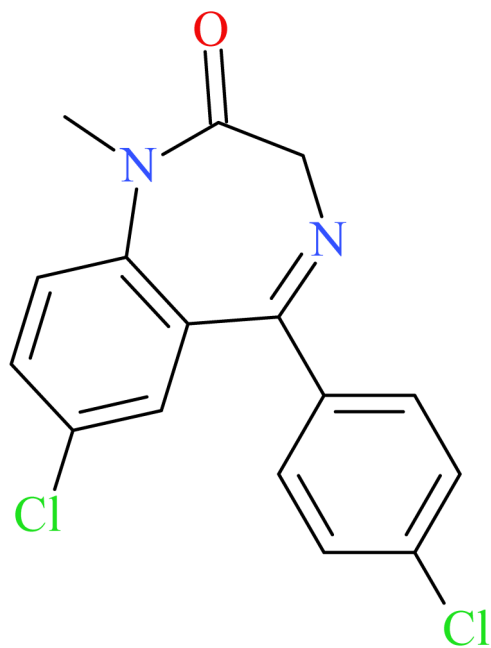




## 4'-Chlorodiazepam



NPS SUBCLASS	Benzodiazepine
REPORT DATE	November 20, 2023
SAMPLE RECEIVED	April 18, 2023
SAMPLE TYPE	Toxicology

Preferred Name	4'-Chlorodiazepam
Synonyms	Ro 5-4864, 4'Cl-Diazepam, 4-Chlorodiazepam
Formal Name	7-chloro-5-(4-chlorophenyl)-1-methyl-3H-1,4-benzodiazepin-2-one
InChI Key	PUMYFTJOWAJIKF-UHFFFAOYSA-N
CAS Number	14439-61-3
Chemical Formula	C <sub>16</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O
Molecular Weight	319.18
Molecular Ion [M <sup>+</sup> ]	318
Exact Mass [M+H] <sup>+</sup>	319.0399

## Characterization & Intelligence

The following information was compiled in November 2023 and is subject to change as new research is conducted and as new information becomes available:

**Description:** 4'-Chlorodiazepam is a novel benzodiazepine bearing structural resemblance to diazepam. 4'-Chlorodiazepam is an isomer of diclazepam (2'-chlorodiazepam); the two were resolved during analysis. 4'-Chlorodiazepam was detected for the first time in the United States by our laboratory in May 2023, and the drug was confirmed in October 2023 after acquiring standard reference material. Of note, this case was collected in 2020.

**Sample Source:** Washoe County Medical Examiner and Coroner, NMS Labs – Toxicology Laboratory

**Sample Appearance:** Liver Specimen, Gastric Fluid

**Pharmacology:** The pharmacology of 4'-chlorodiazepam is extensively published in the literature.<sup>1,2</sup>

**Toxicology:** 4'-Chlorodiazepam has been detected in one toxicology case at the CFSRE.

**Drug Materials:** 4'-Chlorodiazepam has not been identified in drug materials to date at the CFSRE.

**Demographics / Geographics:** The case originated from Nevada.

**Legal Status:** 4'-Chlorodiazepam is not explicitly scheduled in the United States.

### References:

- ▶ Cayman Chemical: [4'-Chlorodiazepam](#)
- ▶ Hoffmann et al. (1964) [Amino substituted benzophenone oximes and derivatives thereof](#)
- ▶ <sup>1</sup>Patel et al. (1982) [Differential effects of GABA on peripheral and central type benzodiazepine binding sites in brain](#)
- ▶ <sup>2</sup>Weissman et al. (1983) [Pharmacological, electrophysiological, and neurochemical actions of the convulsant benzodiazepine Ro 5-4864 \(4'-chlorodiazepam\)](#)

**About:** In collaboration with medical examiner and coroner offices, crime laboratories, clinical partners, and other stakeholders, the Center for Forensic Science Research and Education (CFSRE) is documenting first confirmations of NPS through analysis of drug materials and/or toxicology samples. These reports are generated using comprehensive analytical techniques (e.g., GC-MS, LC-QTOF-MS, NMR) and include available information about the new substances identified at the time of reporting, as well as the analytical data generated during testing. Our new drug monographs are intended to assist with the rapid identification of NPS in forensic casework and related disciplines, and should not be used for confirmatory purposes alone.

