

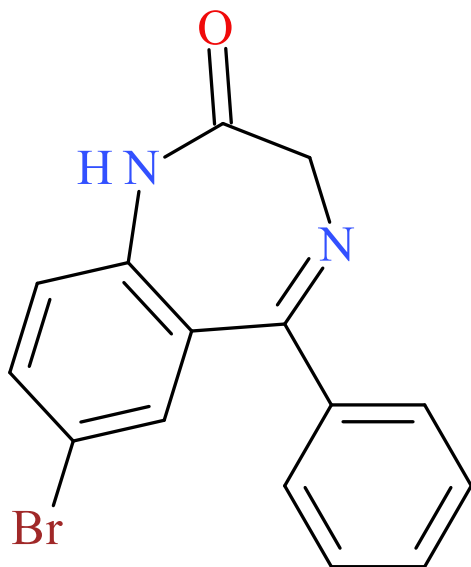
## Desalkylgidazepam

Sample Type: **Toxicology Sample**

Latest Revision: **December 9, 2022**

Date Received: **September 12, 2022**

Date of Report: **December 9, 2022**



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	7-bromo-5-phenyl-1,3-dihydro-1,4-benzodiazepin-2-one
<b>InChI String:</b>	InChI=1S/C15H11BrN2O/c16-11-6-7-13-12(8-11)15(17-9-14(19)18-13)10-4-2-1-3-5-10/h1-8H,9H2,(H,18,19)
<b>CFR:</b>	Not Scheduled (12/2022)
<b>CAS#</b>	2894-61-3
<b>Synonyms:</b>	Bromonordiazepam, Bromo-nordazepam
<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.

**Prepared By:** Alex J. Krotulski, 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

Drug	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Desalkylgidazepam	C <sub>15</sub> H <sub>11</sub> BrN <sub>2</sub> O	315.2	314	315.0128

### 3. BRIEF DESCRIPTION

Desalkylgidazepam 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). Desalkylgidazepam is a metabolite of the prodrug gidazepam but has now emerged on the recreational drug market as a drug on its own. Desalkylgidazepam is structurally similar to nordiazepam. Desalkylgidazepam is not federally controlled in the United States; however, nordiazepam is a Schedule IV drug.

### 4. ADDITIONAL RESOURCES

Andronati SA, Zin'kovskii VG, Totrova MI, Golovenko NI, Stankevich EA, Zhuk OV. (1992) Biokinetics of a new prodrug gidazepam and its metabolite. *Biull Eksp Biol Med.* 113(1):45-7. <https://pubmed.ncbi.nlm.nih.gov/1356504/>

Kolyvanov GB, Zherdev VP, Chirkov AM, Otabekova SG, Litvin AA. (1993) Gidazepam biotransformation and pharmacokinetics in different species of animals and man. *Eksp Klin Farmakol.* 56(3):48-50. <https://pubmed.ncbi.nlm.nih.gov/8106054/>

<https://www.caymanchem.com/product/36608/desalkylgidazepam>

## 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)

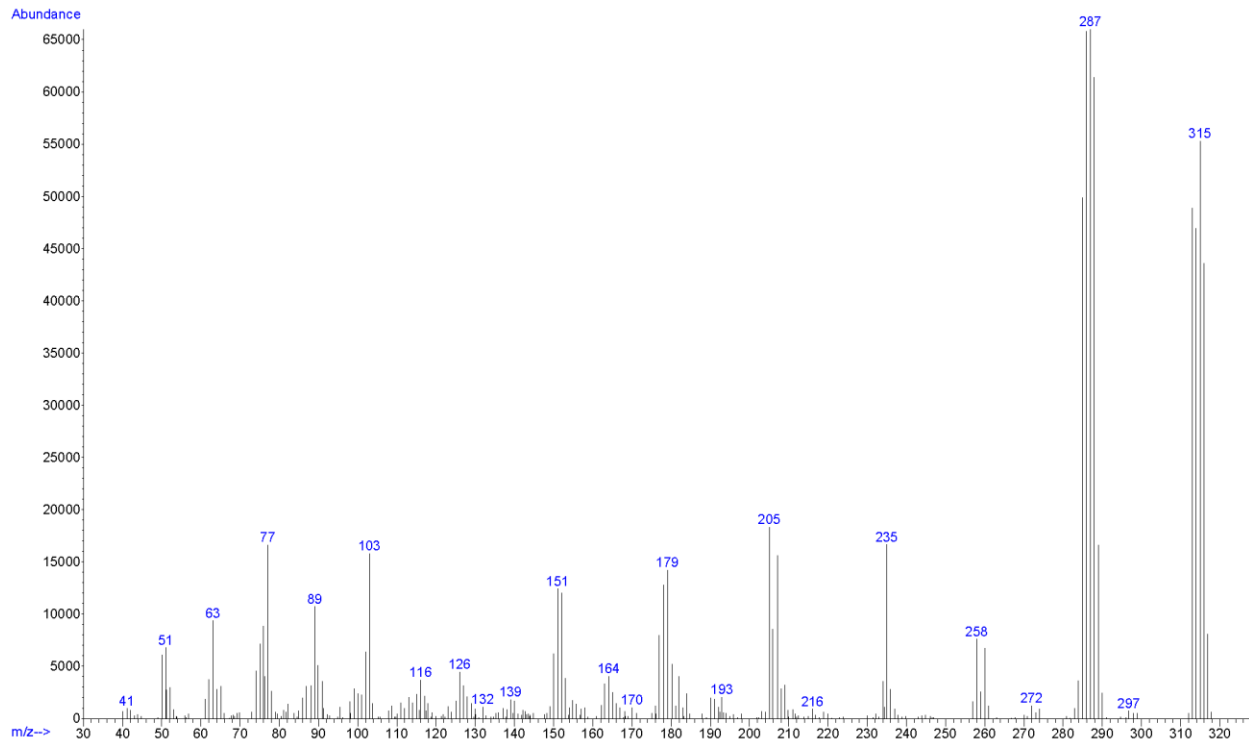
**Sample Preparation:** Standard diluted in methanol

