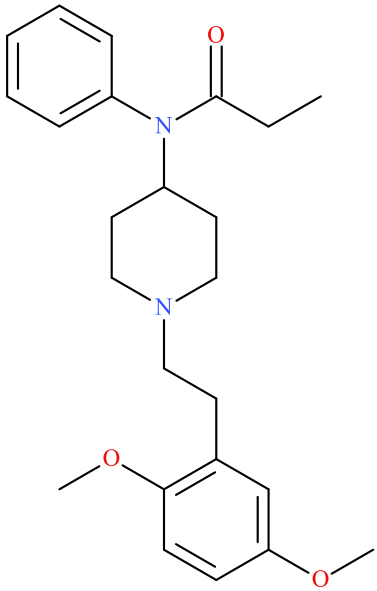
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

2’,5’-Dimethoxyfentanyl



Sample Type: **Seized Material**

Latest Revision: **April 30, 2019**

Date Received: **March 25, 2019**

Date of Report: **April 30, 2019**

1. GENERAL INFORMATION

IUPAC Name:	N-[1-[2-(2,5-dimethoxyphenyl)ethyl]-4-piperidyl]-N-phenyl-propanamide
InChI String:	InChI=1S/C24H32N2O3/c1-4-24(27)26(20-8-6-5-7-9-20)21-13-16-25(17-14-21)15-12-19-18-22(28-2)10-11-23(19)29-3/h5-11,18,21H,4,12-17H2,1-3H3
CFR:	21 CFR 1308: Temporary Placement of Fentanyl-Related Substances in Schedule 1 (02/06/2018)
CAS#	Not Available
Synonyms:	2’,5’-Dimethoxy Fentanyl, 2,5-Dimethoxyfentanyl, Dimethoxy fentanyl
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.*

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{24}H_{32}N_2O_3$	396.5	396	397.2486

3. BRIEF DESCRIPTION

2’,5’-Dimethoxyfentanyl 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. 2’,5’-Dimethoxyfentanyl is not explicitly scheduled by name, but recent legislation has temporarily placed all fentanyl-related substances in Schedule I.

4. ADDITIONAL RESOURCES

No additional resources are available at this time.

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)

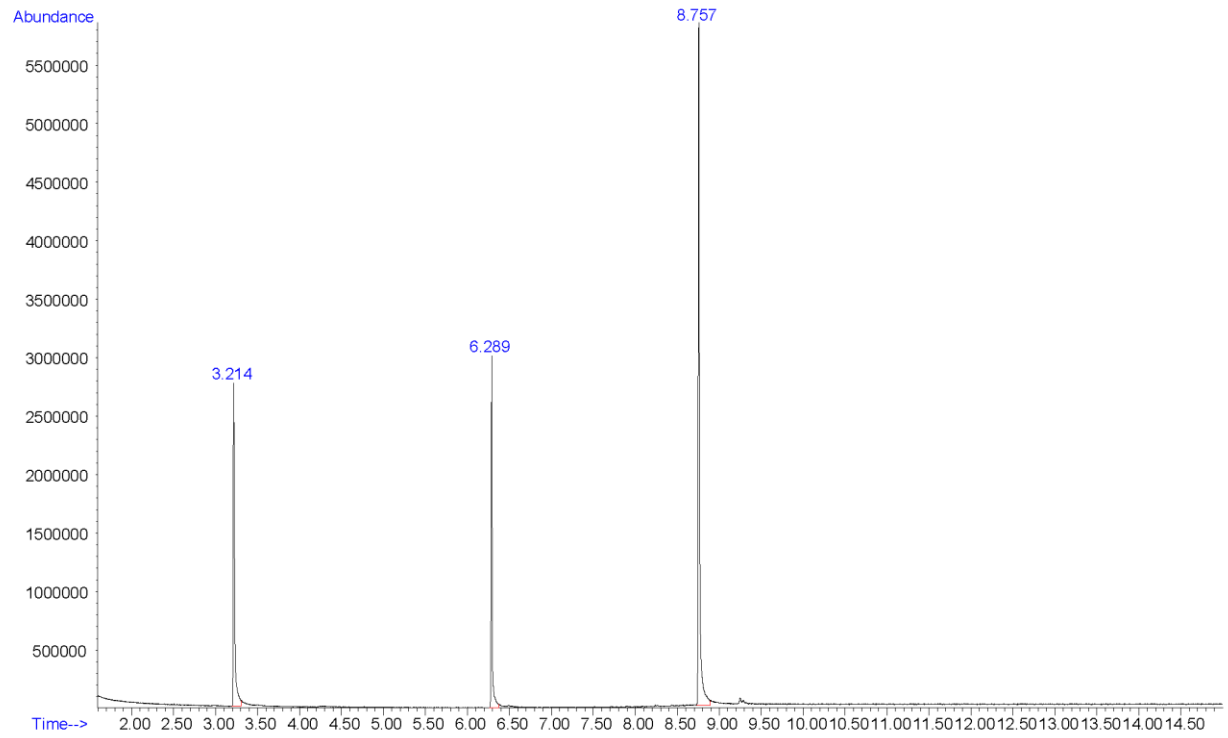
Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

