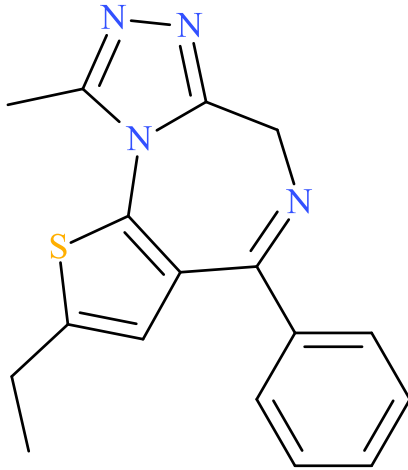


Deschloroetizolam

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 “R 0 3 9”

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

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₁₇ H ₁₆ N ₄ S	308.4	308	309.1168

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

1. Tahara, T.; Mikashima, H.; Terasawa, M; Maruyama, Y. (1987) PAF-antagonistic activity of some thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepines. *Chem. Pharm. Bull.*, **35**, 2119.
2. Nakanishi, M.; Tahara, T.; Araki, K.; Shiroki, M. (1975). Patent US 3904641 - Triazolothienodiazepine compounds. <https://patents.google.com/patent/US3904641>
3. Kitajima, H.; Ehara, S.; Sato, H.; Moriwaki, M.; Onishi, K. (1997) Patent EP 0776892 - Thienylazole compound and thienotriazolodiazepine compound. <https://patents.google.com/patent/EP0776892A1>
4. European Monitoring Centre for Drugs and Drug Addiction. (2015) EMCDDA-Europol 2014 Annual Report on the implementation of Council Decision 2005/387/JHA. *Implementation reports, Publications Office of the European Union, Luxembourg.* <https://www.emcdda.europa.eu/system/files/publications/1018/TDAN15001ENN.pdf>

4. ADDITIONAL RESOURCES (CONTINUED)

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Deschloroetizolam-ID-1174-15-report_final.pdf

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

<https://en.wikipedia.org/wiki/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

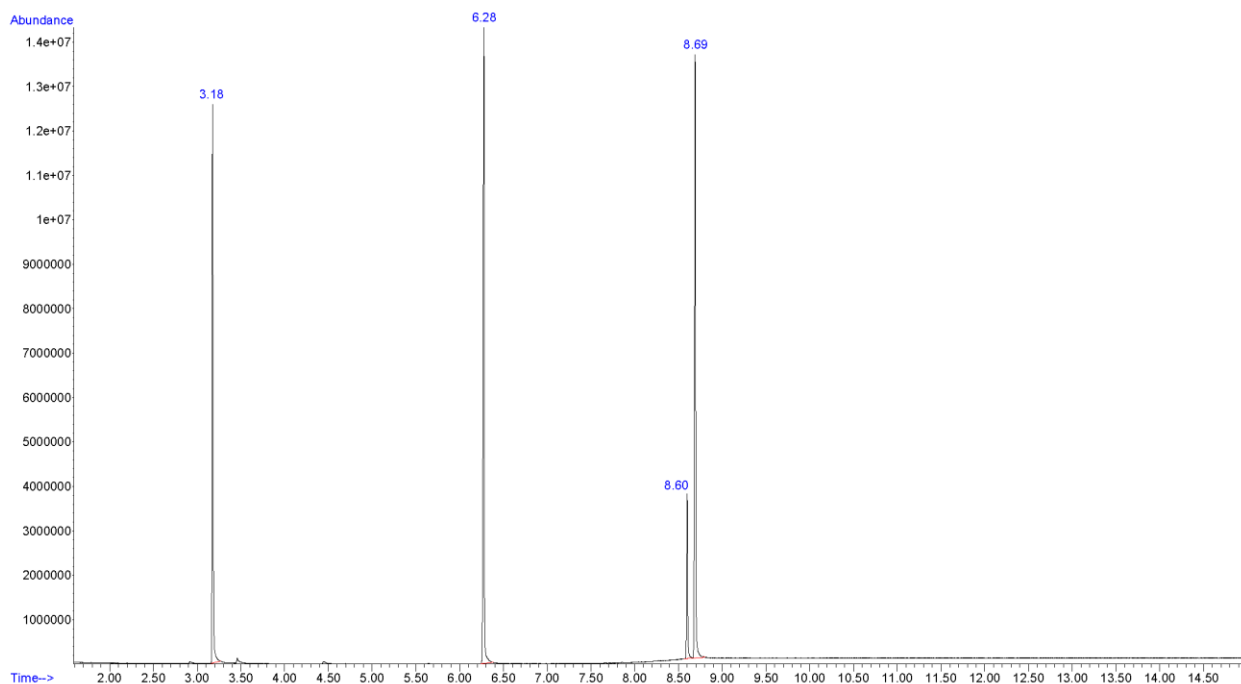
Retention Time: 8.60 min

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.

