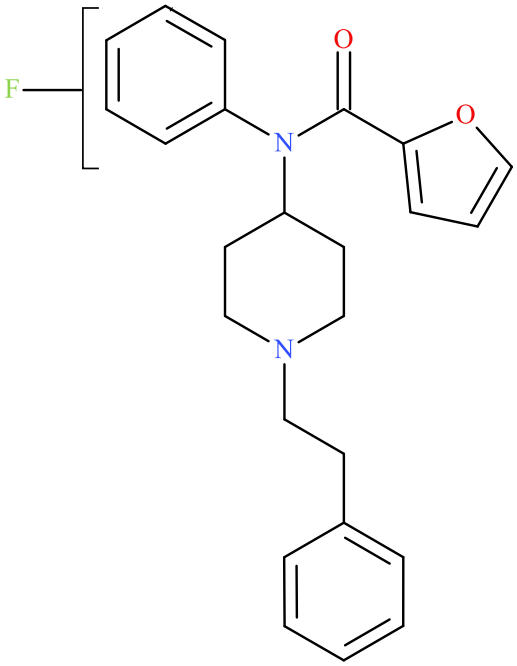
ortho/meta/para-Fluorofuranylfentanyl

Sample Type: **Biological Fluid**



Latest Revision: **January 23, 2019**

Date of Report: **January 23, 2019**

1. GENERAL INFORMATION

IUPAC Name: N-(4-fluorophenyl)-N-[1-(2-phenylethyl)-4-piperidyl]furan-2-carboxamide *(Note: IUPAC Name for para-Fluorofuranylfentanyl)*

InChI String: InChI=1S/C24H25FN2O2/c25-20-8-10-21(11-9-20)27(24(28)23-7-4-18-29-23)22-13-16-26(17-14-22)15-12-19-5-2-1-3-6-19/h1-11,18,22H,12-17H2 *(Note: InChI String for para-Fluorofuranylfentanyl)*

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

CAS# Not Available

Synonyms: *o/m/p*-Fluorofuranylfentanyl, 2/3/4-Fluorofuranylfentanyl, Fluorofuranylfentanyl, Fluoro furanyl fentanyl, Fluoro-FuF

Source: NMS Labs – Toxicology Department

***Important Note**: All identifications were made based on evaluation of analytical data (LC-QTOF) in comparison to analysis of acquired reference material. Due to the isobaric nature of ortho-, meta-, and para-fluorofuranylfentanyl, the position of the fluorine was not confirmed and therefore not reported.*

***Report Prepared By:** Alex J. Krotulski, MSFS, and Barry K. Logan, PhD, F-ABFT*

2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Exact Mass $[M+H]^+$
o/m/p-Fluorofuranylfentanyl	$C_{24}H_{25}FN_2O_2$	392.5	393.1973

3. SAMPLE HISTORY

Fluorofuranylfentanyl has been identified in one case since January 2019. The geographical and demographical breakdown is below:

Geographical Location: Florida

Biological Sample: Cardiac Blood

Date of First Receipt: December 28, 2018

Additional Opioids: Valeryl fentanyl (0.095 ng/mL), Fluoro-4-ANPP

4. BRIEF DESCRIPTION

Fluorofuranylfentanyl 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, furanylfentanyl, and other fentanyl analogues. Fluorofuranylfentanyl is not explicitly scheduled by name, but recent legislation has temporarily placed all fentanyl-related substances in Schedule I. An additional finding in this case was fluoro-4-ANPP, a suspected precursor, metabolite, and/or synthetic by-product in the synthesis of fluorofuranylfentanyl.

5. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/23628

https://www.caymanchem.com/product/22750

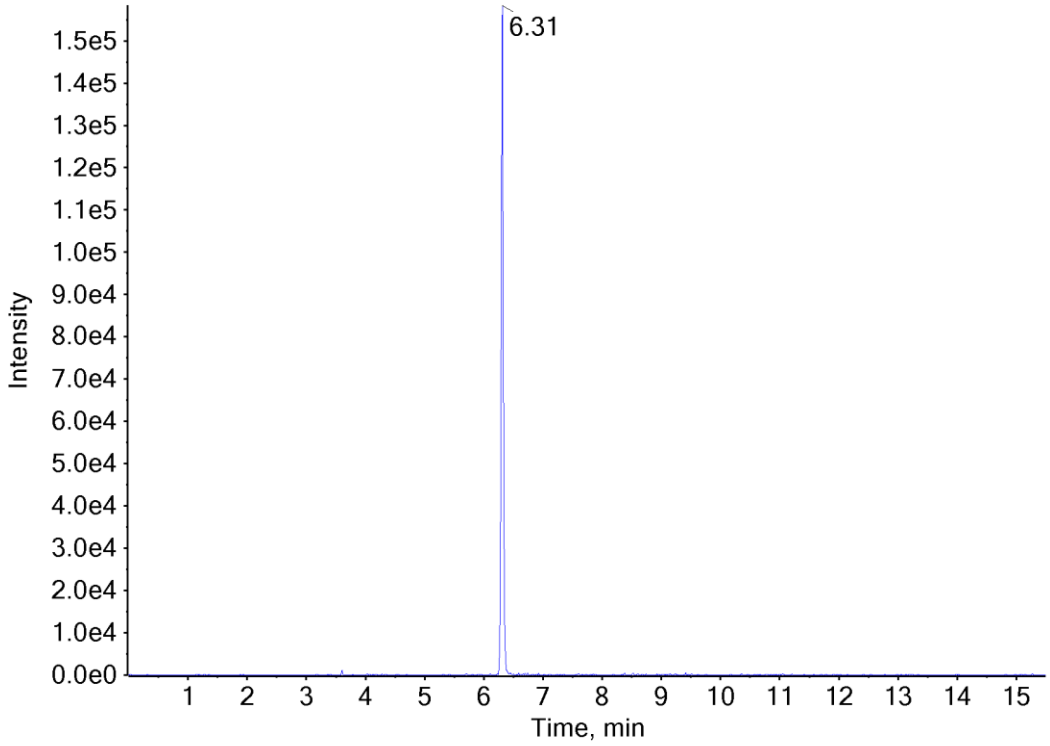
http://www.chemspider.com/Chemical-Structure.44211060.html

