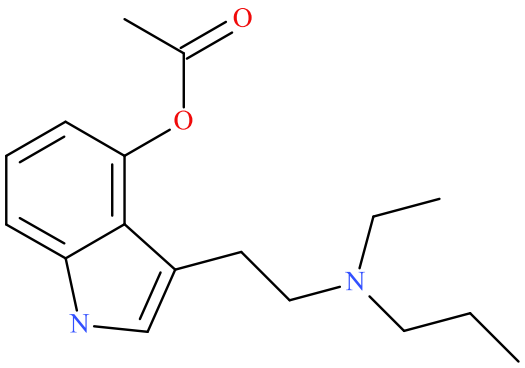
4-AcO-EPT



Sample Type: **Seized Material**

Latest Revision: **June 29, 2021**

Date Received: **March 3, 2021**

Date of Report: **June 29, 2021**

1. GENERAL INFORMATION

IUPAC Name:	[3-[2-[ethyl(propyl)amino]ethyl]-1H-indol-4-yl] acetate
InChI String:	InChI=1S/C17H24N2O2/c1-4-10-19(5-2)11-9-14-12-18-15-7-6-8-16(17(14)15)21-13(3)20/h6-8,12,18H,4-5,9-11H2,1-3H3
CFR:	Not Scheduled (06/2021)
CAS#	Not Available
Synonyms:	4-Acetoxy EPT, 4-acetoxy-N-ethyl-N-propyltryptamine
Source:	NMS Labs – Criminalistic Laboratory
Appearance:	Tan Solid Material

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF-MS, and NMR).*

***Prepared By:** Alex J. Krotulski, PhD; Krystal T Byrd, MSFS; Sarah A. Shuda, MFSF, F-ABC; Melissa F. Fogarty, MSFS, D-ABFT-FT; Sarah E. Decker, BA; 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	$C_{17}H_{24}N_2O_2$	288.4	288	289.1911

3. BRIEF DESCRIPTION

4-AcO-EPT is classified as a novel tryptamine analogue. Tryptamine analogues are modified based on the structure of tryptamine. Tryptamine analogues have been reported to cause hallucinogenic effects, often associated with "psychedelic mushrooms." Tryptamine analogues have caused adverse events, including agitation, tachyarrhythmias, hyperpyrexia, and death, as described in the literature. Structurally similar compounds include psilocin, 4-HO-EPT, and 4-AcO-DPT, among several other tryptamine analogues. Psilocin is a Schedule I substance in the United States.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4-AcO-EPT-ID-2112-19_report.pdf

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)

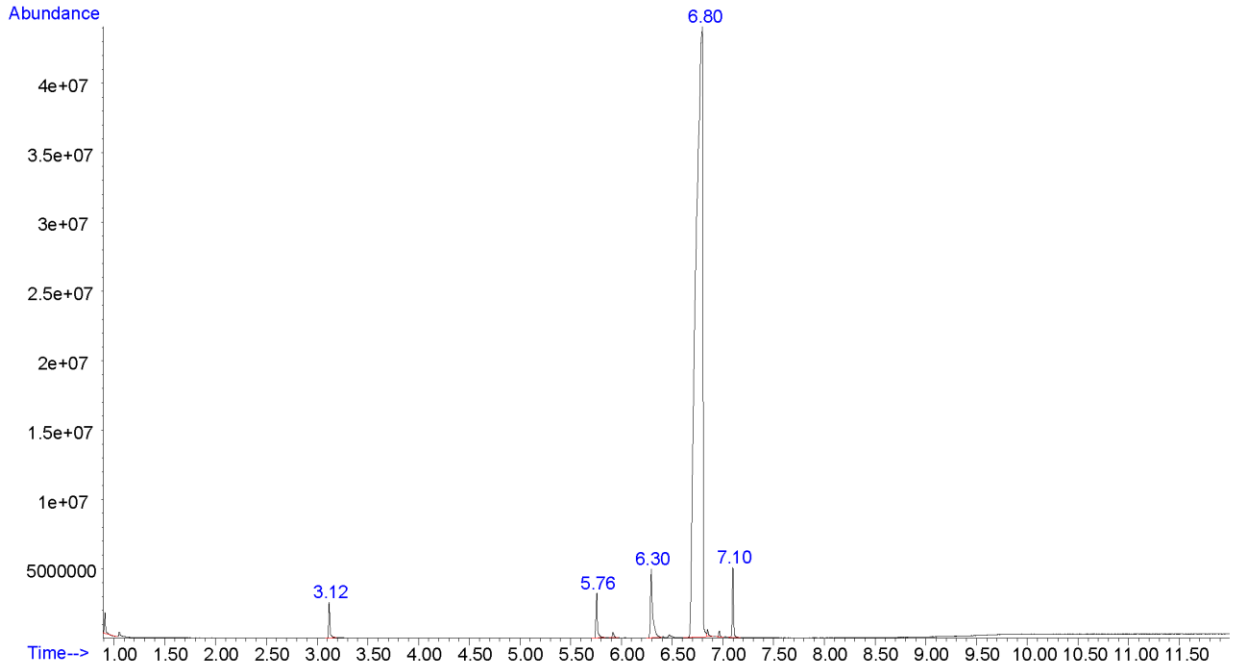
Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

