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☙ Characterization – NMR spectra

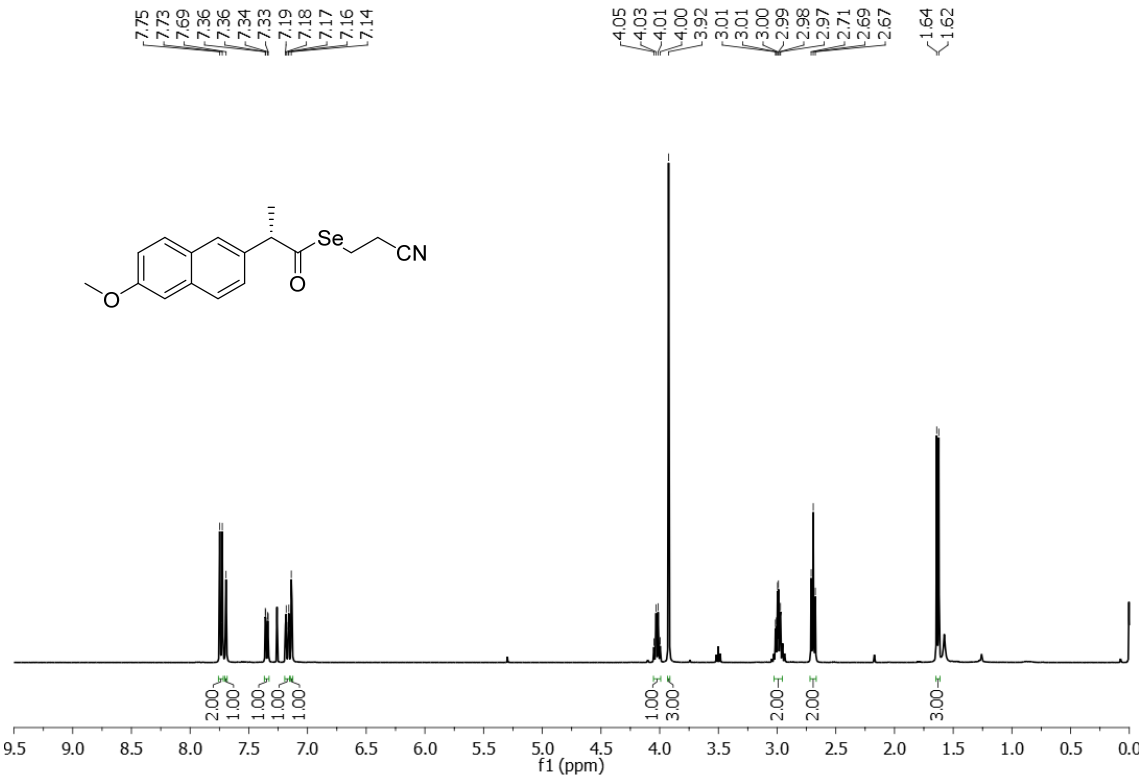


Figure S1. ^{1}H-NMR spectrum of compound **I.3e**.

