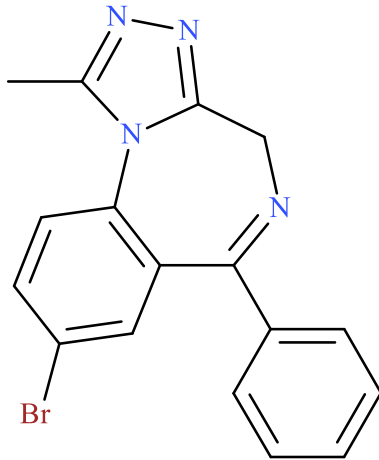


## Bromazolam



Sample Type: **Seized Material & Biological Fluid**

Latest Revision: **May 1, 2020**

Date Received: **March 3, 2020**  
(Seized Material)

Date of Report: **May 1, 2020**

### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	8-bromo-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine
<b>InChI String:</b>	InChI=1S/C17H13BrN4/c1-11-20-21-16-10-19-17(12-5-3-2-4-6-12)14-9-13(18)7-8-15(14)22(11)16/h2-9H,10H2,1H3
<b>CFR:</b>	Not Scheduled (04/2020)
<b>CAS#</b>	71368-80-4
<b>Synonyms:</b>	XLI-268
<b>Source:</b>	Department of Homeland Security (Seized Material) NMS Labs – Toxicology Department (Biological Fluid)
<b>Appearance:</b>	Orange round tablet, Singly-score, Monogrammed “LL” (Seized Material)

**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 <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>17</sub> H <sub>13</sub> BrN <sub>4</sub>	353.2	352	353.0396

### 3. BRIEF DESCRIPTION

Bromazolam is classified as a novel benzodiazepine. Limited peer reviewed literature is available describing bromazolam. Confirmatory data for its activity and potency have not been reported. Benzodiazepines are central nervous system depressants. Novel benzodiazepines, often pirated from early drug discovery or pharmaceutical studies, have appeared on the 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). Bromazolam is structurally similar to traditional benzodiazepines, including alprazolam (replacing the chlorine with a bromine) and bromazepam (addition of triazole ring). Alprazolam and bromazepam are Schedule IV substances in the United States; bromazolam is not explicitly scheduled. To date, bromazolam has been identified in at least one blood sample from a forensic toxicology case.

### 4. SAMPLE HISTORY (BIOLOGICAL FLUID)

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

<b>Case Type:</b>	DUID Investigation (n=1)
<b>Geographical Location:</b>	Pennsylvania (n=1)
<b>Gender:</b>	Not Available
<b>Age Range:</b>	Not Available
<b>Biological Sample:</b>	Blood (n=1)
<b>Date of First Collection:</b>	January 2020
<b>Additional Findings:</b>	No additional NPS or benzodiazepines identified

## 5. ADDITIONAL RESOURCES

Manchester et al. (2018) The Emergence of New Psychoactive Substance (NPS) Benzodiazepines: A Review. *Drug Testing and Analysis*. **10** (1), 37-53.

Waters et al. (2018) The use of a quantitative structure-activity relationship (QSAR) model to predict GABA-A receptor binding of newly emerging benzodiazepines. *Science & Justice*. **58** (3), 219-225.

[http://www.emcdda.europa.eu/system/files/publications/4724/TDAN17001ENN\\_PDFWEB.pdf](http://www.emcdda.europa.eu/system/files/publications/4724/TDAN17001ENN_PDFWEB.pdf)