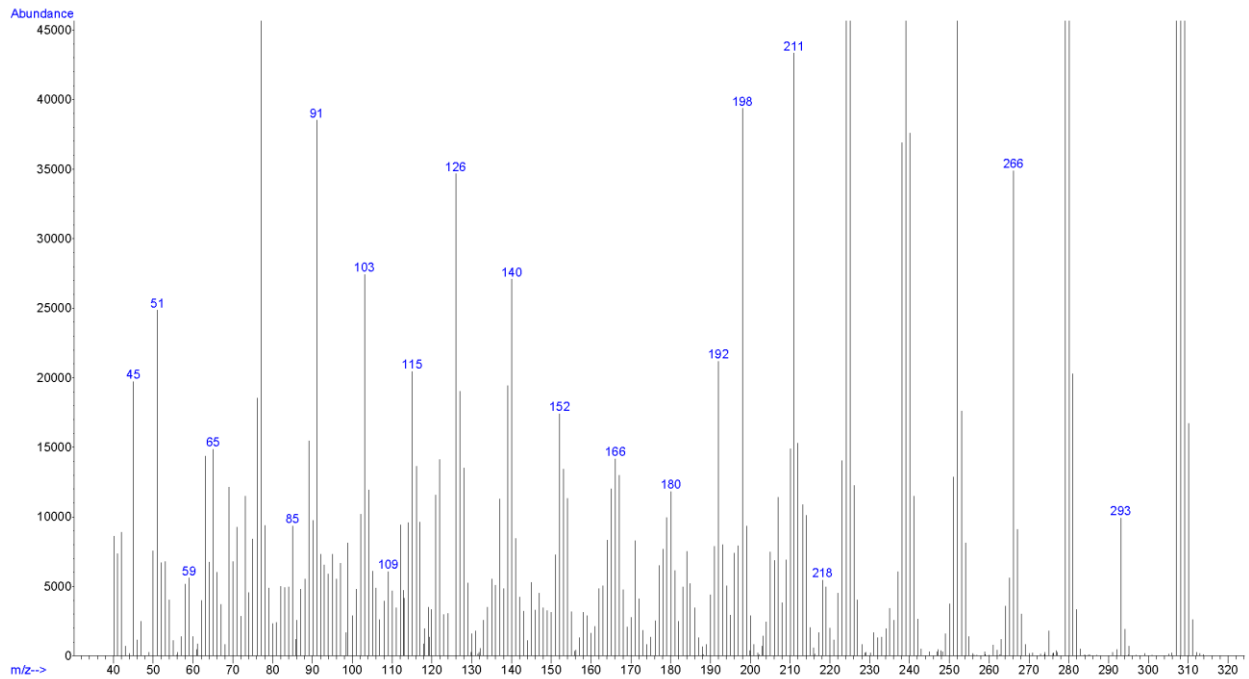
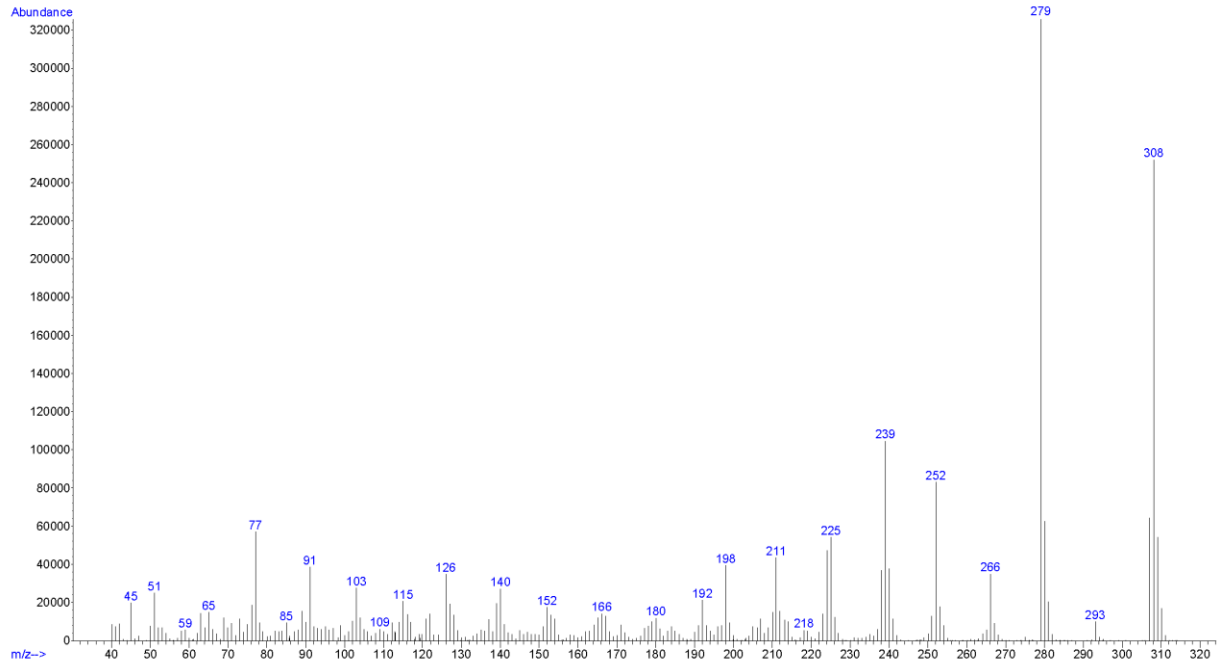
<https://www.caymanchem.com/product/23107/deschloroetizolam>

