Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Synthesis of Novel Seven-membered Carbasugars and Evaluation of their Glycosidase Inhibition Potential

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Single Crystal X-Ray Diffraction (SCXRD) Data:

Data measurements were done at 298 K on a Bruker-KAPPA APEX II CCD diffractometer with graphite-monochromatized (MoK = 0.71073 Å) radiation. The X-ray data collection was analysed by SMART program (Bruker, version 5.631, 2004). All the data were corrected for Lorentzian, polarization and absorption effects using SAINTPLUS and SADABS programs (Bruker, 2004). SHELXT and SHELXL-2014 were used for structure solution and full matrix least-squares refinement on F^2.

1. Table S1: Crystal data of Compound 15: Compound **15** was crystallised from mixture of methanol:chloroform (1:19, v/v).

CCDC No.	2046641
Empirical formula	$C_{16}H_{34}O_9$
Formula weight	370.43
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C 2
Unit cell dimensions	a = 14.4368(11) Å, b = 4.9452(4) Å, c = 12.9747(10) Å, α = 90°, β = 94.740(4)°, γ = 90°
Volume	923.13(12) $Å^3$
Z	2
Density (calculated)	1.333 g/cm^3
Absorption coefficient	0.108 mm^{-1}
F(000)	404
Crystal size	0.250 x 0.100 x 0.100 mm^3
Theta range for data collection	2.832 to 25.980°.
Index ranges	-17<=h<=17, -5<=k<=6, -
Reflections collected	3993
Independent reflections	1748 [R(int) = 0.1379]
Completeness to theta =	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9886 and 0.9719
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1748 / 2 / 124
Goodness-of-fit on F^2	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0593, wR2 = 0.1522
R indices (all data)	R1 = 0.0663, wR2 = 0.1570
Absolute structure parameter	-2(2)
Largest diff. peak and hole	0.298 and -0.193 $e.Å^{-3}$

2. **Table S2.** Bond angles and torsional angles of the seven-membered ring of compound **15.**

Sequence of atoms taken to calculate bond angle	**Bond angle (°)**	**Sequence of atoms taken to calculate the torsional angle**	**Torsional angle (°)**	**Torsional angles of cycloheptane ring in a twist chair conformation**
C7-C1-C2	110.98	C1-C2-C3-C4	-35.25	-39
C1-C2-C3	119.14	C2-C3-C4-C5	-39.67	-39
C2-C3-C4	118.25	C3-C4-C5-C6	82.85	88
C3-C4-C5	115.19	C4-C5-C6-C7	-73.97	-72
C4-C5-C6	112.78	C5-C6-C7-C1	61.28	54
C5-C6-C7	116.43	C6-C7-C1-C2	-73.11	-72
C6-C7-C1	114.49	C7-C1-C2-C3	82.55	88

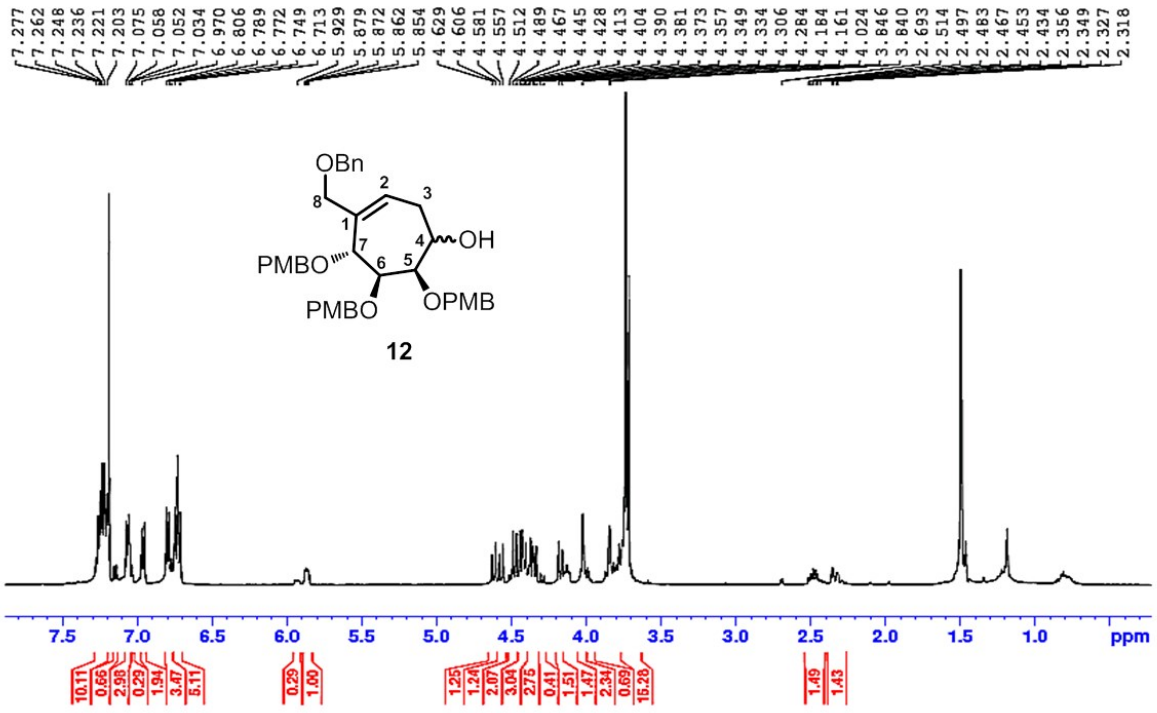
3. Table S3. Crystal Data of Compound 23: Compound **23** was crystallised from a solution of 2% methanol/ethylacetate.

CCDC No.	2046642
Empirical formula	$C_{15}H_{22}O_6$
Formula weight	298.32
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21
Unit cell dimensions	a = 4.7565(2) Å, b = 25.9753(13) Å, c = 6.1401(3) Å, α= 90°, β= 94.072(3)°, γ= 90°
Volume	756.70(6) $Å^3$
Z	2
Density (calculated)	1.309 g/cm^3
Absorption coefficient	0.101 mm^{-1}
F(000)	320
Crystal size	0.200 x 0.150 x 0.150 mm^3

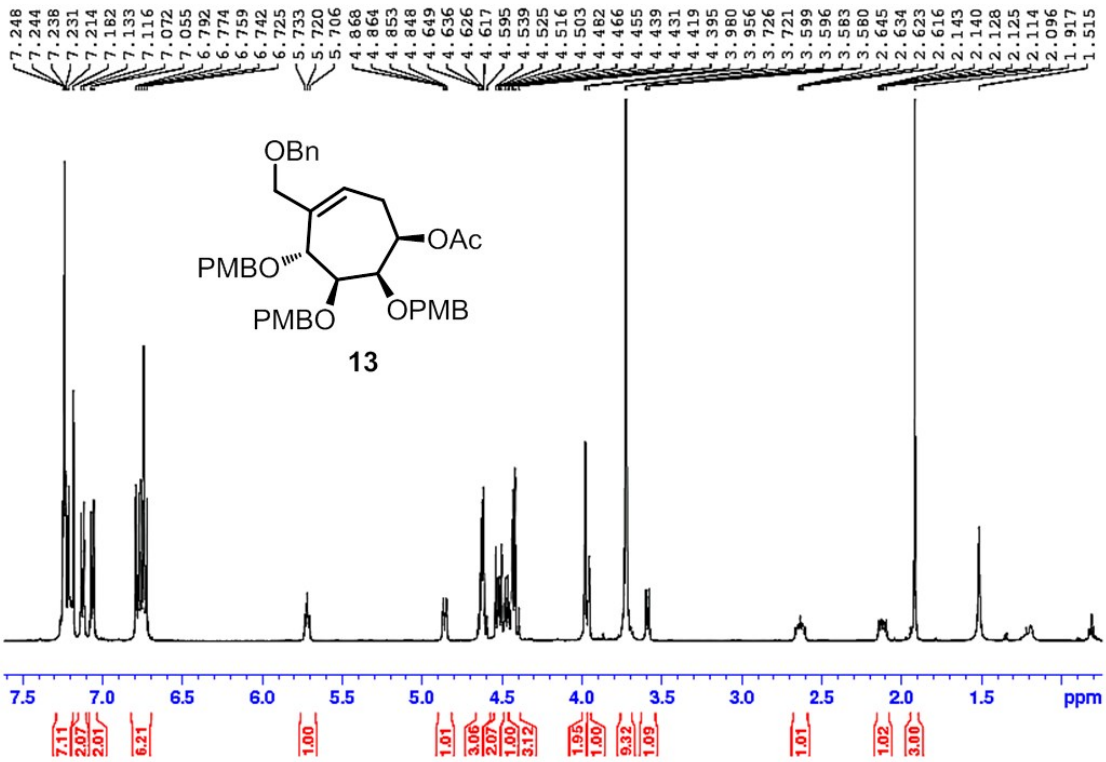
Theta range for data collection	3.137 to 25.999°.
Index ranges	-5<=h<=5, -32<=k<=32, -
Reflections collected	6338
Independent reflections	2695 [R(int) = 0.0171]
Completeness to theta = 25.242°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.985 and 0.980
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2695 / 3 / 203
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.1183
R indices (all data)	R1 = 0.0509, wR2 = 0.1240
Absolute structure parameter	0.4(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.581 and -0.201 e.Å^{-3}

4. NMR spectra

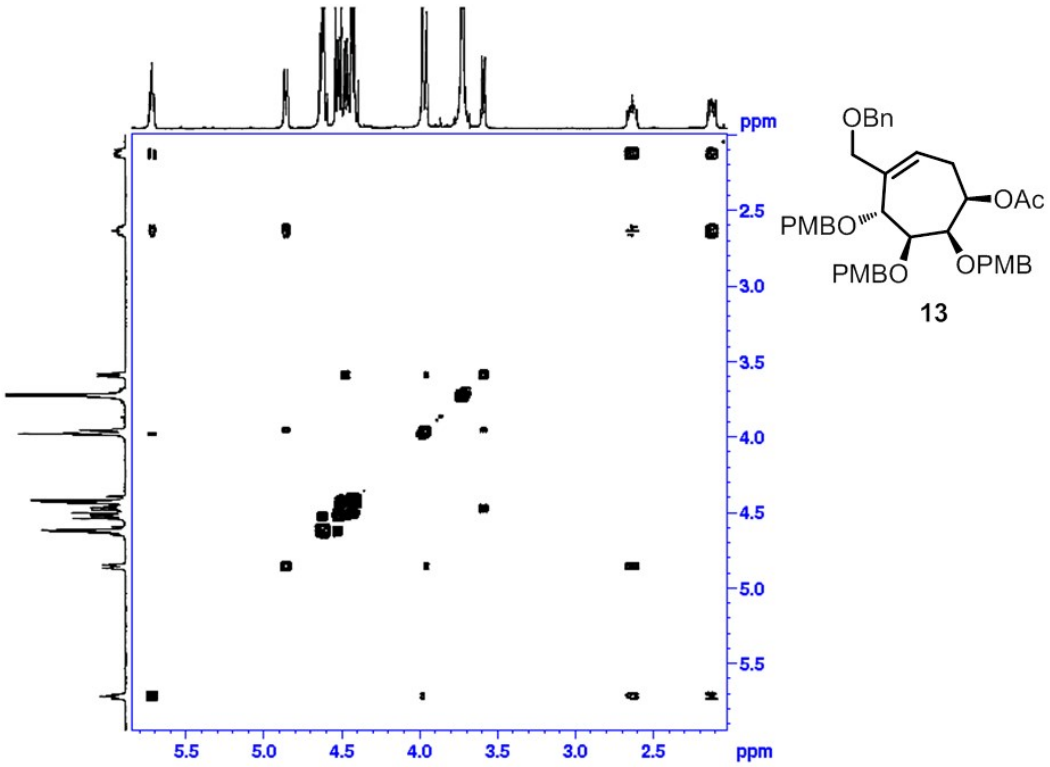
^{1}H NMR spectra of mixture of diastereomers **12** (1:0.3 ratio) recorded in $CDCl_3$



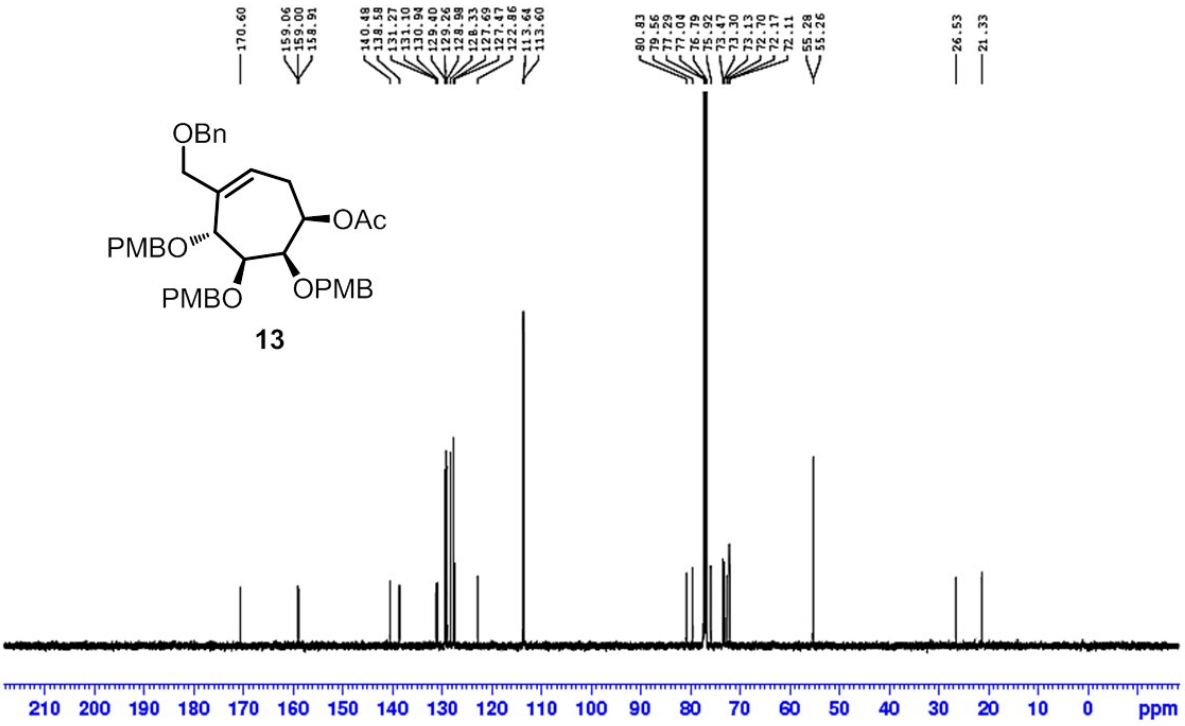
^{1}H NMR spectrum of compound **13** recorded in $CDCl_3$



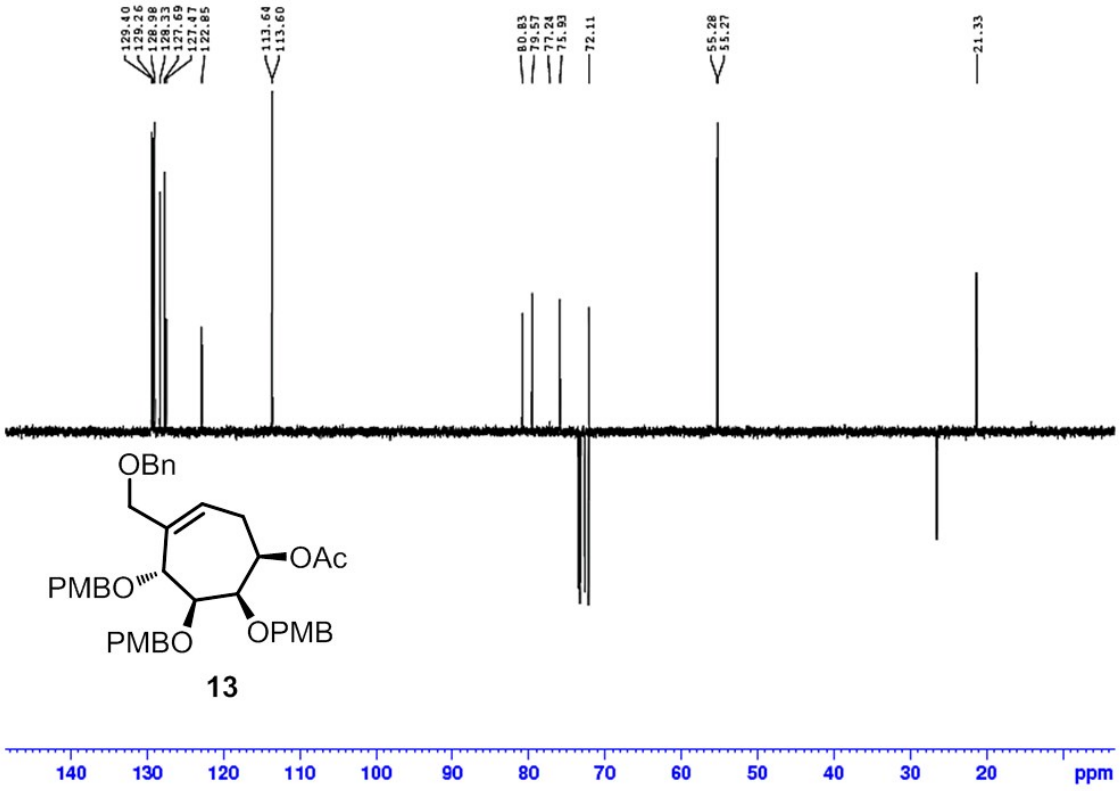
COSY spectrum of compound **13** recorded in $CDCl_3$



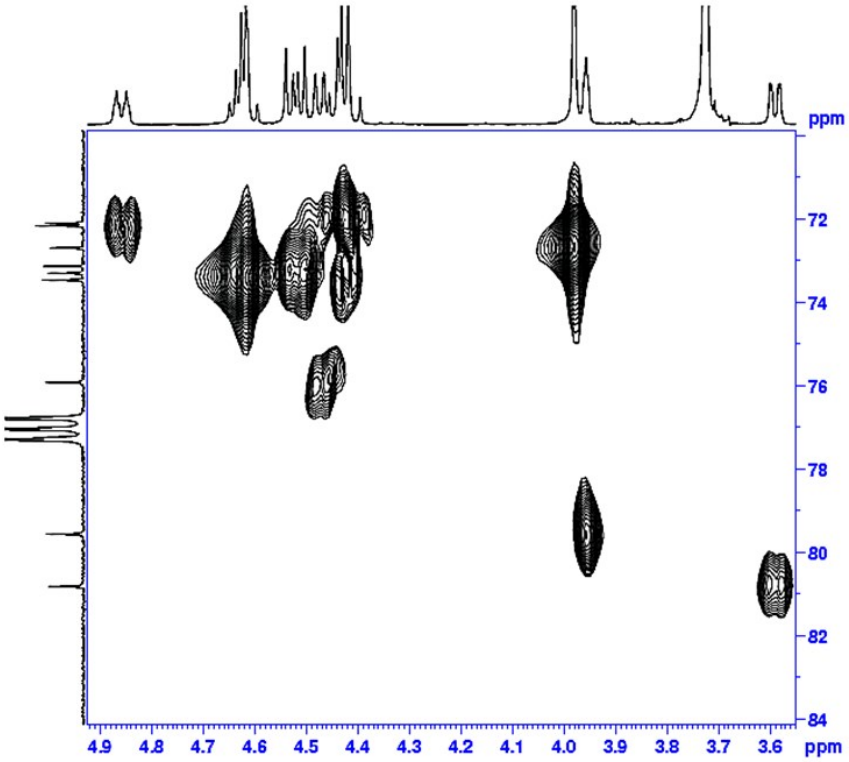
^{13}C spectrum of **13** recorded in $CDCl_3$

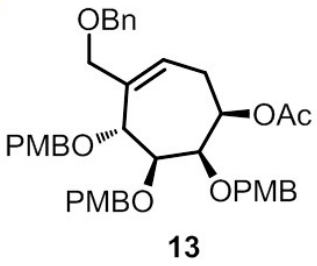


DEPT spectrum of compound **13** recorded in $CDCl_3$



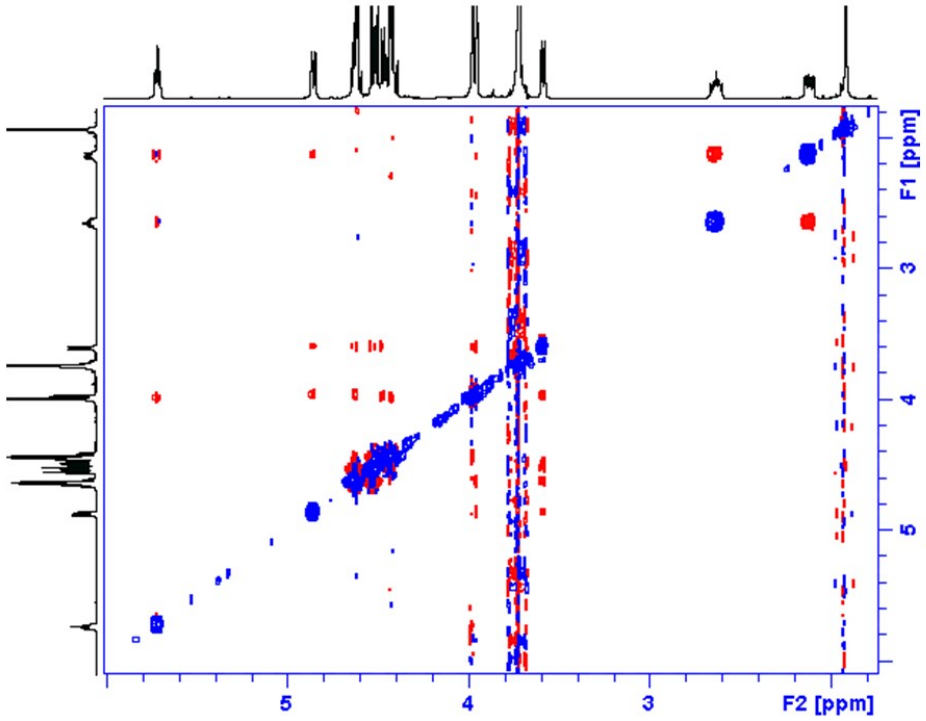
HMQC spectrum of compound **13** recorded in $CDCl_3$

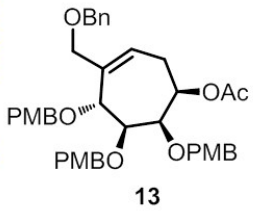




13

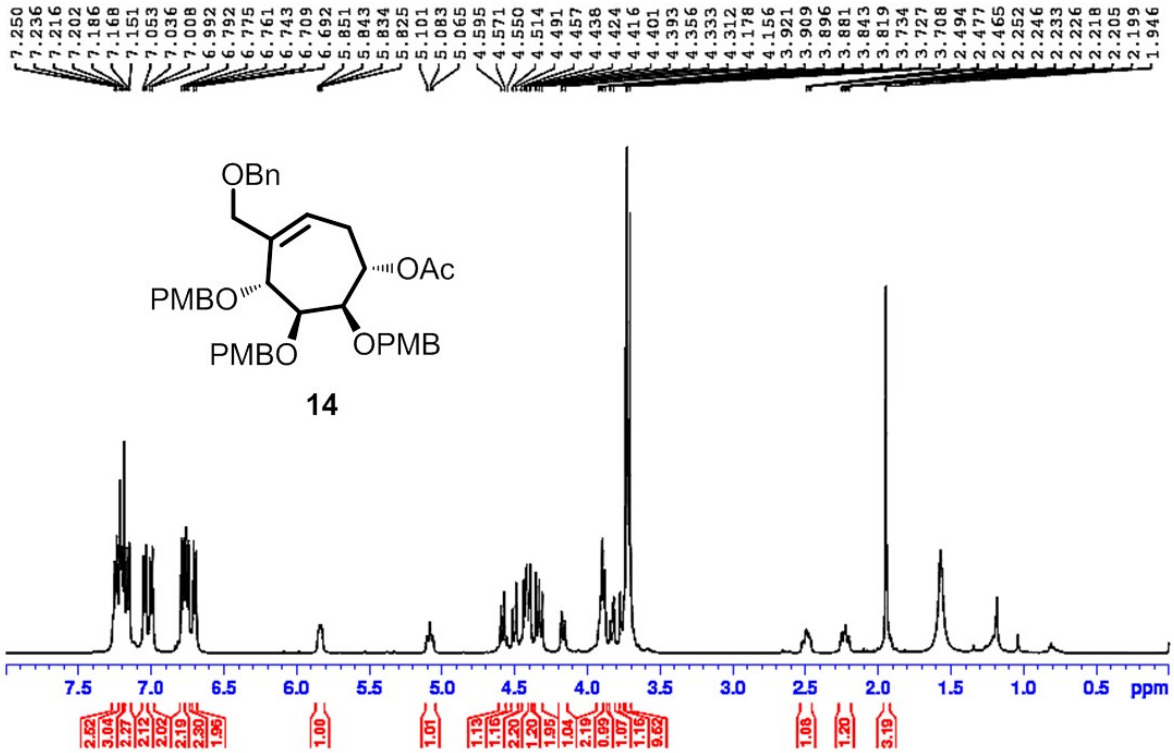
NOESY spectrum of compound **13** recorded in $CDCl_3$



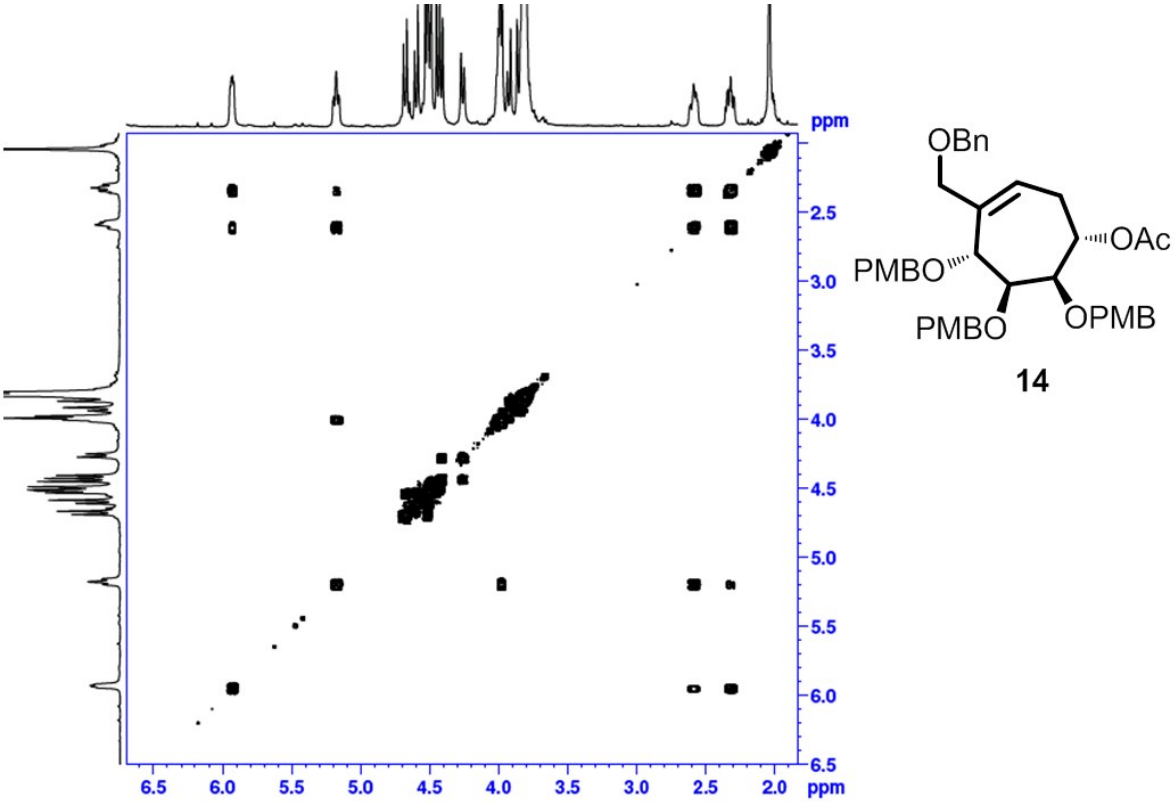


13

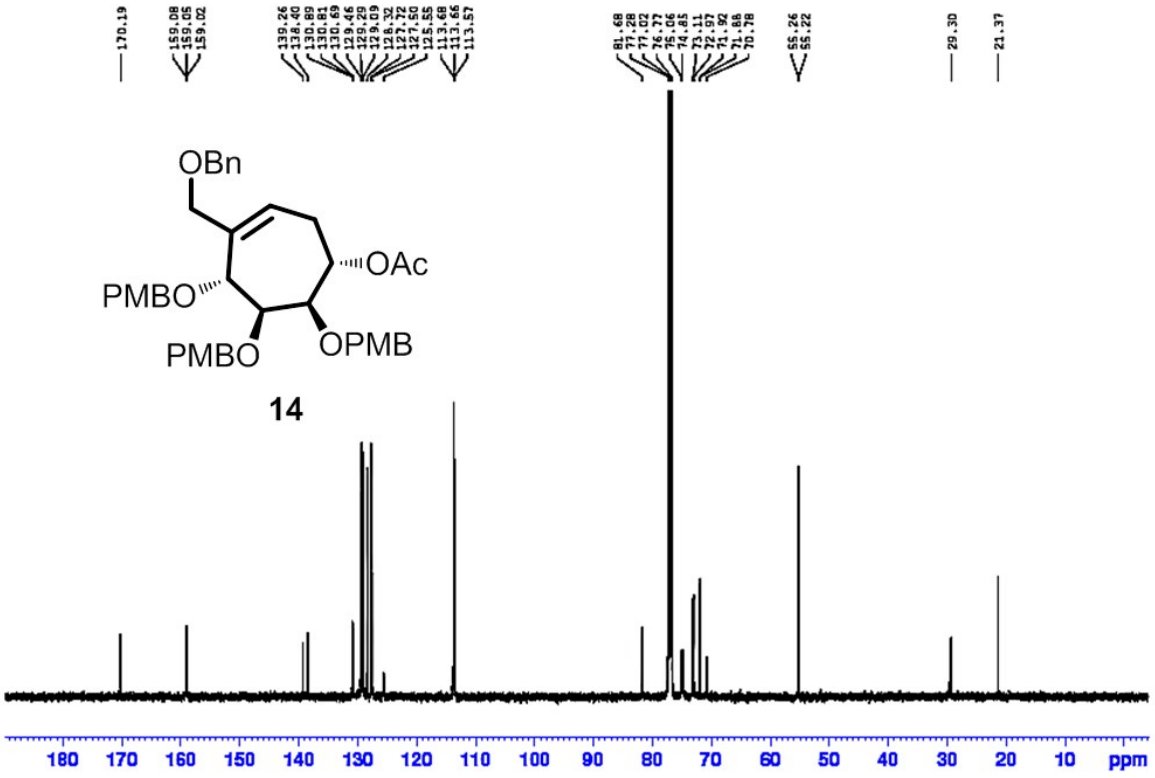
^{1}H NMR spectrum of compound **14** recorded in $CDCl_3$



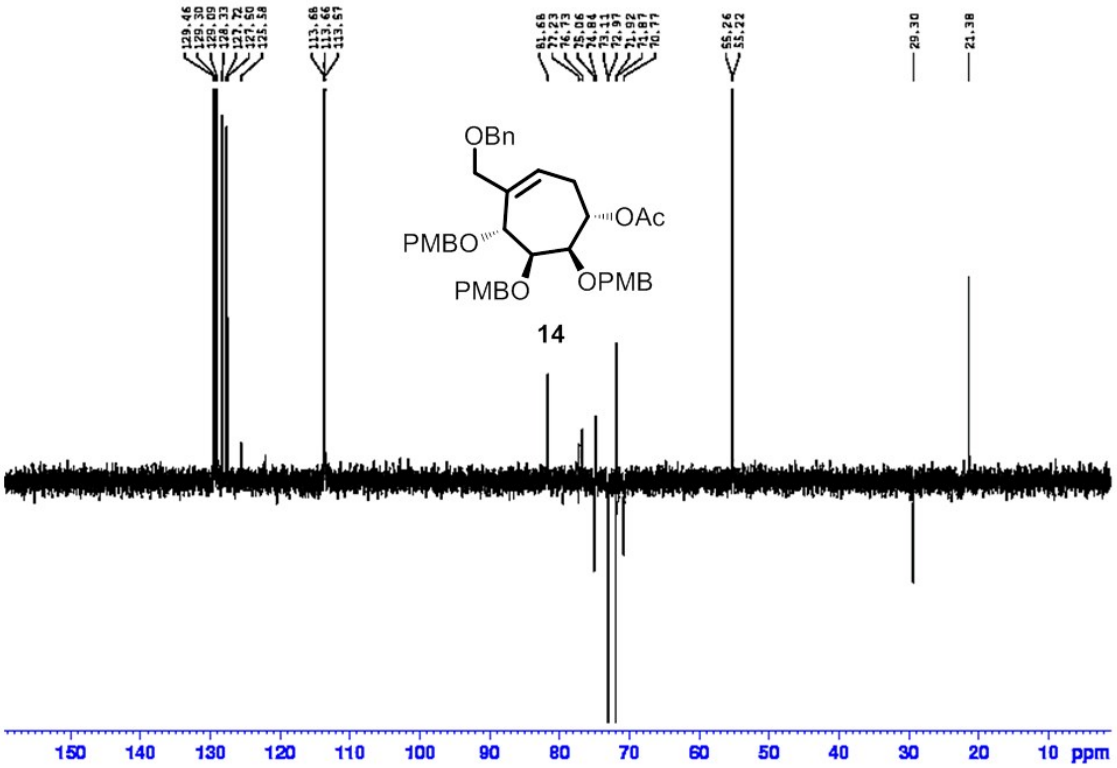
COSY spectrum of compond **14** recorded in $CDCl_3$



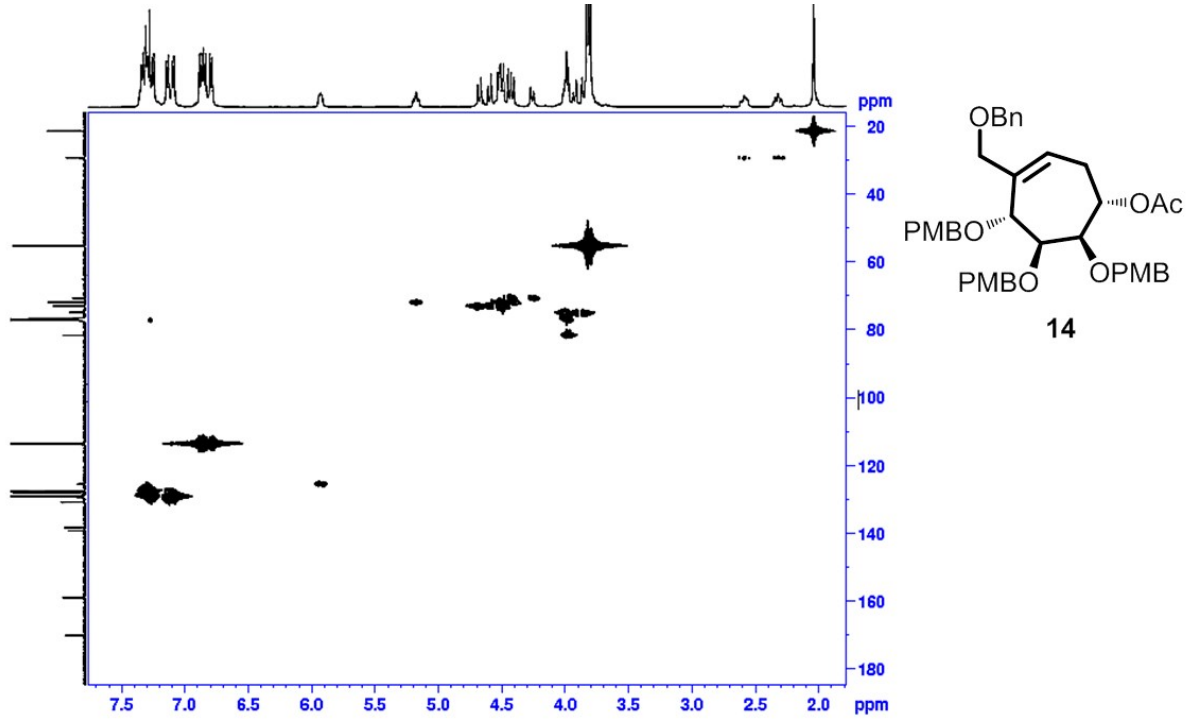
^{13}C spectrum of compound **14** recorded in $CDCl_3$



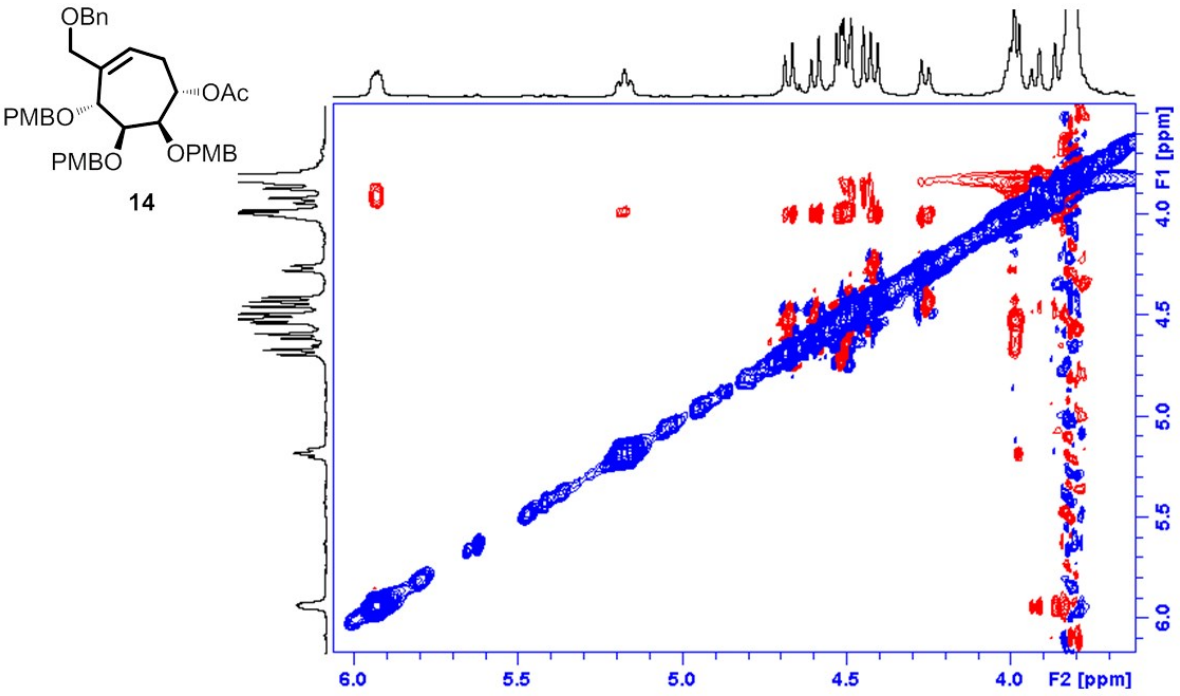
DEPT spectrum of compound **14** recorded in $CDCl_3$



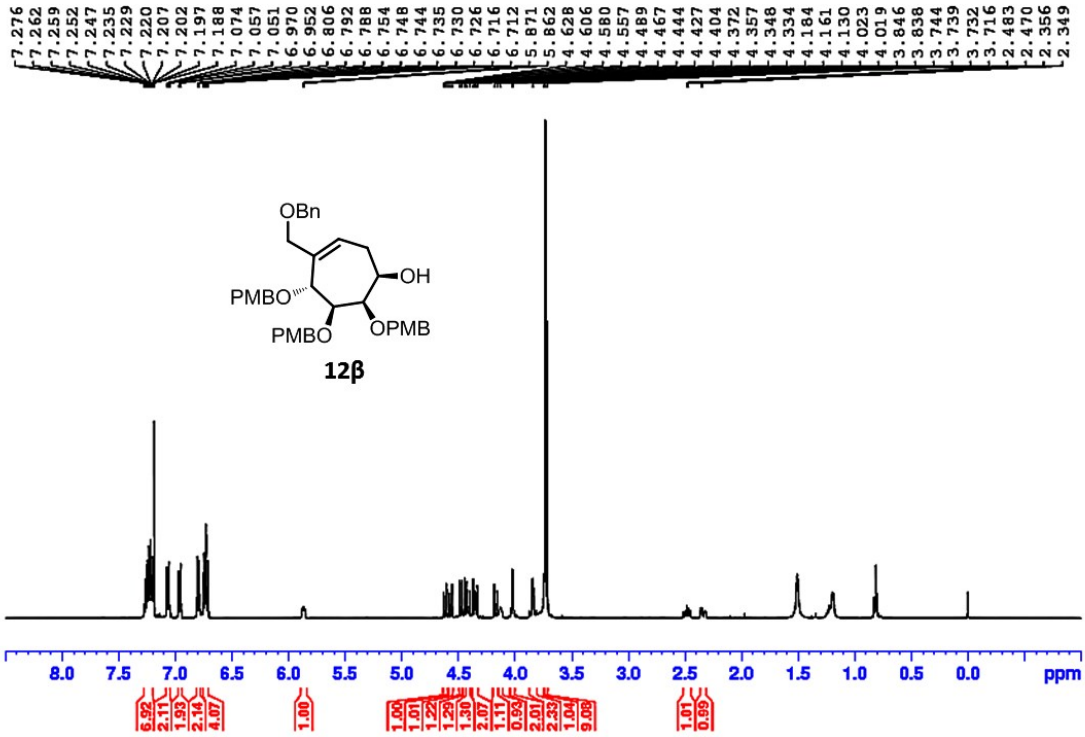
HMQC spectrum of compound **14** recorded in $CDCl_3$



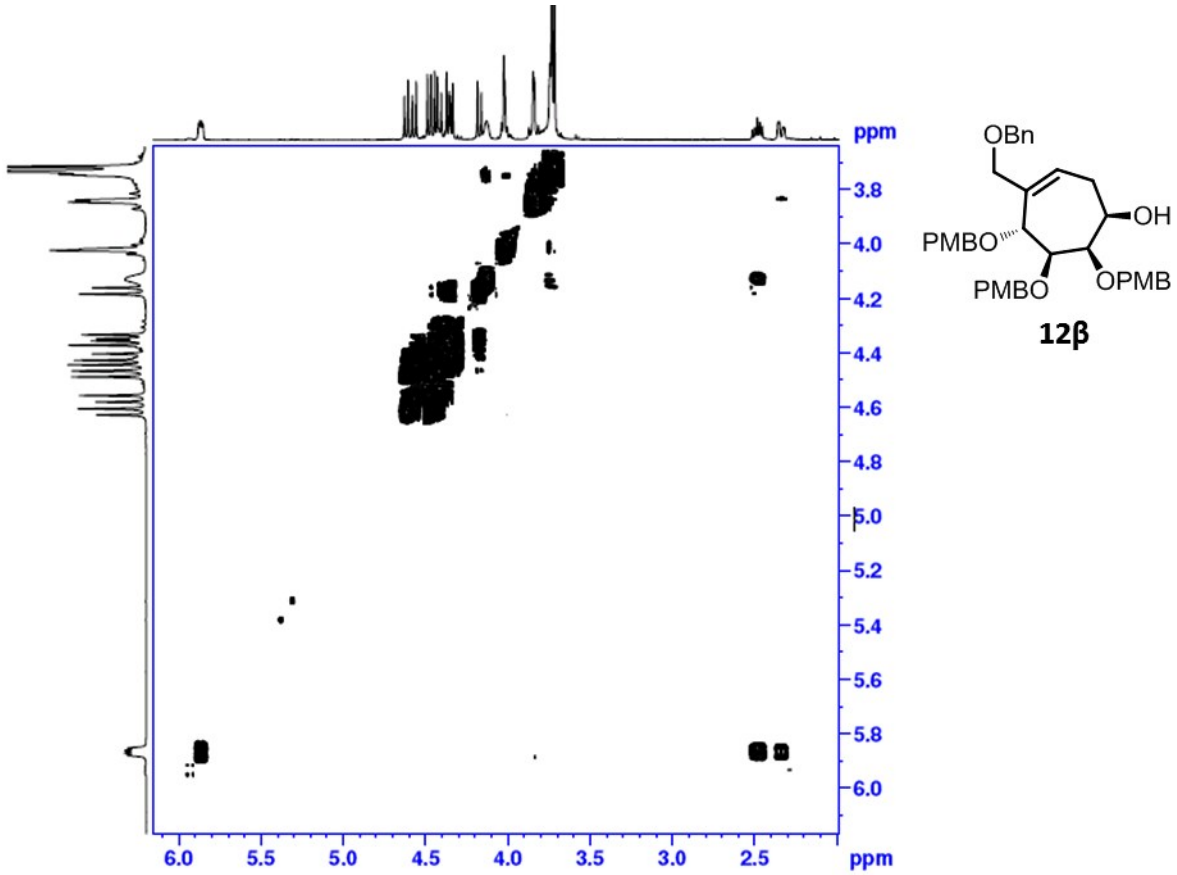
NOESY spectrum of compound **14** recorded in $CDCl_3$



