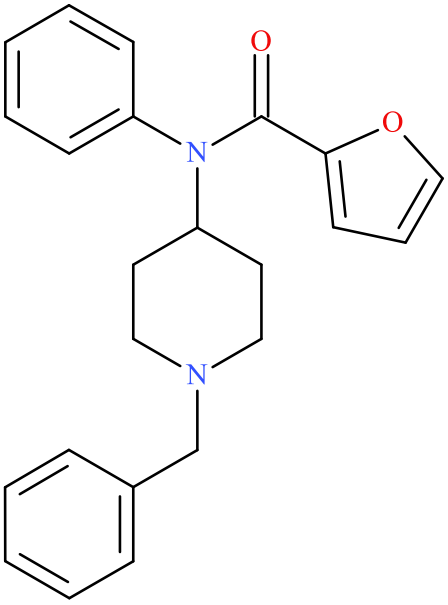
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

Benzylfuranylfentanyl

Sample Type: **Seized Material**



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

Date Received: **March 23rd, 2018**

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

1. GENERAL INFORMATION

IUPAC Name:	N-(1-benzyl-4-piperidyl)-N-phenyl-furan-2-carboxamide
InChI String:	InChI=1S/C23H24N2O2/c26-23(22-12-7-17-27-22)25(20-10-5-2-6-11-20)21-13-15-24(16-14-21)18-19-8-3-1-4-9-19/h1-12,17,21H,13-16,18H2
CFR:	Not Scheduled (04/2018)
CAS#	Not Available
Synonyms:	Benzyl Furanyl Fentanyl, Benzyl Fu-F
Source:	Department of Homeland Security
Appearance:	White Solid Material

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.*

***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	$C_{23}H_{24}N_2O_2$	360.45	360	361.1911

3. BRIEF DESCRIPTION

Benzylfuranylfentanyl is classified as a suspected fentanyl analogue precursor. Fentanyl analogue precursors are modified based on the structure of fentanyl or its analogues with the absence of notable functional groups or structural features. Fentanyl analogue precursors are often used in the synthesis of a variety of fentanyl analogues. Benzylfuranylfentanyl is not a scheduled substance in the United States.

4. ADDITIONAL RESOURCES

Diouf, O.; Gadeau, S.; Chelle, F.; Gelbcke, M.; Talaga, P.; Christophe, B.; Gillard, M.; Massingham, R.; Guyaux, M. (2002) A New Series of M3 Muscarinic Antagonists Based on the 4-Amino-piperidine Scaffold. *Bioorg Med Chem Lett*. **12**. 2535 – 2539.

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)

