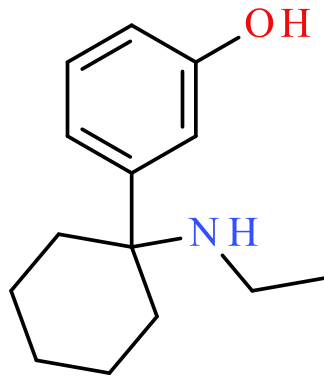


3-HO-PCE

Sample Type: **Seized Material**



Latest Revision: **December 12, 2019**

Date Received: **October 3, 2019**

Date of Report: **December 12, 2019**

1. GENERAL INFORMATION

IUPAC Name:	3-[1-(ethylamino)cyclohexyl]phenol
InChI String:	InChI=1S/C14H21NO/c1-2-15-14(9-4-3-5-10-14)12-7-6-8-13(16)11-12/h6-8,11,15-16H,2-5,9-10H2,1H3
CFR:	Not Scheduled (12/2019)
CAS#	Not Available
Synonyms:	3-Hydroxy PCE, 3-OH-PCE, 3-Hydroxyeticyclidine
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-MS, and NMR).

Prepared By: Alex J. Krotulski, PhD, 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 ₁₄ H ₂₁ NO	219.3	219	220.1696

3. BRIEF DESCRIPTION

3-HO-PCE is classified as a novel hallucinogen. Novel hallucinogens have been reported to cause effects similar to ketamine and phencyclidine (PCP). Novel hallucinogens have caused adverse events, including deaths, as described in the literature. Structurally similar compounds include eticyclidine (PCE) and 3-MeO-PCE. PCE is a Schedule I substance in the United States.

4. ADDITIONAL RESOURCES

[https://www.caymanchem.com/product/26877/3-hydroxy-pce-\(hydrochloride\)](https://www.caymanchem.com/product/26877/3-hydroxy-pce-(hydrochloride))

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/3-HO-PCE-ID-1959-18_report.pdf

<https://psychonautwiki.org/wiki/3-HO-PCE>

<https://isomerdesign.com/PiHKAL/explore.php?id=968>

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: Zebtron™ 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

