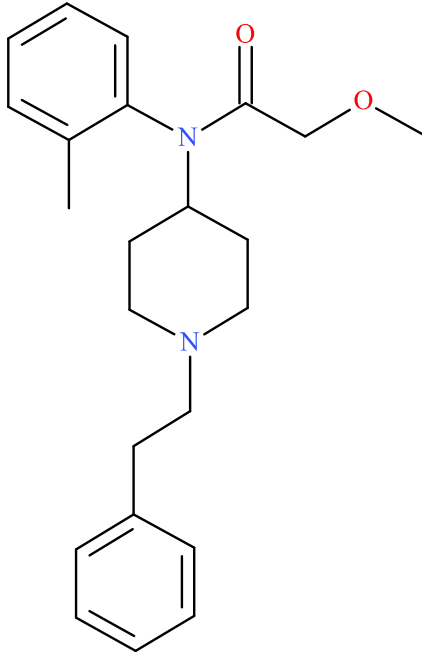


***ortho*-Methylmethoxyacetylfentanyl**



Sample Type: **Seized Material**

Latest Revision: **May 18th, 2018**

Date Received: **January 22nd, 2018**

Date of Report: **March 27th, 2018**

1. GENERAL INFORMATION

IUPAC Name: 2-methoxy-N-(*o*-tolyl)-N-[1-(2-phenylethyl)-4-piperidyl]acetamide

InChI String: InChI=1S/C23H30N2O2/c1-19-8-6-7-11-22(19)25(23(26)18-27-2)21-13-16-24(17-14-21)15-12-20-9-4-3-5-10-20/h3-11,21H,12-18H2,1-2H3

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

CAS# Not available

Synonyms: *ortho*-Methyl Methoxyacetylfentanyl, *ortho*-Methyl-Methoxyacetylfentanyl, *o*-Methyl Methoxyacetylfentanyl, 2-Methyl Methoxyacetylfentanyl, *ortho*-Me-MeO-Ace-Fentanyl

Source: Department of Homeland Security

Appearance: White Solid Material.

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

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

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₂₃ H ₃₀ N ₂ O ₂	366.50	366	367.2380

3. BRIEF DESCRIPTION

ortho-Methylmethoxyacetylfentanyl 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 methoxyacetylfentanyl. Fentanyl is a Schedule II substance and methoxyacetylfentanyl is a Schedule I substance in the United States, although recent legislation has temporarily placed all fentanyl-related substances in Schedule I.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/22977>

5. QUALITATIVE DATA

5.1 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

Column: Zebtron™ Inferno™ ZB-35HT (15 m x 250 μm x 0.25 μm)

Carrier Gas: Helium (Flow: 1 mL/min)