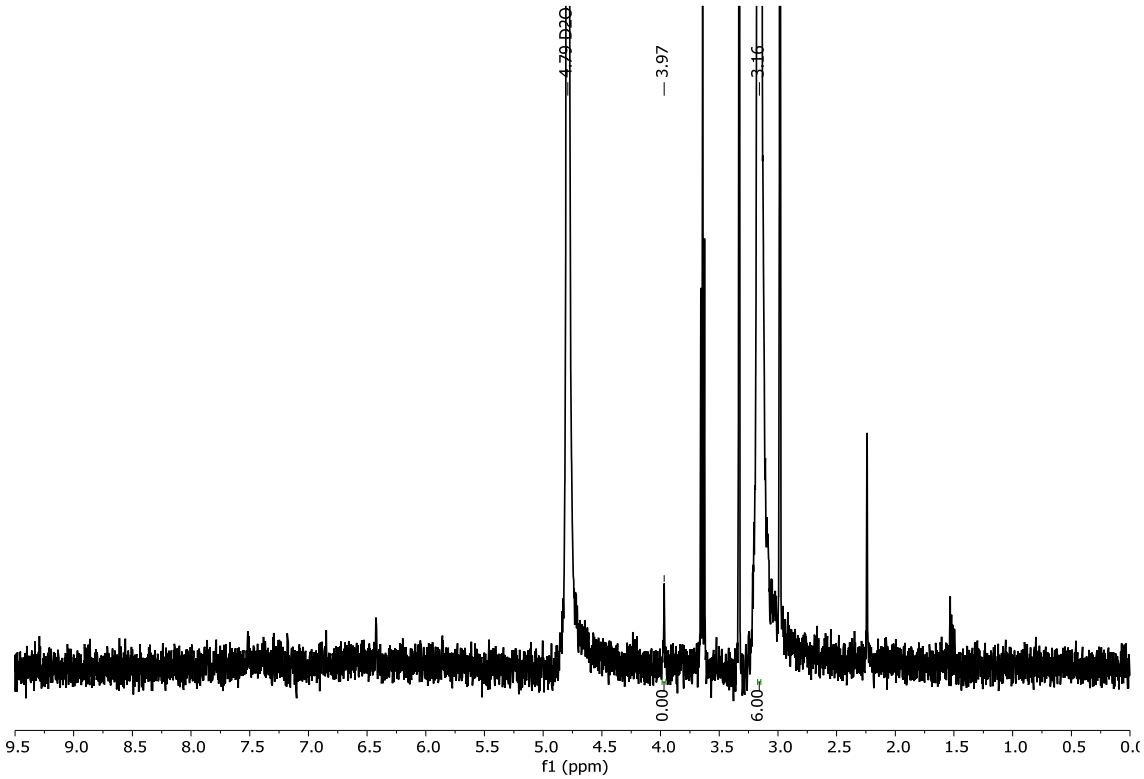


Figure S2. ^{1}H-NMR spectrum of compound **I.3e** and dimethyl sulfone.

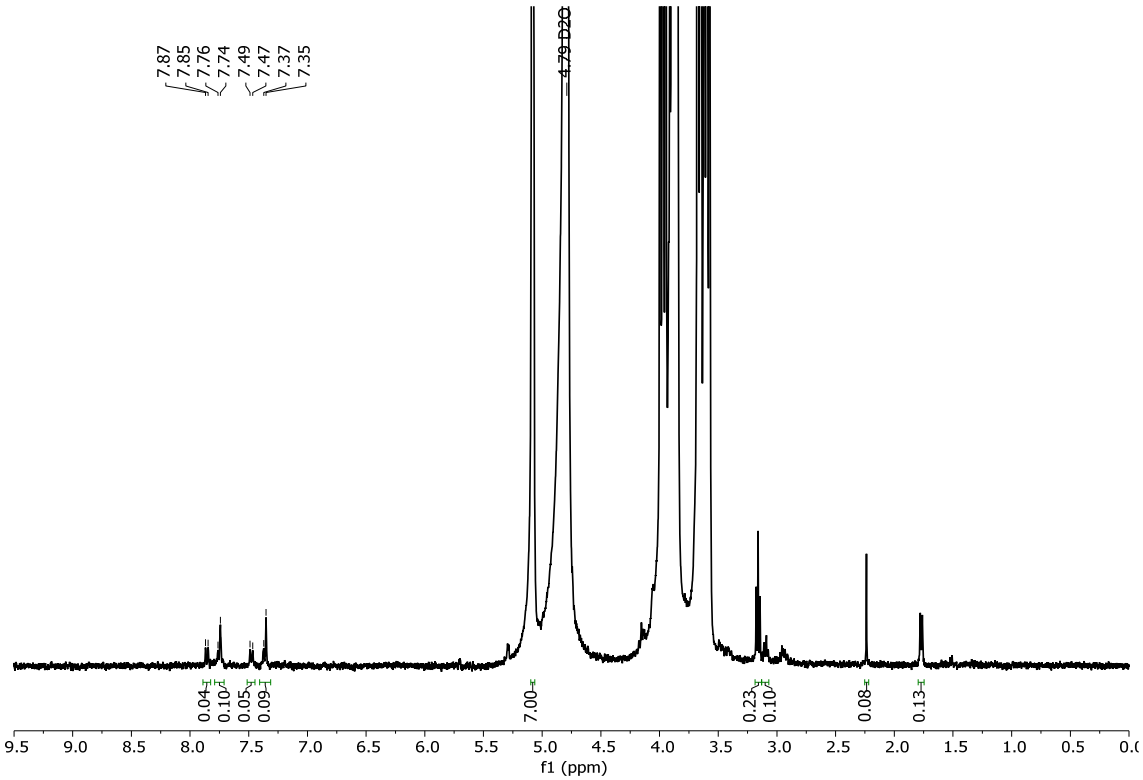


Figure S3. ^{1}H-NMR spectrum of compound **I.3e** and β-CD.

