

Supplementary Material

A bis-glycosylamine strategy for the synthesis of dimeric iminosugars based on a DAB-1 scaffold

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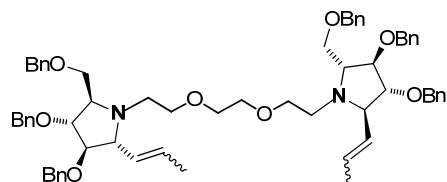
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Content :

1. Analytical data of **18d** (page S2)
2. ¹H NMR and ¹³C NMR spectra of new compounds (pages S3-S34)
3. Comparative ¹H NMR and ¹³C NMR data of **19d(R,R)** and **19d(S,S)** (pages S35)

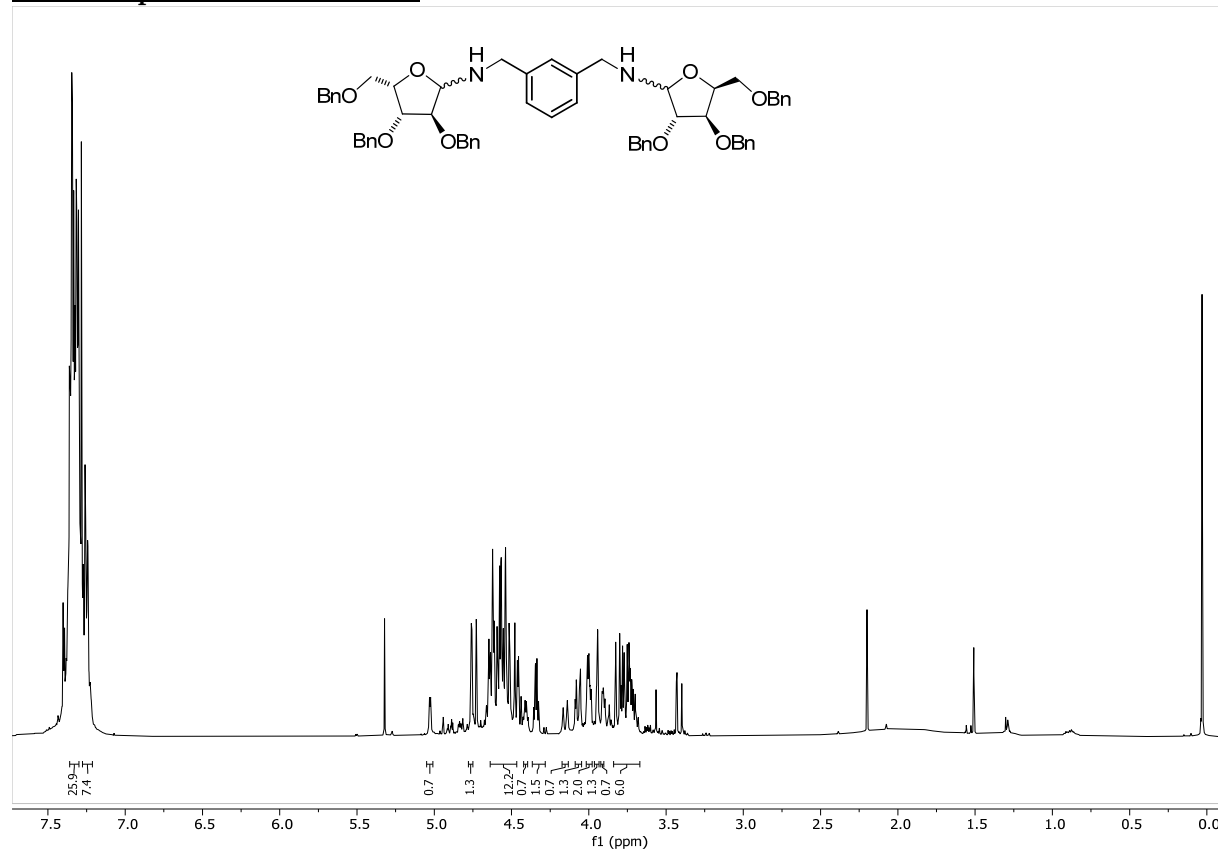
1. Characterizations of 18d



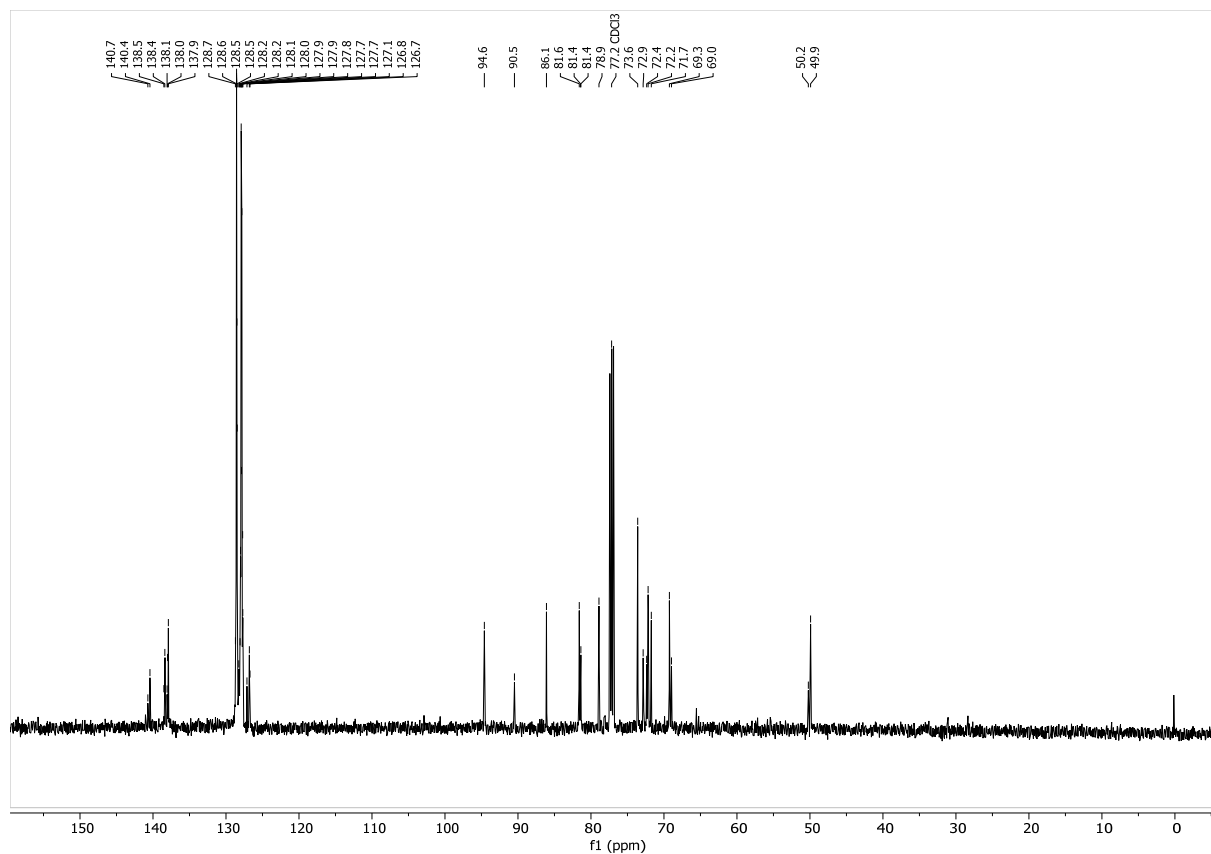
^1H NMR (500 MHz, CDCl_3): δ 7.34 – 7.29 (m, 30 H, Ar-H), 5.73 – 5.64 (m, 2 H, 2 x 1a- H^{maj} + 2 x 1a- H^{min}), 5.4 – 5.45 (m, 2 H, 2 x 2a- H^{maj} + 2 x 2a- H^{min}), 4.58 – 4.46 (m, 12 H, 6 x $\text{CH}_2\text{-Ph}$), 4.00 – 3.94 (m, 2 H, 2 x 4- H^{maj} + 2 x 4- H^{min}), 3.79 – 3.76 (m, 2 H, 2 x 3- H^{maj} + 2 x 3- H^{min}), 3.68 – 3.50 (m, 14 H, 2 x 6- H^{maj} + 2 x 6- H^{min} + 2 x 2- H^{maj} + 2 x 2- H^{min} + 4 x CH_2), 3.35 – 3.31 (m, 2 H, 2 x 5- H^{maj} + 2 x 5- H^{min}), 2.91 – 2.81 (m, 4 H, 2 x $\text{NH-CH}_2^{\text{maj}}$ + 2 x $\text{NH-CH}_2^{\text{min}}$), 1.74 – 1.70 (m, 6 H, 2 x 3a- H^{maj} + 2 x 3a- H^{min}) ppm; ^{13}C NMR (125 MHz, CDCl_3): δ 138.5 (C^{IV}), 138.5 (C^{IV}), 130.8 (C-2a $^{\text{maj}}$), 130.1 (C-2a $^{\text{min}}$), 129.6 (C-1a $^{\text{maj}}$), 128.4, 128.3, 127.9, (C-Ar), 127.9 (C-1a $^{\text{min}}$), 127.8, 127.7, 127.7, 127.6 (C-Ar), 88.5 (C-3 $^{\text{min}}$), 88.2 (C-3 $^{\text{maj}}$), 85.8 (C-4 $^{\text{min}}$), 85.6 (C-4 $^{\text{maj}}$), 73.3 ($\text{CH}_2\text{-Ph}$), 71.7 ($\text{CH}_2\text{-Ph}$), 71.4 ($\text{CH}_2\text{-Ph}$), 70.4 (CH_2), 70.2 (CH_2), 70.0 (C-2 $^{\text{maj}}$ + C-2 $^{\text{min}}$), 69.1 (C-6 $^{\text{min}}$), 68.9 (C-6 $^{\text{maj}}$), 65.6 (C-5 $^{\text{min}}$), 65.5 (C-5 $^{\text{maj}}$), 46.8 ($\text{NH-CH}_2^{\text{min}}$), 46.7 ($\text{NH-CH}_2^{\text{maj}}$), 18.0 (C-3a $^{\text{maj}}$), 13.4 (C-3a $^{\text{min}}$) ppm; $[\alpha]_D^{25} = -30.8$ (c 1, CHCl_3). HRMS (ESI) m/z calcd for $[\text{C}_{64}\text{H}_{76}\text{N}_2\text{O}_8 + \text{H}]^+$: 1001.5680, found 1001.5671.

1. ^1H NMR and ^{13}C NMR spectra of new compounds

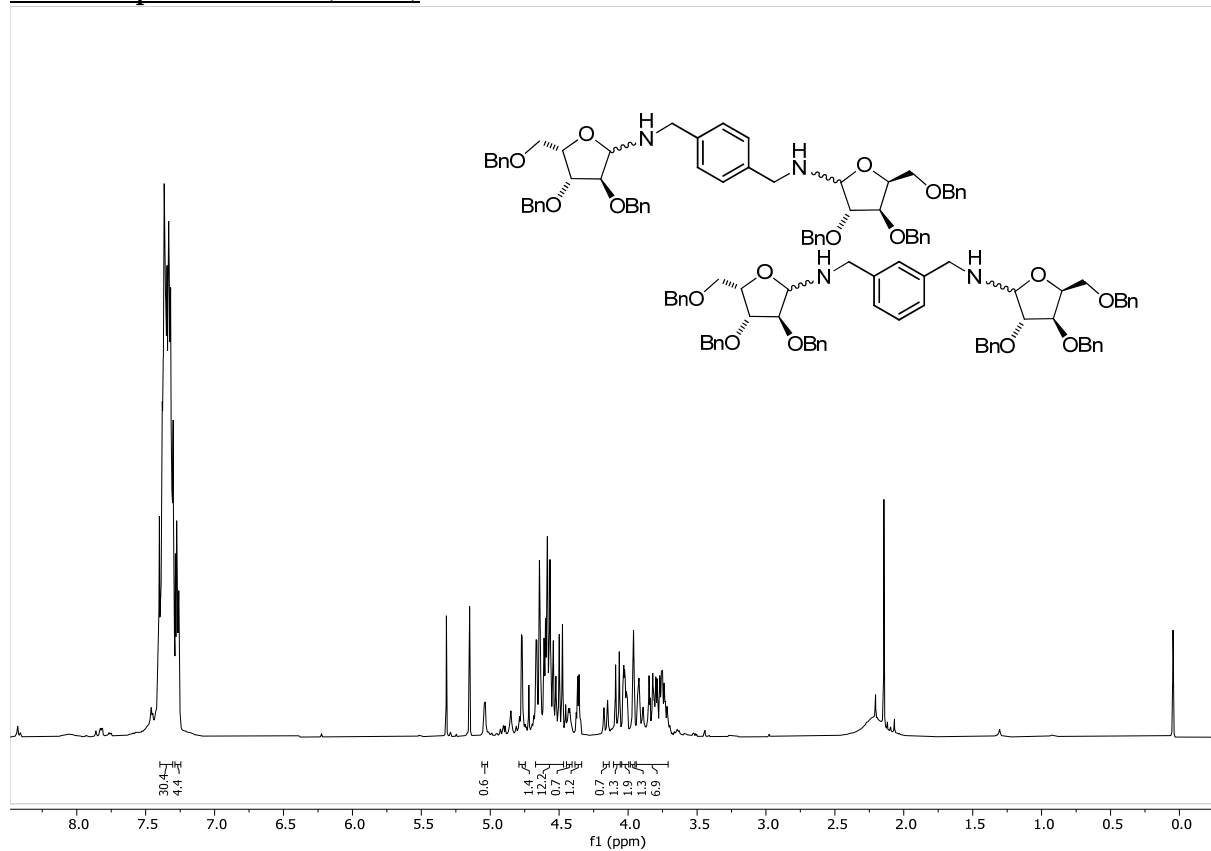
¹H-NMR spectrum of 10a (CDCl₃)



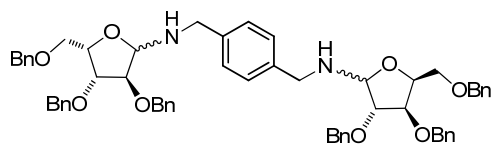
¹³C-NMR spectrum of 10a (CDCl₃)



¹H-NMR spectrum of 10b (CDCl₃)



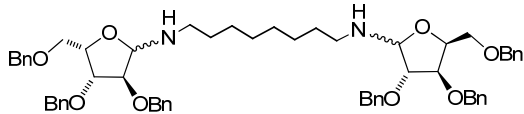
¹³C-NMR spectrum of 10b (CDCl₃)



Chemical structure of the compound is shown above the spectrum. The structure is a symmetrical molecule consisting of two 2,3,4-tri-O-benzyl-5-O-((9-oxo-9H-fluoren-2-ylideneamino)oxy)pentofuranose units linked by a 1,6-hexanediyl chain. The structure is drawn with stereochemistry indicating the anomeric configuration of the sugar units.

¹H NMR spectrum (CDCl₃) of the compound. The x-axis is labeled f1 (ppm) and ranges from 0.0 to 10.0. The spectrum shows a large solvent peak at 7.26 ppm (CDCl₃), a cluster of peaks between 3.5 and 5.5 ppm corresponding to the sugar protons, and a sharp peak at 0.0 ppm (TMS). Integration values are provided below the baseline: 0.7, 1.3, 12.7, 0.7, 1.2, 1.9, 1.9, 4.1, 2.1, 2.4, and 14.2.

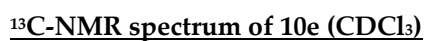
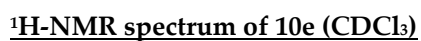
¹³C-NMR spectrum of 10c (CDCl₃)

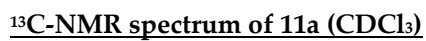
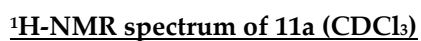


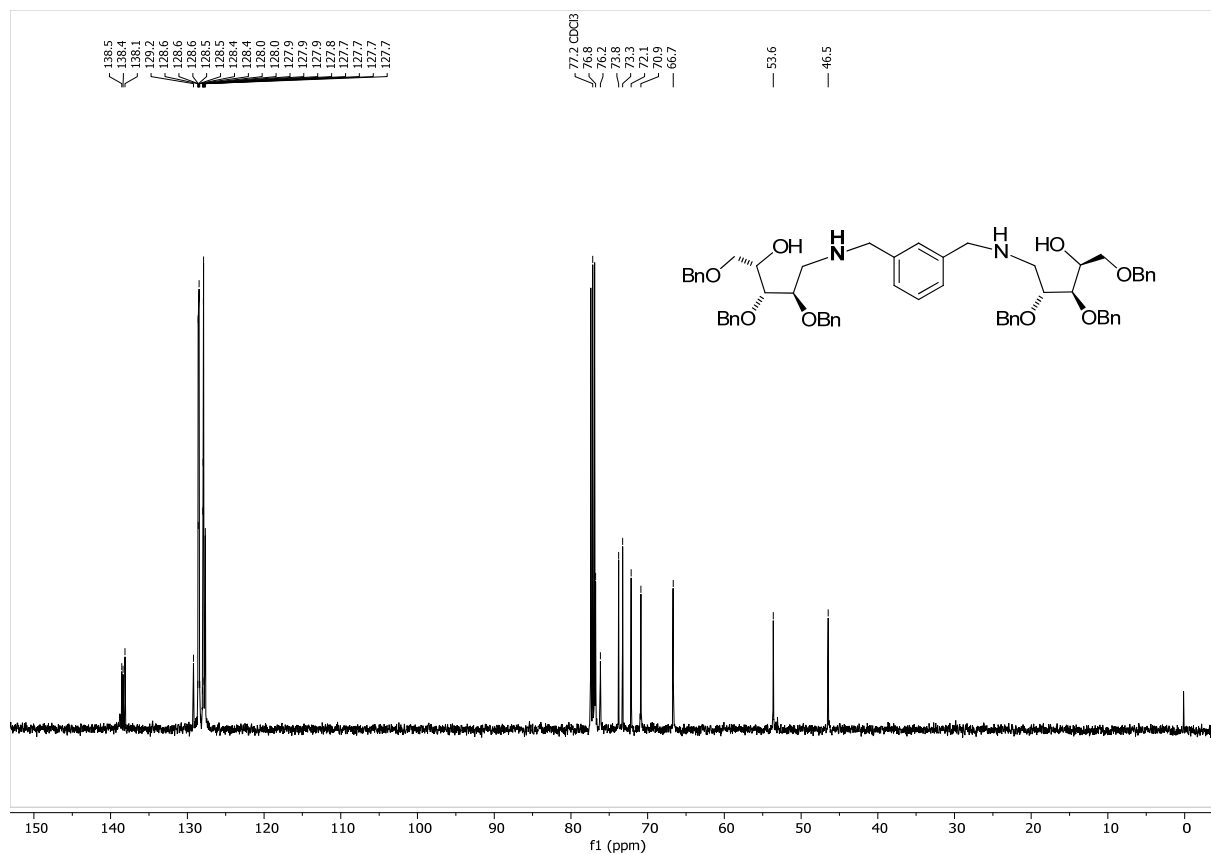
Chemical structure of the compound is shown above the spectrum. The spectrum displays peaks corresponding to the structure, with integration values provided below the baseline.