Temperatures: Injection Port: 265 °C
Transfer Line: 300 °C
MS Source: 230 °C

MS Quad: 150 °C

Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

Injection Parameters: Injection Type: Splitless

Injection Volume: 1 µL

MS Parameters: Mass Scan Range: 40-550 m/z

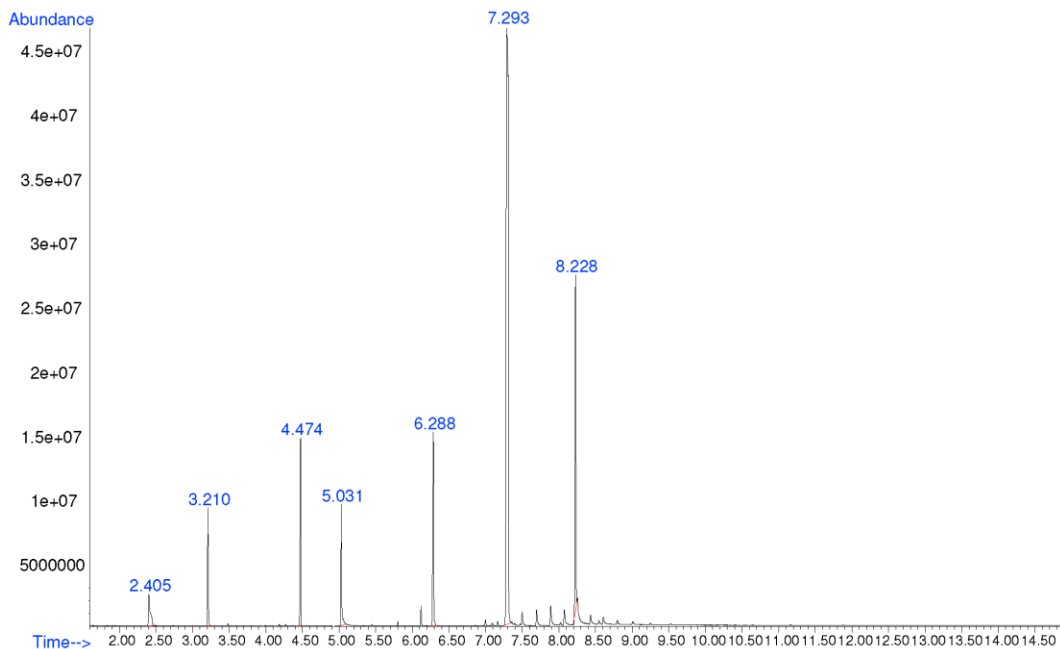
Threshold: 250

Retention Time: 8.228 min

Standard Comparison: Reference material for *ortho*-methoxymethoxyacetylfentanyl (Batch: 0513077-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *ortho*-methoxymethoxyacetylfentanyl, based on retention time (8.222 min) and mass spectral data.

