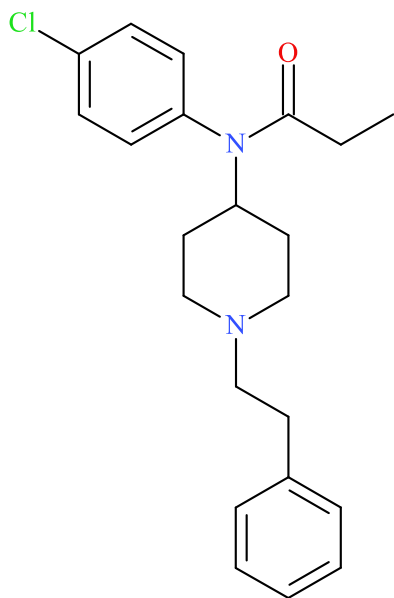


Chlorofentanyl

Sample Type: **Biological Fluid**

Latest Revision: **December 17, 2020**

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



1. GENERAL INFORMATION

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

InChI String: InChI=1S/C22H27ClN2O/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# 117994-27-1

Synonyms: *ortho*-Chlorofentanyl, *meta*-Chlorofentanyl, *para*-Chlorofentanyl, 2-Chlorofentanyl, 3-Chlorofentanyl, 4-Chlorofentanyl, Chloro fentanyl, CF

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-chloro*” configuration was used for structural purposes; however, position of the chlorine 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 ⁺]	Exact Mass [M+H] ⁺
Base	C ₂₂ H ₂₇ ClN ₂ O	370.9	370	371.1885

3. SAMPLE HISTORY

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

4. BRIEF DESCRIPTION

Chlorofentanyl 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. *para*-Chlorofentanyl is an active synthetic opioid with reported potency less than fentanyl.¹ Structurally similar compounds include fentanyl, fluorofentanyl, bromofentanyl, and other fentanyl analogues. Chlorofentanyl 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

1. Hassanien, SH; Bassman, JR; Perrien Naccarato, CM; Twarozynski, JJ; Traynor, JR; Iula, DM; Anand, JP. In vitro pharmacology of fentanyl analogs at the human mu opioid receptor and their spectroscopic analysis. *Drug Testing and Analysis*. 2020.

<https://onlinelibrary.wiley.com/doi/abs/10.1002/dta.2822>

[https://www.caymanchem.com/product/20034/para-chlorofentanyl-\(hydrochloride\)](https://www.caymanchem.com/product/20034/para-chlorofentanyl-(hydrochloride))

[https://www.caymanchem.com/product/31039/meta-chlorofentanyl-\(hydrochloride\)](https://www.caymanchem.com/product/31039/meta-chlorofentanyl-(hydrochloride))

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

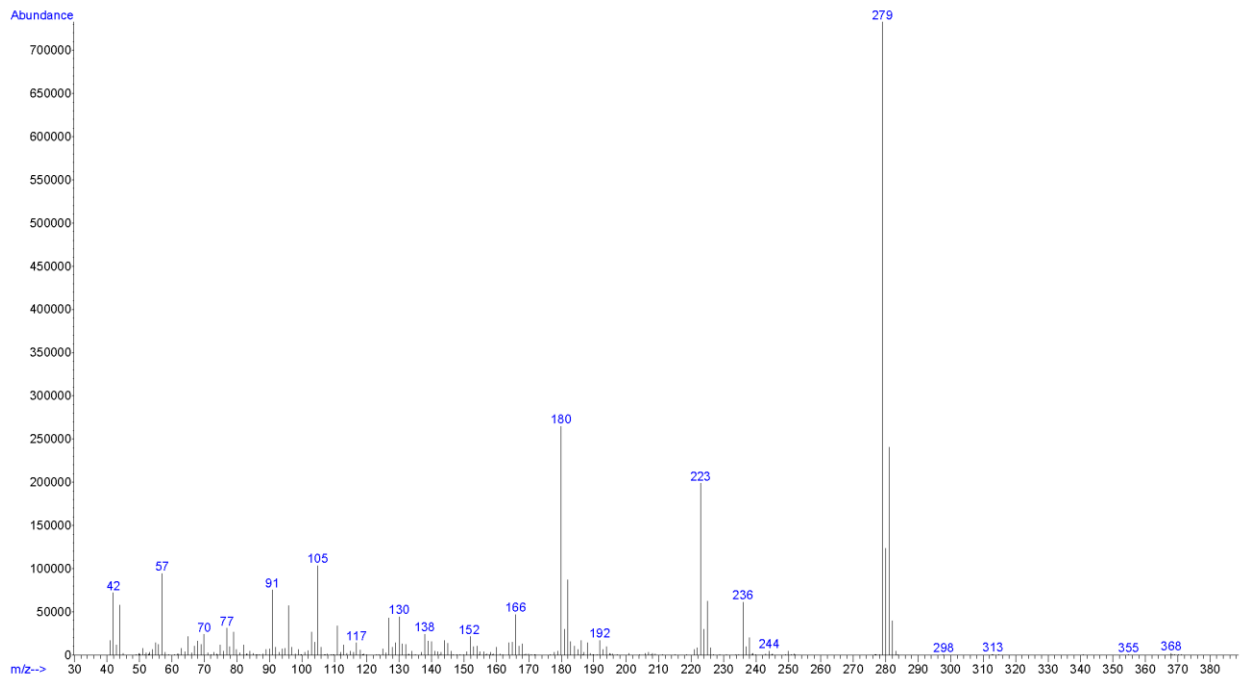
Testing Performed At: NMS Labs (Willow Grove, PA)