Chemical Shift (ppm)	Integration
7.2 (solvent)	31.8
5.1 (NH)	0.6
4.6-4.8 (sugar protons)	1.4, 1.2, 0.7, 1.2
3.8-4.1 (linker protons)	1.9, 1.3, 0.7, 4.1
3.5-3.7 (sugar protons)	8.0
2.8-3.2 (benzyloxy protons)	2.0, 2.3

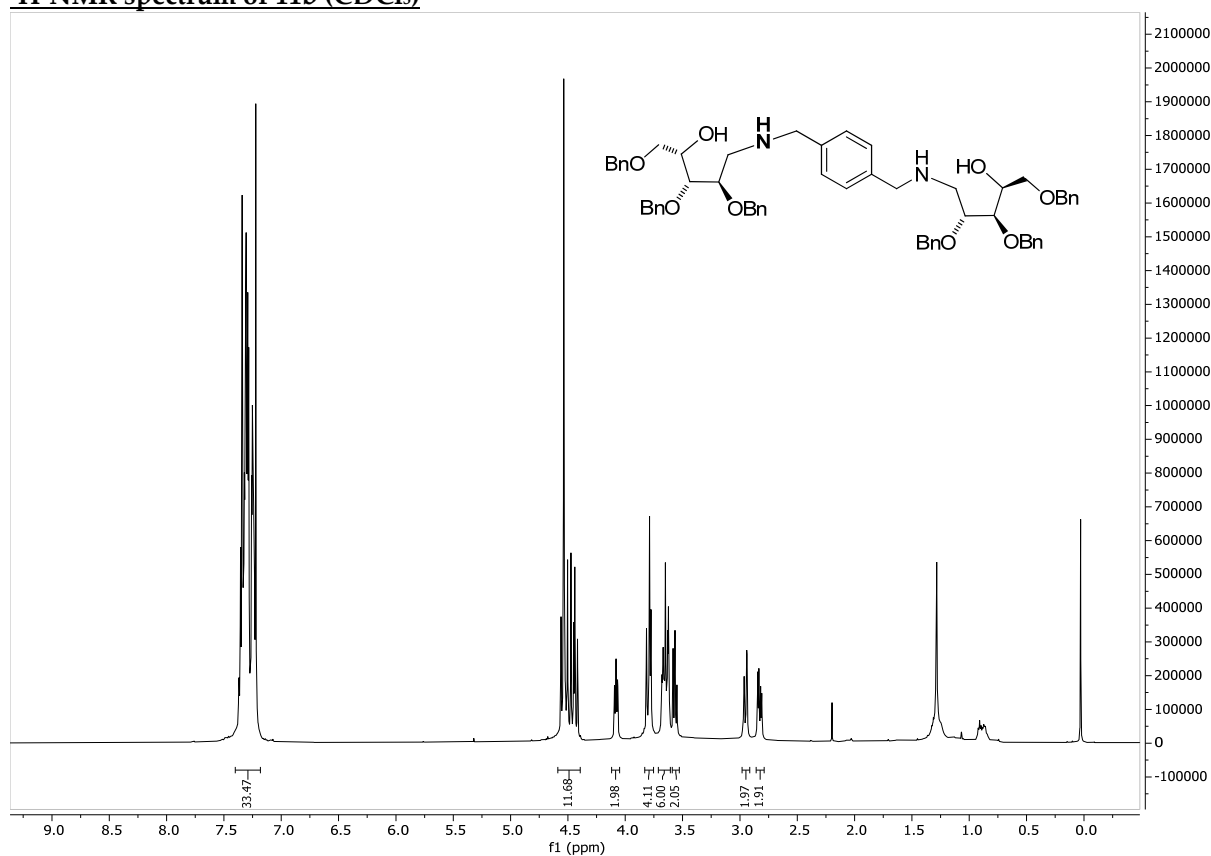
S7



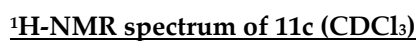


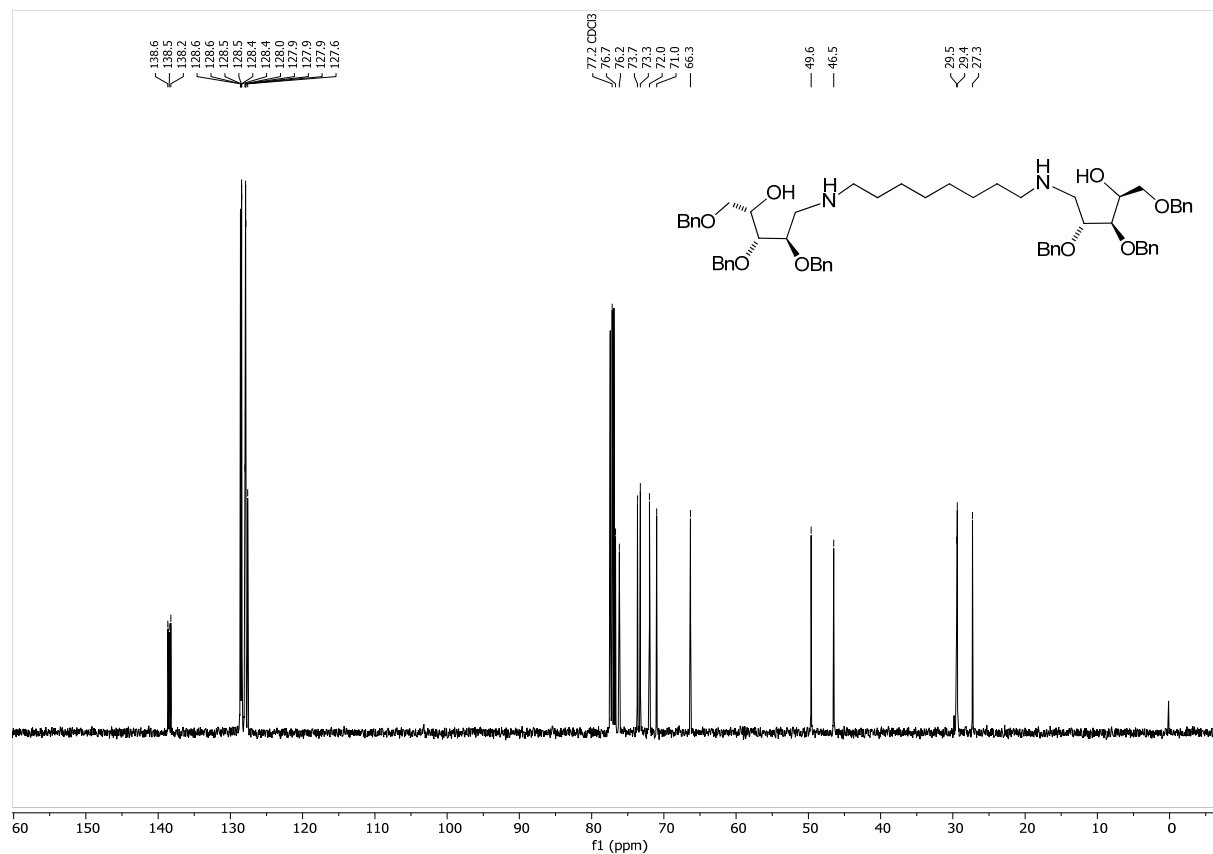


¹H-NMR spectrum of 11b (CDCl₃)

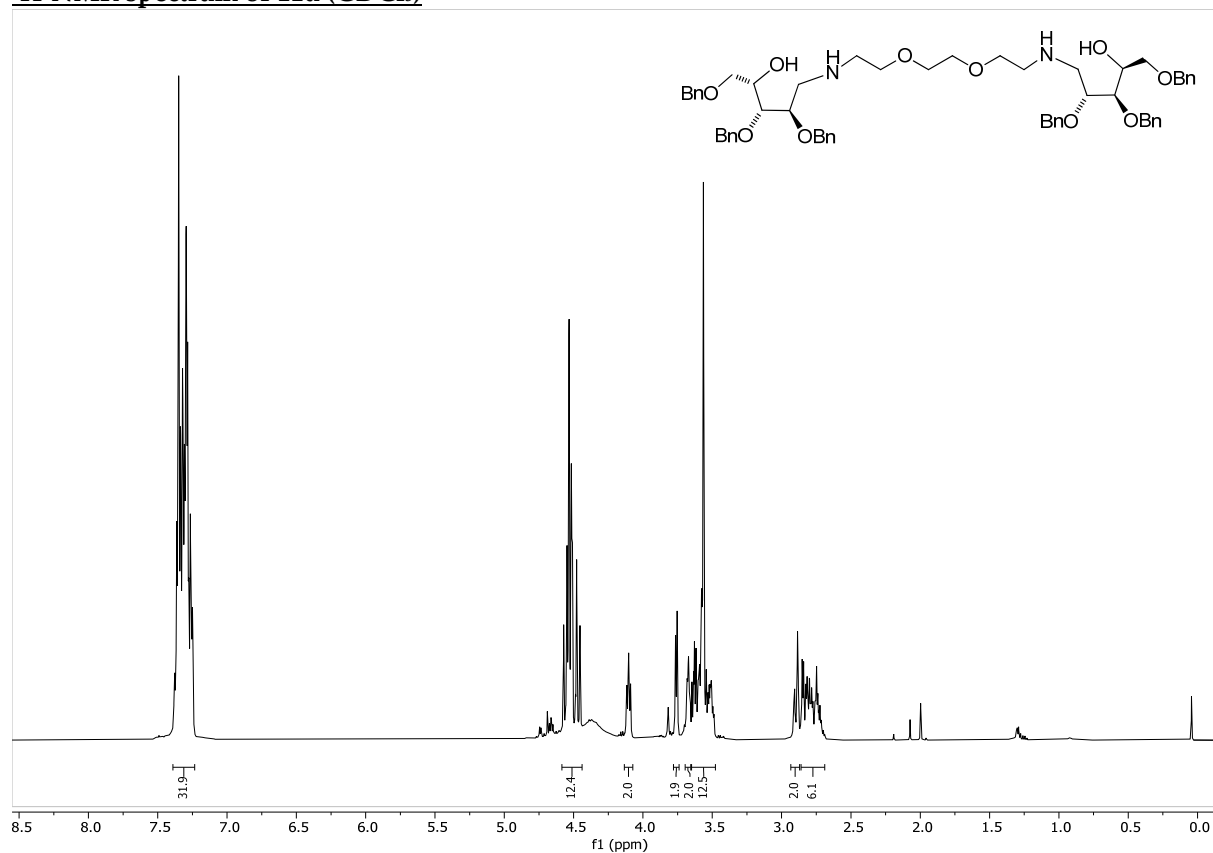


¹³C-NMR spectrum of 11b (CDCl₃)

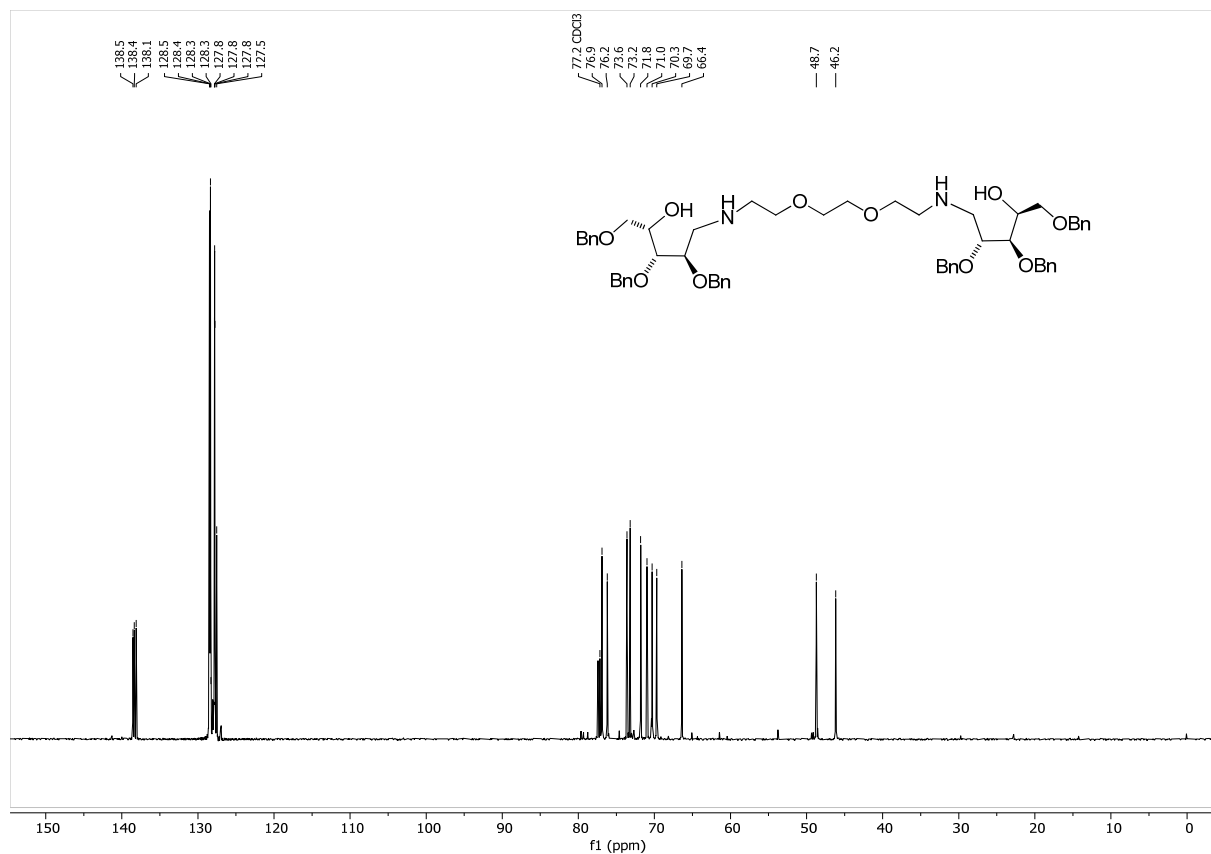




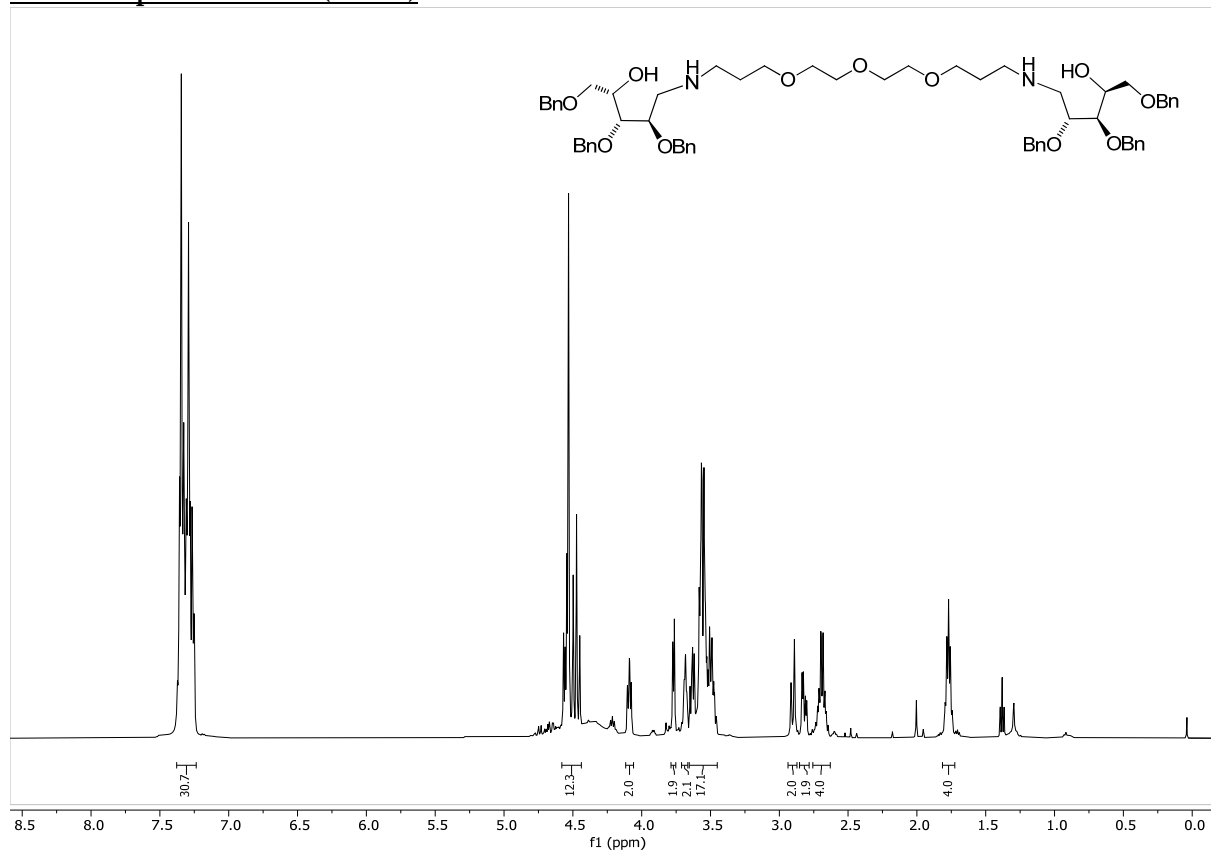
¹H-NMR spectrum of 11d (CDCl₃)