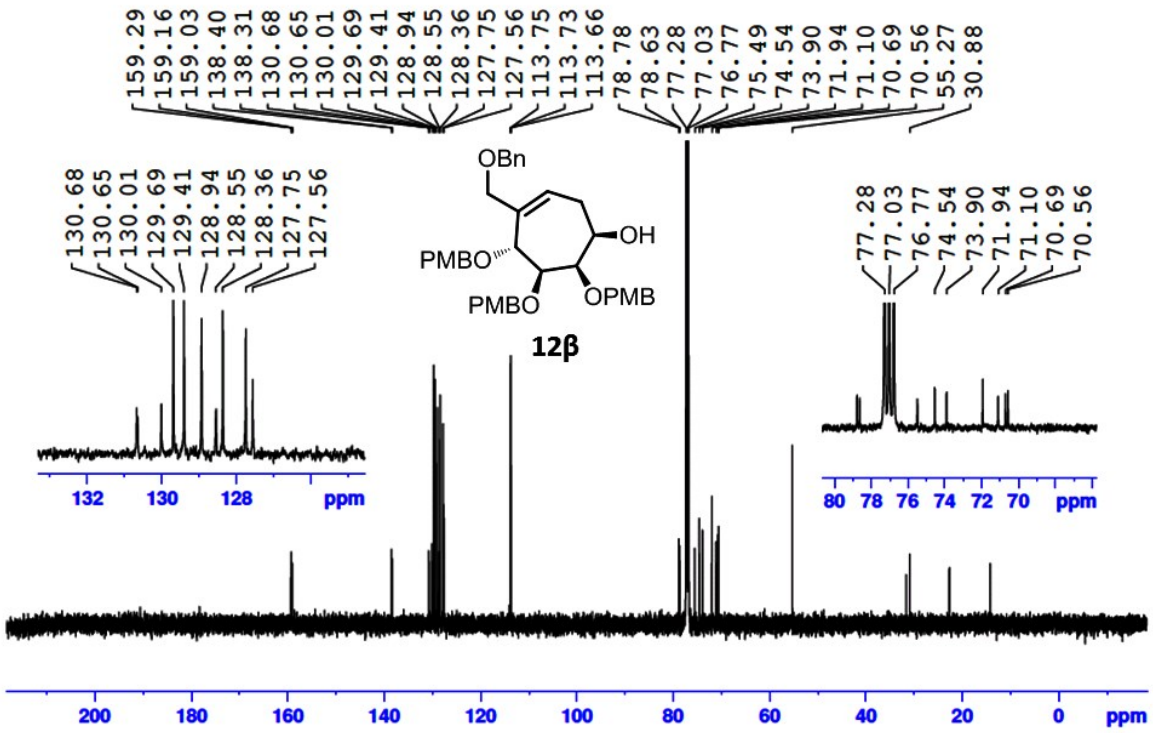
^{1}H NMR spectrum of compound **12β** recorded in $CDCl_3$



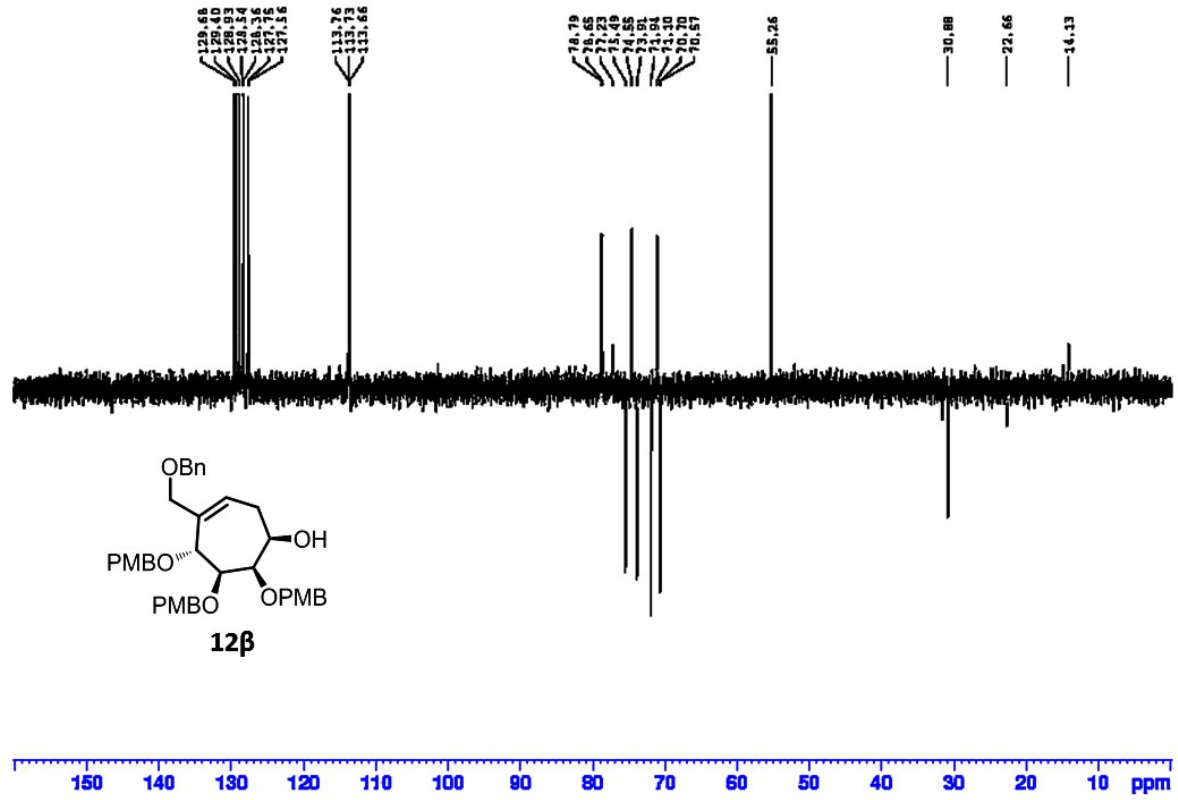
COSY spectra of compound **12β** recorded in $CDCl_3$



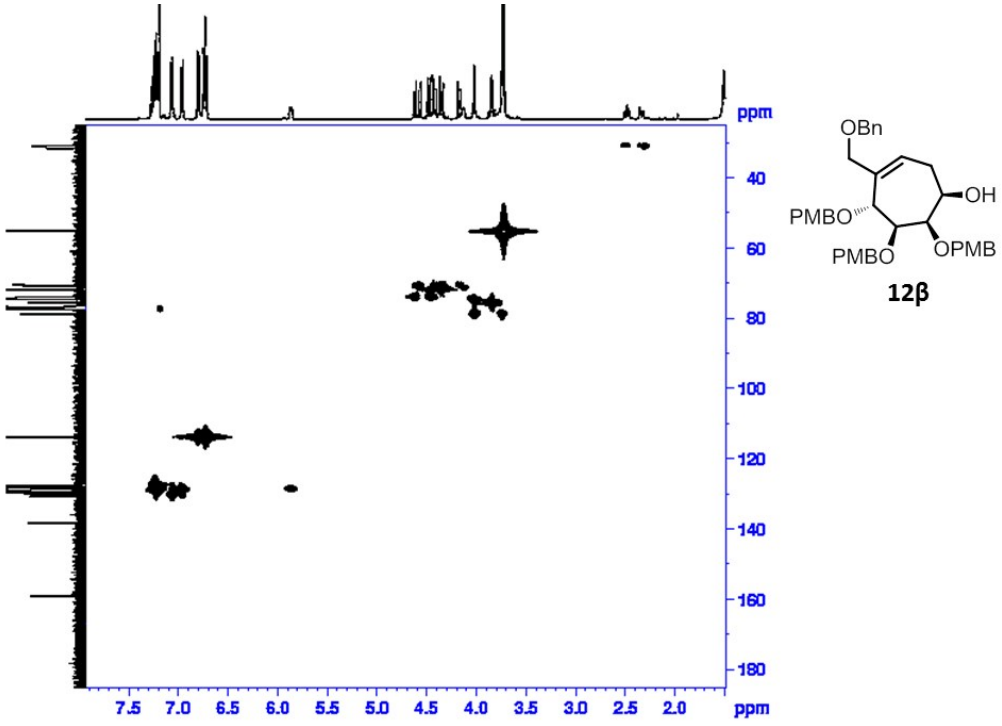
^{13}C NMR spectrum of compound **12β** recorded in $CDCl_3$



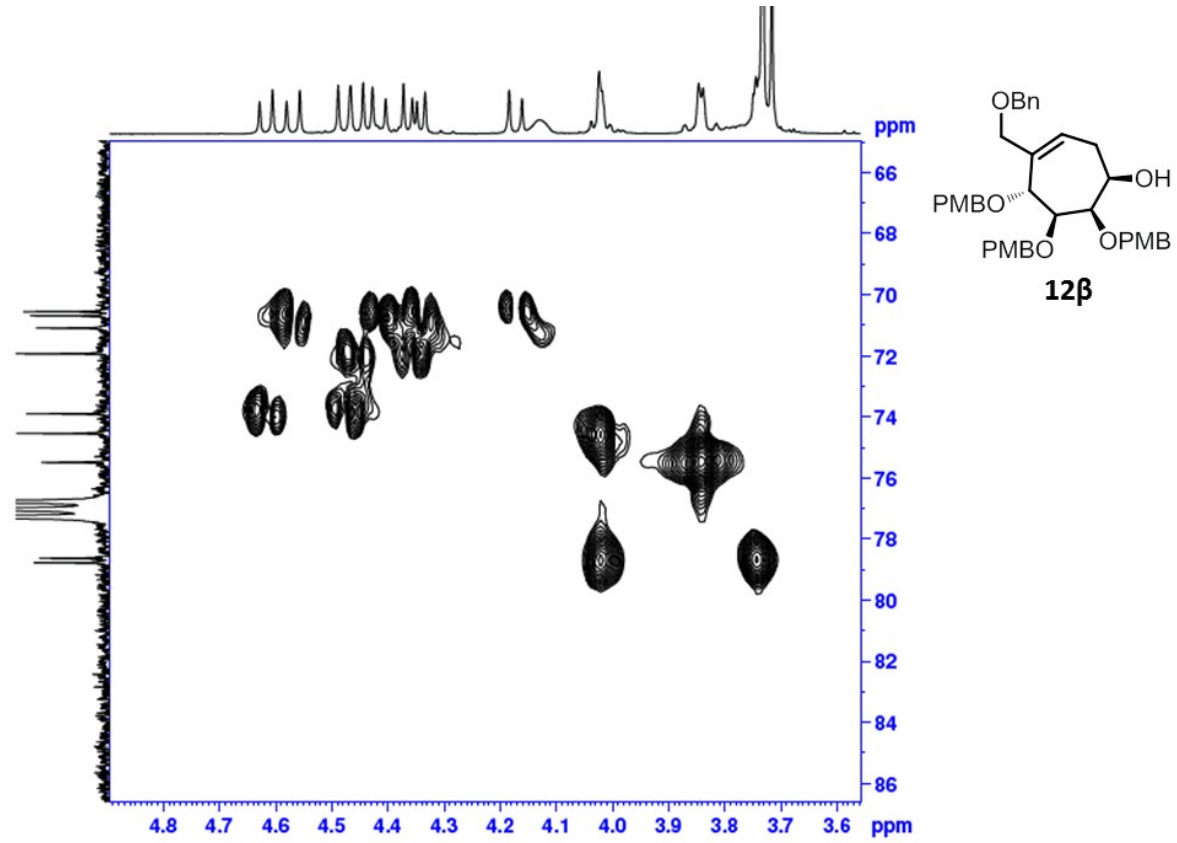
DEPT spectrum of compound **12β** recorded in $CDCl_3$



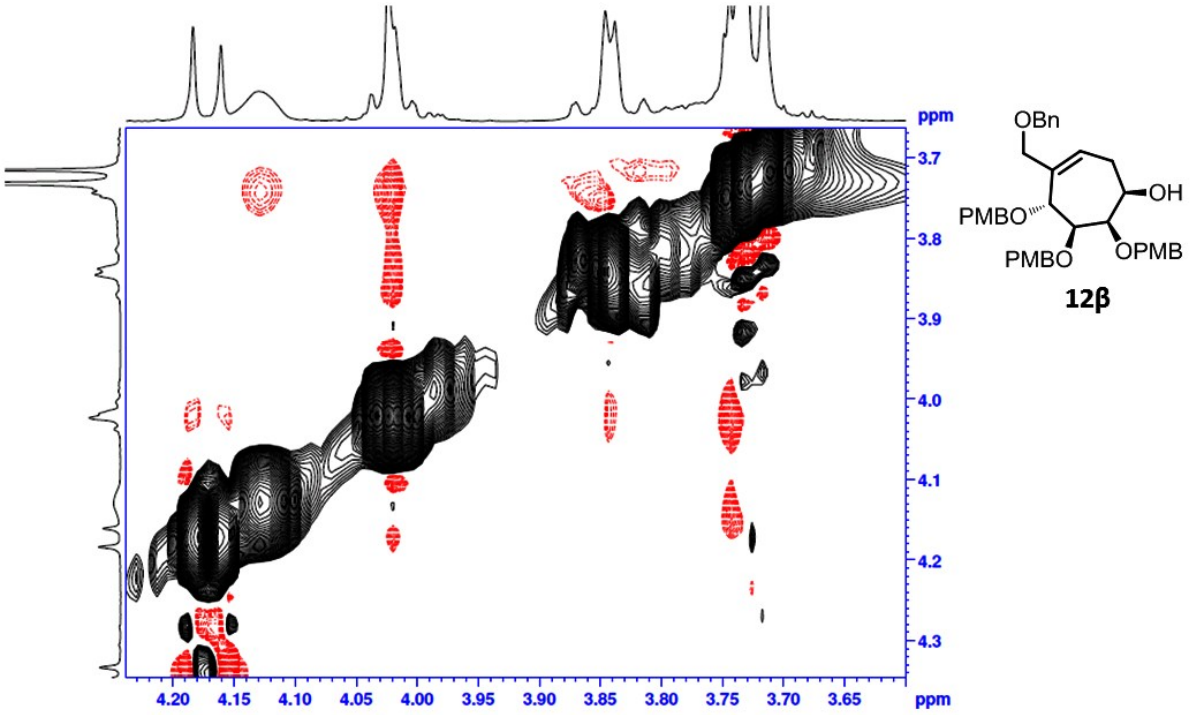
HMQC spectrum of compound **12β** recorded in $CDCl_3$



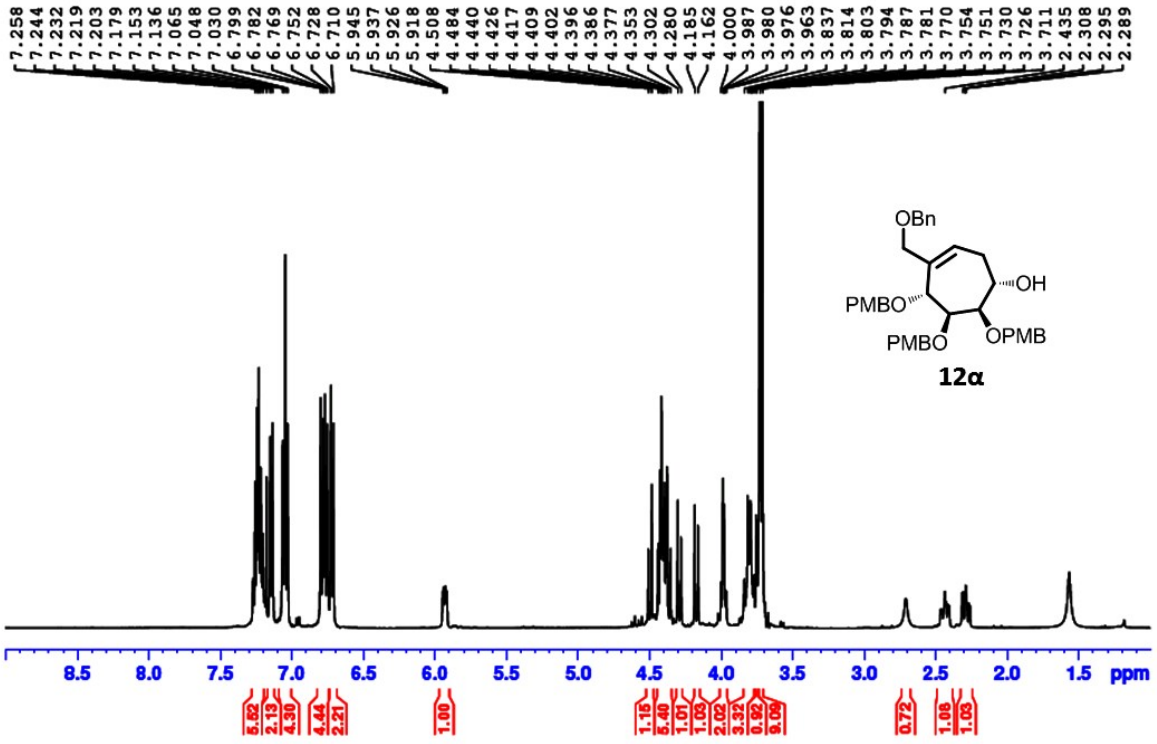
Expanded HMQC spectrum of compound **12β** recorded in $CDCl_3$



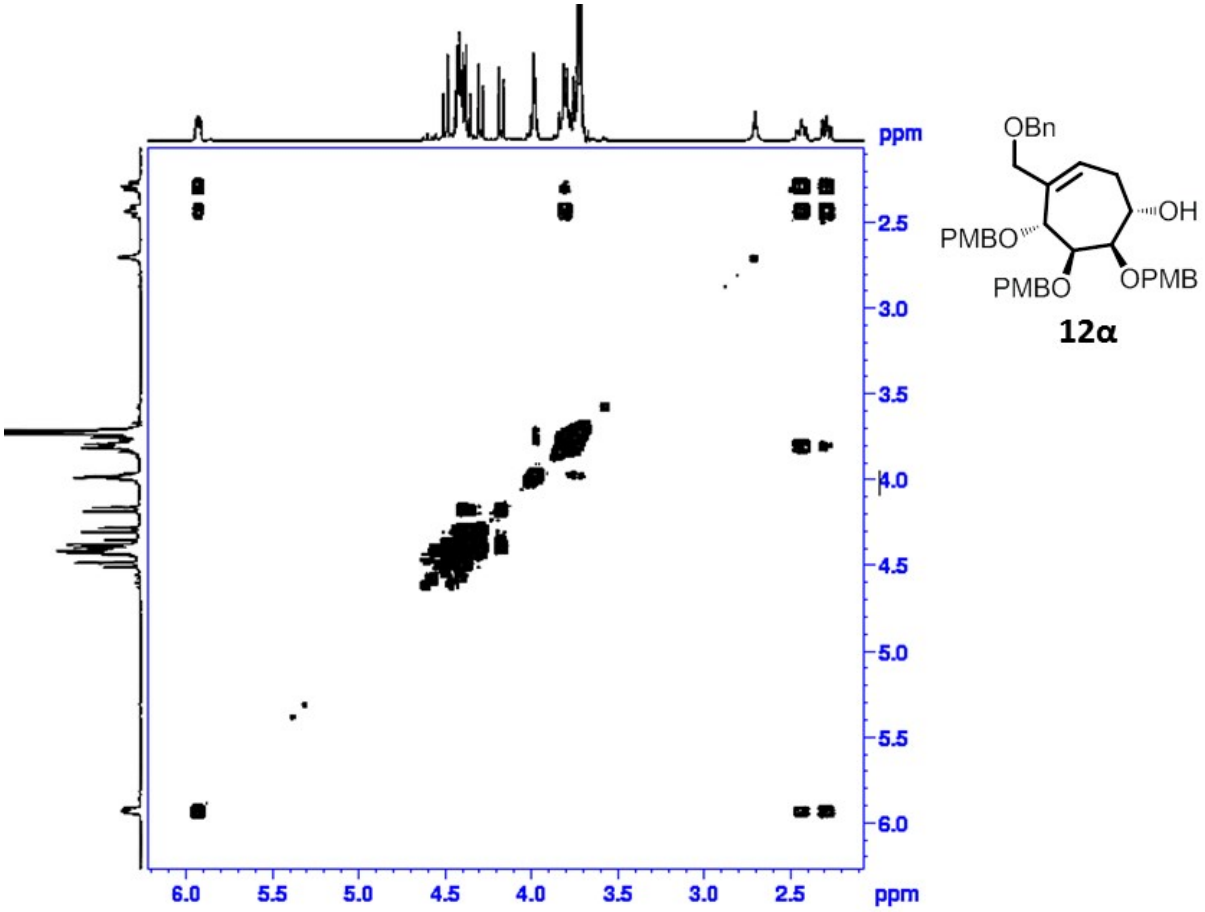
NOESY spectrum of compound **12β** recorded in $CDCl_3$



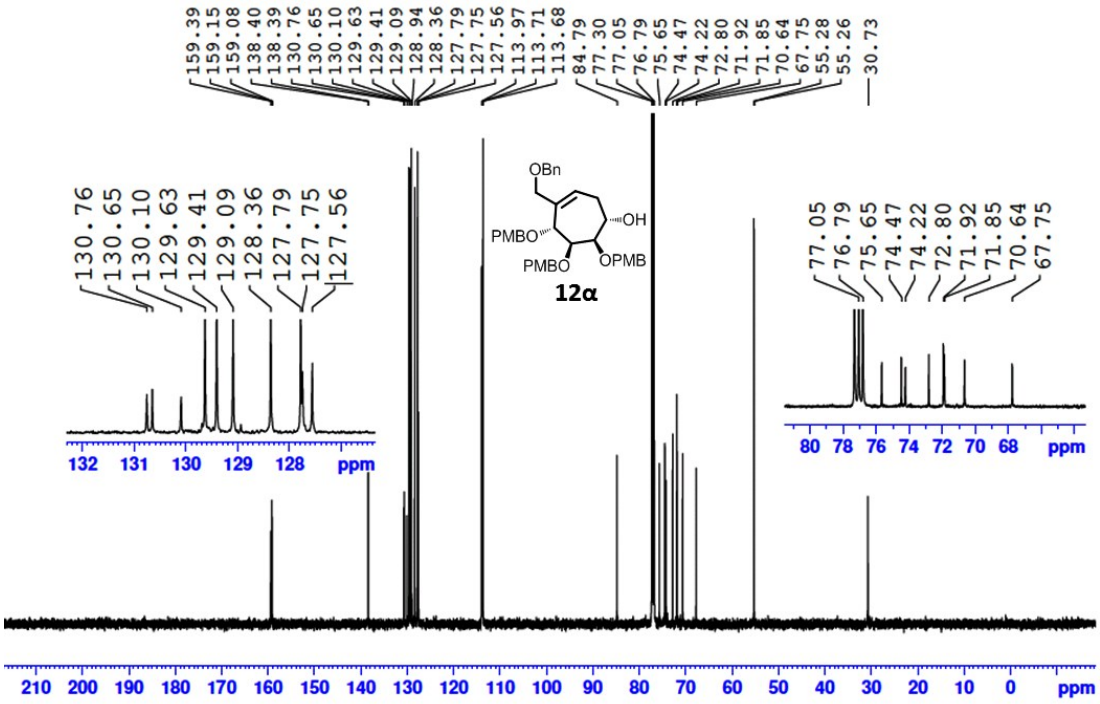
^{1}H NMR spectrum of compound **12α** recorded in $CDCl_3$



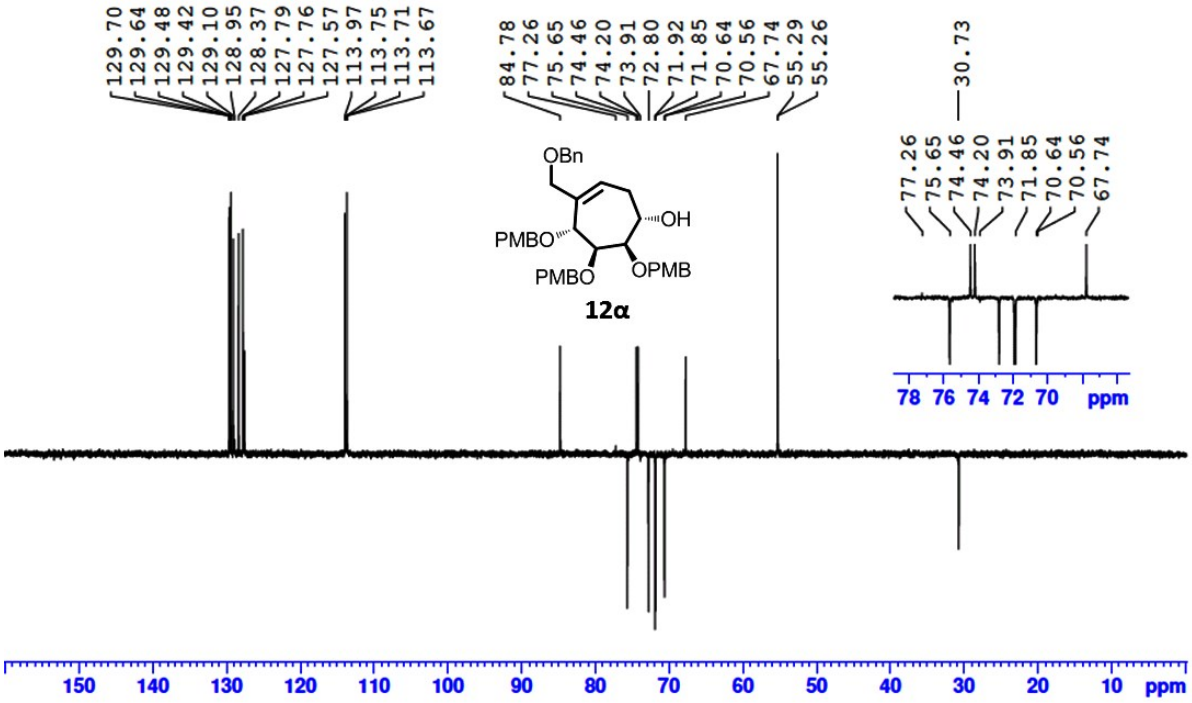
COSY spectrum of compound **12α** recorded in $CDCl_3$



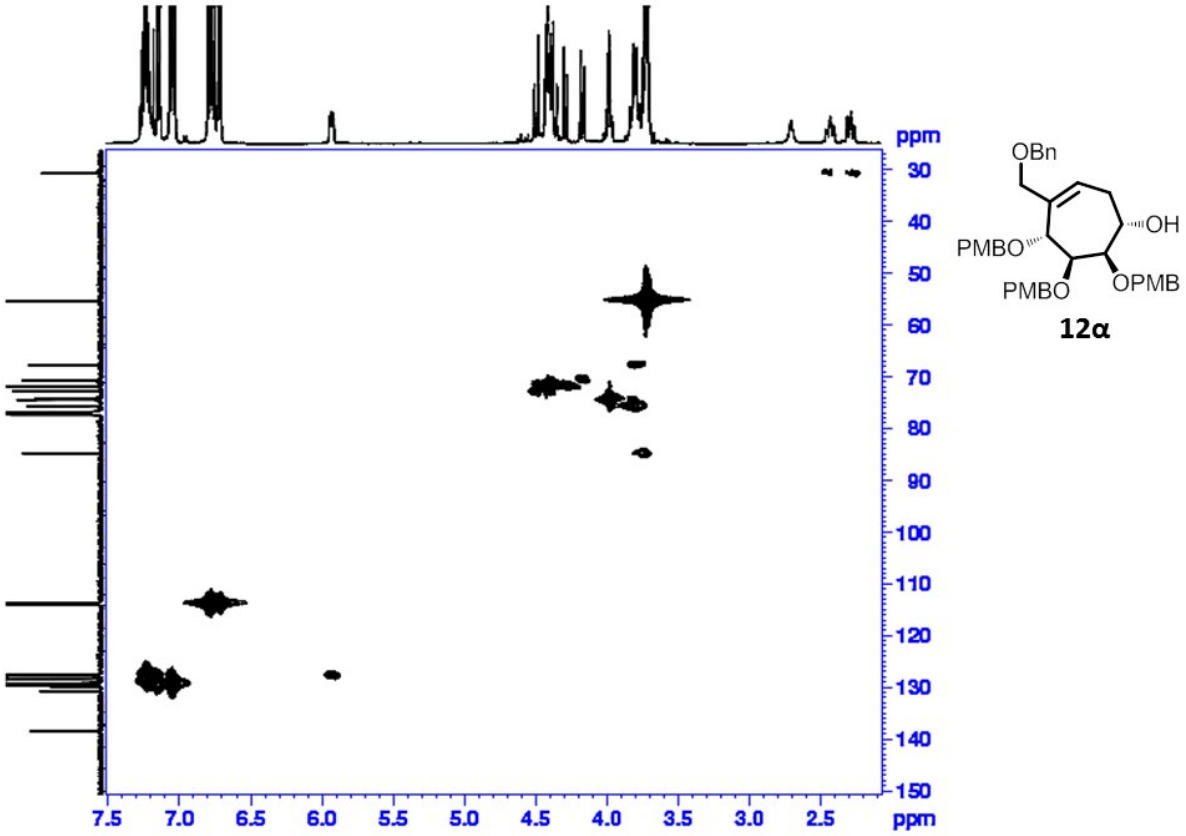
^{13}C spectrum of compound **12α** recorded in $CDCl_3$



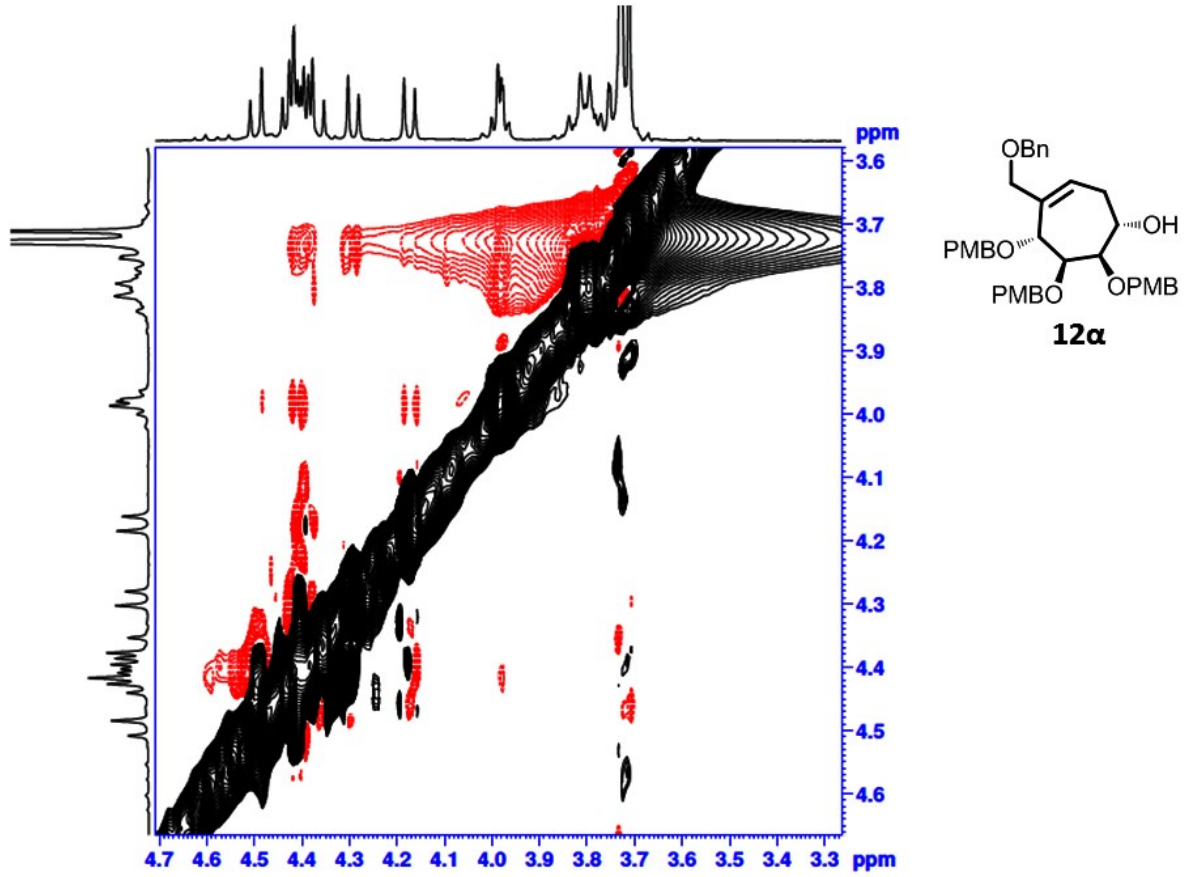
DEPT spectrum of compound **12α** recorded in $CDCl_3$



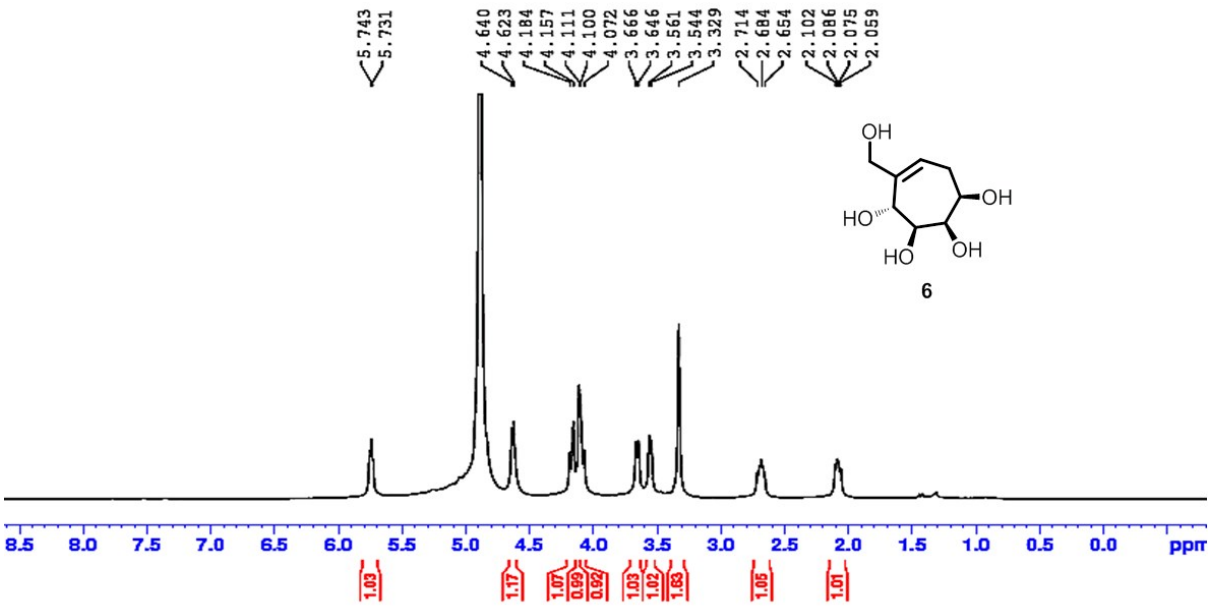
HMQC spectrum of compound **12α** recorded in $CDCl_3$



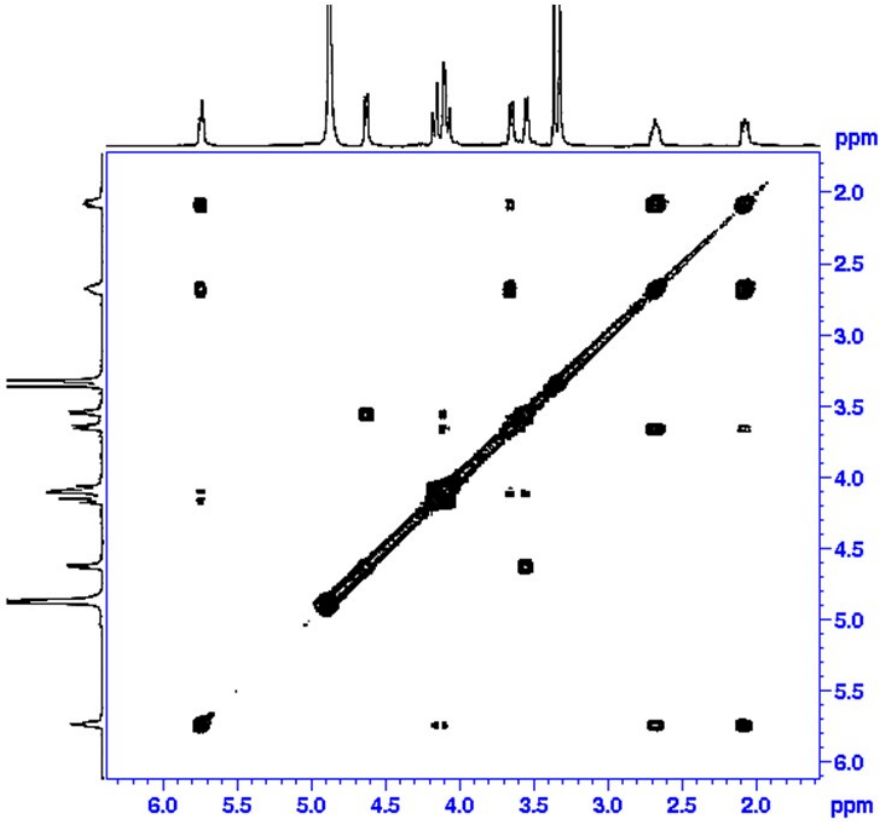
Expanded NOESY spectrum of compound **12α** recorded in $CDCl_3$

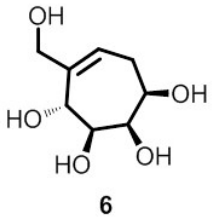


^{1}H NMR spectrum of compound **6** recorded in CD_3OD



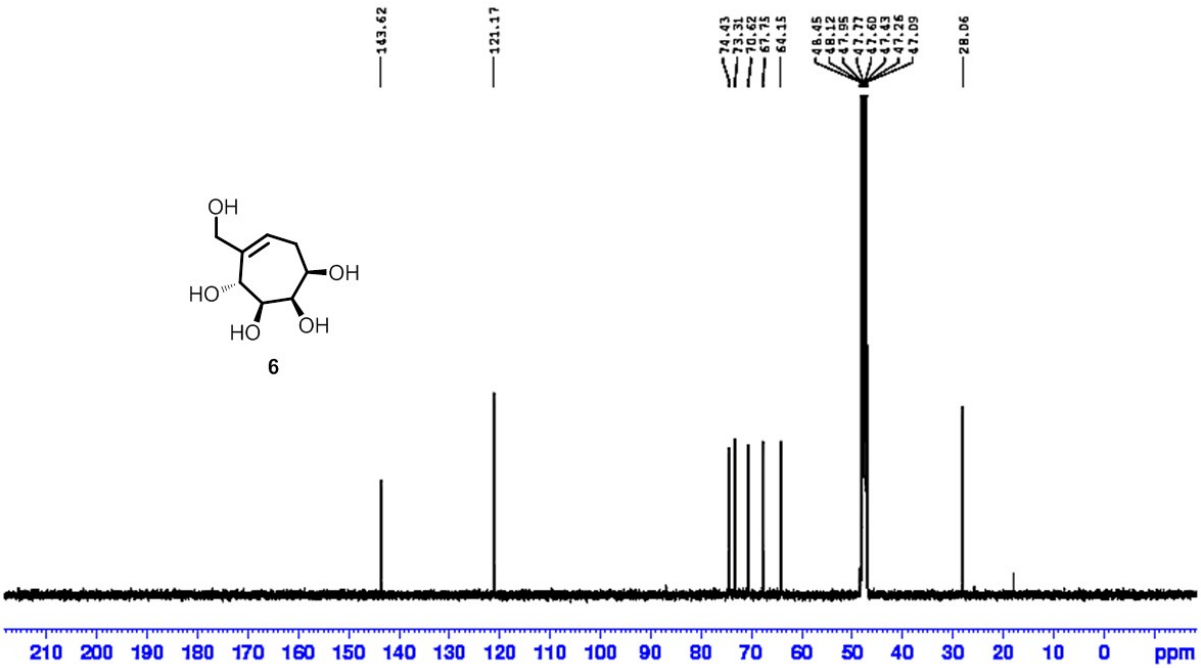
COSY spectrum of compound **6** recorded in CD_3OD



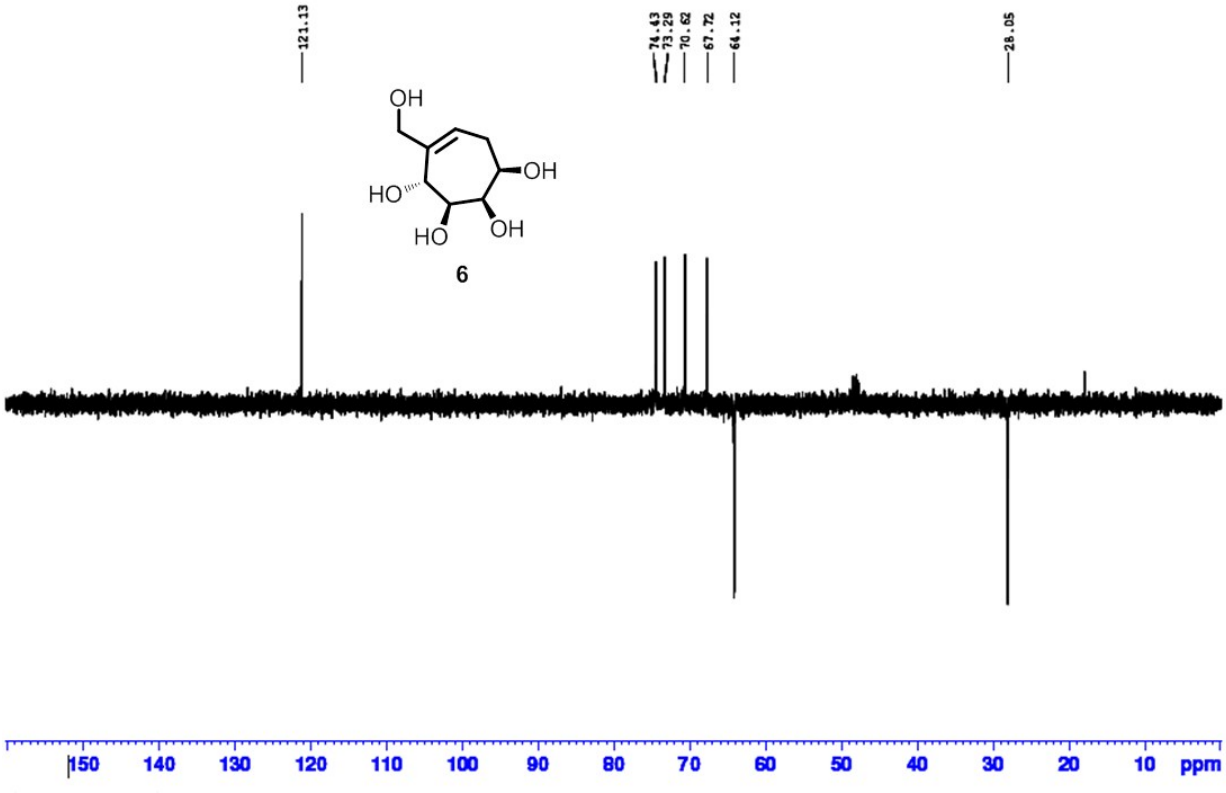


6

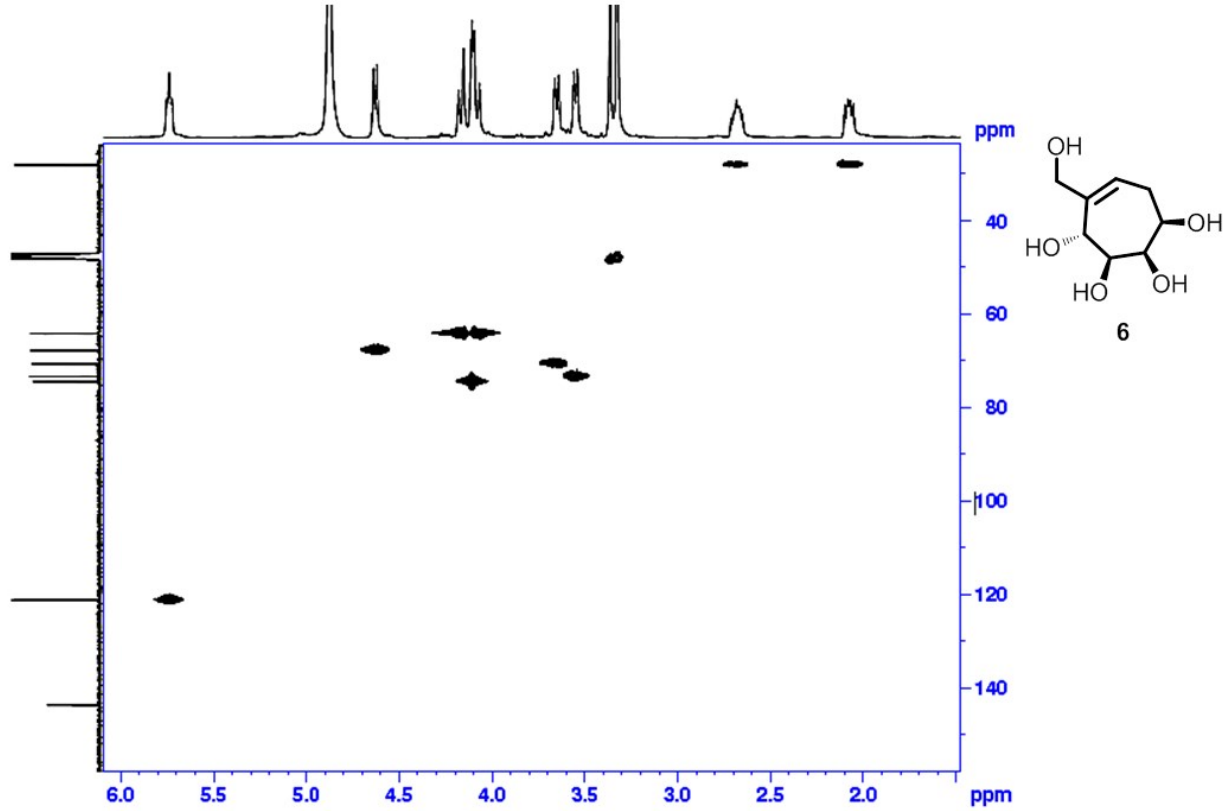
^{13}C NMR spectrum of compound **6** recorded in CD_3OD