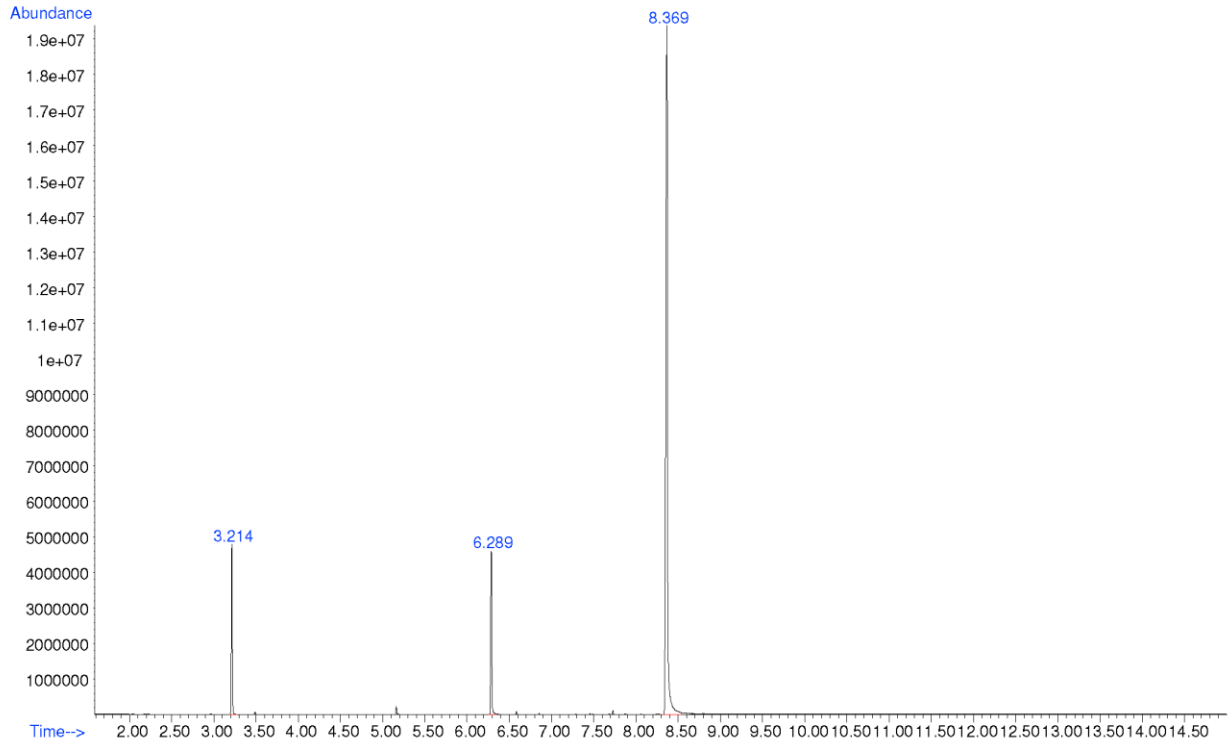
Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

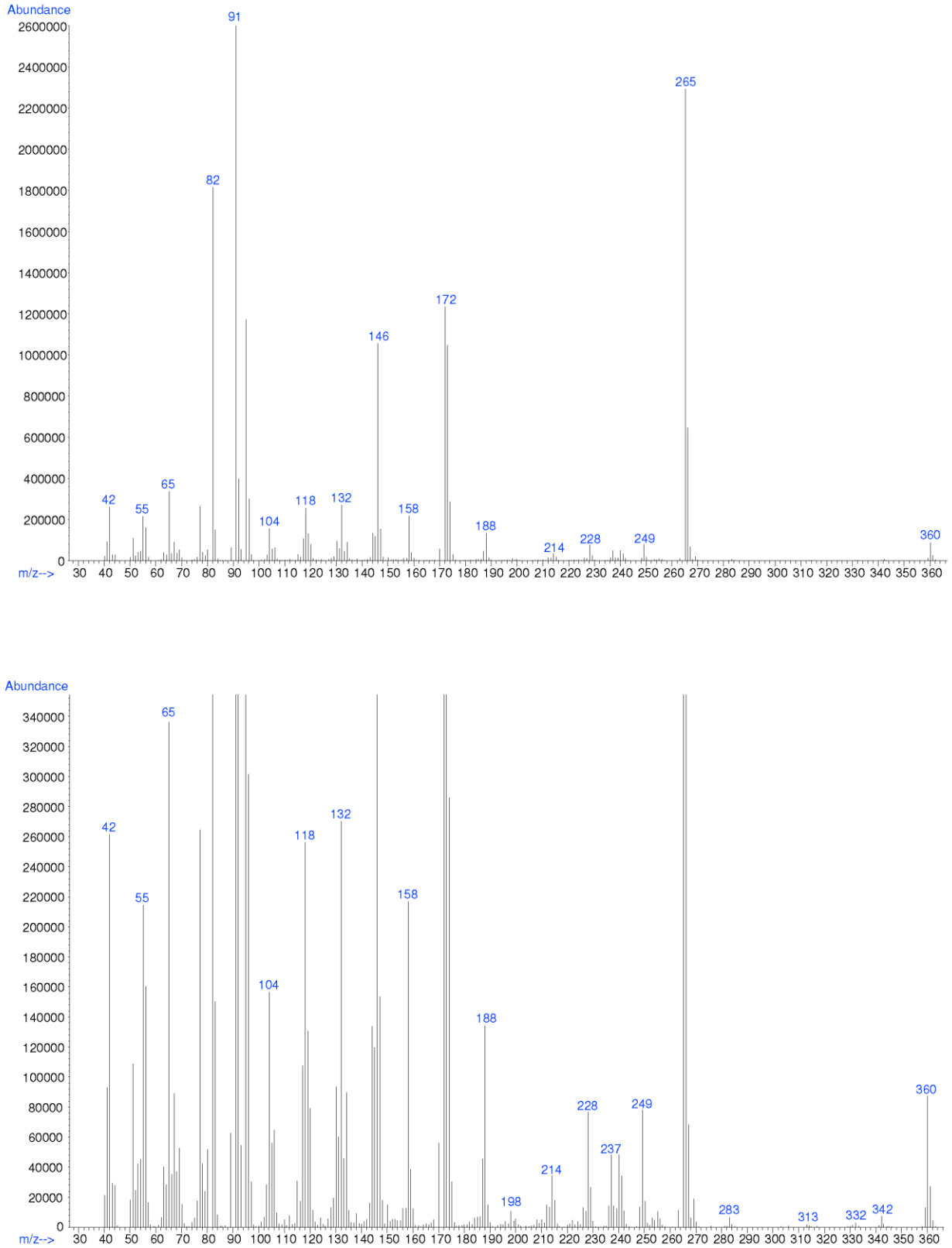
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	8.369 min