<https://www.caymanchem.com/product/22665/bromazolam>

## 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

**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

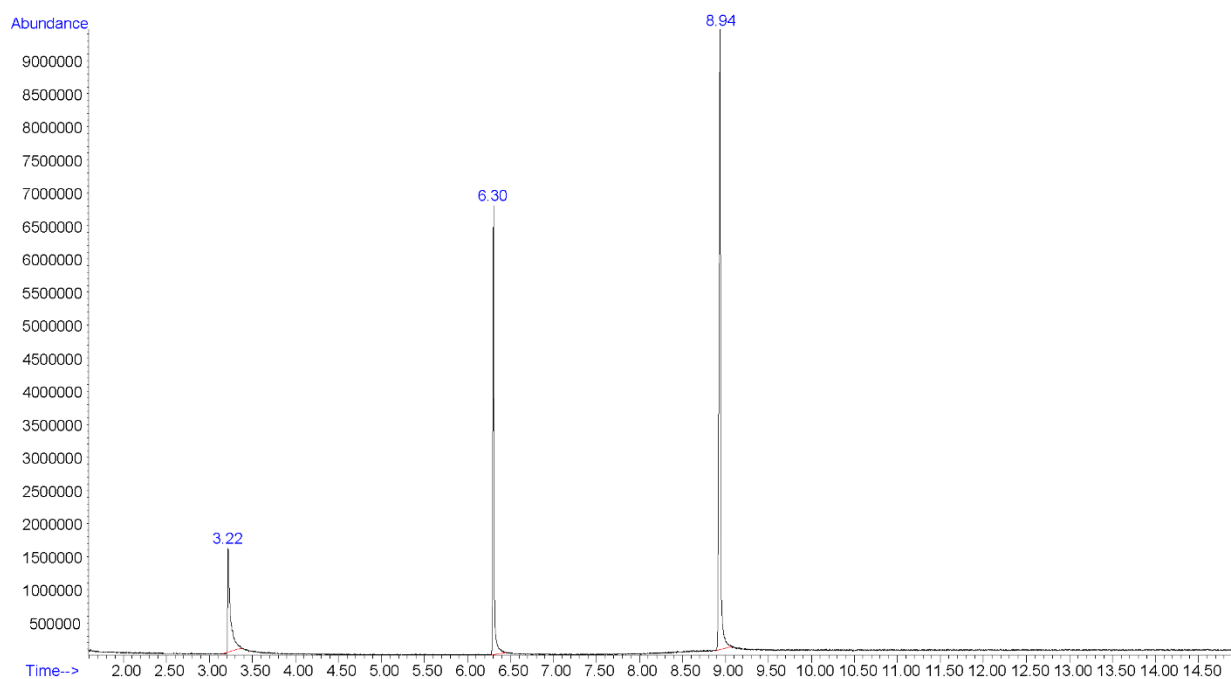
**Injection Parameters:** Injection Type: Splitless  
Injection Volume: 1 μL