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

**Standard:** Reference material for desalkylgidazepam (Batch: 0641974-5) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA).

<https://www.caymanchem.com/product/36608/desalkylgidazepam>

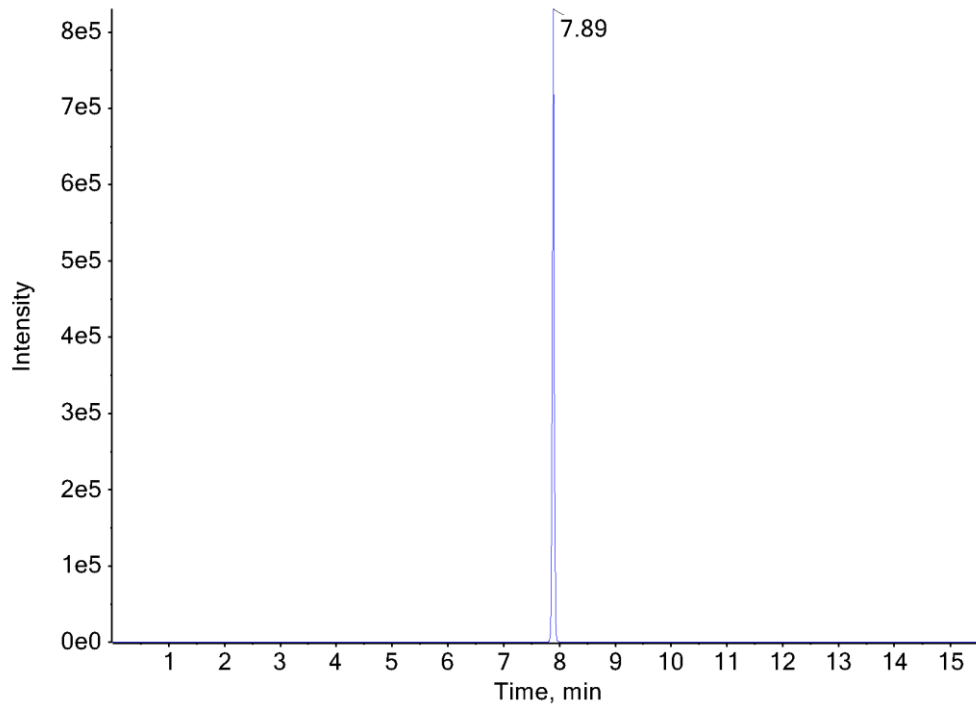
#### EI (70 eV) Mass Spectrum: Desalkylgidazepam (Standard)



