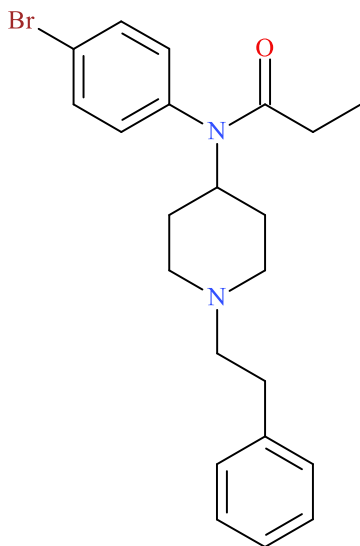


## Bromofentanyl

Sample Type: **Biological Fluid**

Latest Revision: **December 17, 2020**

Date of Report: **December 17, 2020**



### 1. GENERAL INFORMATION

**IUPAC Name:** N-(4-bromophenyl)-N-[1-(2-phenylethyl)-4-piperidyl]propanamide

**InChI String:** InChI=1S/C22H27BrN2O/c1-2-22(26)25(20-10-8-19(23)9-11-20)21-13-16-24(17-14-21)15-12-18-6-4-3-5-7-18/h3-11,21H,2,12-17H2,1H3

**CFR:** 21 CFR 1308: Temporary Placement of Fentanyl-Related Substances in Schedule 1 (02/06/2018)

**CAS#** 117994-23-7

**Synonyms:** *ortho*-Bromofentanyl, *meta*-Bromofentanyl, *para*-Bromofentanyl, 2-Bromofentanyl, 3-Bromofentanyl, 4-Bromofentanyl, Bromo fentanyl, BF

**Important Notes:** All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. The “*para*-bromo” configuration was used for structural purposes; however, position of the bromine atom was not confirmed during analysis.

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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>22</sub> H <sub>27</sub> BrN <sub>2</sub> O	415.4	414	415.1380

### 3. SAMPLE HISTORY

<b>Case Type:</b>	Antemortem (n=1)
<b>Geographical Location:</b>	Pennsylvania (n=1)
<b>Biological Sample:</b>	Oral Fluid (n=1)
<b>Date of Collection:</b>	March 2020
<b>Additional Findings:</b>	Fentanyl (n=1)

### 4. BRIEF DESCRIPTION

Bromofentanyl is classified as a fentanyl analogue and novel opioid. Fentanyl analogues are modified based on the structure of fentanyl. Fentanyl analogues have been reported to cause psychoactive effects, similar to fentanyl and other opioids. Fentanyl analogues have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include fentanyl, fluorofentanyl, chlorofentanyl, and other fentanyl analogues. Bromofentanyl is not explicitly scheduled by name, but legislation has temporarily placed all fentanyl-related substances in Schedule I in the United States.

### 5. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/27536/para-bromofentanyl>

## 6. QUALITATIVE DATA

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

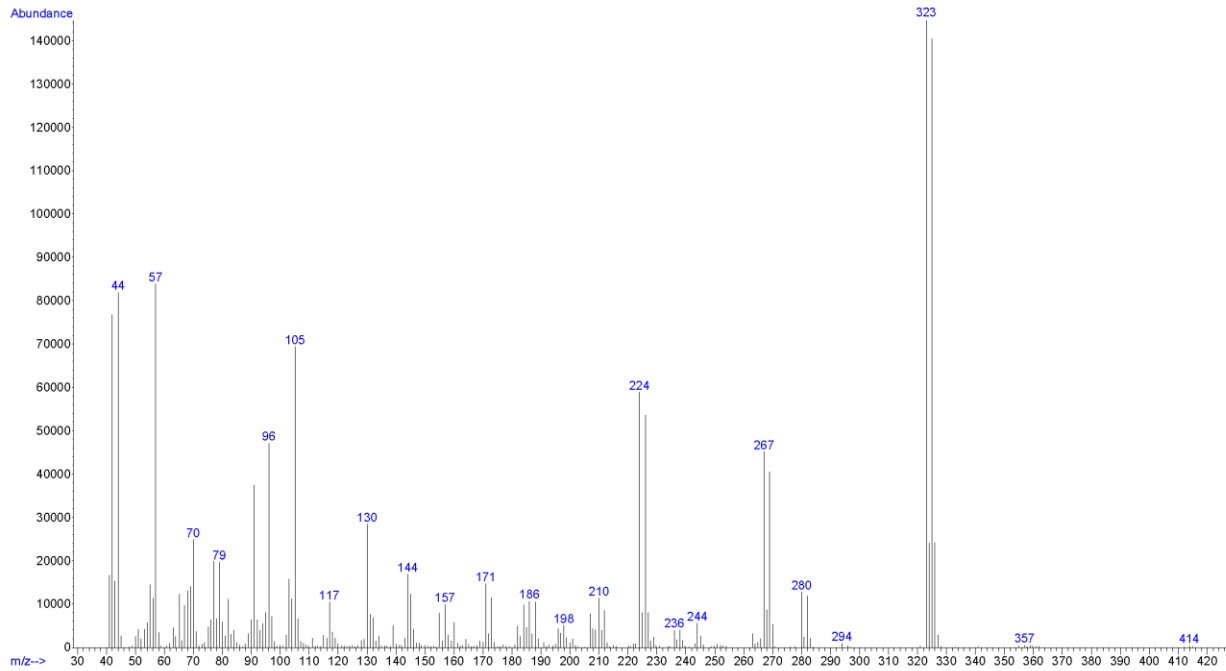
**Testing Performed At:** The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

