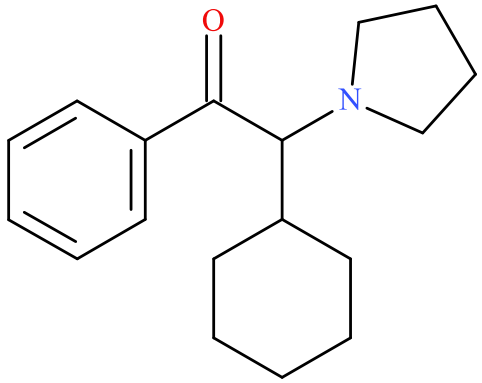
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

alpha-PCYP

Sample Type: **Seized Material**



Latest Revision: **May 27, 2020**

Date Received: **March 3, 2019**

Date of Report: **May 27, 2020**

1. GENERAL INFORMATION

IUPAC Name:	2-cyclohexyl-1-phenyl-2-pyrrolidin-1-yl-ethanone
InChI String:	InChI=1S/C18H25NO/c20-18(16-11-5-2-6-12-16)17(19-13-7-8-14-19)15-9-3-1-4-10-15/h2,5-6,11-12,15,17H,1,3-4,7-10,13-14H2
CFR:	Not Scheduled (05/2020)
CAS#	1803168-16-2
Synonyms:	α-PCYP, alpha-Pyrrolidinocyclohexylphenone, alpha-Pyrrolidinocyclohexanophenone
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	$C_{18}H_{25}NO$	271.4	271	272.2009

3. BRIEF DESCRIPTION

Alpha-PCYP is classified as a novel stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause stimulant-like effects, similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include alpha-pyrrolidinopentiophenone (alpha-PVP), alpha-pyrrolidinobutiophenone (alpha-PBP), alpha-pyrrolidinohexanophenone (alpha-PHP), and alpha-pyrrolidinoisohexanophenone (alpha-PiHP). Alpha-PVP, alpha-PHP, and alpha-PBP are Schedule I substances in the United States; alpha-PCYP is not explicitly scheduled. The potency of alpha-PCYP was previously studied alongside similar pyrrolidine cathinone analogues, in which alpha-PCYP was found to be twice as potent as alpha-PVP.[1]

4. ADDITIONAL RESOURCES

1. Kolanos R, Sakloth F, Jain AD, Partilla JS, Baumann MH, Glennon RA. (2015) "Structural Modification of the Designer Stimulant α-Pyrrolidinovalerophenone (α-PVP) Influences Potency at Dopamine Transporters". *ACS Chemical Neuroscience*. **6** (10): 1726–31.

https://www.caymanchem.com/product/30241/%CE%B1-pyrrolidinocyclohexanophenone-(hydrochloride)

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

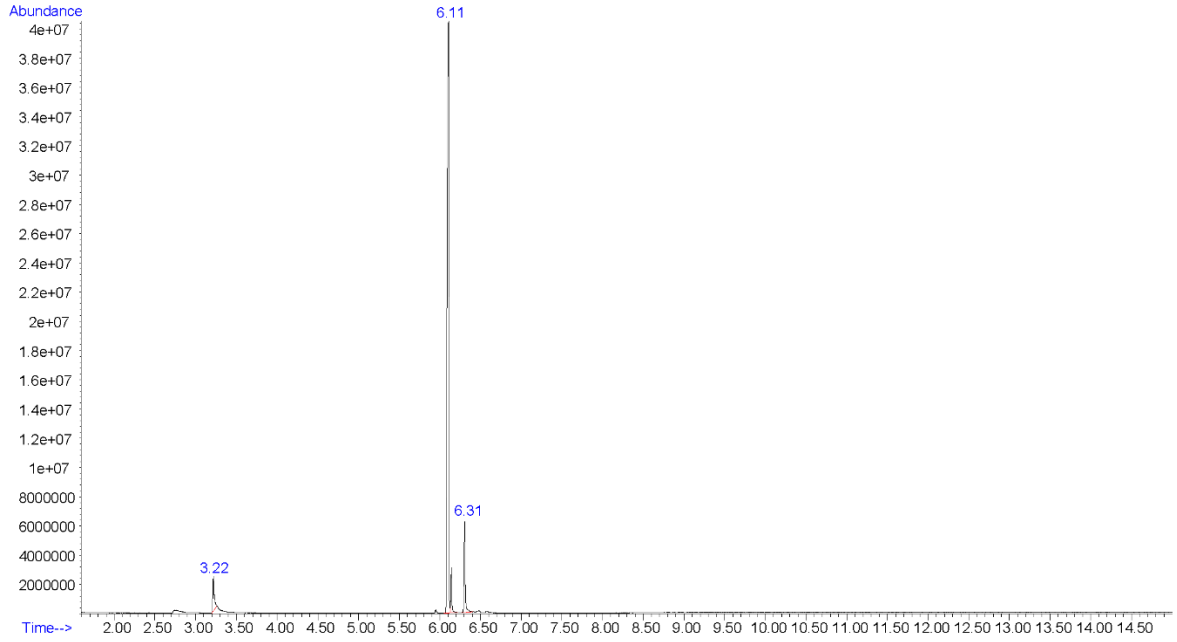
Sample Preparation: Acid/Base extraction

