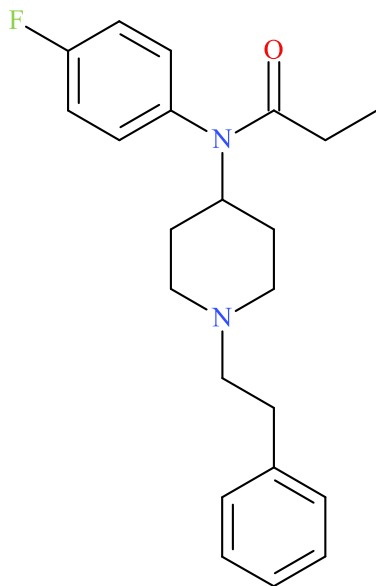


Fluorofentanyl

Sample Type: **Biological Fluid**

Latest Revision: **December 17, 2020**

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



1. GENERAL INFORMATION

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

InChI String: InChI=1S/C22H27FN2O/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# 117332-92-0

Synonyms: *ortho*-Fluorofentanyl, *meta*-Fluorofentanyl, *para*-Fluorofentanyl, 2-Fluorofentanyl, 3-Fluorofentanyl, 4-Fluorofentanyl, Fluorofentanyl, FF, NIH 10491

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*-fluoro” configuration was used for structural purposes; however, position of the fluorine 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 FN ₂ O	354.5	354	355.2180

3. SAMPLE HISTORY

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

4. BRIEF DESCRIPTION

Fluorofentanyl 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. Fluorofentanyl is a potent synthetic opioid.¹ Fluorofentanyl has been linked to at least 16 deaths in the United States, commonly found in combination with fentanyl.² Structurally similar compounds include fentanyl, chlorofentanyl, bromofentanyl, and other fentanyl analogues. Both *ortho*- and *para*-fluorofentanyl are explicitly Schedule I substances 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>

2. Papsun, DM; Krotulski, AJ; Mohr, ALA; Menendez, MJ; Logan, BK. Fluorofentanyl Identified in Forensic Casework as Wave of Fentanyl-Related Substances Appears in the United States. *NPS Discovery – Public Alert*. 2020. https://www.npsdiscovery.org/wp-content/uploads/2020/12/Public-Alert_Fluorofentanyl_NPS-Discovery_120320.pdf

Fogarty, MF; Papsun, DM; Logan, BK. Analysis of Fentanyl and 18 Novel Fentanyl Analogs and Metabolites by LC–MS–MS, and report of Fatalities Associated with Methoxyacetylfentanyl and Cyclopropylfentanyl. *Journal of Analytical Toxicology*. 2018, 42, 592-604.

<https://academic.oup.com/jat/article/42/9/592/4994607>

The World Health Organization. https://www.who.int/medicines/access/controlled-substances/Annex_1_41_ECDD_recommendations_NPS_and_medicines_22012019.pdf

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/2-Fluorofentanyl-ID-1701_16_report.pdf

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/3-Fluorofentanyl-ID-1751-16_report.pdf

[https://www.caymanchem.com/product/15496/para-fluorofentanyl-\(hydrochloride\)](https://www.caymanchem.com/product/15496/para-fluorofentanyl-(hydrochloride))

[https://www.caymanchem.com/product/19424/meta-fluorofentanyl-\(hydrochloride\)](https://www.caymanchem.com/product/19424/meta-fluorofentanyl-(hydrochloride))

[https://www.caymanchem.com/product/19425/ortho-fluorofentanyl-\(hydrochloride\)](https://www.caymanchem.com/product/19425/ortho-fluorofentanyl-(hydrochloride))

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

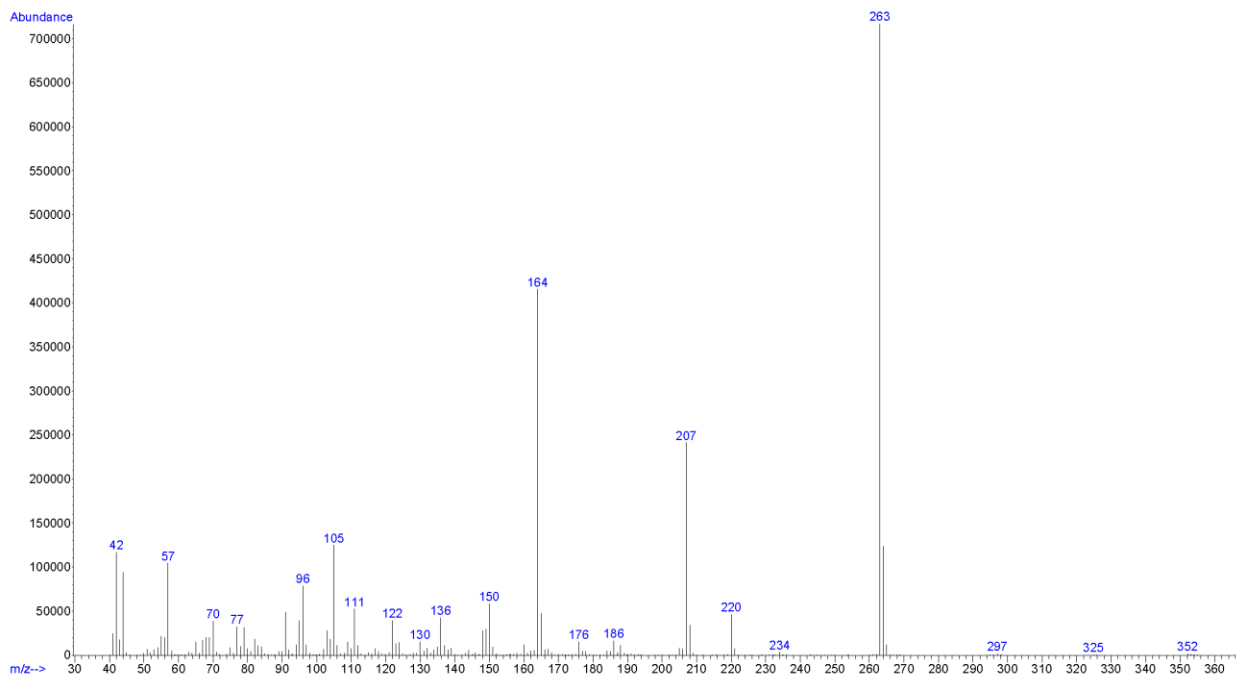
Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Standard diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Standard: Reference material for *ortho*-Fluorofentanyl (Batch: 0490394-11) was purchased from Cayman Chemical (Ann Arbor, MI, USA). ([https://www.caymanchem.com/product/19425/ortho-fluorofentanyl-\(hydrochloride\)](https://www.caymanchem.com/product/19425/ortho-fluorofentanyl-(hydrochloride)))