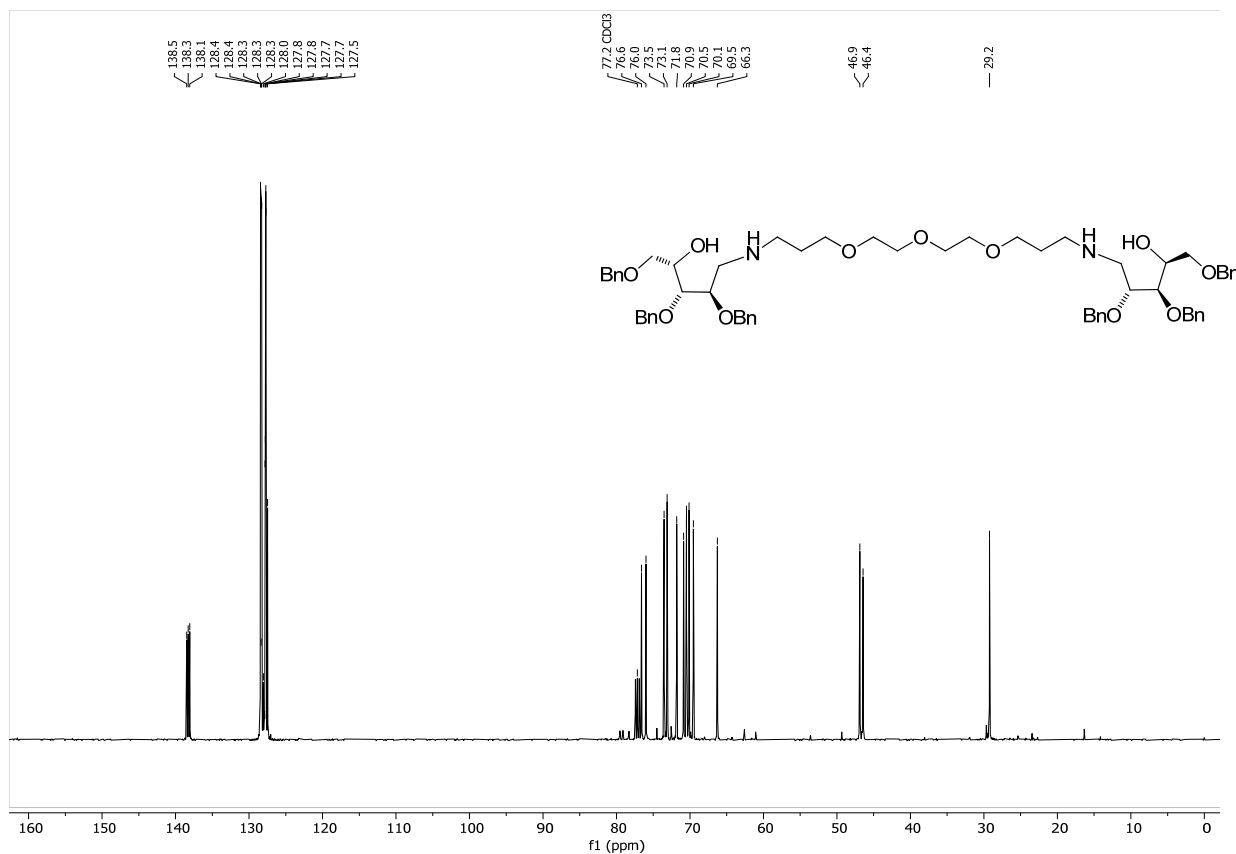
¹³C-NMR spectrum of 11d (CDCl₃)



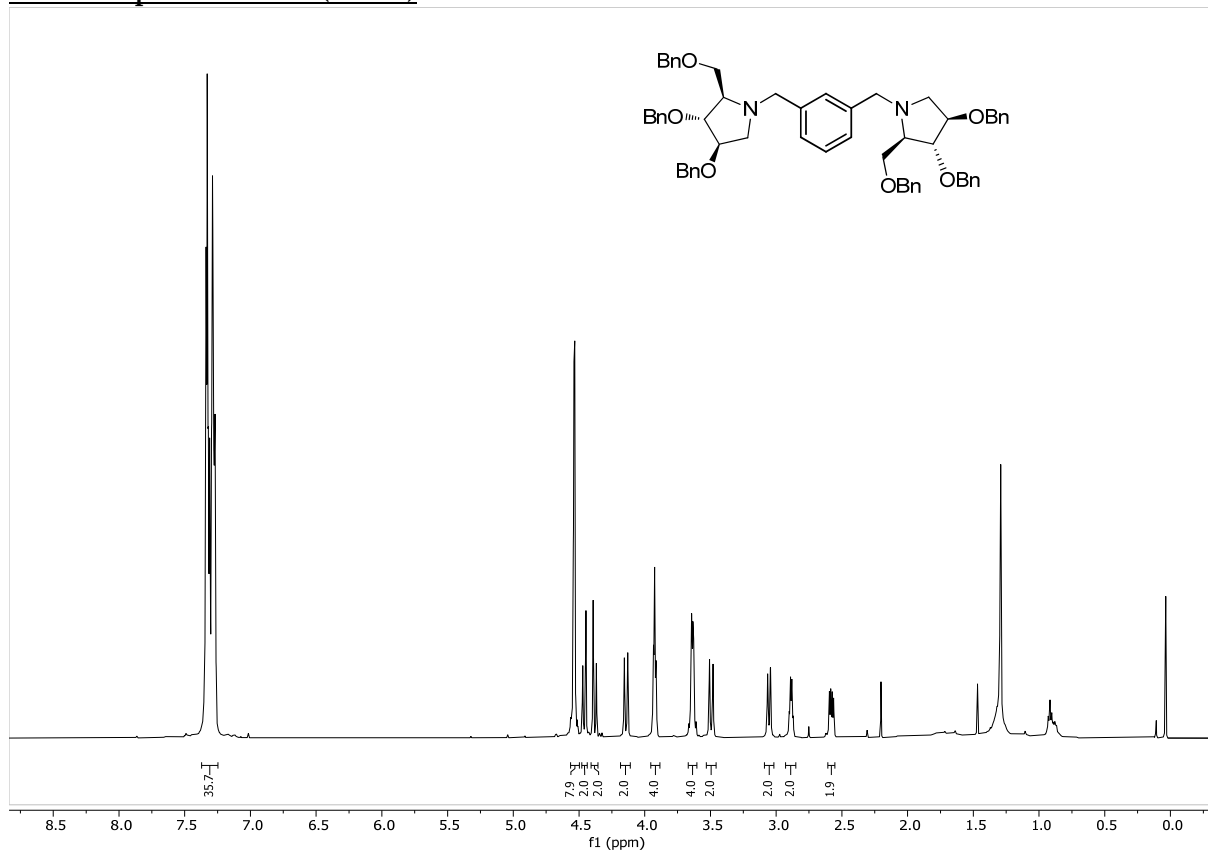
¹H-NMR spectrum of 11e (CDCl₃)



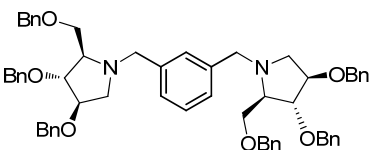
¹³C-NMR spectrum of 11e (CDCl₃)



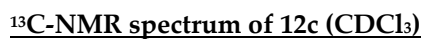
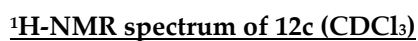
¹H-NMR spectrum of 12a (CDCl₃)

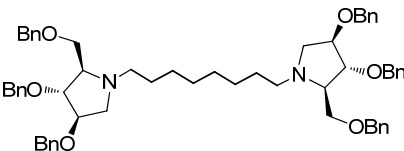


¹³C-NMR spectrum of 12a (CDCl₃)

[illegible]

S15





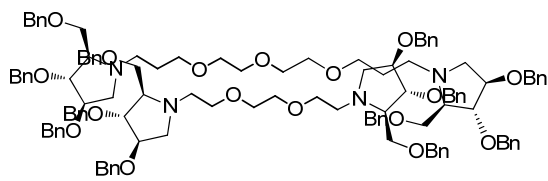
Chemical structure of the compound is shown above the spectrum. The structure is a bis-oxazoline derivative, specifically 2,2'-(1,3-bis(methoxyethoxy))bis(2,2-dimethoxy-1,3-oxazoline). The structure consists of two 2,2-dimethoxy-1,3-oxazoline rings connected by a 1,3-bis(methoxyethoxy) linker. The chemical structure is shown with stereochemistry: the methoxy groups on the oxazoline rings are in the (R) configuration.

¹H NMR spectrum (CDCl₃) showing peaks from 0.0 to 9.0 ppm. The spectrum displays several multiplets and singlets corresponding to the protons in the molecule. Key peaks are labeled with their chemical shifts (ppm) and integration values:

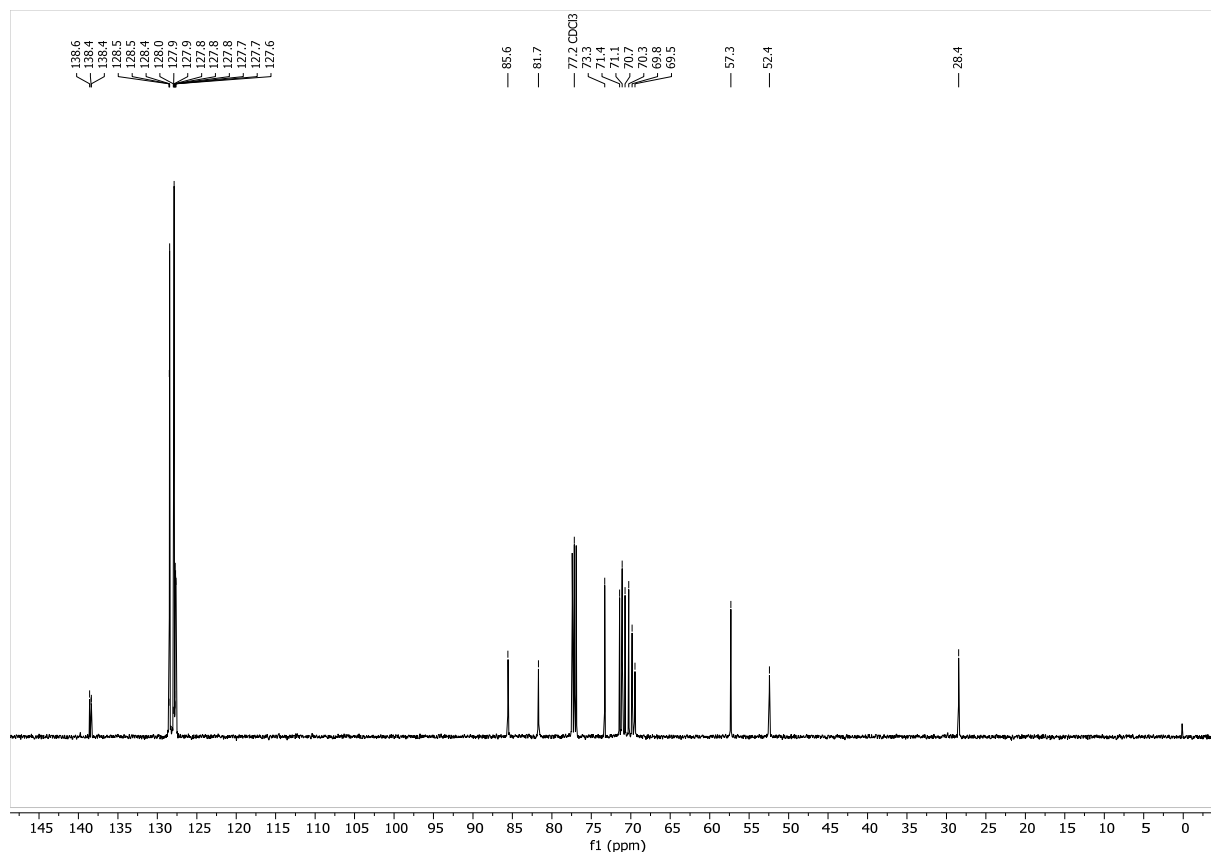
- 7.32 ppm (s, 1H, integration 32.15)
- 4.52 ppm (m, 4H, integration 10.22)
- 4.02 ppm (m, 4H, integration 2.05)
- 3.72 ppm (m, 4H, integration 1.99)
- 3.52 ppm (m, 4H, integration 12.91)
- 3.32 ppm (m, 4H, integration 1.92)
- 3.12 ppm (m, 4H, integration 2.04)
- 2.92 ppm (m, 4H, integration 2.01)
- 2.72 ppm (m, 4H, integration 1.98)
- 2.52 ppm (m, 4H, integration 2.00)

The spectrum shows a complex pattern of peaks, indicating the presence of multiple proton environments in the molecule. The integration values provide a quantitative measure of the relative areas under the peaks, which can be used to determine the relative concentrations of the different proton environments.

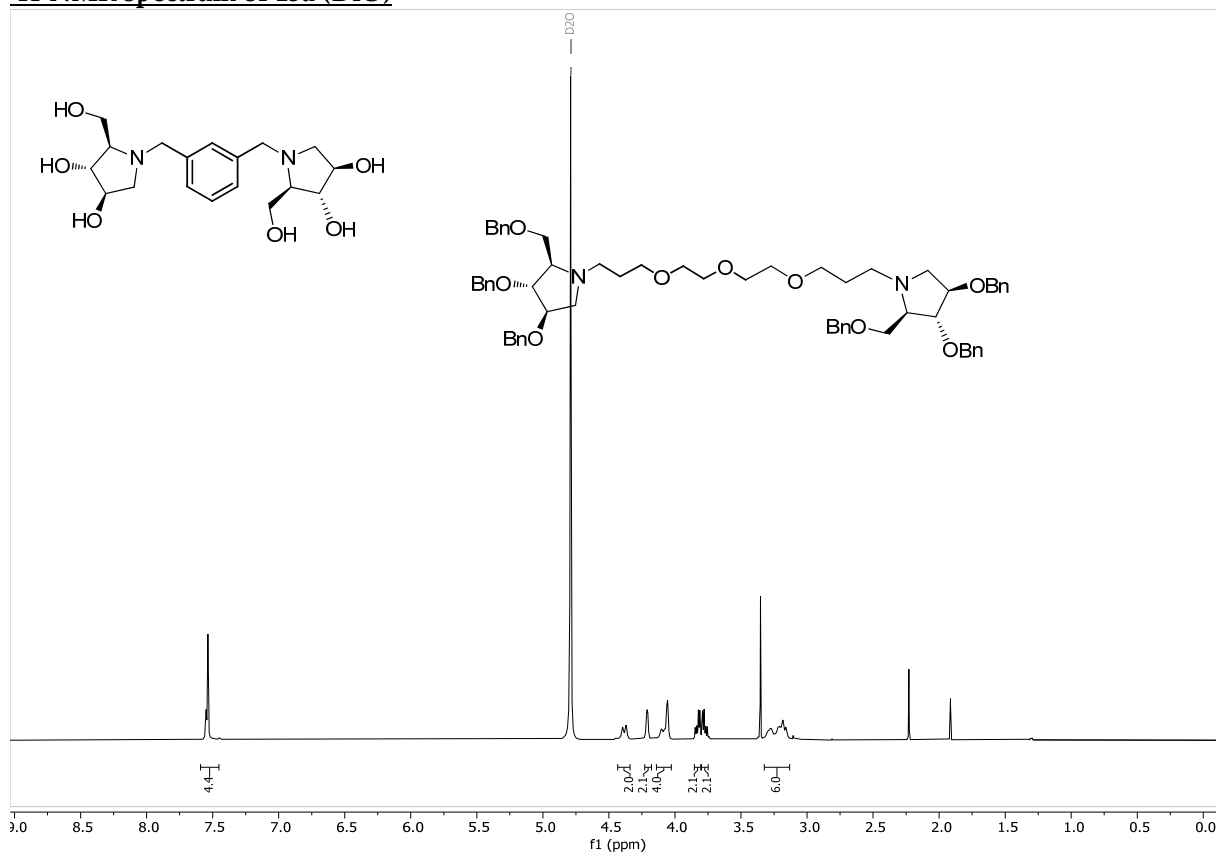
S17



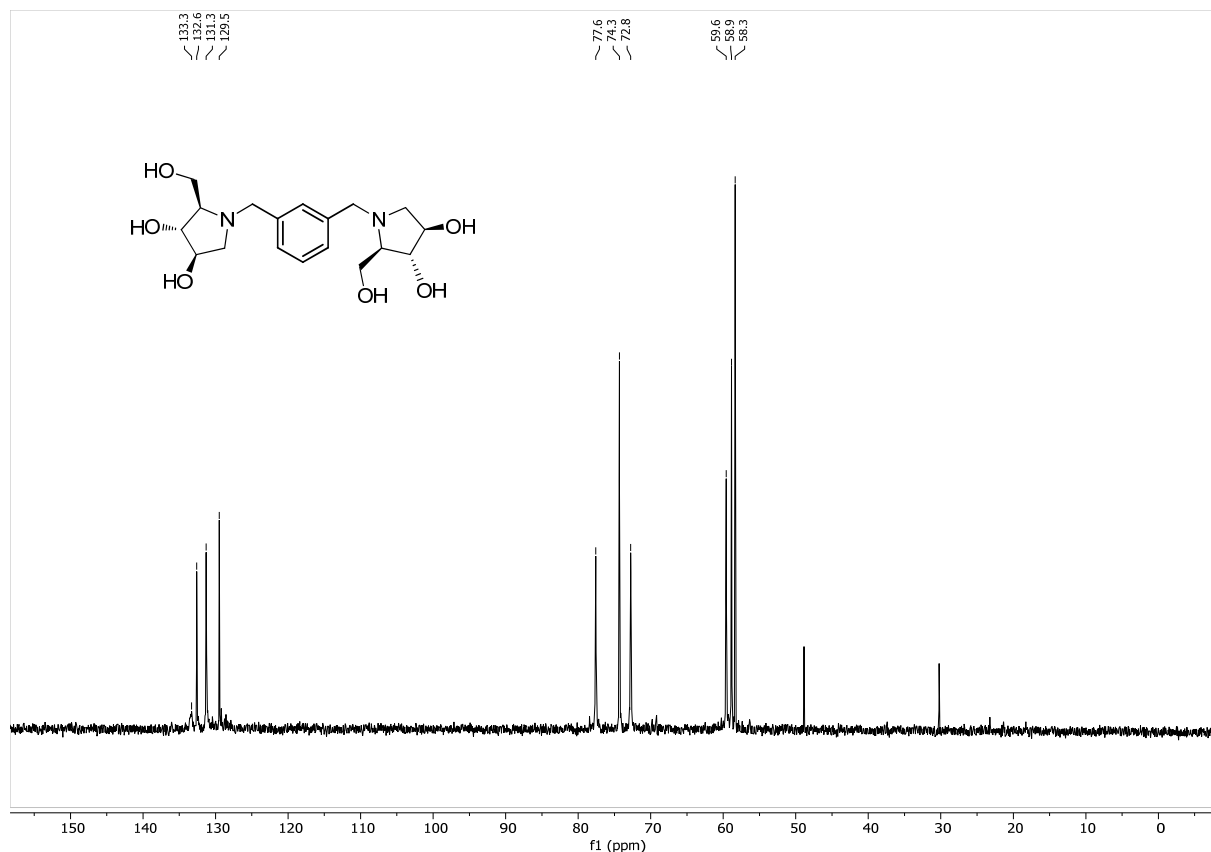
S18



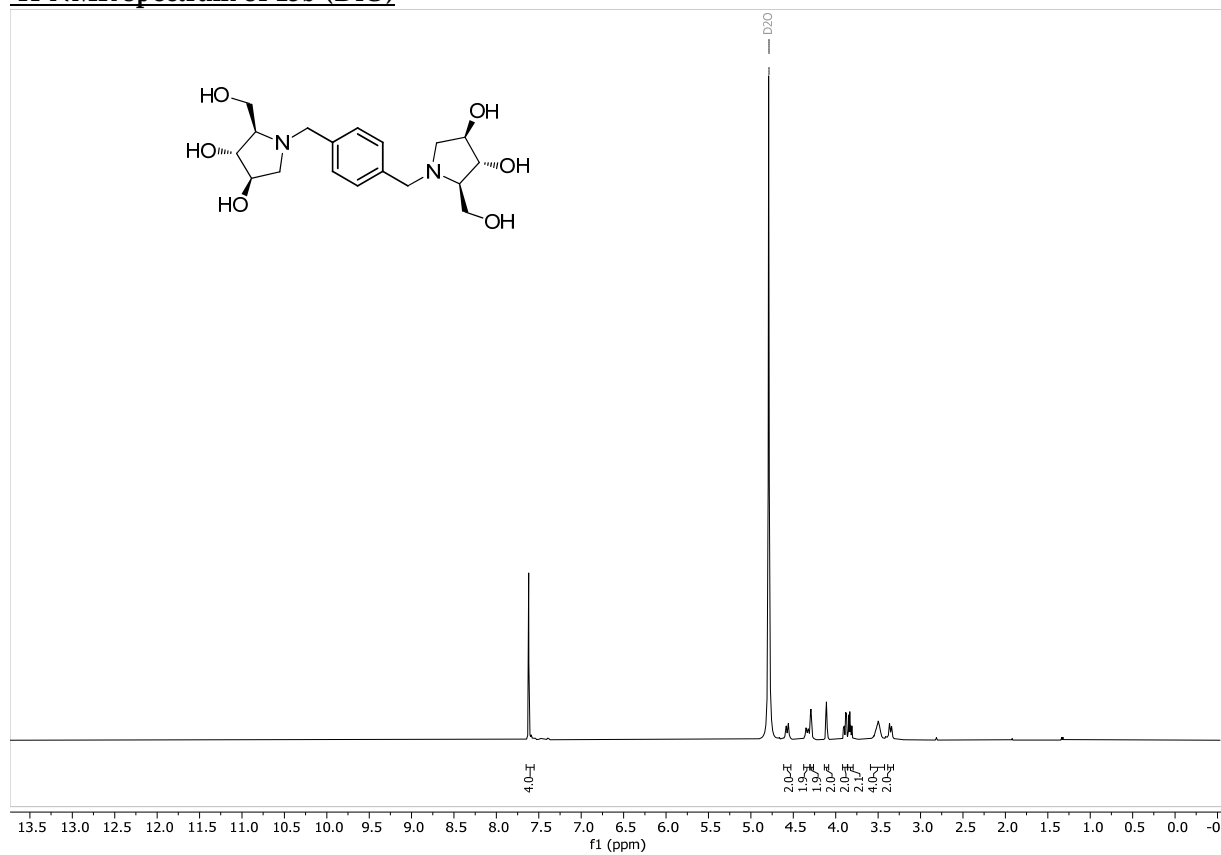
¹H-NMR spectrum of 13a (D₂O)