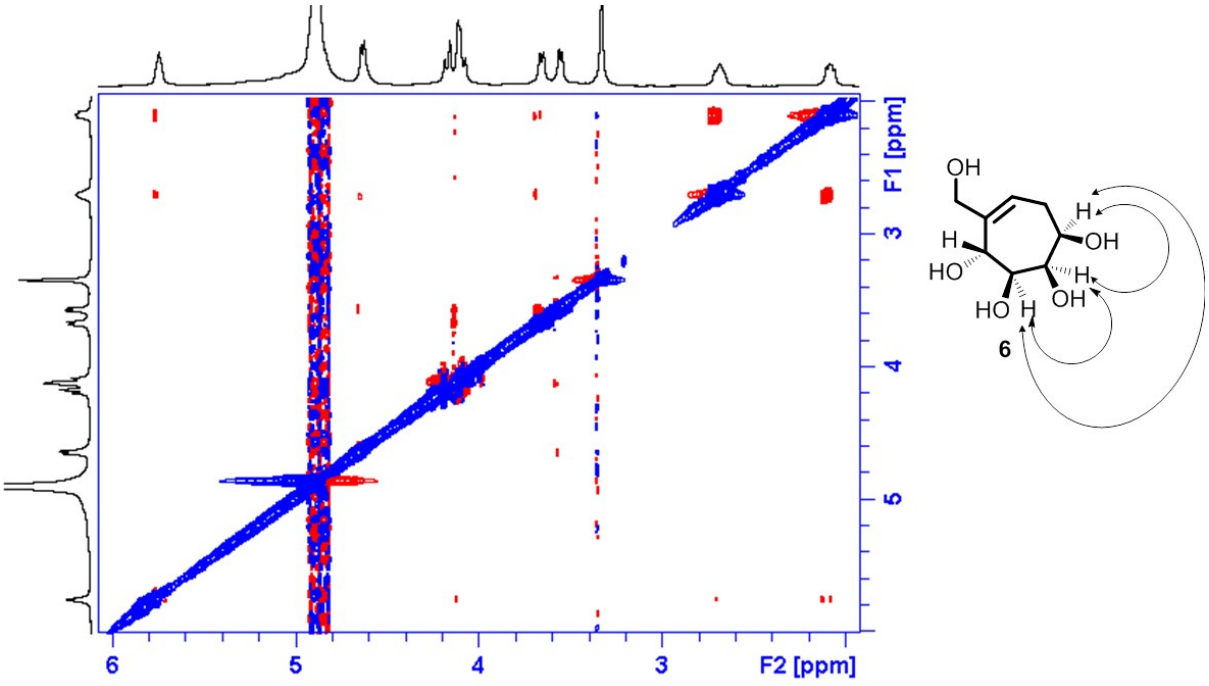
DEPT spectrum of compound **6** recorded in CD_3OD



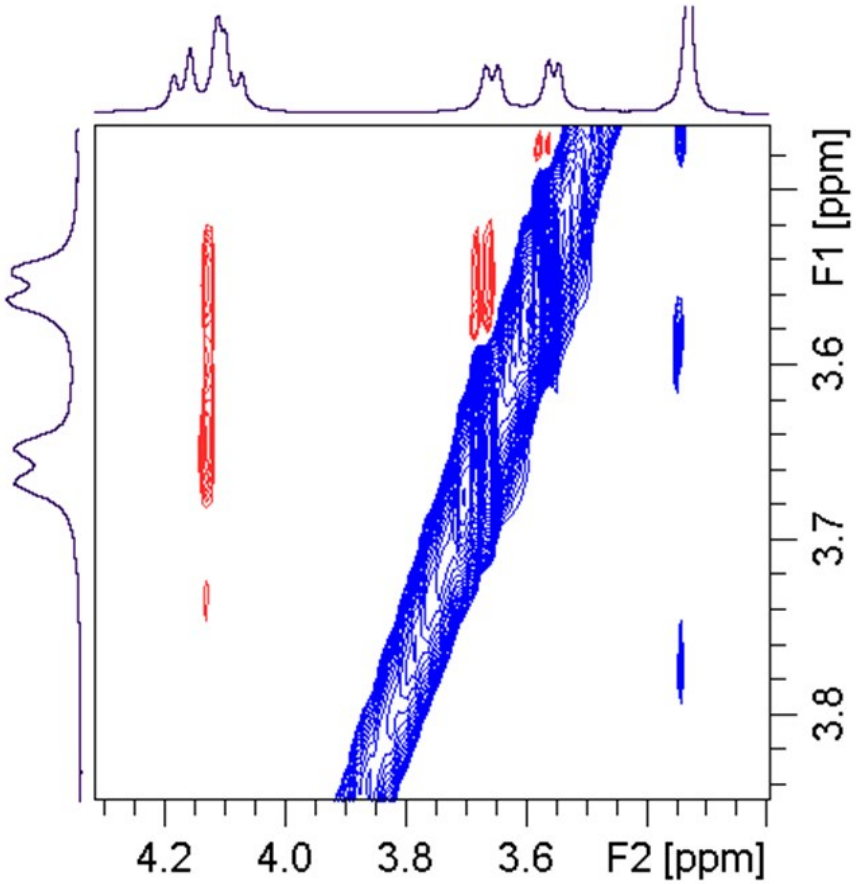
HMQC spectrum of compound **6** recorded in CD_3OD



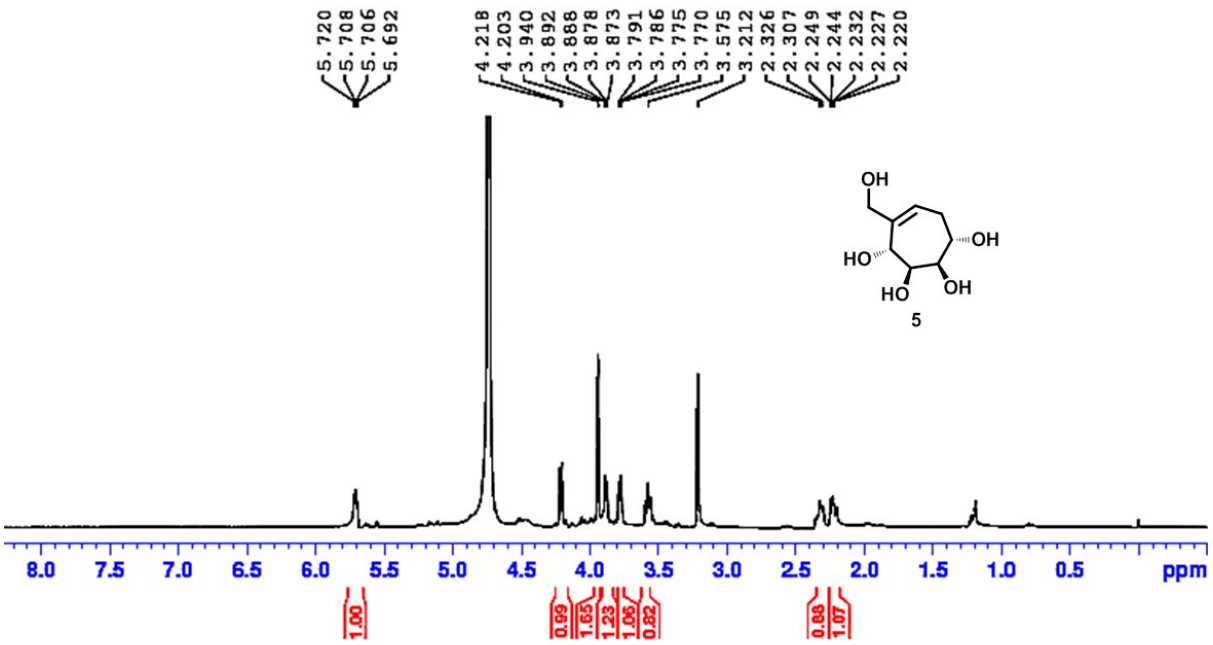
NOESY spectrum of compound **6** recorded in CD_3OD



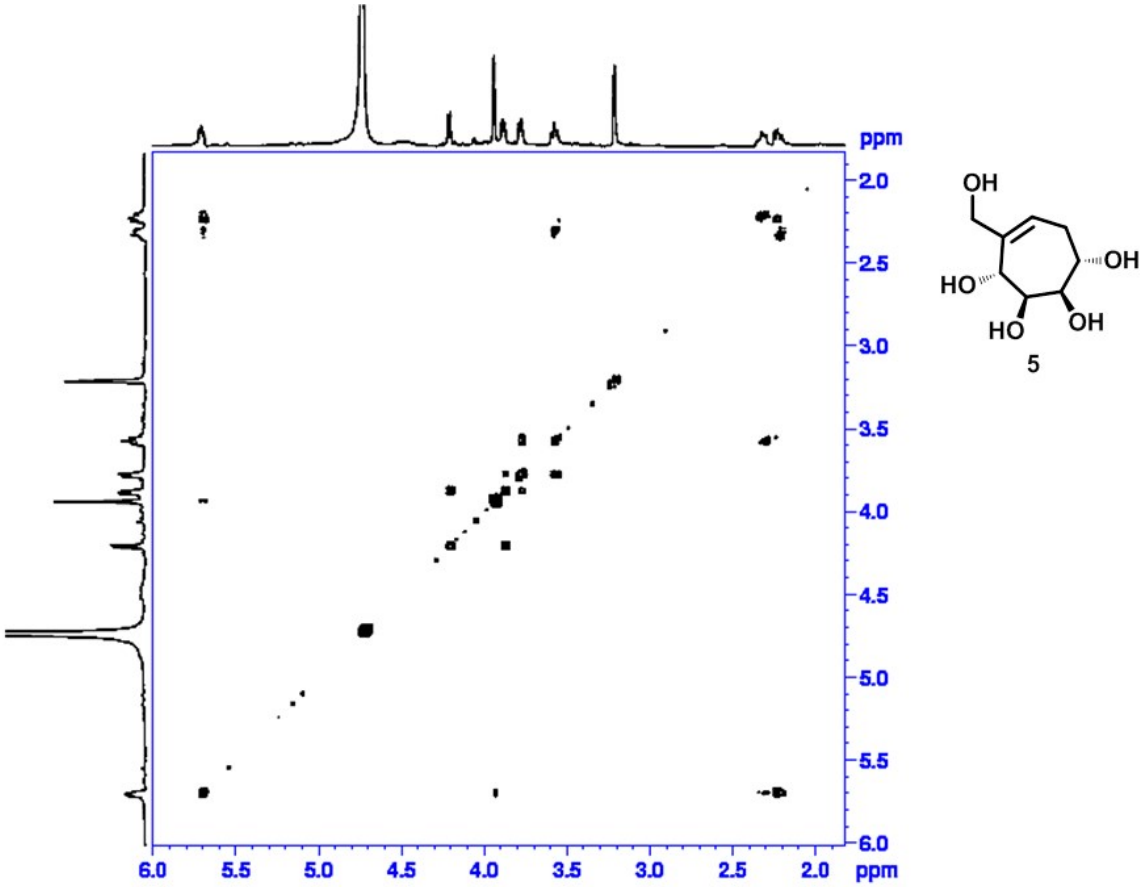
Expanded NOESY spectrum of compound **6** recorded in CD_3OD



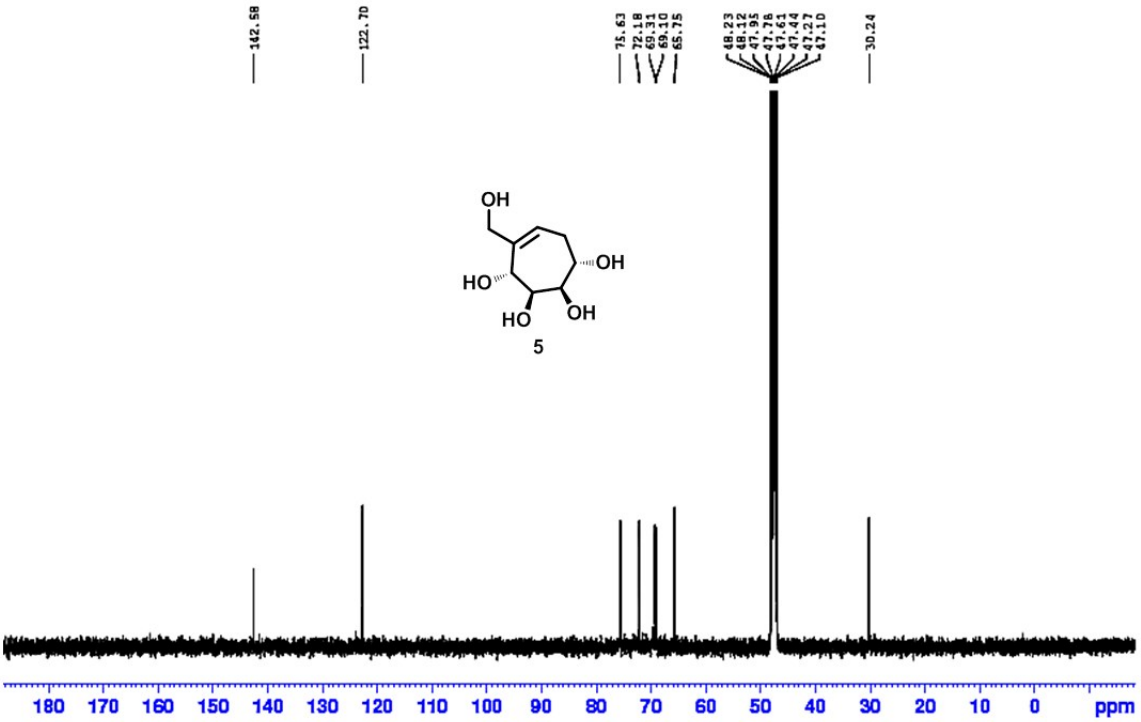
^{1}H NMR spectrum of compound **5** recorded in CD_3OD



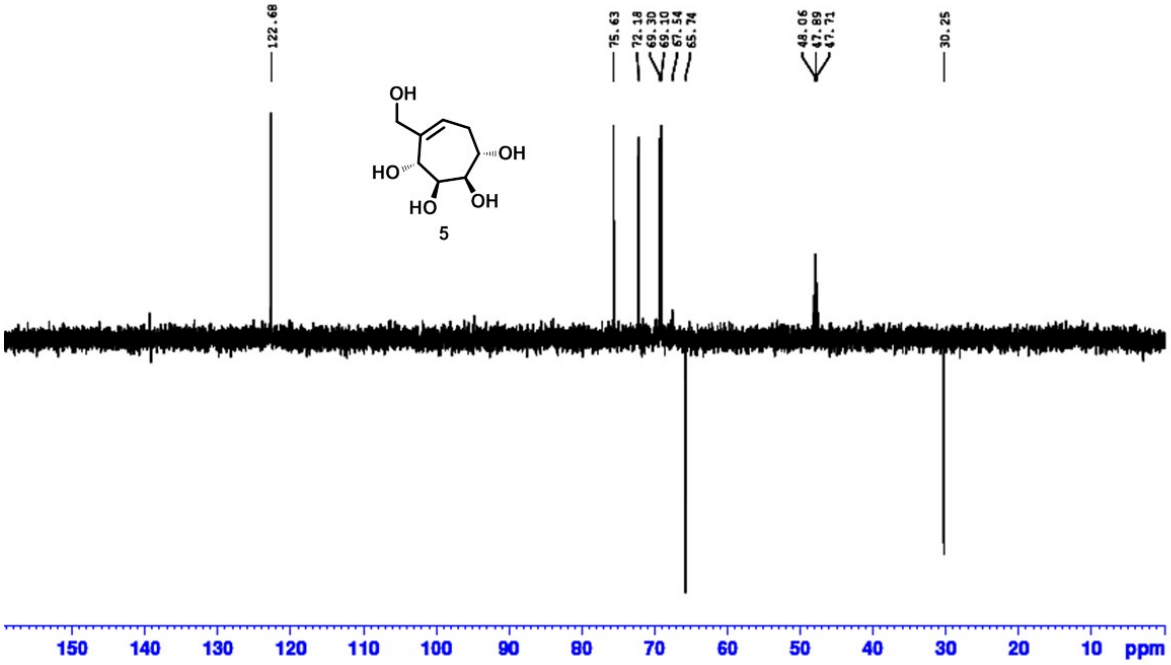
COSY spectrum of compound **5** recorded in CD_3OD



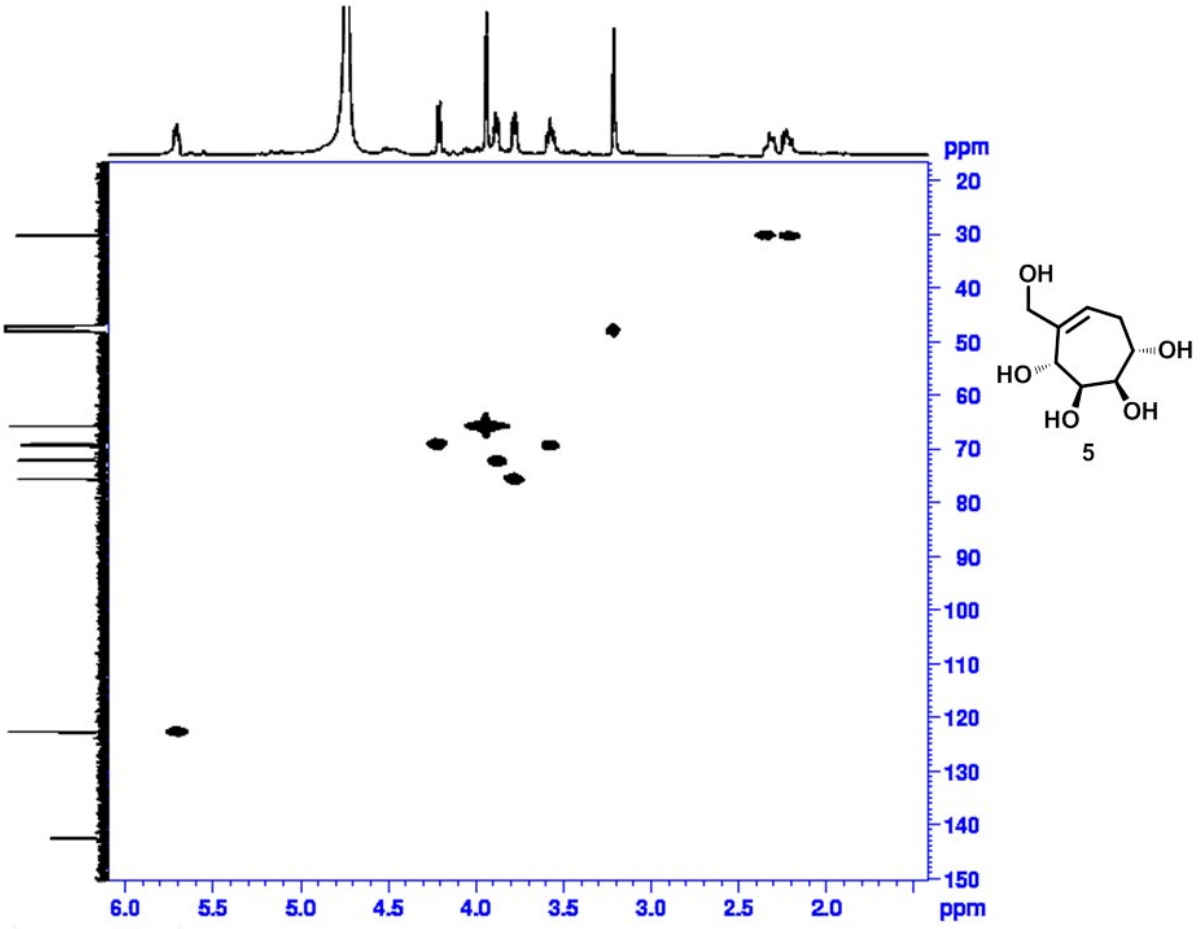
^{13}C spectrum of compound **5** recorded in CD_3OD



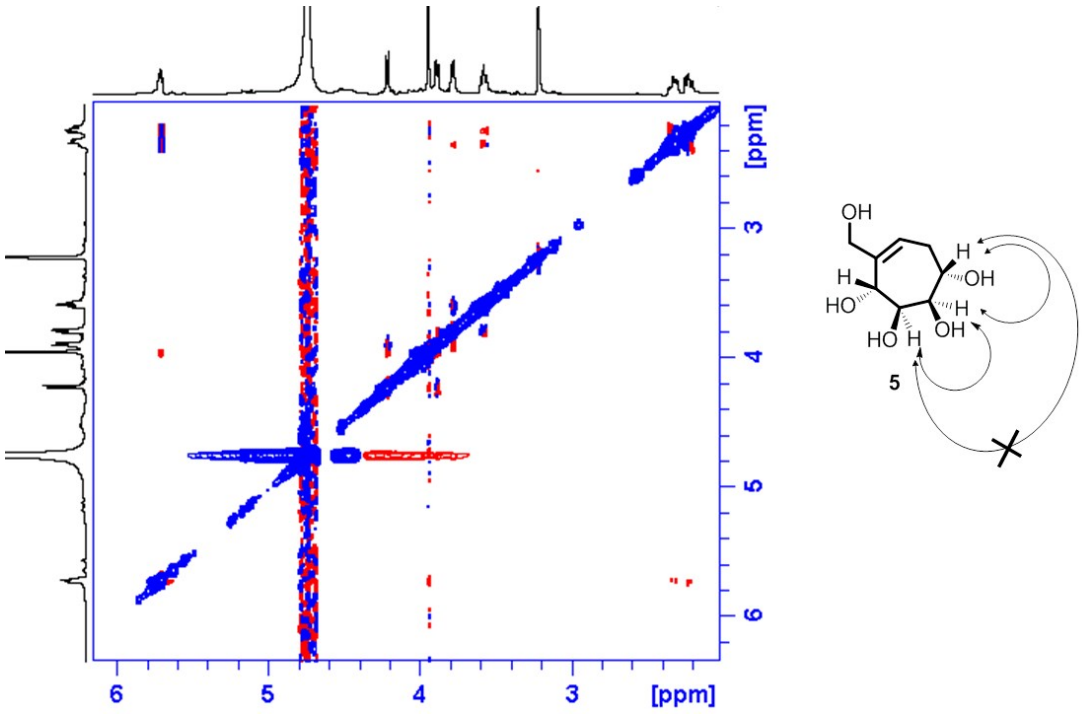
DEPT spectrum compound **5** recorded in CD_3OD



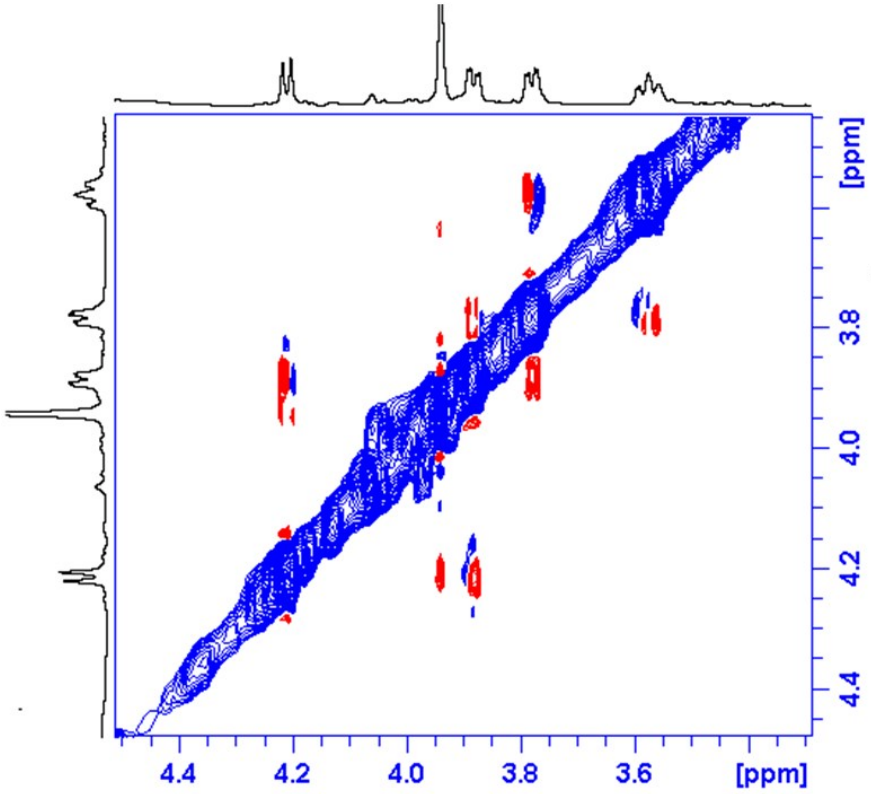
HMQC spectrum compound **5** recorded in CD_3OD



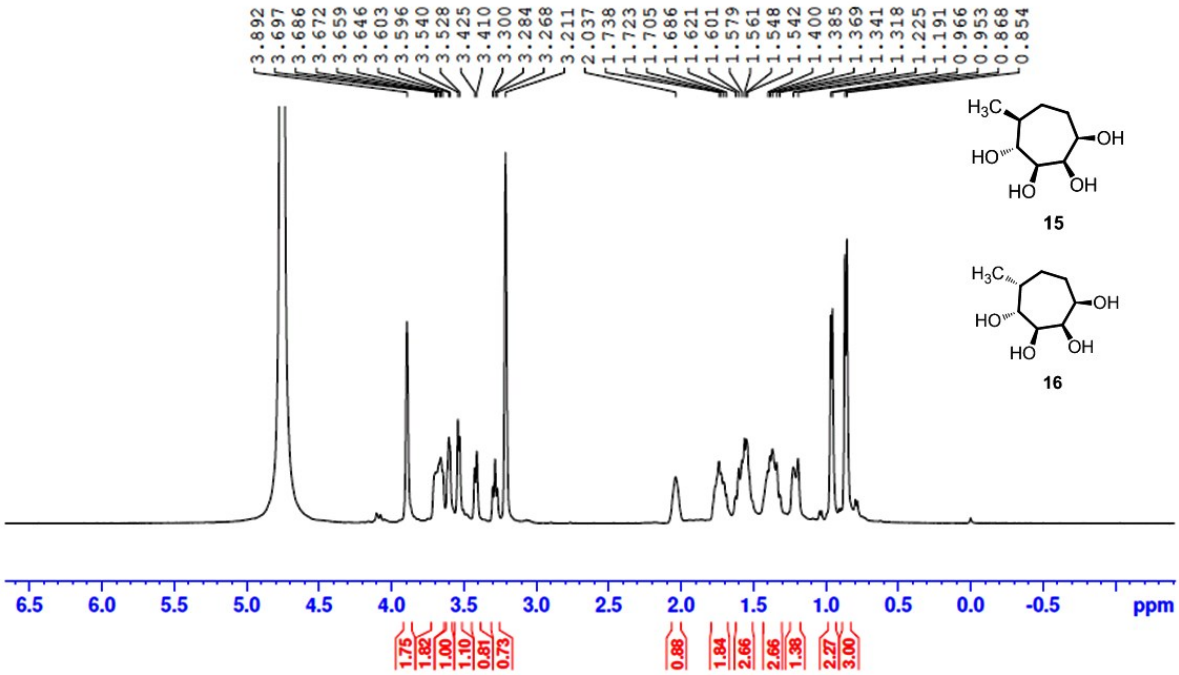
NOESY spectrum compound **5** recorded in CD_3OD



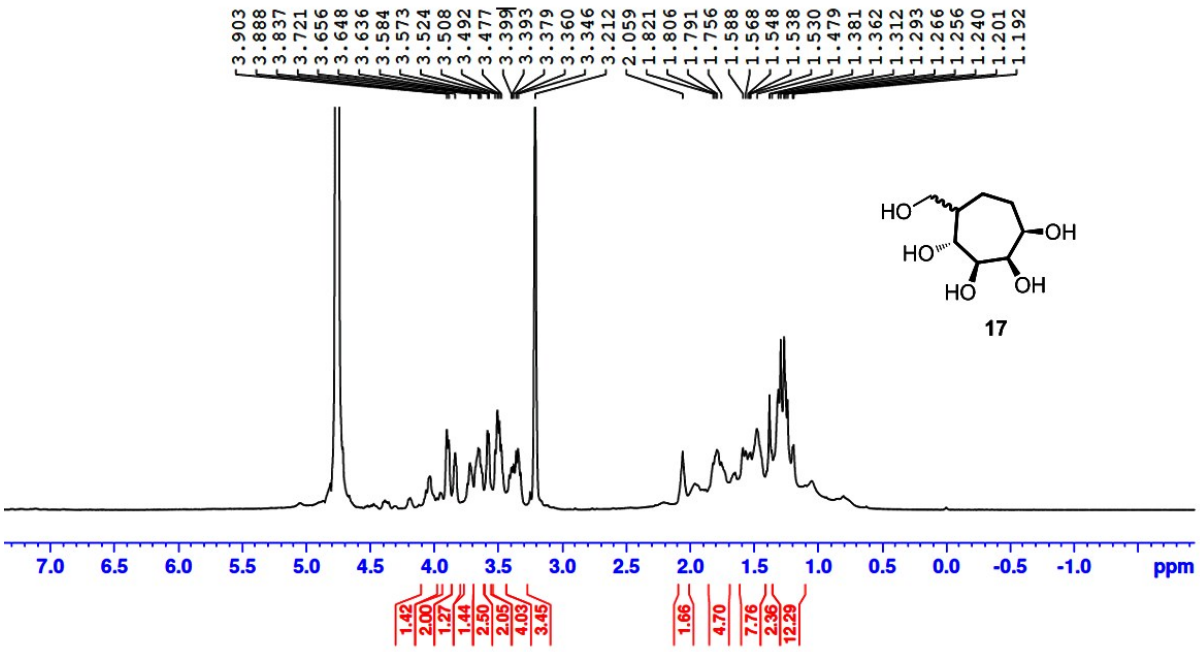
Expanded NOESY spectrum compound **5** recorded in CD_3OD



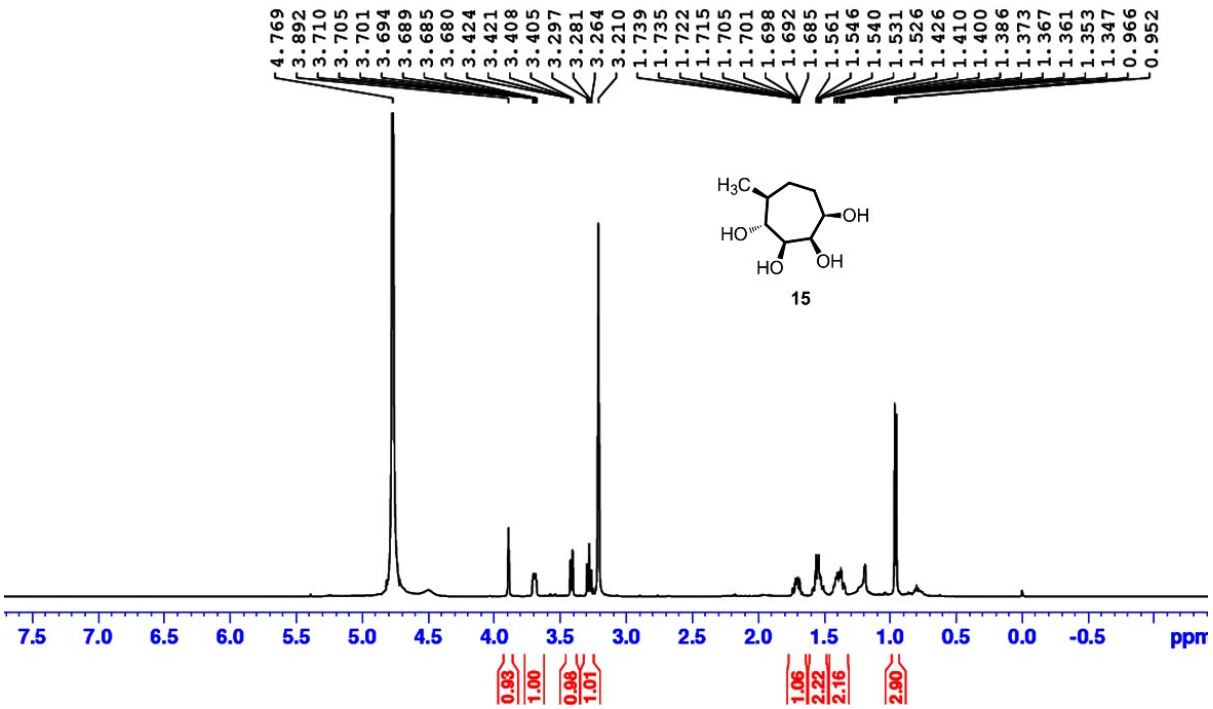
^{1}H NMR spectrum of mixture of compounds **15** (major) and **16** (minor) recorded in CD_3OD



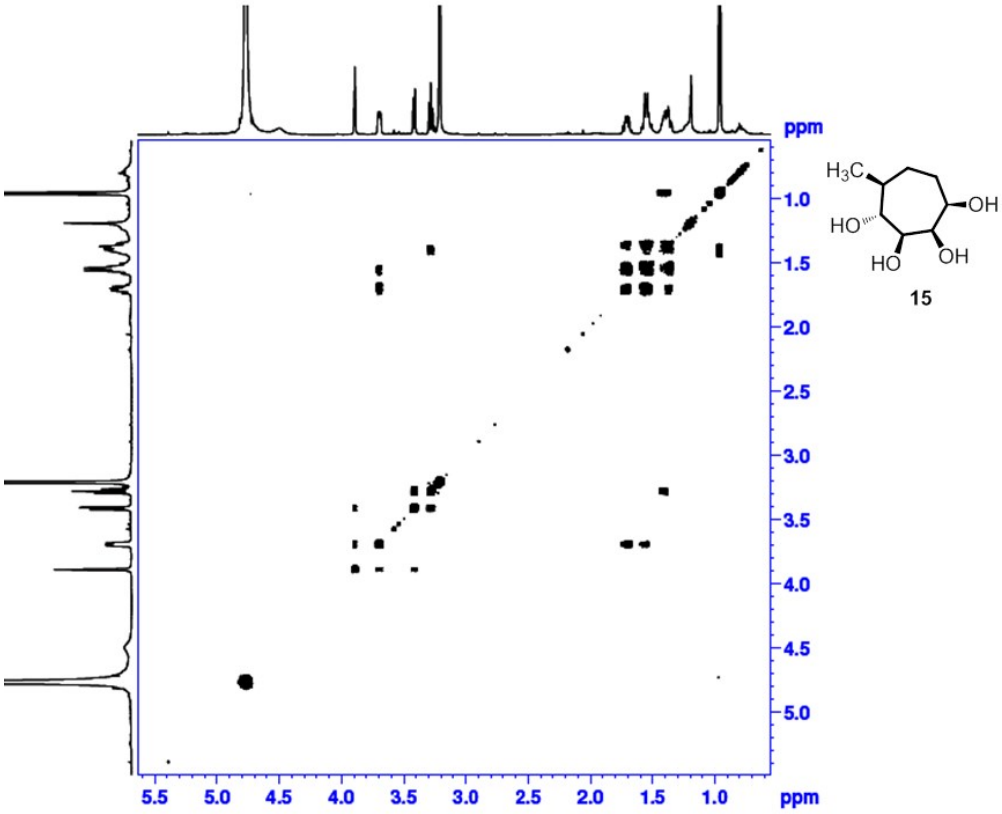
^{1}H NMR spectrum of inseparable mixture of diastereomers **17** recorded in CD_3OD



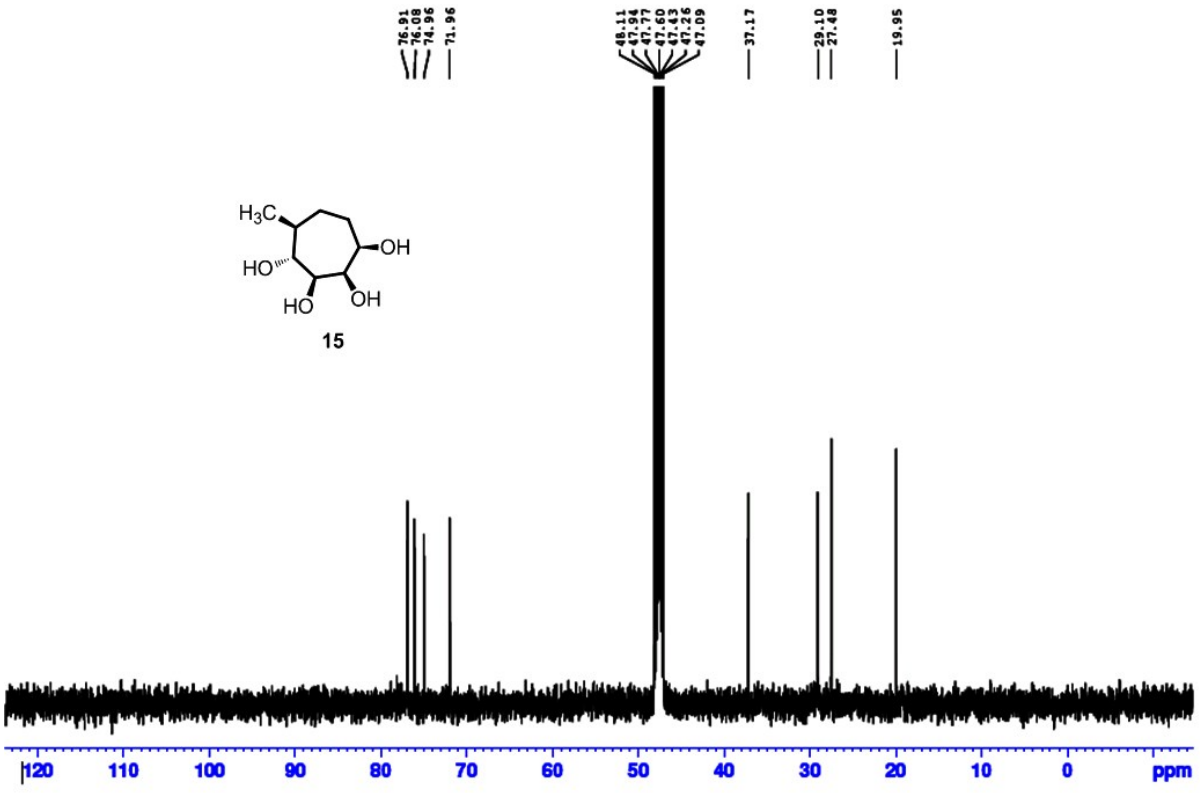
^{1}H NMR spectrum of compound **15** recorded in CD_3OD



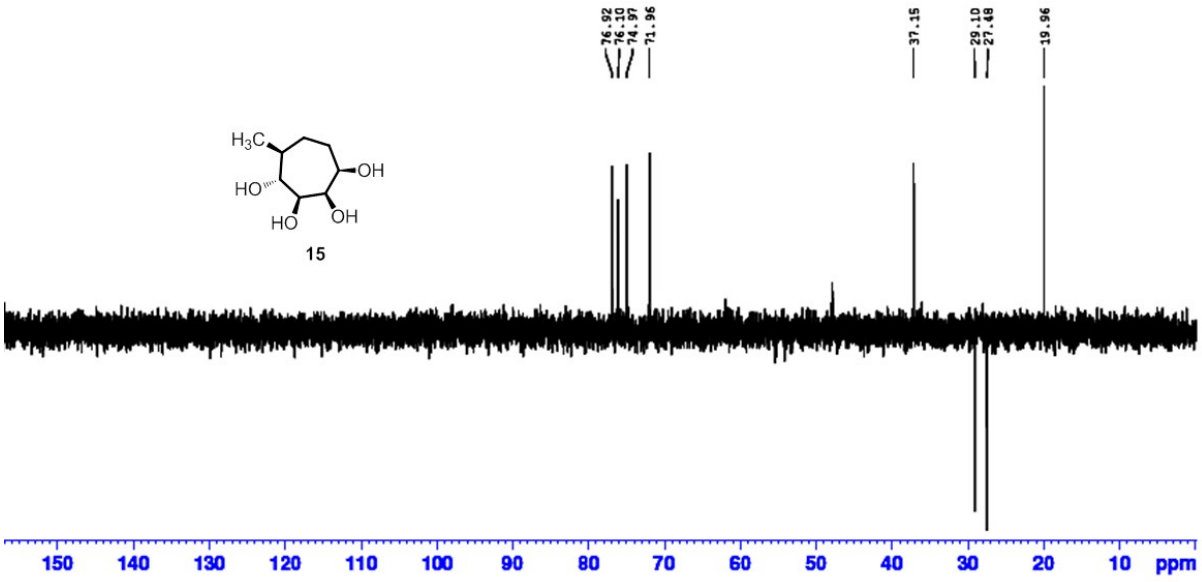
COSY spectrum of compound **15** recorded in CD_3OD