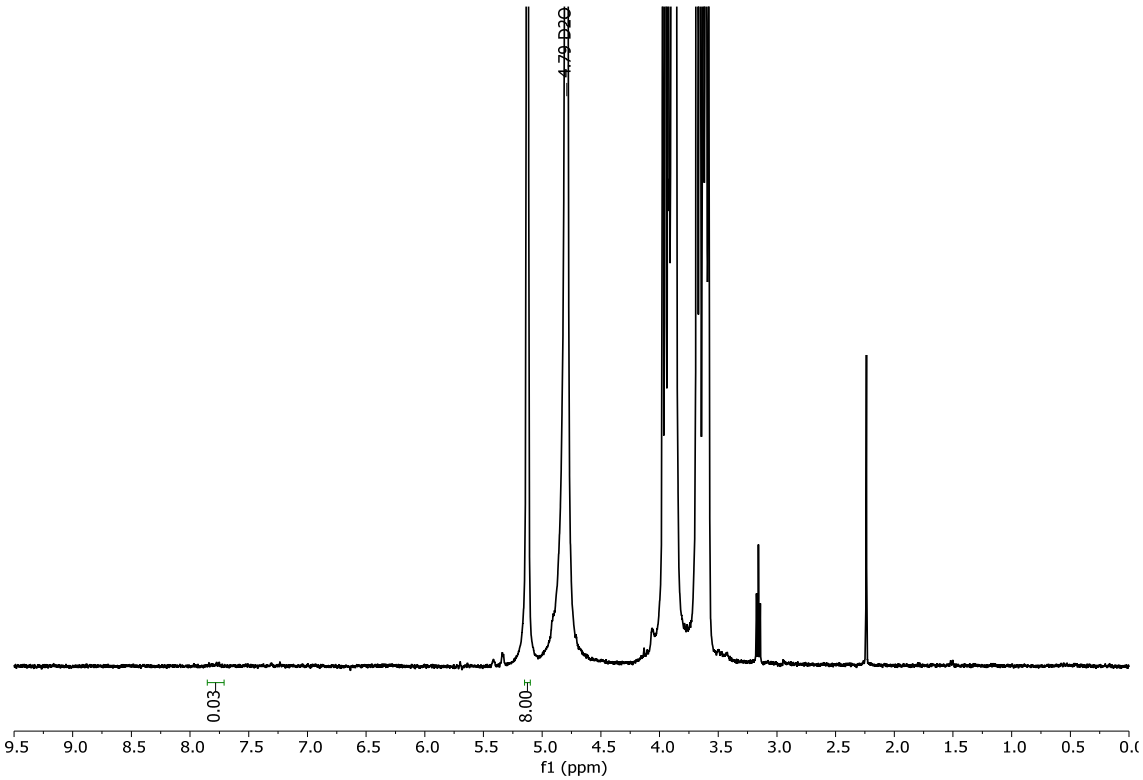


Figure S4. ^{1}H-NMR spectrum of compound **I.3e** and γ-CD.