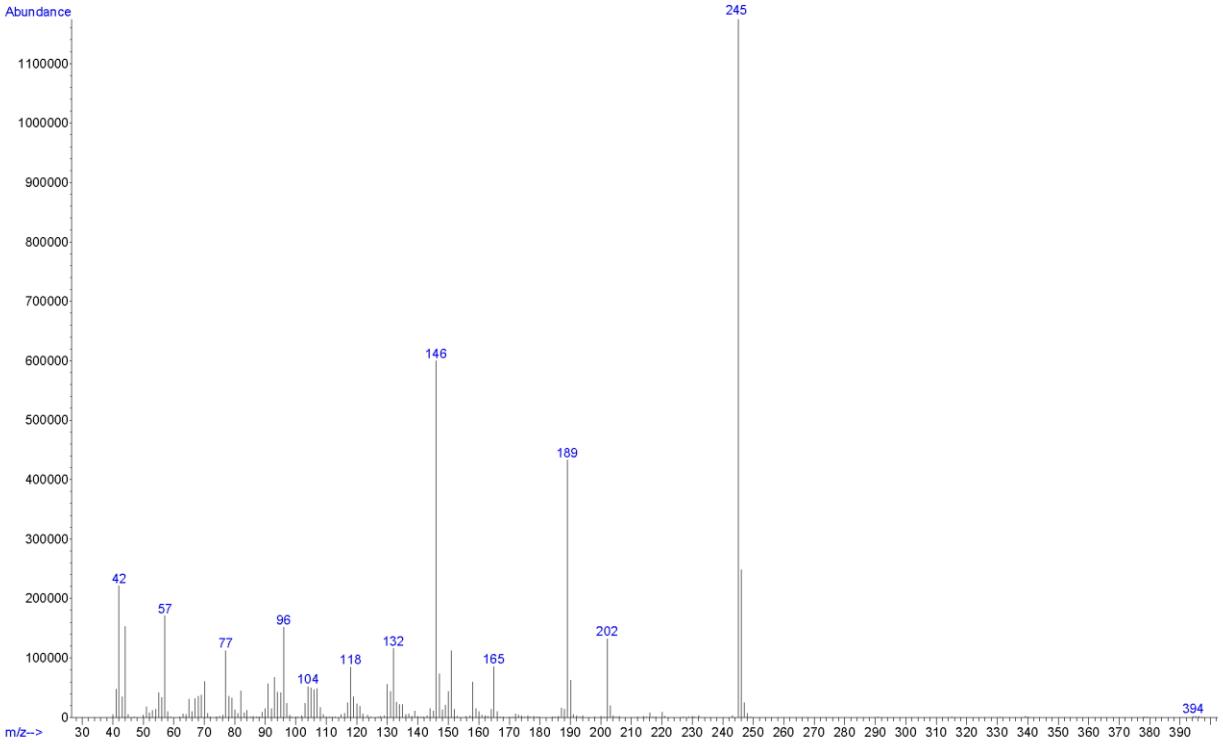
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	8.757 min