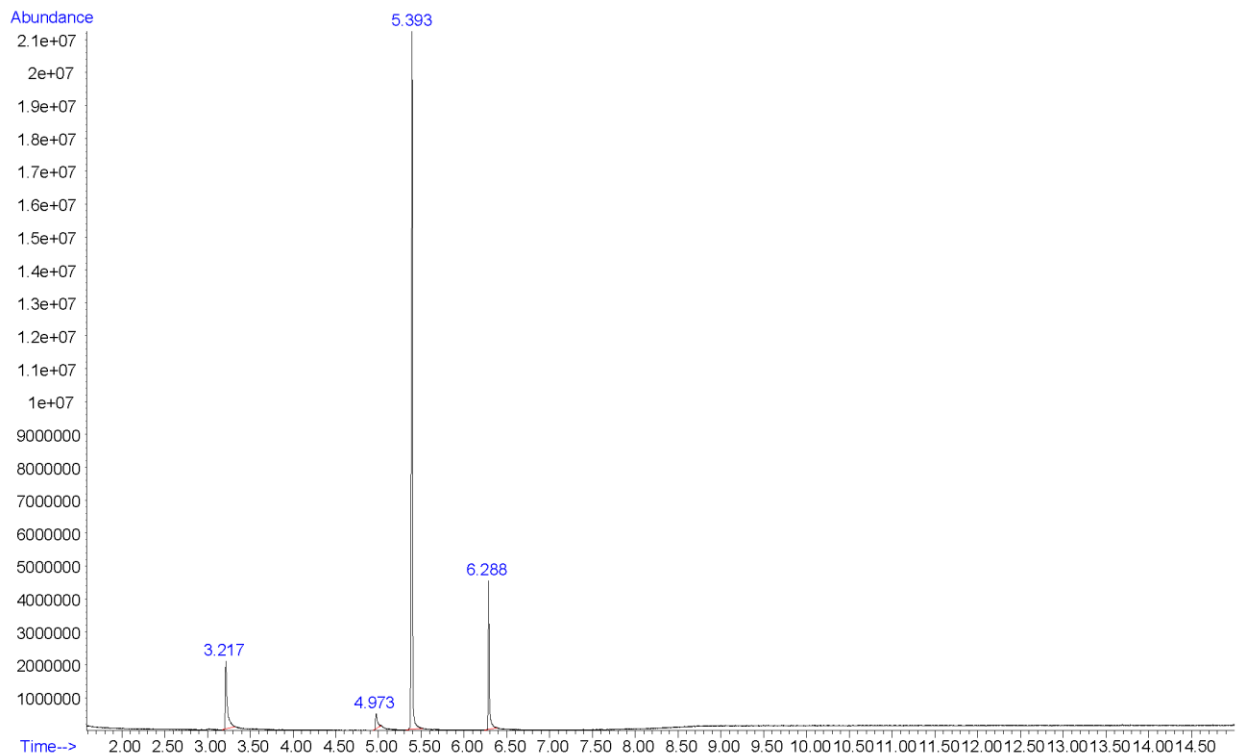
Injection Volume: 1 µL

MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

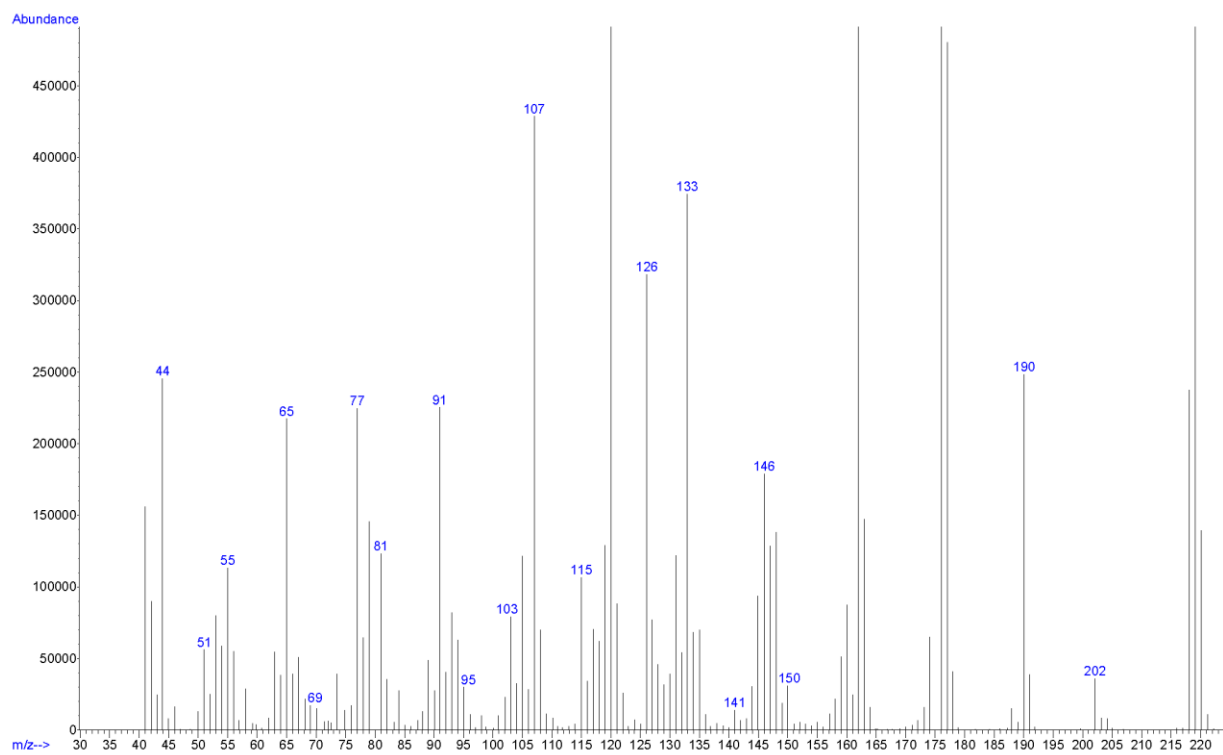
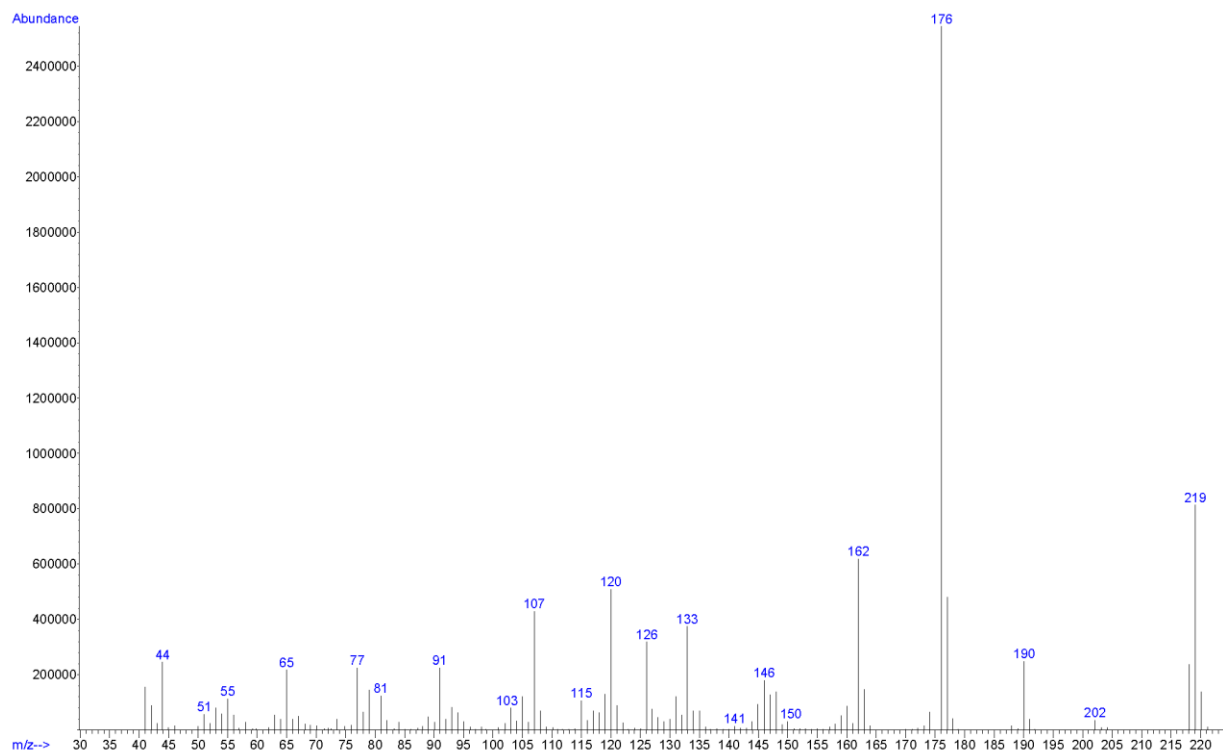
Retention Time: 5.393 min

Chromatogram: 3-HO-PCE



Additional peaks present in chromatogram: internal standard (3.217 min), not a controlled substance (4.973 min), and internal standard (6.288 min)