Chromatogram: Deschloroetizolam



Additional peaks present in chromatogram: internal standards (3.18 min and 6.28 min) and flubromazolam (8.69 min)

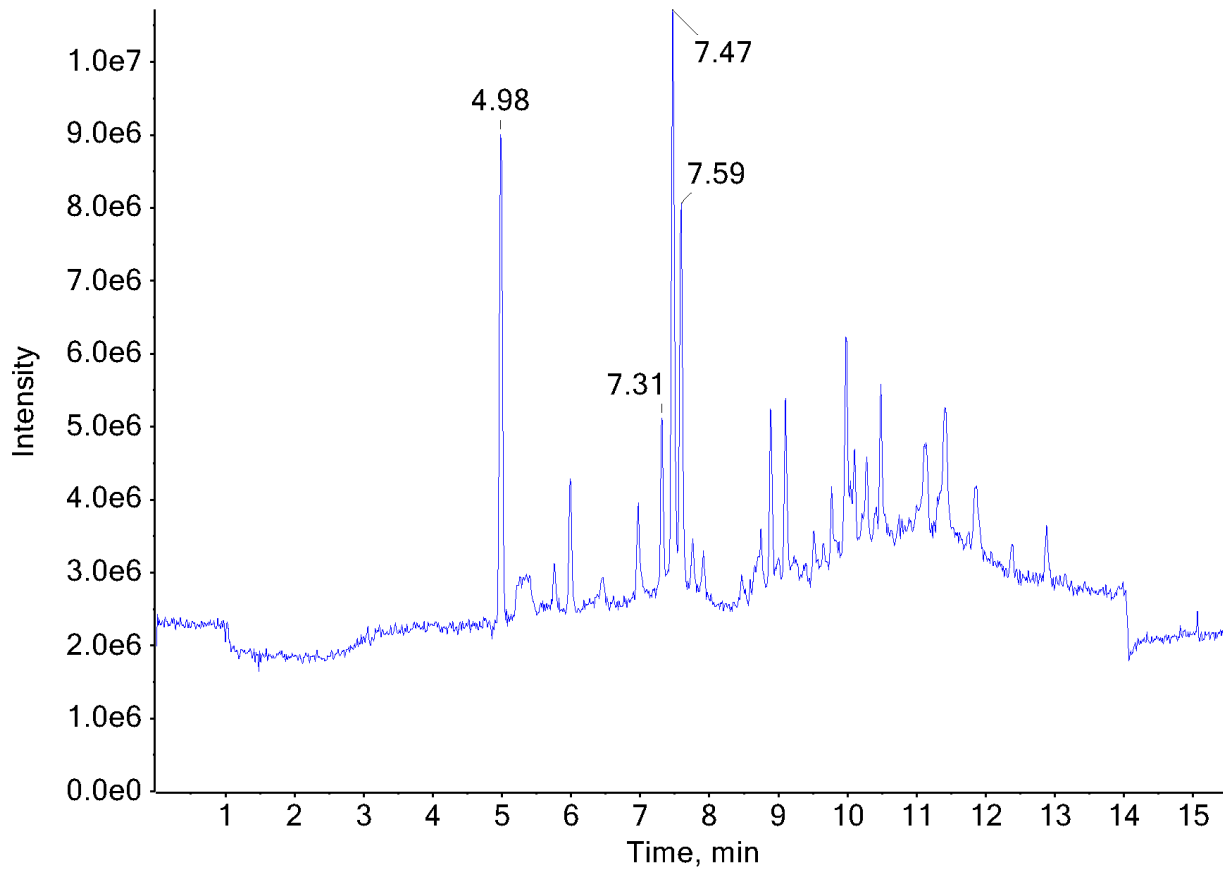
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Deschloroetizolam



