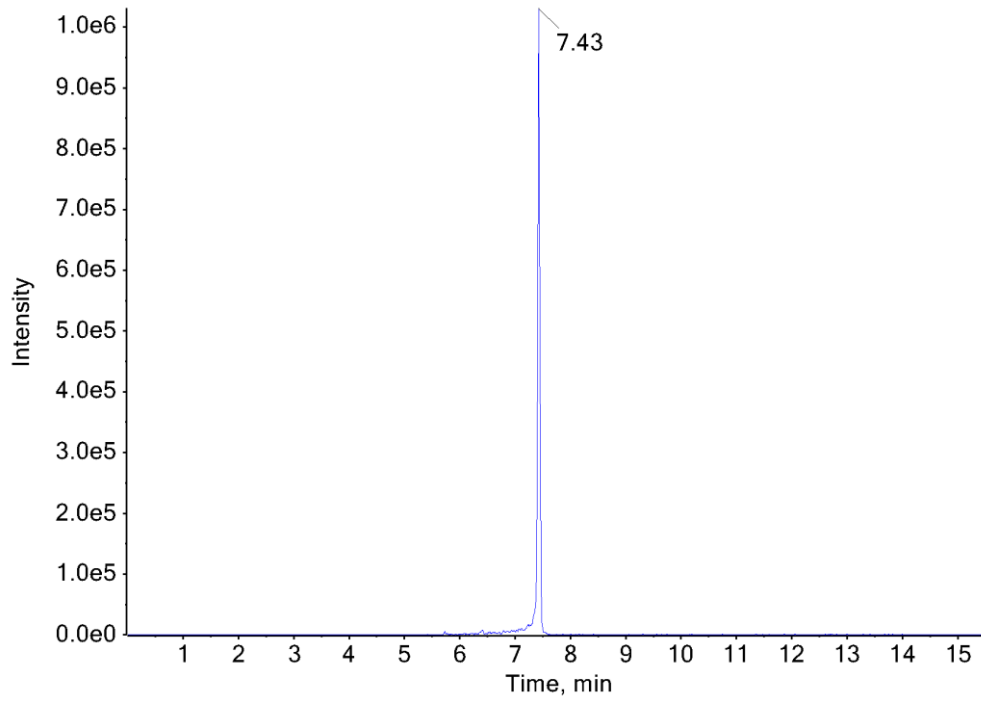
#### EI (70 eV) Mass Spectrum: 4'-Cl-Deschloroalprazolam (Standard)



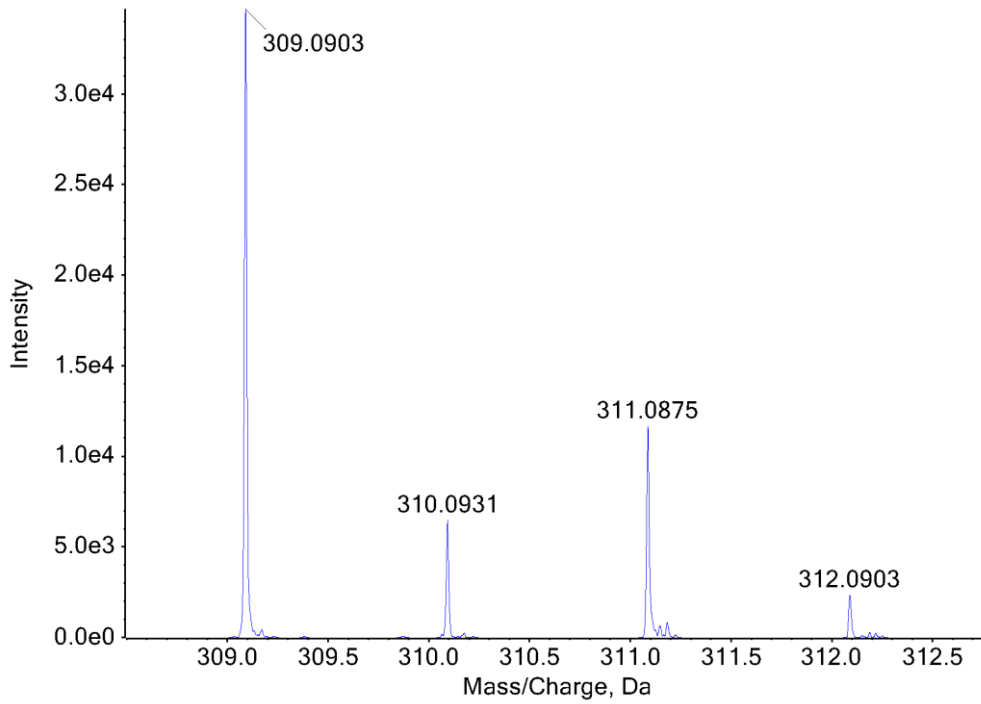
## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