Instrument: Agilent 5975 Series GC/MSD System

Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)

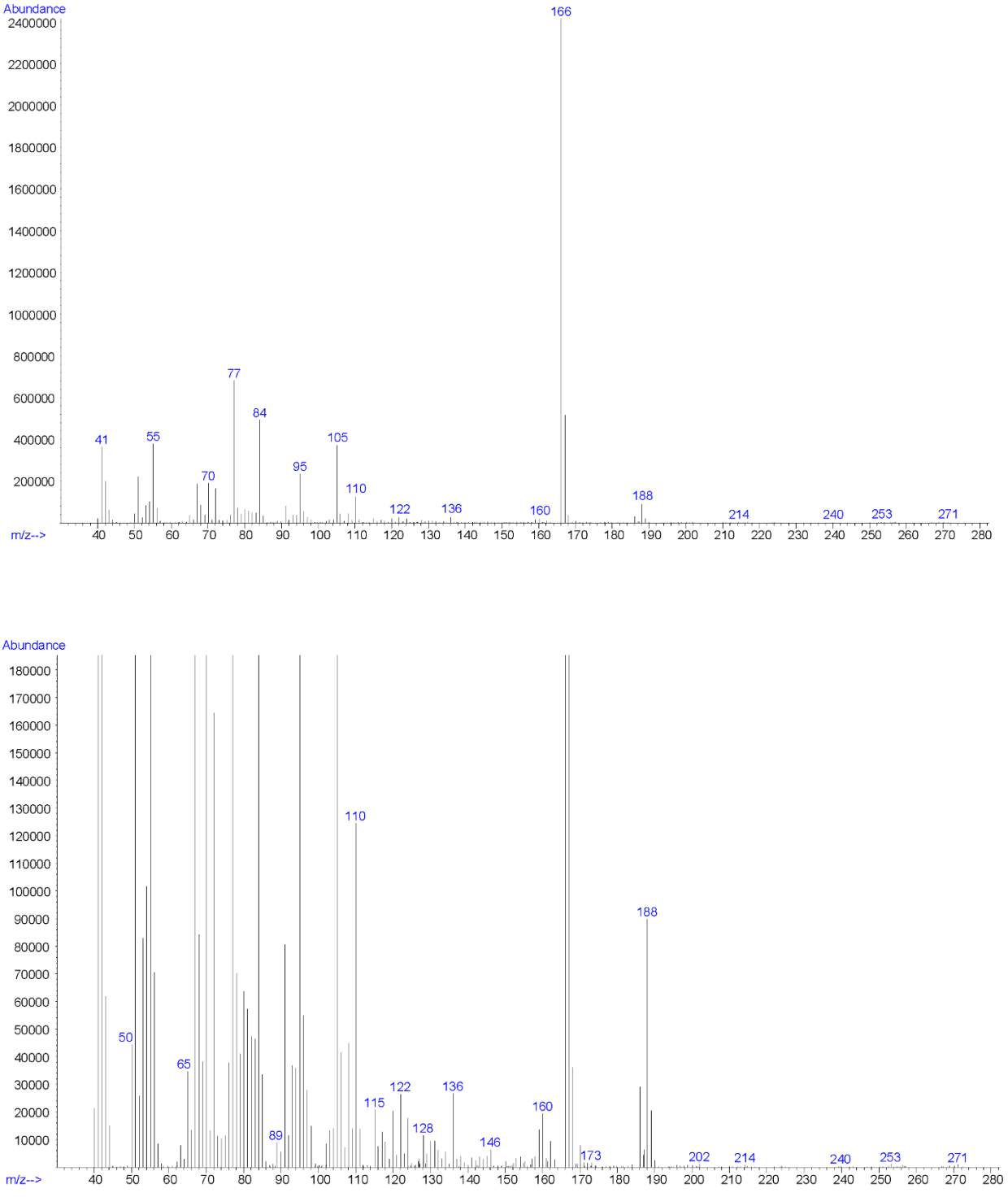
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	6.11 min