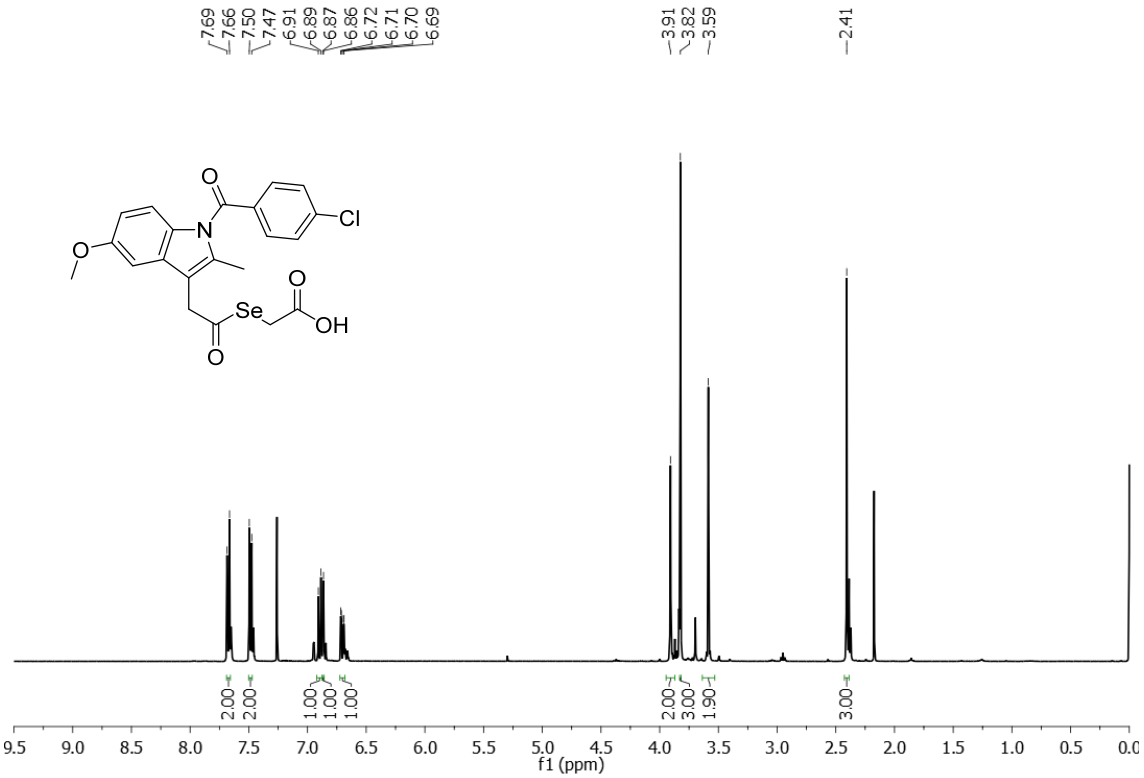


Figure S5. ^{1}H-NMR spectrum of compound **I.4a**.

