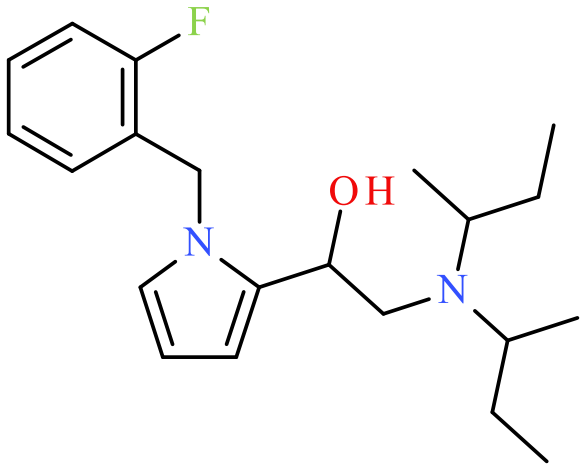
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

2F-Viminol

Sample Type: **Seized Material**



Latest Revision: **December 4, 2019**

Date Received: **October 3, 2019**

Date of Report: **November 15, 2019**

1. GENERAL INFORMATION

IUPAC Name:	2-(disec-butylamino)-1-[1-[(2-fluorophenyl)methyl]pyrrol-2-yl]ethanol
InChI String:	InChI=1S/C21H31FN2O/c1-5-16(3)24(17(4)6-2)15-21(25)20-12-9-13-23(20)14-18-10-7-8-11-19(18)22/h7-13,16-17,21,25H,5-6,14-15H2,1-4H3
CFR:	Not Scheduled (11/2019)
CAS#	Not Available
Synonyms:	2-Fluoro Viminol, Viminol Fluoro Analogue
Source:	Department of Homeland Security
Appearance:	Off-White Solid Material

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

***Prepared By:** Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, D-ABFT-FT, 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	$C_{21}H_{31}FN_2O$	346.5	346	347.2493

3. BRIEF DESCRIPTION

2F-Viminol is classified as a novel opioid. Novel opioids have been reported to cause effects similar to heroin and fentanyl. Novel opioids have caused adverse events, including deaths, as described in the literature. 2F-Viminol is unlike other novel opioids (e.g. fentanyl analogues, U-series analogues) previously characterized. Viminol, the 2-position chlorinated molecule, is structurally similar to 2F-Viminol. Viminol (or Dividol) was first synthetized in the 1960s.[1] Viminol exists as six stereoisomers and is described to have potent analgesic activity with minimal dependence liability.[2] One stereoisomer of Viminol is reported to be 3.5 times more potent than morphine.[2,3] 2F-Viminol was later synthesized in the 1970s and is reported to be more potent than Viminol with relative decreased toxicity potential.[4] Viminol and 2F-Viminol are not approved by the FDA for use within the United States.[5] Viminol and 2F-Viminol are not scheduled substances in the United States.

4. ADDITIONAL RESOURCES

1. Teotino, UM; Bella, DD. (10 November 1970). "Patent US3539589A – 1-(alpha-pyrryl)-2-amino ethanols." https://patents.google.com/patent/US3539589

2. Shook, JE; Kallman, MJ; Dewet, WL. (1984) The discriminative stimulus properties of the R2 isomer of viminol. *Pharmacology Biochemistry and Behavior*, **20**, 59-62. https://www.sciencedirect.com/science/article/pii/0091305784901011?via%3Dihub

3. Bella, D; Veneziani, C; Chiarino, D; Teotino, U. (31 December 1974). "Patent US3857857A – Stereoisomers of 1-(1{40 (-o-chlorobenzyl)-2{40 -pyrryl)-2-disec. butylamino-ethanol." https://patents.google.com/patent/US3857857

4. Conti, F. (10 April 1979). "Patent US4148907A – Stereoisomers of 1-(1'benzyl-2'pyrryl)-2-di-sec.-butylaminoethanol and pharmaceutical compositions comprising same." https://patents.google.com/patent/US4148907