Chromatogram: Alpha-PCYP



Additional peaks present in chromatogram: internal standard (3.22 min) and internal standard (6.31 min)

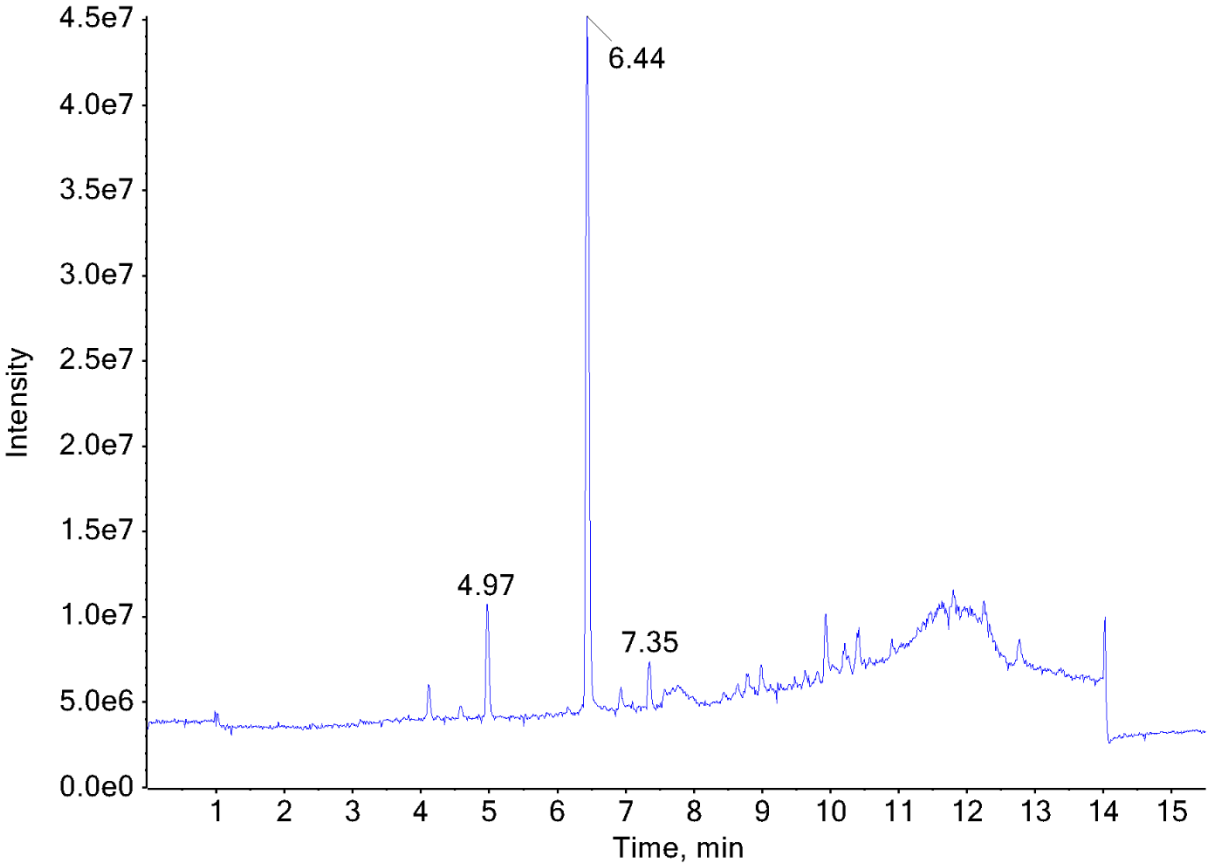
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Alpha-PCYP