6. QUALITATIVE DATA

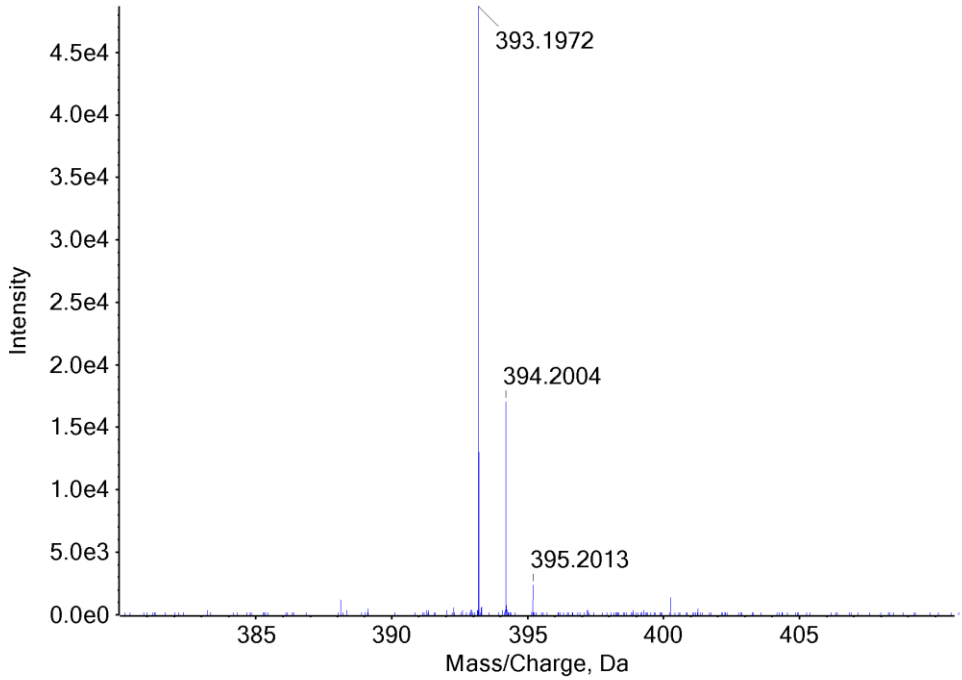
6.1 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	6.31 min
Standard Comparison:	Reference material for ortho-Fluorofuranylfentanyl (Batch: 0528616-1) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Fluorofuranylfentanyl, based on retention time (6.43 min) and mass spectral data. (https://www.caymanchem.com/product/23628)

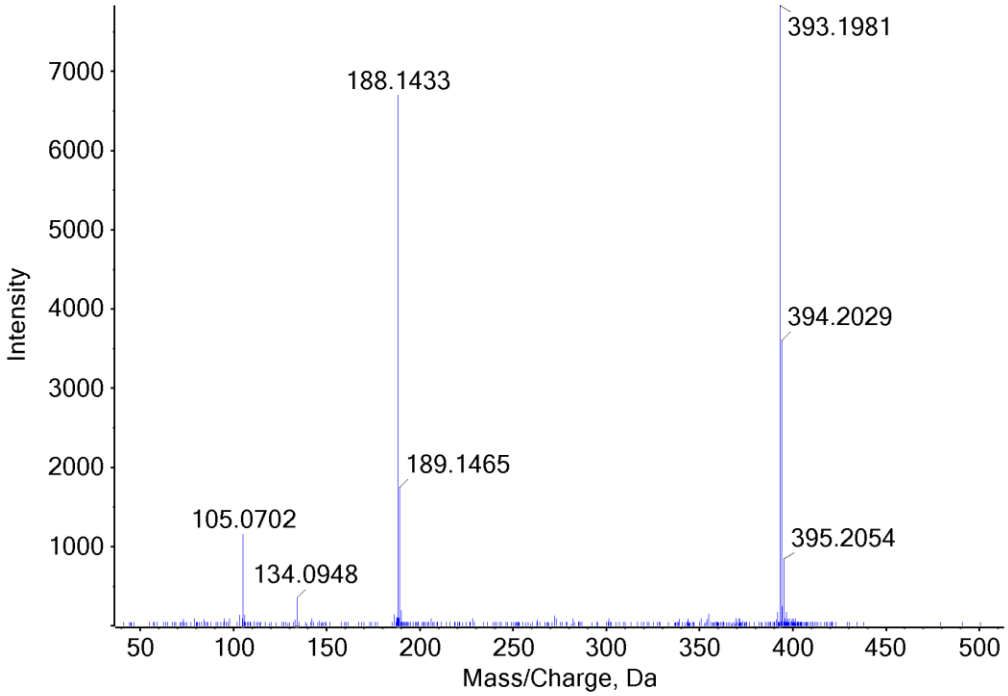
Extracted Ion Chromatogram: Fluorofuranylfentanyl



TOF MS Spectrum: Fluorofuranylfentanyl



MS/MS Spectrum: Fluorofuranylfentanyl



7. FUNDING

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