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

**Acknowledgements:** This report was prepared by Alex J. Krotulski, Sara E. Walton, Donna M. Papsun, Melissa F. Fogarty, and Barry K. Logan at the Center for Forensic Science Research and Education (CFSRE) at the Fredric Rieders Family Foundation. The authors acknowledge scientists at the CFSRE and NMS Labs for their involvements and contributions. For more information, contact [npsdiscovery@cfsre.org](mailto:npsdiscovery@cfsre.org) or visit [www.npsdiscovery.org](http://www.npsdiscovery.org).

**Funding:** CFSRE's NPS Discovery is supported by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 15PNIJ-22-GG-04434-MUMU, "Implementation of NPS Discovery – An Early Warning System for Novel Drug Intelligence, Surveillance, Monitoring, Response, and Forecasting using Drug Materials and Toxicology Populations in the US"). 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.

**Suggested Citation:** Krotulski, AJ; Walton, SE; Papsun, DM; Fogarty, MF; Logan, BK. (2023) *4'-Chlorodiazepam — NPS Discovery New Drug Monograph*, Center for Forensic Science Research and Education, United States.

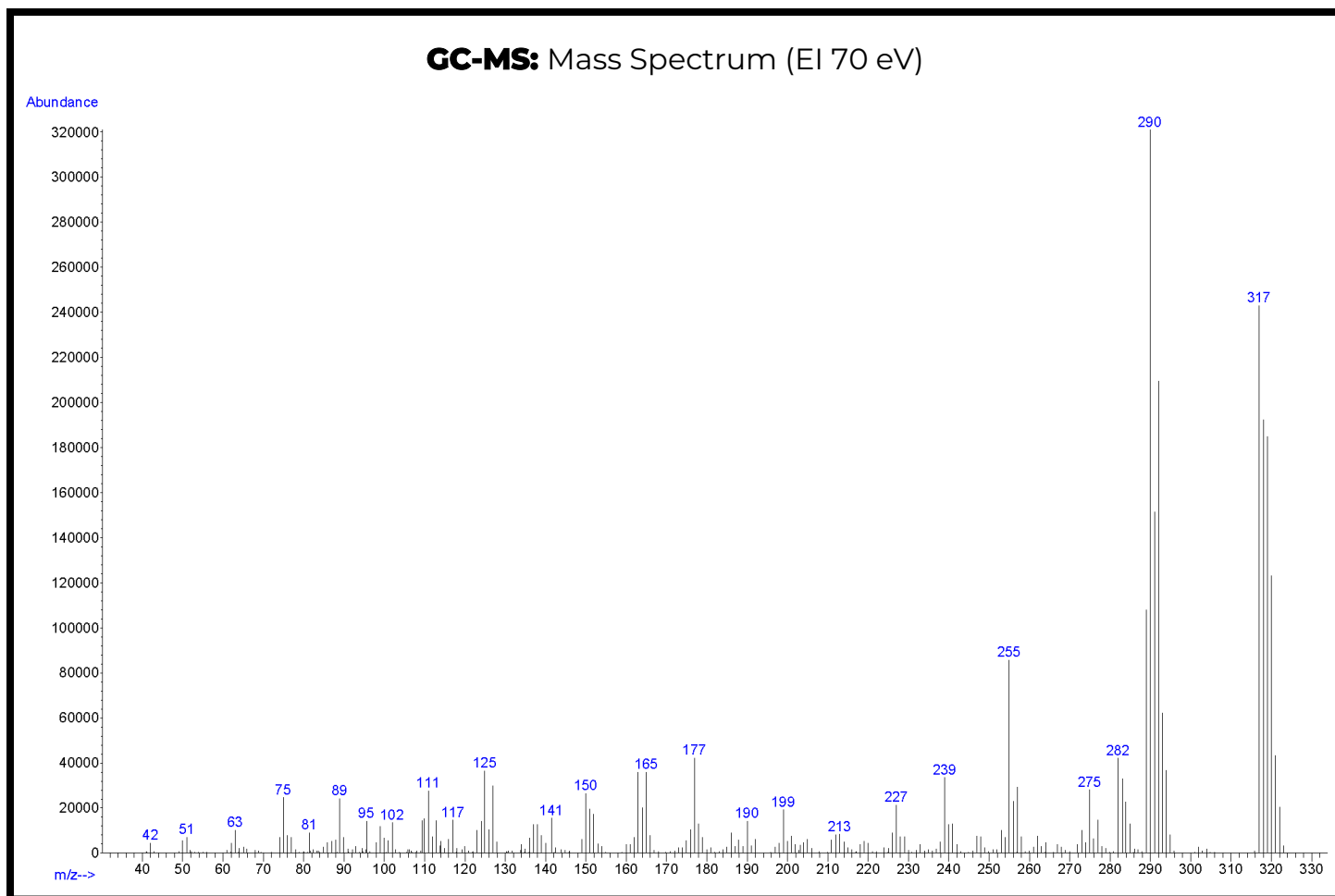
## Gas Chromatography Mass Spectrometry (GC-MS)

