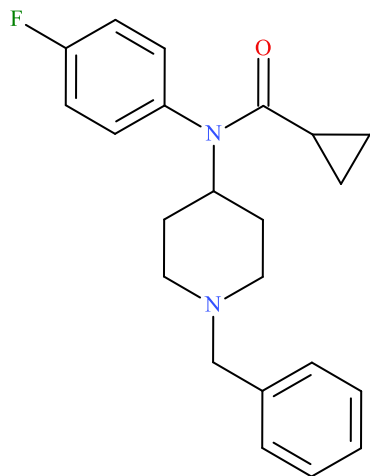


## ***para*-Fluorocyclopropylbenzylfentanyl & Despropionyl *para*-Fluorobenzylfentanyl**

***para*-Fluorocyclopropylbenzylfentanyl**

Sample Type: **Seized Material**

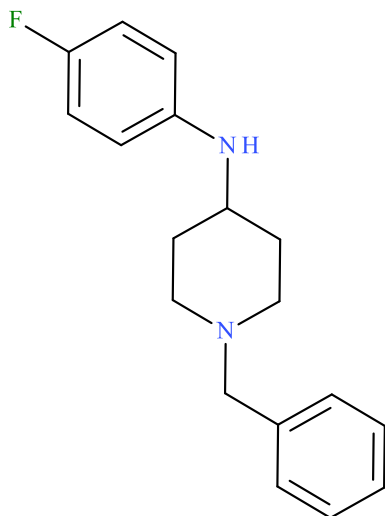


Latest Revision: **October 5, 2018**

Date Received: **June 27, 2018**

Date of Report: **October 5, 2018**

***Despropionyl para*-Fluorobenzylfentanyl**



**Important Note:** Identification of *para*-Fluorocyclopropylbenzylfentanyl was made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material. Identification of Despropionyl *para*-Fluorobenzylfentanyl was made based on evaluation of analytical data only (GC-MS and LC-QTOF).

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

## 1. GENERAL INFORMATION

### *1.1 para-Fluorocyclopropylbenzylfentanyl*

<b>IUPAC Name:</b>	N-(1-benzyl-4-piperidyl)-N-(4-fluorophenyl) cyclopropanecarboxamide
<b>InChI String:</b>	InChI=1S/C22H25FN2O/c23-19-8-10-20(11-9-19)25(22(26)18-6-7-18)21-12-14-24(15-13-21)16-17-4-2-1-3-5-17/h1-5,8-11,18,21H,6-7,12-16H2
<b>CFR:</b>	Not Scheduled (10/2018)
<b>CAS#</b>	Not Available
<b>Synonyms:</b>	<i>N</i> -benzyl <i>para</i> -fluoro Cyclopropyl norfentanyl, p-FCBF
<b>Source:</b>	Department of Homeland Security
<b>Appearance:</b>	White Solid Material

### *1.2 Despropionyl para-Fluorobenzylfentanyl*

<b>IUPAC Name:</b>	1-benzyl-N-(4-fluorophenyl)piperidin-4-amine
<b>InChI String:</b>	InChI=1S/C18H21FN2/c19-16-6-8-17(9-7-16)20-18-10-12-21(13-11-18)14-15-4-2-1-3-5-15/h1-9,18,20H,10-14H2
<b>CFR:</b>	Not Scheduled (10/2018)
<b>CAS#</b>	Not Available
<b>Synonyms:</b>	<i>para</i> -Fluoro 4-ANBP, 4-Fluoro 4-ANBP
<b>Source:</b>	Department of Homeland Security
<b>Appearance:</b>	White Solid Material

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
<i>para</i> -Fluorocyclopropylbenzylfentanyl	C <sub>22</sub> H <sub>25</sub> FN <sub>2</sub> O	352.4	352	353.2024
Despropionyl <i>para</i> -Fluorobenzylfentanyl	C <sub>18</sub> H <sub>21</sub> FN <sub>2</sub>	284.4	284	285.1762