Chromatogram: Benzylfuranylfentanyl



Additional peaks present in chromatogram: internal standard 1 (3.214 min) and internal standard 2 (6.289 min)

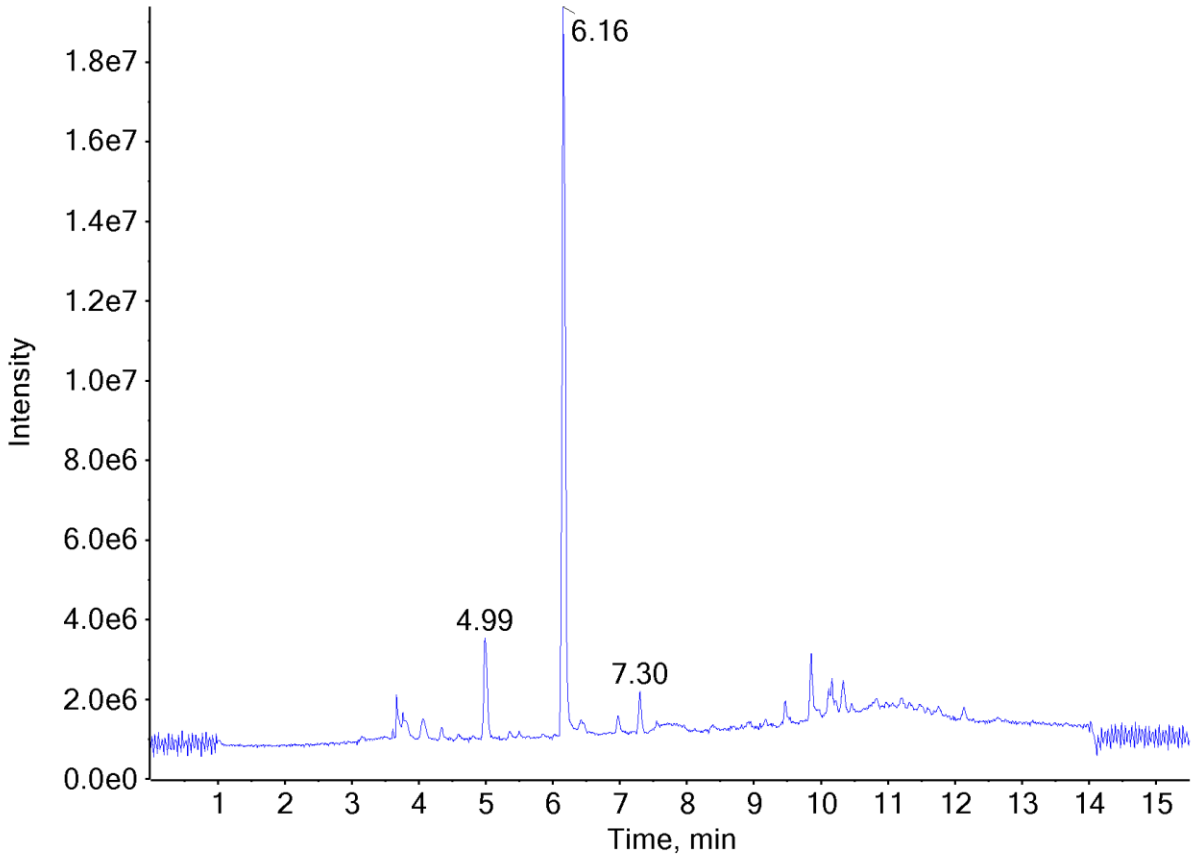
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Benzylfuranylfentanyl