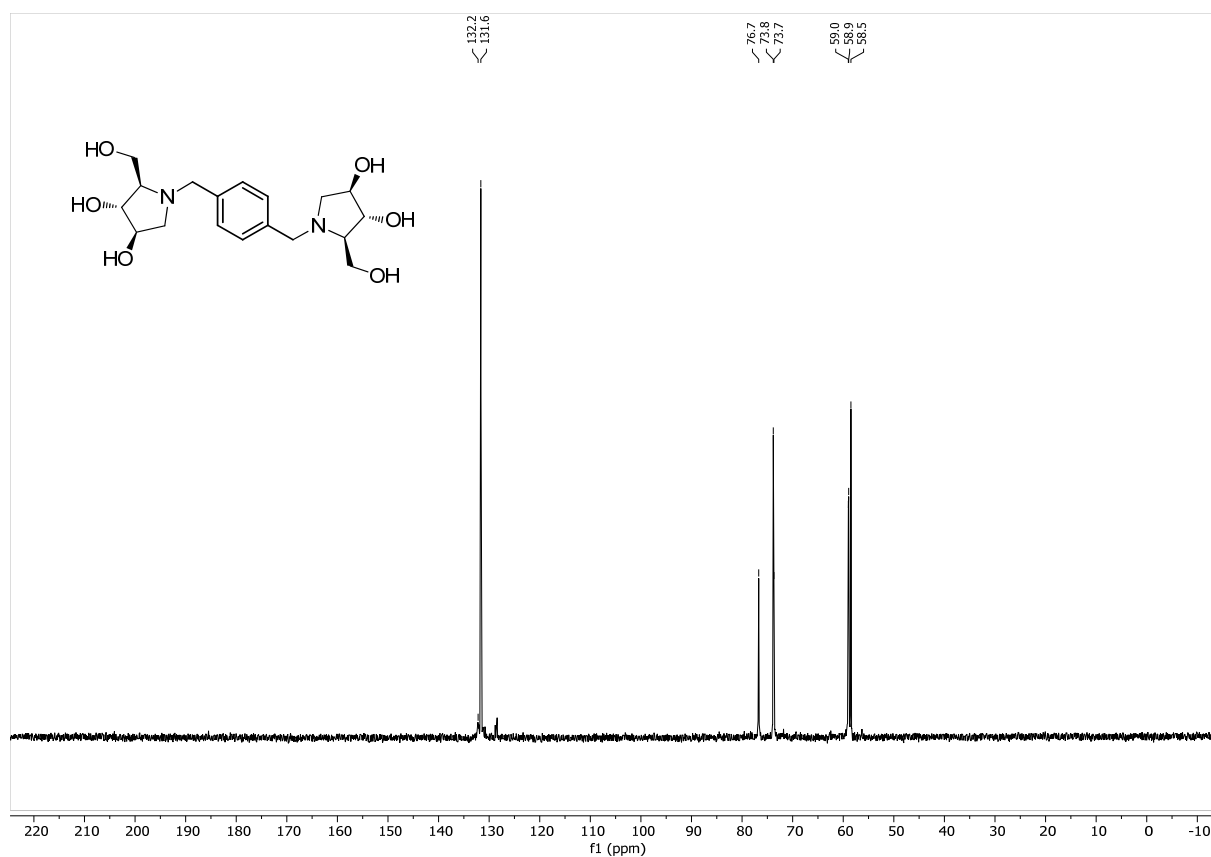
¹³C-NMR spectrum of 13a (D₂O)



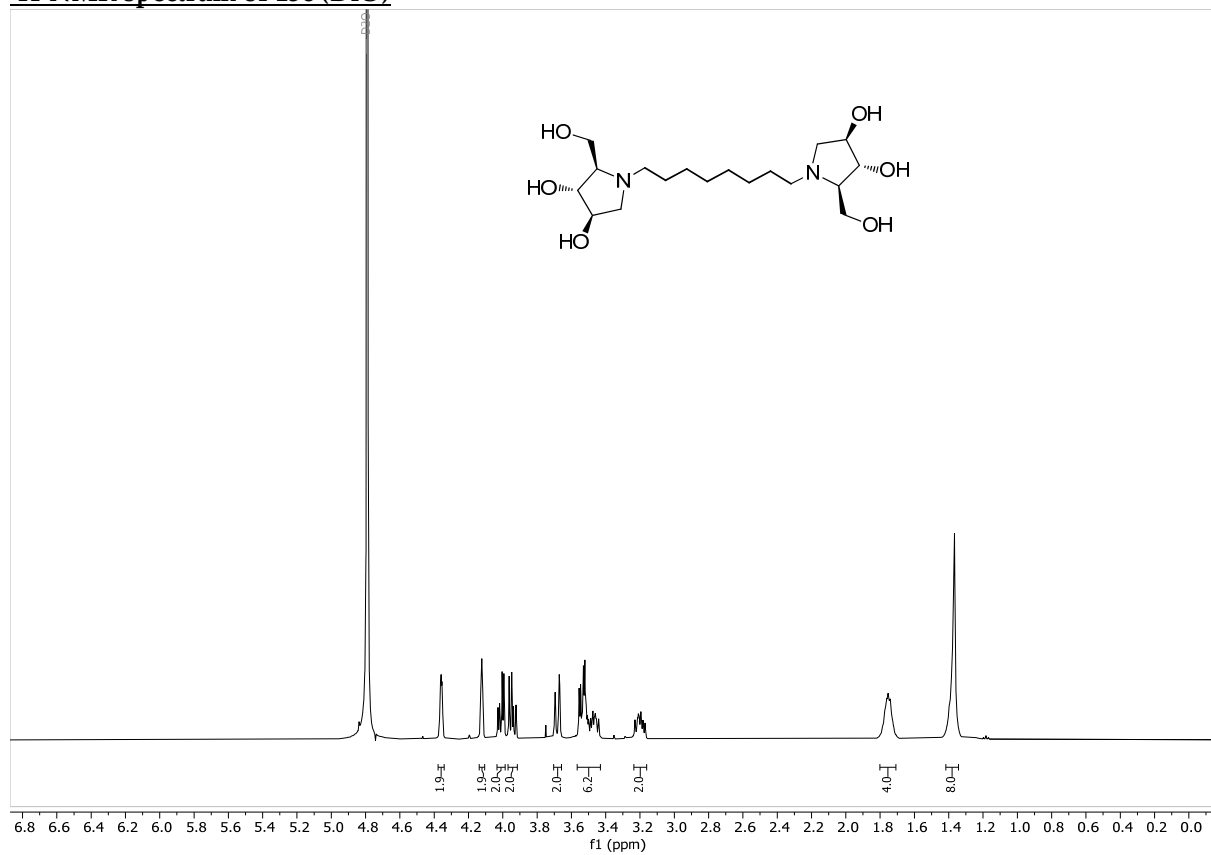
¹H-NMR spectrum of 13b (D₂O)



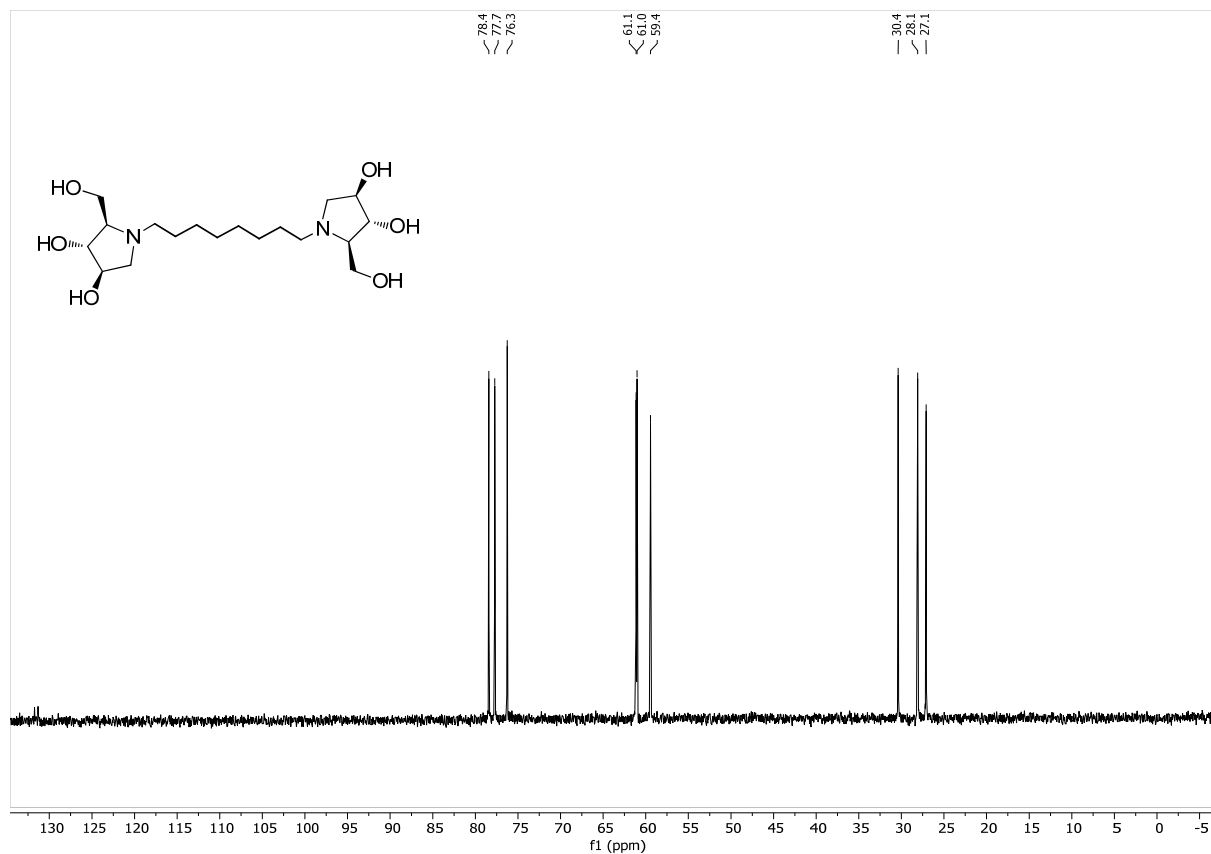
¹³C-NMR spectrum of 13b (D₂O)



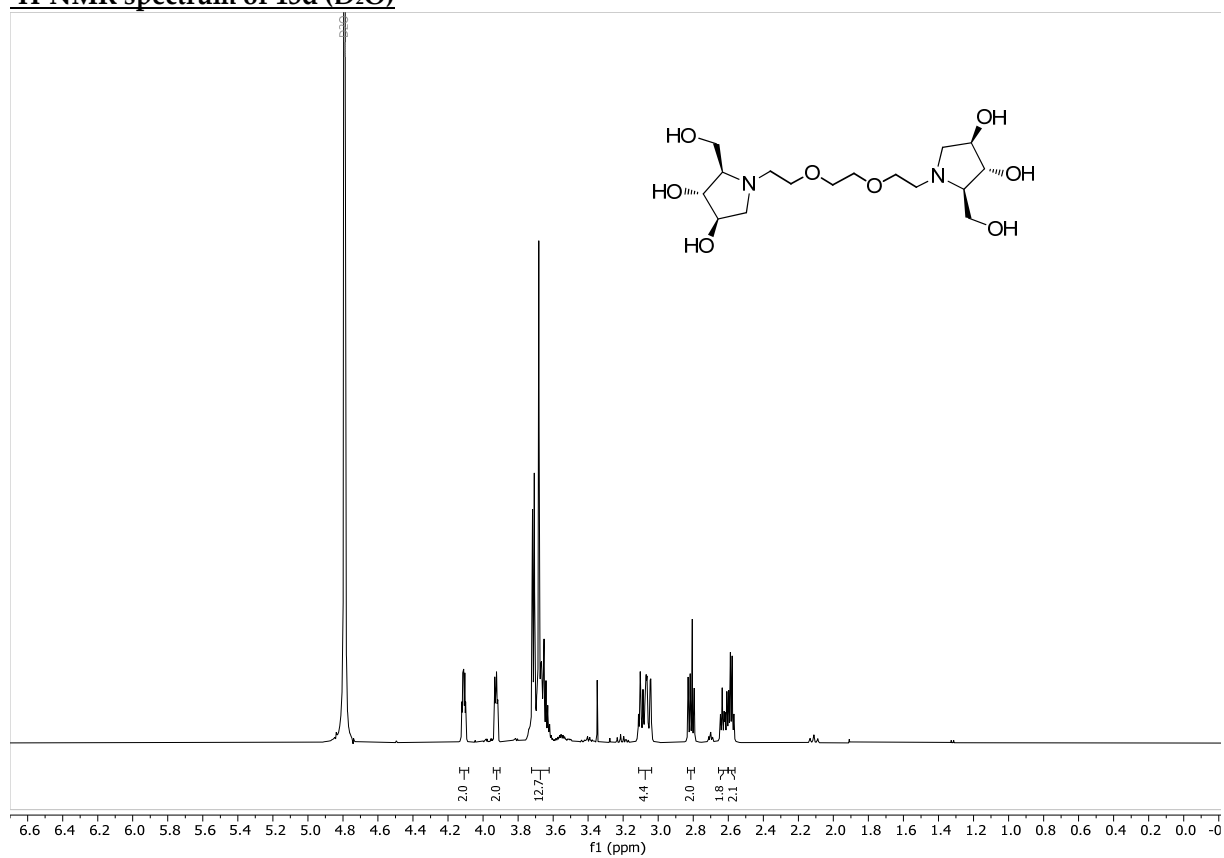
¹H-NMR spectrum of 13c (D₂O)



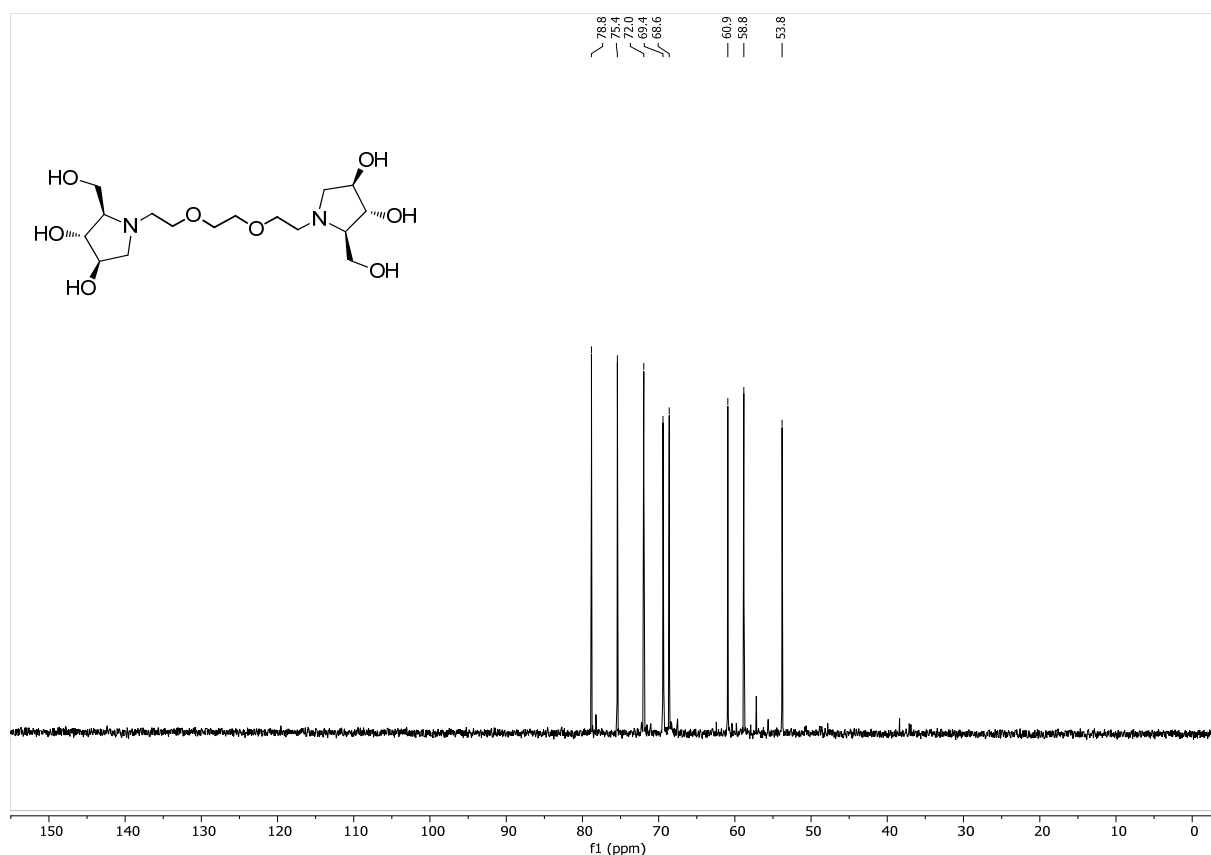
¹³C-NMR spectrum of 13c (D₂O)