### 3. BRIEF DESCRIPTION

*para*-Fluorocyclopropylbenzylfentanyl and Despropionyl *para*-Fluorobenzylfentanyl are classified as suspected fentanyl analogue precursors. Both compounds were detected in a single exhibit of white powder seized at the United States border. These substances are benzyl and despropionyl benzyl analogues of fentanyl related substances. Both compounds are structurally related to benzylfentanyl, which demonstrates minimal opioid receptor agonist activity and is not scheduled in the United States. Benzyl and despropionyl analogues have utility as potential precursors for fentanyl and fentanyl analogue synthesis. The presence of Despropionyl *para*-Fluorobenzylfentanyl in this exhibit may be due to its unconsumed nature during the synthesis of *para*-Fluorocyclopropylbenzylfentanyl. *para*-Fluorocyclopropylbenzylfentanyl and Despropionyl *para*-Fluorobenzylfentanyl are not scheduled substances in the United States.

### 4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/25238>

### 5. QUALITATIVE DATA

#### 5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

**Testing Performed At:** NMS Labs (Willow Grove, PA)

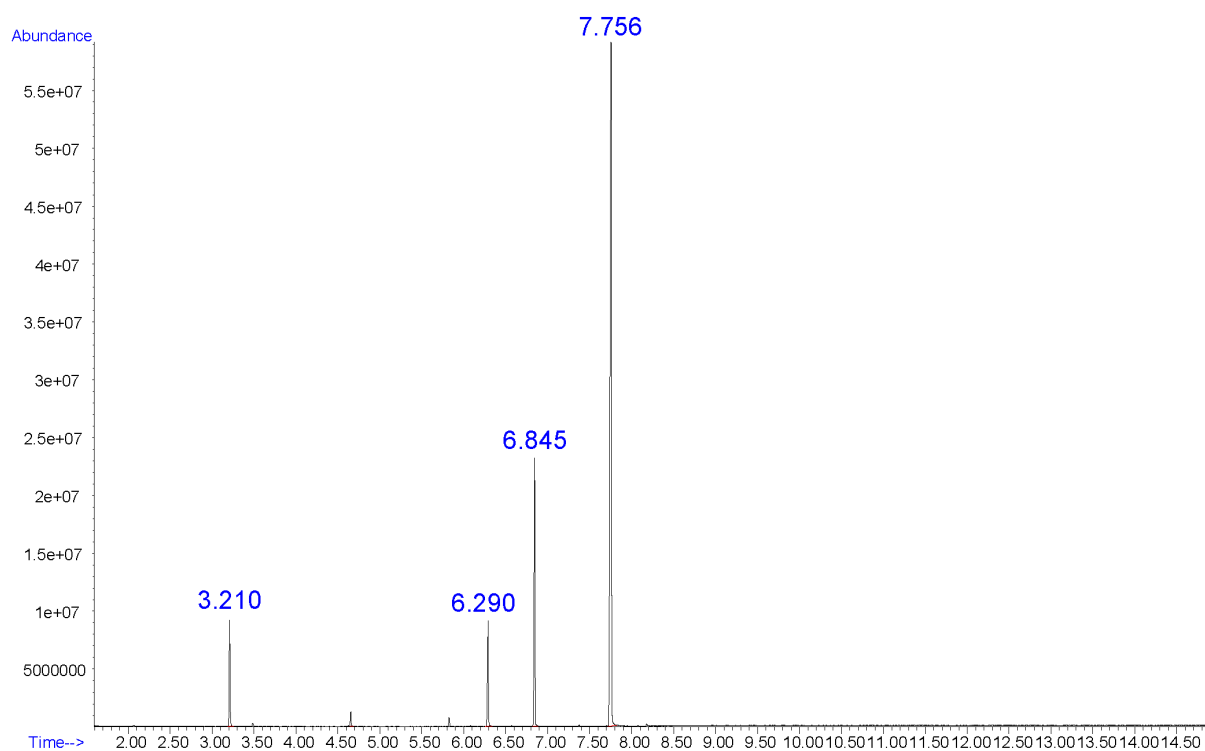
**Sample Preparation:** Acid/base extraction