**Laboratory:** Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

**Instrument:** Agilent 5975 Series GC/MSD

**Sample Preparation:** Standard diluted in methanol

**Methods:** [www.cfsre.org/nps-discovery/monographs](http://www.cfsre.org/nps-discovery/monographs)  
[GC-MS Method Details](#)



# Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (LC-QTOF-MS)

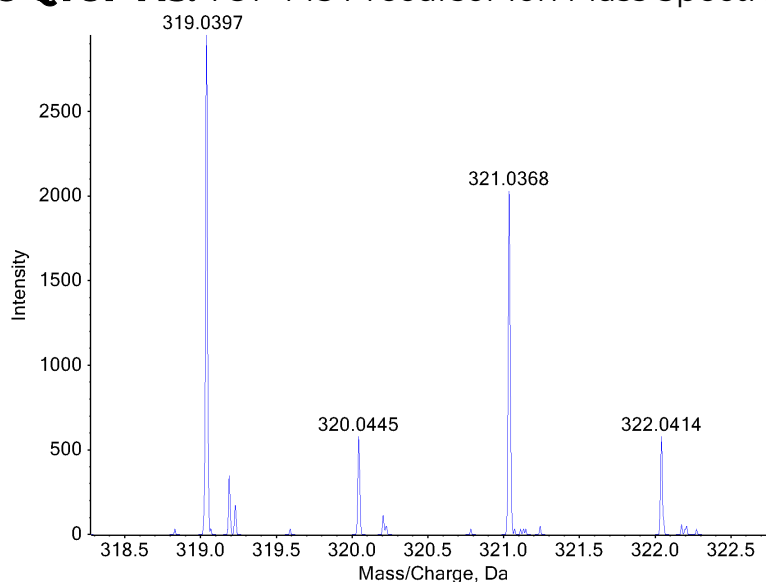
**Laboratory:** Center for Forensic Science Research and Education (CFSRE, Willow Grove, PA, USA)

**Instrument:** Sciex X500R LC-QTOF-MS

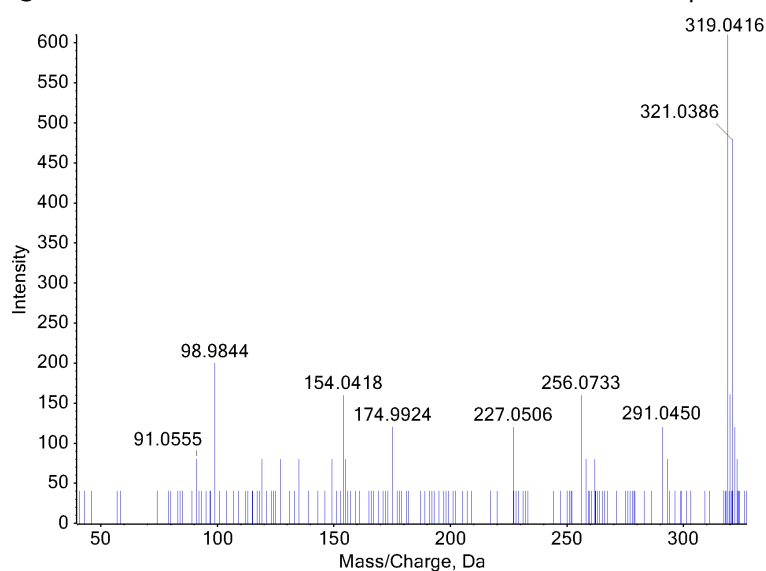
**Sample Preparation:** Liquid-liquid extraction

**Methods:** [www.cfsre.org/nps-discovery/monographs](http://www.cfsre.org/nps-discovery/monographs)  
[LC-QTOF-MS Method Details](#)

**LC-QTOF-MS: TOF-MS Precursor Ion Mass Spectrum**



**LC-QTOF-MS: TOF-MS/MS Product Ion Mass Spectrum**



**Confirmation Using Drug Standard:** Reference material (Batch: 0681851-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). The analyte was confirmed to be 4'-chlorodiazepam based on retention time (sample: 8.94 min vs. standard: 8.95 min) and mass spectral data comparisons.