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

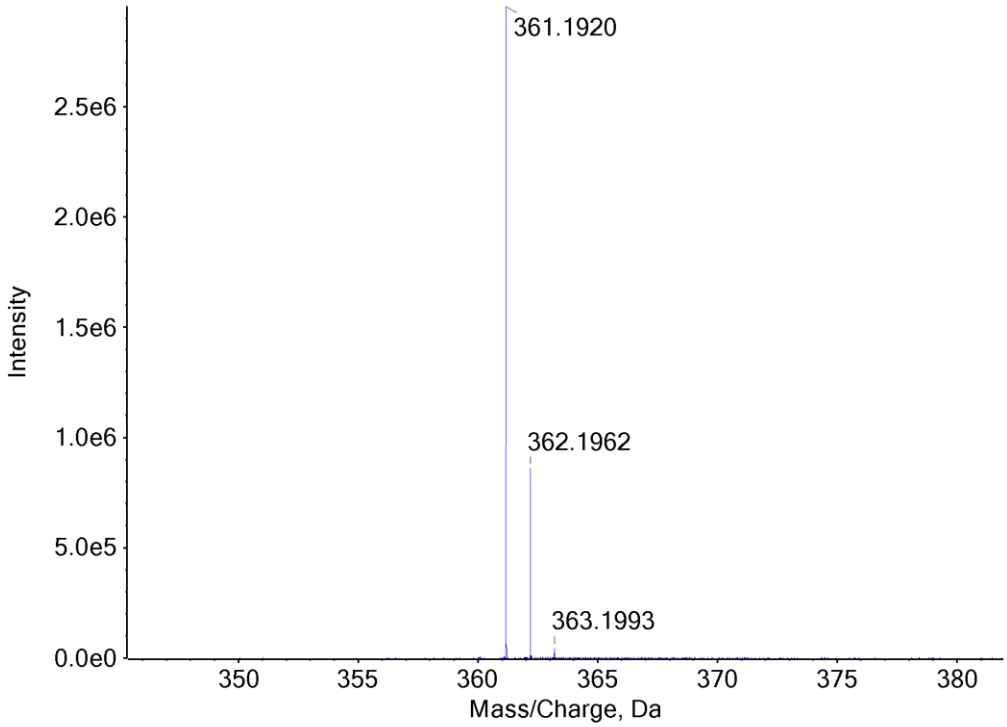
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	6.16 min