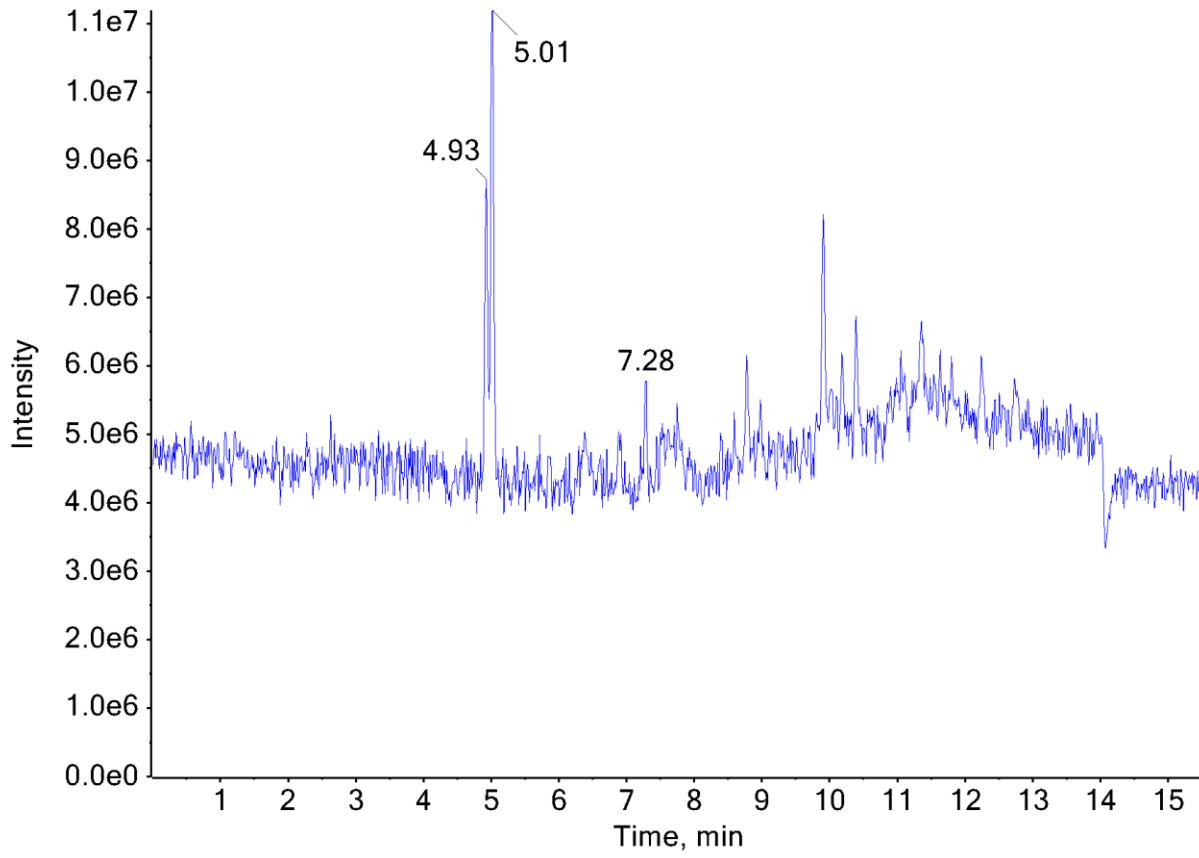
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 3-HO-PCE