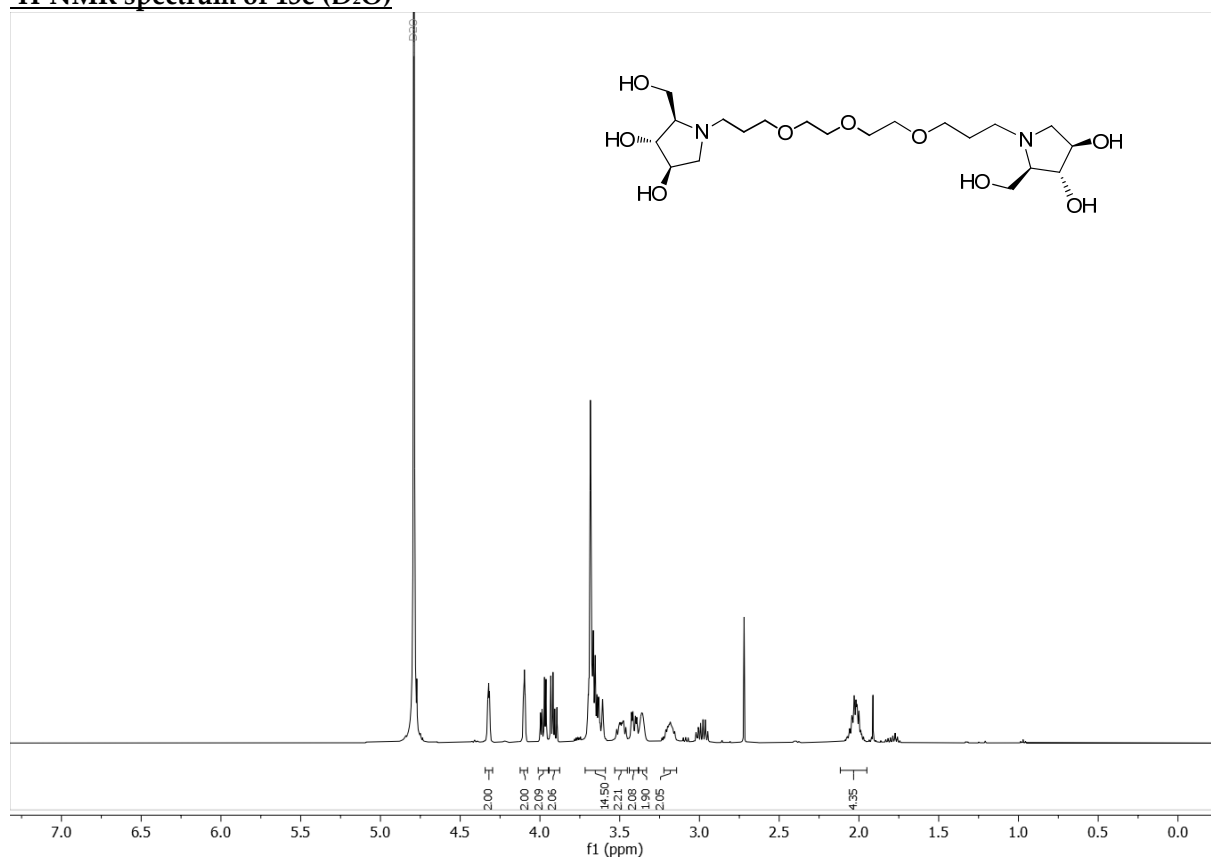
¹H-NMR spectrum of 13d (D₂O)



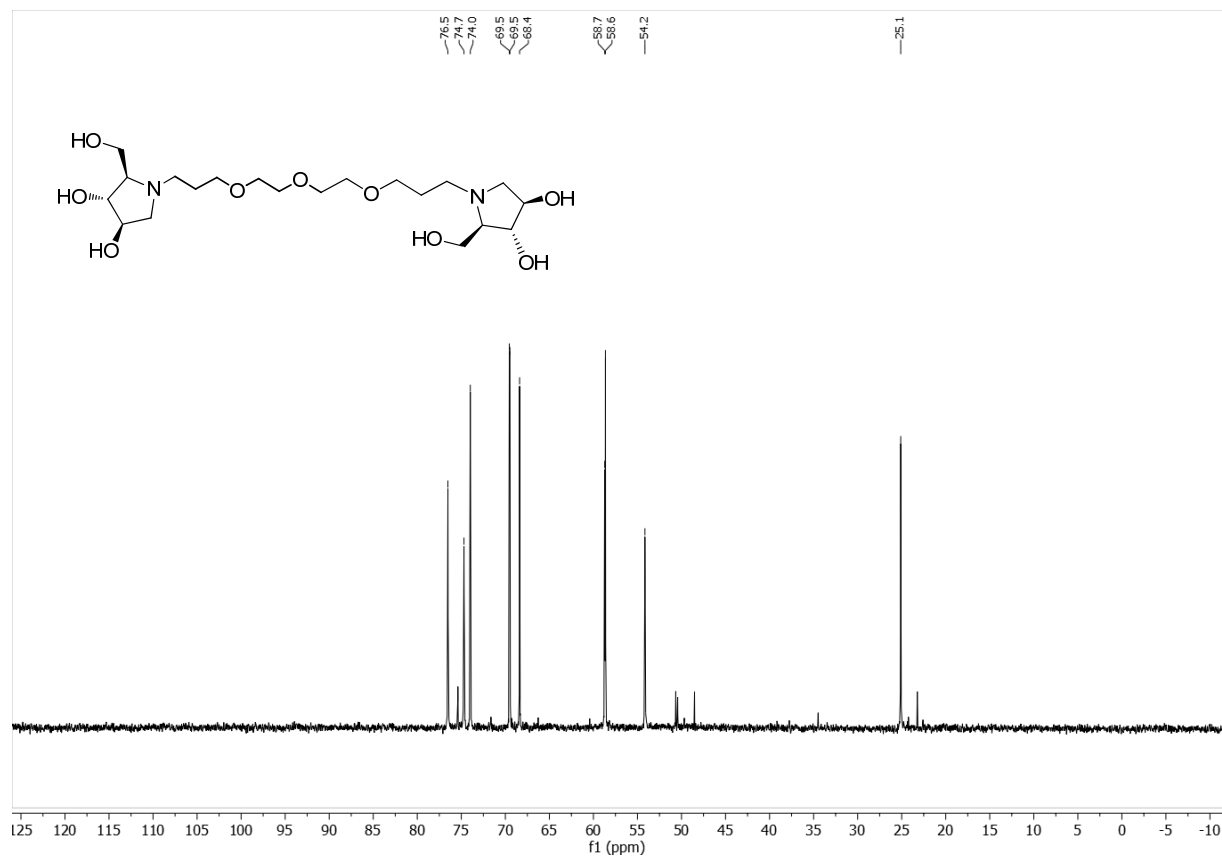
¹³C-NMR spectrum of 13d (D₂O)



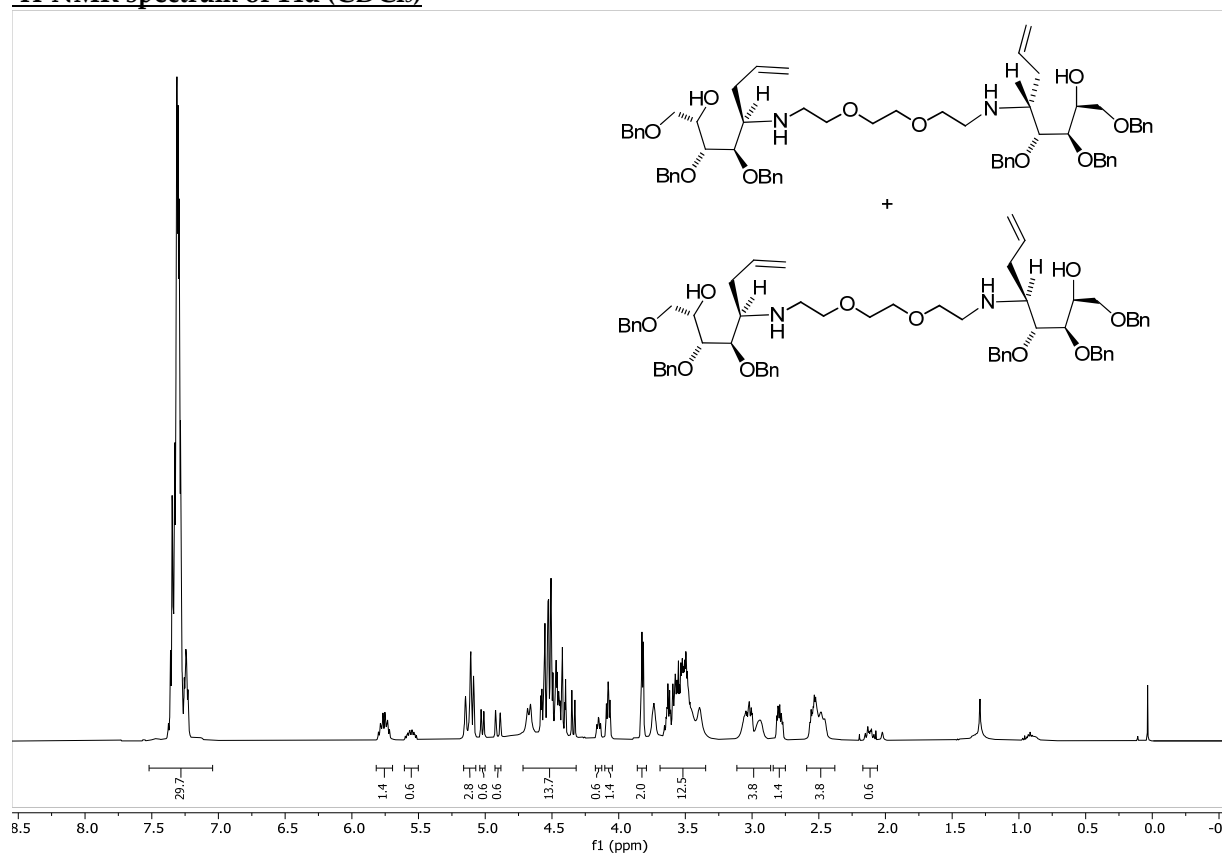
¹H-NMR spectrum of 13e (D₂O)



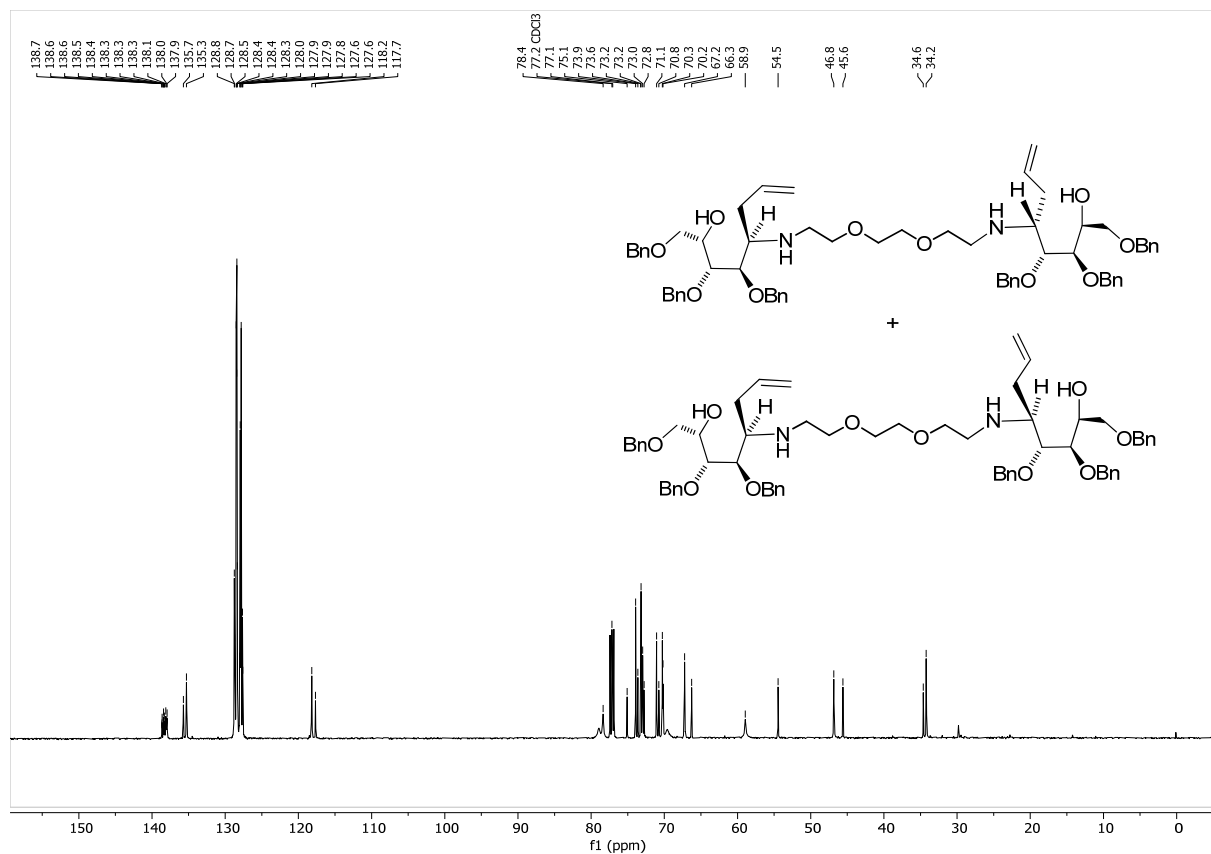
¹³C-NMR spectrum of 13e (D₂O)



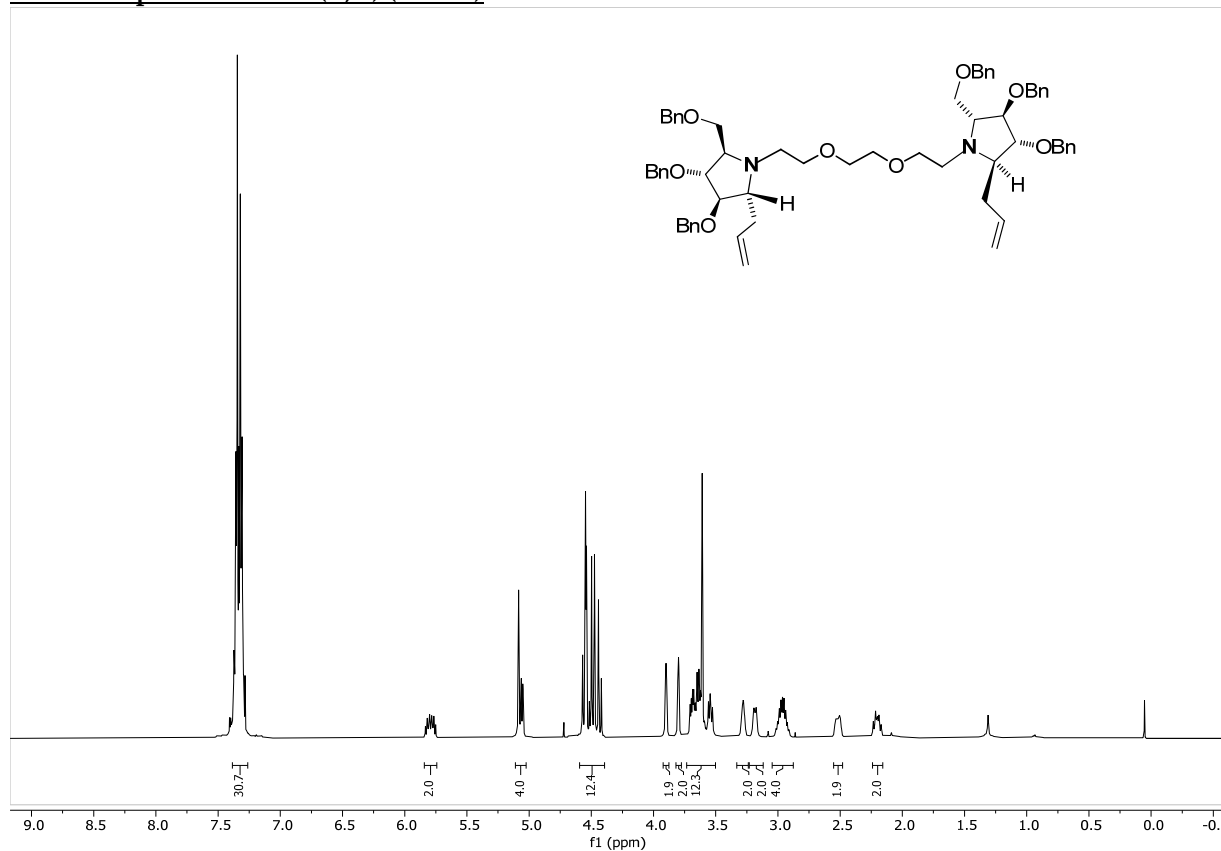
¹H-NMR spectrum of 14d (CDCl₃)



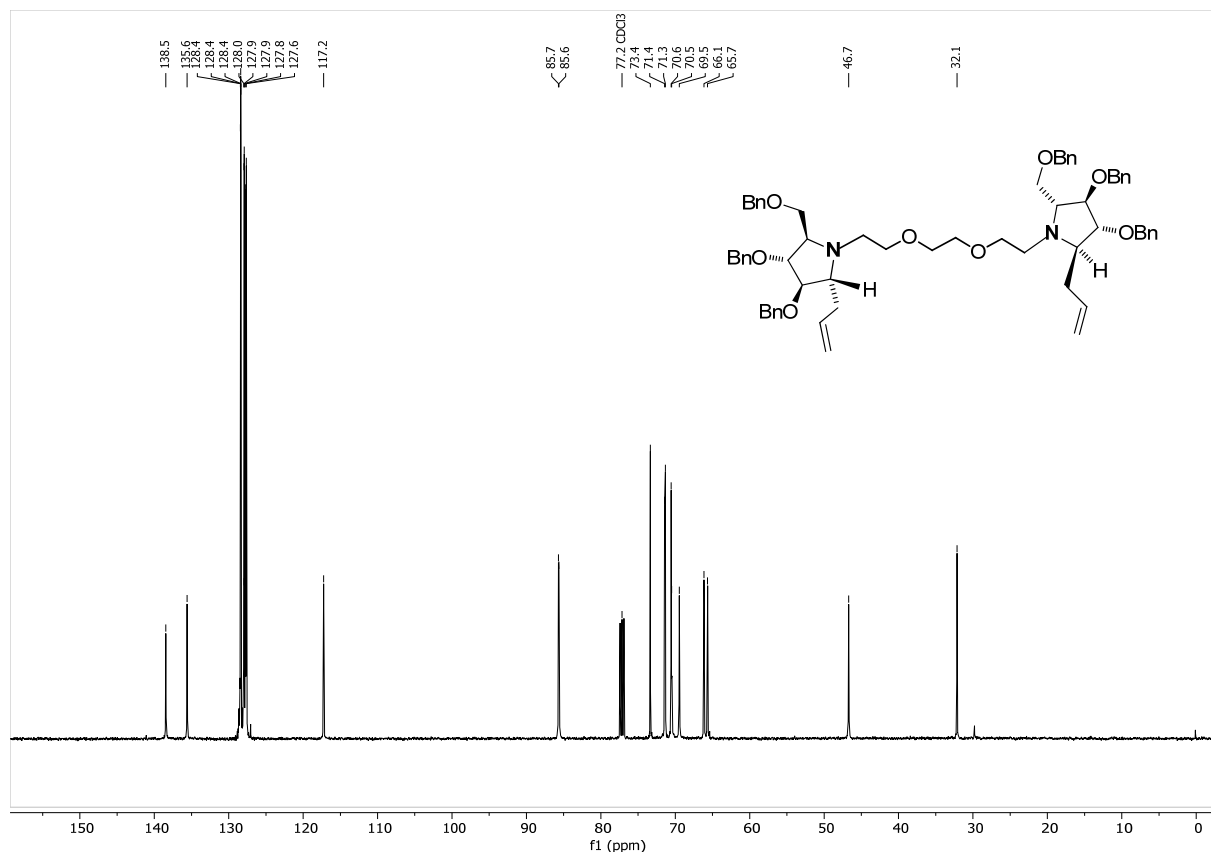
¹³C-NMR spectrum of 14d (CDCl₃)