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

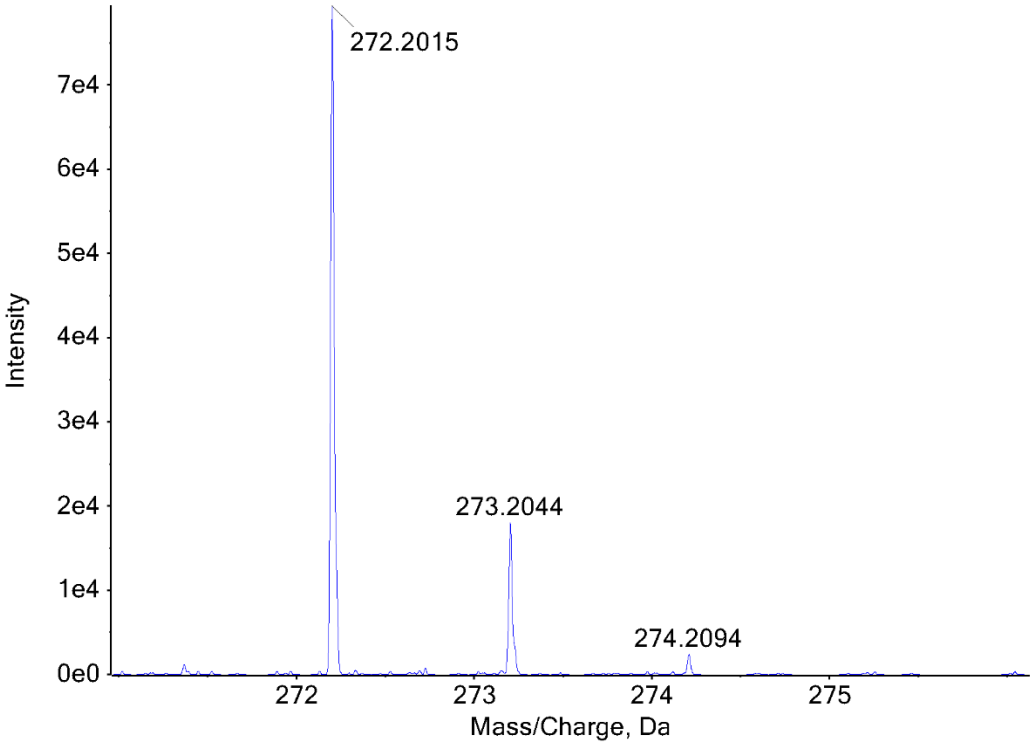
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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:	6.44 min