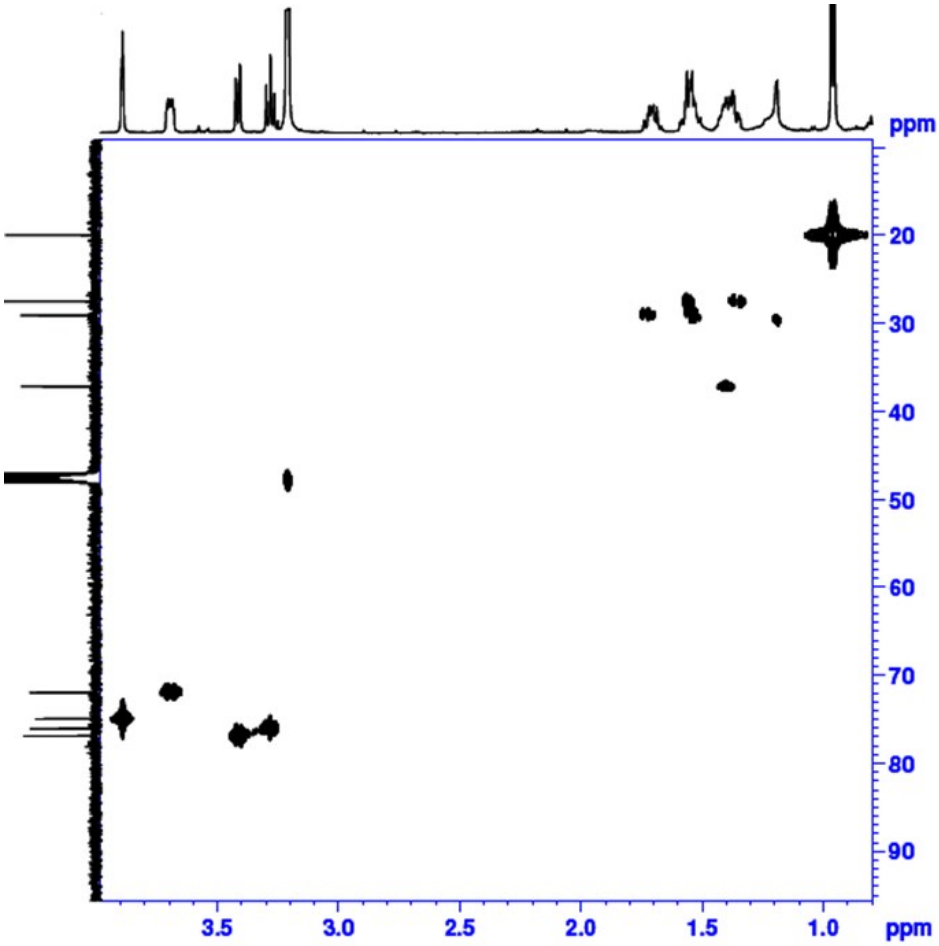
^{13}C spectrum of compound **15** recorded in CD_3OD

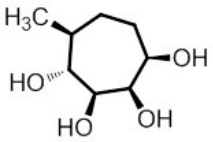


DEPT spectrum of compound **15** recorded in CD_3OD



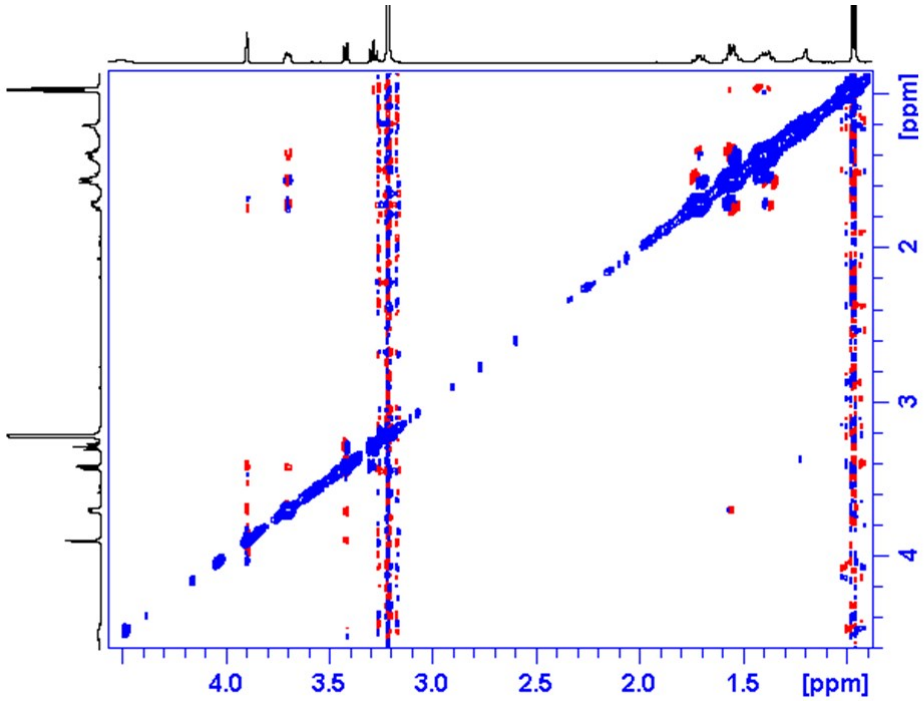
HMQC spectrum of compound **15** recorded in CD_3OD

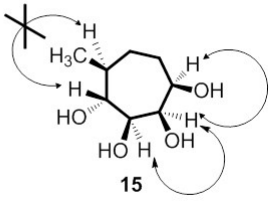




15

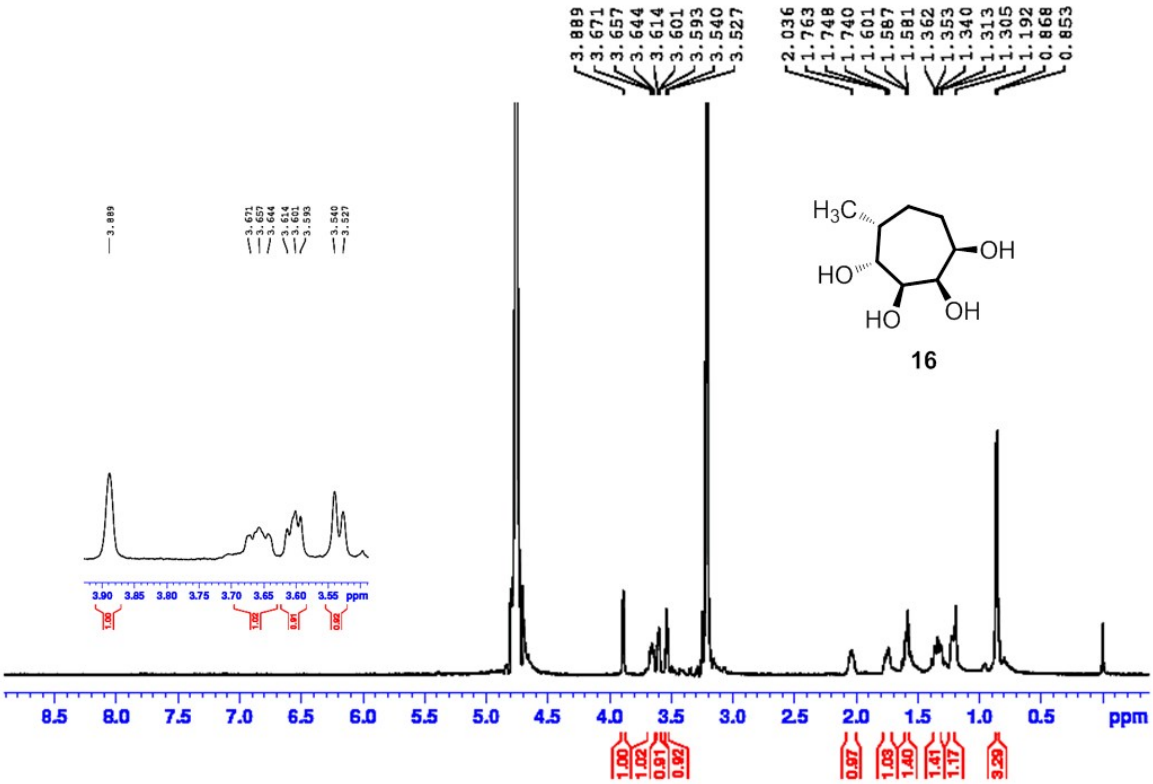
NOESY spectrum of compound **15** recorded in CD_3OD



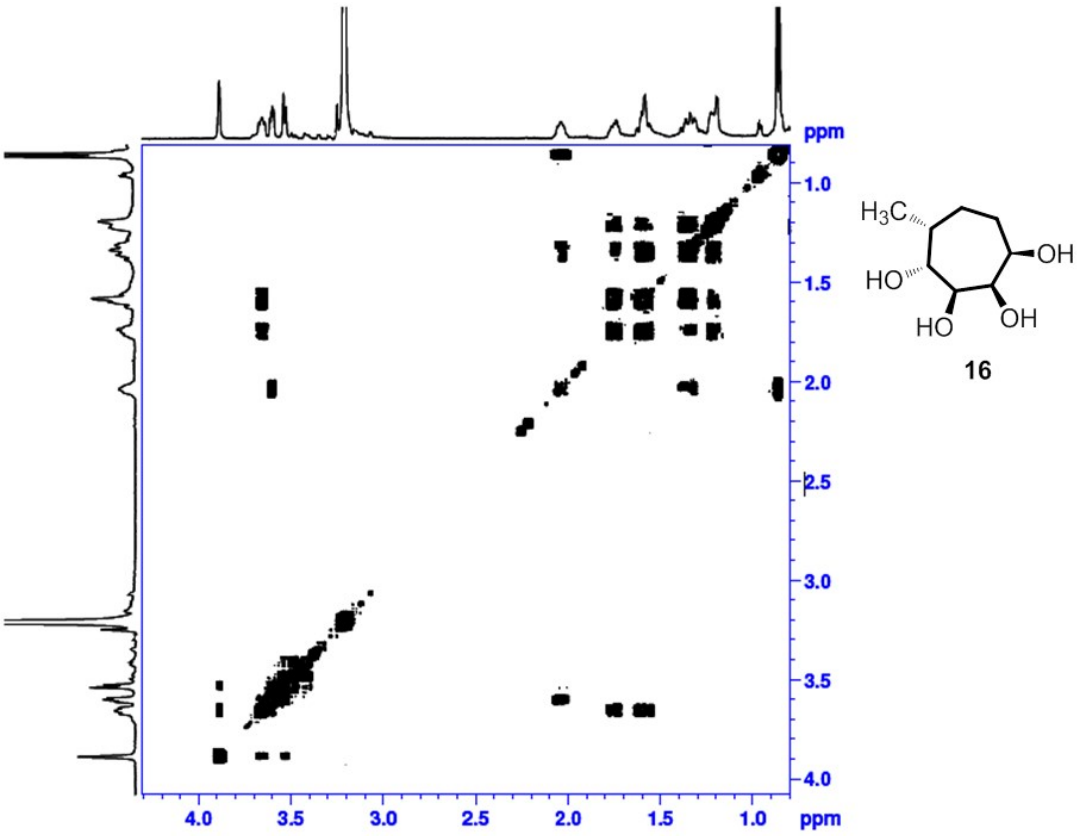


15

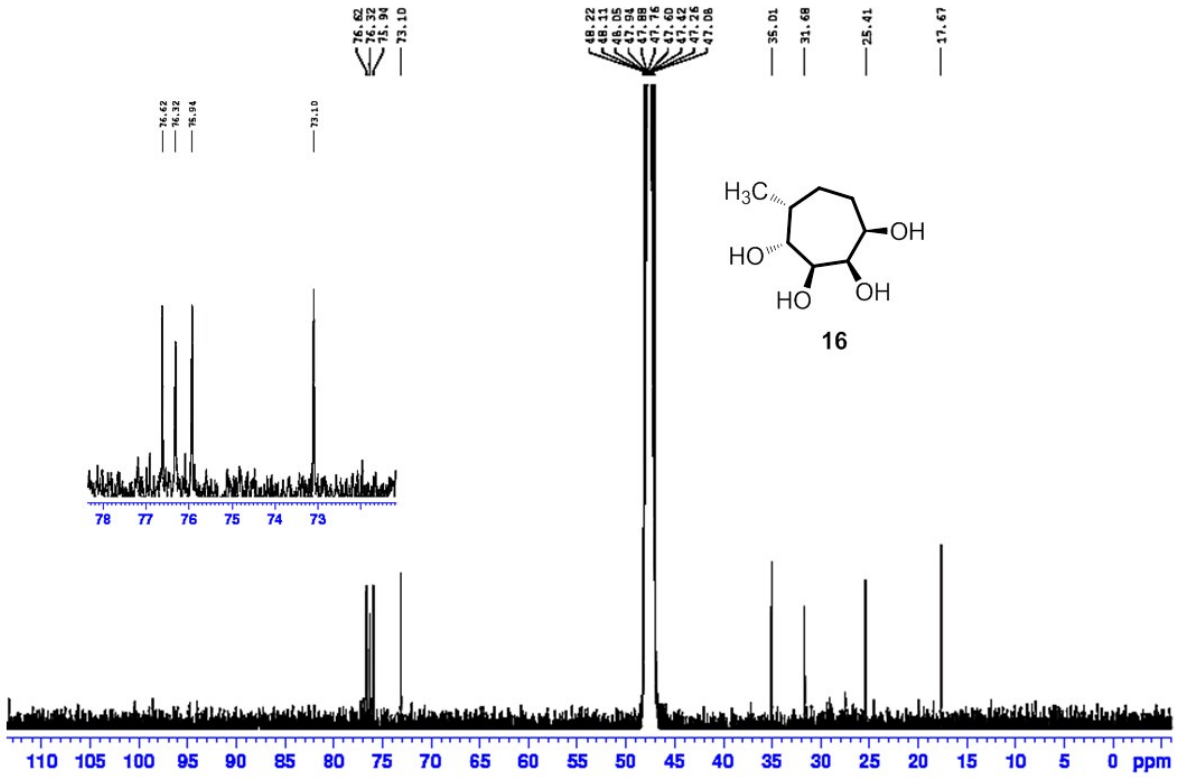
^{1}H spectrum of compound **16** recorded in CD_3OD



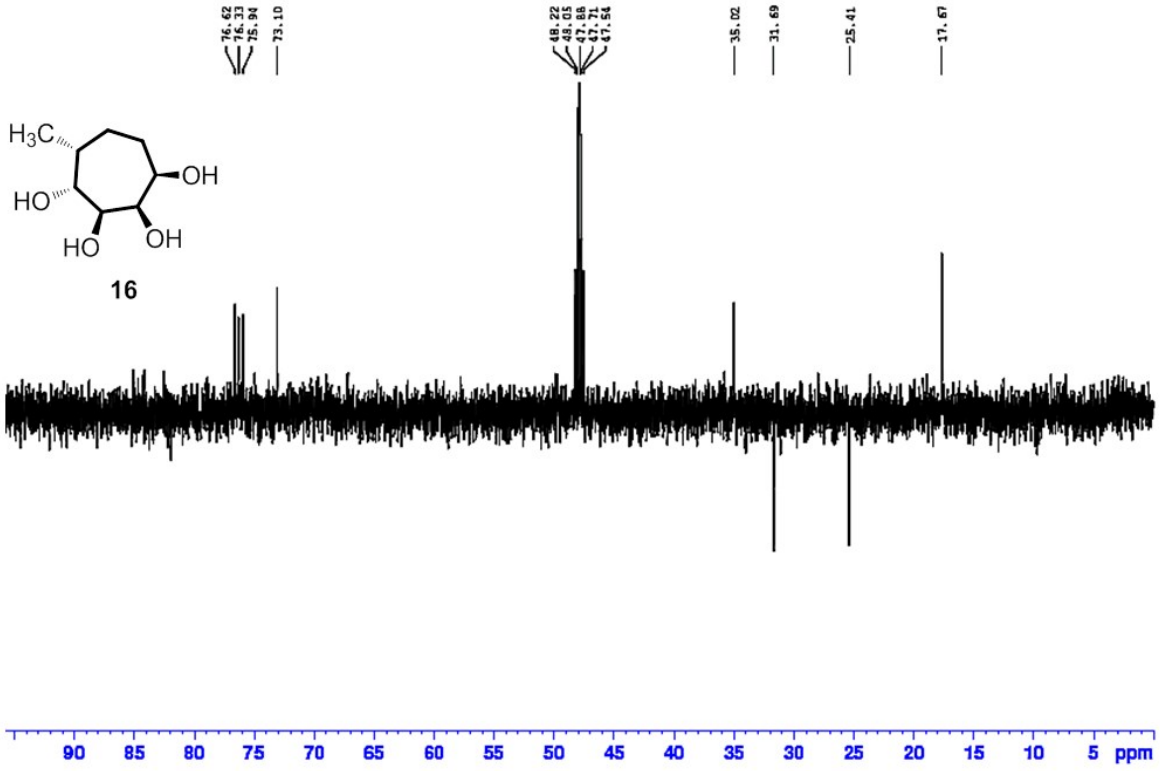
COSY spectrum of compound **16** recorded in CD_3OD



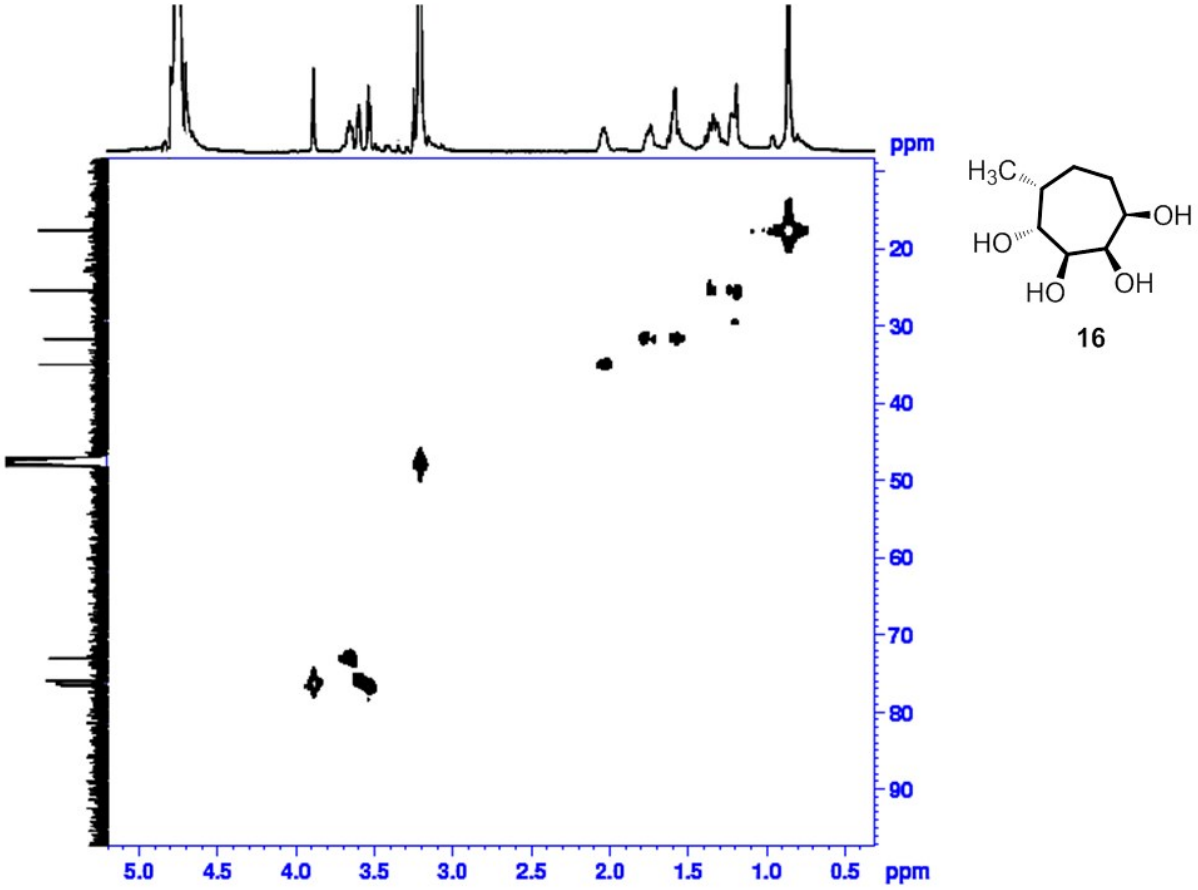
^{13}C NMR spectrum of compound **16** recorded in CD_3OD



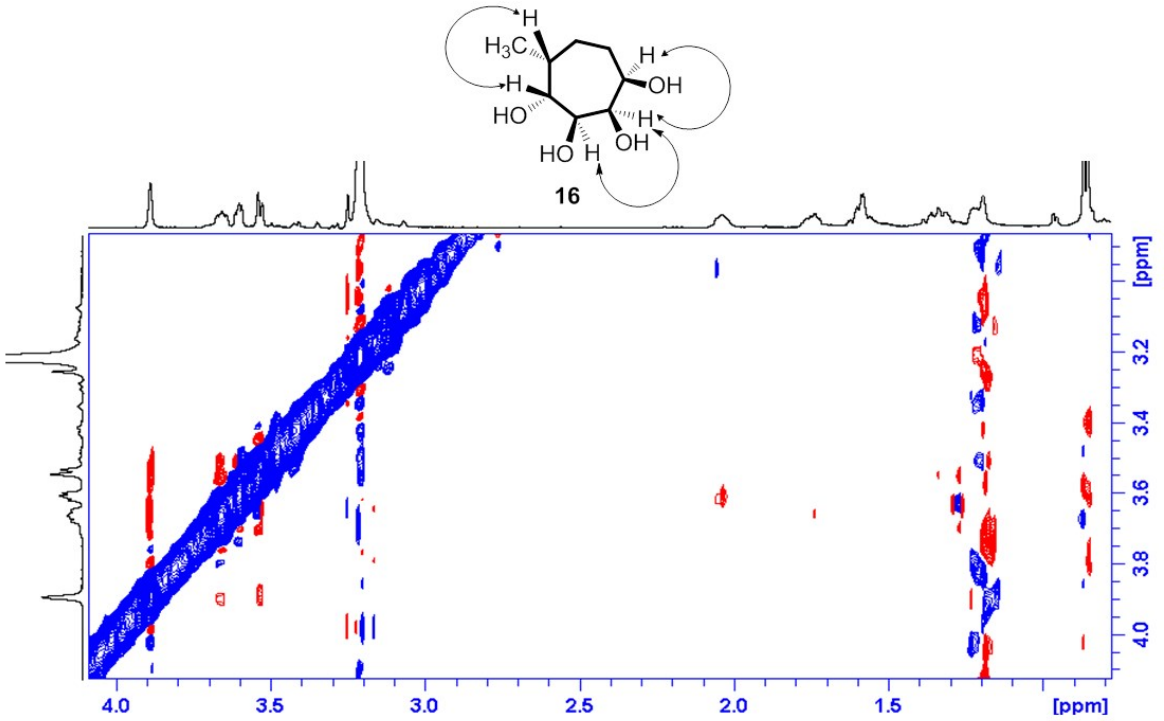
DEPT spectrum of compound **16** recorded in CD_3OD



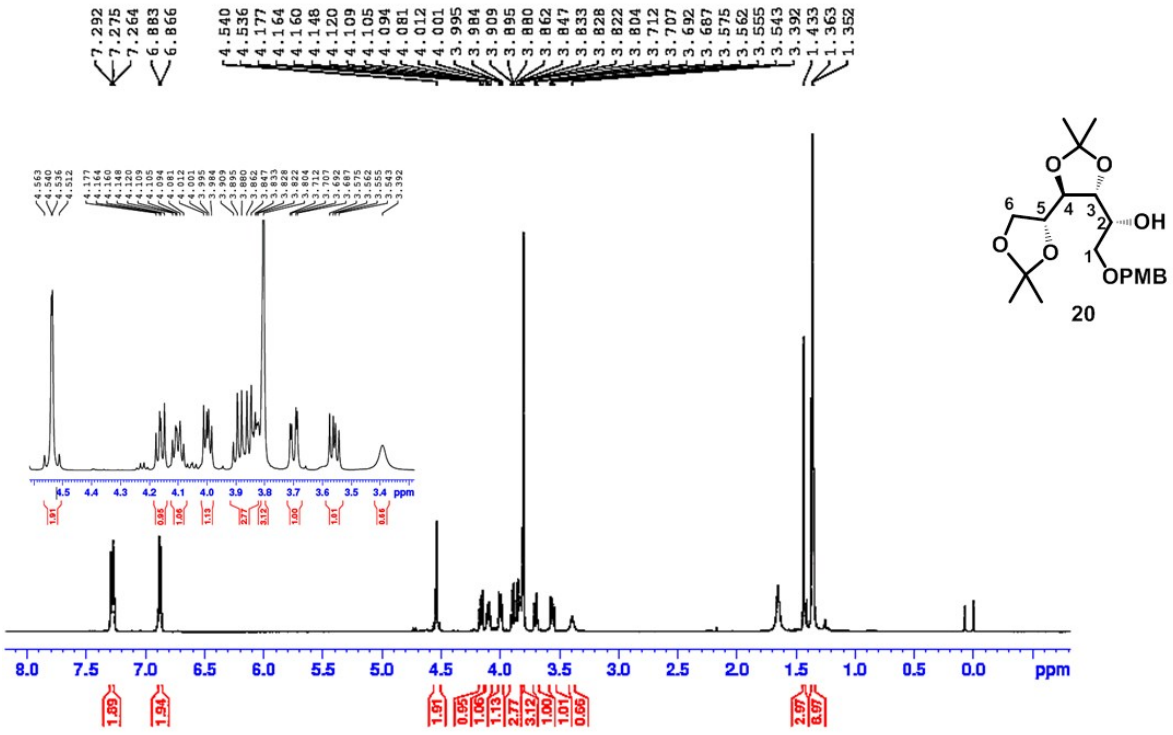
HMQC spectrum of compound **16** recorded in CD_3OD



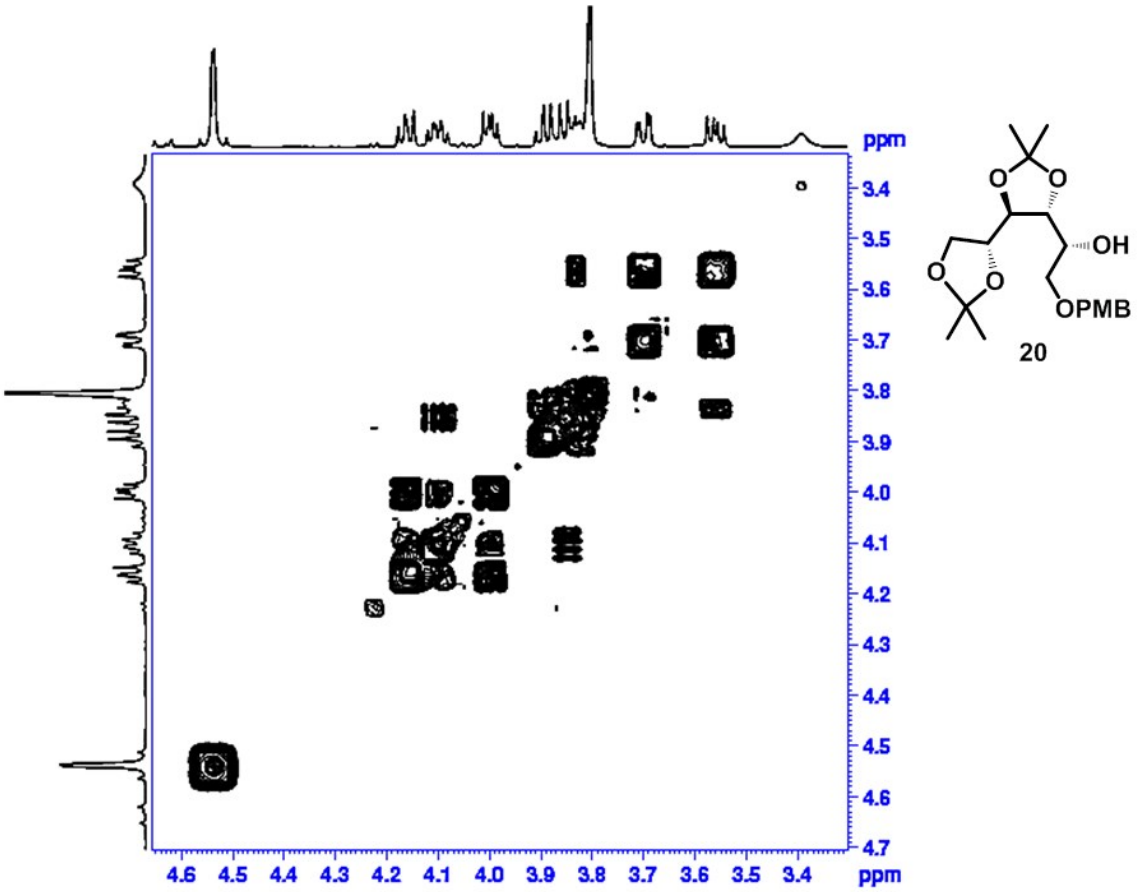
NOESY spectrum of compound **16** recorded in CD_3OD



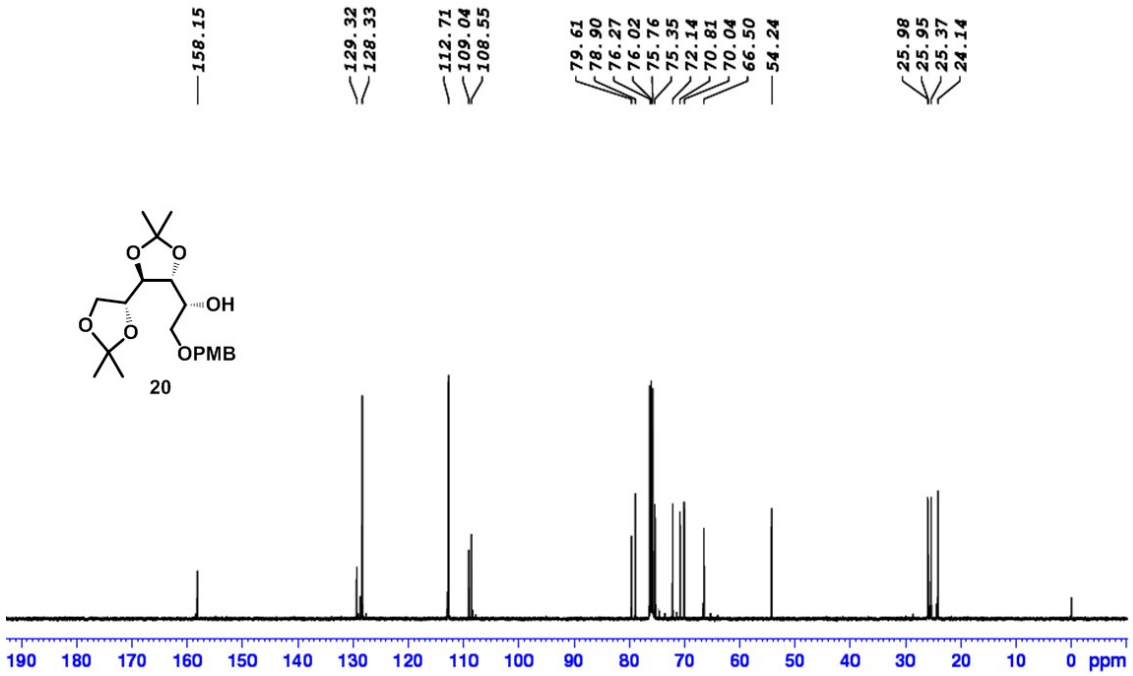
^1H NMR spectrum of compound **20** recorded in $CDCl_3$



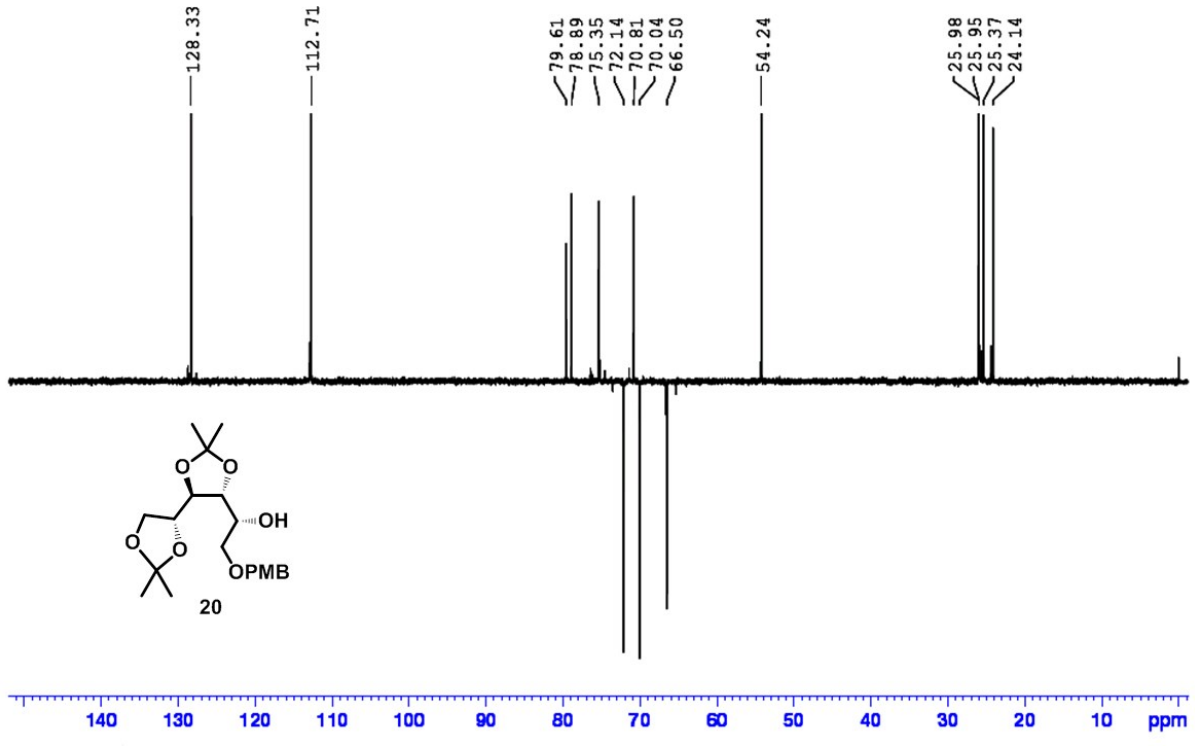
COSY spectrum of compound **20** recorded in $CDCl_3$



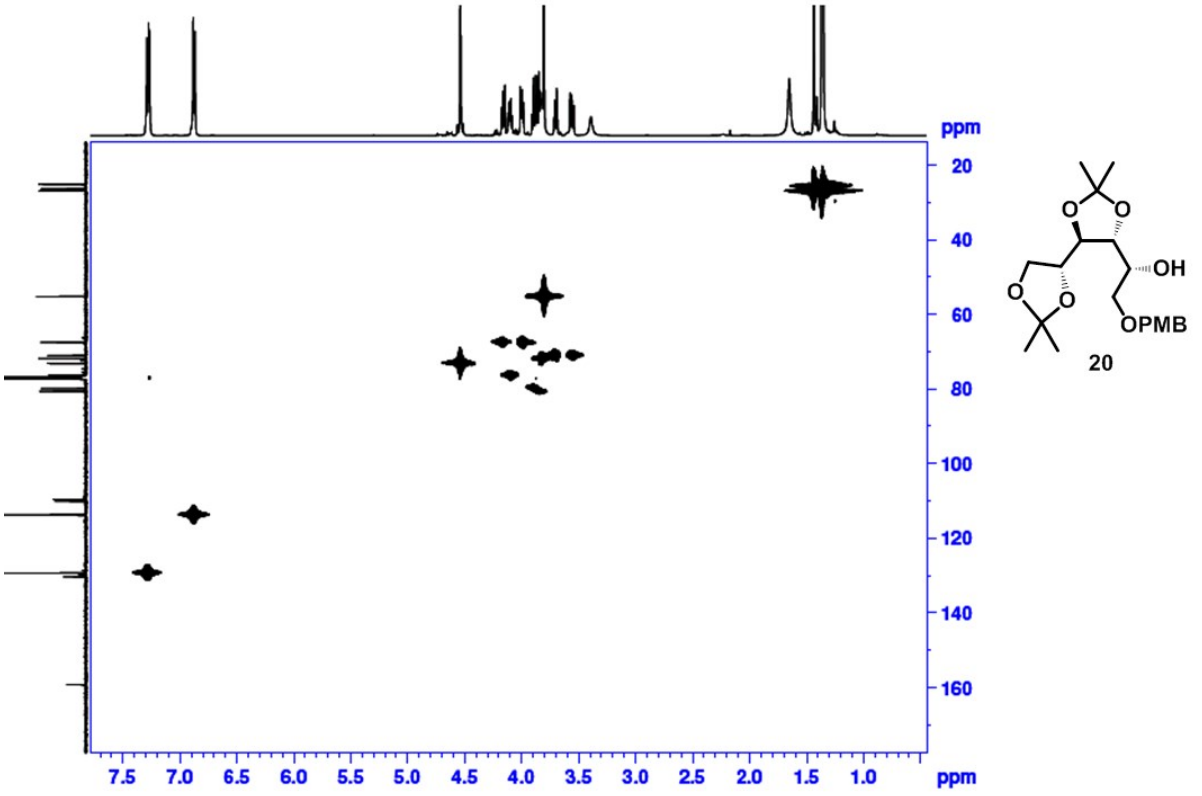
^{13}C spectrum of compound **20** recorded in $CDCl_3$



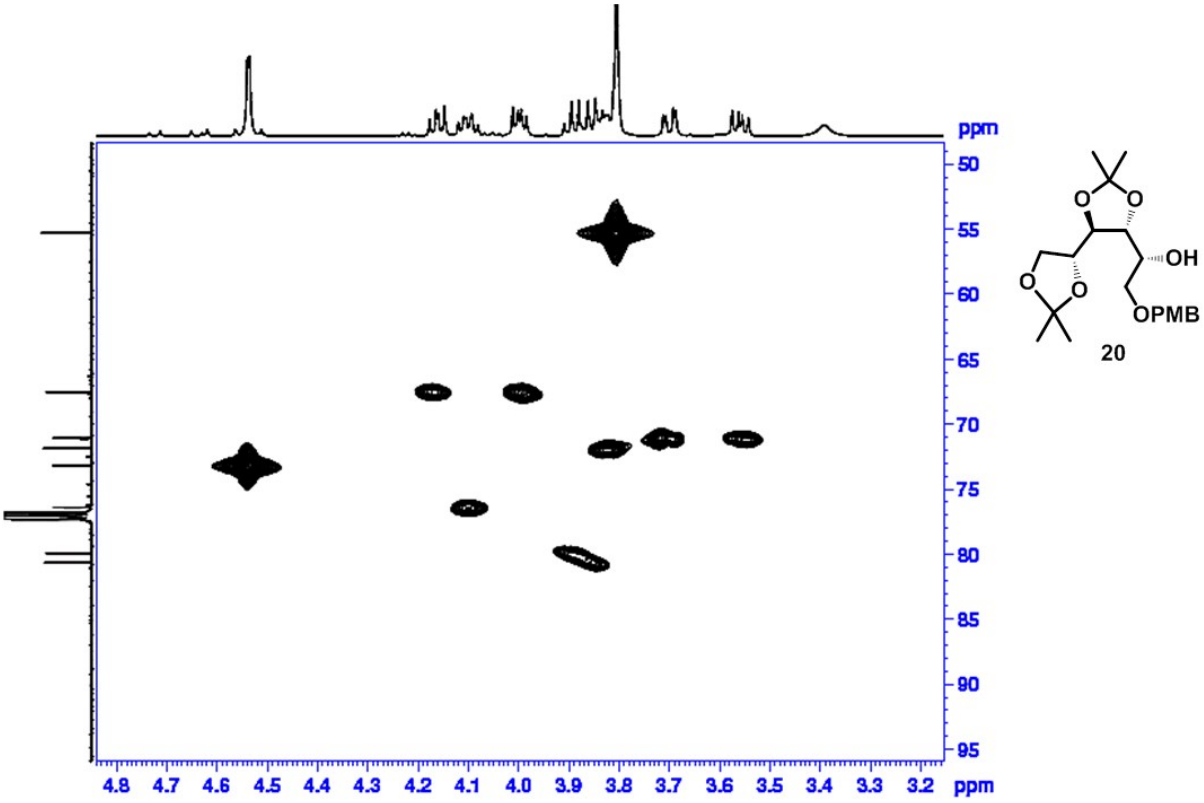
DEPT spectrum of compound **20** recorded in $CDCl_3$



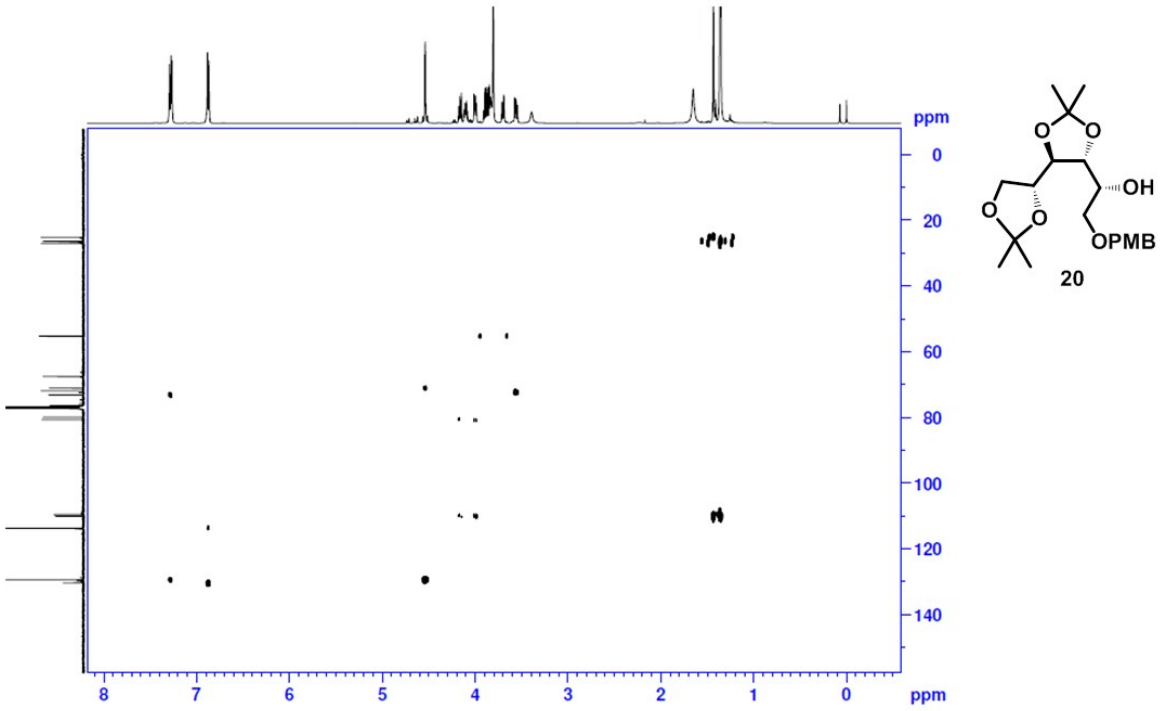
HMQC spectrum of compound **20** recorded in $CDCl_3$



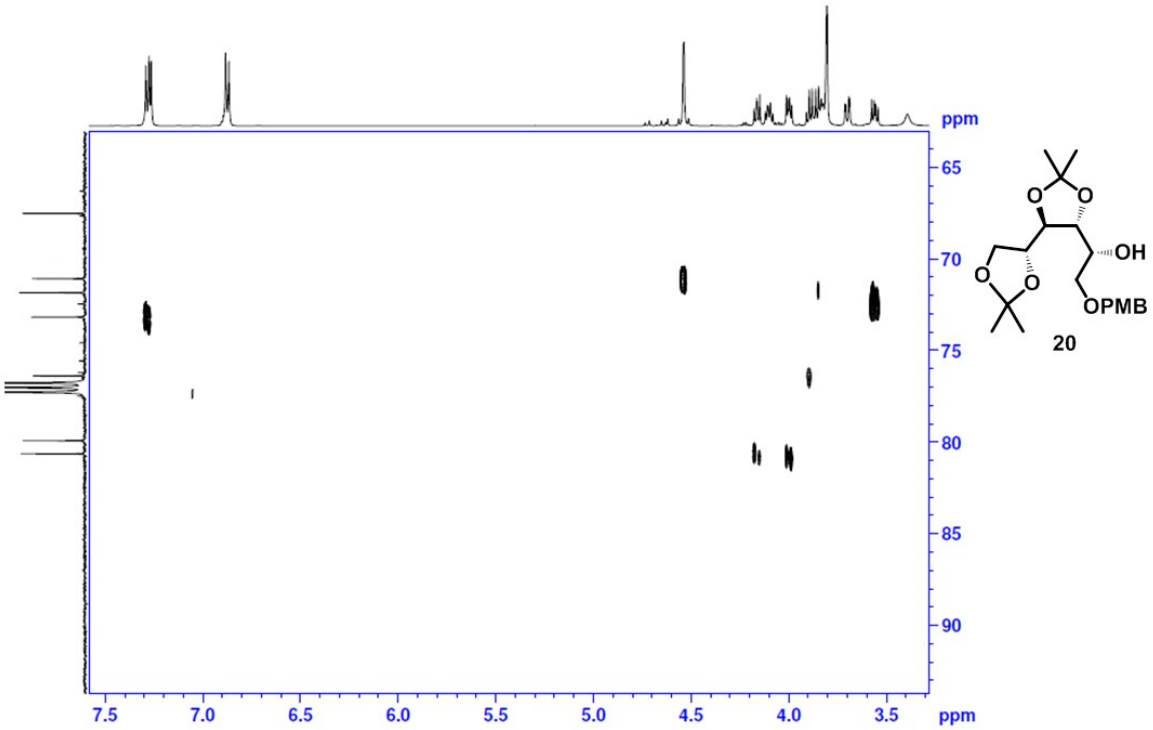
Expanded HMQC spectrum of compound **20** recorded in $CDCl_3$