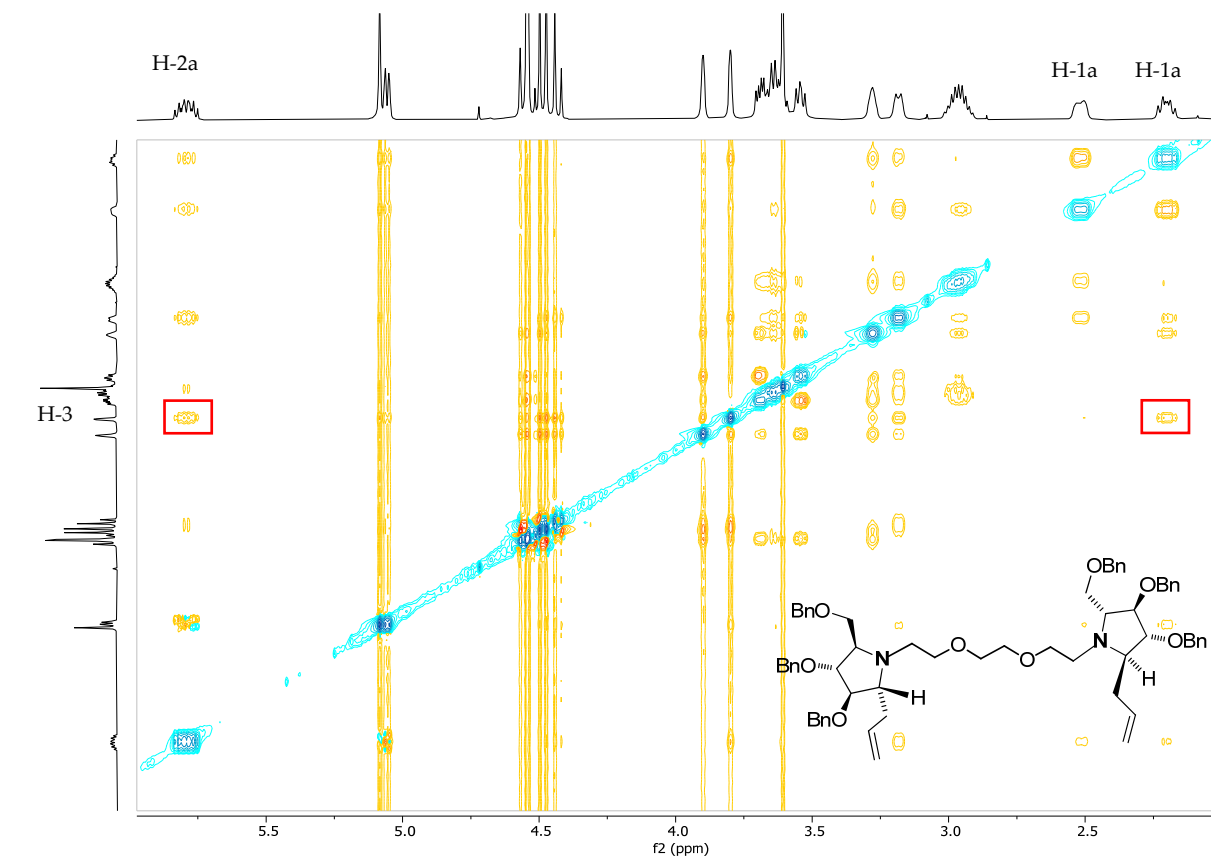
¹H-NMR spectrum of 15d(*R,R*) (CDCl₃)



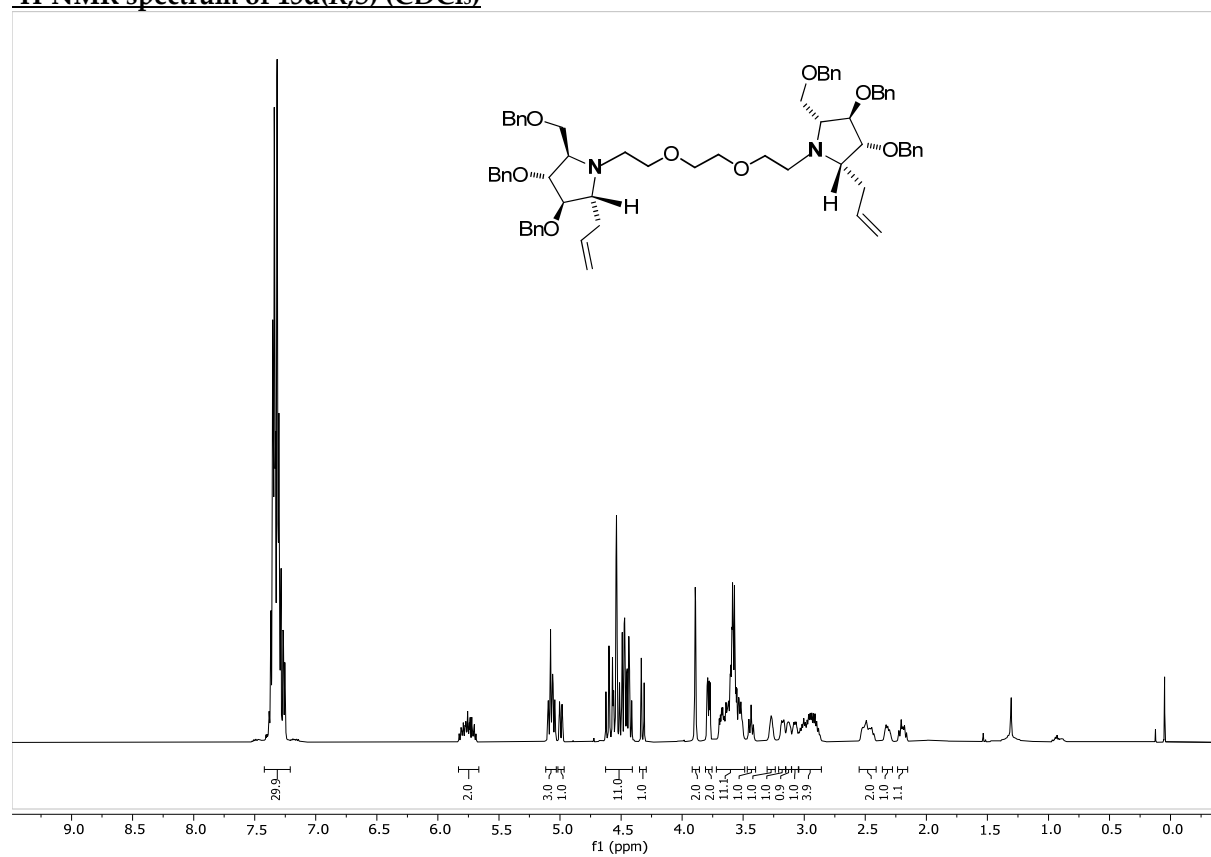
¹³C-NMR spectrum of 15d(*R,R*) (CDCl₃)



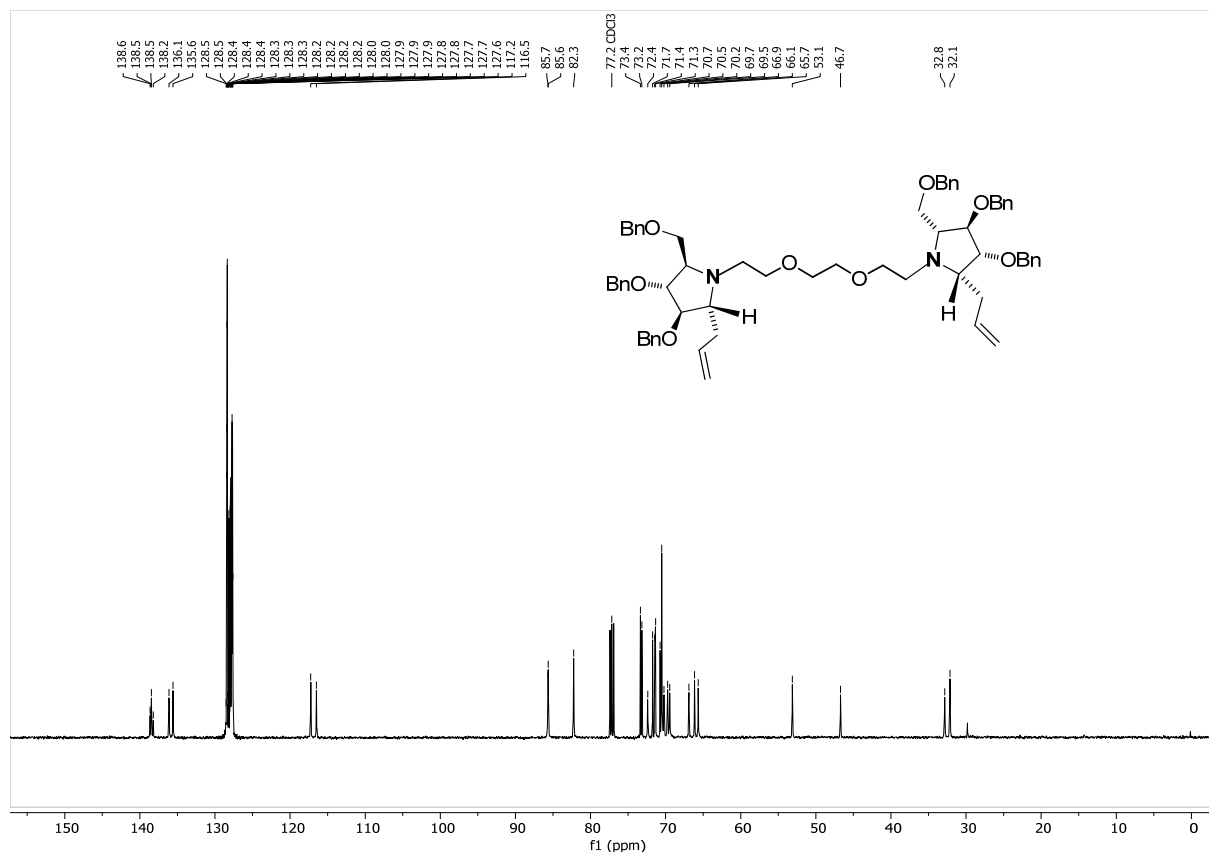
NOESY 2D NMR spectrum of 15d(*R,R*) (CDCl₃)



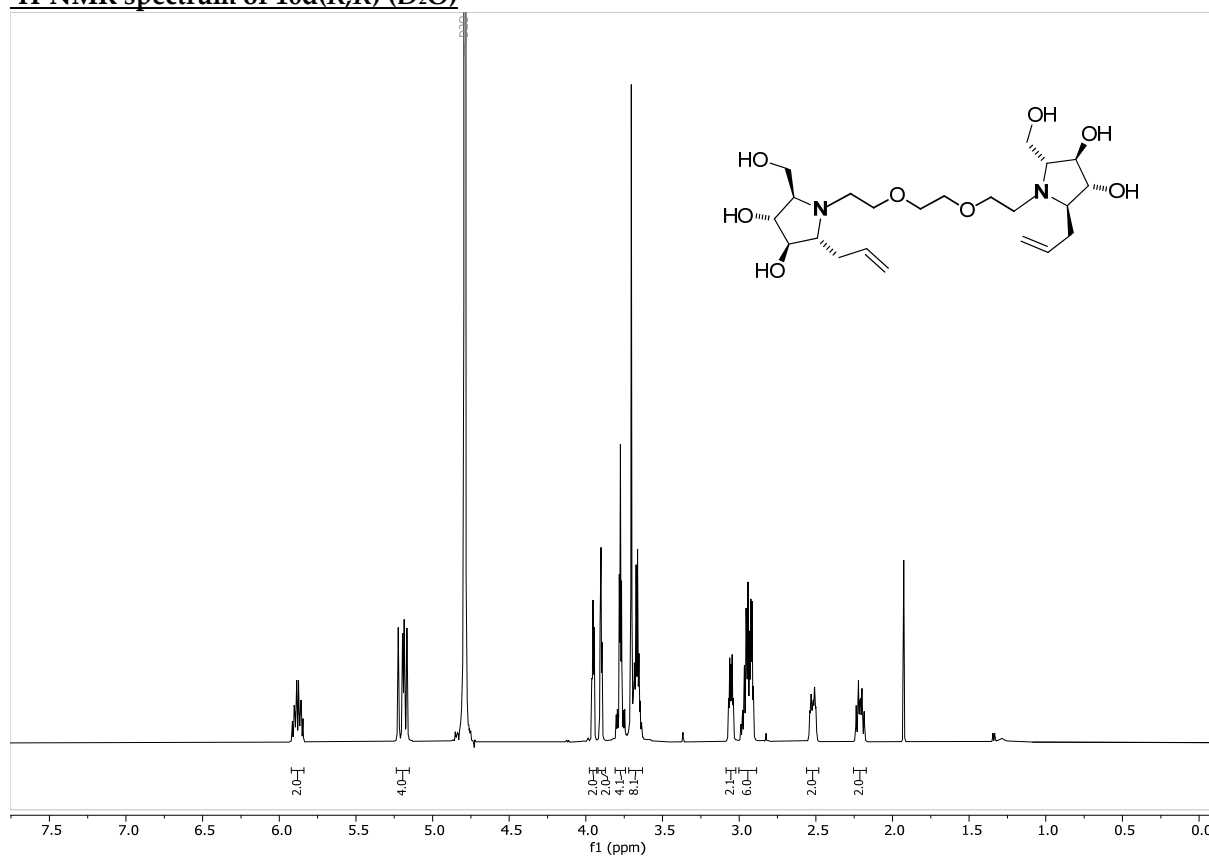
^1H -NMR spectrum of 15d(*R,S*) (CDCl_3)



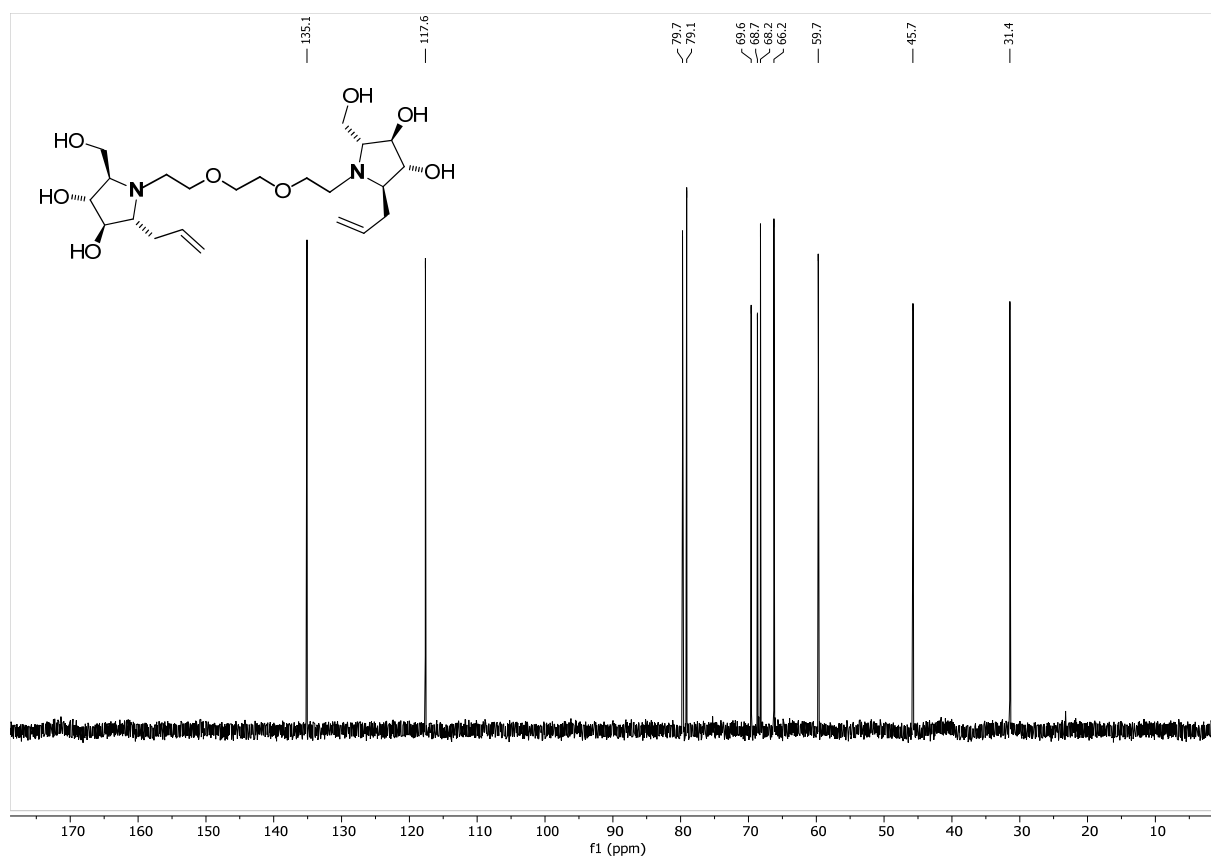
^{13}C -NMR spectrum of 15d(*R,S*) (CDCl_3)