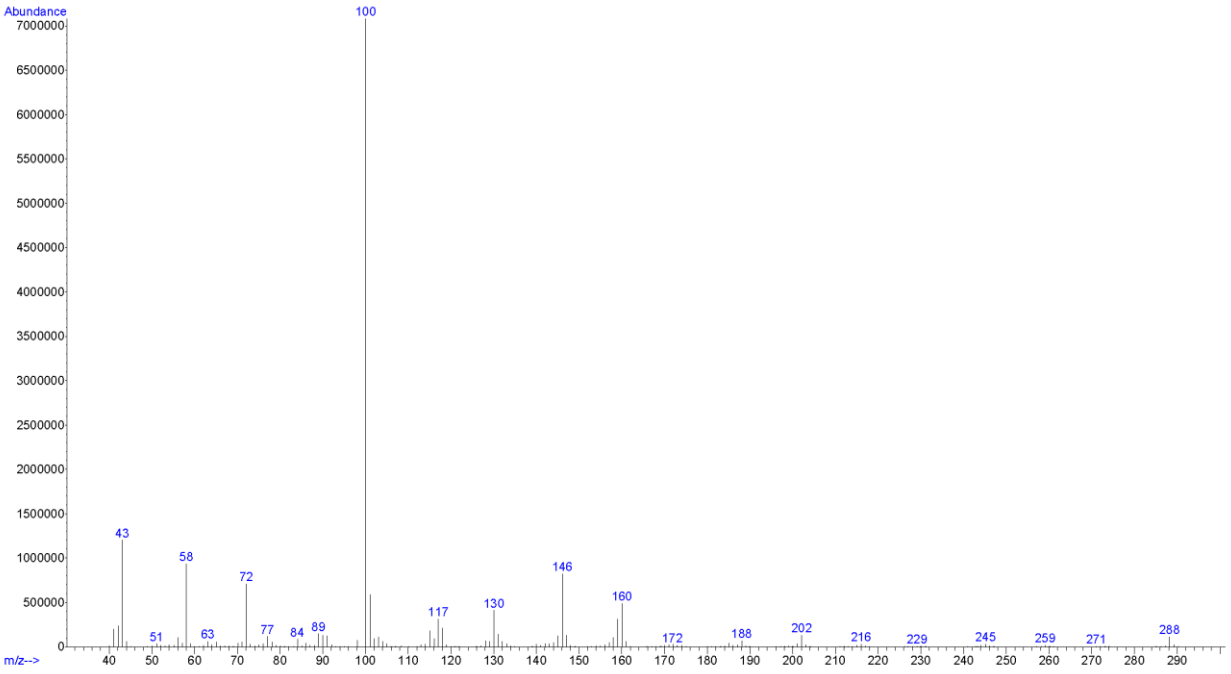
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	6.80 min