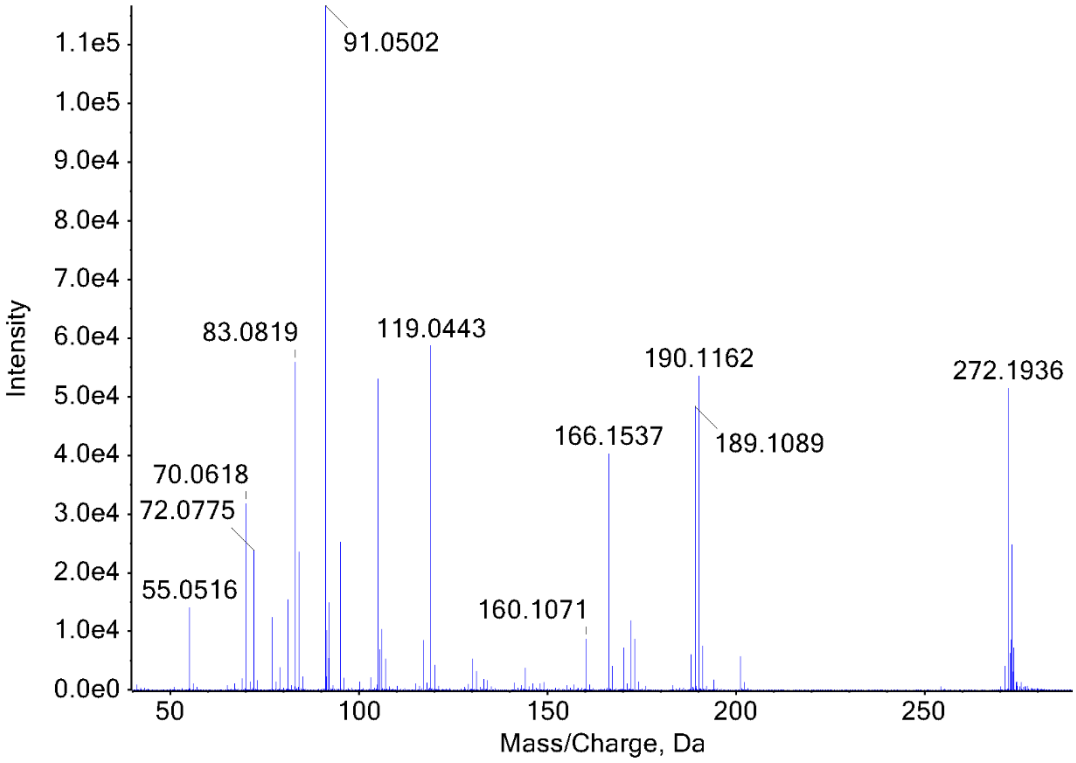
Chromatogram: Alpha-PCYP



Additional peaks present in chromatogram: internal standards (4.97 min and 7.35 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Alpha-PCYP