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

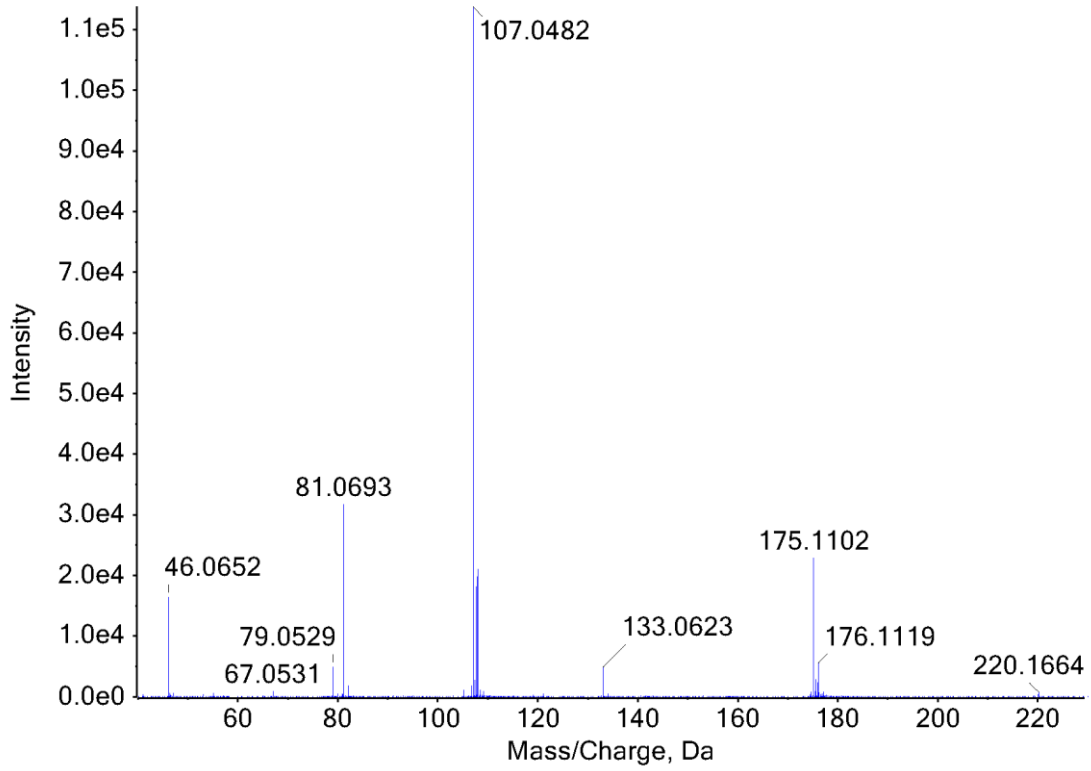
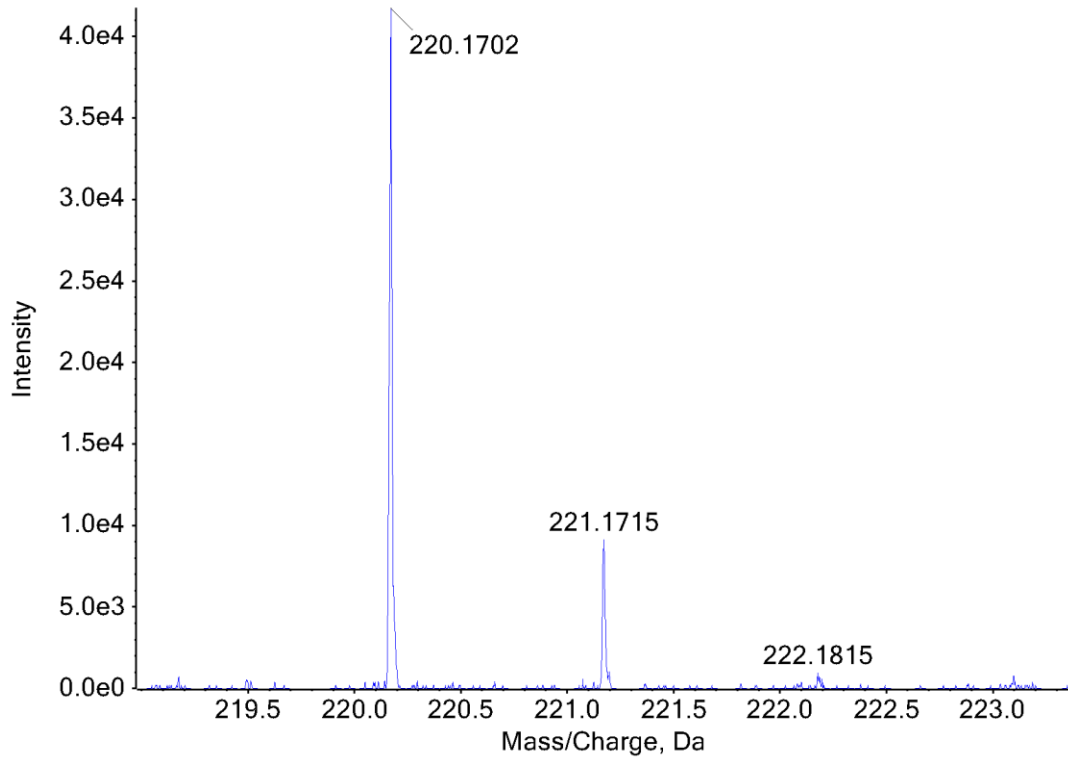
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	5.01 min