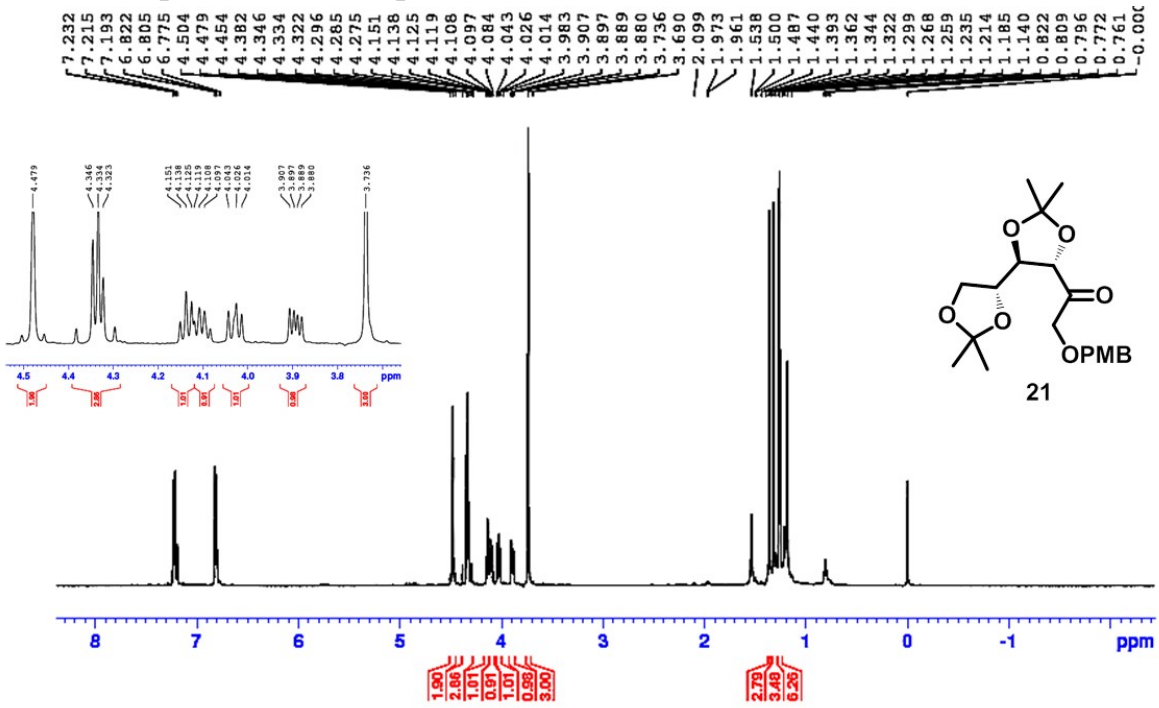
HMBC spectrum of compound **20** recorded in $CDCl_3$



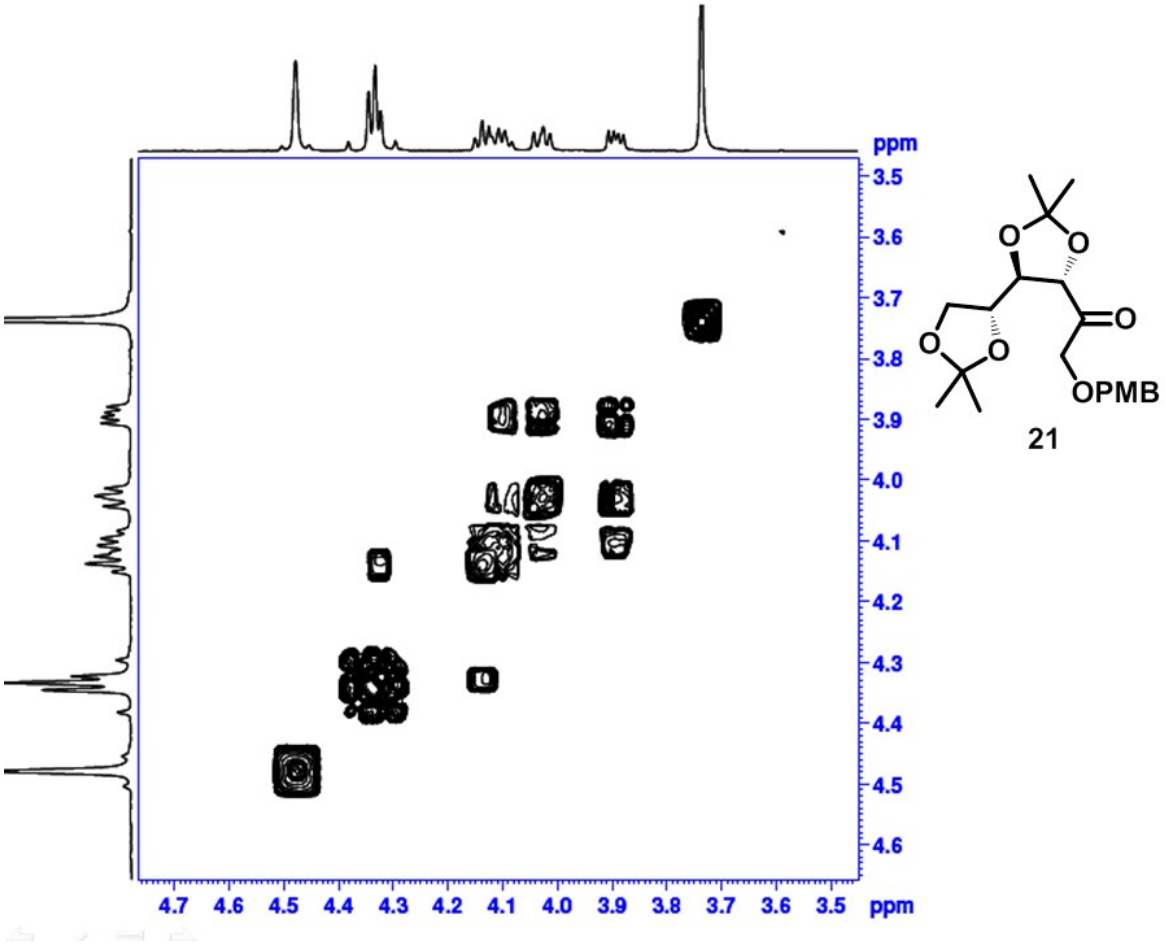
Expanded HMBC spectrum of compound **20** recorded in $CDCl_3$



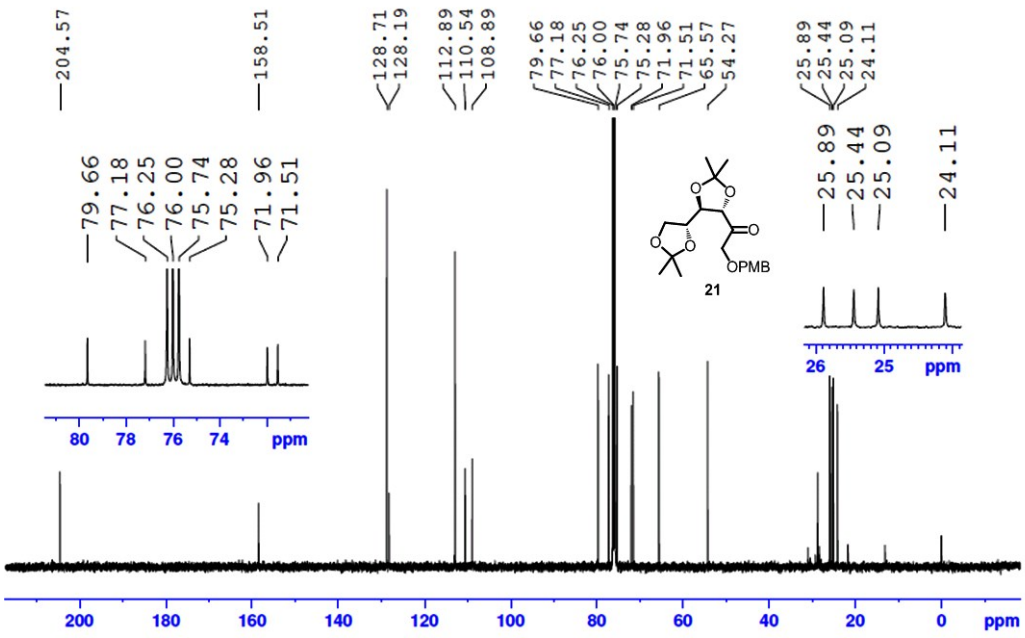
^{1}H NMR spectrum of compound **21** recorded in $CDCl_3$



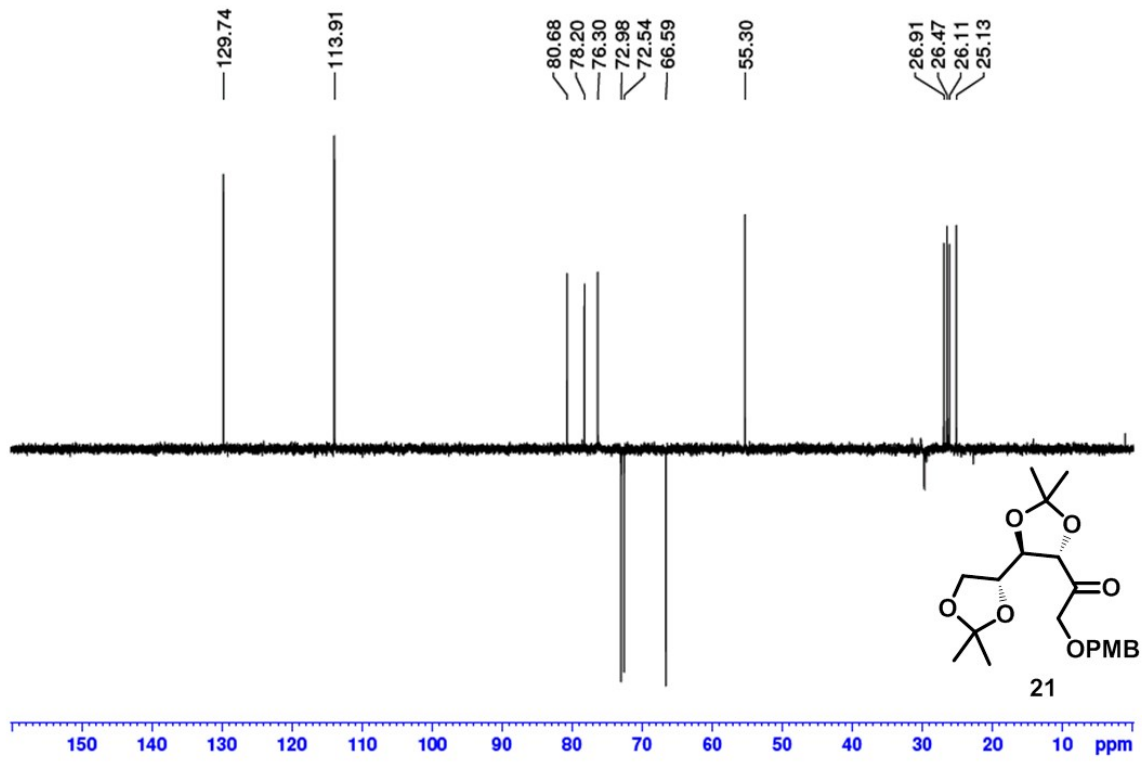
COSY spectrum of compound **21** recorded in $CDCl_3$



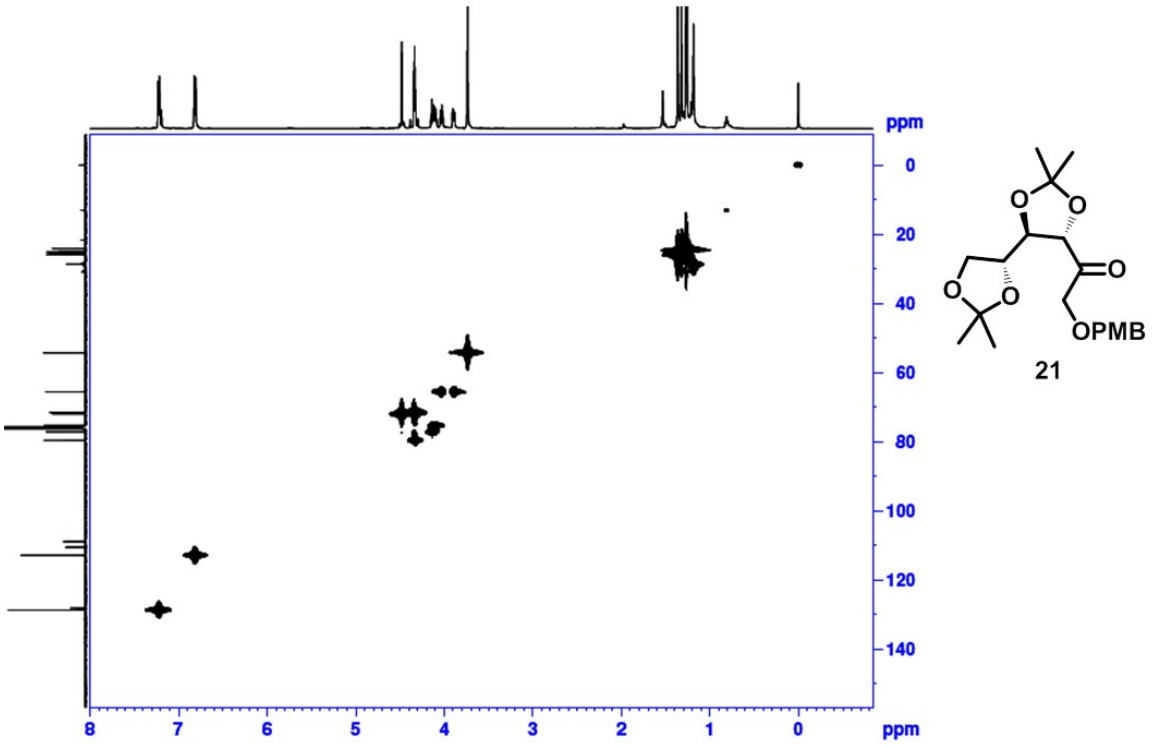
^{13}C spectrum of compound **21** recorded in $CDCl_3$



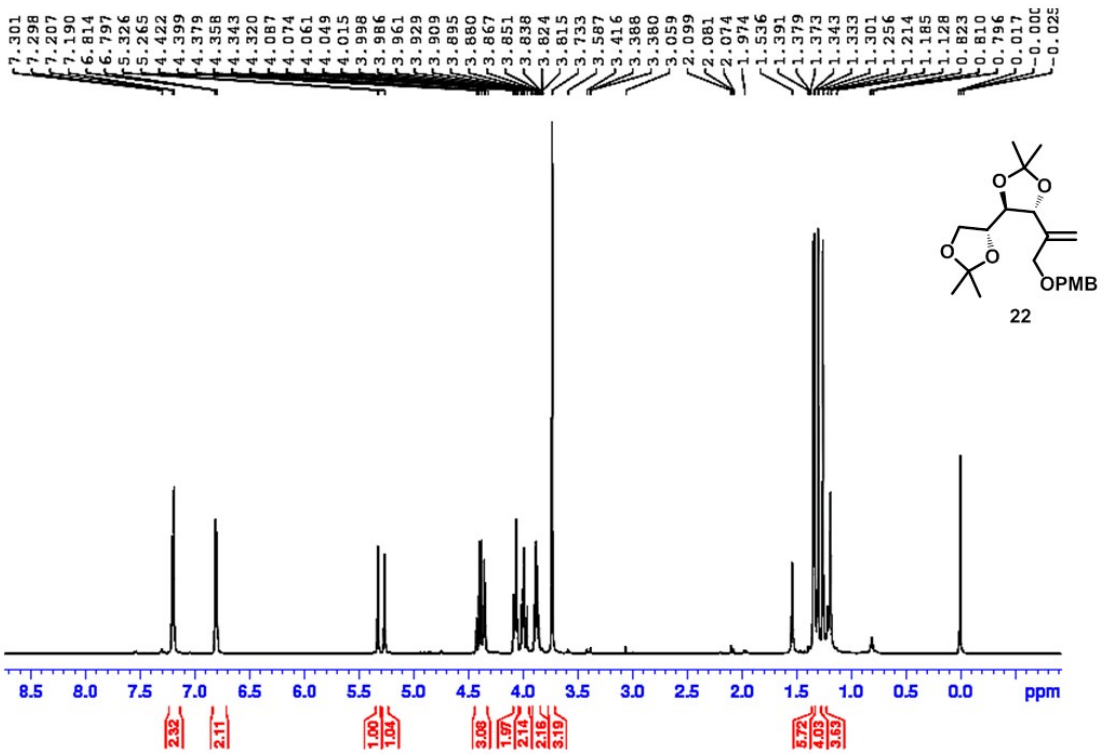
DEPT spectrum of compound **21** recorded in $CDCl_3$



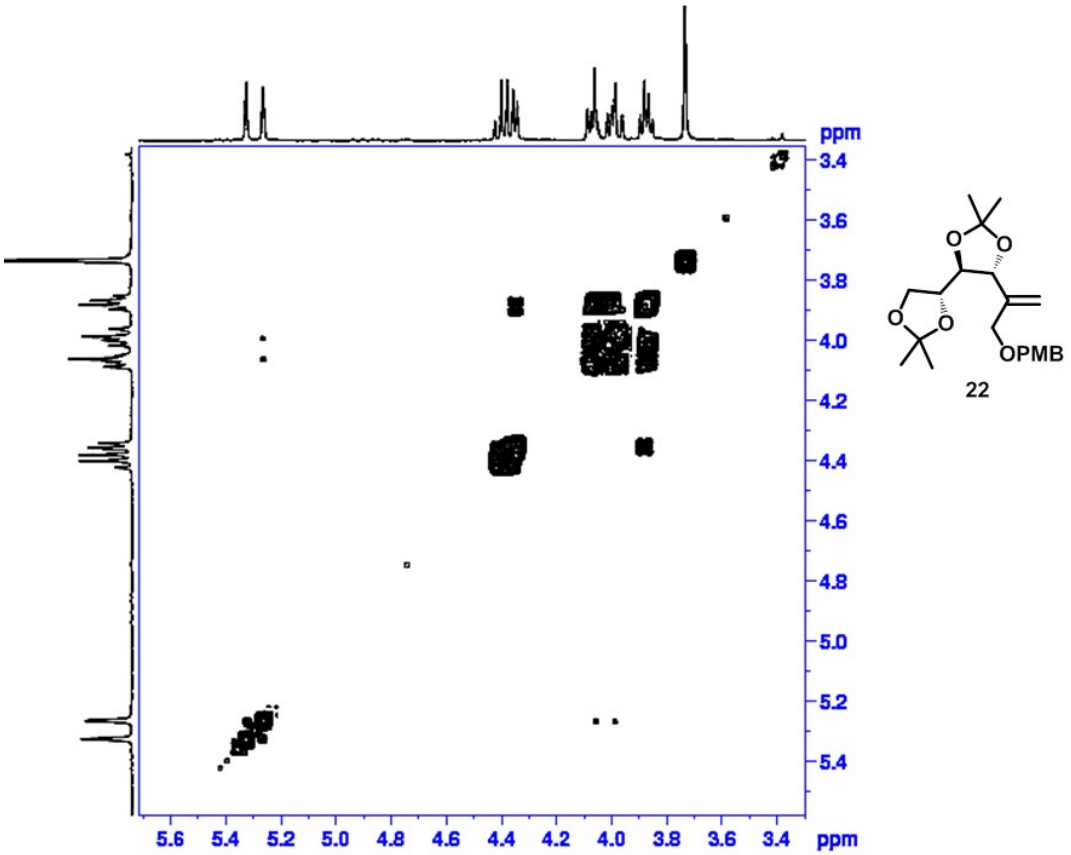
HMQC spectrum of compound **21** recorded in $CDCl_3$



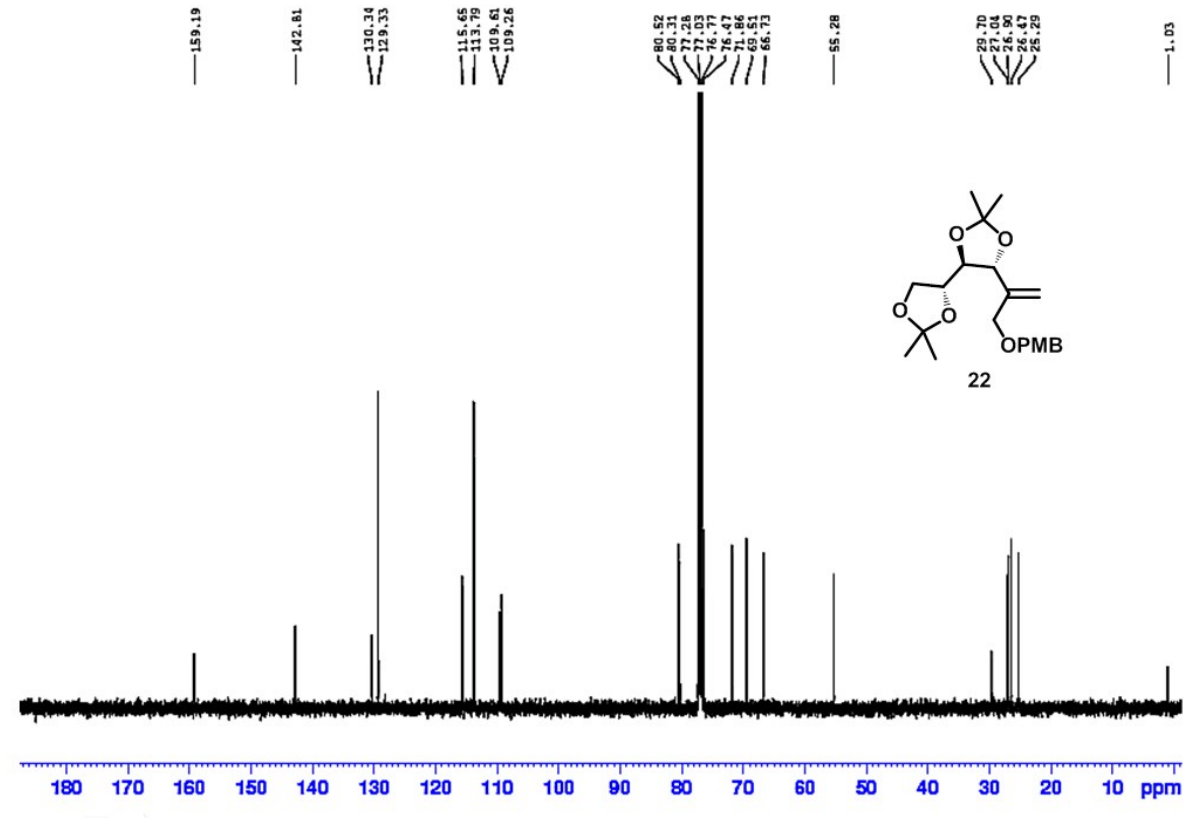
^{1}H NMR spectrum of compound **22** recorded in $CDCl_3$



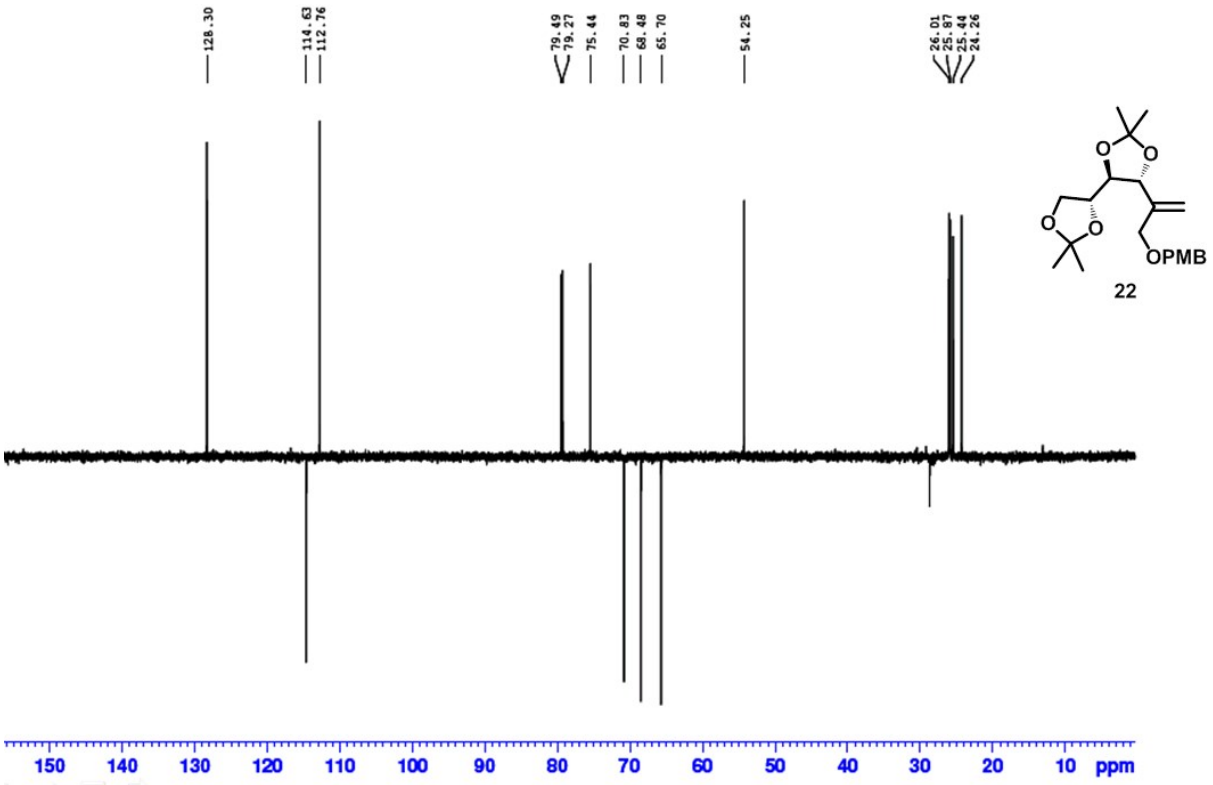
COSY spectrum of compound **22** recorded in $CDCl_3$



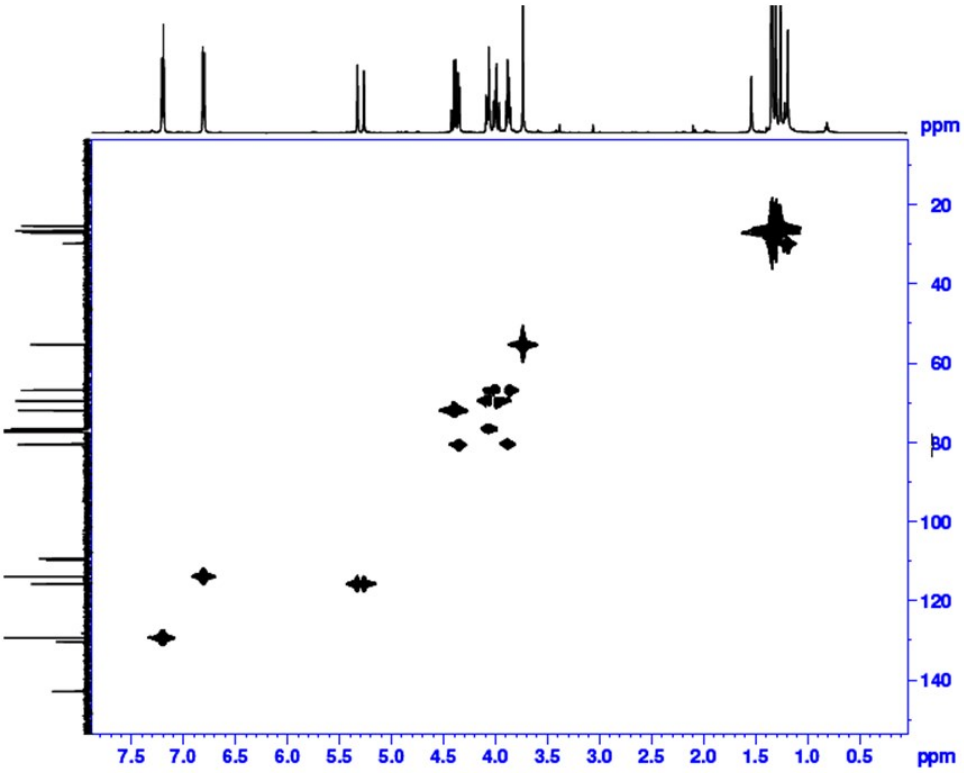
^{13}C spectrum of compound **22** recorded in $CDCl_3$

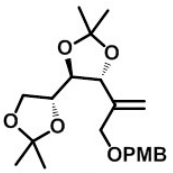


DEPT spectrum of compound **22** recorded in $CDCl_3$



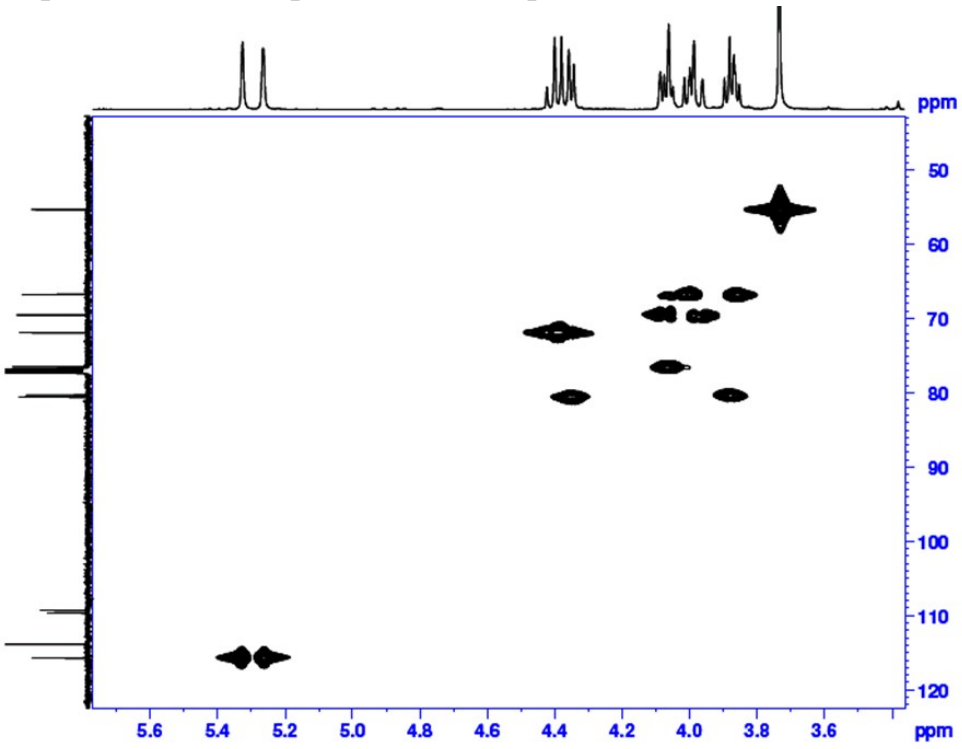
HMQC spectrum of compound **22** recorded in $CDCl_3$

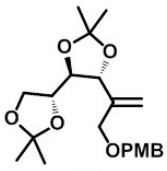




22

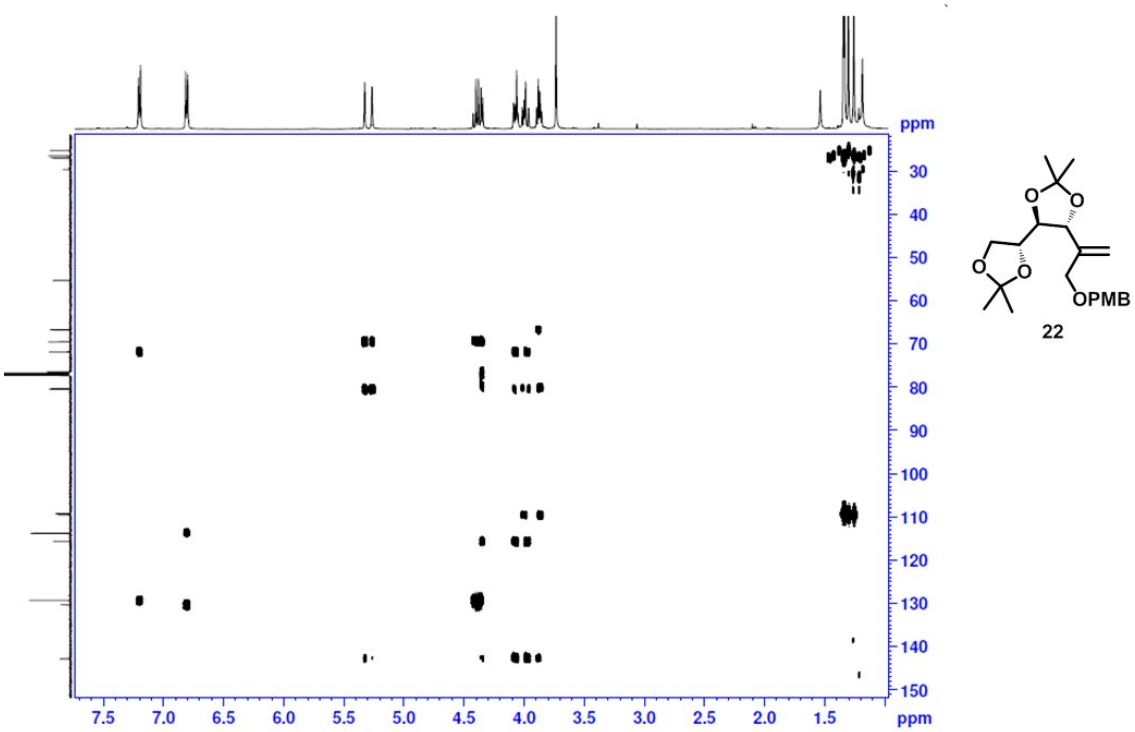
Expanded HMQC spectrum of compound **22** recorded in $CDCl_3$



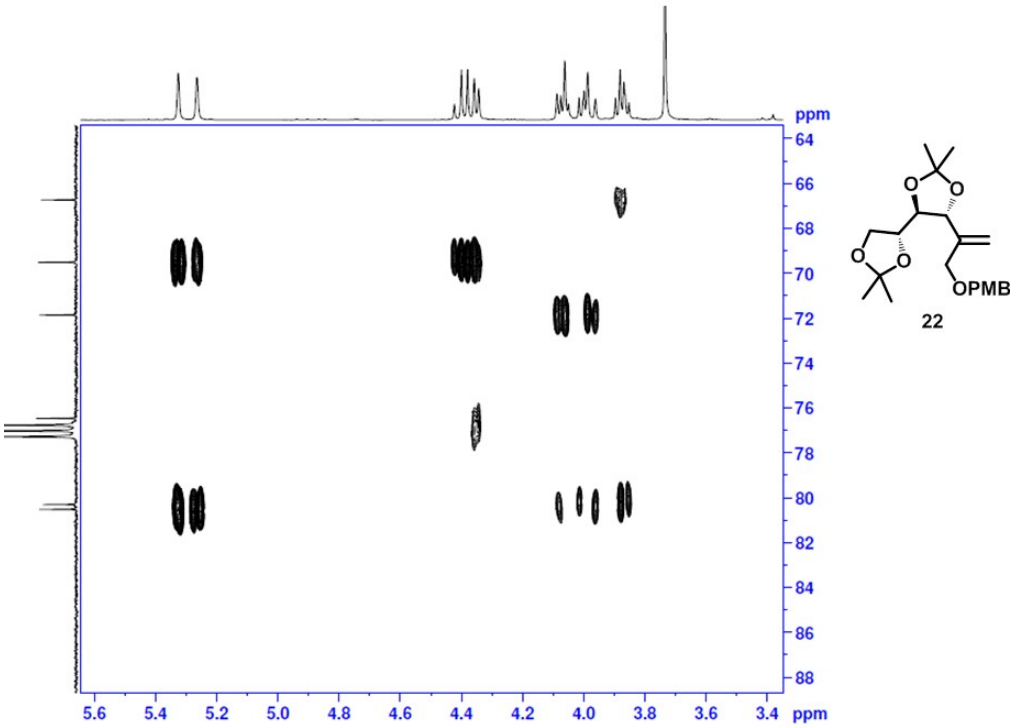


22

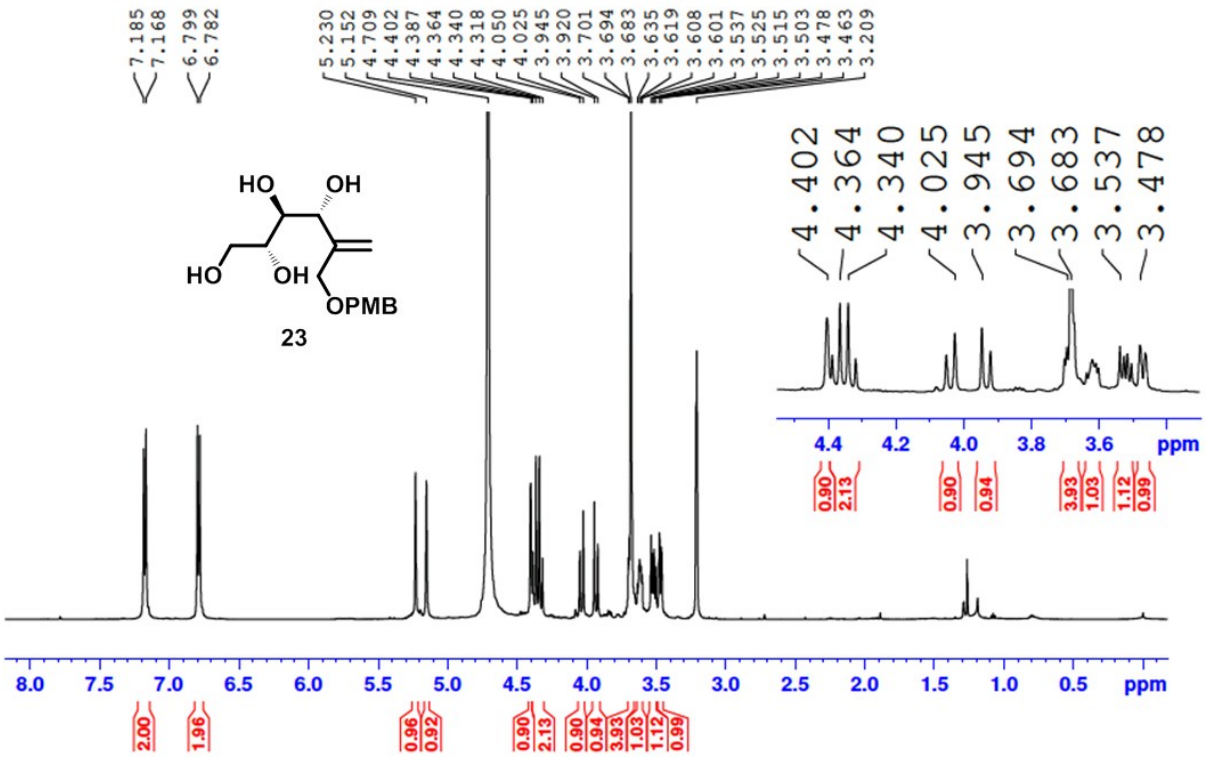
HMBC spectrum of compound **22** recorded in $CDCl_3$



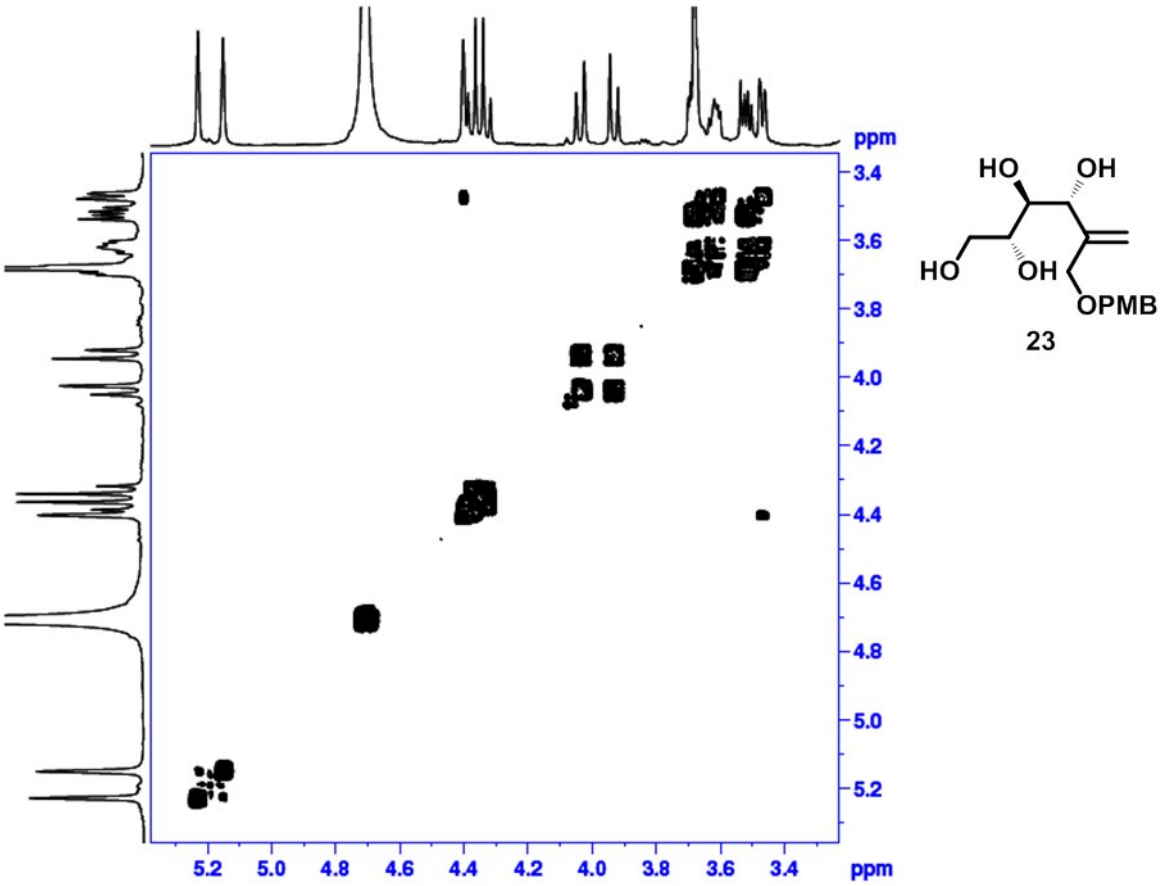
Expanded HMBC spectrum of compound **22** recorded in $CDCl_3$



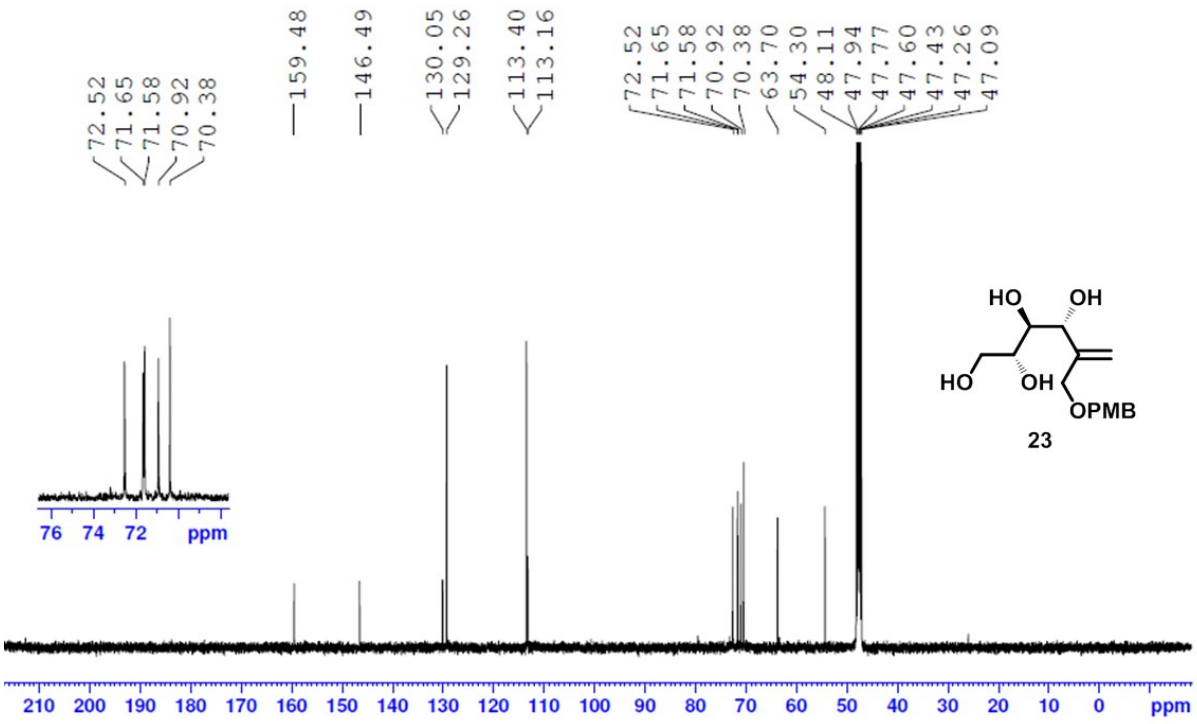
^{1}H NMR spectrum of compound **23** recorded in CD_3OD