5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in $CDCl_3$

Instrument: 600 MHz Bruker AVANCE™ III Spectrometer

Parameters: Pulse Sequence: Proton

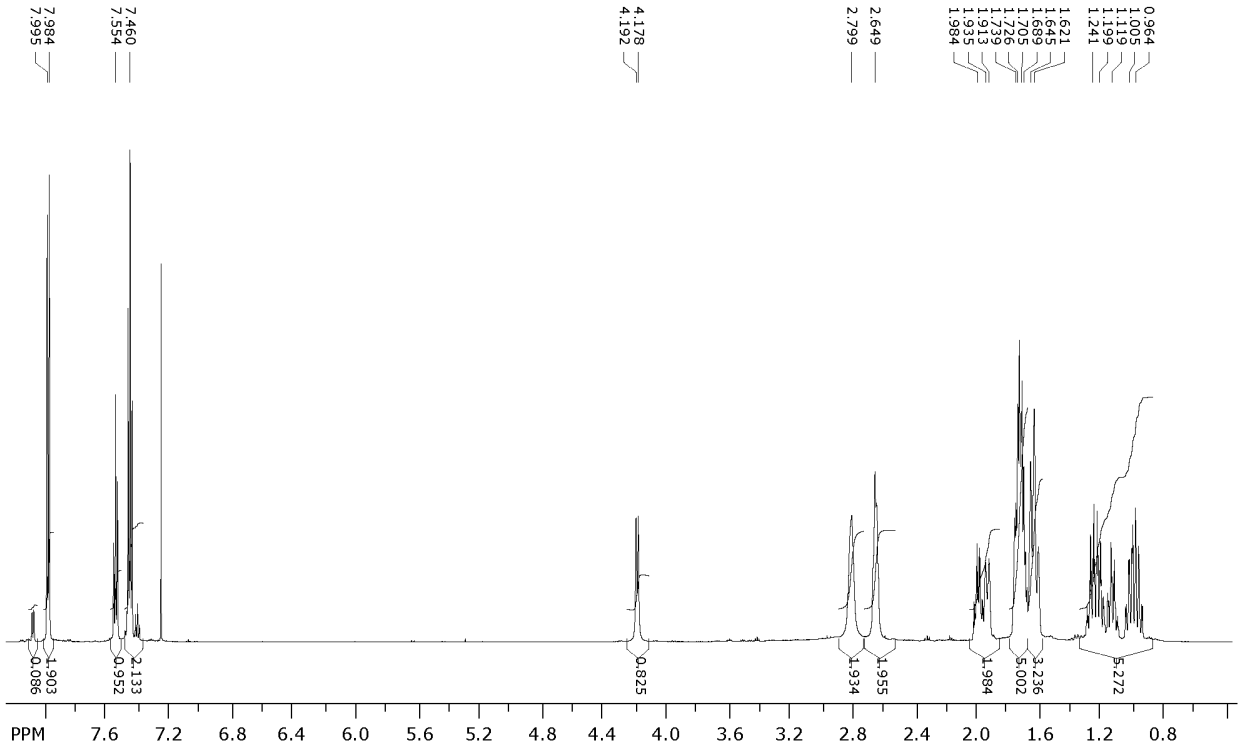
Solvent: $CDCl_3$

Spectral Width: 12019.23 Hz = 20.0276 ppm = 0.183399 Hz/pt for ^{1}H; 36231.88 Hz = 240.0768 ppm = 0.552855 Hz/pt for ^{13}C; 5980.86 Hz = 9.9659 ppm = 2.9203 Hz/pt for COSY; 5980.86 Hz = 9.9659 ppm = 2.9203 Hz/pt for HSQC; 5980.86 Hz = 9.9659 ppm = 1.9469 Hz/pt for HSQC

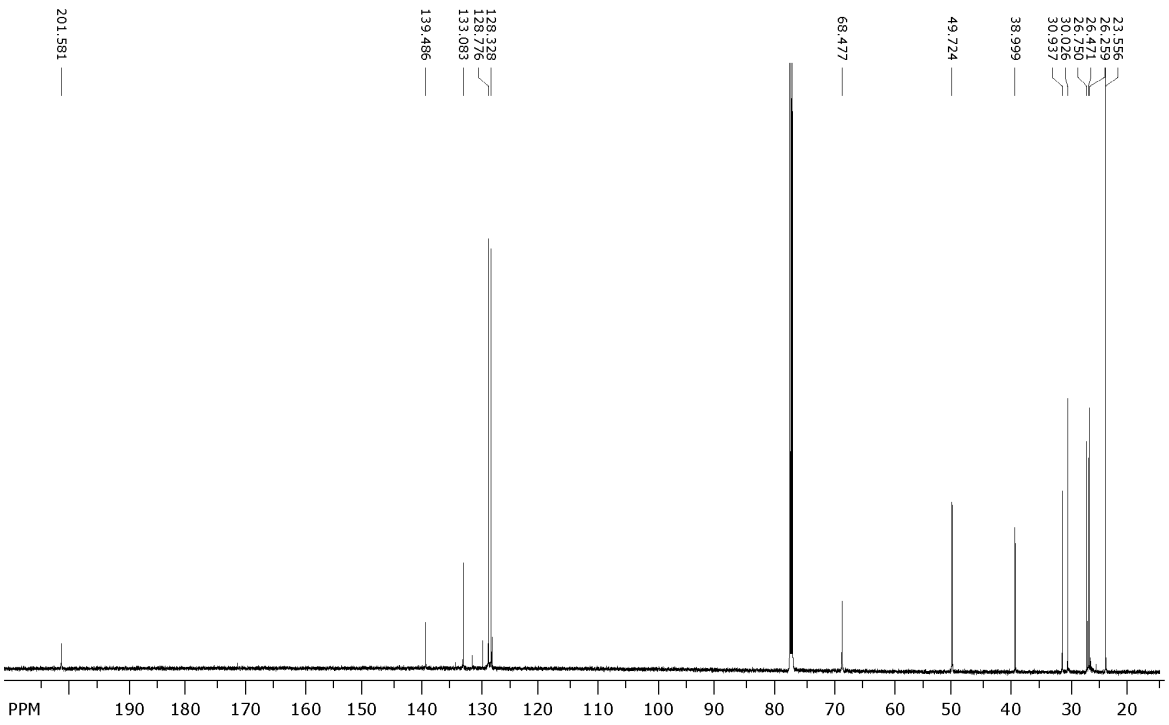
Number of Scans: 16 for ^{1}H; 256 for ^{13}C; 2 for COSY; 4 for HSQC; 10 for HMBC