Chromatogram: 3-HO-PCE



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

TOF MS (Top) and MS/MS (Bottom) Spectra: 3-HO-PCE



5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in CD₃OD

Instrument: 600 MHz Bruker AVANCE™ III Spectrometer

Parameters: Pulse Sequence: Proton

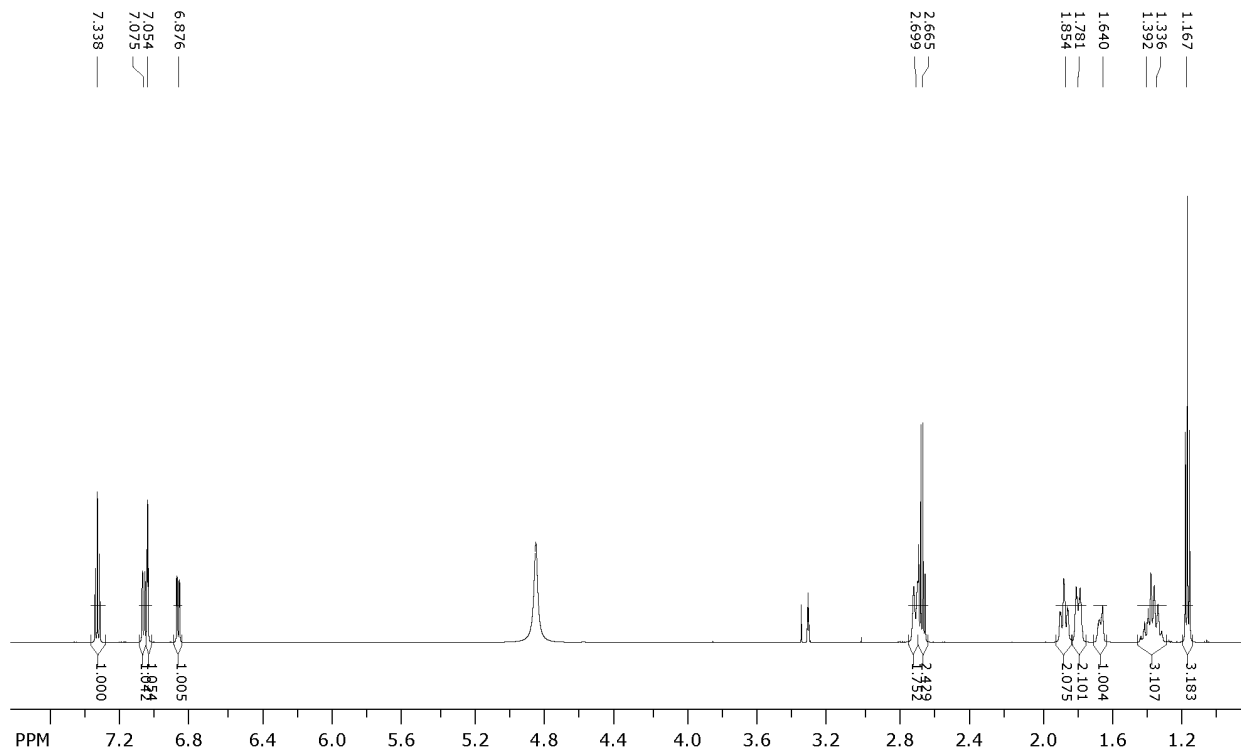
Solvent: CD₃OD

Spectral Width: 12019.23 Hz = 20.0276 ppm = 0.183399 Hz/pt for ¹H; 5733.9 Hz, 2484.9 Hz offset, 2048 pts for HMBC; 5733.9 Hz, 2484.9 Hz offset, 1024 pts for HSQC; 5733.9 Hz, 2484.9 Hz offset, 1536 pts for COSY