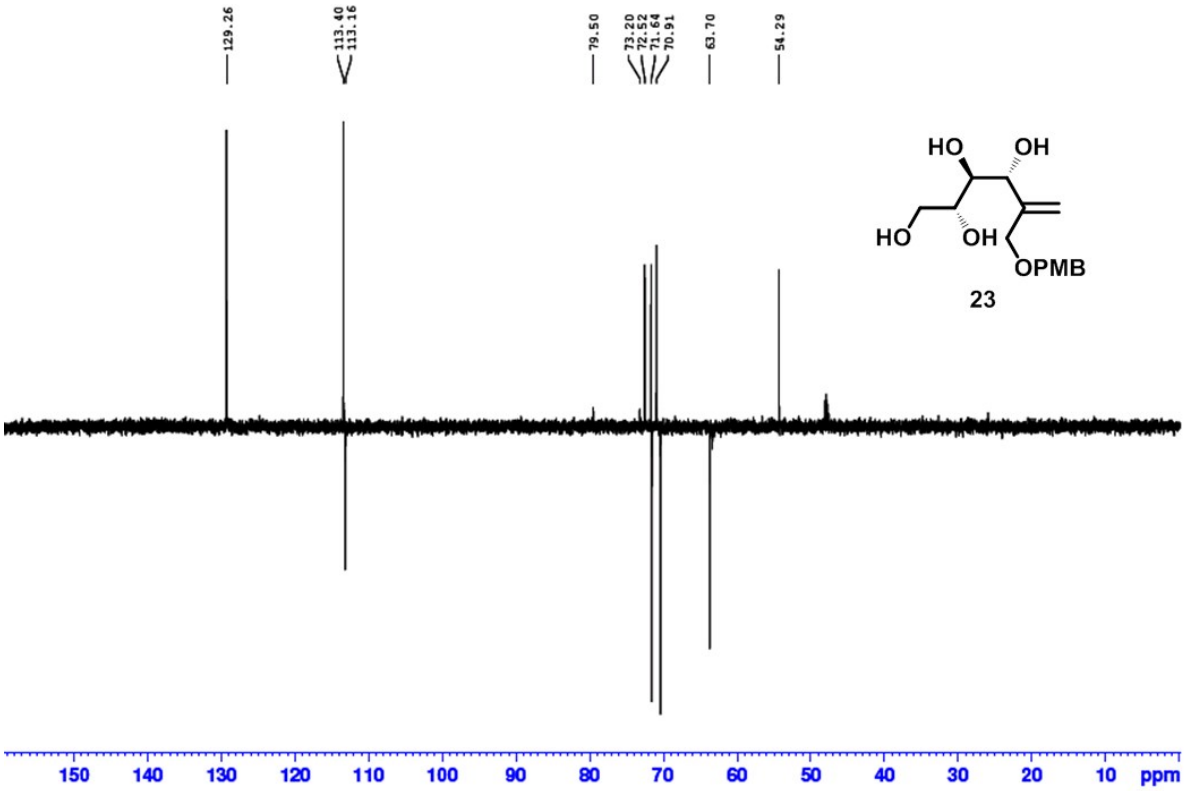
COSY spectrum of compound **23** recorded in CD_3OD



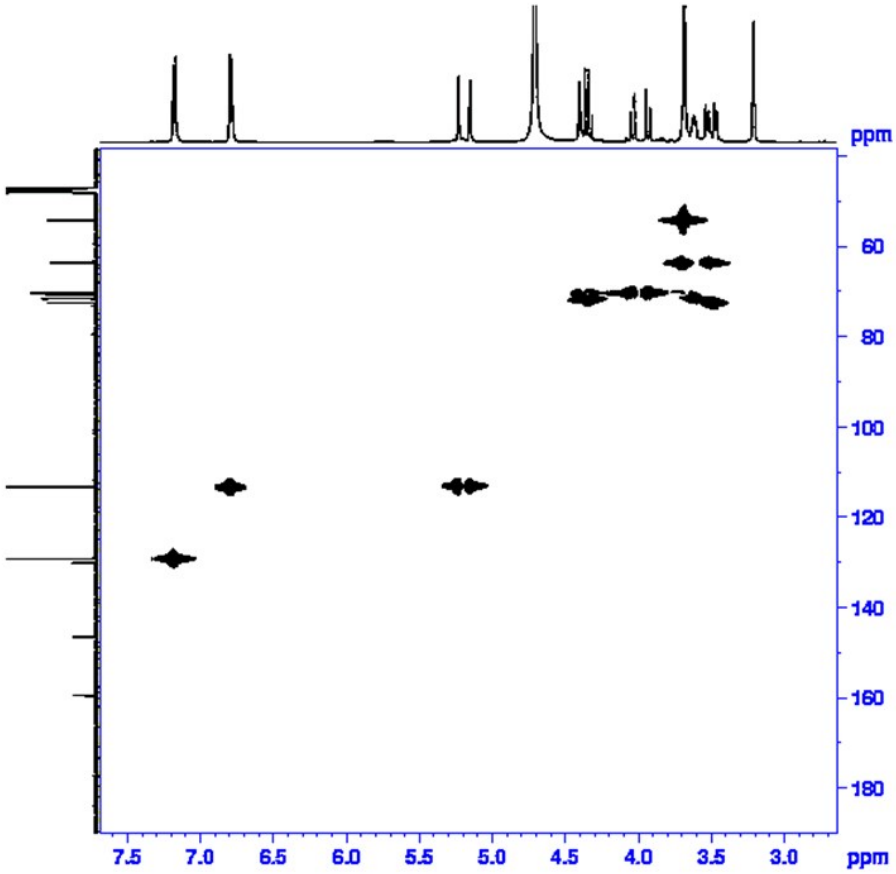
^{13}C spectrum of compound **23** recorded in CD_3OD



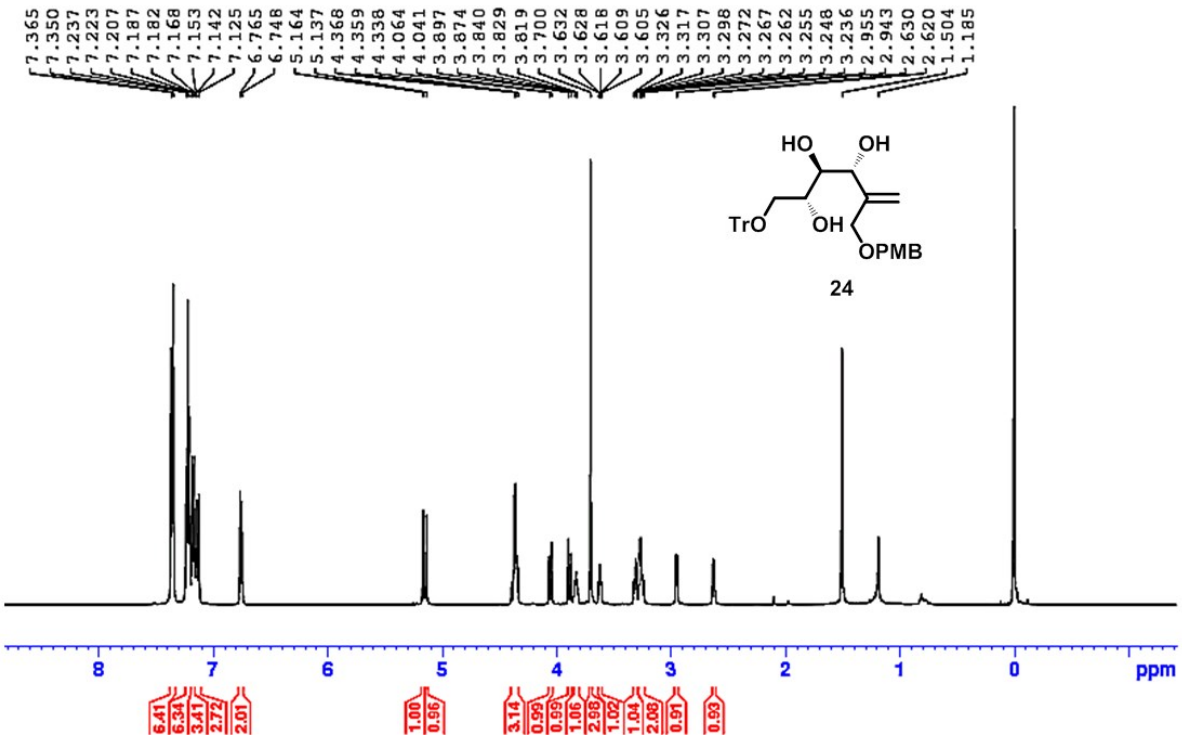
DEPT spectrum of compound **23** recorded in CD3OD



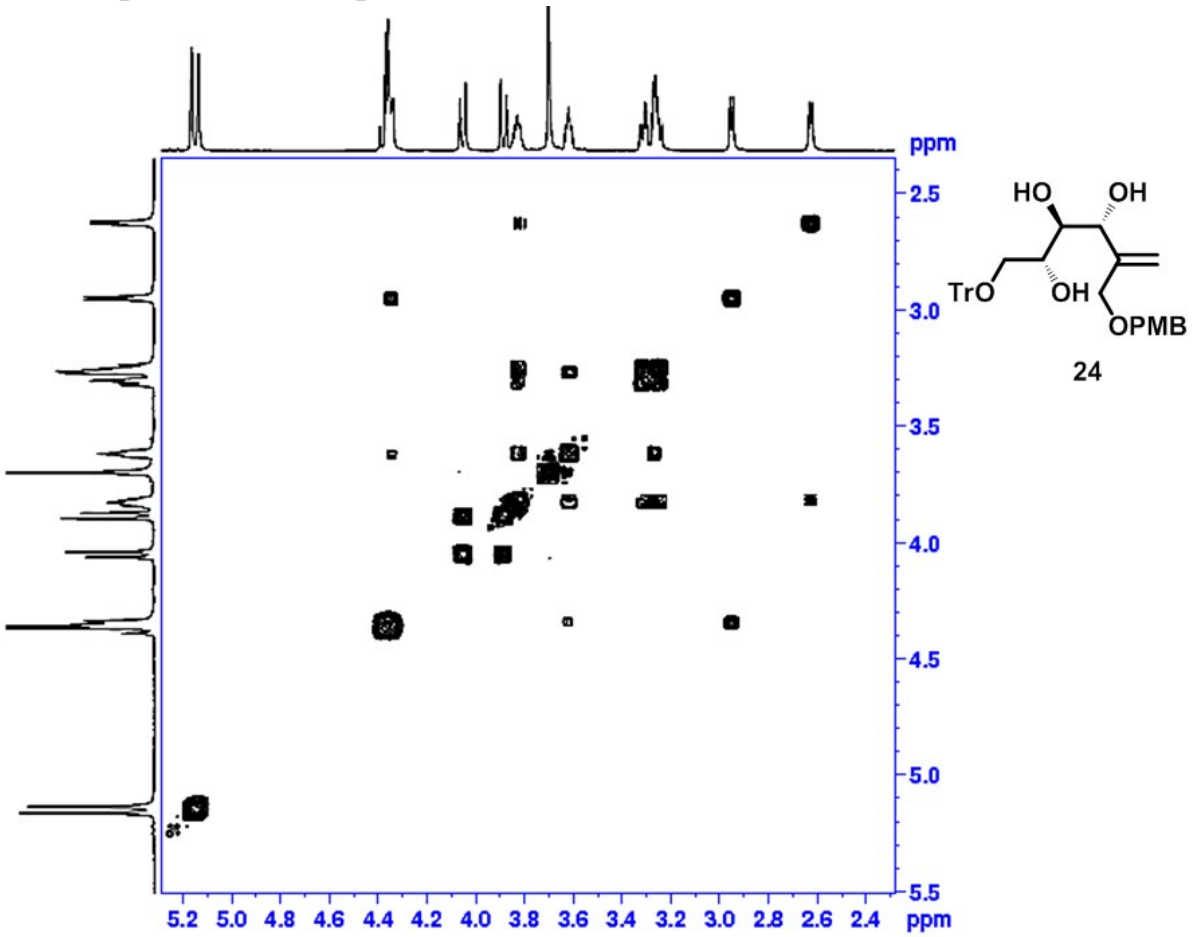
HMQC spectrum of compound **23** recorded in CD_3OD



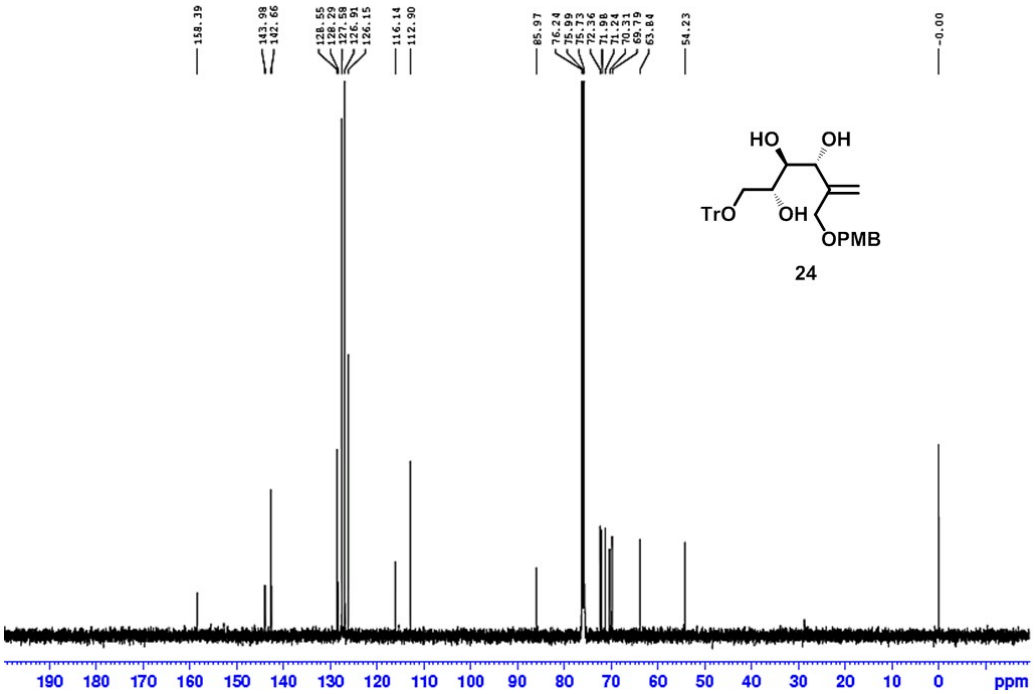
^{1}H NMR spectrum of compound **24** recorded in $CDCl_3$



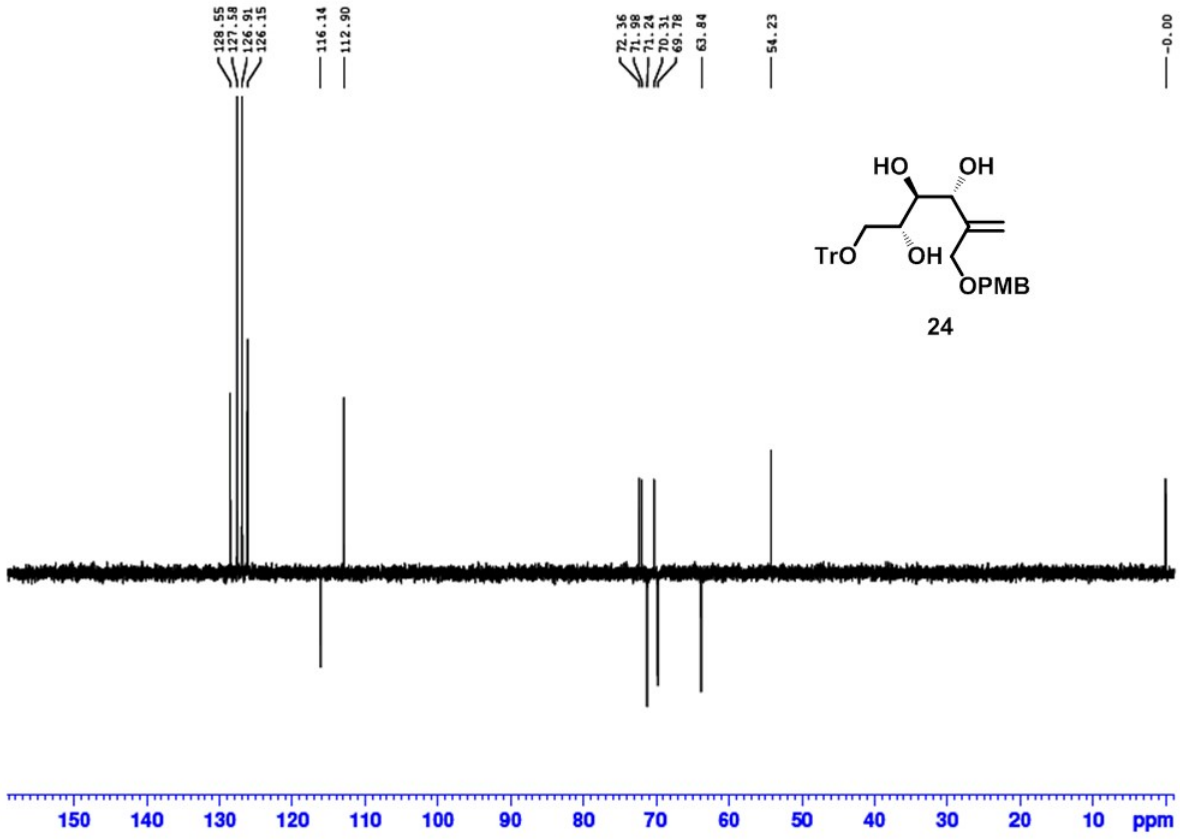
COSY spectrum of compound **24** recorded in $CDCl_3$



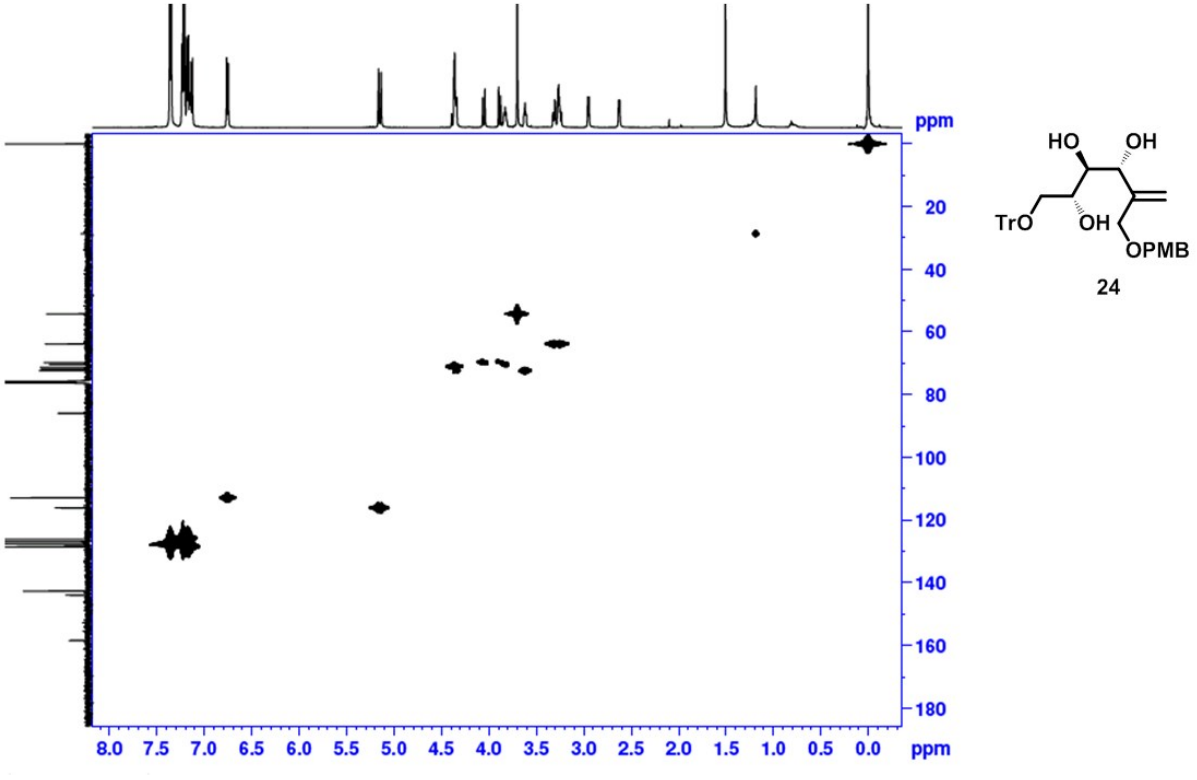
^{13}C spectrum of compound **24** recorded in $CDCl_3$



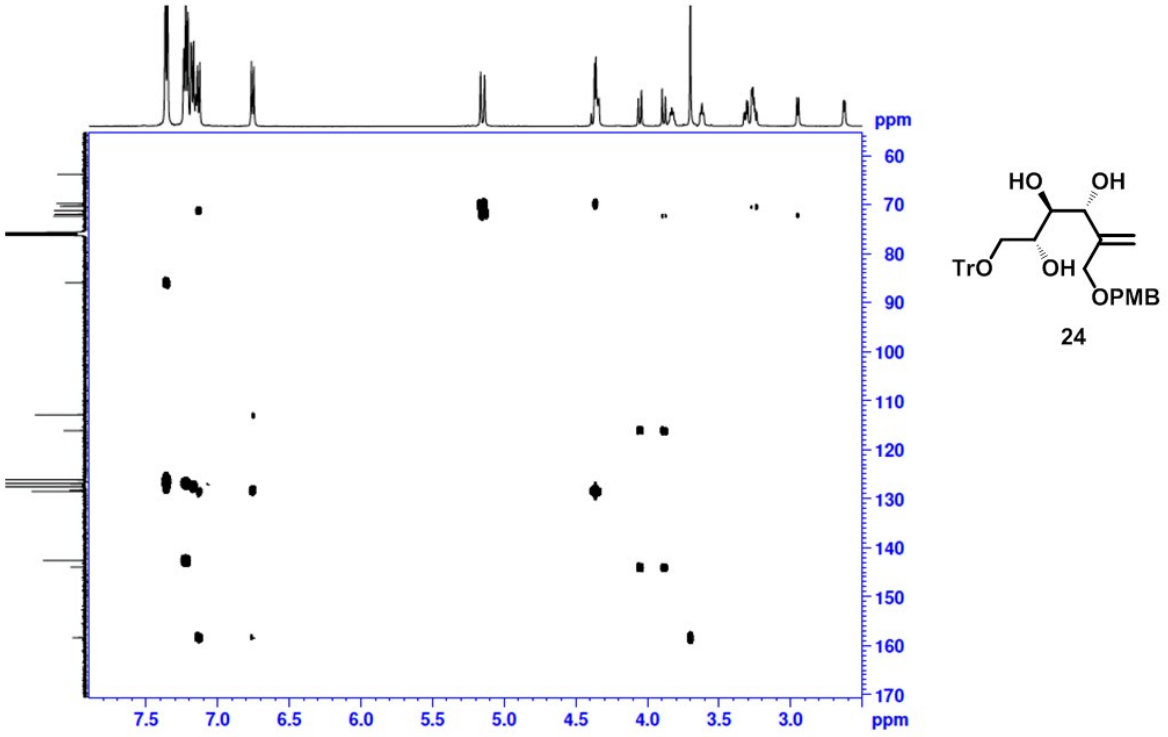
DEPT spectrum of compound **24** recorded in $CDCl_3$



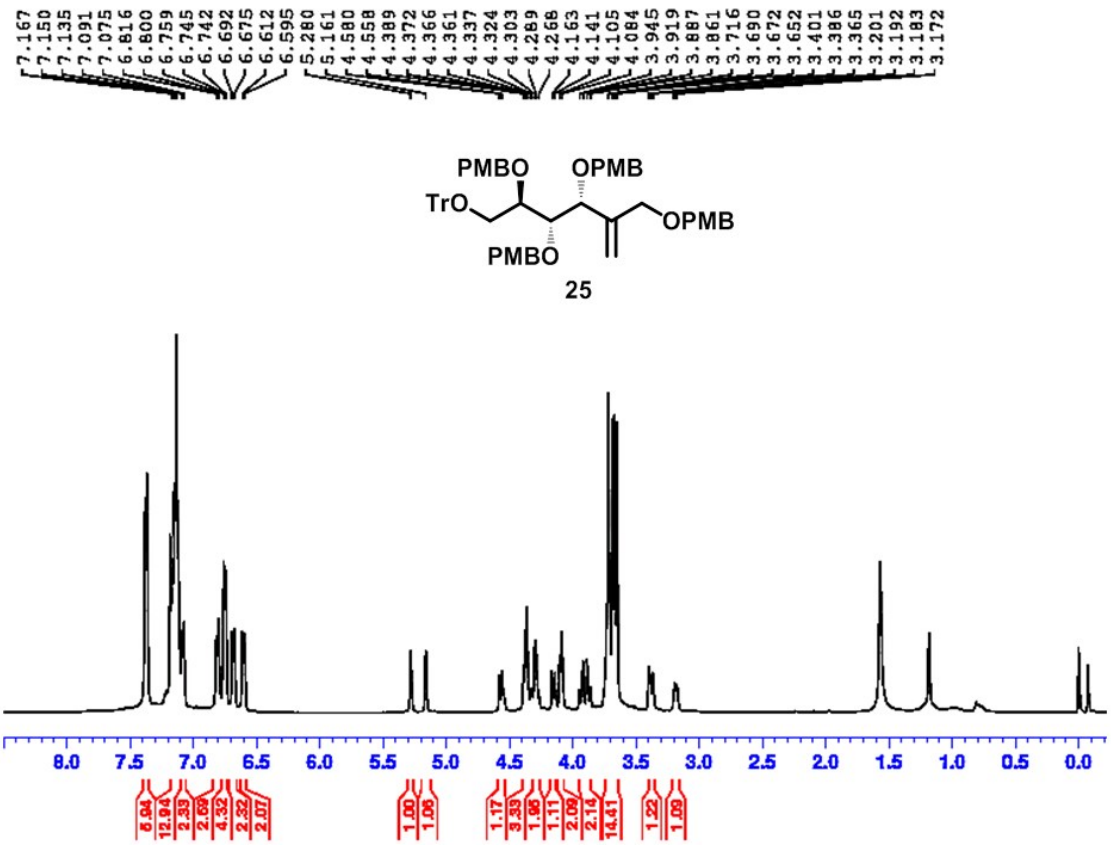
HMQC spectrum of compound **24** recorded in $CDCl_3$



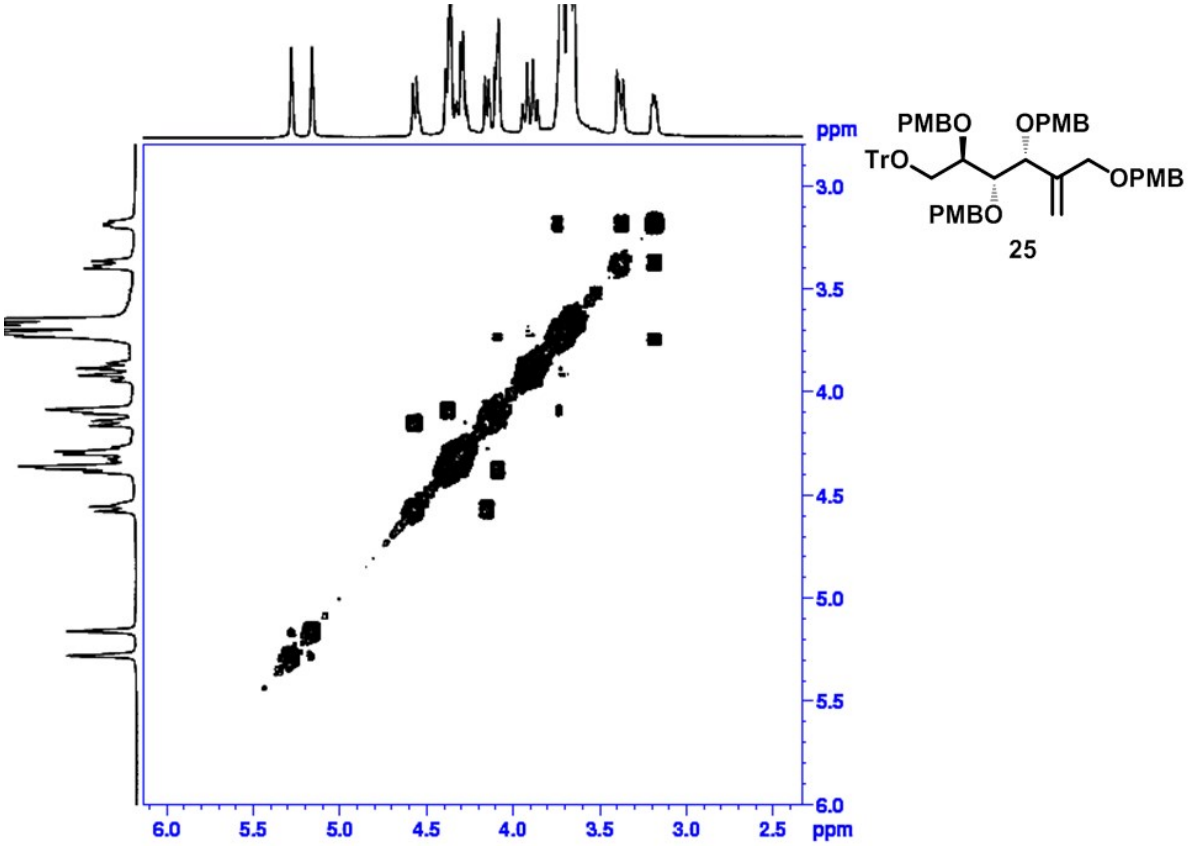
HMBC spectrum of compound **24** recorded in $CDCl_3$



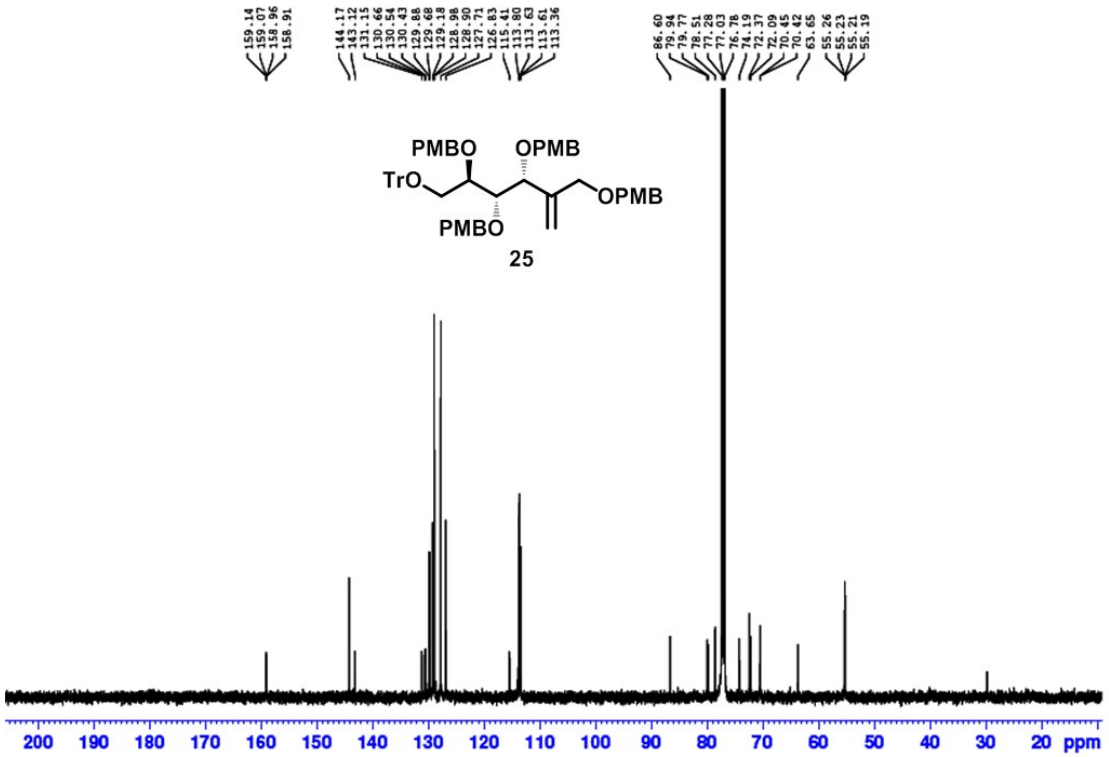
^{1}H NMR spectrum of compound **25** recorded in $CDCl_3$



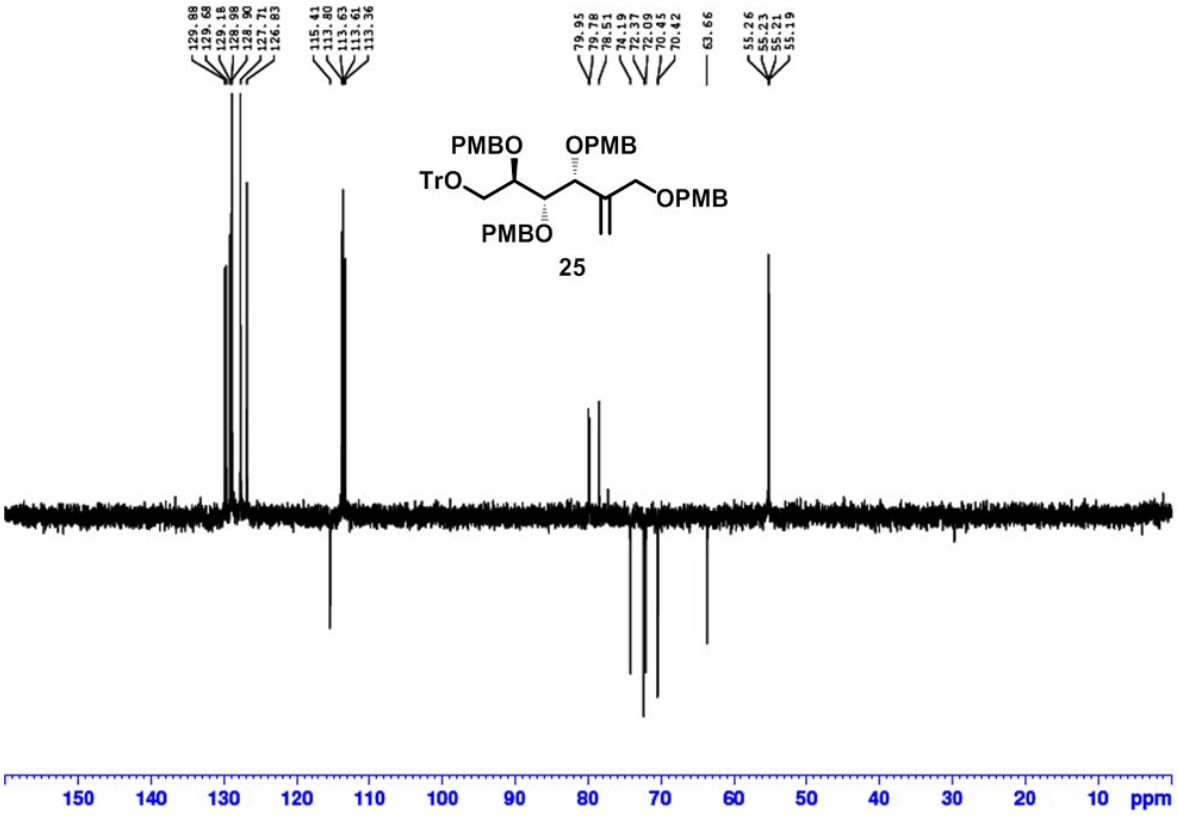
COSY spectrum of compound **25** recorded in $CDCl_3$



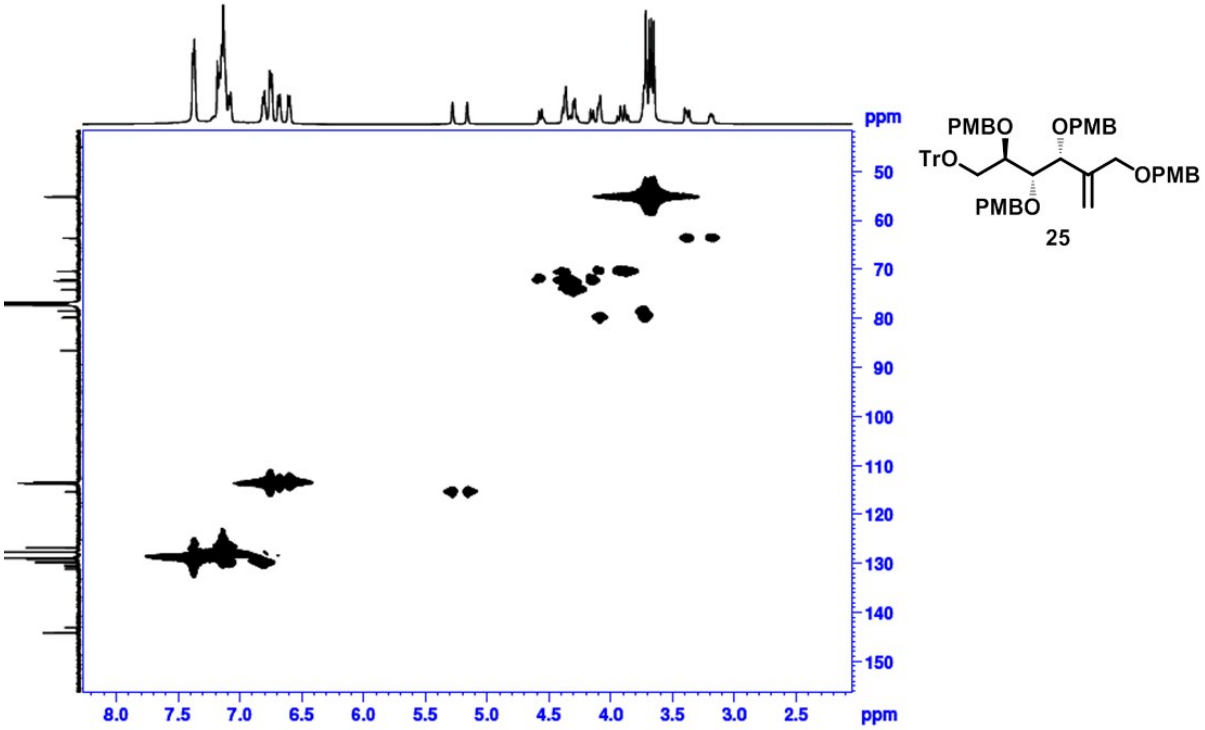
^{13}C NMR spectrum of compound **25** recorded in $CDCl_3$



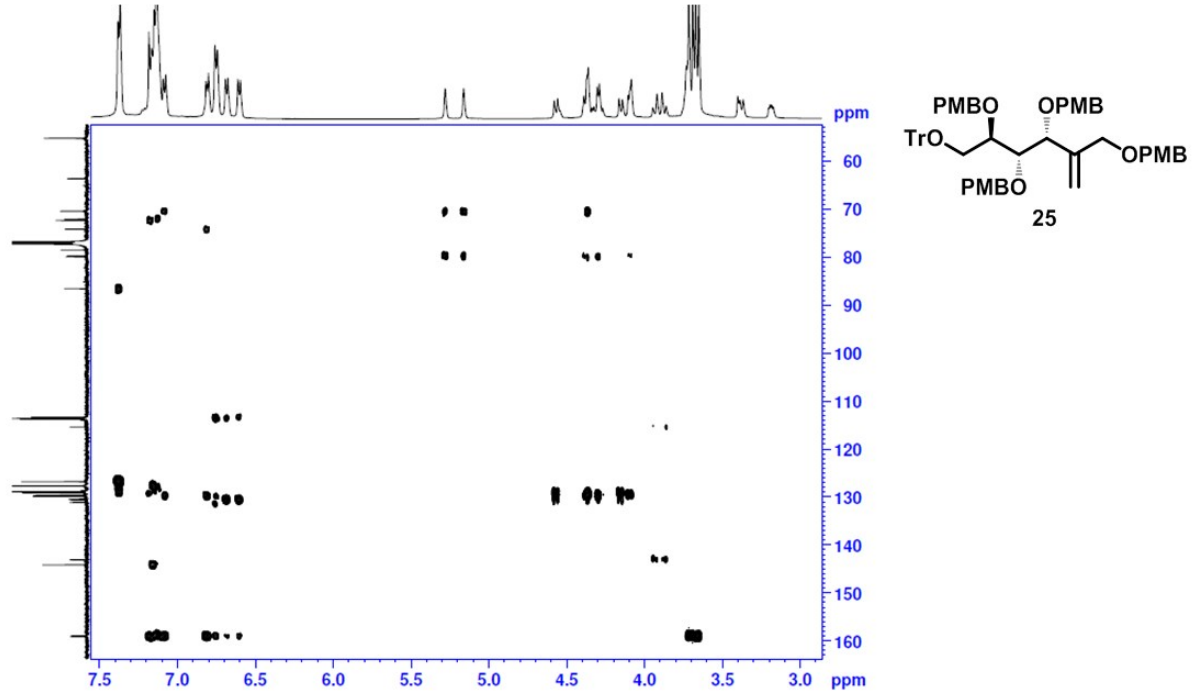
DEPT spectrum of compound **25** recorded in $CDCl_3$



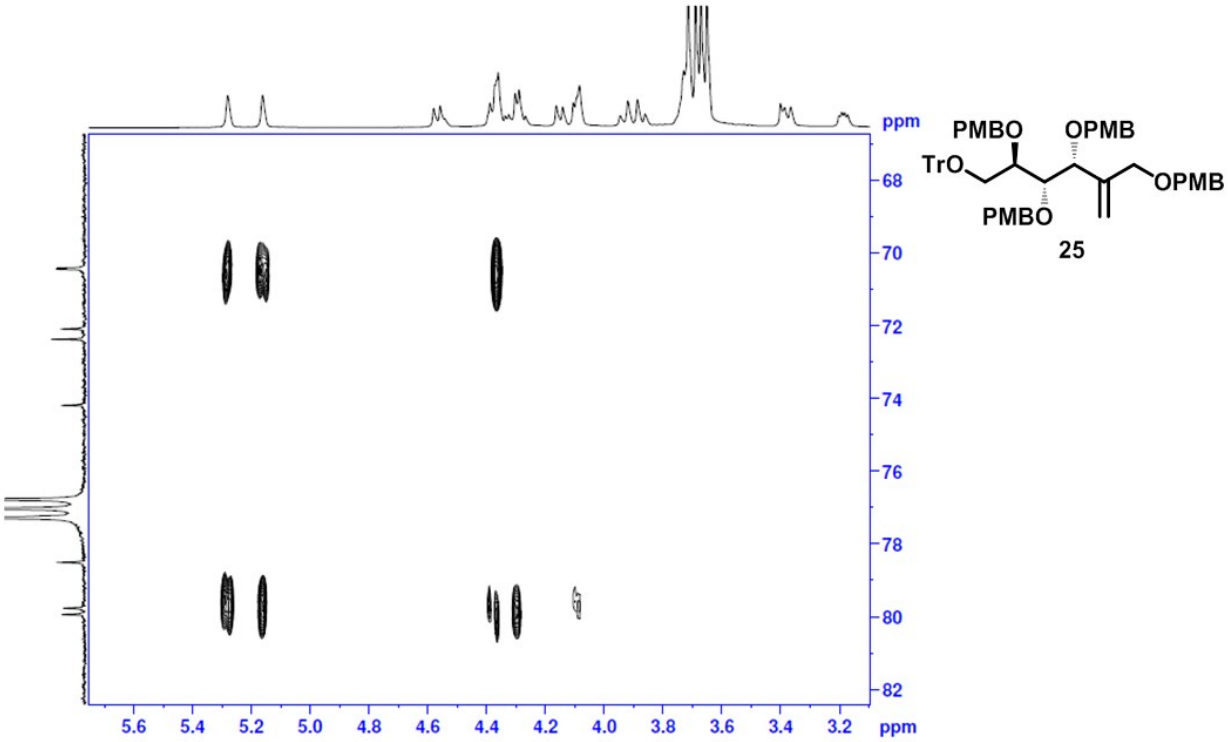
HMQC spectrum of compound **25** recorded in $CDCl_3$