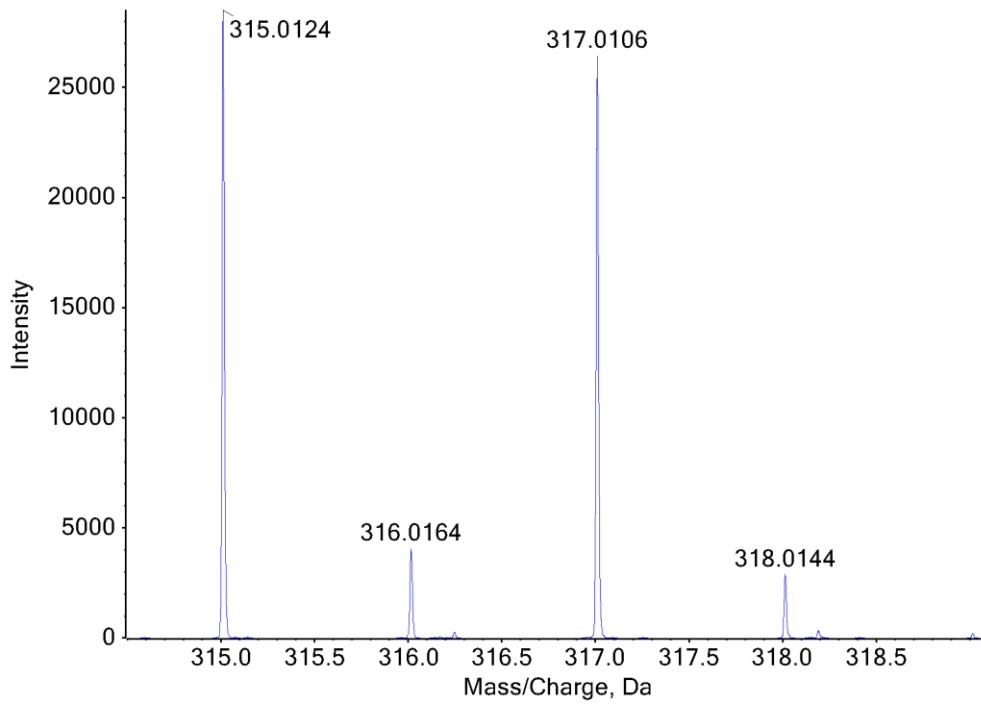
## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

<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 X500R, Sciex ExionLC
<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>	7.89 min
<b>Standard Comparison:</b>	Reference material for desalkylgidazepam (Batch: 0641974-5) 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 desalkylgidazepam, based on retention time (7.90 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/36608/desalkylgidazepam">https://www.caymanchem.com/product/36608/desalkylgidazepam</a> )

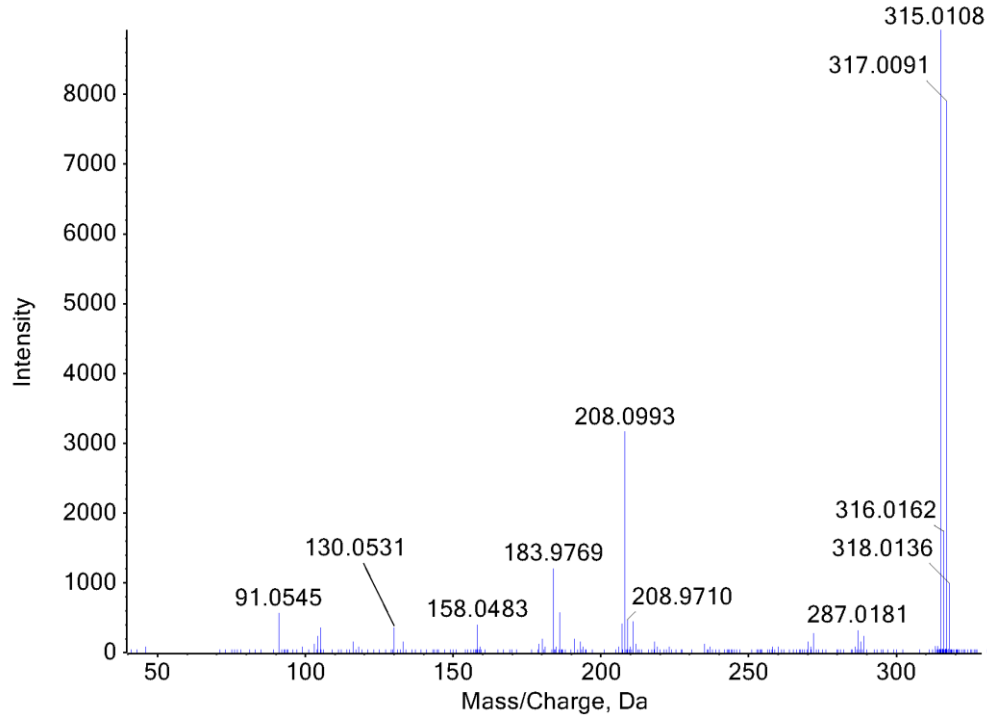
### Extracted Ion Chromatogram: Desalkylgidazepam



### TOF MS Spectra: Desalkylgidazepam



## MS/MS Spectra: Desalkylgidazepam



## 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.