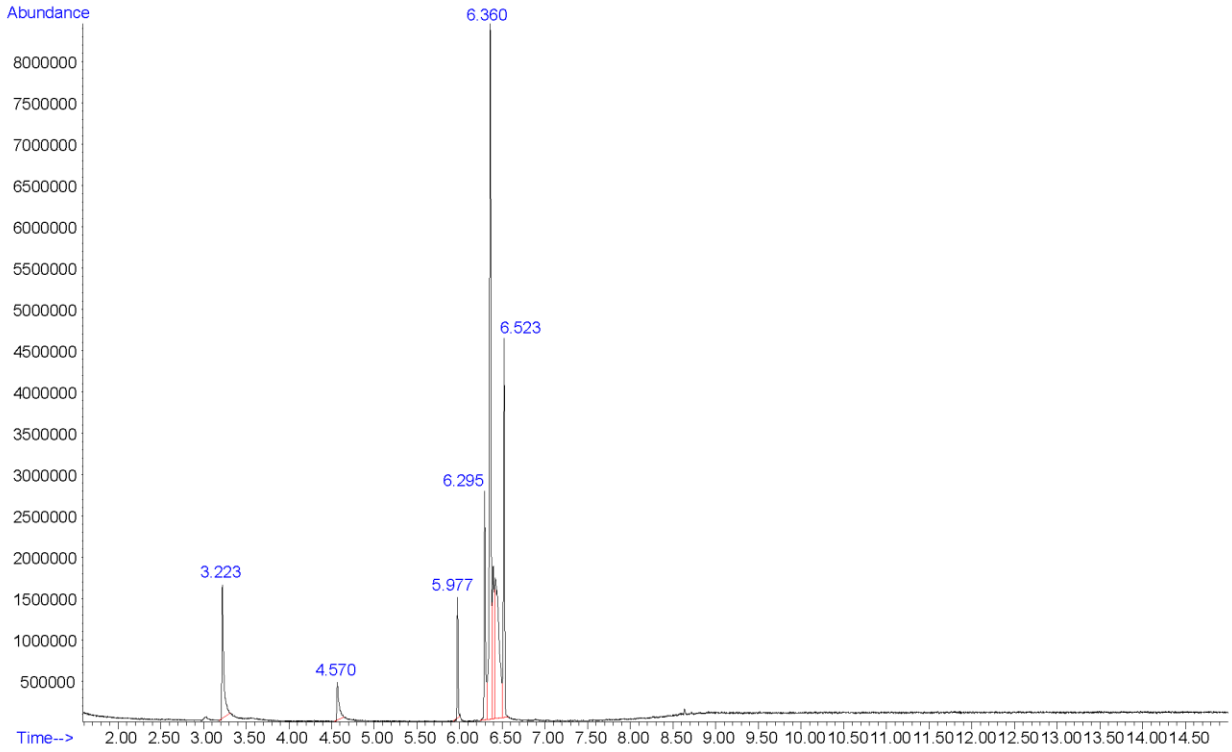
5. U.S. Food & Drug Administration. Drugs@FDA: FDA Approved Drug Products. https://www.accessdata.fda.gov/scripts/cder/daf/