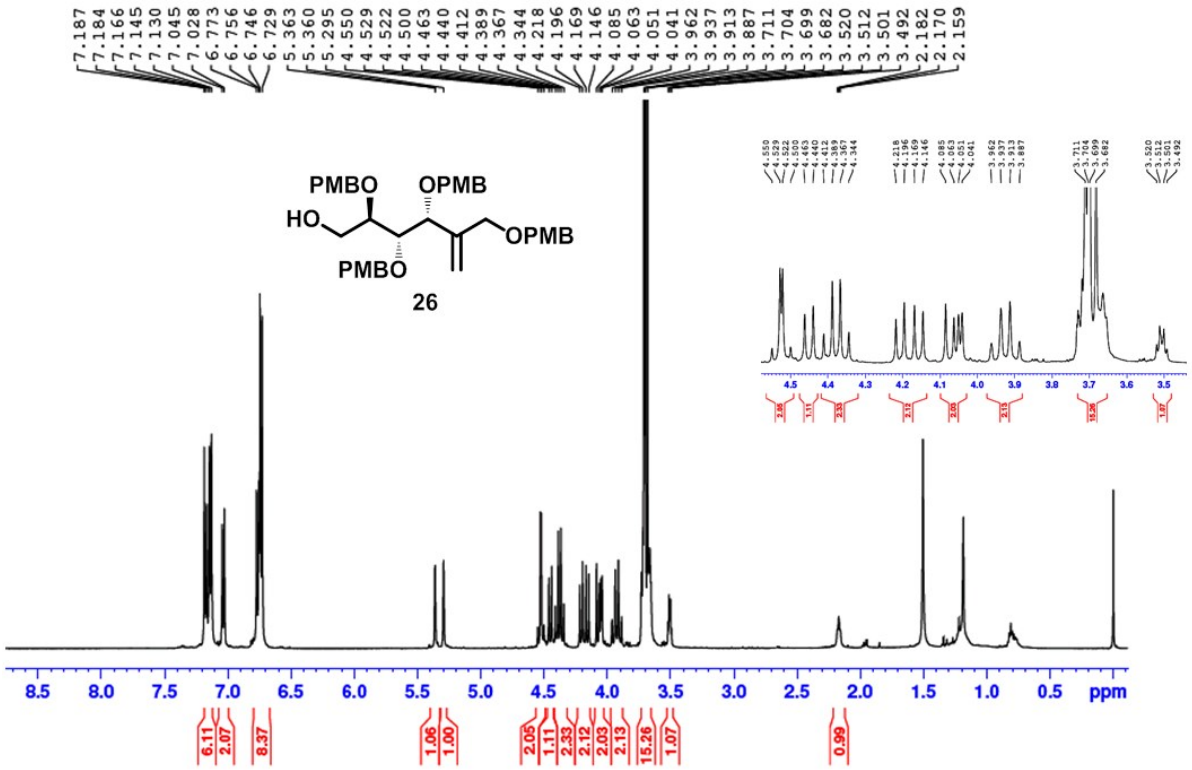
HMBC spectrum of compound **25** recorded in $CDCl_3$



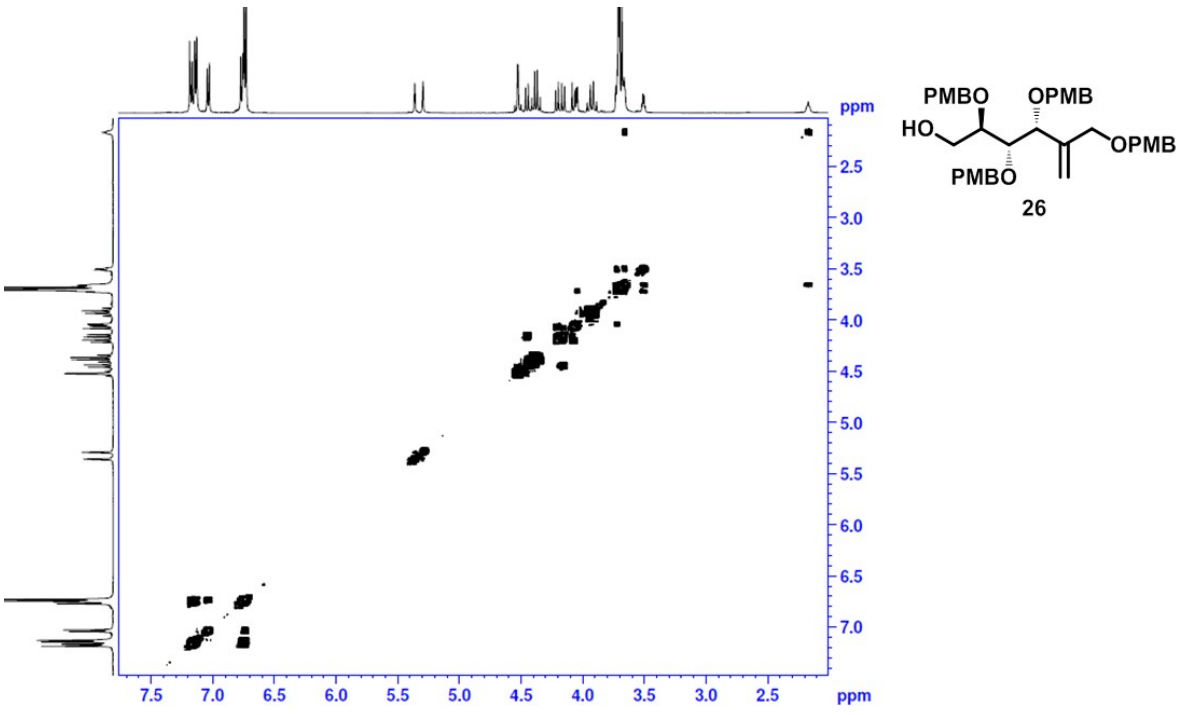
Expanded HMBC spectrum of compound **25** recorded in $CDCl_3$



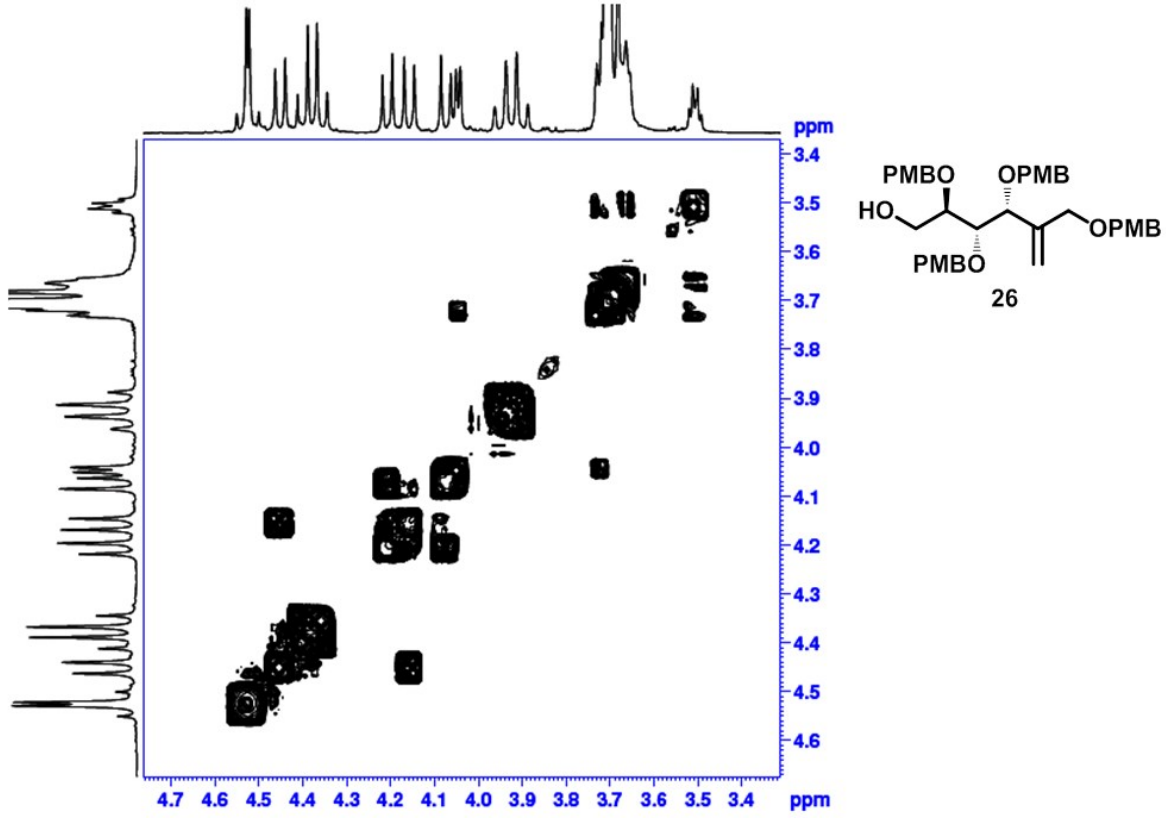
^{1}H NMR spectrum of compound **26** recorded in $CDCl_3$



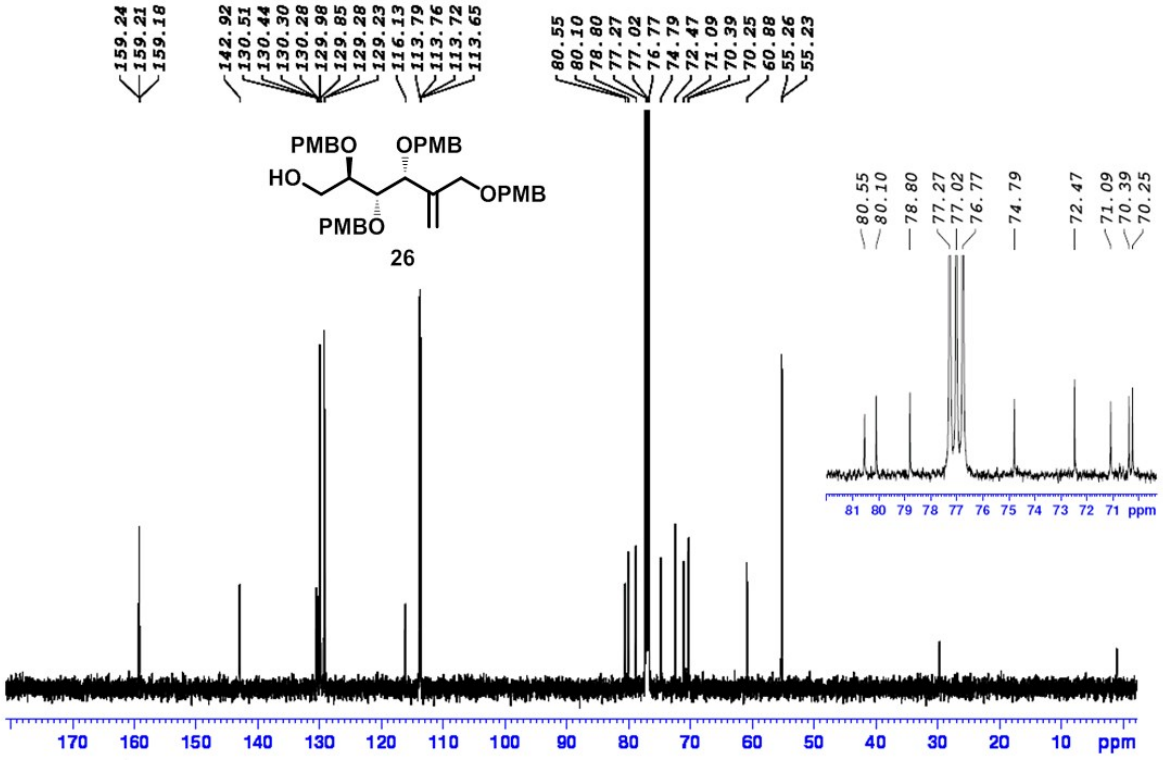
COSY spectrum of compound **26** recorded in $CDCl_3$



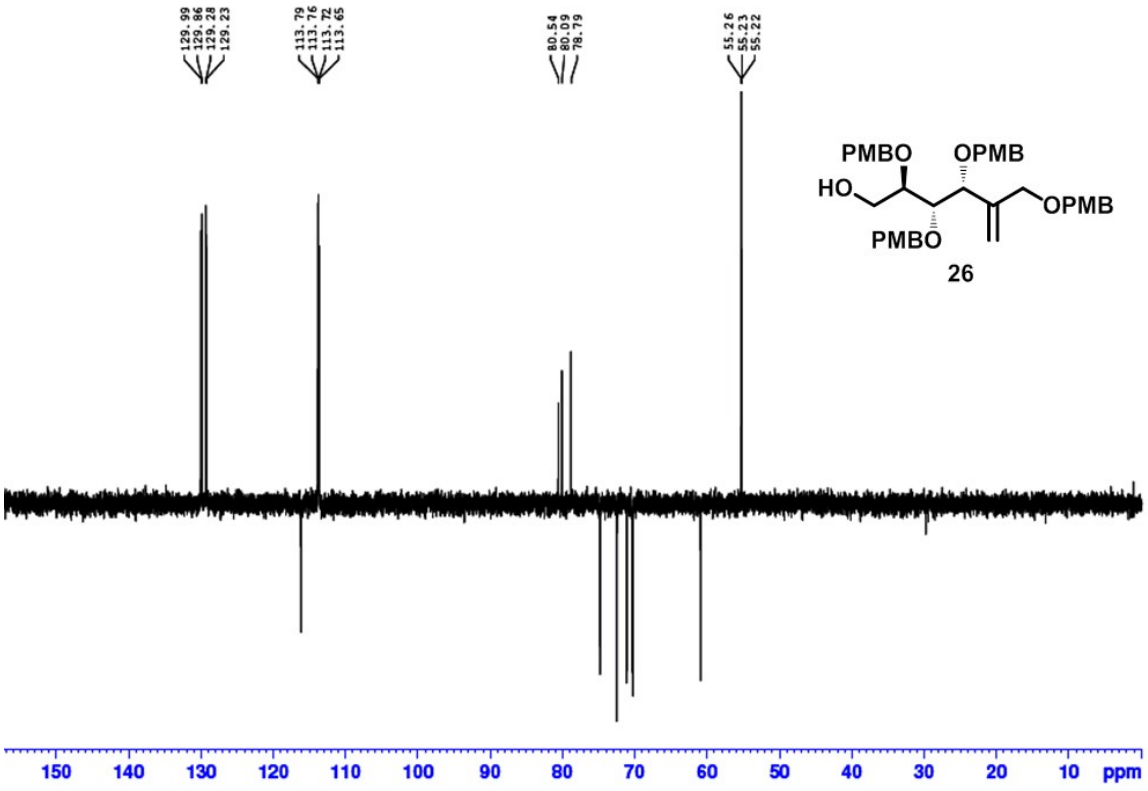
Expanded COSY spectrum of compound **26** recorded in $CDCl_3$



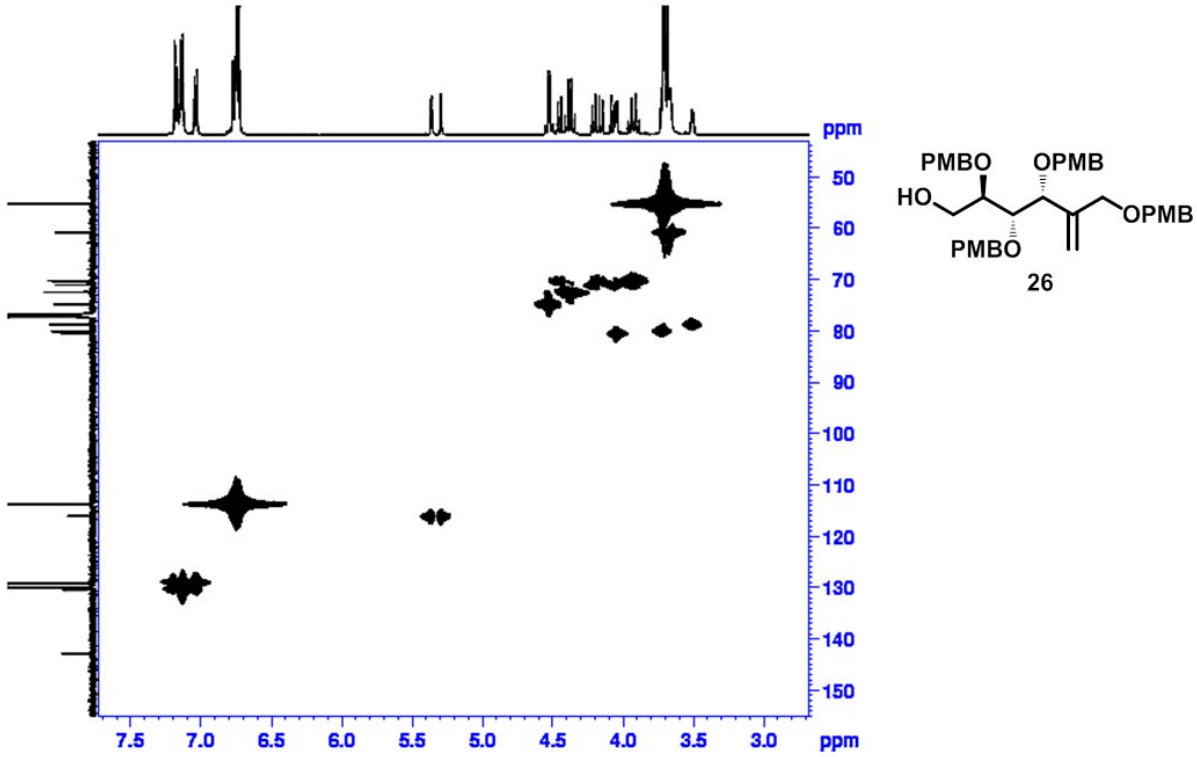
^{13}C spectrum of compound **26** recorded in $CDCl_3$



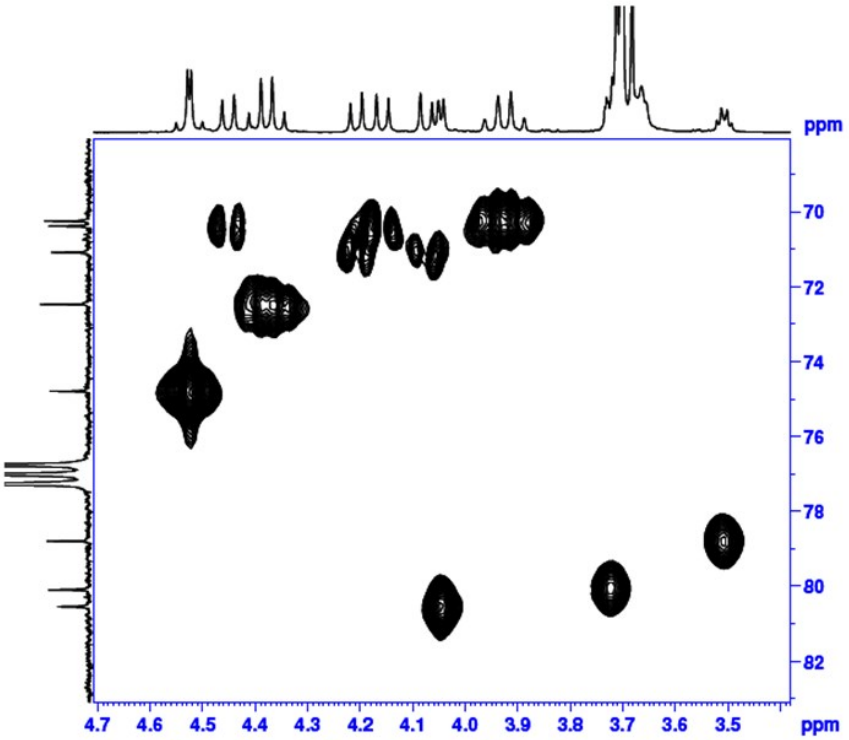
DEPT spectrum of compound **26** recorded in $CDCl_3$

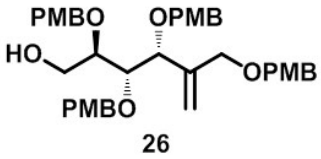


HMQC spectrum of compound **26** recorded in $CDCl_3$

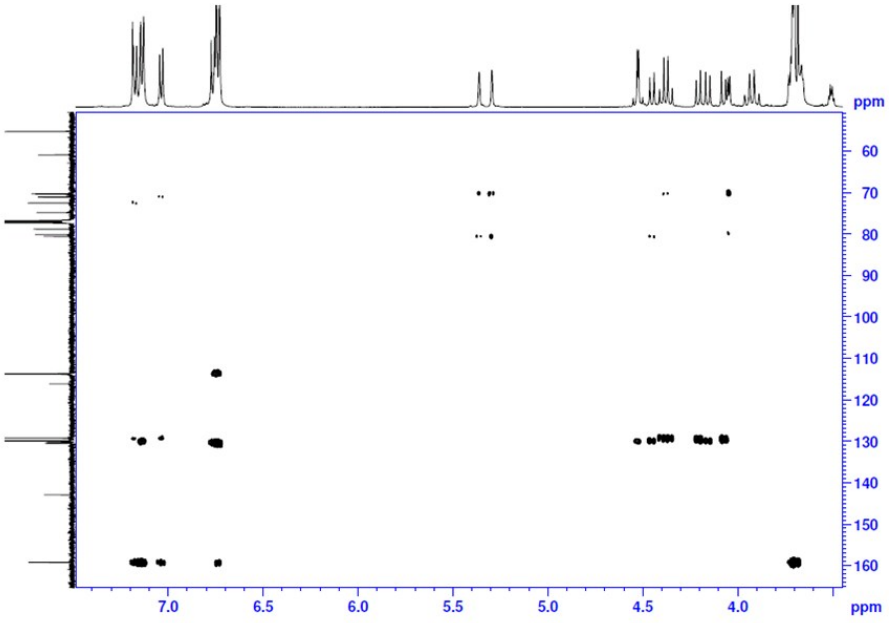


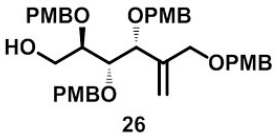
Expanded spectrum of compound **26** recorded in $CDCl_3$



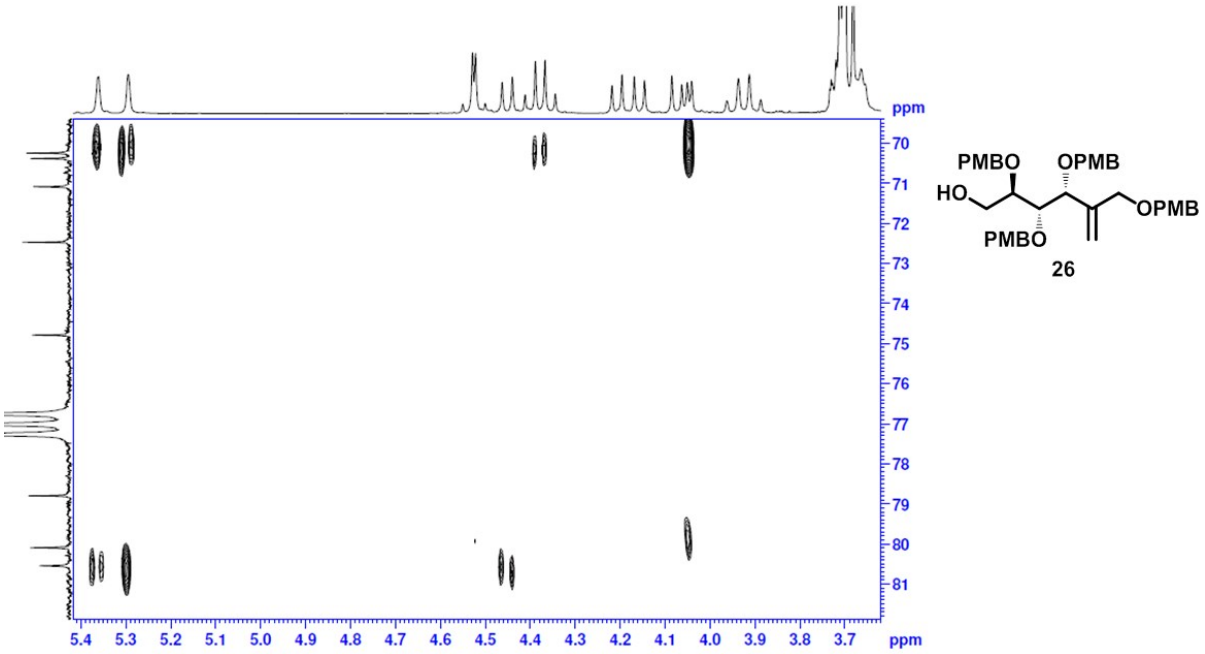


HMBC spectrum of compound **26** recorded in $CDCl_3$

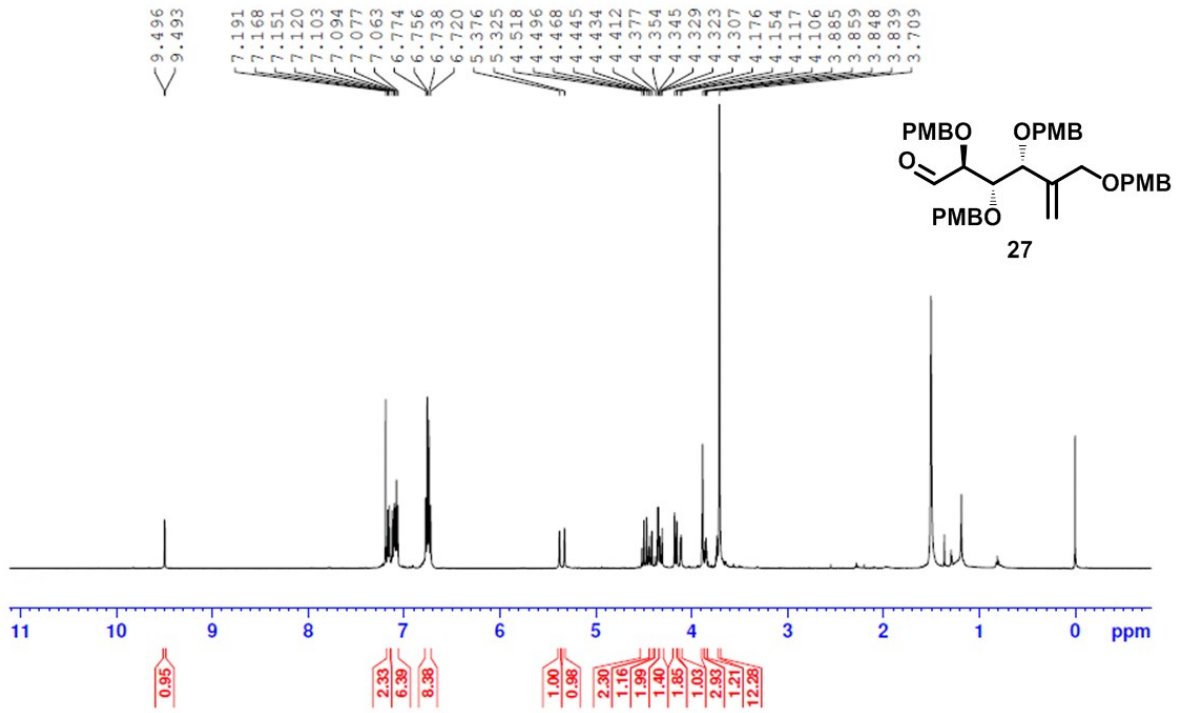




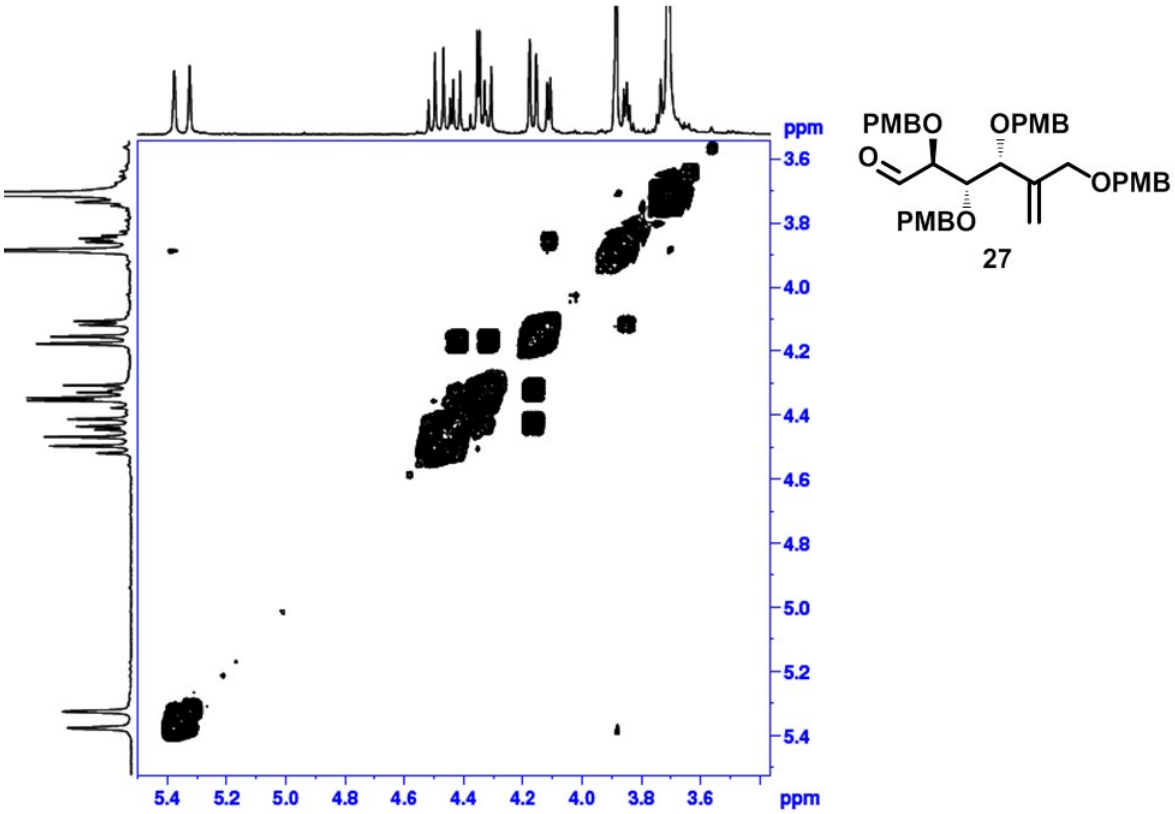
Expanded HMBC spectrum of compound **26** recorded in $CDCl_3$



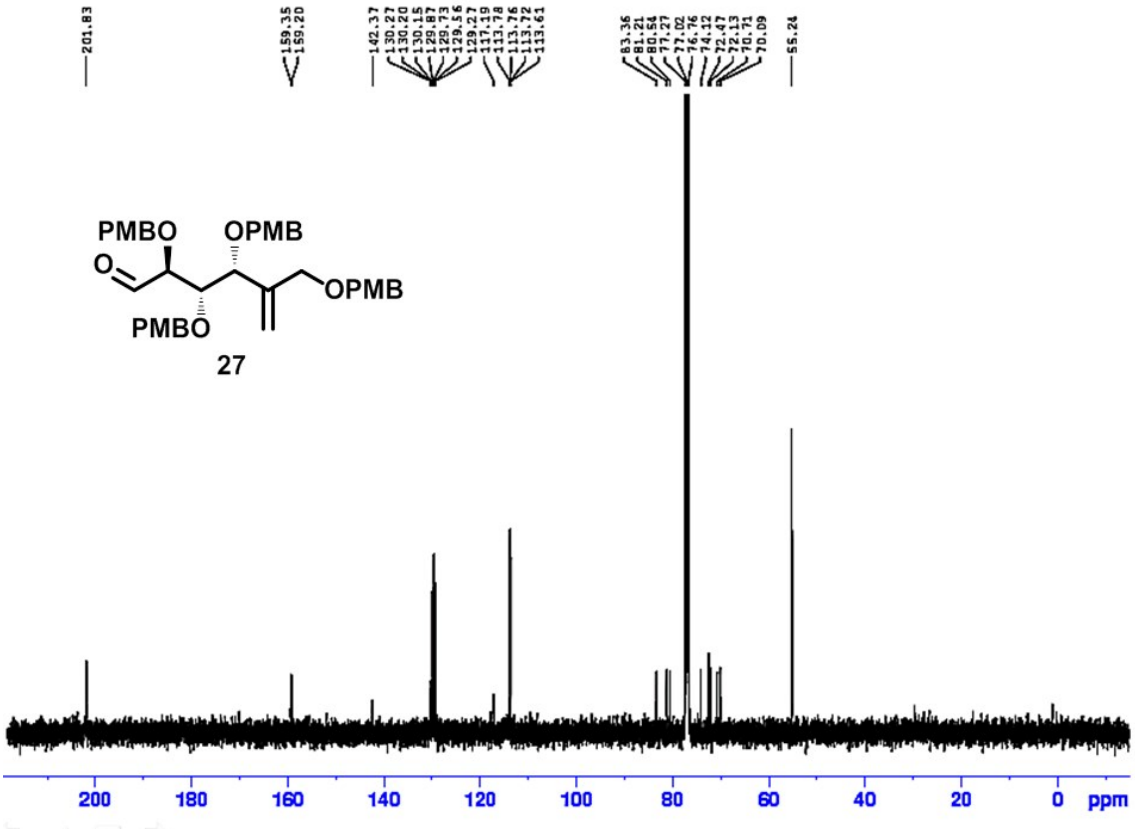
^1H NMR spectrum of compound **27** recorded in $CDCl_3$



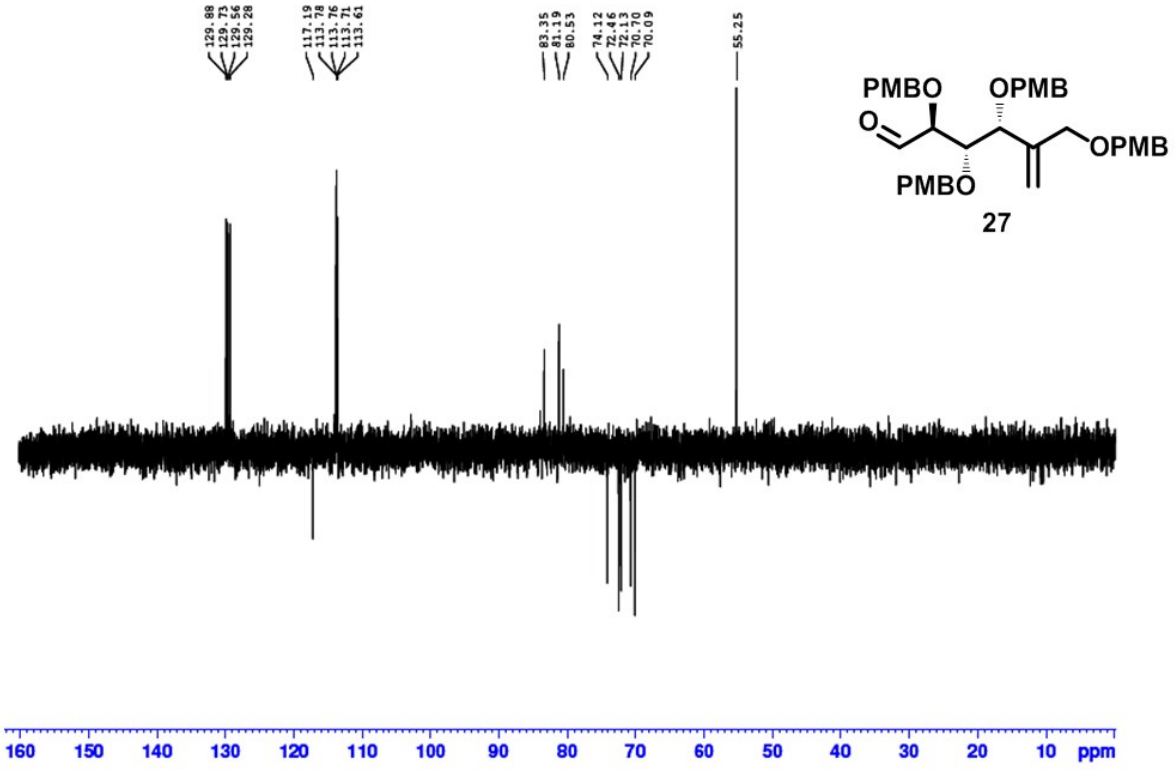
COSY spectrum of compound **27** recorded in $CDCl_3$



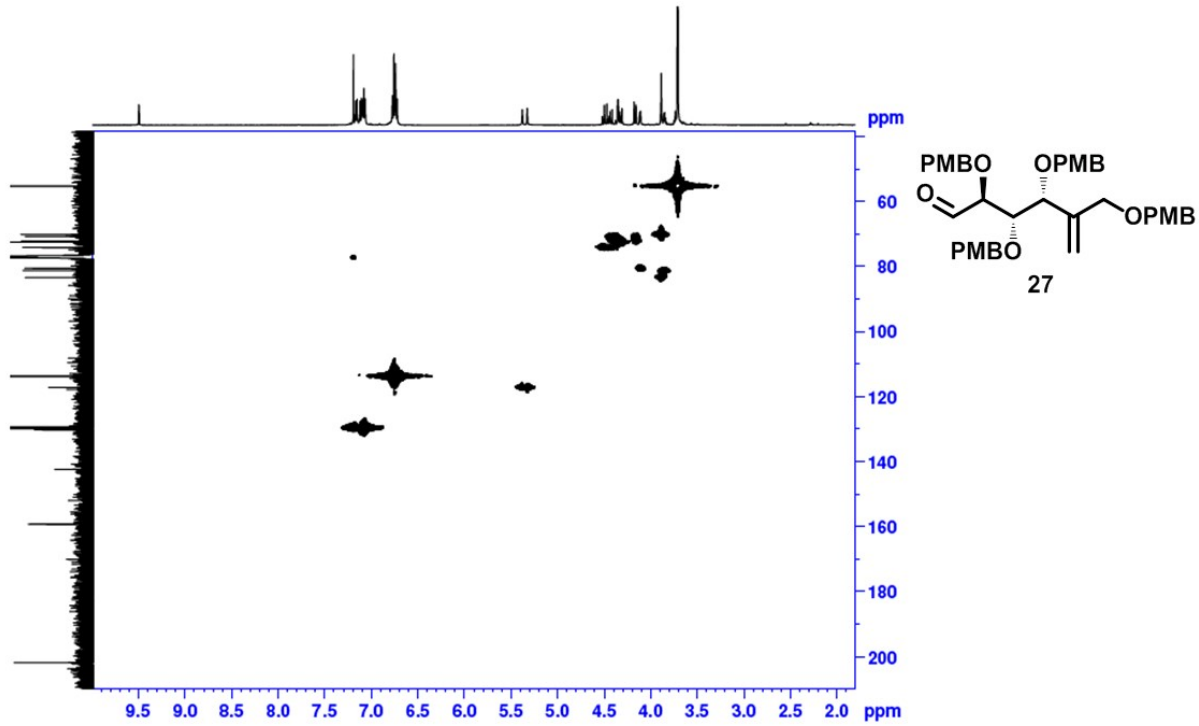
^{13}C NMR spectrum of compound **27** recorded in $CDCl_3$



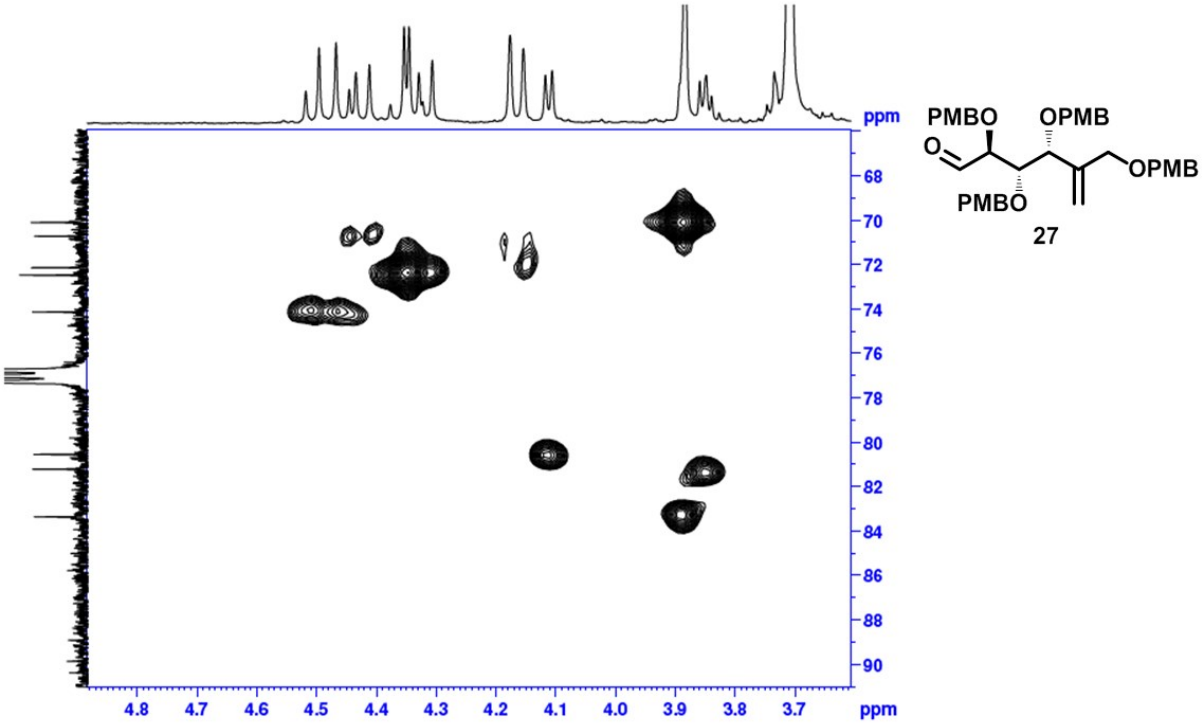
DEPT spectrum of compound **27** recorded in $CDCl_3$



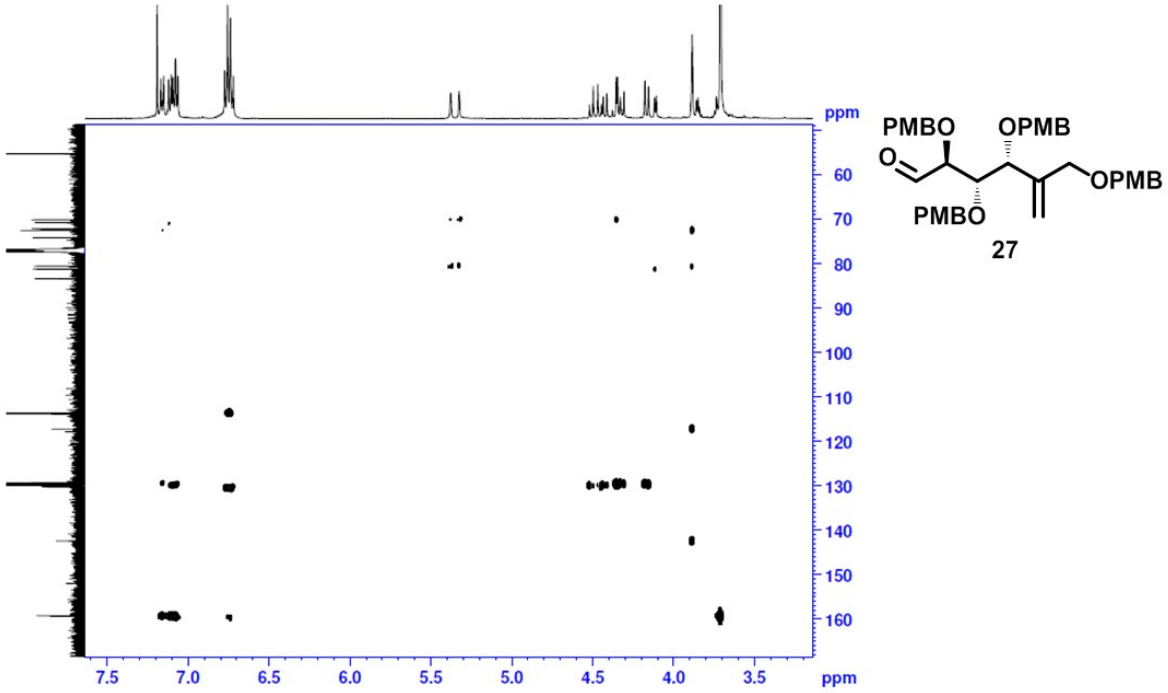
HMQC spectrum of compound **27** recorded in $CDCl_3$