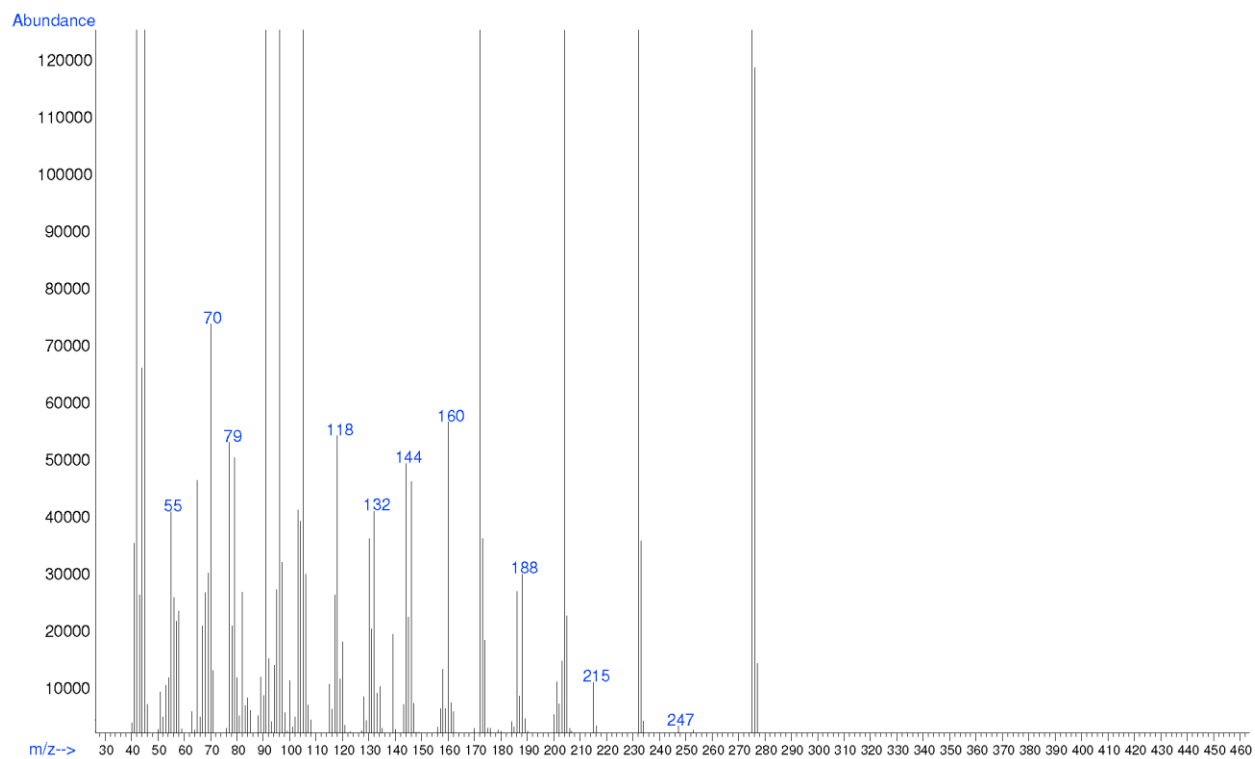
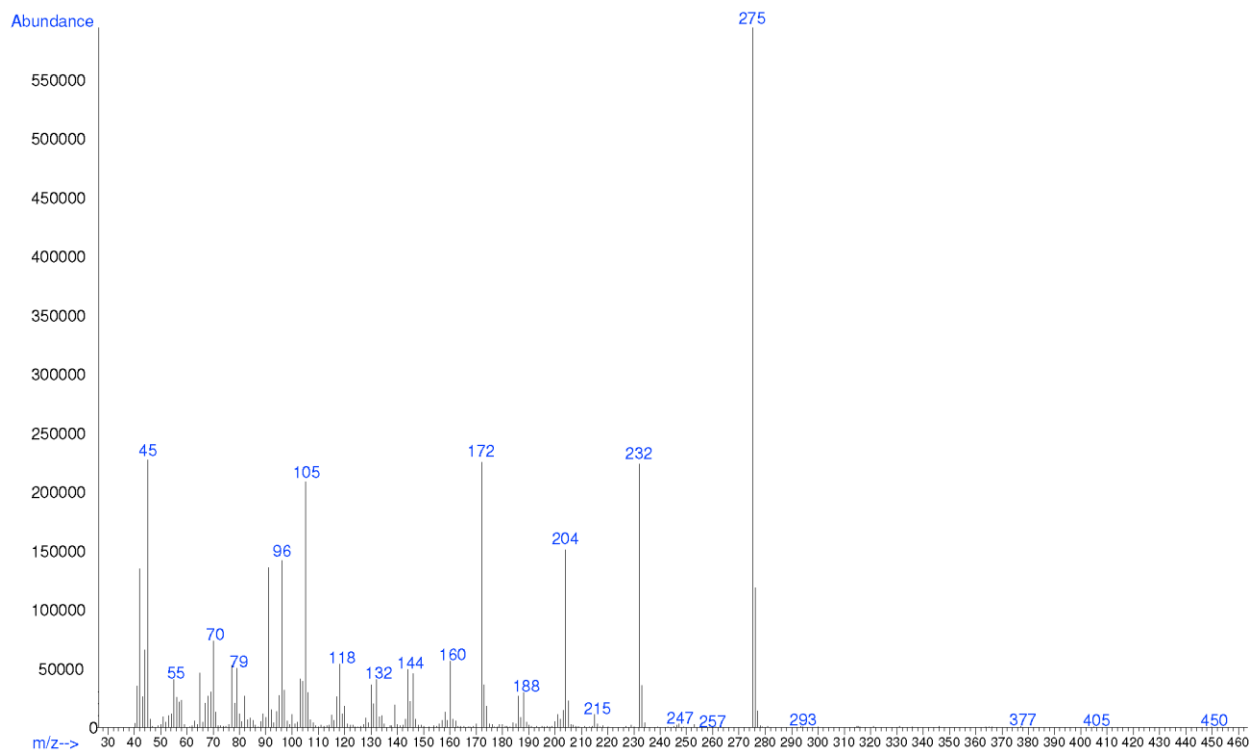
<https://www.caymanchem.com/product/22977>