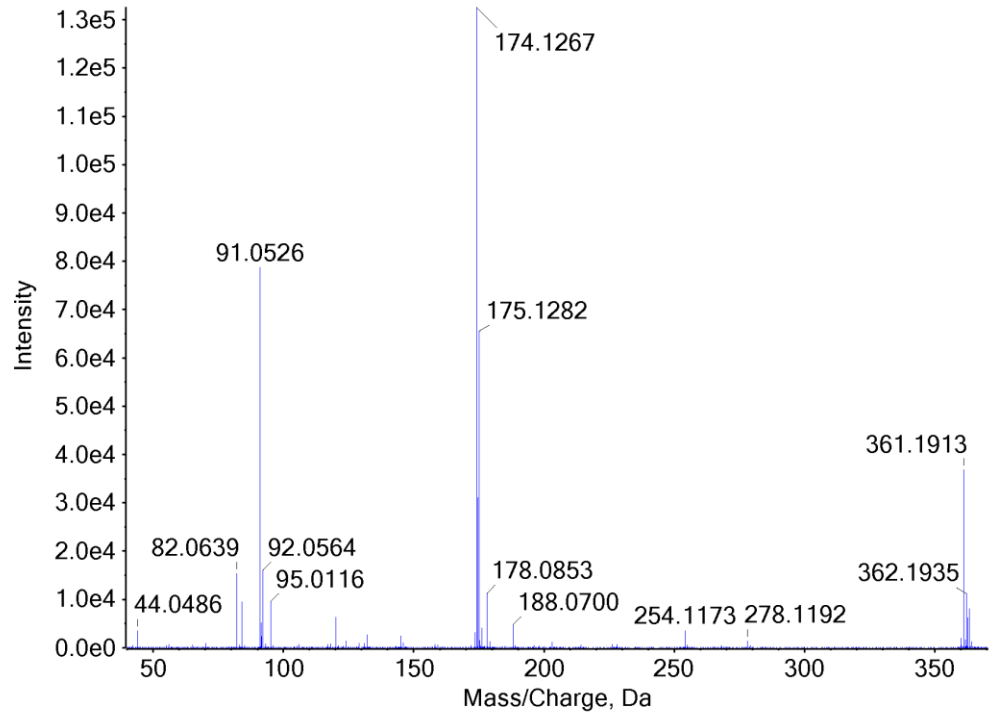
Chromatogram: Benzylfuranylfentanyl



Additional peaks present in chromatogram: internal standard 1 (4.99 min) and internal standard 2 (7.30 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Benzylfuranylfentanyl





5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in methylene chloride (5 mL), washed with 2 N NaOH (2 mL) and brine, evaporated, and dissolved in DMSO