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

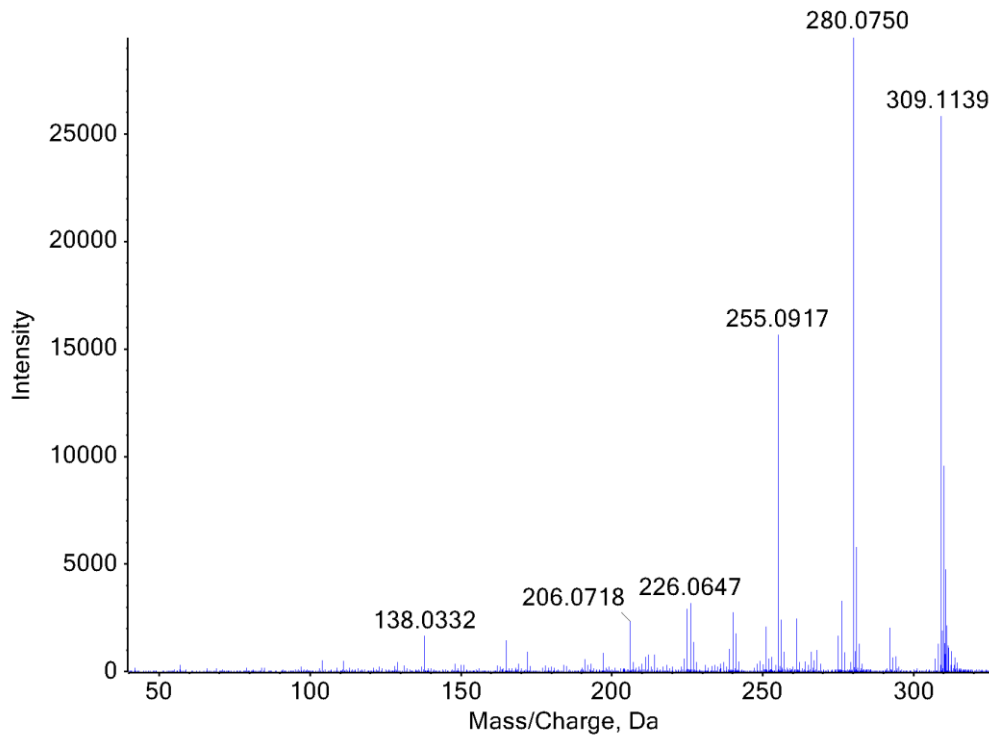
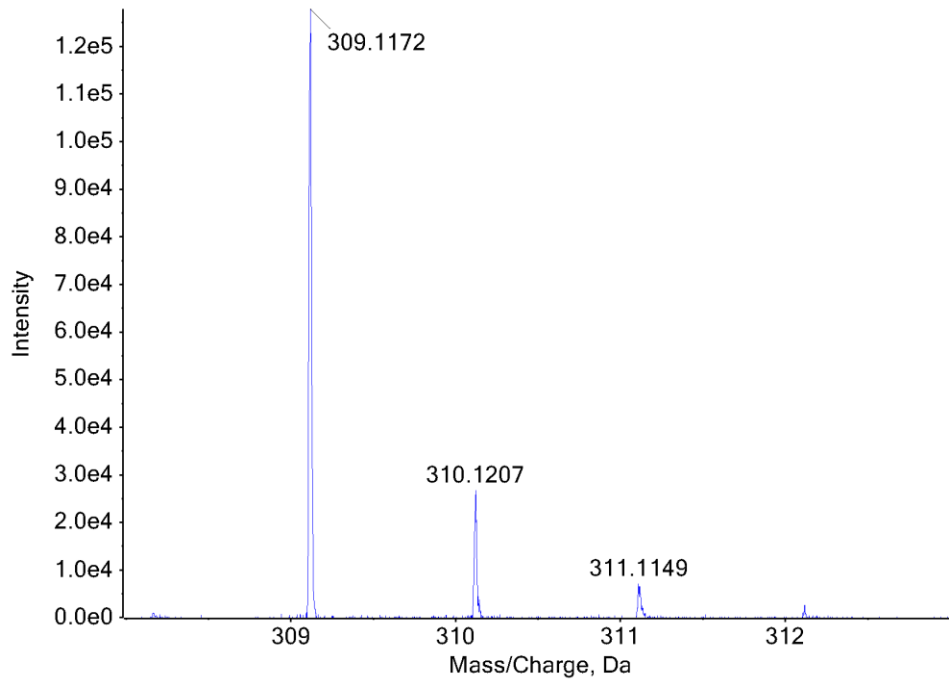
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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: Collision 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

NPS Discovery at the Center for Forensic Science Research and Education (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 reflect those of the Department of Justice.