Chromatogram: *ortho*-Methoxymethoxyacetylfentanyl



Additional peaks present in chromatogram: not a controlled substance (2.405 min), internal standard 1 (3.210 min), not a controlled substance (4.474 min), not a controlled substance (5.031 min), internal standard 2 (6.288 min), despropionyl ortho-methylfentanyl (7.293 min)

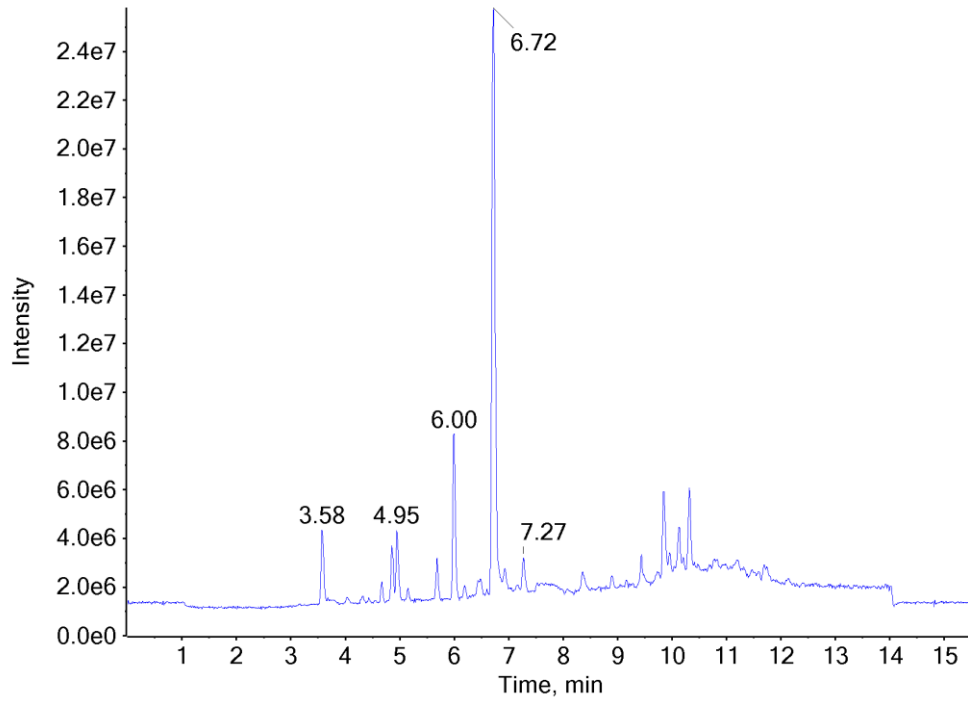
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *ortho*-Methylmethoxyacetylfentanyl



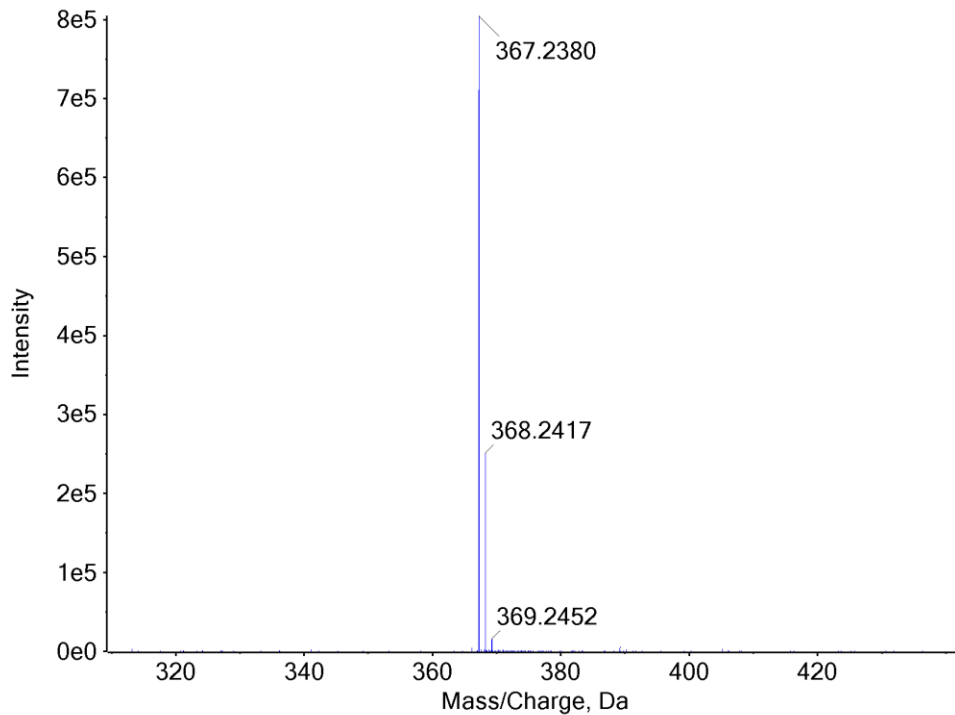
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