Instrument: 300 MHz INOVA VARIAN Spectrometer

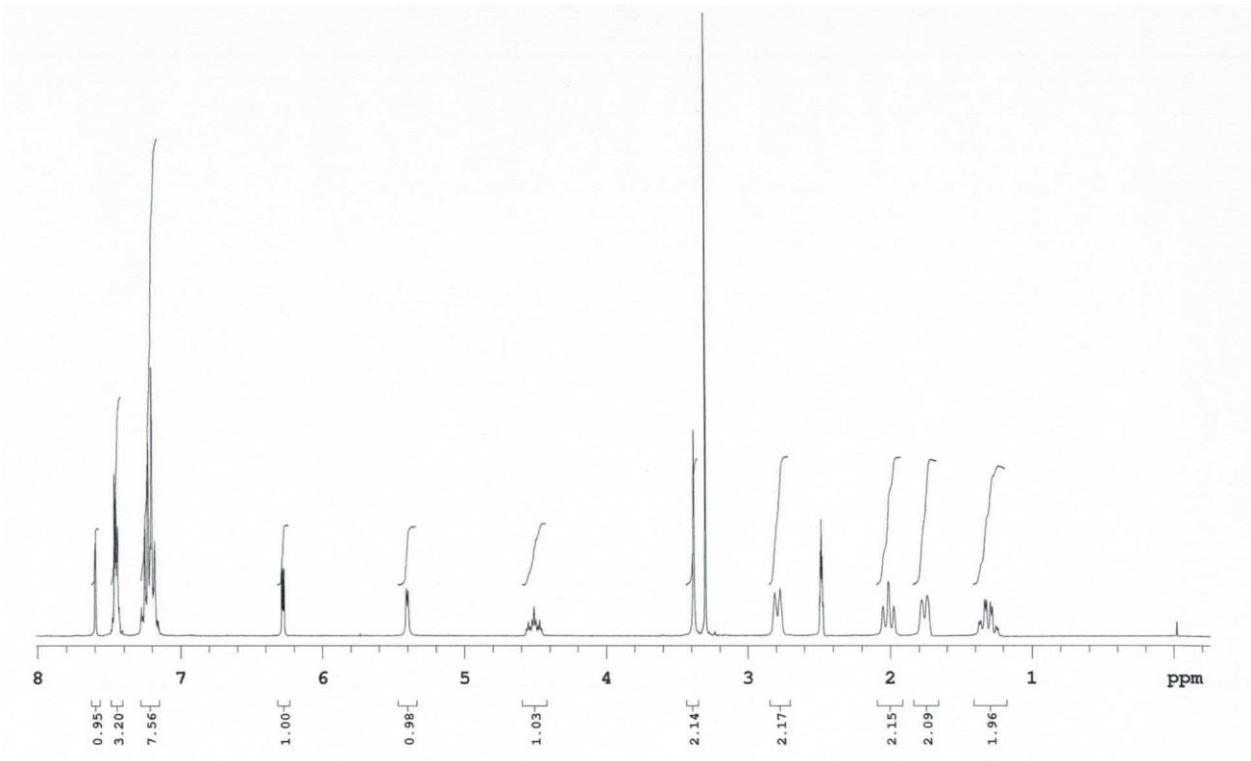
Parameters: Pulse Sequence: Proton