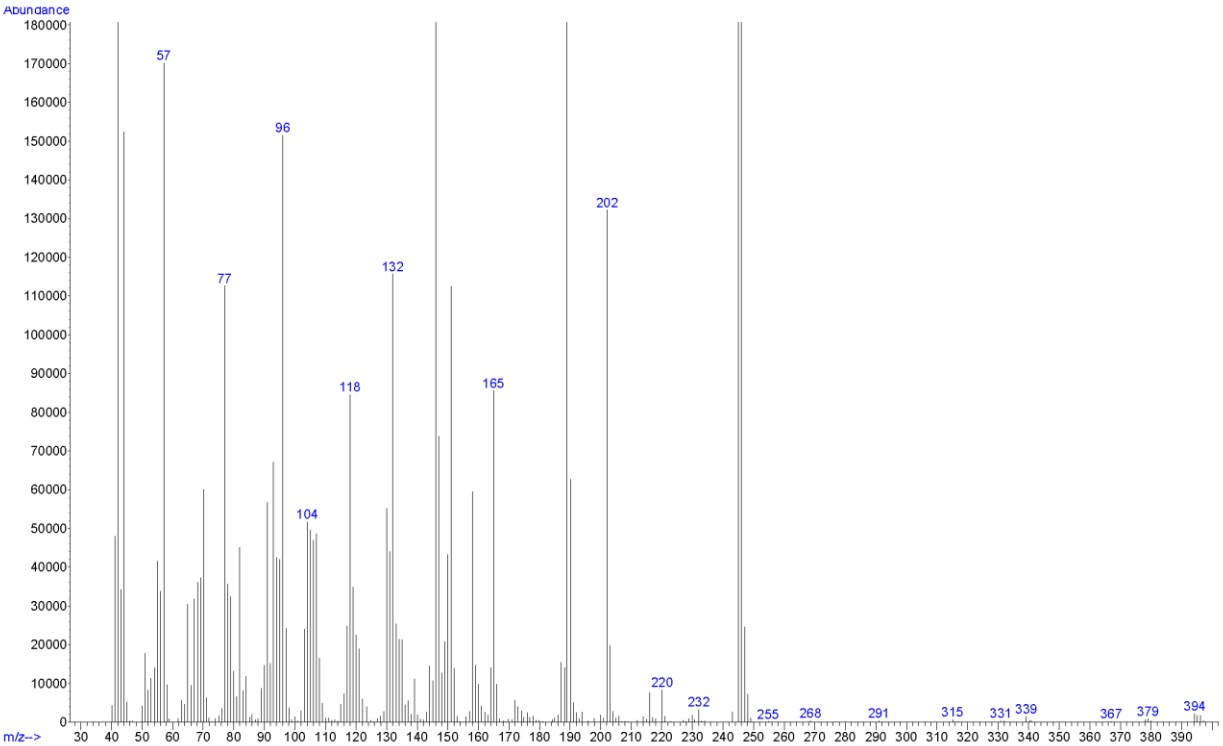
Chromatogram: 2',5'-Dimethoxyfentanyl



Additional peaks present in chromatogram: internal standards (3.214 min and 6.289 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 2',5'-Dimethoxyfentanyl

