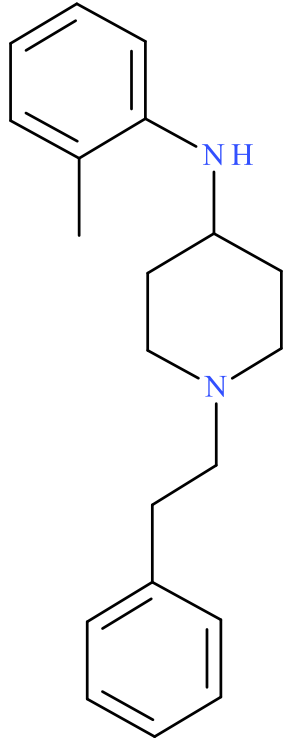


Despropionyl *ortho*-Methylfentanyl

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: N-(*o*-tolyl)-1-(2-phenylethyl)piperidin-4-amine

InChI String: InChI=1S/C20H26N2/c1-17-7-5-6-10-20(17)21-19-12-15-22(16-13-19)14-11-18-8-3-2-4-9-18/h2-10,19,21H,11-16H2,1H3

CFR: Not Scheduled (03/2018)

CAS# 28456-18-0

Synonyms: Despropionyl *o*-Methylfentanyl Despropionyl 2-Methylfentanyl, *ortho*-Methyl 4-ANPP

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 ₂₀ H ₂₆ N ₂	294.43	294	295.2169

3. BRIEF DESCRIPTION

Despropionyl *ortho*-Methylfentanyl is classified as an analogue of the fentanyl precursor 4-anilino-N-phenethylpiperidine (4-ANPP). Fentanyl precursors are modified based on the structure of 4-ANPP and are often used in the synthesis of fentanyl analogues. 4-ANPP is a Schedule II substance in the United States.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/24279>

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: Zebron™ 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 μ L

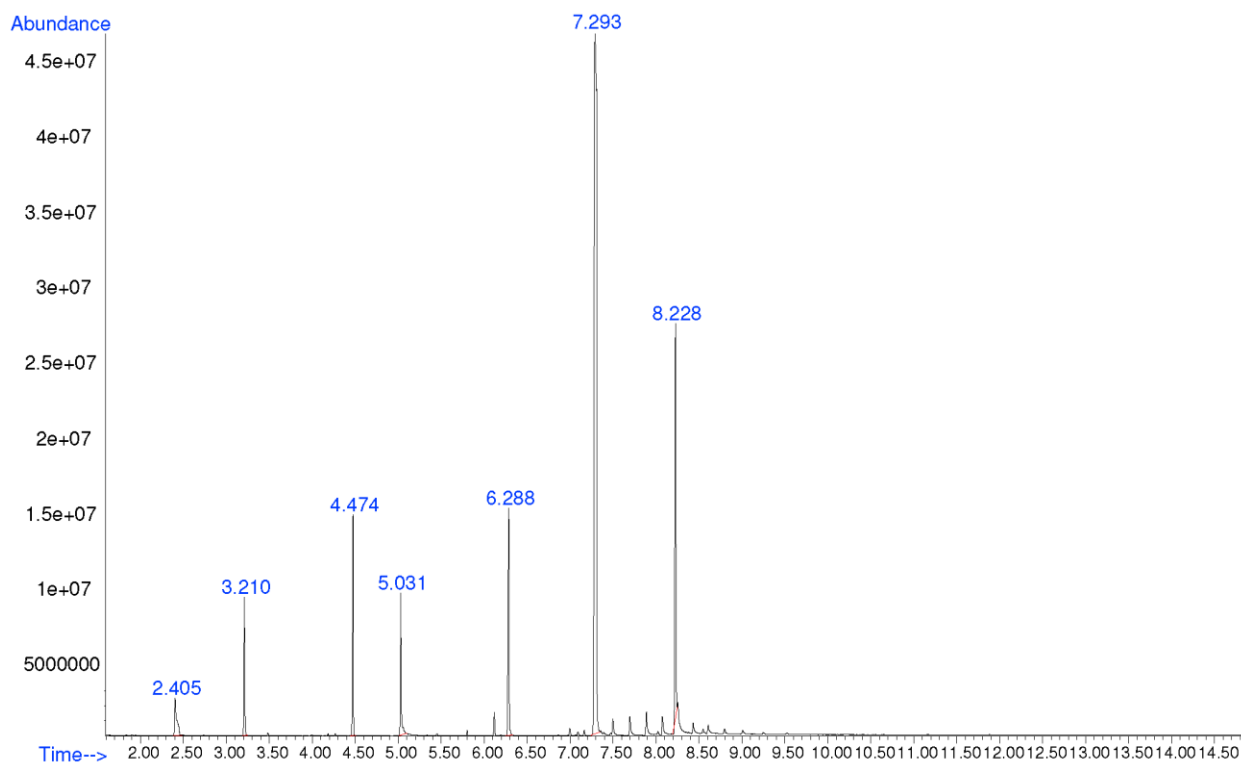
MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 7.293 min