**MS Parameters:** Mass Scan Range: 40-550 m/z  
Threshold: 250

**Retention Time:** 8.94 min

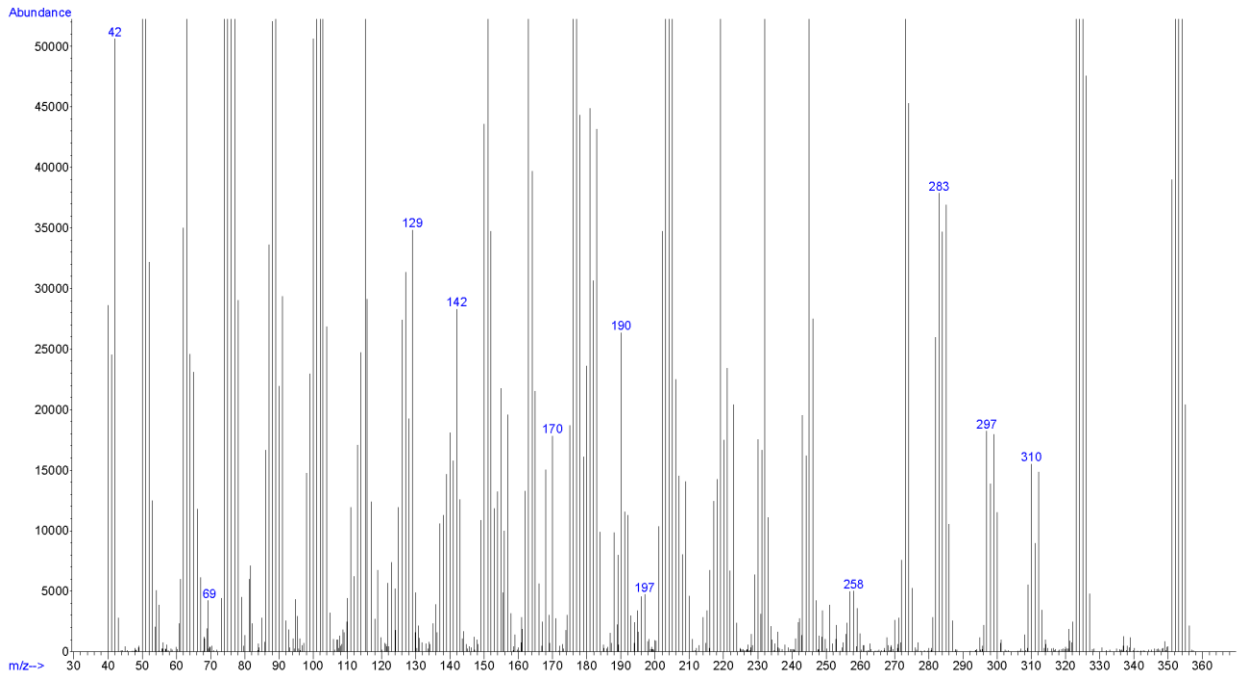
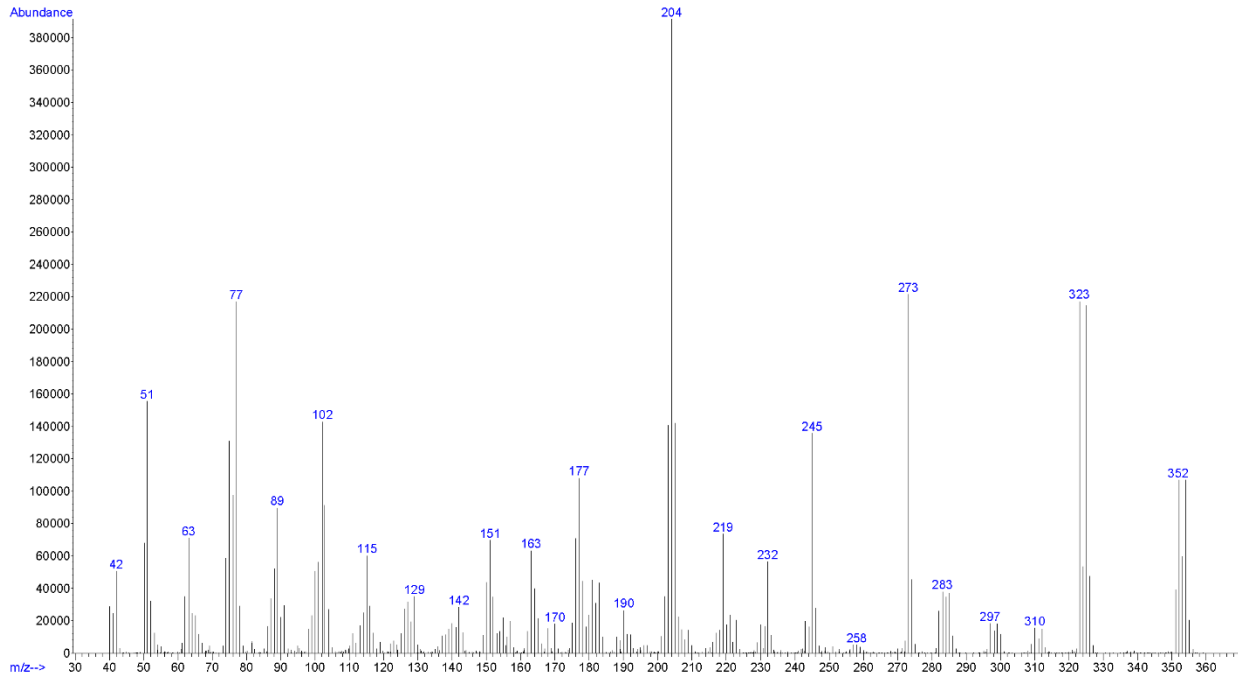
**Standard Comparison:** Reference material for Bromazolam (Batch: 0545063-11) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Bromazolam, based on retention time (8.92 min) and mass spectral data.  
(<https://www.caymanchem.com/product/22665/bromazolam>)