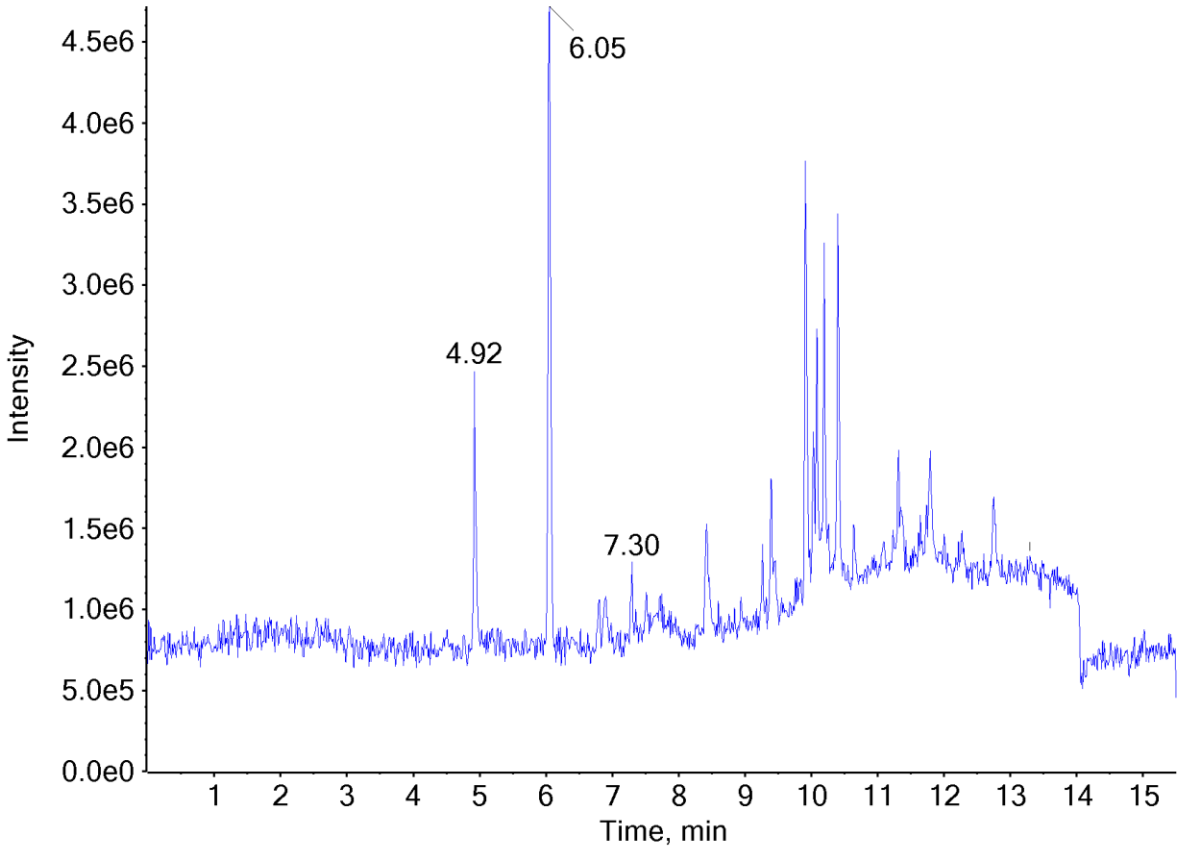




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

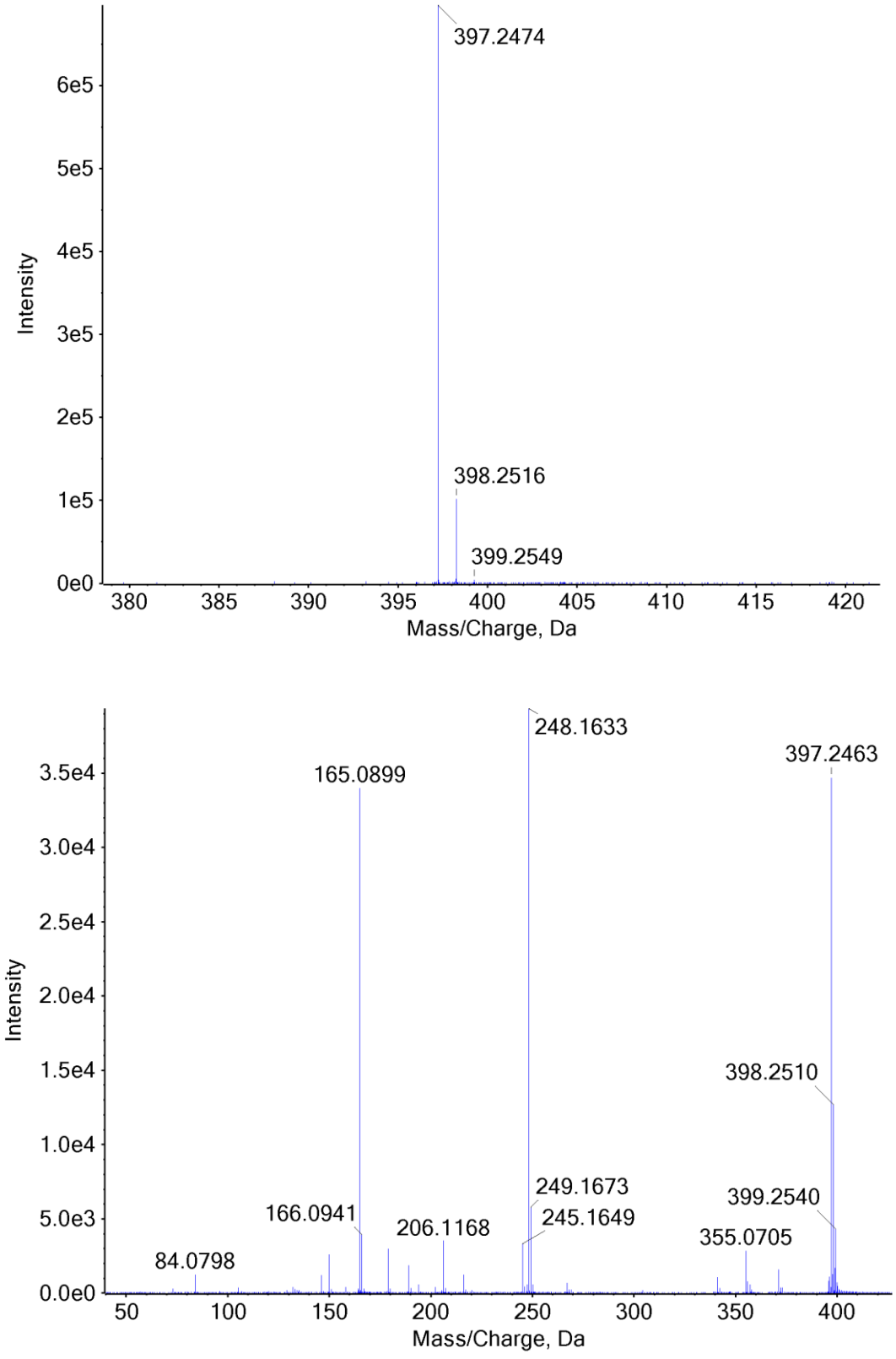
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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:	6.05 min