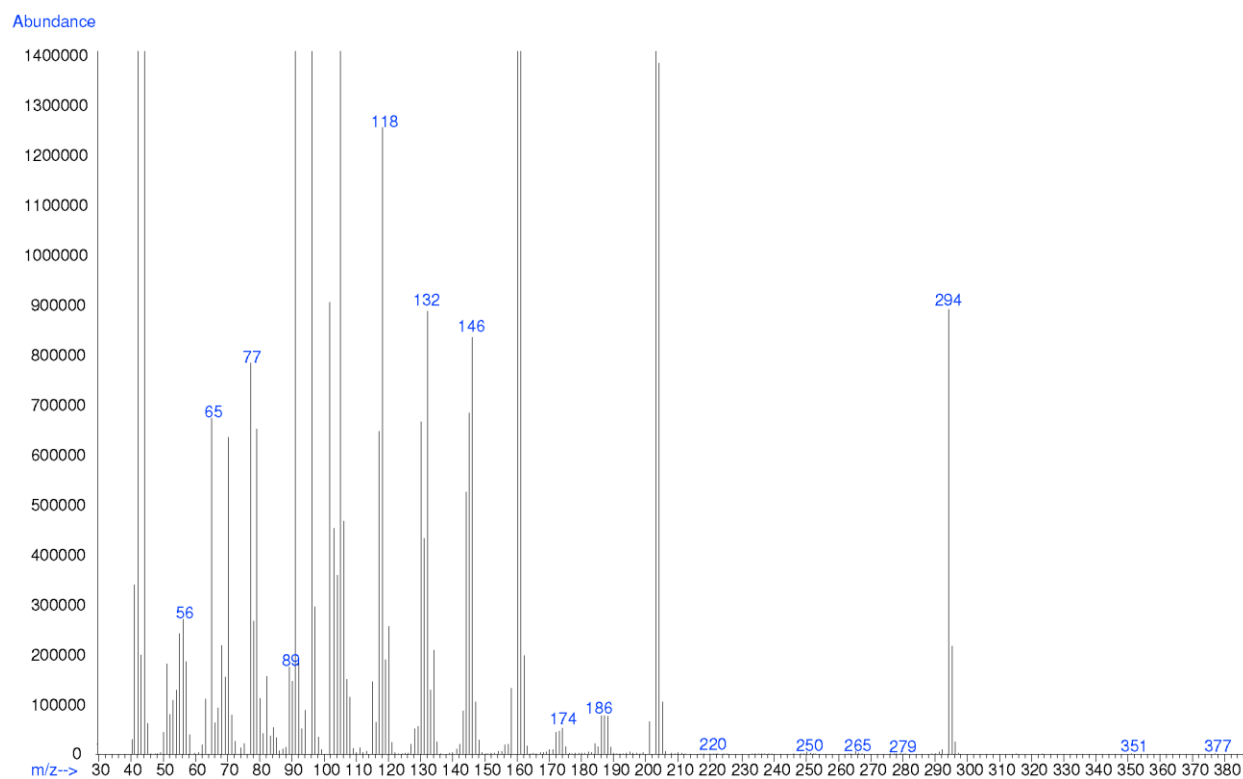
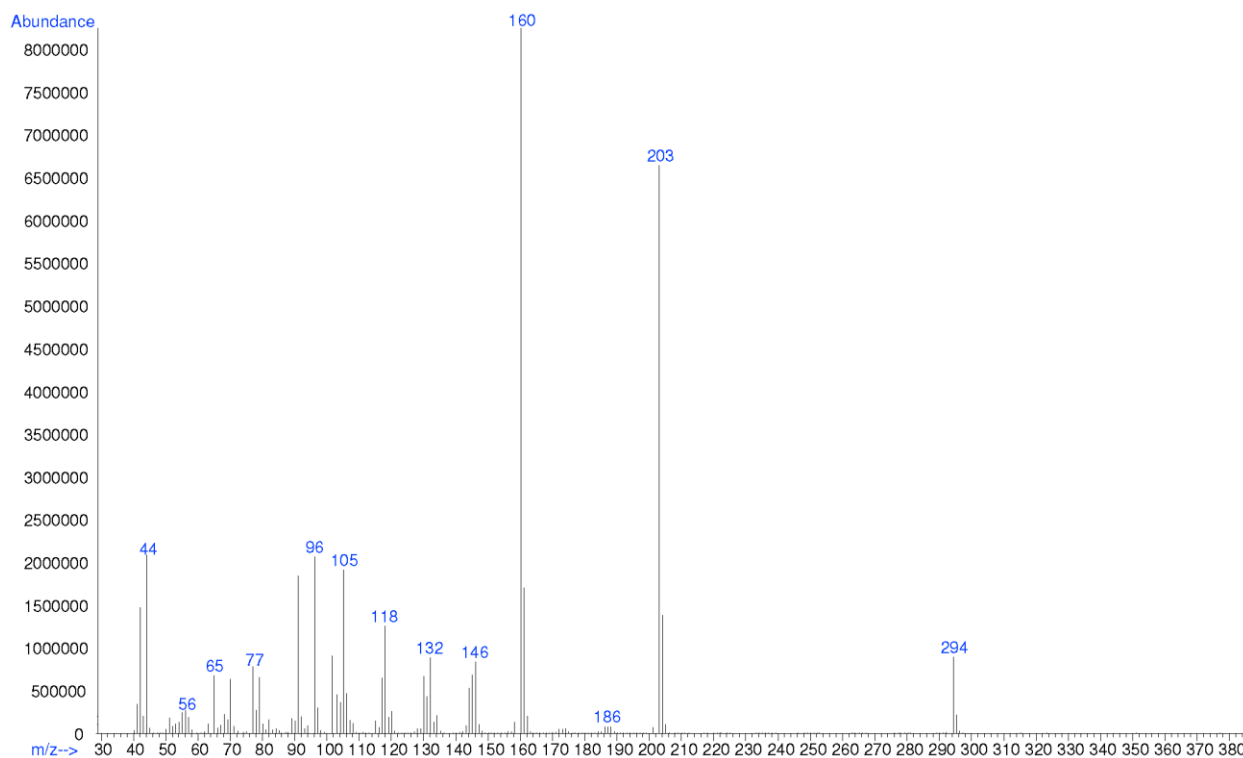
Standard Comparison: Reference material for despropionyl *ortho*-methylfentanyl (Batch: 0521837-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as despropionyl *ortho*-methylfentanyl, based on retention time (7.290 min) and mass spectral data. (<https://www.caymanchem.com/product/24279>)