**Instrument:** Agilent 5975 Series GC/MSD System

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

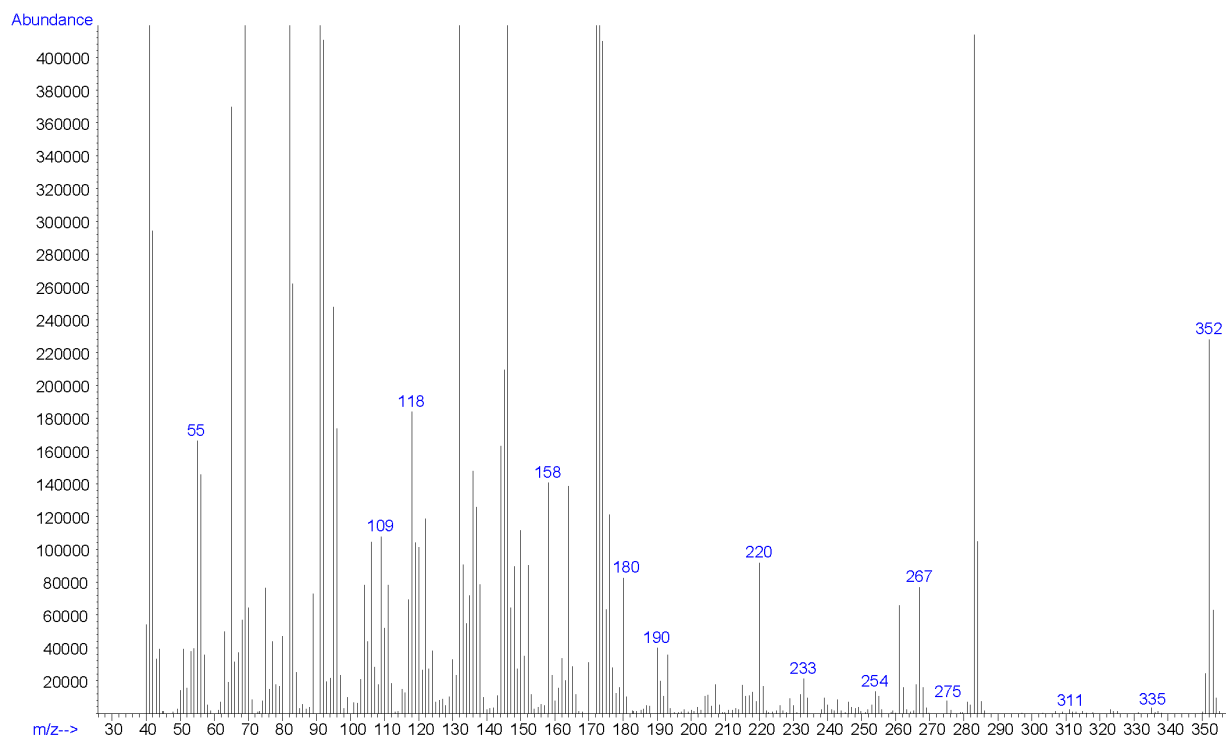
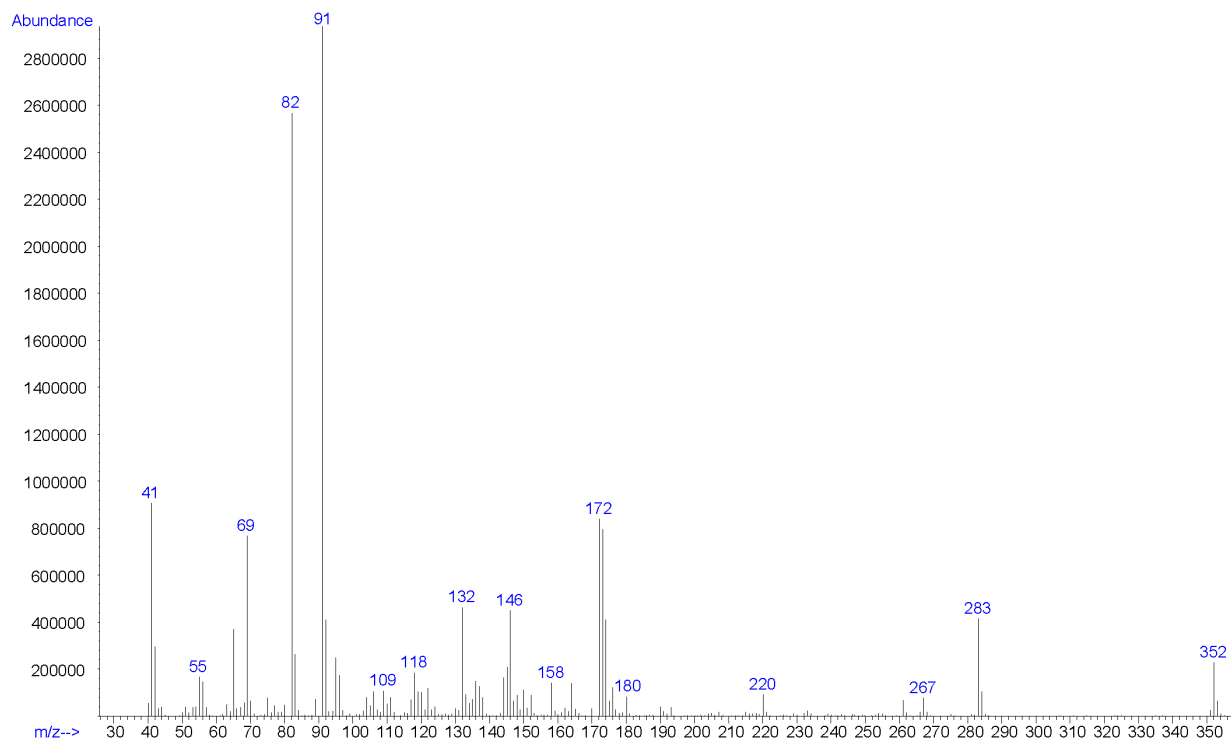
<b>Carrier Gas:</b>	Helium (Flow: 1 mL/min)
<b>Temperatures:</b>	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
<b>Injection Parameters:</b>	Injection Type: Splitless
	Injection Volume: 1 µL
<b>MS Parameters:</b>	Mass Scan Range: 40-550 m/z
	Threshold: 250
<b>Retention Time:</b>	<i>Despropionyl para-Fluorobenzylfentanyl</i> : 6.845 min
	<i>para-Fluorocyclopropylbenzylfentanyl</i> : 7.756 min
<b>Standard Comparison:</b>	Reference material for <i>para</i> -Fluorocyclopropylbenzylfentanyl (Batch: 0531312-6) 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>para</i> -Fluorocyclopropylbenzylfentanyl, based on retention time (7.737 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/25238">https://www.caymanchem.com/product/25238</a> )

