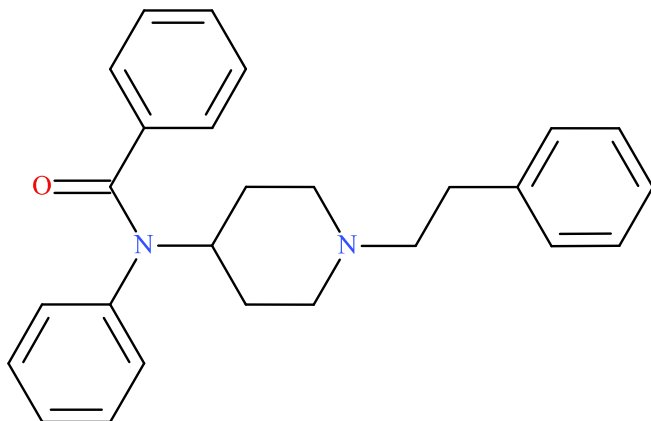


Phenylfentanyl

Sample Type: **Biological Fluid**



Latest Revision: **September 4, 2018**

Date of Report: **September 4, 2018**

1. GENERAL INFORMATION

- IUPAC Name:** N-phenyl-N-[1-(2-phenylethyl)-4-piperidyl]benzamide
- InChI String:** InChI=1S/C26H28N2O/c29-26(23-12-6-2-7-13-23)28(24-14-8-3-9-15-24)25-17-20-27(21-18-25)19-16-22-10-4-1-5-11-22/h1-15,25H,16-21H2
- CFR:** 21 CFR 1308: Temporary Placement of Fentanyl-Related Substances in Schedule 1 (02/06/2018)
- CAS#** Not Available
- Synonyms:** Phenyl fentanyl, Benzoylfentanyl, Benzoyl fentanyl
- Source:** NMS Labs – Toxicology Department

2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Exact Mass [M+H] ⁺
Phenylfentanyl	C ₂₆ H ₂₈ N ₂ O	384.5	385.2274

Important Note: All identifications were made based on evaluation of analytical data (LC-QTOF) in comparison to analysis of acquired reference material.

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

3. SAMPLE HISTORY

Phenylfentanyl has been identified in three case since June 2018. The geographical and demographical breakdown is below:

Geographical Location:	Ohio (n=3)
Biological Sample:	Femoral Blood (n=1), Antemortem Urine (n=2)
Date of First Collection:	Not Available
Date of First Receipt:	June 29, 2018
Additional NPS:	Cyclopropylfentanyl (n=3), Methoxyacetylfentanyl (n=3), 4-ANPP (n=3), Tetrahydrofurfanylfentanyl (n=2)

4. BRIEF DESCRIPTION

Phenylfentanyl 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 and other fentanyl analogues. Fentanyl is a Schedule II substance in the United States while several fentanyl analogues are explicitly Schedule I substances, although recent legislation has temporarily placed all fentanyl-related substances in Schedule I.

5. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/22551>

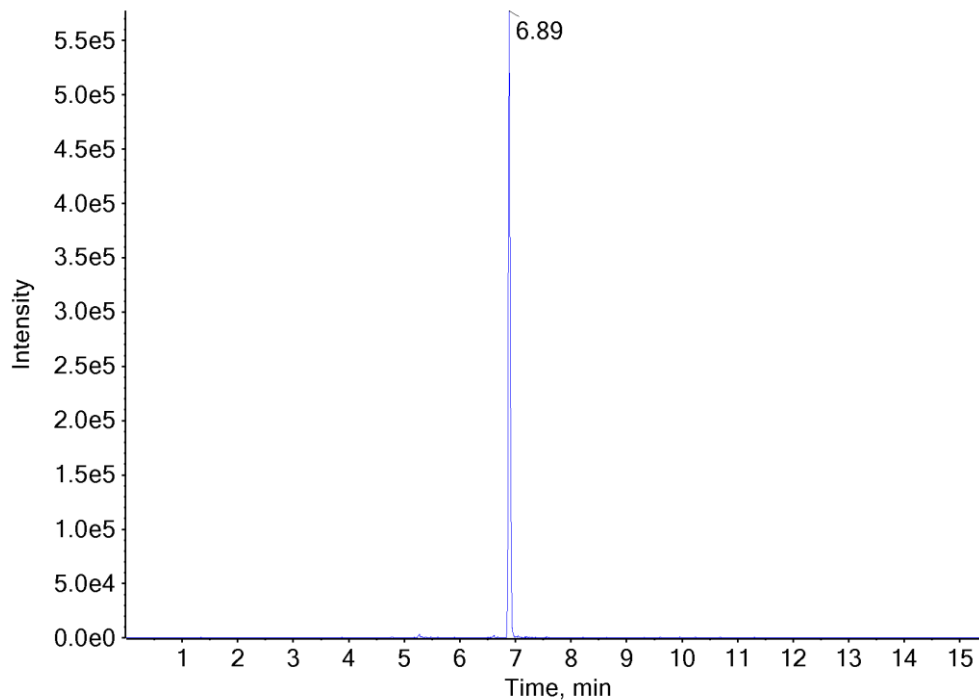
http://www.emcdda.europa.eu/system/files/publications/9282/20183924_TDAN18001ENN_PD_F.pdf