Chromatogram: Despropionyl *ortho*-Methylfentanyl



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), ortho-methyl methoxyacetylfentanyl (8.228 min)

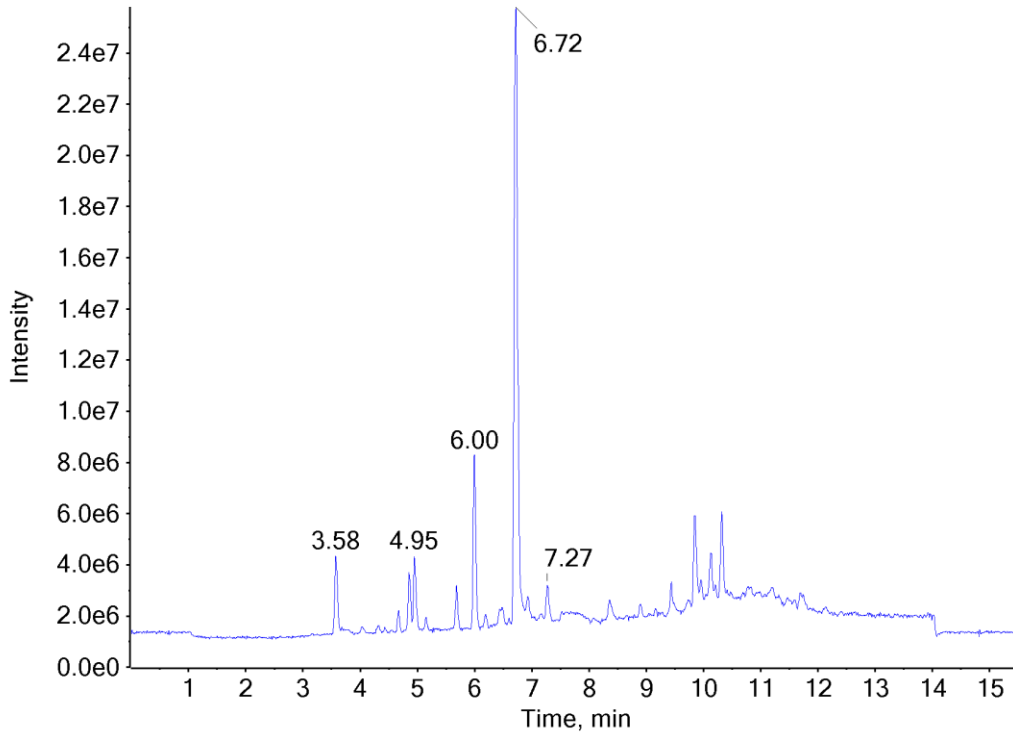
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Despropionyl *ortho*-Methylfentanyl