**Chromatogram: *para*-Fluorocyclopropylbenzylfentanyl &  
Despropionyl *para*-Fluorobenzylfentanyl**

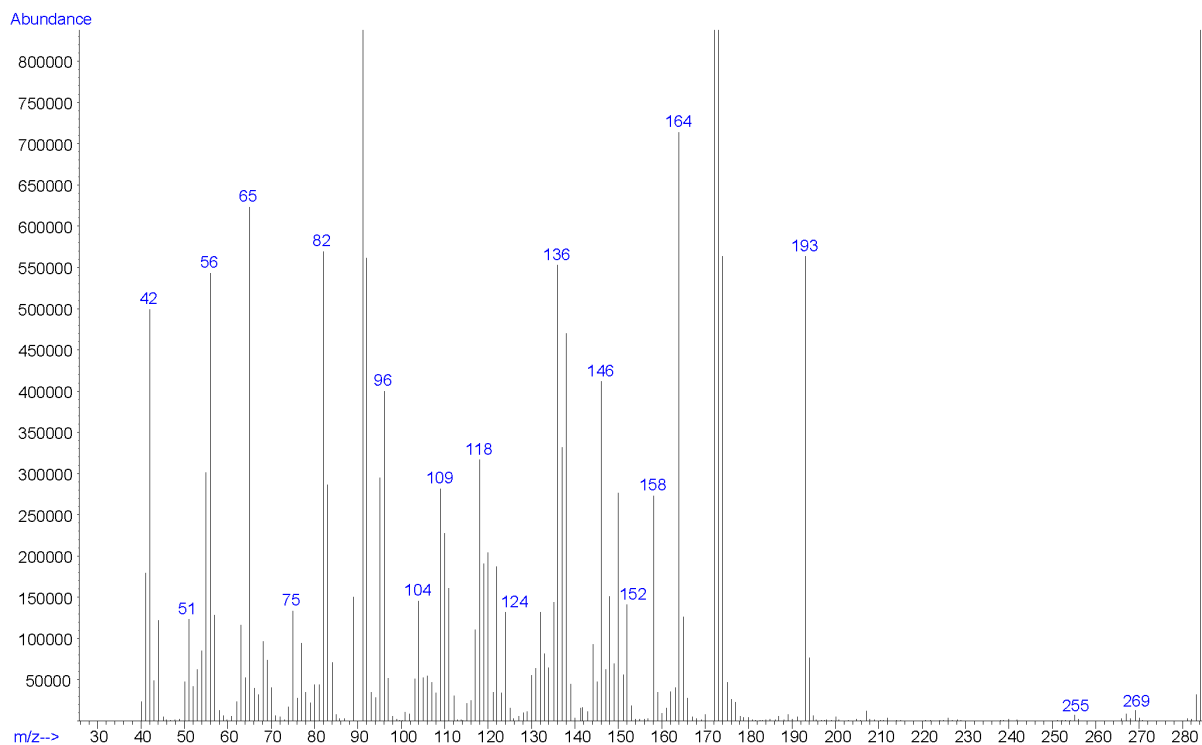
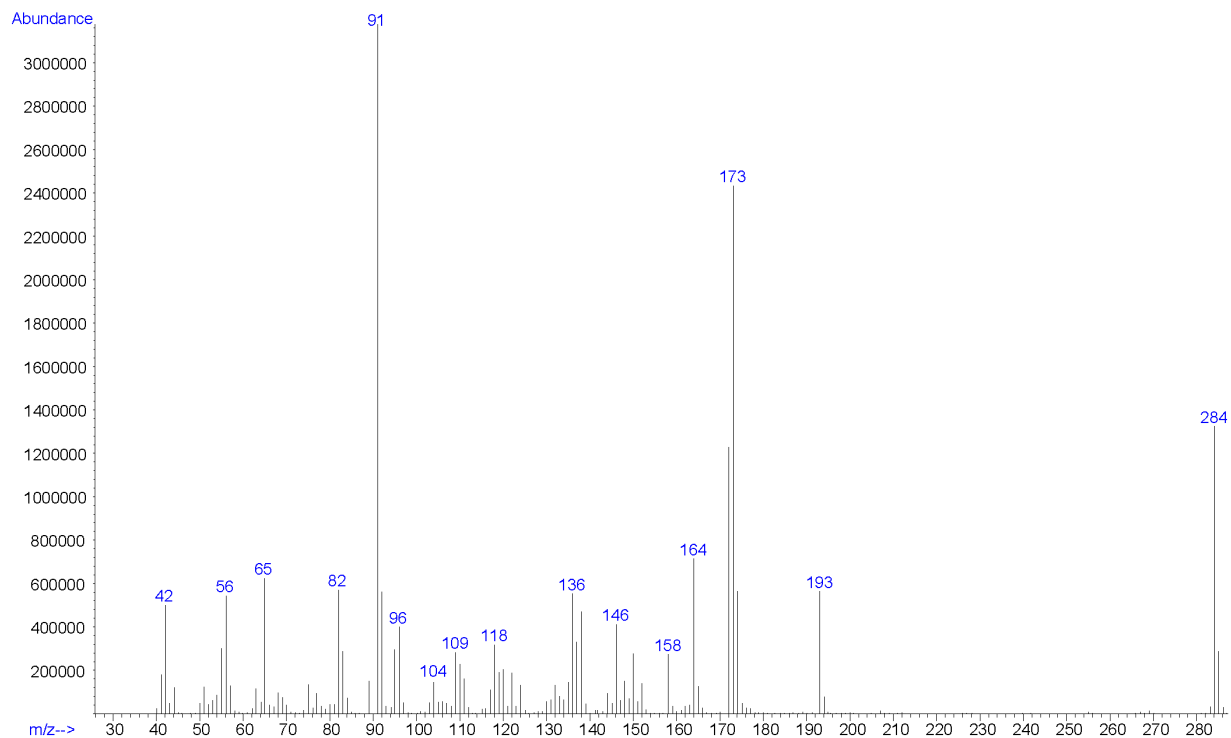