Sample Preparation: Acid/base extraction

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for *para*-Chlorofentanyl (Batch: 0489672-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). ([https://www.caymanchem.com/product/20034/para-chlorofentanyl-\(hydrochloride\)](https://www.caymanchem.com/product/20034/para-chlorofentanyl-(hydrochloride)))

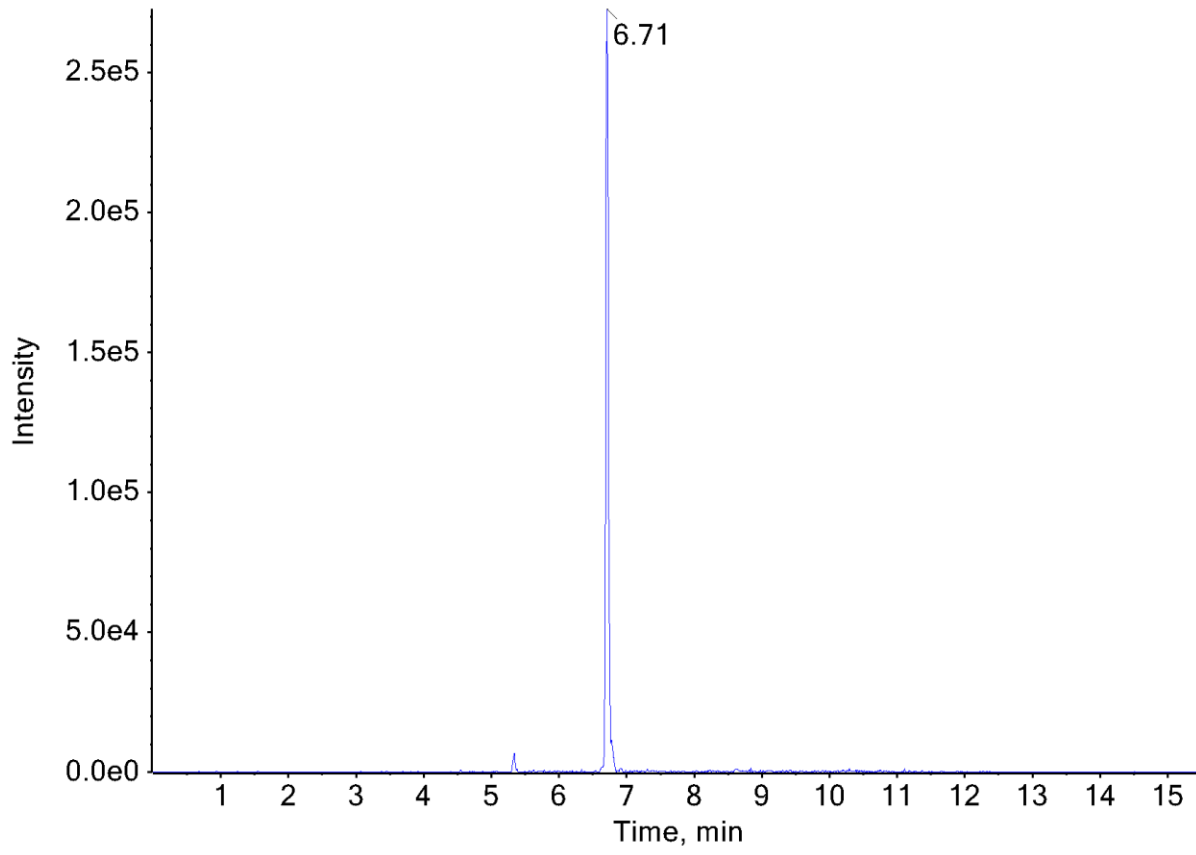
EI (70 eV) Mass Spectrum: Chlorofentanyl



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 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:	6.71 min
Standard Comparison:	Reference material for <i>para</i> -Chlorofentanyl (Batch: 0489672-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Chlorofentanyl, based on retention time (6.88 min) and mass spectral data; however, absolute configuration of the structure as <i>para</i> -Chlorofentanyl was not determined. (https://www.caymanchem.com/product/20034/para-chlorofentanyl-(hydrochloride))

Extracted Ion Chromatogram (XIC): Chlorofentanyl



TOF MS (Top) and MS/MS (Bottom) Spectra: Chlorofentanyl