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

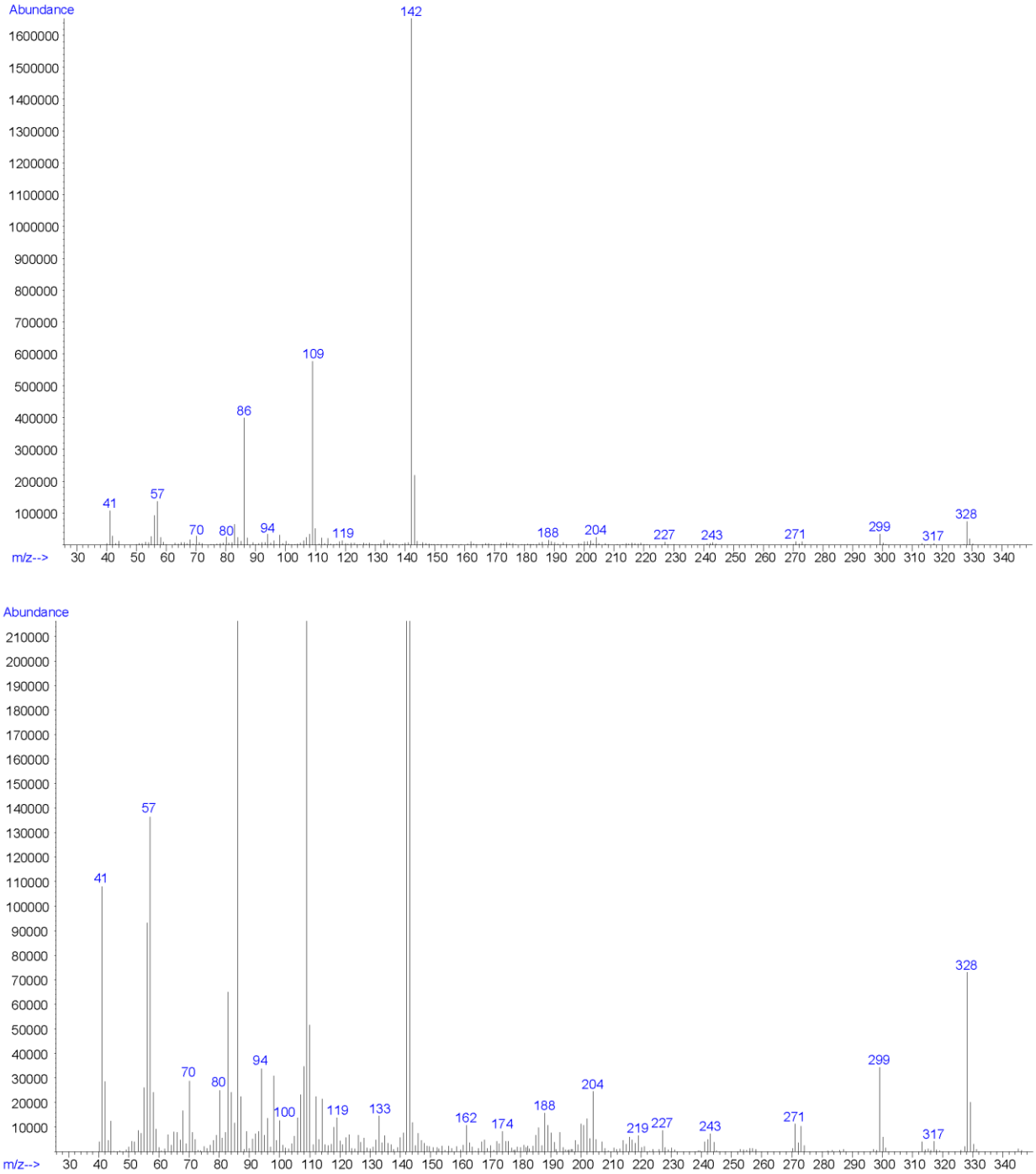
Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 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:	6.523 min

Chromatogram: 2F-Viminol



Additional peaks present in chromatogram: internal standard (3.223 min), not a controlled substance (4.570 min), suspected breakdown product (5.977 min), internal standard (6.295 min), suspected breakdown product (6.360 min)

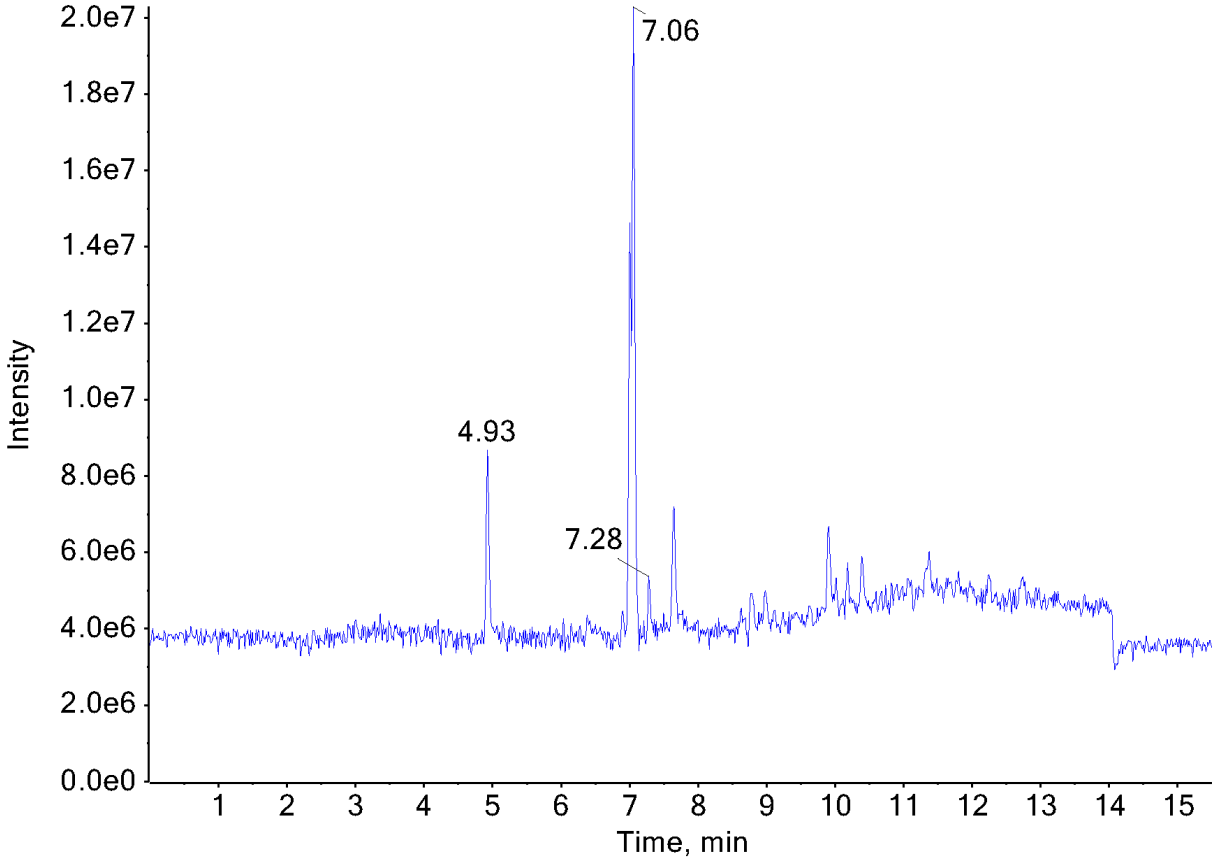
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 2F-Viminol