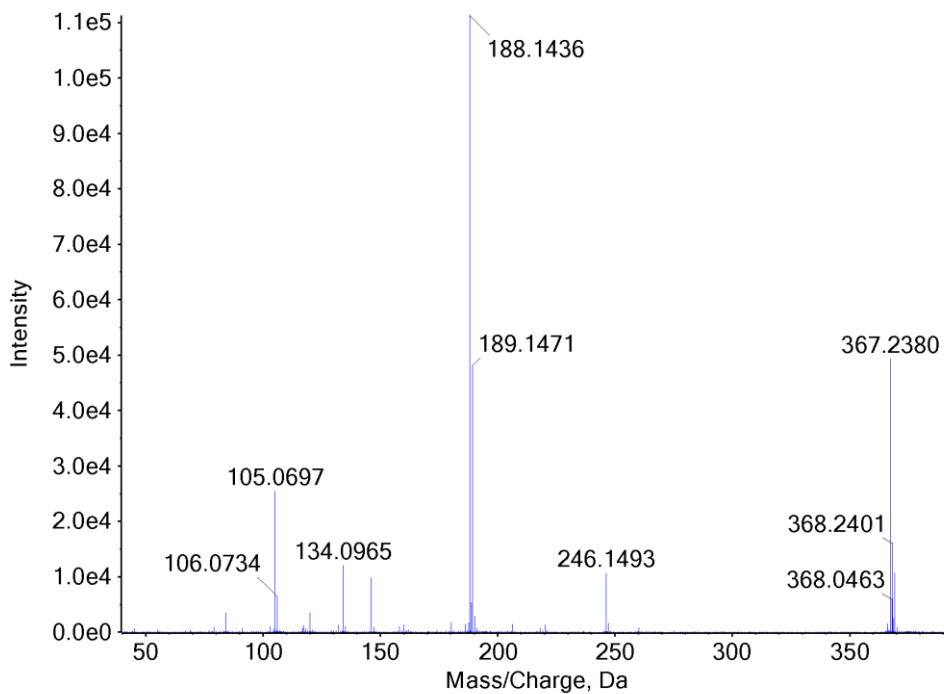
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	6.00 min
Standard Comparison:	Reference material for <i>ortho</i> -methylethoxyacetylfentanyl (Batch: 0513077-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as <i>ortho</i> -methylethoxyacetylfentanyl, based on retention time (5.988 min) and mass spectral data. https://www.caymanchem.com/product/22977

Chromatogram: *ortho*-Methylmethoxyacetylfentanyl



TOF MS (Top) and MS/MS (Bottom) Spectra: *ortho*-Methylmethoxyacetylfentanyl





6. REVISION HISTORY

<u>Date</u>	<u>Revision</u>
05/18/2018	Added "Sample Type: Seized Material" to Page 1.
05/18/2018	Added "Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT" to Page 1 footer.