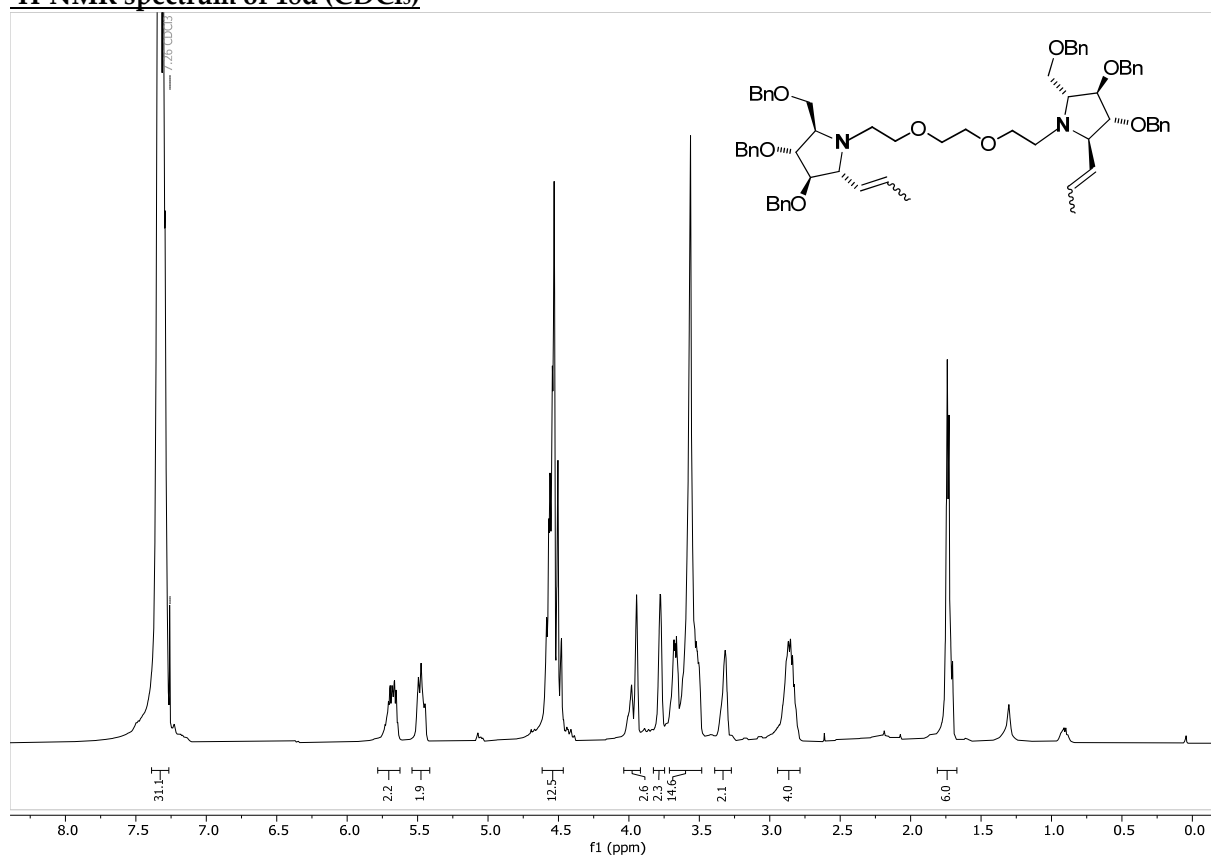
¹H-NMR spectrum of 16d(R,R) (D₂O)



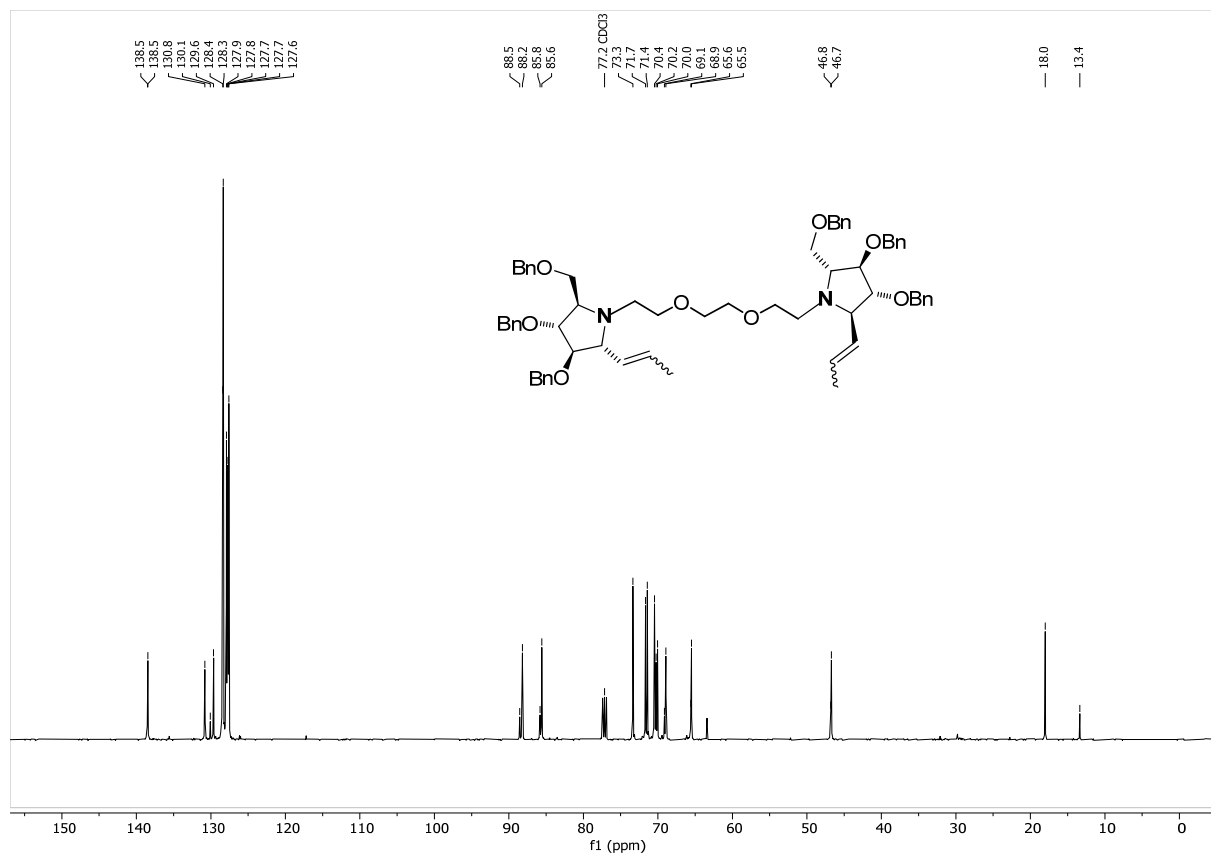
¹³C-NMR spectrum of 16d(R,R) (D₂O)



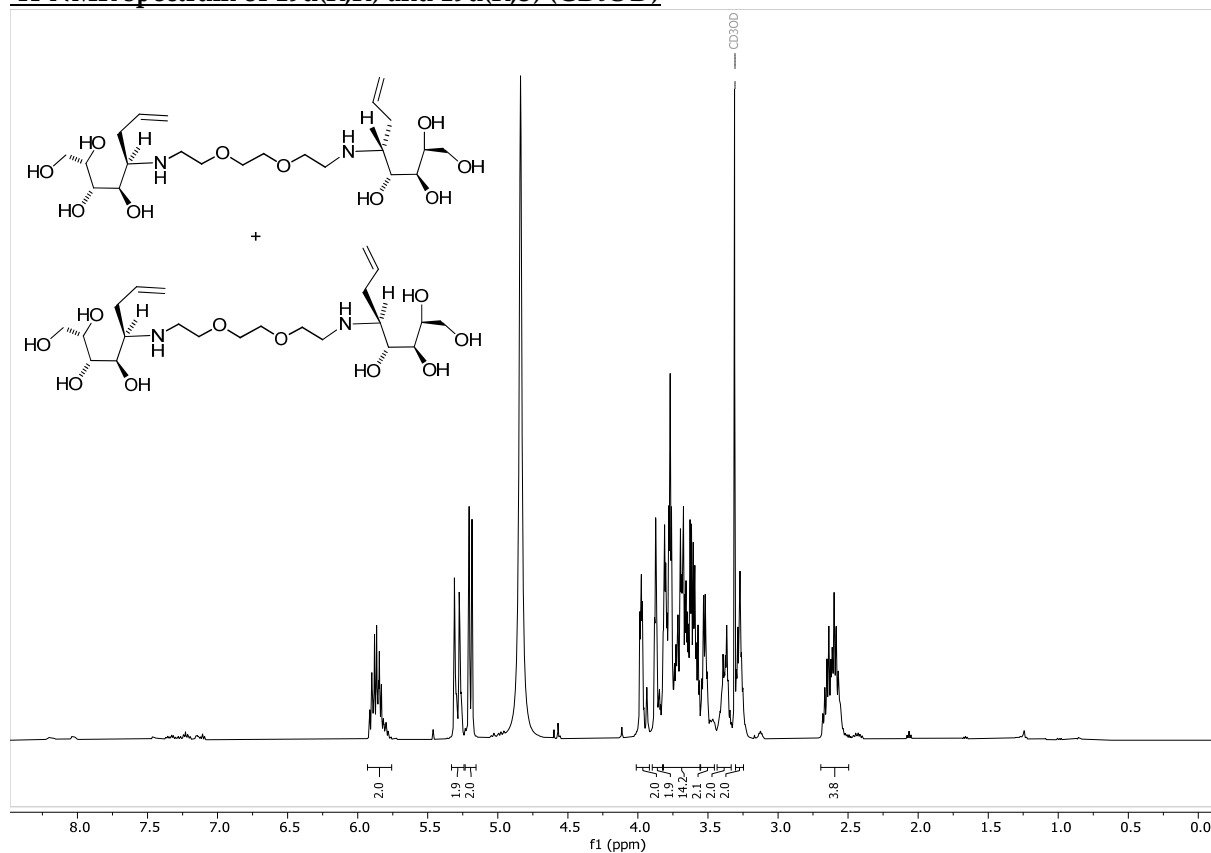
¹H-NMR spectrum of 18d (CDCl₃)



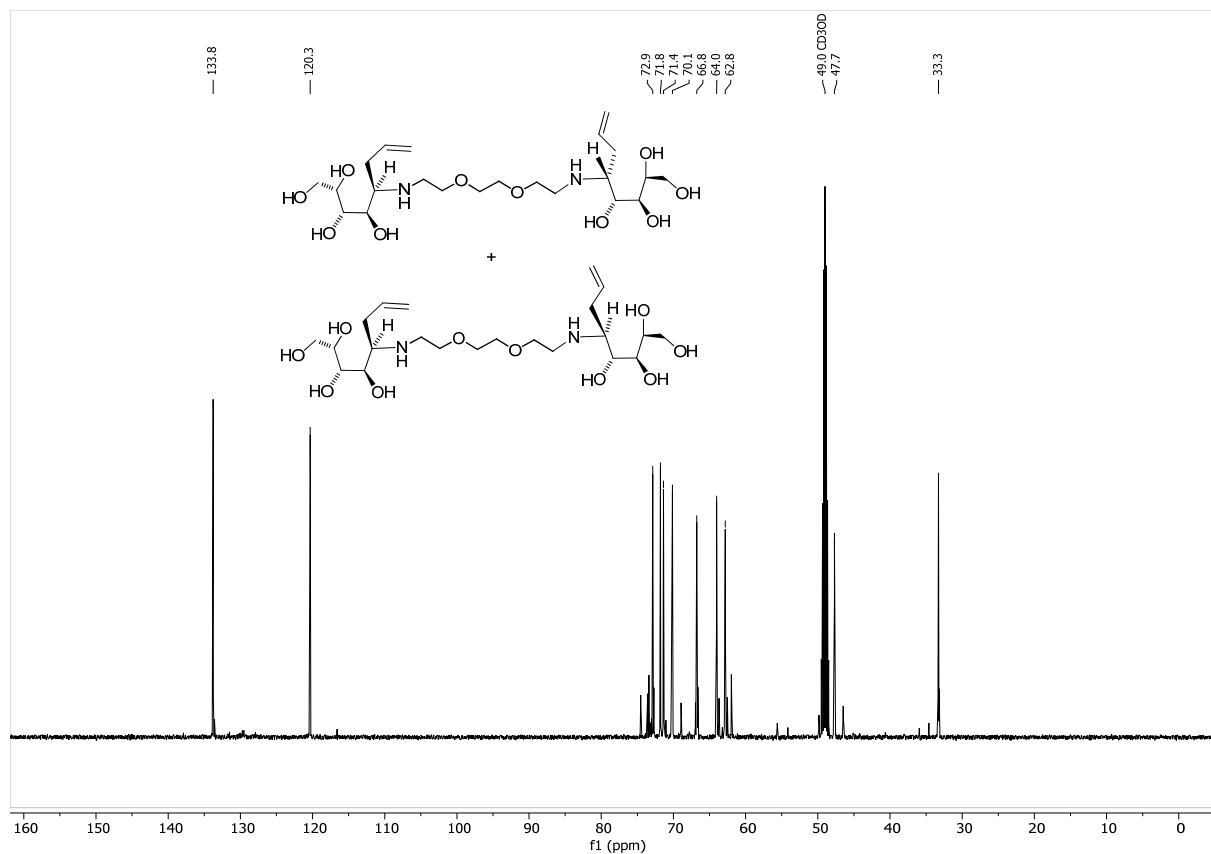
¹³C-NMR spectrum of 18d (CDCl₃)



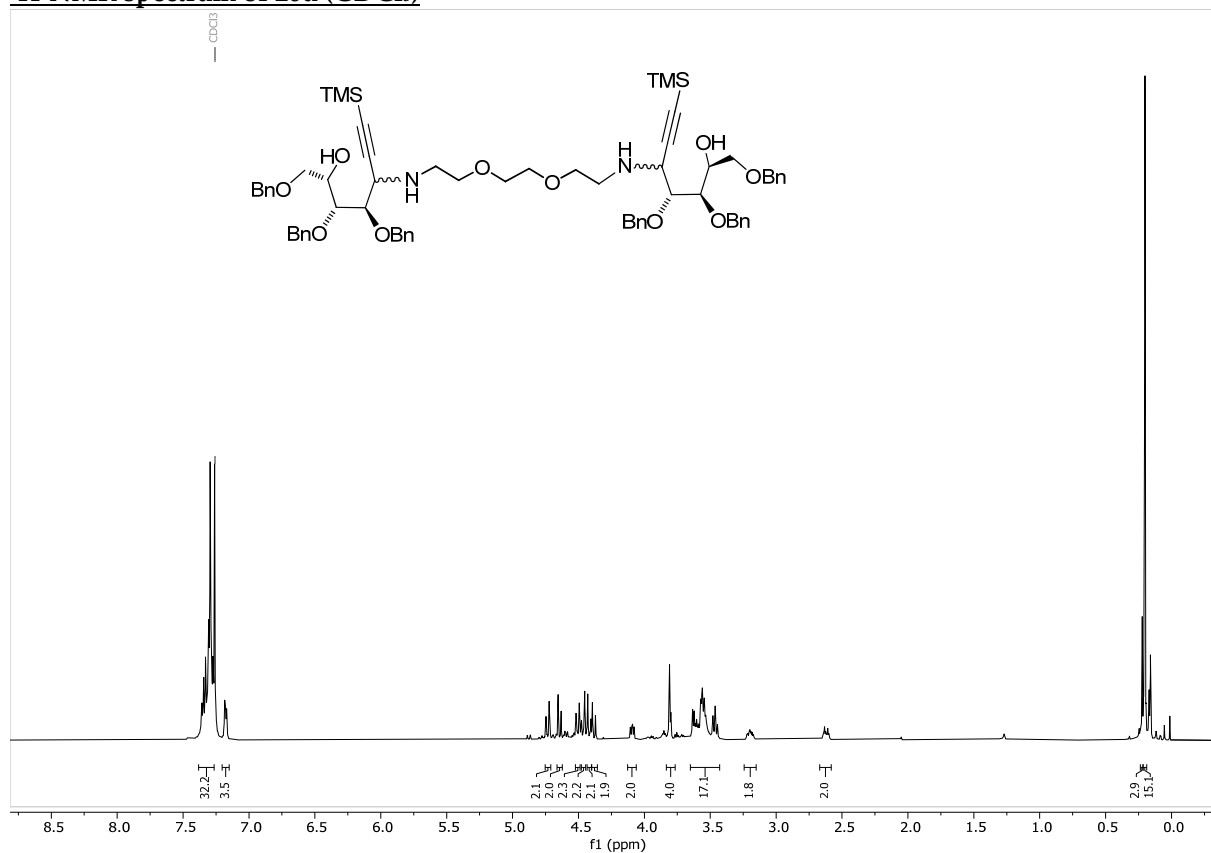
¹H-NMR spectrum of 19d(*R,R*) and 19d(*R,S*) (CD₃OD)



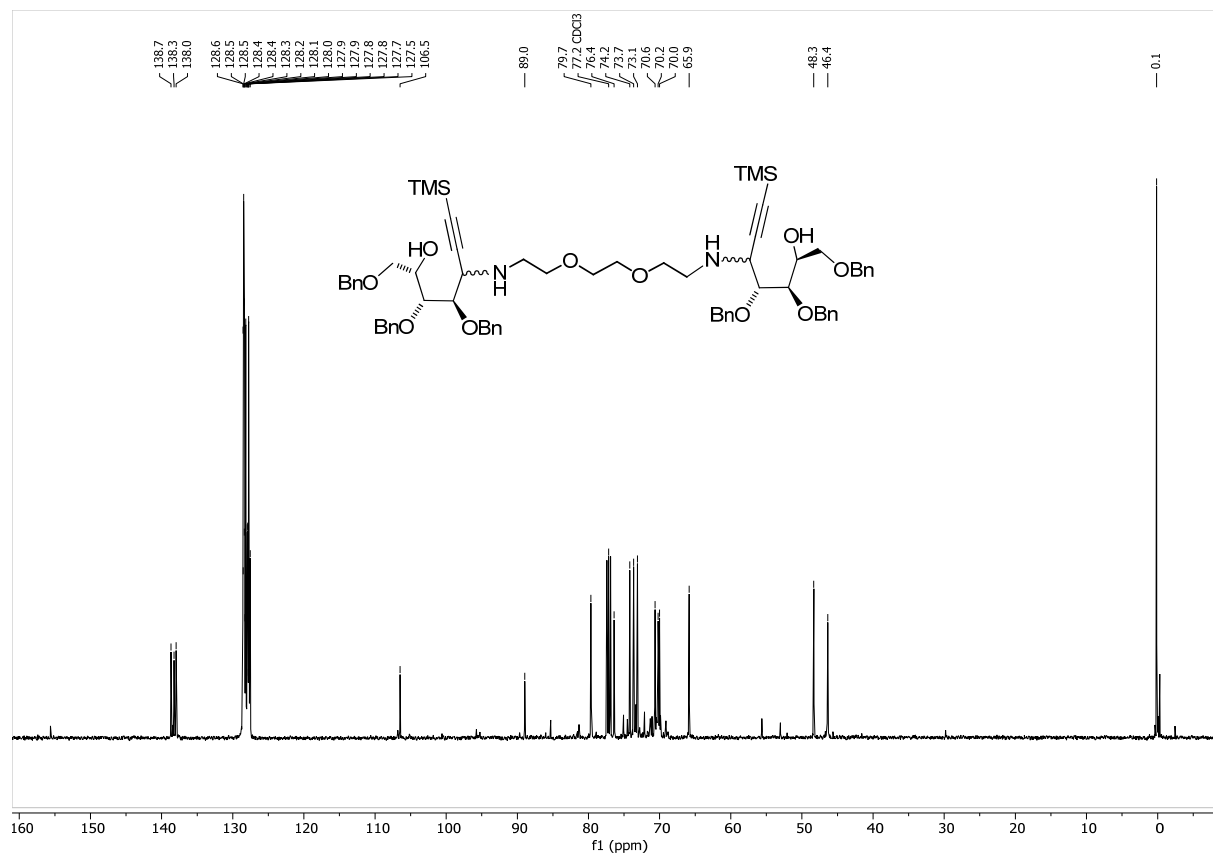
¹³C-NMR spectrum of 19d(*R,R*) and 19d(*R,S*) (CD₃OD)