**Sample Preparation:** Standard diluted in methanol

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

**Standard:** Reference material for *para*-Bromofentanyl (Batch: 0560956-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). (<https://www.caymanchem.com/product/27536/para-bromofentanyl>)

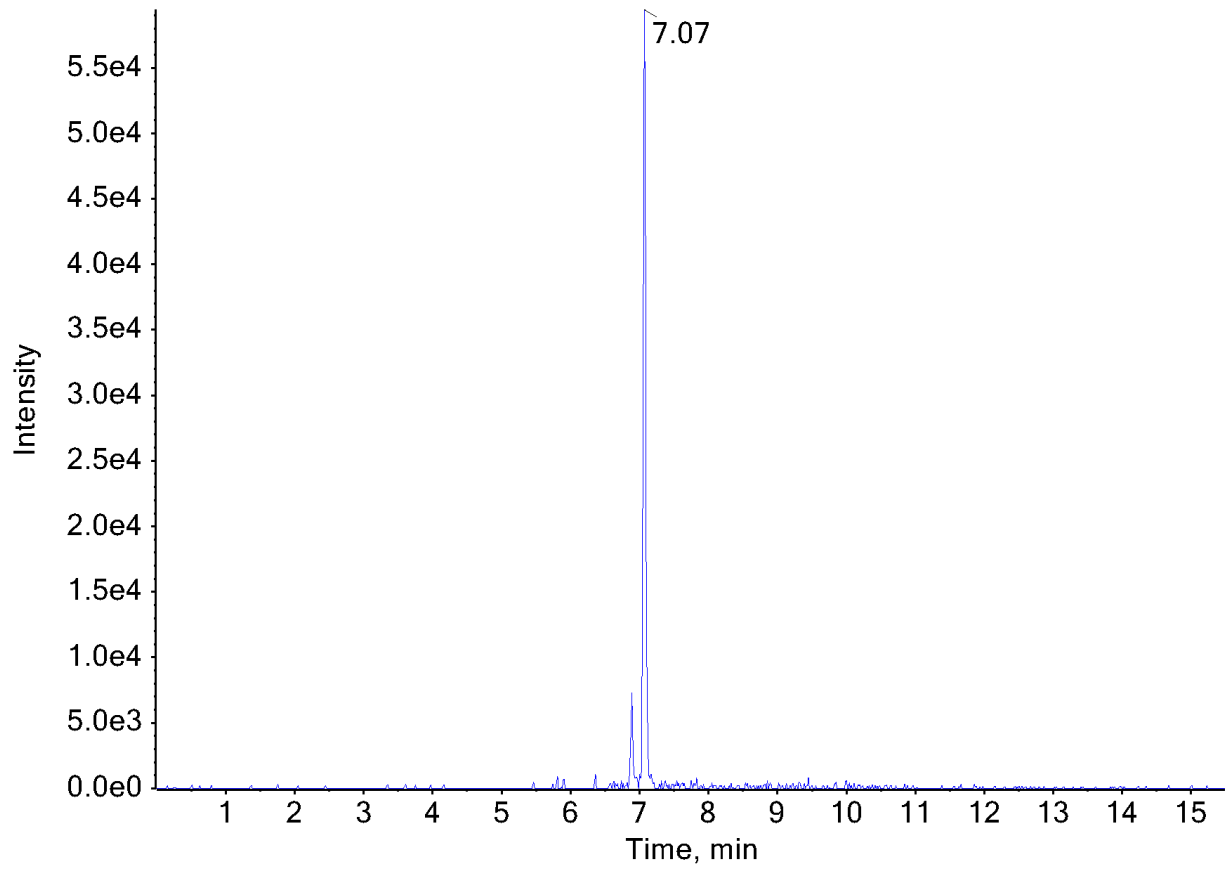
#### EI (70 eV) Mass Spectrum: Bromofentanyl



## 6.2 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>	No additional preparation - direct analysis of sample extract
<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>	7.07 min
<b>Standard Comparison:</b>	Reference material for <i>para</i> -Bromofentanyl (Batch: 0560956-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Bromofentanyl, based on retention time (6.98 min) and mass spectral data; however, absolute configuration of the structure as <i>para</i> -Bromofentanyl was not determined. ( <a href="https://www.caymanchem.com/product/27536/para-bromofentanyl">https://www.caymanchem.com/product/27536/para-bromofentanyl</a> )

**Extracted Ion Chromatogram (XIC): Bromofentanyl**



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