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

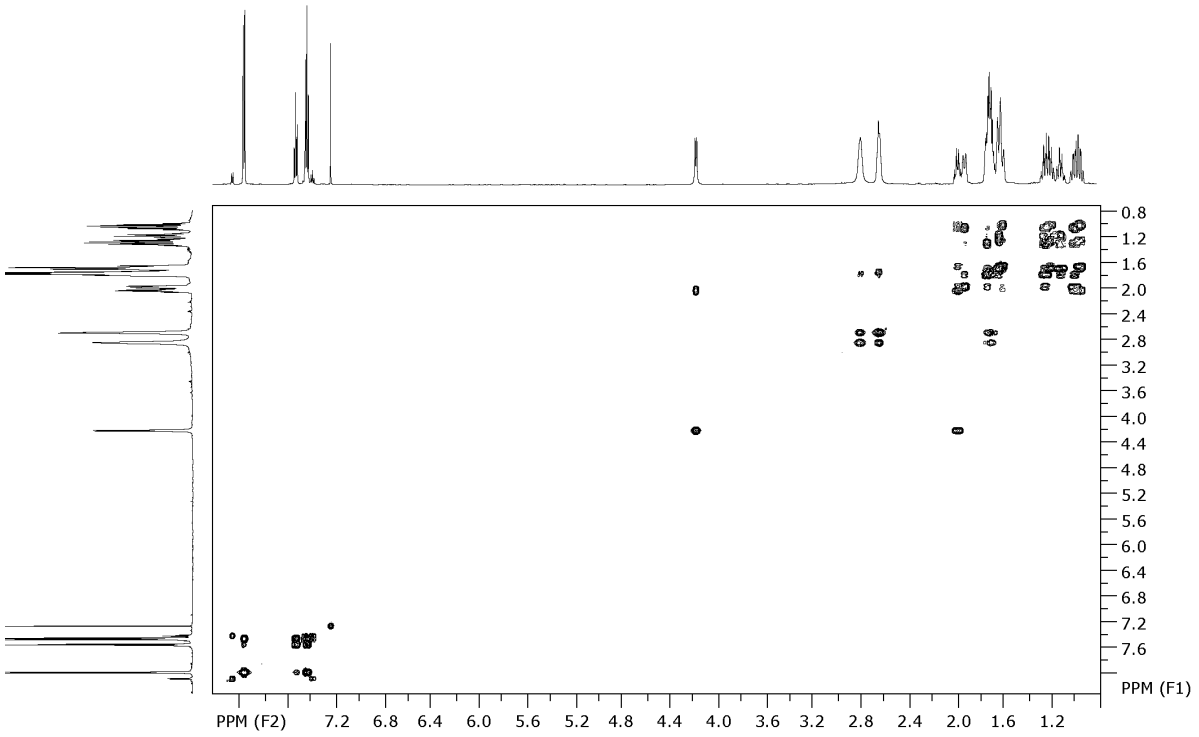
^{1}H NMR: Alpha-PCYP



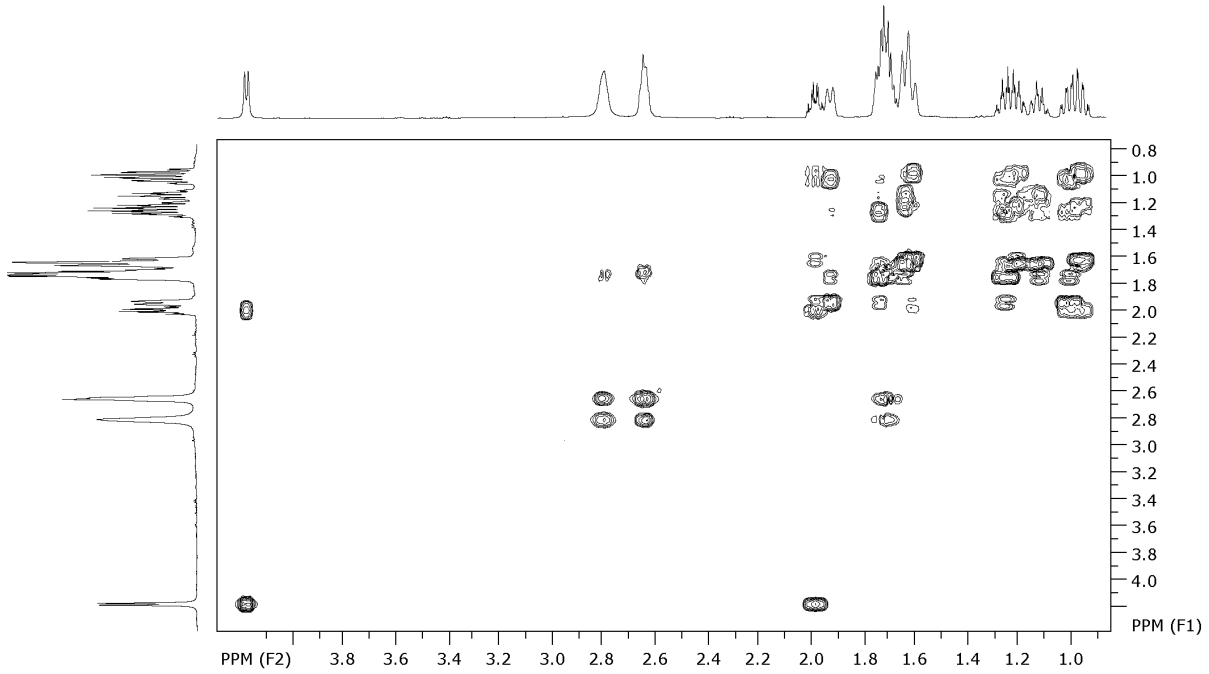