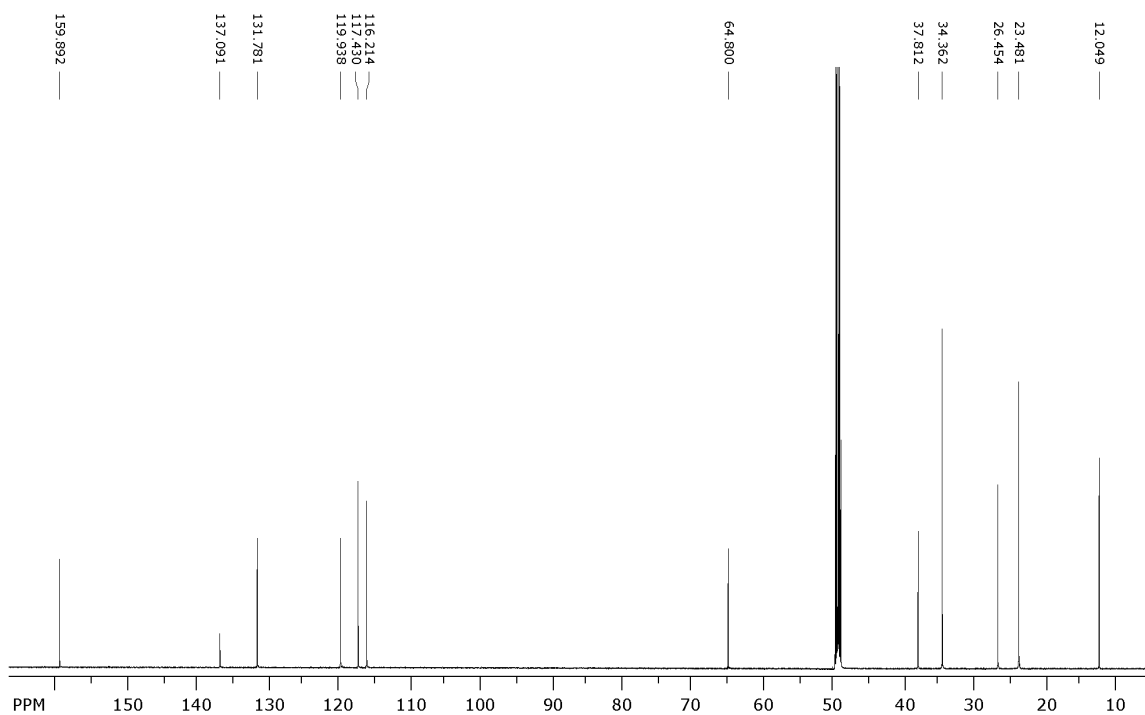
Number of Scans: 8

Delay Between Pulses: 1.000 second for ¹H, 2.000 seconds for ¹³C

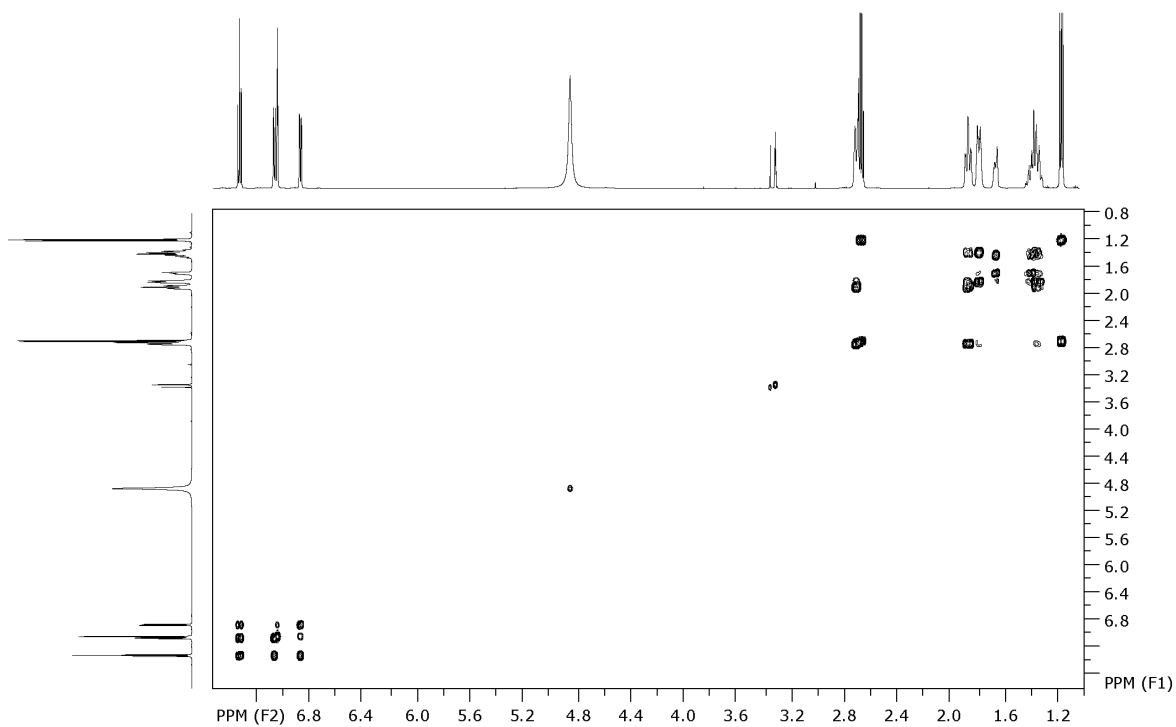