<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>	Liquid-liquid extraction (LLE)
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	TOF MS Scan Range: 100-510 Da Precursor Isolation: SWATH® acquisition (27 windows) Fragmentation: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
<b>Retention Time:</b>	7.43 min
<b>Standard Comparison:</b>	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. ( <a href="https://www.caymanchem.com/product/36057/4'-chloro-deschloroalprazolam">https://www.caymanchem.com/product/36057/4'-chloro-deschloroalprazolam</a> )

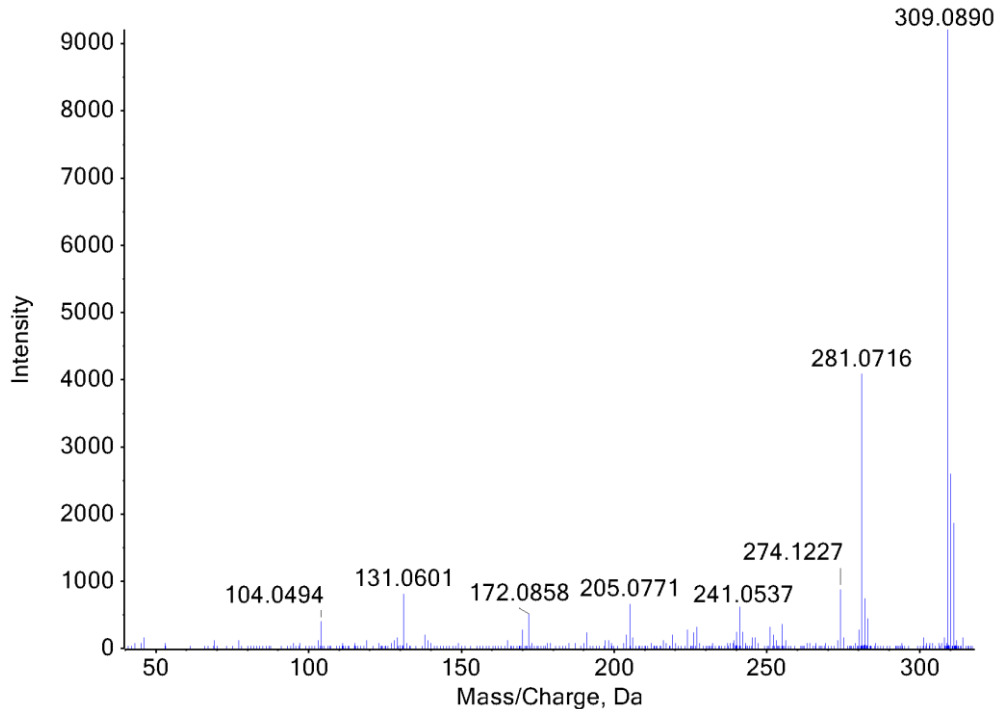
### Extracted Ion Chromatogram: 4'-Cl-Deschloroalprazolam



### TOF MS Spectra: 4'-Cl-Deschloroalprazolam



## MS/MS Spectra: 4'-Cl-Deschloroalprazolam



## 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.