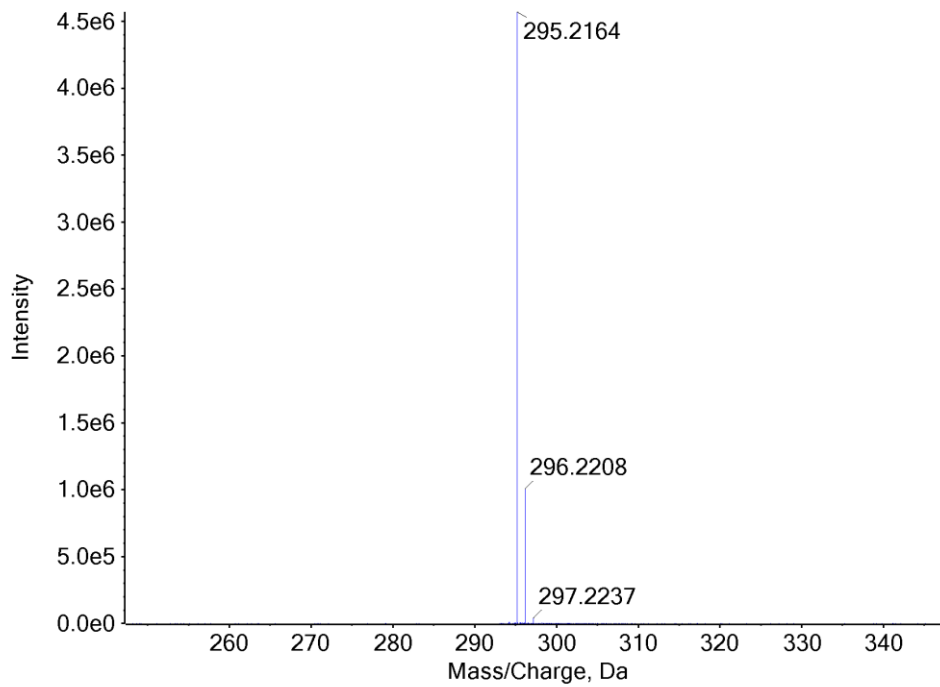
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

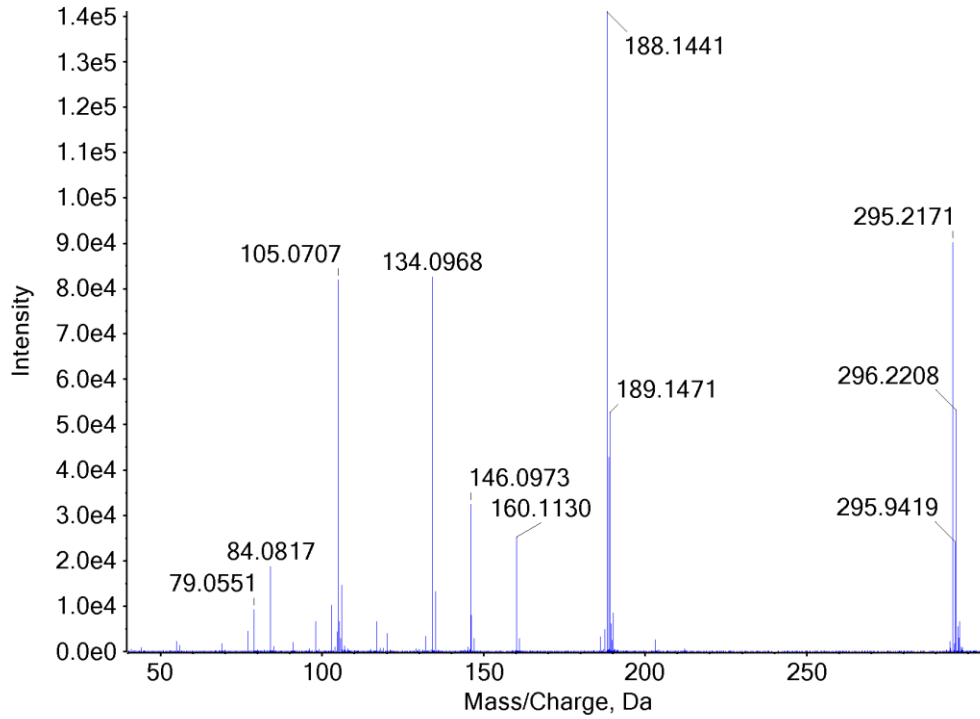
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	6.72 min
Standard Comparison:	Reference material for despropionyl <i>ortho</i> -methylfentanyl (Batch: 0521837-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as despropionyl <i>ortho</i> -methylfentanyl, based on retention time (6.723 min) and mass spectral data. (https://www.caymanchem.com/product/24279).

Chromatogram: Despropionyl *ortho*-Methylfentanyl



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





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.