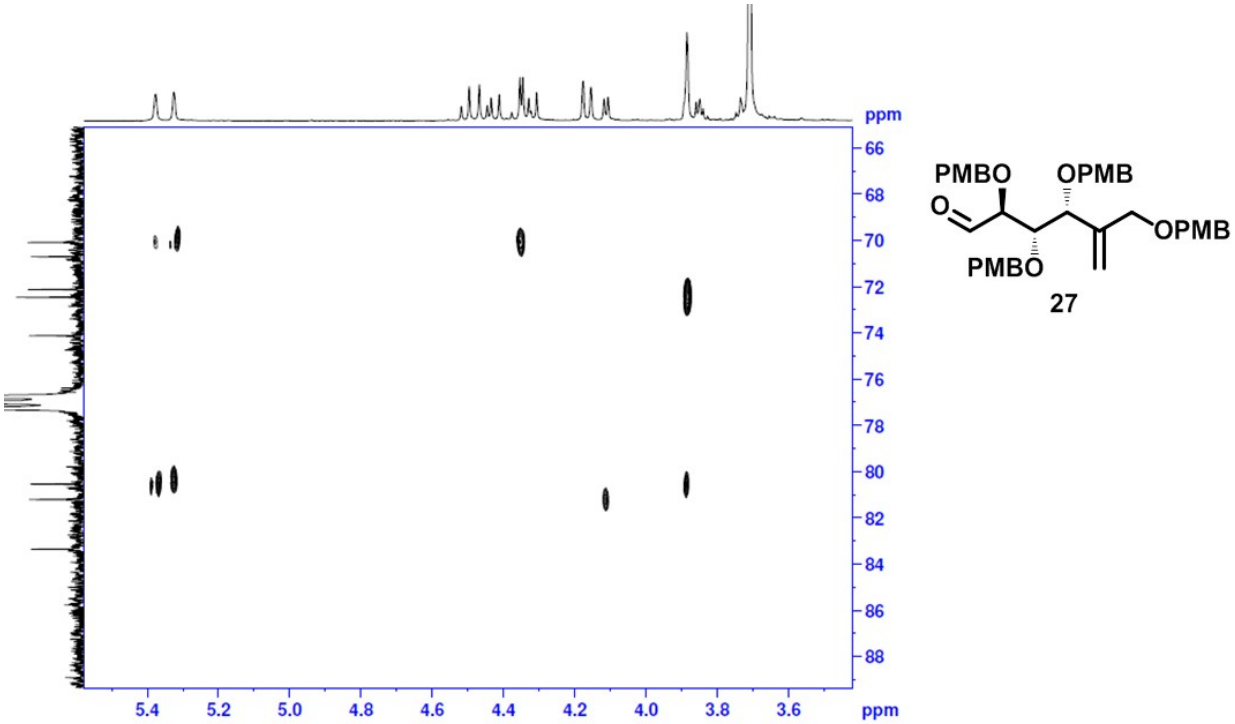
Expanded HMQC spectrum of compound **27** recorded in $CDCl_3$



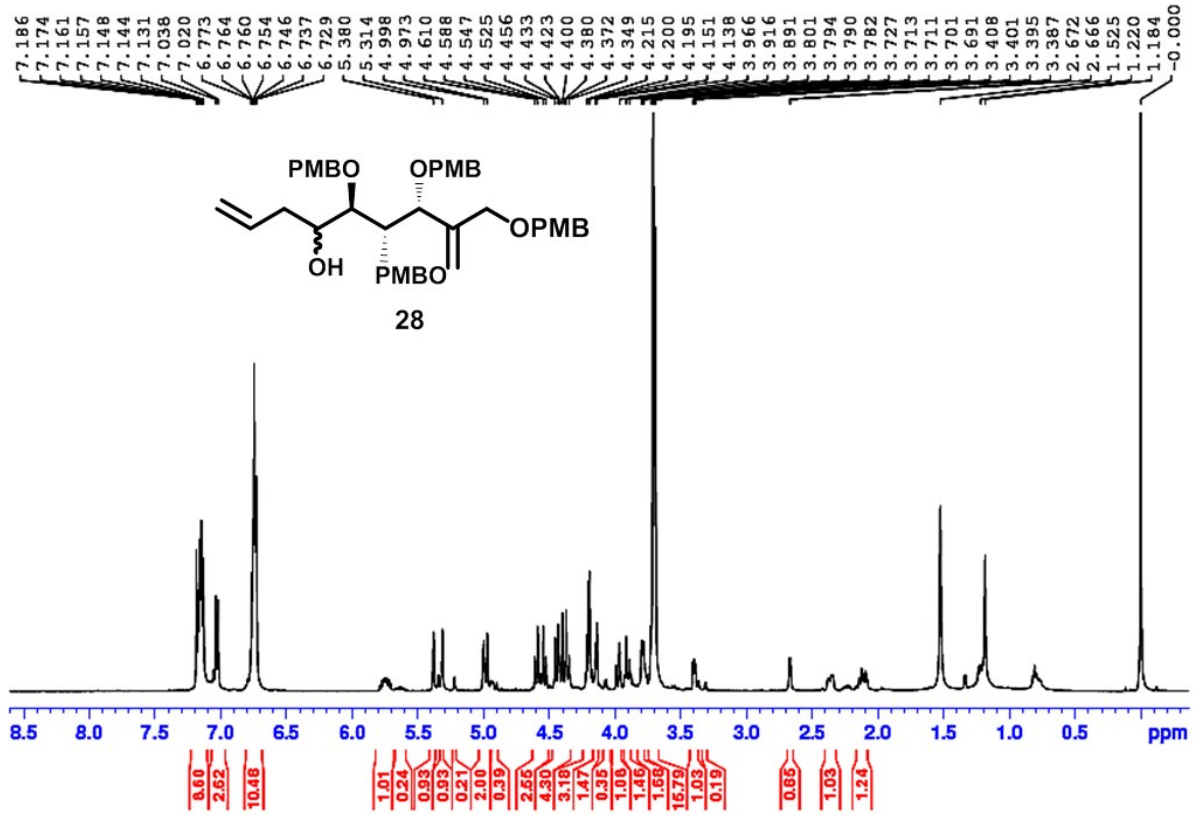
HMBC spectrum of compound **27** recorded in $CDCl_3$



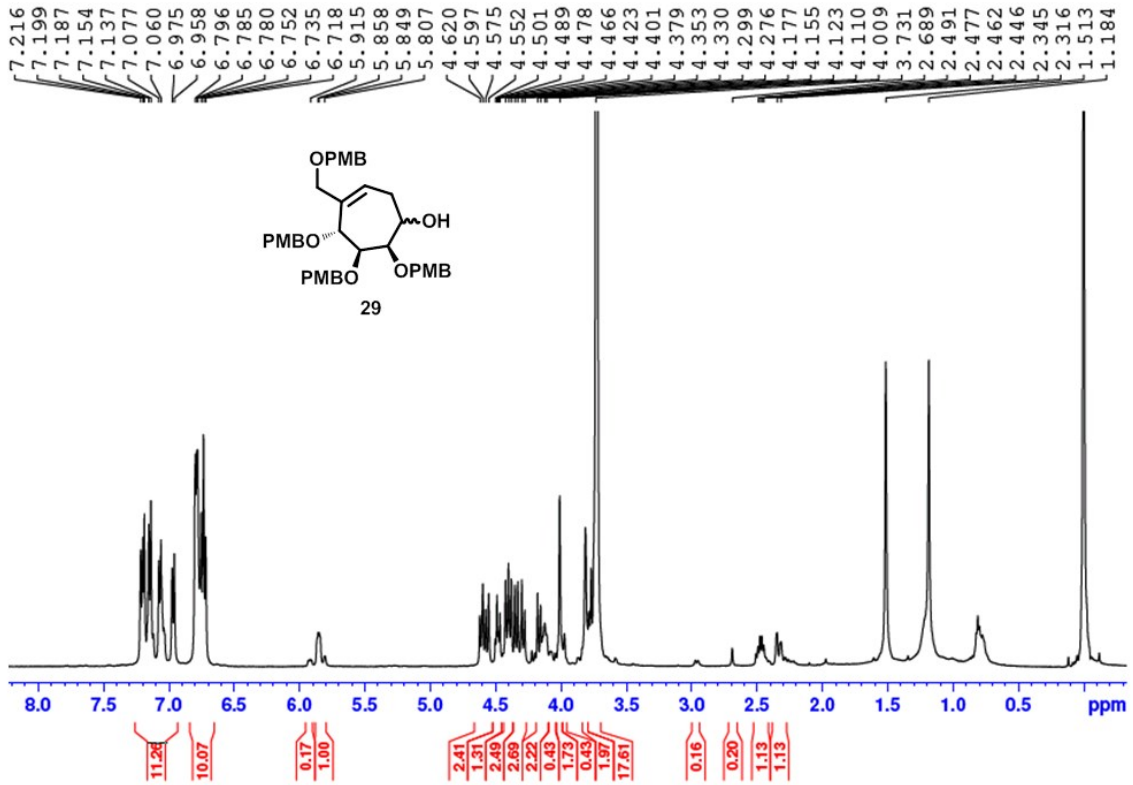
Expanded HMBC spectrum of compound **27** recorded in $CDCl_3$



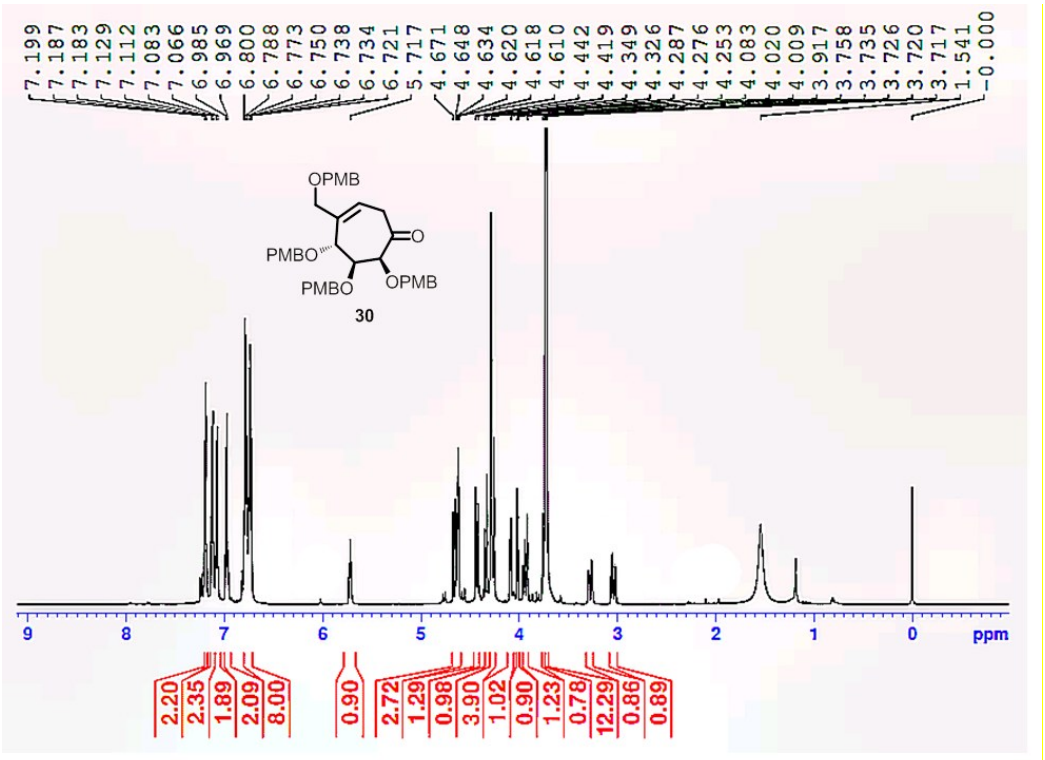
^1H spectrum of the mixture of diastereomers **28** recorded in $CDCl_3$



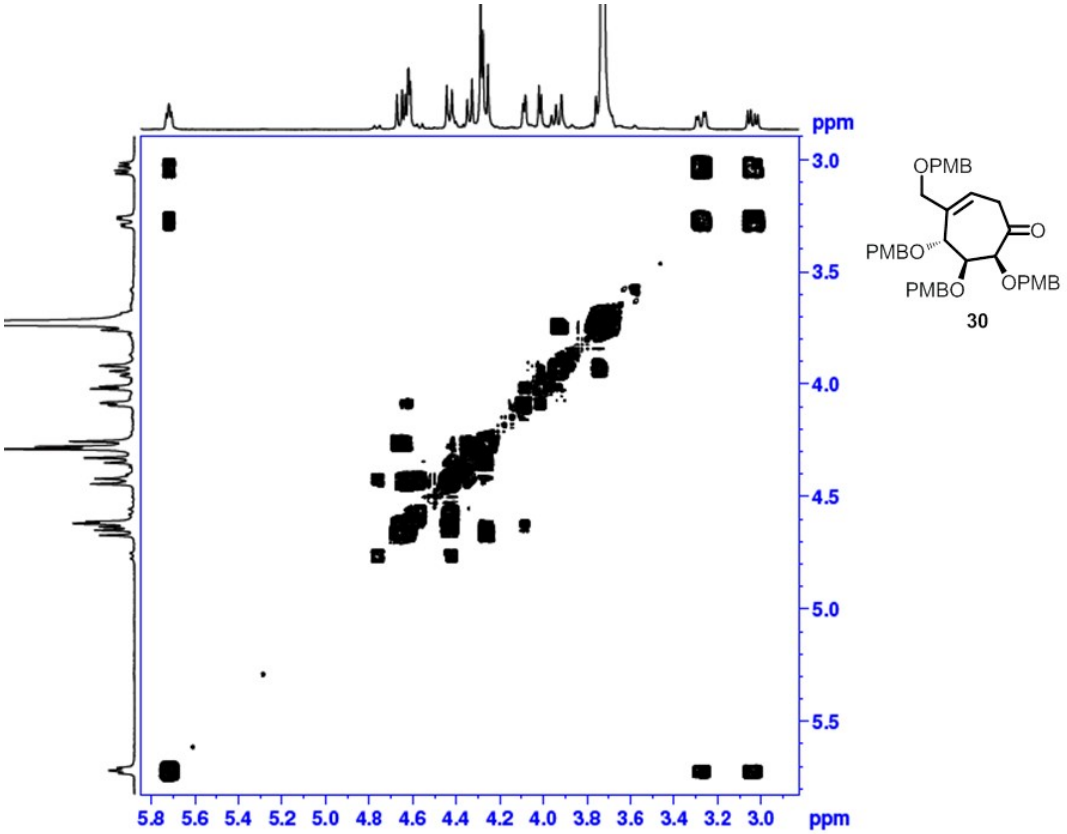
^{1}H spectrum of the mixture of diastereomers **29** recorded in $CDCl_3$



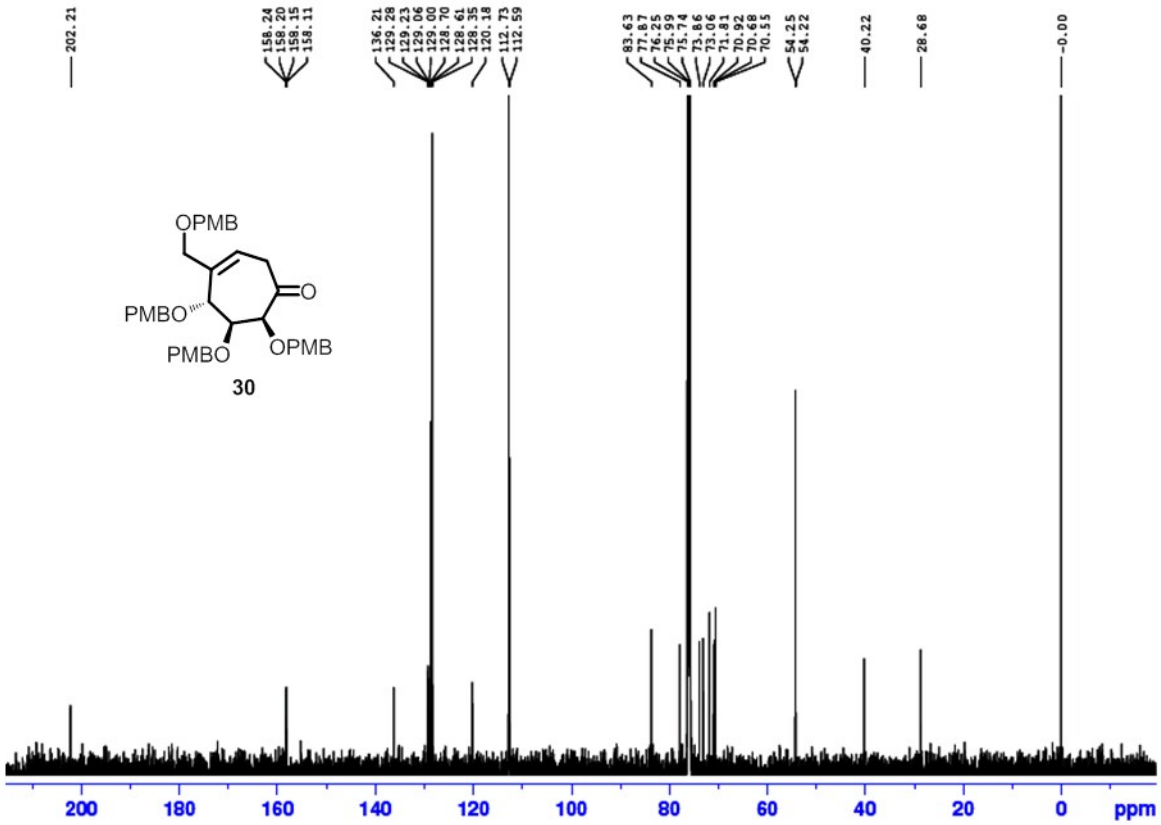
^{1}H spectrum of cyclic ketone **30** recorded in $CDCl_3$



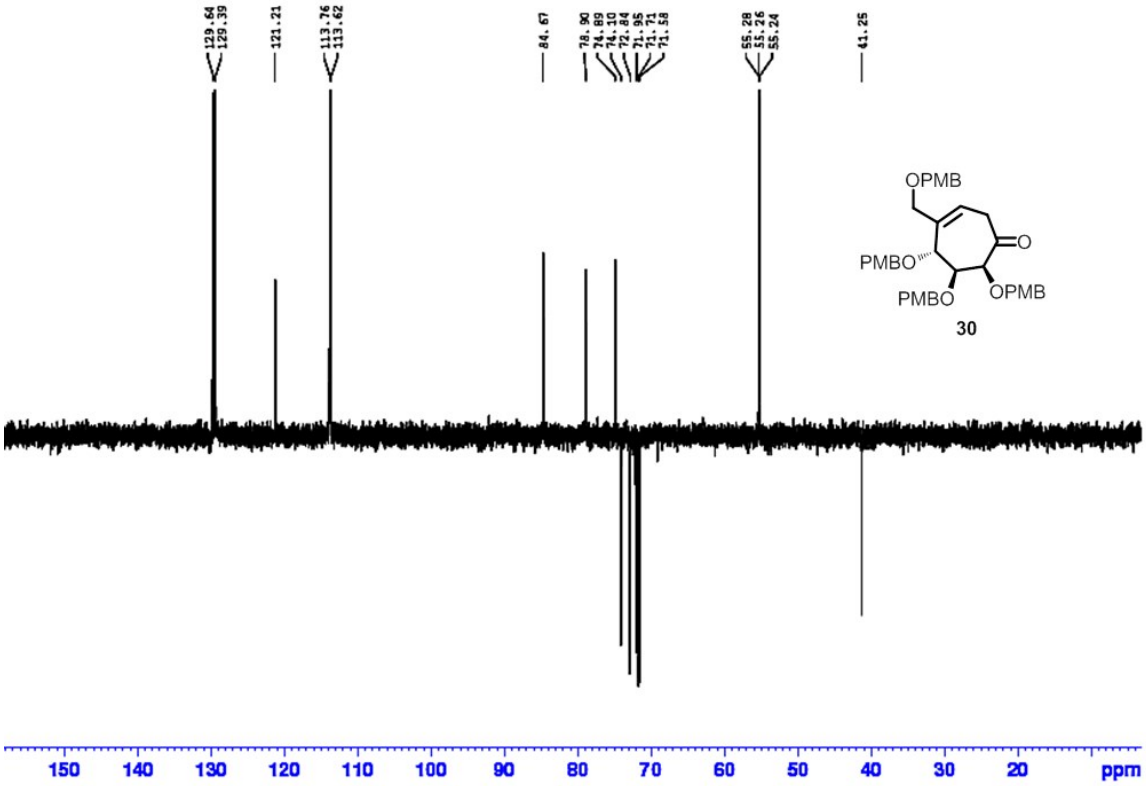
COSY spectrum of cyclic ketone **30** recorded in $CDCl_3$



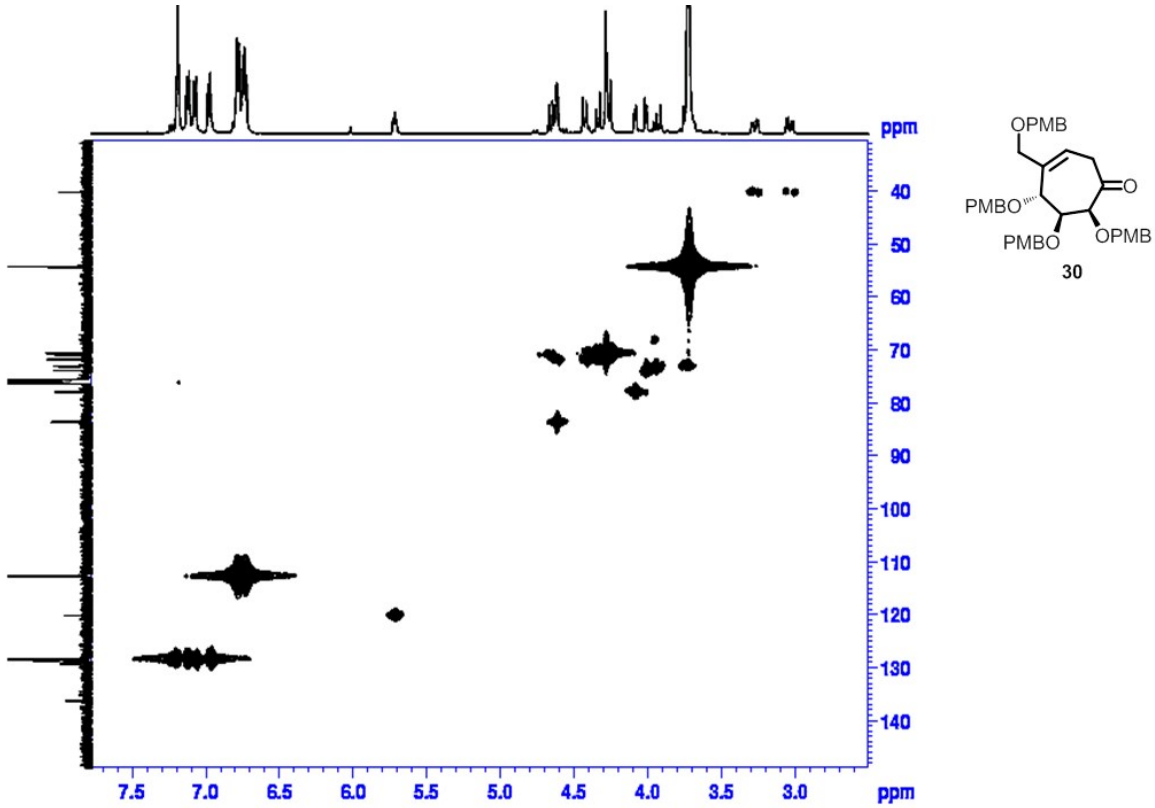
^{13}C NMR spectrum of cyclic ketone **30** recorded in $CDCl_3$



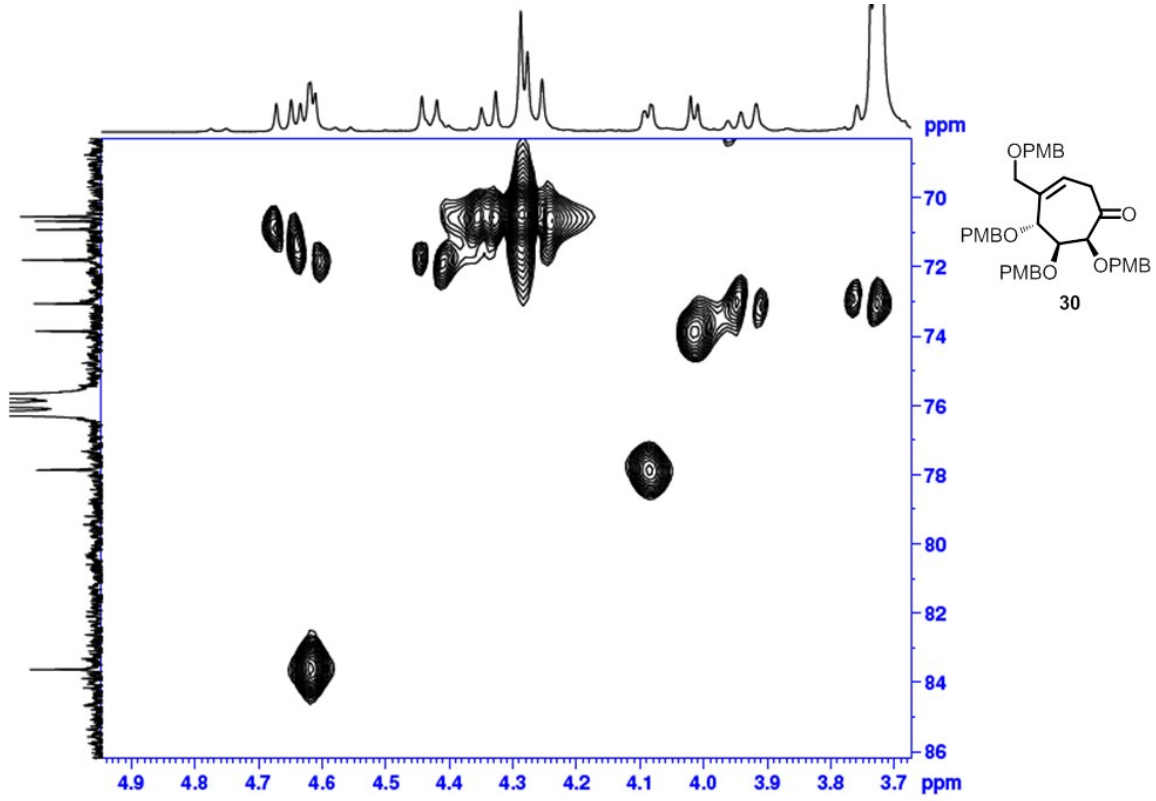
DEPT spectrum of cyclic ketone **30** recorded in $CDCl_3$



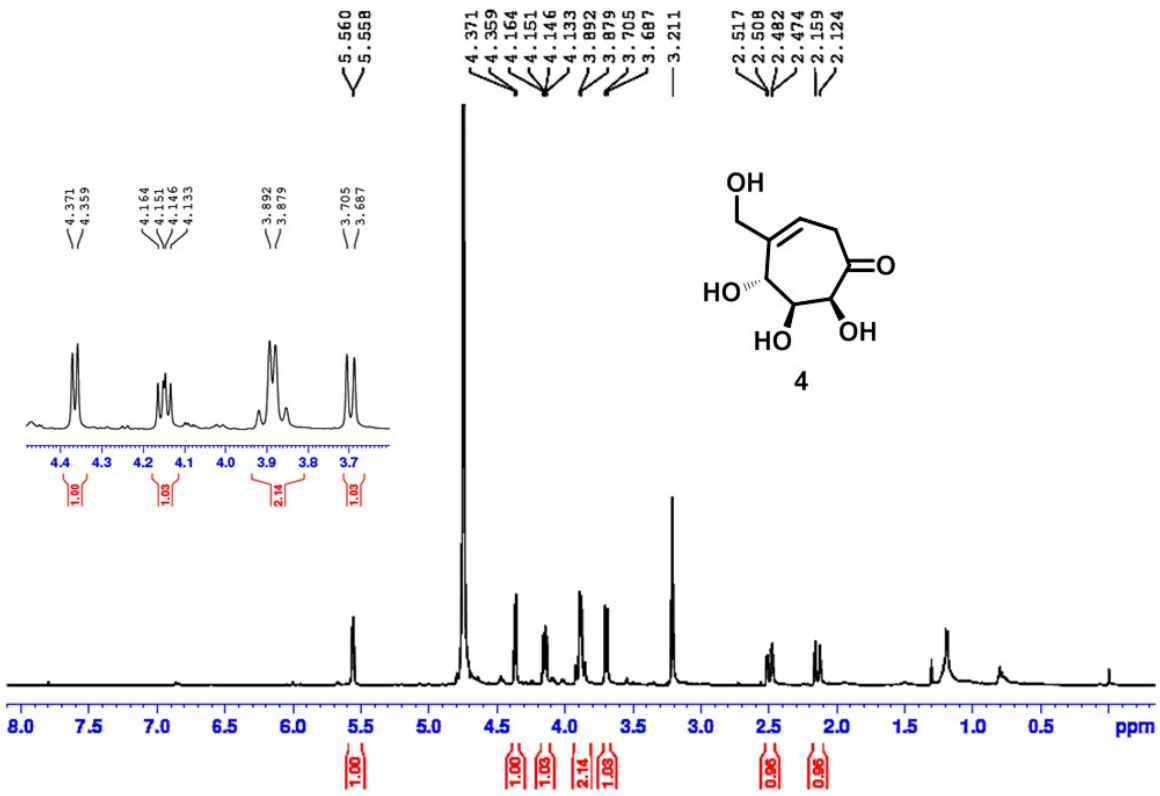
HMQC spectrum of cyclic ketone **30** recorded in $CDCl_3$



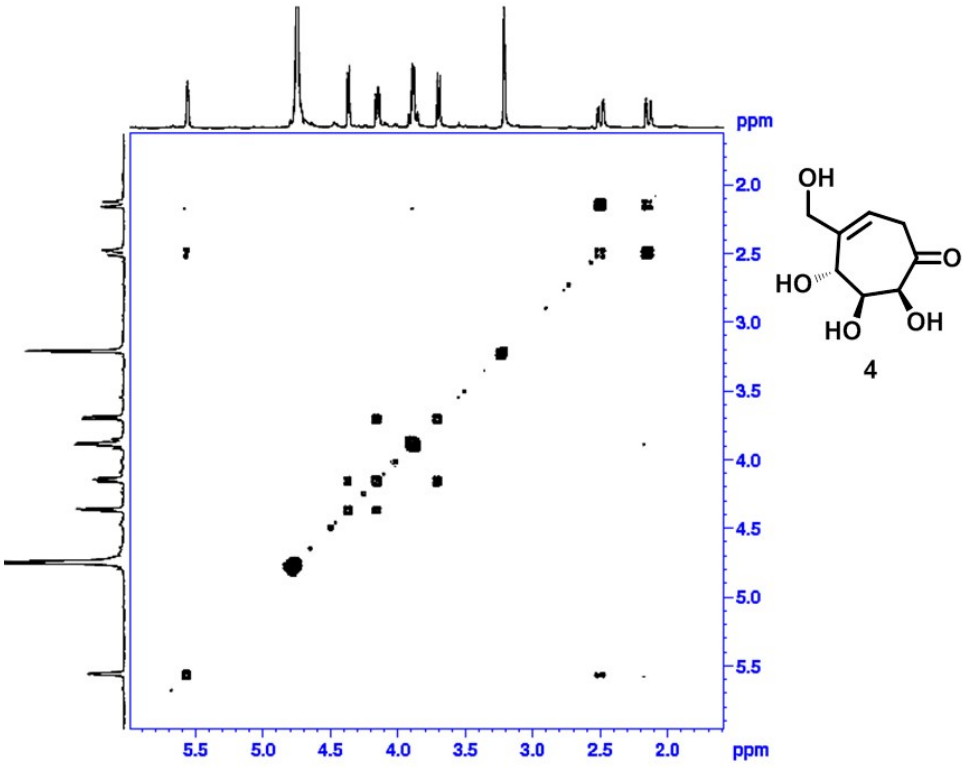
Expanded HMQC spectrum of cyclic ketone **30** recorded in $CDCl_3$



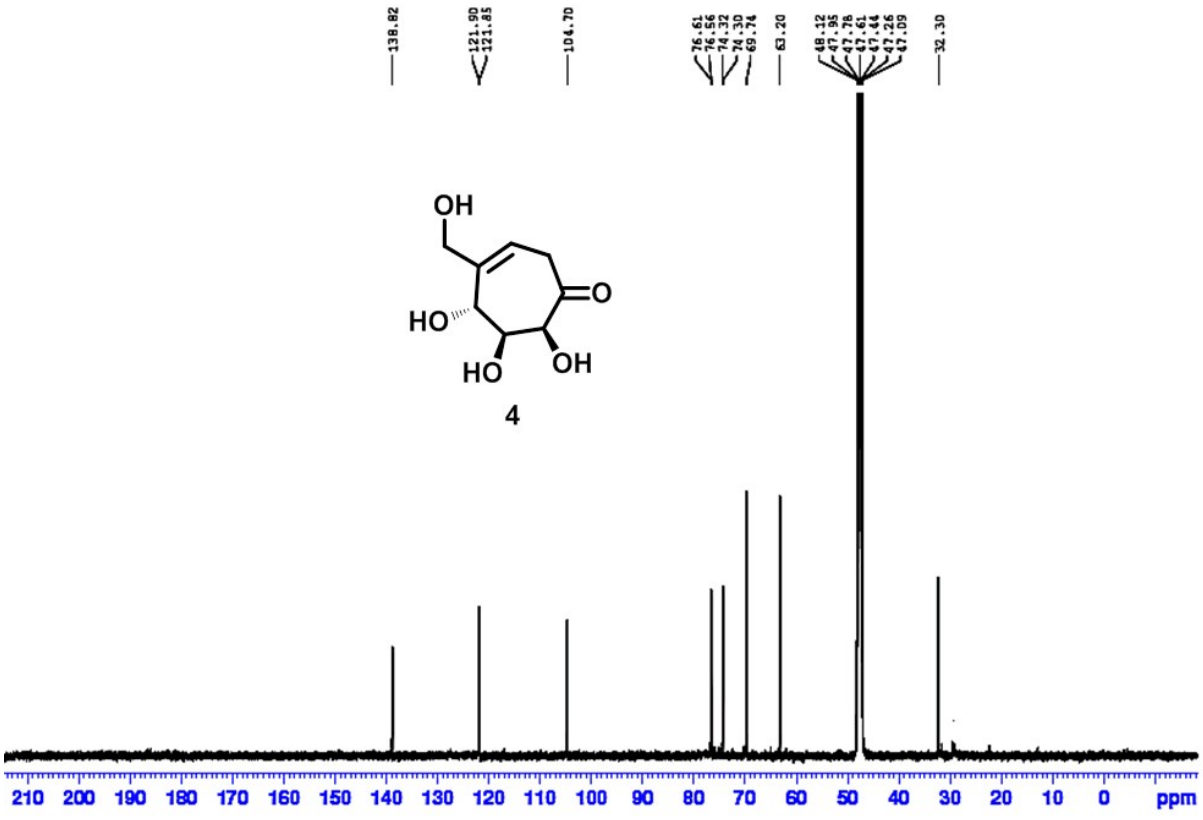
^{1}H NMR spectrum of compound **4** recorded in CD_3OD



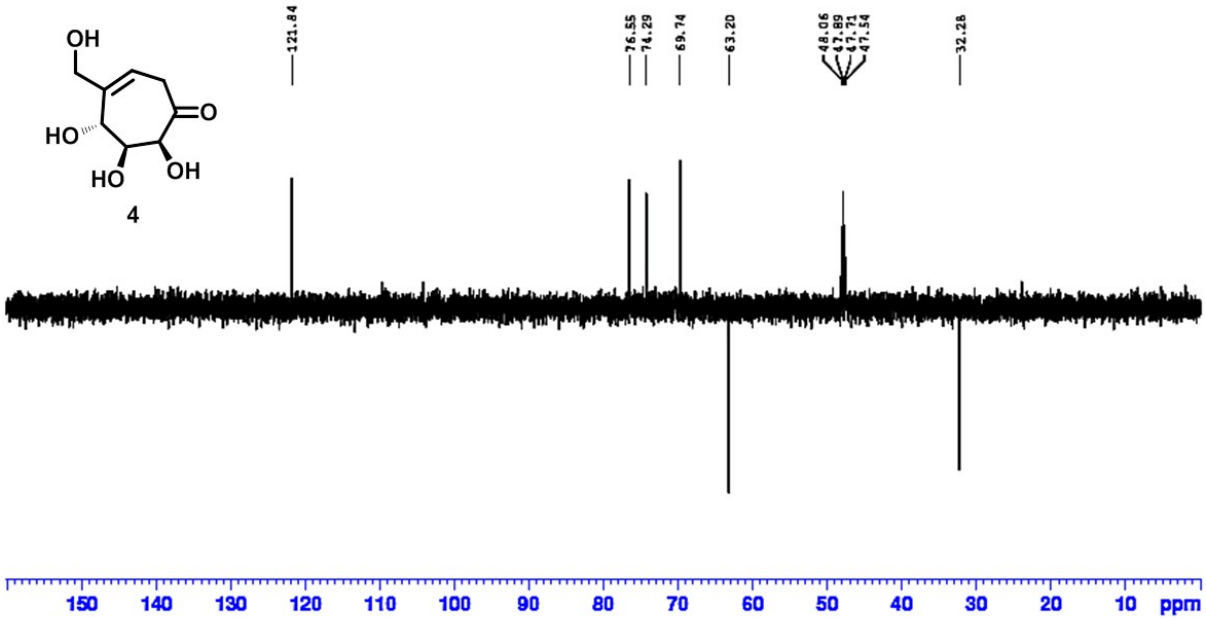
COSY spectrum of compound **4** recorded in CD_3OD



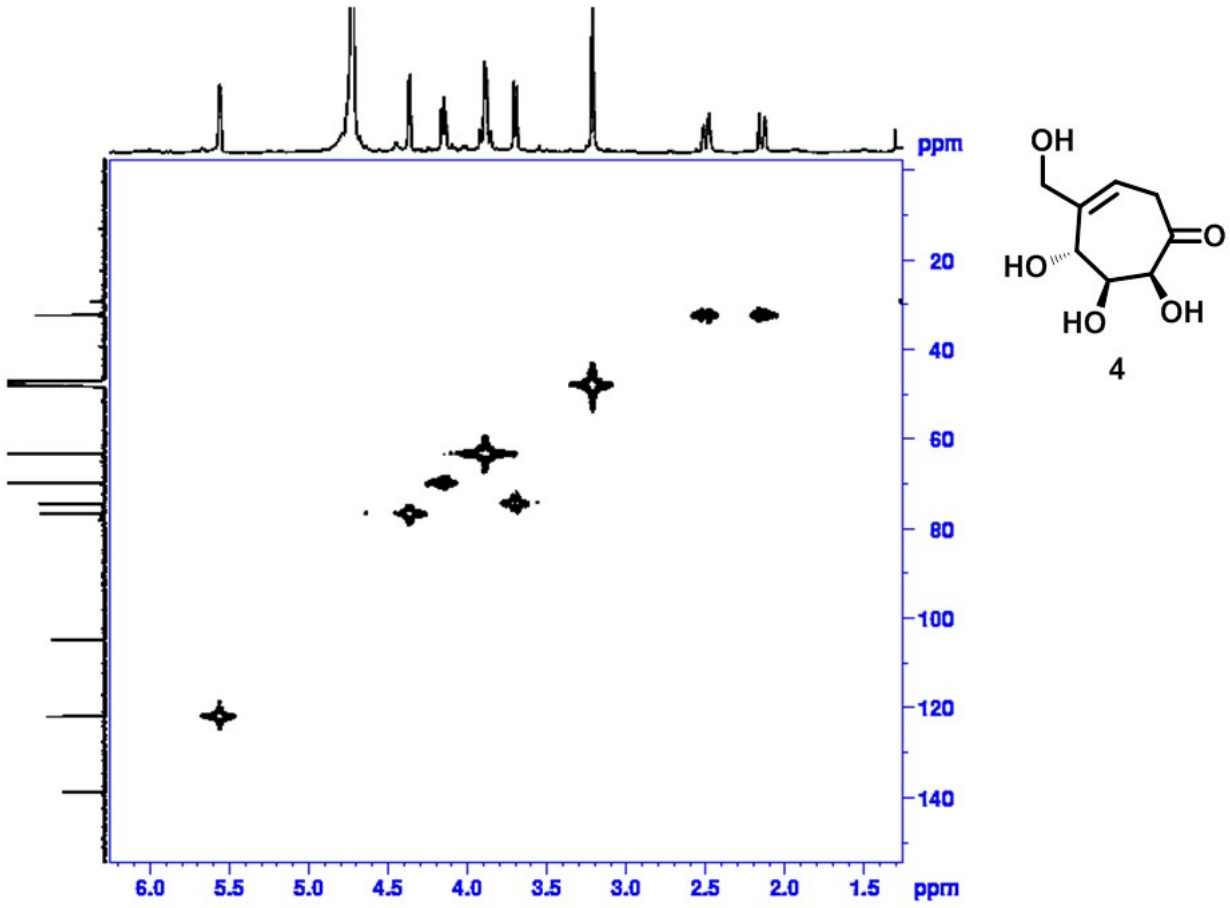
^{13}C NMR spectrum of compound **4** recorded in CD_3OD



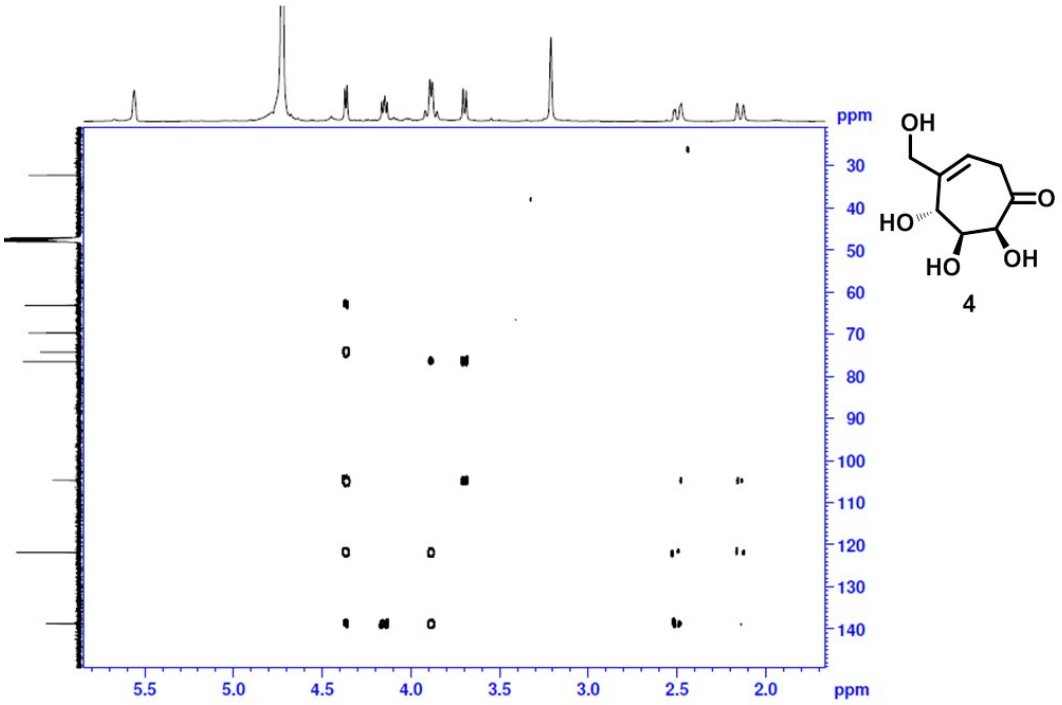
DEPT spectrum of compound **4** recorded in CD_3OD



HMQC spectrum of compound **4** recorded in CD_3OD



HMBC spectrum of compound **4** recorded in CD_3OD



NOESY spectrum of compound **4** recorded in CD_3OD