6. QUALITATIVE DATA

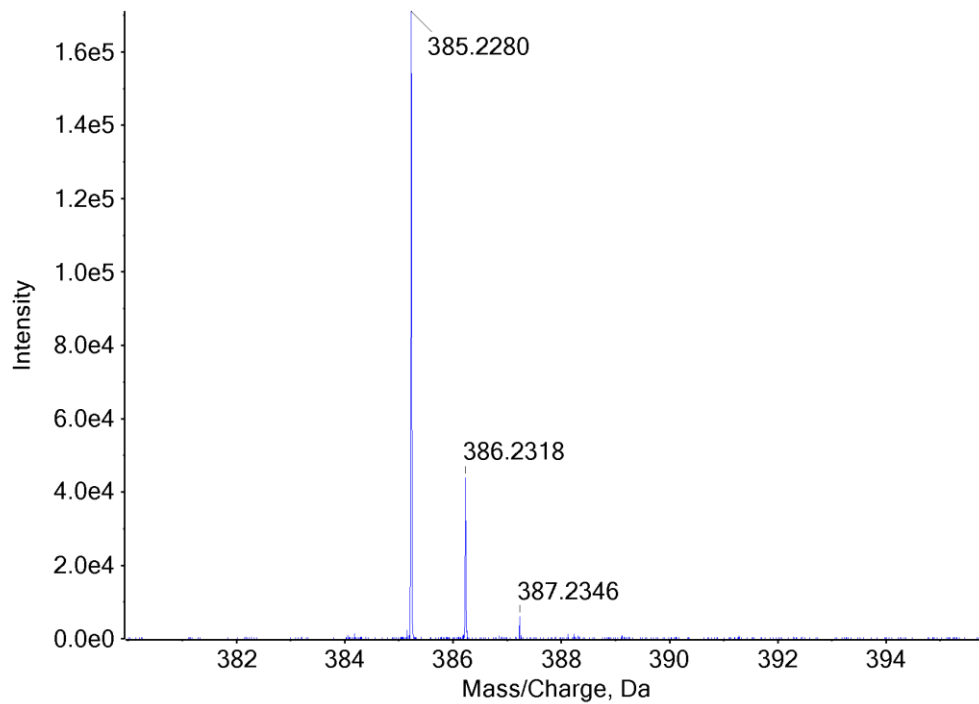
6.1 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	6.89 min
Standard Comparison:	Reference material for Phenylfentanyl (Batch: 0508384-16) 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 Phenylfentanyl, based on retention time (6.78 min) and mass spectral data. (https://www.caymanchem.com/product/22551)

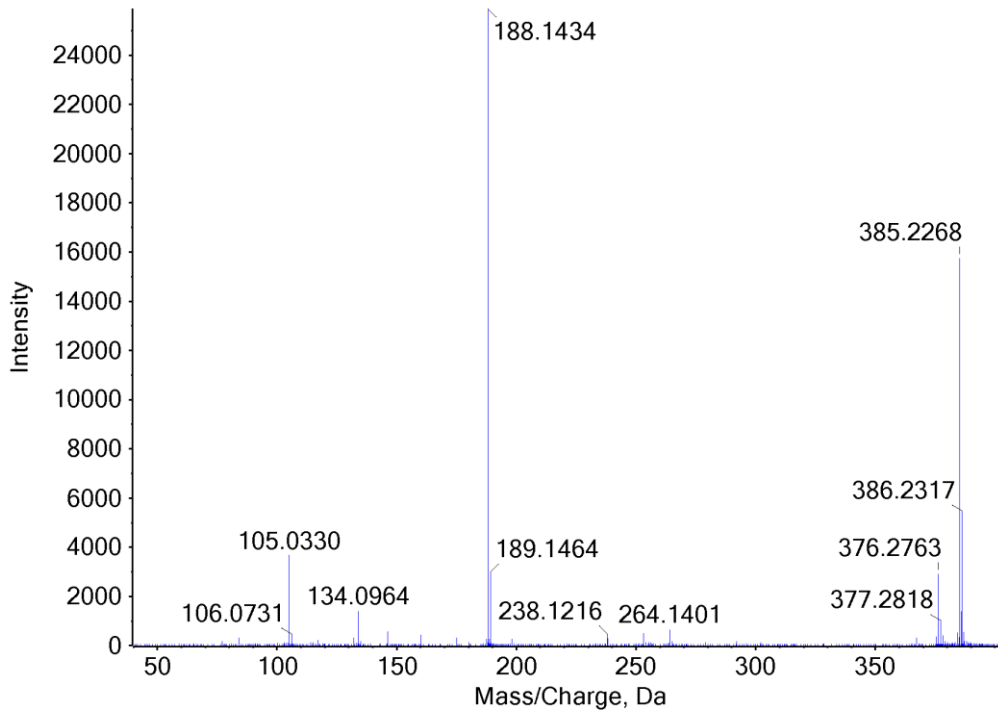
Extracted Ion Chromatogram: Phenylfentanyl



TOF MS Spectrum: Phenylfentanyl



MS/MS Spectrum: Phenylfentanyl



7. FUNDING

This project was supported by Award Number 2017-R2-CX-0002, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this publication, program, or exhibition are those of the author(s) and do not necessarily reflect those of the Department of Justice.