*Additional peaks present in chromatogram: internal standards (3.210 and 6.290 mins)*

**EI (70 eV) Mass Spectrum (Top) and 10x (Bottom):  
*para*-Fluorocyclopropylbenzylfentanyl**



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

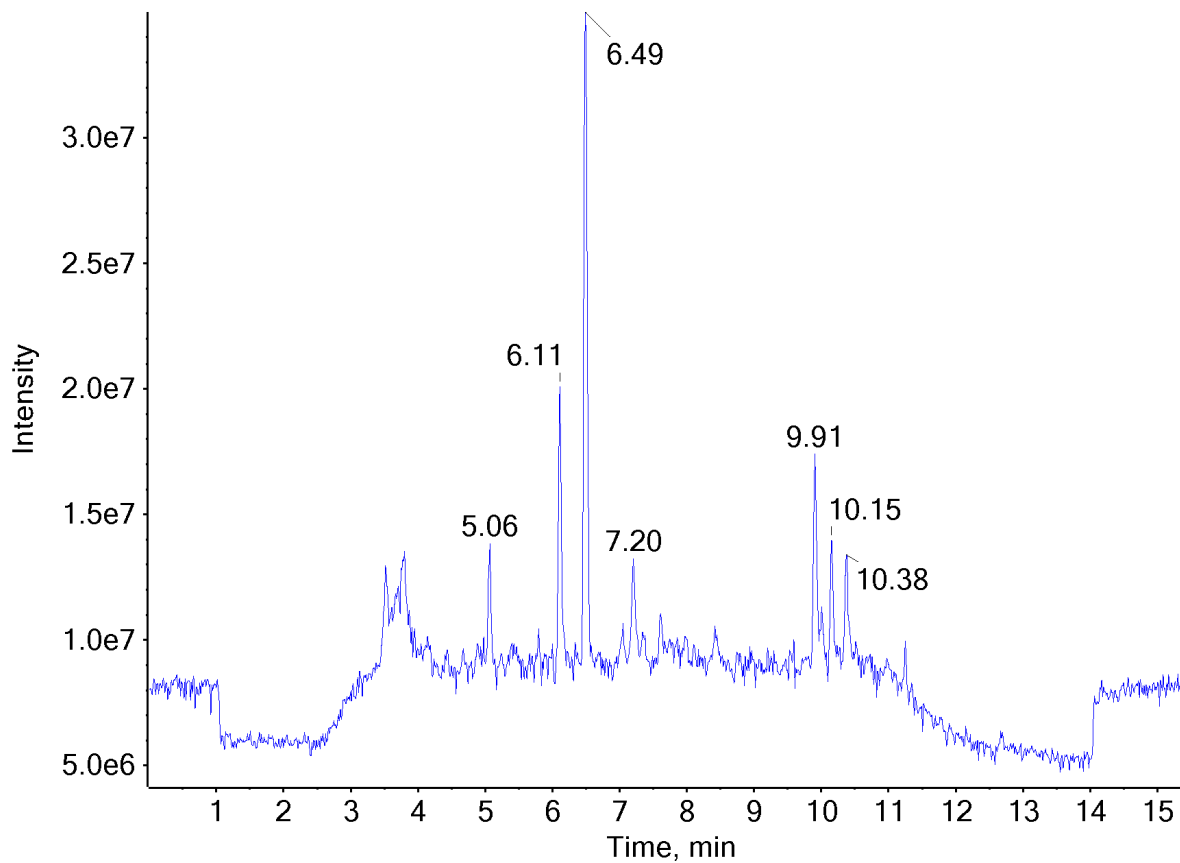


## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	1:100 dilution of acid/base extraction in mobile phase
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	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
<b>Retention Time:</b>	<i>Despropionyl para-Fluorobenzylfentanyl</i> : 6.11 min <i>para-Fluorocyclopropylbenzylfentanyl</i> : 6.49 min
<b>Standard Comparison:</b>	Reference material for <i>para</i> -Fluorocyclopropylbenzylfentanyl (Batch: 0531312-6) 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>para</i> -Fluorocyclopropylbenzylfentanyl, based on retention time (6.33 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/25238">https://www.caymanchem.com/product/25238</a> )