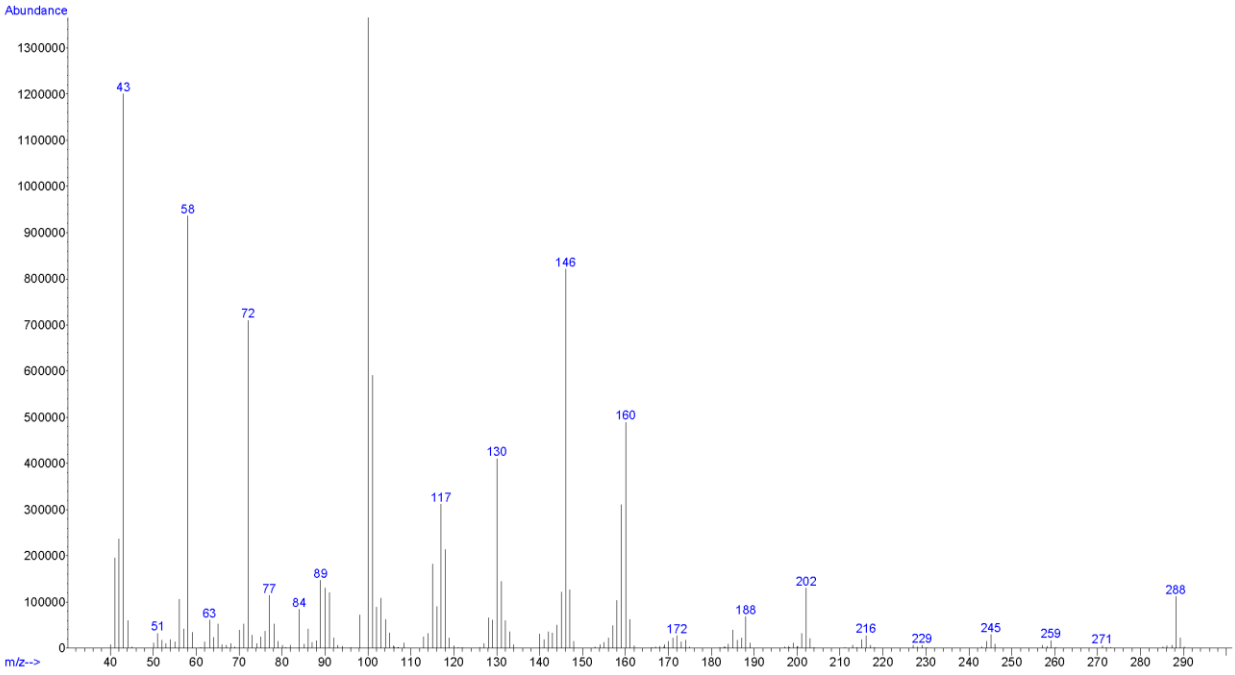
Chromatogram: 4-AcO-EPT



Additional peaks present in chromatogram: internal standard (3.12 min), not a controlled substance (5.76 min), internal standard (6.30 min) and not a controlled substance (7.10 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4-AcO-EPT