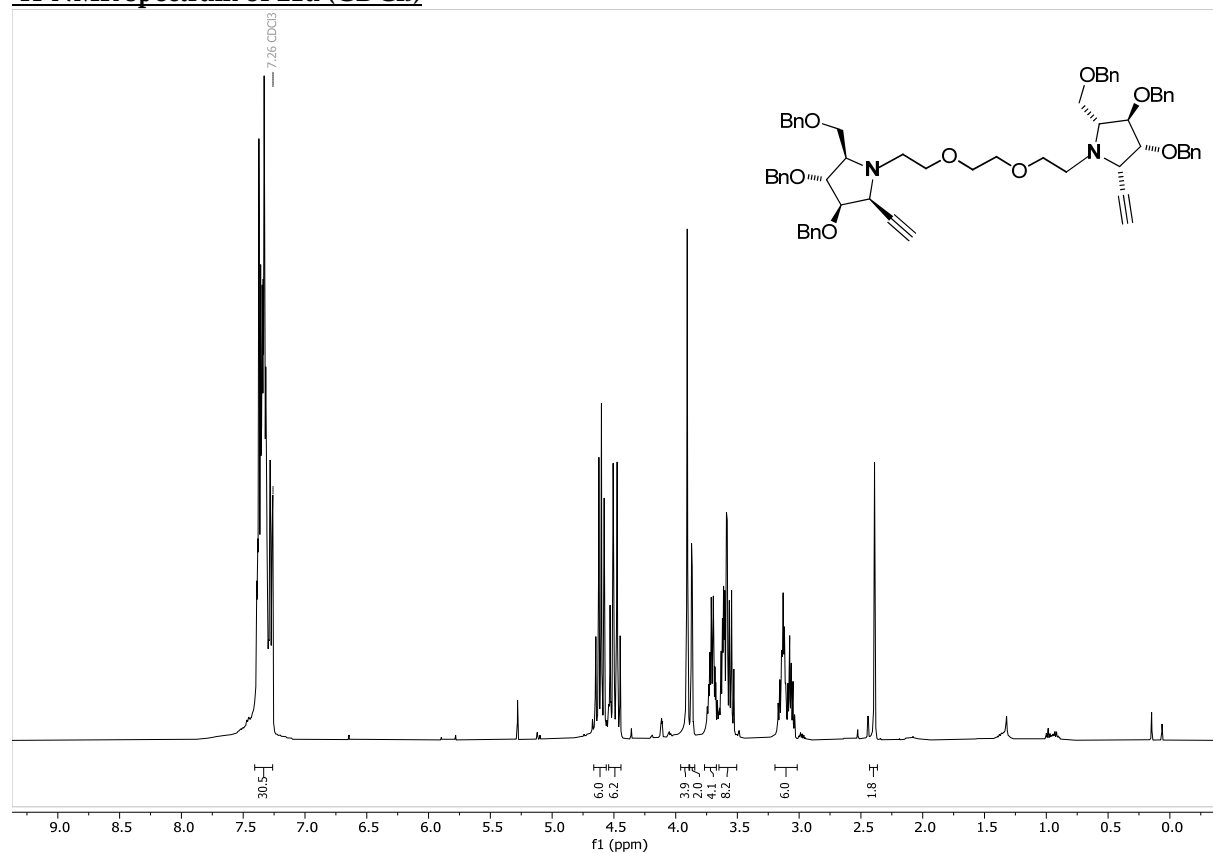
¹H-NMR spectrum of 20d (CDCl₃)



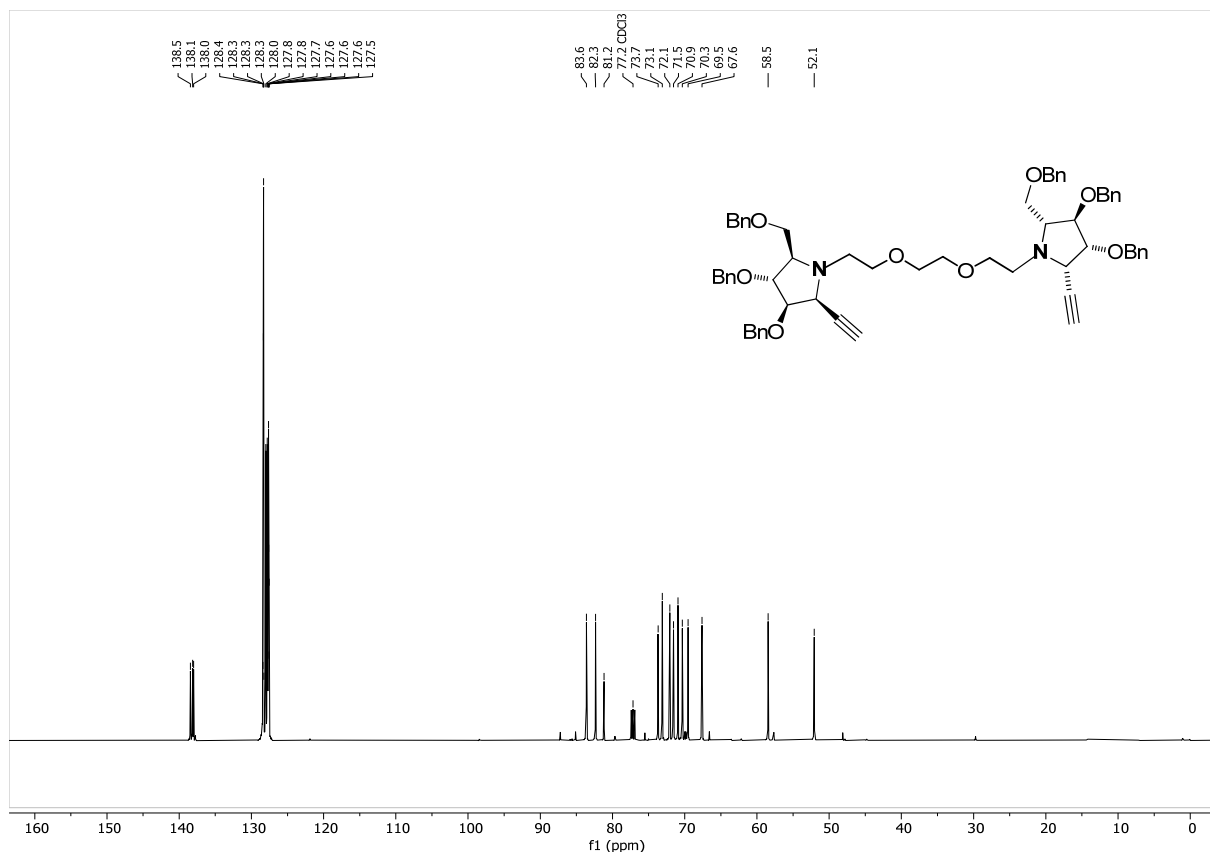
¹³C-NMR spectrum of 20d (CDCl₃)



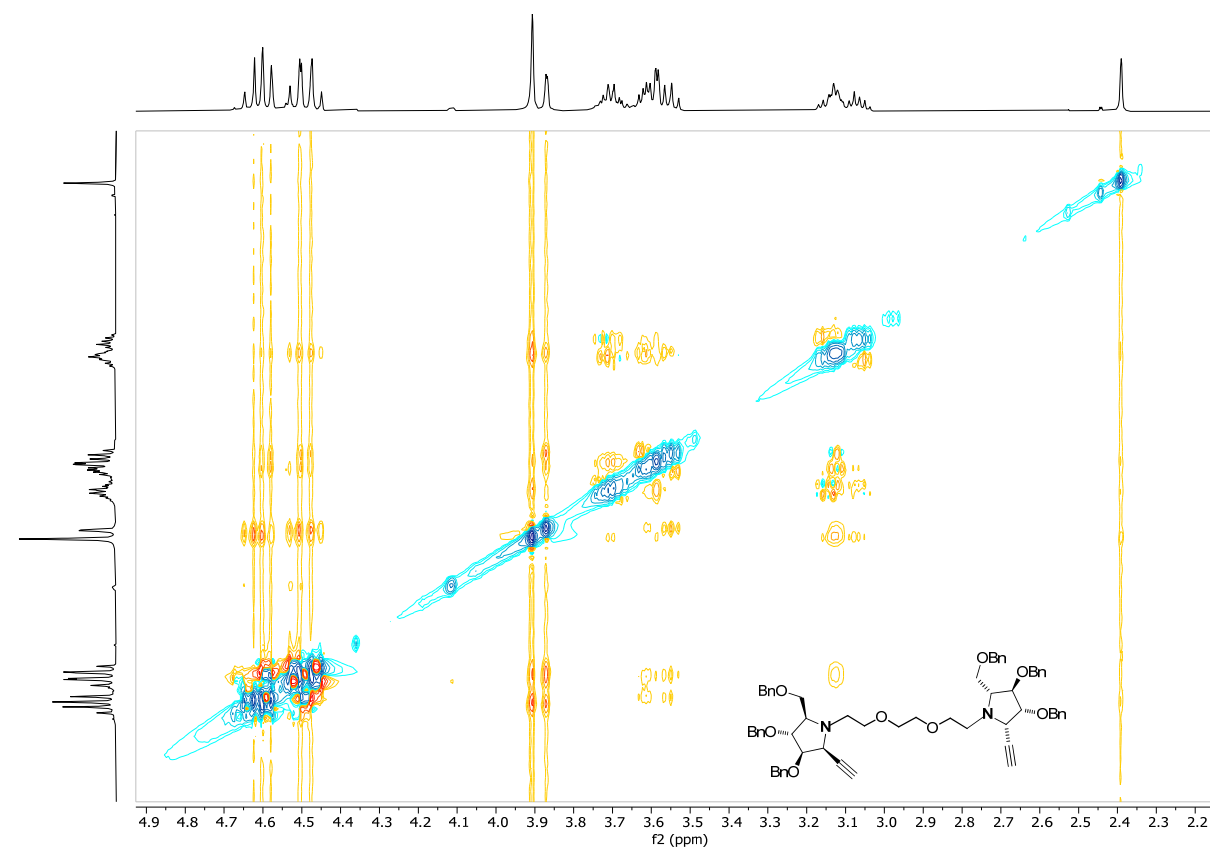
¹H-NMR spectrum of 21d (CDCl₃)



¹³C-NMR spectrum of 21d (CDCl₃)



NOESY 2D NMR spectrum of 21d (CDCl₃)

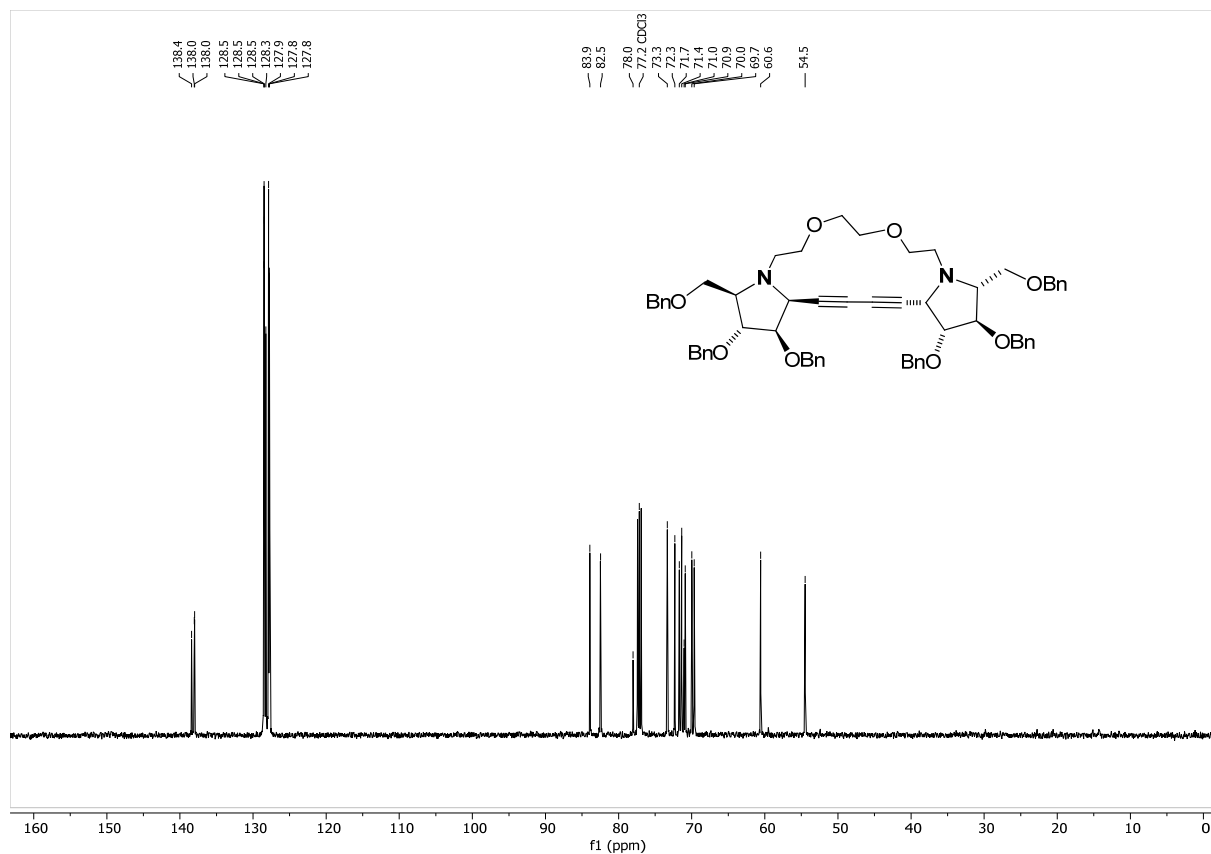


Chemical structure of the compound is shown above the spectrum. The structure is a dimeric molecule consisting of two 2,3,4-tri-O-benzyl-5-(benzyloxymethyl)pyrrolidine rings connected by a 1,4-bis(benzyloxymethyl)oxy linker. The molecule is shown in its chair conformation.

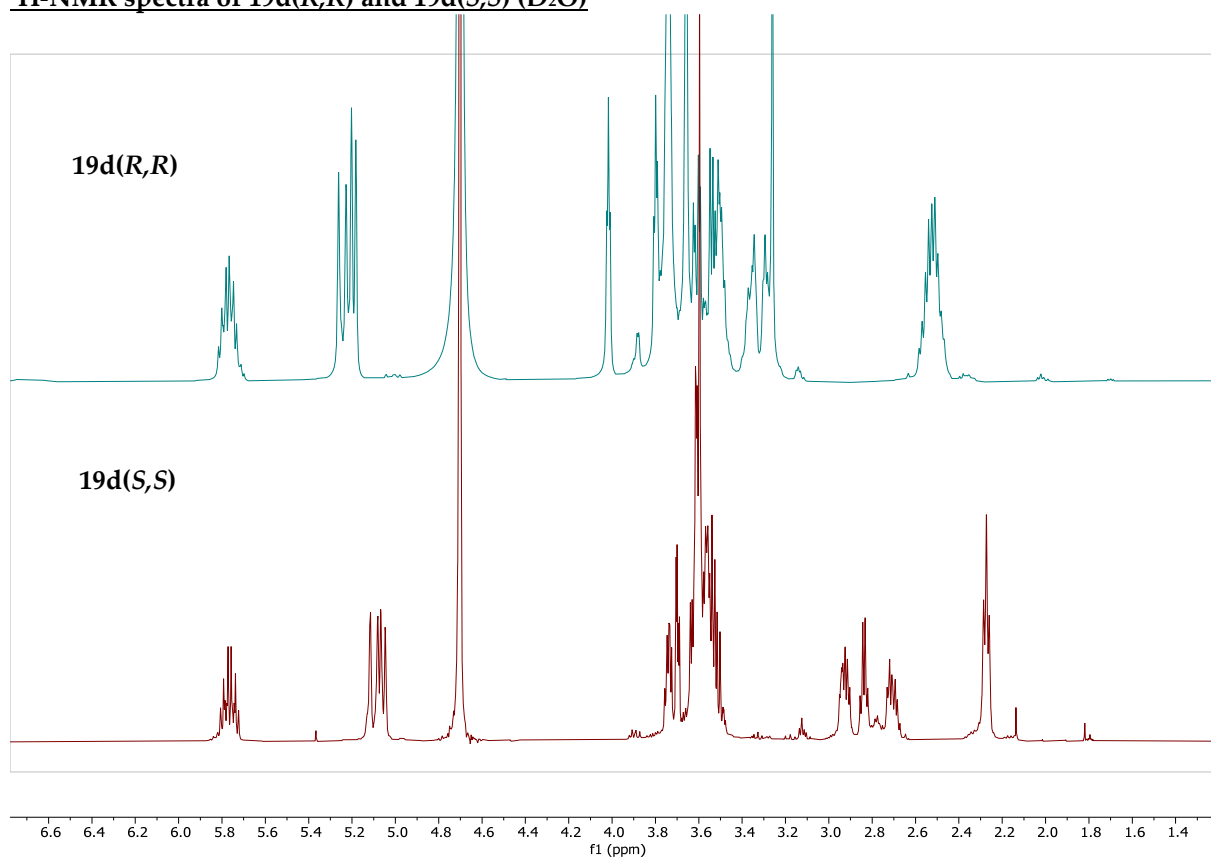
¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 0.0 to 9.0. The spectrum shows several peaks corresponding to the structure, including aromatic protons (7.0-7.5 ppm), aliphatic protons (2.5-4.5 ppm), and a small peak at 0.0 ppm (TMS). Integration values are provided below the baseline.

Chemical Shift (ppm)	Integration
7.26	26.0
7.1-7.5	4.0
4.5-4.8	2.0, 2.0, 2.0, 2.0, 4.1
3.5-4.0	4.0, 2.0, 2.0, 6.0, 6.1
2.5-3.0	2.0, 4.0

S34



¹H-NMR spectra of 19d(*R,R*) and 19d(*S,S*) (D₂O)



¹³C-NMR spectra of 19d(*R,R*) and 19d(*S,S*) (D₂O)