¹H NMR: 3-HO-PCE



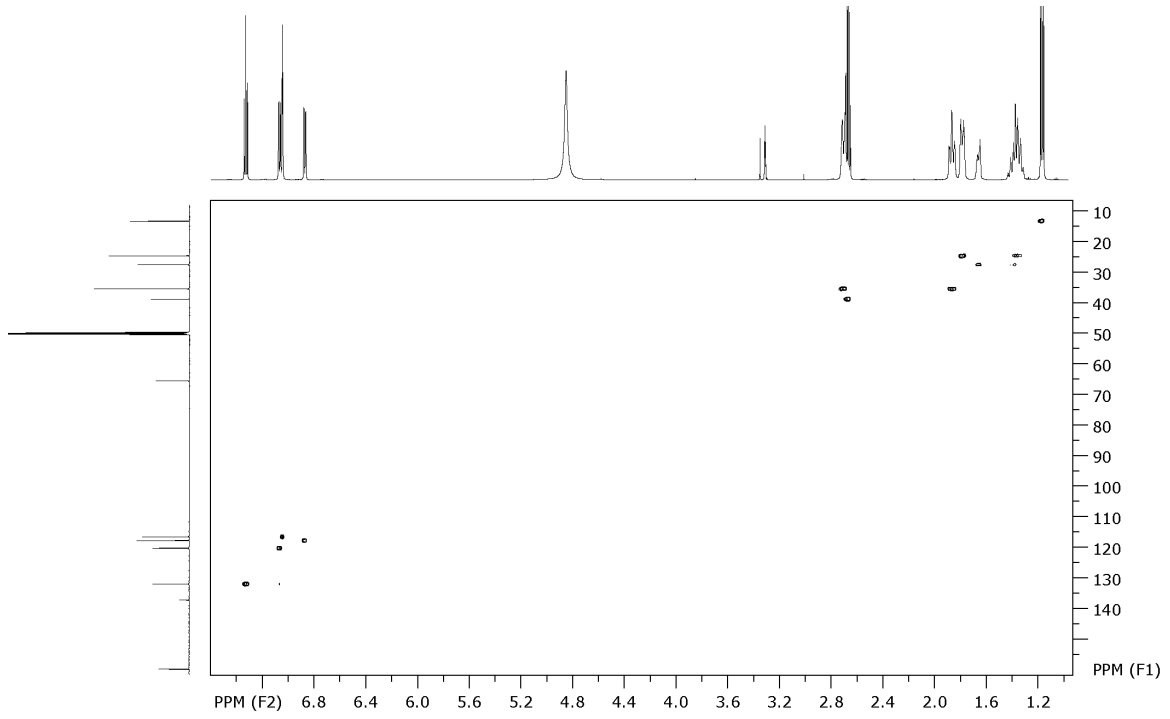
¹³C NMR: 3-HO-PCE



COSY NMR: 3-HO-PCE



HSQC NMR: 3-HO-PCE



HMBC NMR: 3-HO-PCE