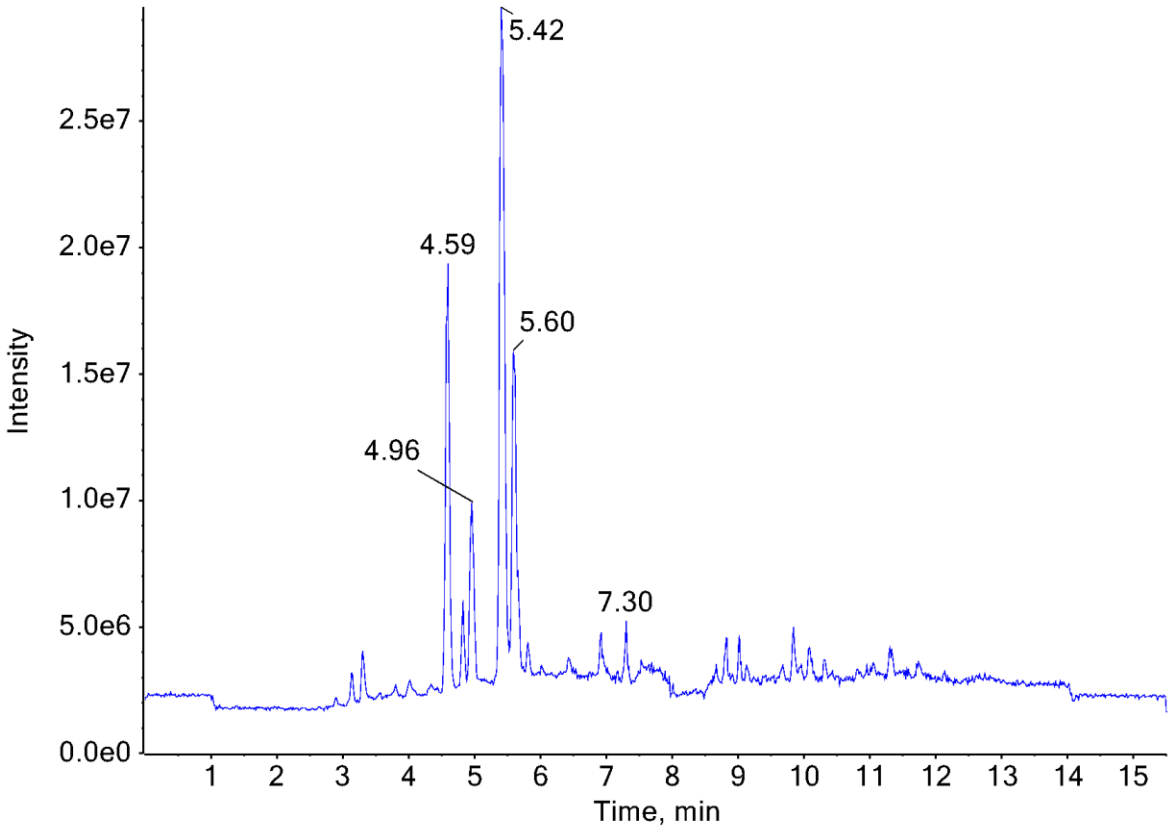




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

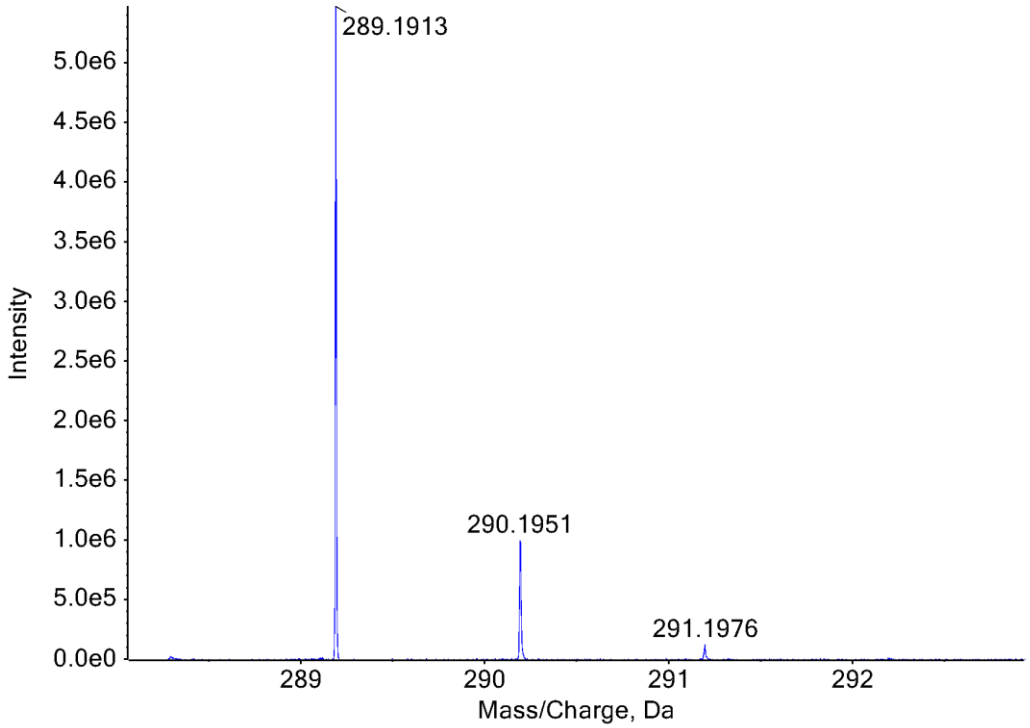
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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:	5.42 min