### Chromatogram: Bromazolam



*Additional peaks present in chromatogram: internal standards (3.22 min and 6.30 min)*

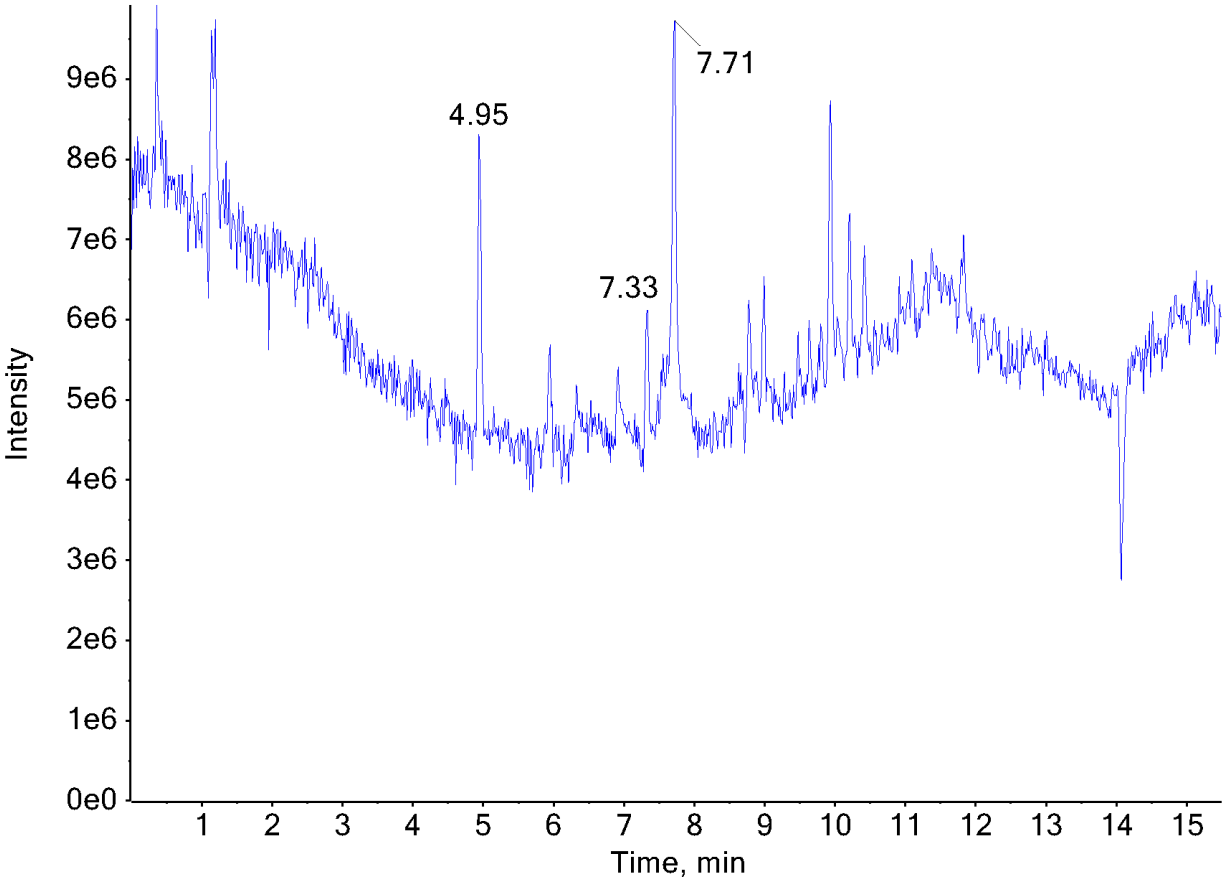
# EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Bromazepam



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

<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>	1:100 dilution of acid/base extract in mobile phase
<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>	7.71 min
<b>Standard Comparison:</b>	Reference material for Bromazolam (Batch: 0545063-11) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Bromazolam, based on retention time (7.72 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/22665/bromazolam">https://www.caymanchem.com/product/22665/bromazolam</a> )

**Chromatogram: Bromazolam**



*Additional peaks present in chromatogram: internal standards (4.95 min and 7.33 min)*

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