Chromatogram: 2’,5’-Dimethoxyfentanyl



Additional peaks present in chromatogram: internal standards (4.92 min and 7.30 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 2',5'-Dimethoxyfentanyl



5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in $CDCl_3$

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

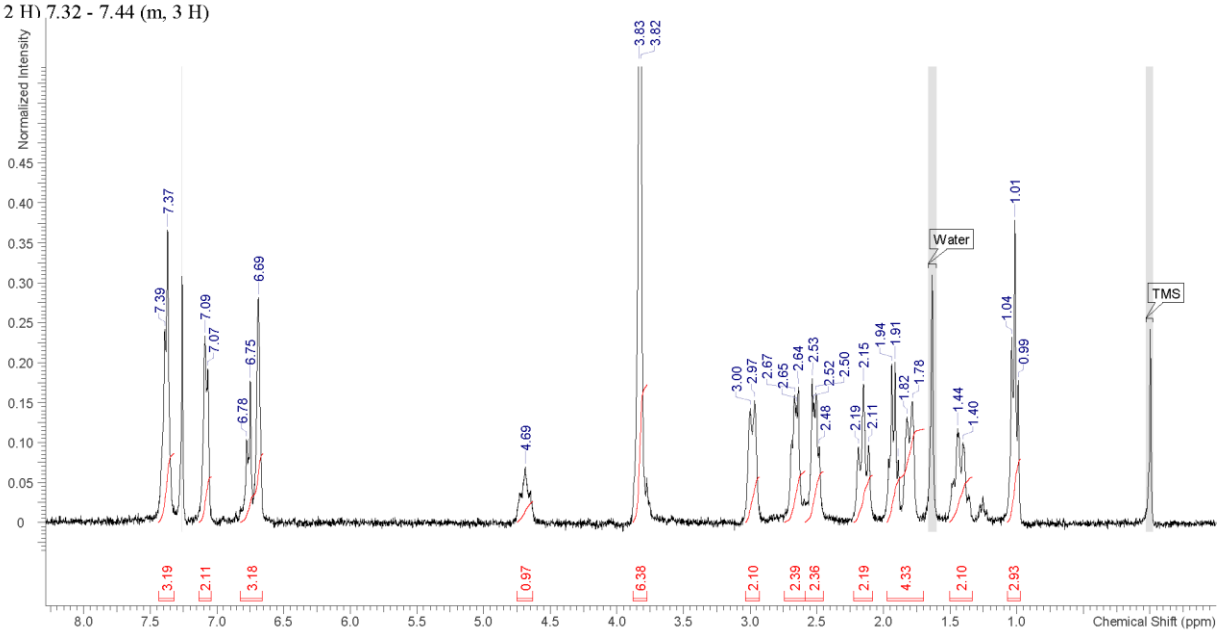
Solvent: $CDCl_3$

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: 2',5'-Dimethoxyfentanyl

^{1}H NMR (300 MHz, CHLOROFORM-*d*) δ ppm 0.97 - 1.07 (m, 3 H) 1.42 (br d, *J*=12.30 Hz, 2 H) 1.70 - 1.97 (m, 4 H) 2.15 (br t, *J*=11.72 Hz, 2 H) 2.45 - 2.59 (m, 2 H) 2.59 - 2.74 (m, 3 H) 2.98 (br d, *J*=9.96 Hz, 2 H) 3.77 - 3.88 (m, 6 H) 4.69 (br s, 1 H) 6.66 - 6.82 (m, 3 H) 7.08 (br d, *J*=5.86 Hz, 2 H) 7.32 - 7.44 (m, 3 H)



COSY NMR: 2',5'-Dimethoxyfentanyl