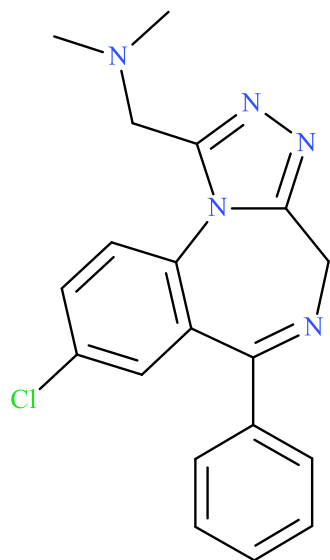


## Adinazolam

Sample Type: **Biological Fluid**

Latest Revision: **August 11, 2020**

Date of Report: **August 11, 2020**



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-(8-chloro-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepin-1-yl)-N,N-dimethyl-methanamine
<b>InChI String:</b>	InChI=1S/C19H18ClN5/c1-24(2)12-18-23-22-17-11-21-19(13-6-4-3-5-7-13)15-10-14(20)8-9-16(15)25(17)18/h3-10H,11-12H2,1-2H3
<b>CFR:</b>	Not Scheduled (07/2020)
<b>CAS#</b>	37115-32-5
<b>Synonyms:</b>	Deracyn®
<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

Form	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>19</sub> H <sub>18</sub> ClN <sub>5</sub>	351.8	351	352.1323

### 3. SAMPLE HISTORY

Adinazolam has been identified in at least three toxicology cases since April 2020. The geographical and demographical breakdown is below:

<b>Case Type:</b>	Postmortem (n=3)
<b>Geographical Location:</b>	Michigan (n=1), Mississippi (n=1), Rhode Island (n=1)
<b>Gender:</b>	Female (n=1), Male (n=1), Unknown (n=1)
<b>Age Range:</b>	20-40 years
<b>Biological Sample:</b>	Blood (n=3)
<b>Date of First Collection:</b>	April 2020
<b>Additional Findings:</b>	Flualprazolam (n=2), Etizolam (n=2), Fentanyl (n=2)

### 4. BRIEF DESCRIPTION

Adinazolam is classified as a novel benzodiazepine due to its recent emergence among forensic investigations (n=3) in the United States. Benzodiazepines are central nervous system depressants. Novel benzodiazepines, often pirated from early drug discovery or pharmaceutical studies, have appeared on novel and illicit drug markets in recent years. These substances 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). Unlike some novel benzodiazepines, there exist several published reports involving adinazolam. Adinazolam was first synthesized in 1980 by researchers at the Upjohn Company.<sup>1</sup> Pharmacological studies show adinazolam exhibits anxiolytic and antidepressant activity.<sup>1-4</sup> The metabolism of adinazolam has been extensively studied, showing conversion to *N*-desmethyl adinazolam, *N,N*-didesmethyl adinazolam, and *alpha*-hydroxy alprazolam.<sup>2,5</sup> Adinazolam is structurally distinct from traditional benzodiazepines; however, its structure may be considered most similar to alprazolam, the difference being the addition of an aminoalkyl- group to the triazole ring. Adinazolam is not a scheduled substance in the United States.

## 5. ADDITIONAL RESOURCES

1. Hester, JB; Rudzik, AD; VonVoigtlander, PF. (1980) 1-(Aminoalkyl)-6-aryl-4H-s-triazolo [4, 3-a][1, 4] benzodiazepines with antianxiety and antidepressant activity. *J. Med. Chem.* 23, 392-402.
2. Sethy, VH; Collins, RJ; Daniels, EG. (1984) Determination of biological activity of adinazolam and its metabolites. *J. Pharm. Pharmacol.* 36, 546-548
3. Pyke, R; Cohn, J; Feighner, J; Smith, W. (1983) Open-label studies of adinazolam in severe depression. *Psychopharmacol Bull.* 19, 96-98.
4. Lathi, RA; Sethy, VH; Barsuhn, C; Hester, JB. (1983) Pharmacological profile of the antidepressant adinazolam, a triazolobenzodiazepine. *Neuropharmacol.* 22, 1277-82.
5. Venkatakrisnan, K; von Moltke, LL; Duan, SX; Fleishaker, JC; Shader, RI; Greenblatt, DJ. (1998) Kinetic Characterization and Identification of the Enzymes Responsible for the Hepatic Biotransformation of Adinazolam and N-desmethyadinazolam in Man. *J Pharm Pharmacol.* 50(3): 265-274.

<https://www.caymanchem.com/product/18205/adinazolam>

[https://www.policija.si/apps/nfl\\_response\\_web/0\\_Analytical\\_Reports\\_final/ADINAZOLAM-ID-1277-15-report\\_final.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/ADINAZOLAM-ID-1277-15-report_final.pdf)