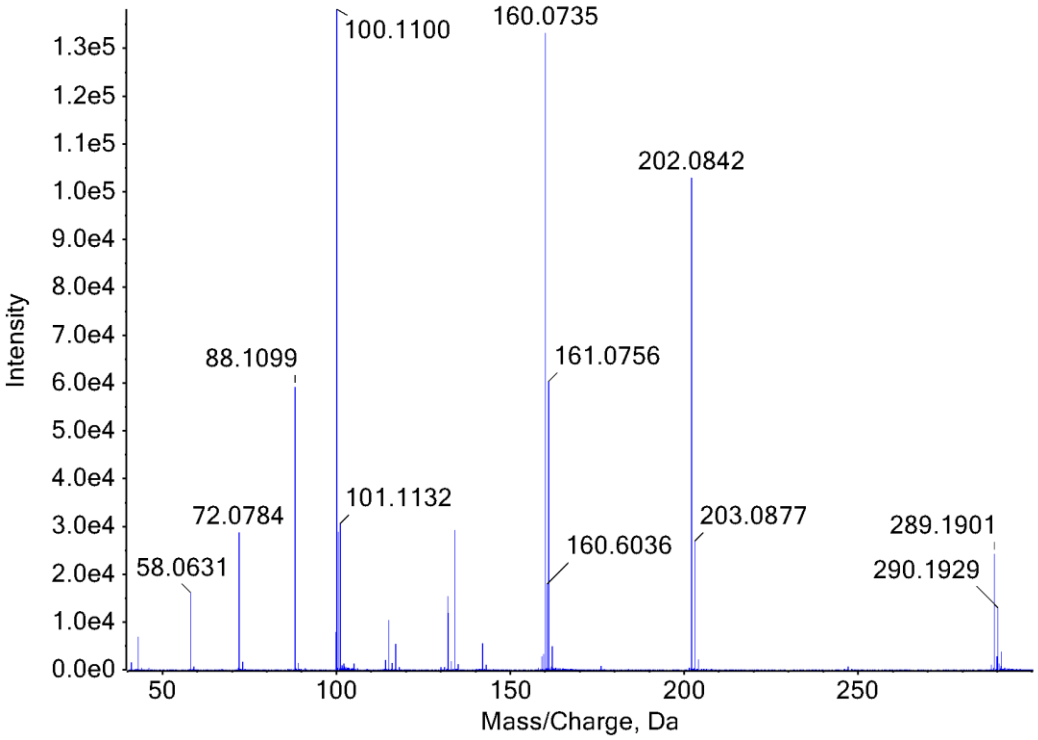
Chromatogram: 4-AcO-EPT



Additional peaks present in chromatogram: not a controlled substance (4.59 min), internal standard (4.96 min), not a controlled substance (5.60 min), and internal standard (7.30 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 4-AcO-EPT