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

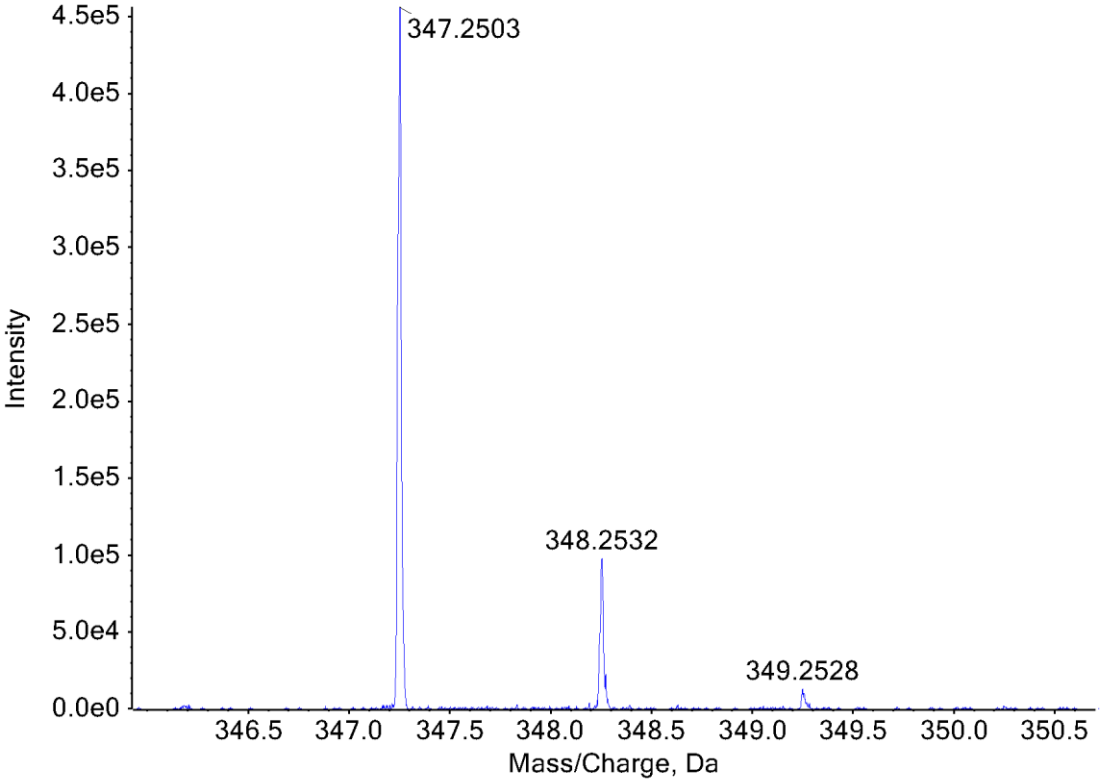
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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:	7.06 min