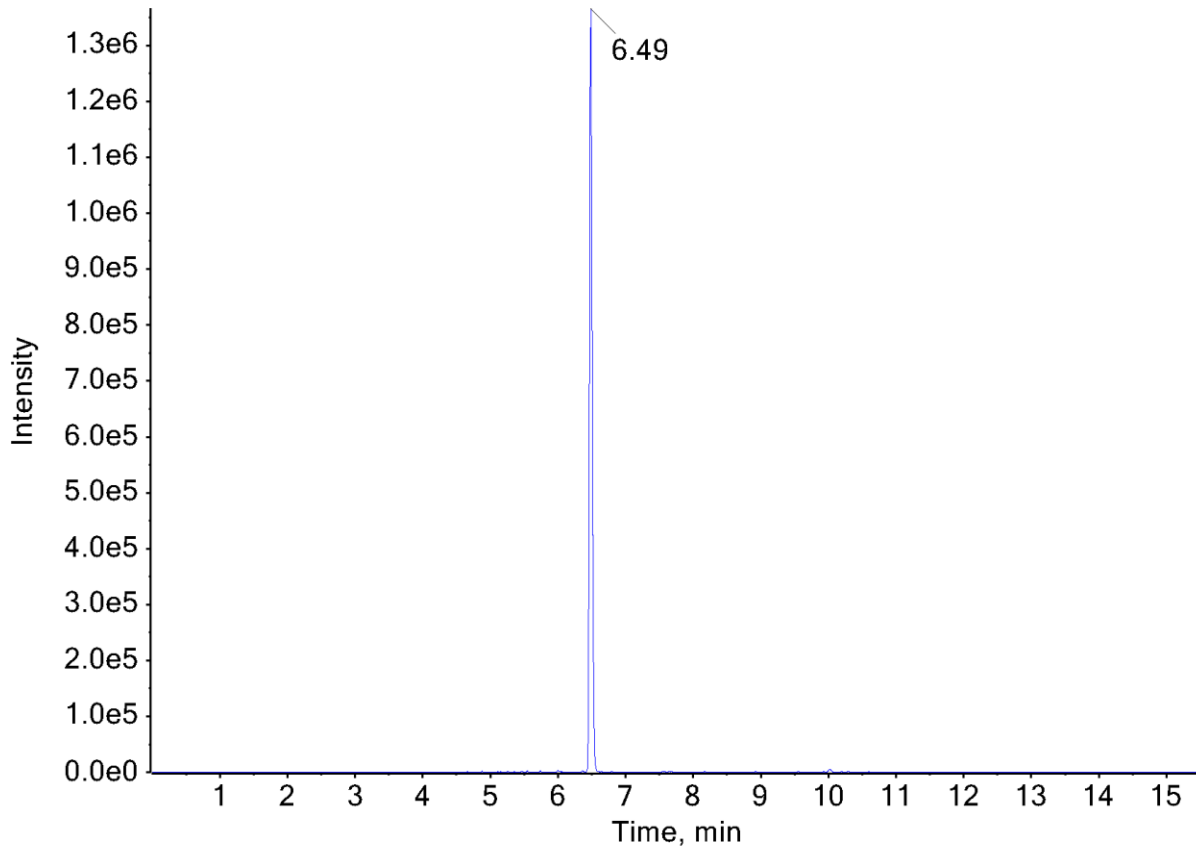
EI (70 eV) Mass Spectrum: Fluorofentanyl



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:	6.49 min
Standard Comparison:	Reference material for <i>ortho</i> -Fluorofentanyl (Batch: 0490394-11) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Fluorofentanyl, based on retention time (6.35 min) and mass spectral data; however, absolute configuration of the structure as <i>ortho</i> -Fluorofentanyl was not determined. (https://www.caymanchem.com/product/19425/ortho-fluorofentanyl-(hydrochloride))

Extracted Ion Chromatogram (XIC): Fluorofentanyl



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