Solvent: DMSO

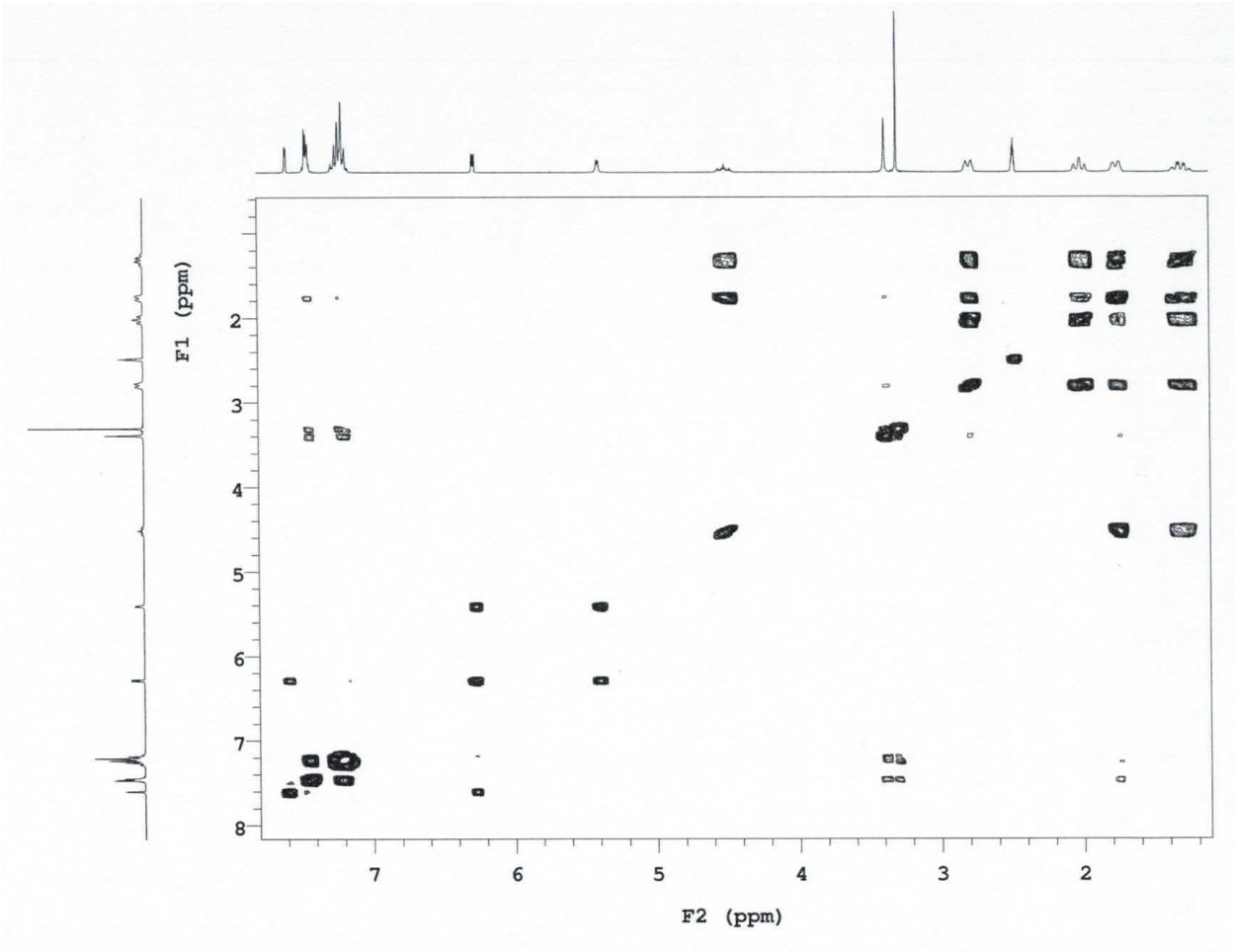
Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