<http://swgdrug.org/Monographs/Adinazolam.pdf>

## 6. QUALITATIVE DATA

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

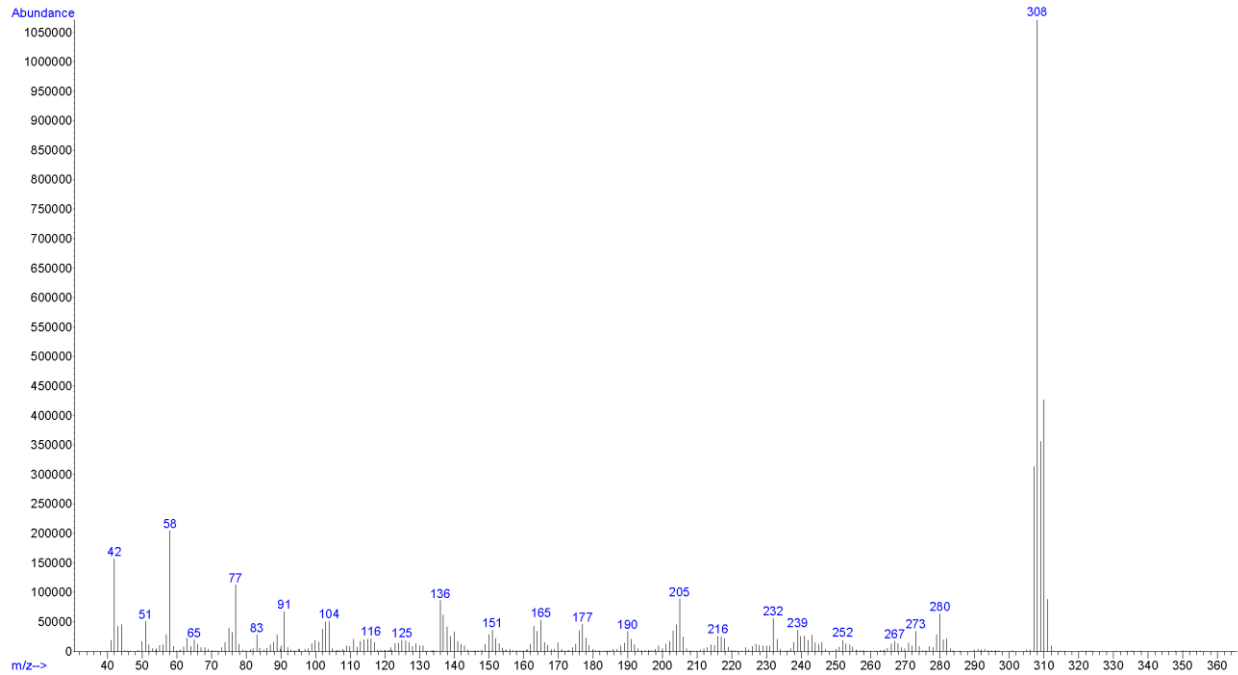
**Testing Performed At:** NMS Labs (Willow Grove, PA)

**Sample Preparation:** Acid/base extraction

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

**Standard:** Reference material for Adinazolam (Batch: 0579199-7) was purchased from Cayman Chemical (Ann Arbor, MI, USA).  
(<https://www.caymanchem.com/product/18205/adinazolam>)

## EI (70 eV) Mass Spectrum: Adinazolam



### 6.2 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:** No additional preparation - direct analysis of sample extract

**Instrument:** Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

**Column:** Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6  $\mu$ m)

**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)

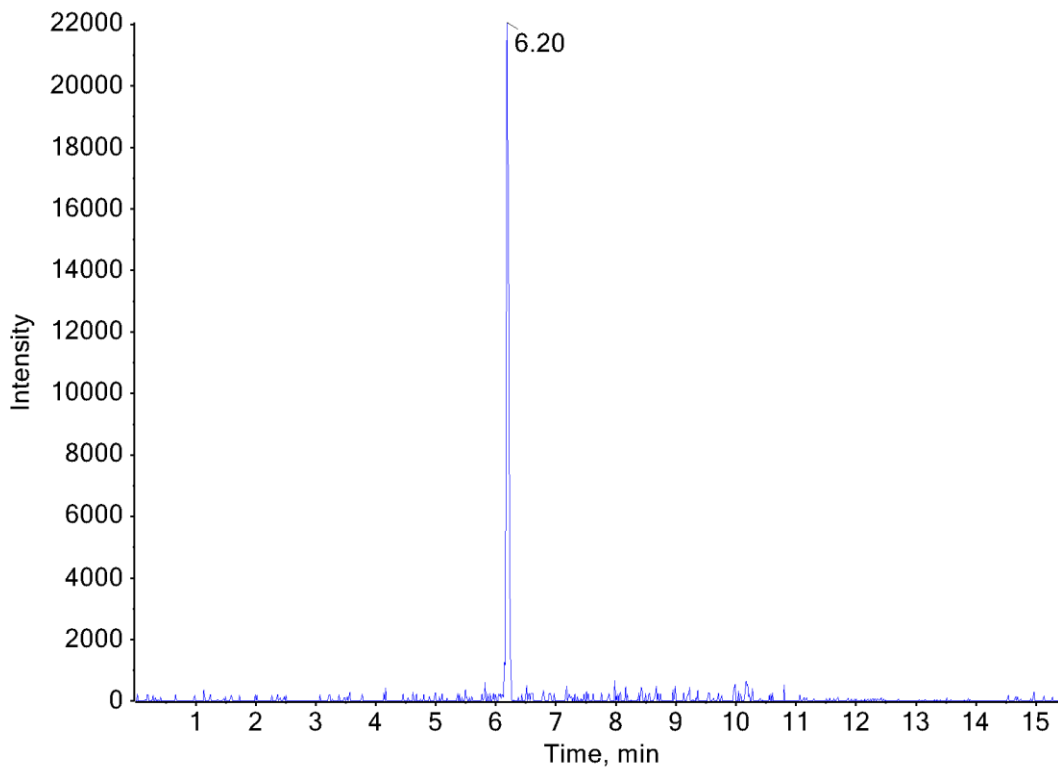
MS/MS Scan Range: 50-510 Da

**Retention Time:** 6.20 min

**Standard Comparison:** Reference material for Adinazolam (Batch: 0579199-7) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Adinazolam, based on retention time (6.04 min) and mass spectral data.

<https://www.caymanchem.com/product/18205/adinazolam>

### Extracted Ion Chromatogram (XIC): Adinazolam



**TOF MS (Top) and MS/MS (Bottom) Spectra: Adinazolam**