^{13}C NMR: Alpha-PCYP



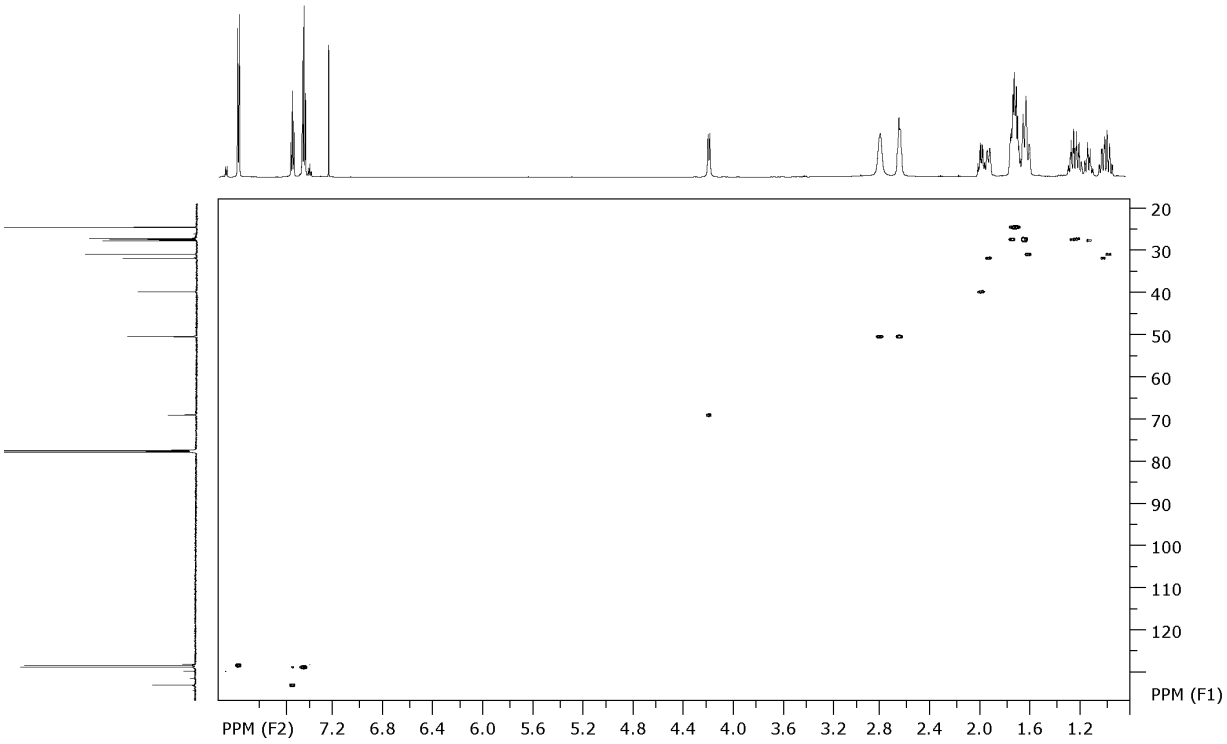
COSY NMR: Alpha-PCYP



COSY NMR (Zoom): Alpha-PCYP



HSQC NMR: Alpha-PCYP



HMBC NMR: Alpha-PCYP