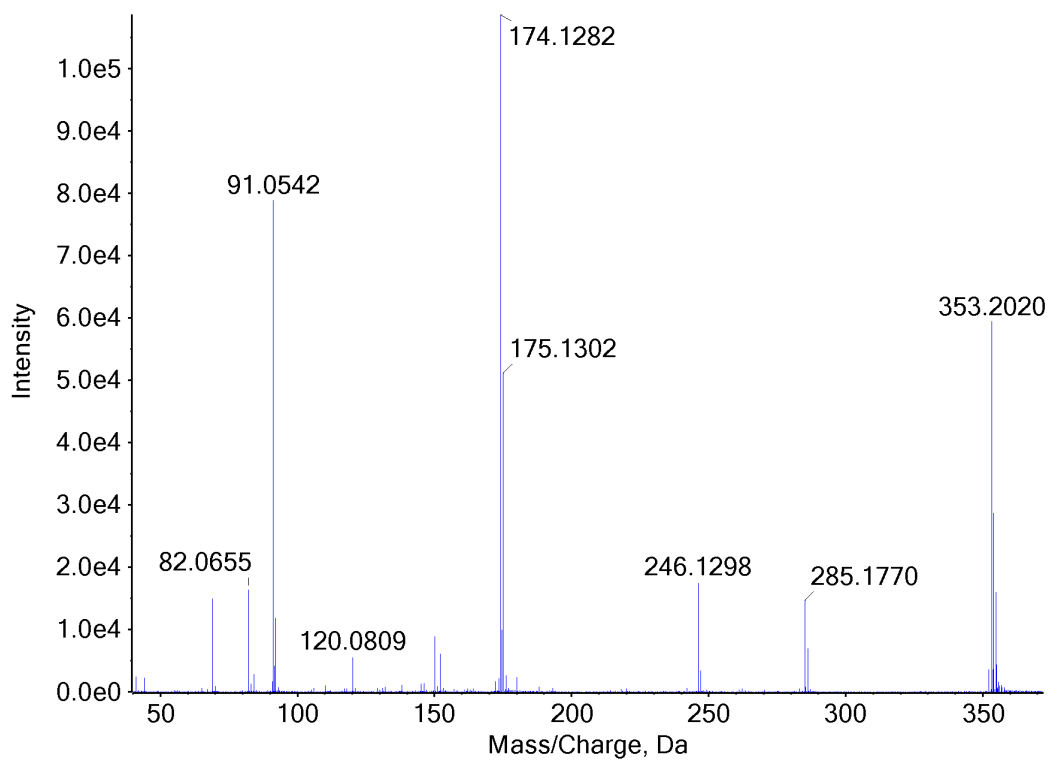
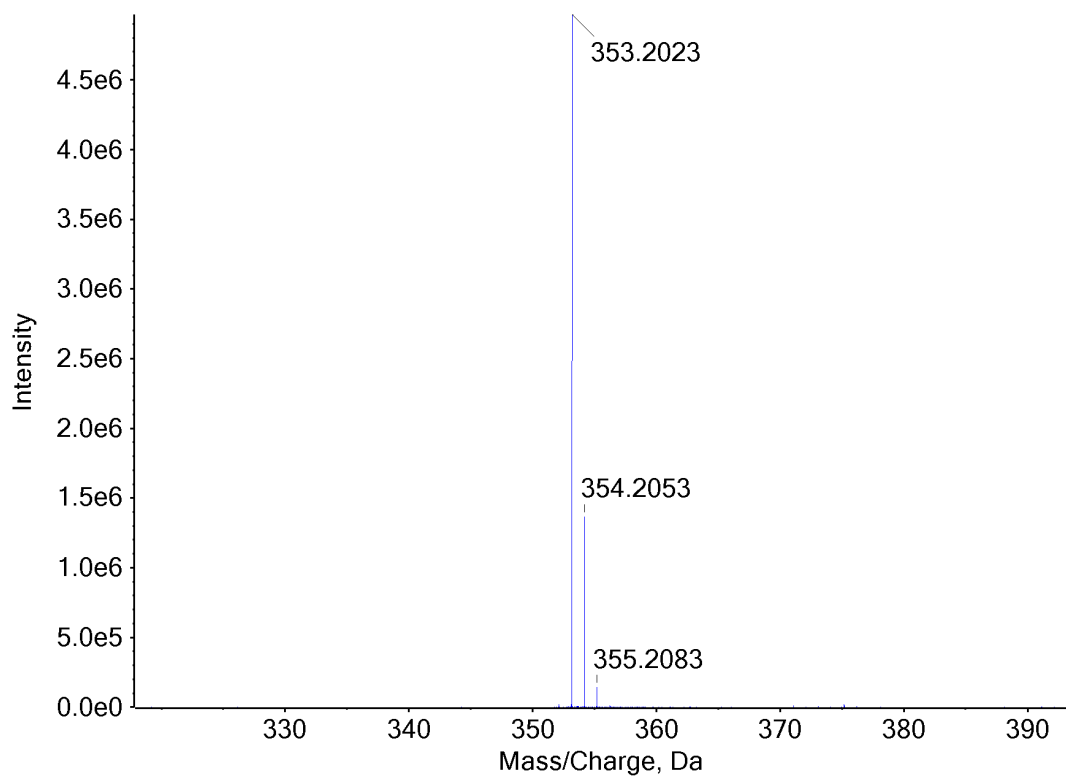


**Chromatogram: *para*-Fluorocyclopropylbenzylfentanyl and  
Despropionyl *para*-Fluorobenzylfentanyl**



*Additional peaks present in chromatogram: internal standard (5.06 min), not a controlled substance (7.20 min), not a controlled substance (9.91 min), not a controlled substance (10.15 min), not a controlled substance (10.38 min)*

**TOF MS (Top) and MS/MS (Bottom) Spectra: *para*-Fluorocyclopropylbenzylfentanyl**



**TOF MS (Top) and MS/MS (Bottom) Spectra: Despropionyl *para*-Fluorobenzylfentanyl**