5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in $CDCl_3$

Instrument: 300 MHz INOVA VARIAN Spectrometer

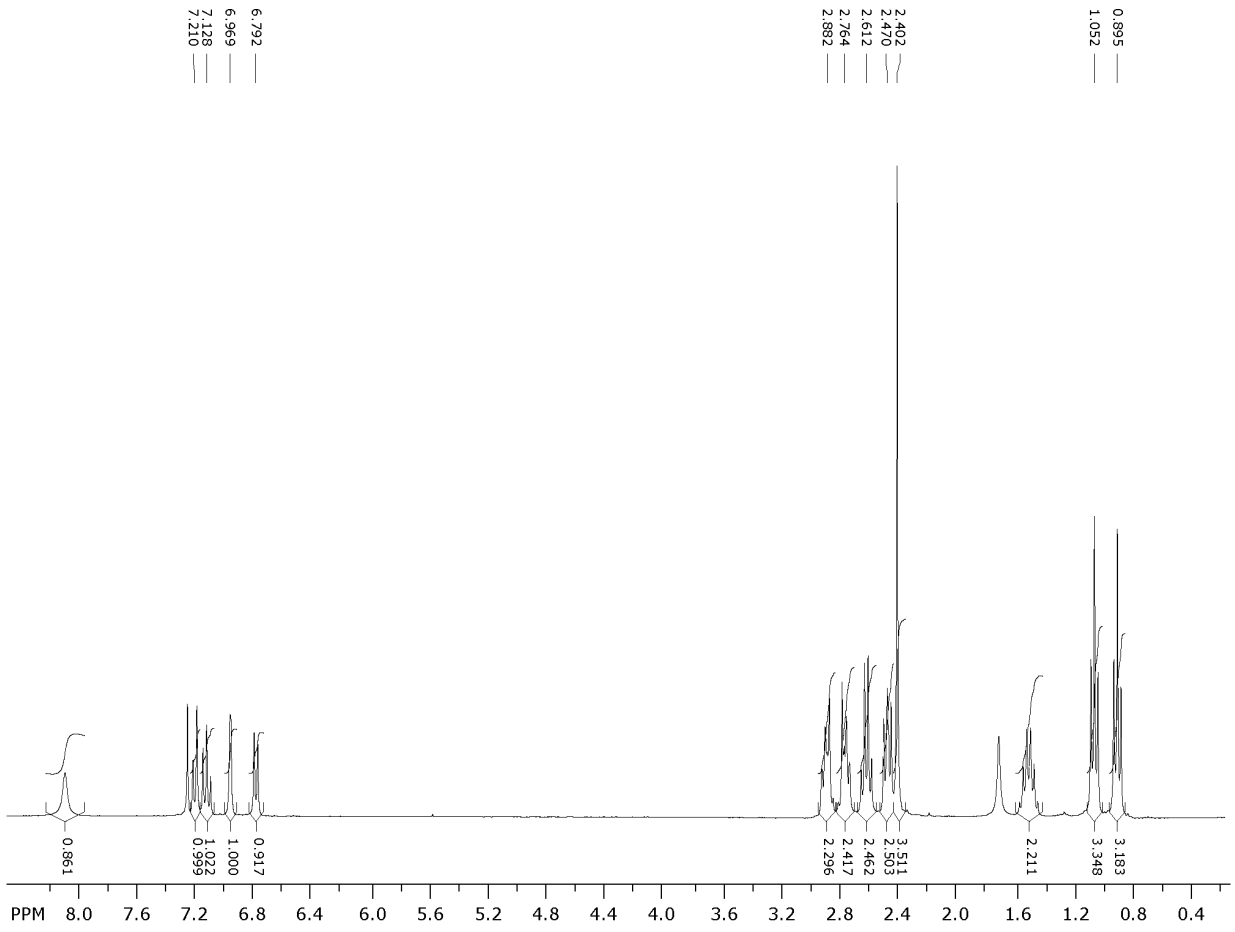
Parameters: Pulse Sequence: Proton

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: 4-AcO-EPT



6. FUNDING

NPS Discovery at the Center for Forensic Science Research and Education (CFSRE) is supported in part by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 2020-DQ-BX-0007, “Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS)”). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect those of the Department of Justice.