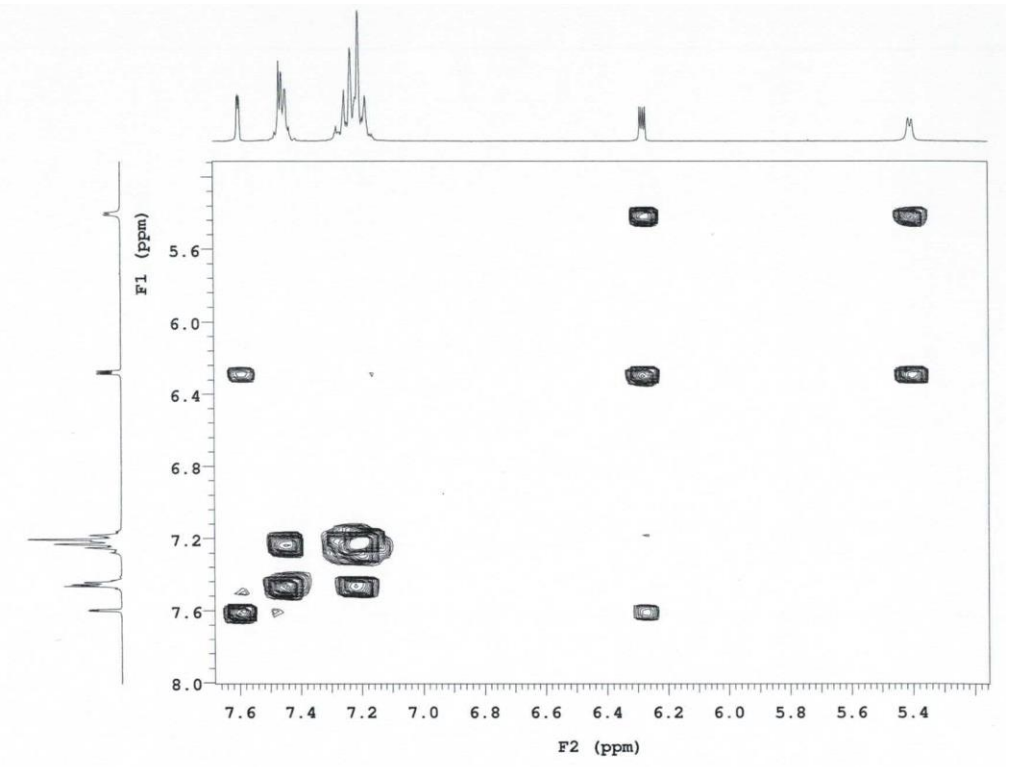
^{1}H NMR: Benzylfuranylfentanyl

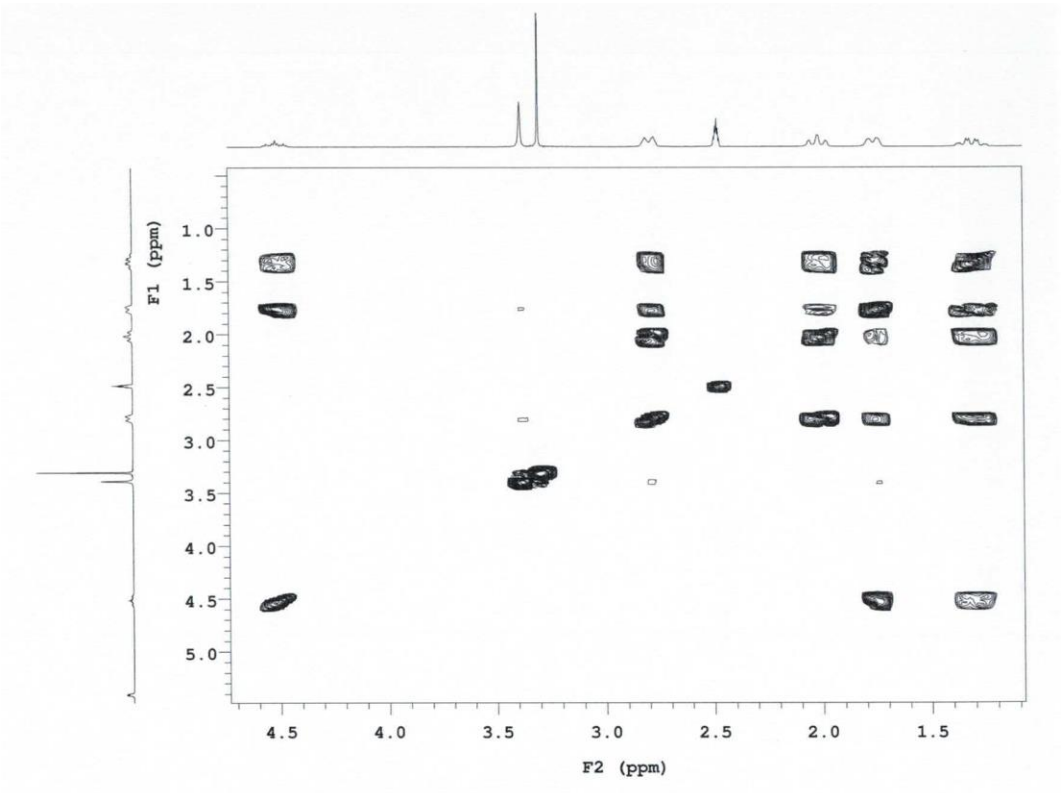


gCOSY: Benzylfuranylfentanyl



gCOSY (2x Zoom): Benzylfuranylfentanyl





6. REVISION HISTORY

Date	Revision
05/01/2018	Section 5.3: Sample preparation revised ("Dilute powder in $CDCl_3$" changed to "Powder dissolved in methylene chloride [5 mL], washed with 2 N NaOH [2 mL] and brine, evaporated, and dissolved in DMSO"). Parameters revised ("$CDCl_3$" changed to "DMSO").
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.