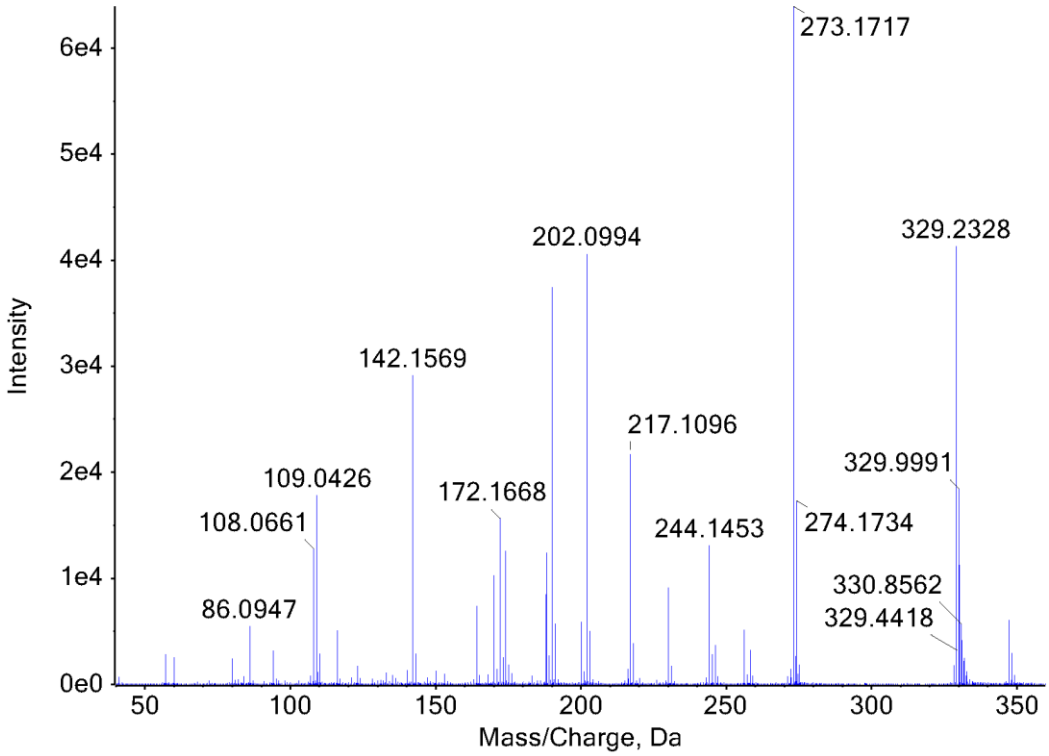
Chromatogram: 2F-Viminol



Additional peaks present in chromatogram: internal standards (4.93 min and 7.28 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 2F-Viminol





5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in DMSO-D6

Instrument: 300 MHz INOVA VARIAN Spectrometer

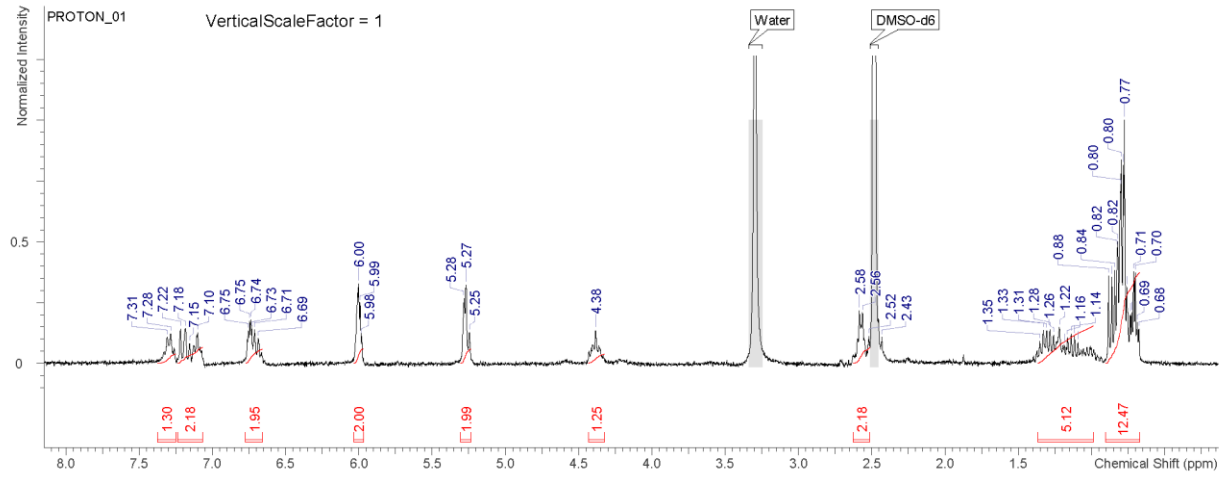
Parameters: Pulse Sequence: Proton

Solvent: DMSO-D6

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: 2F-Viminol



6. REVISION HISTORY

Date	Revision
12/4/2019	GC-MS data (mass spectra) were revised due to the discovery of breakdown