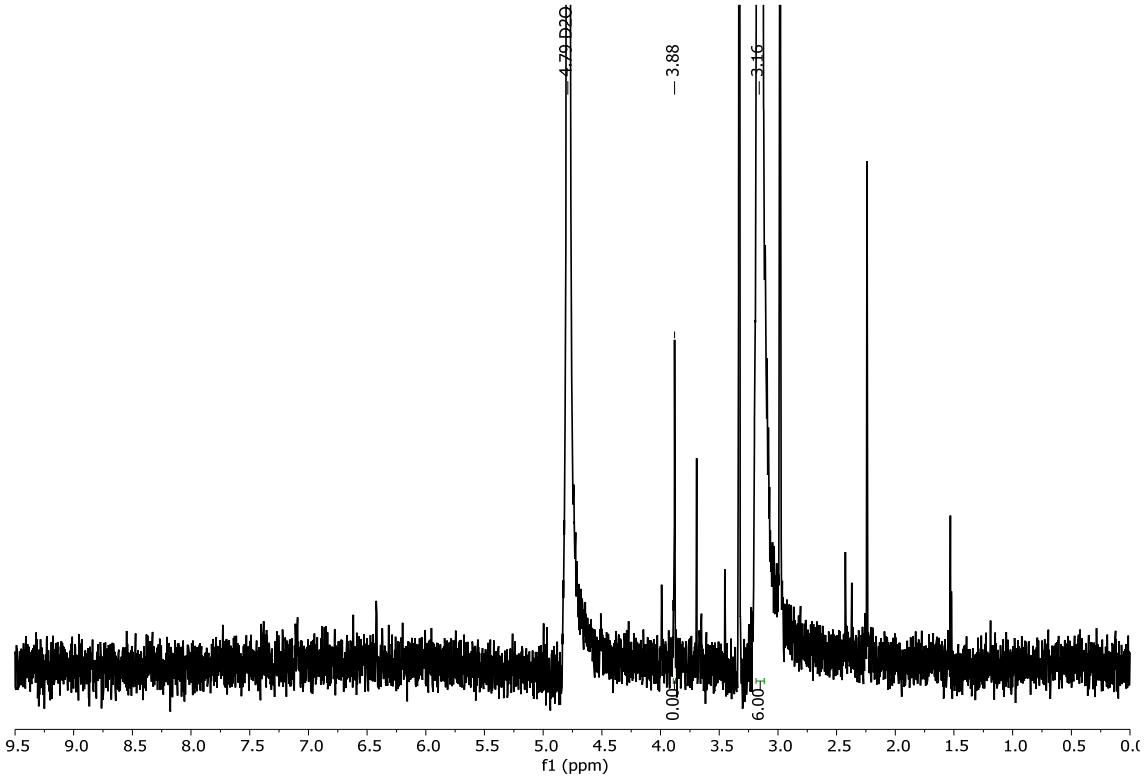


Figure S6. ^{1}H-NMR spectrum of compound **I.4a** and dimethyl sulfone.

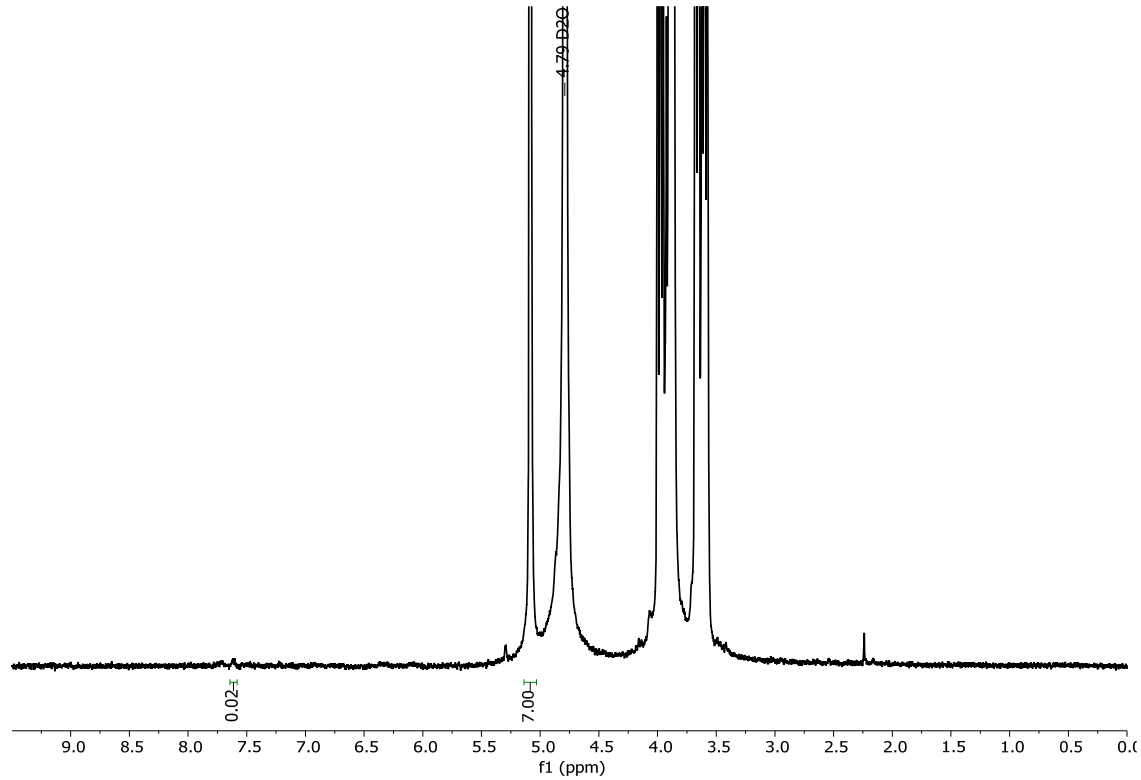


Figure S7. ^{1}H-NMR spectrum of compound **I.4a** and β-CD.

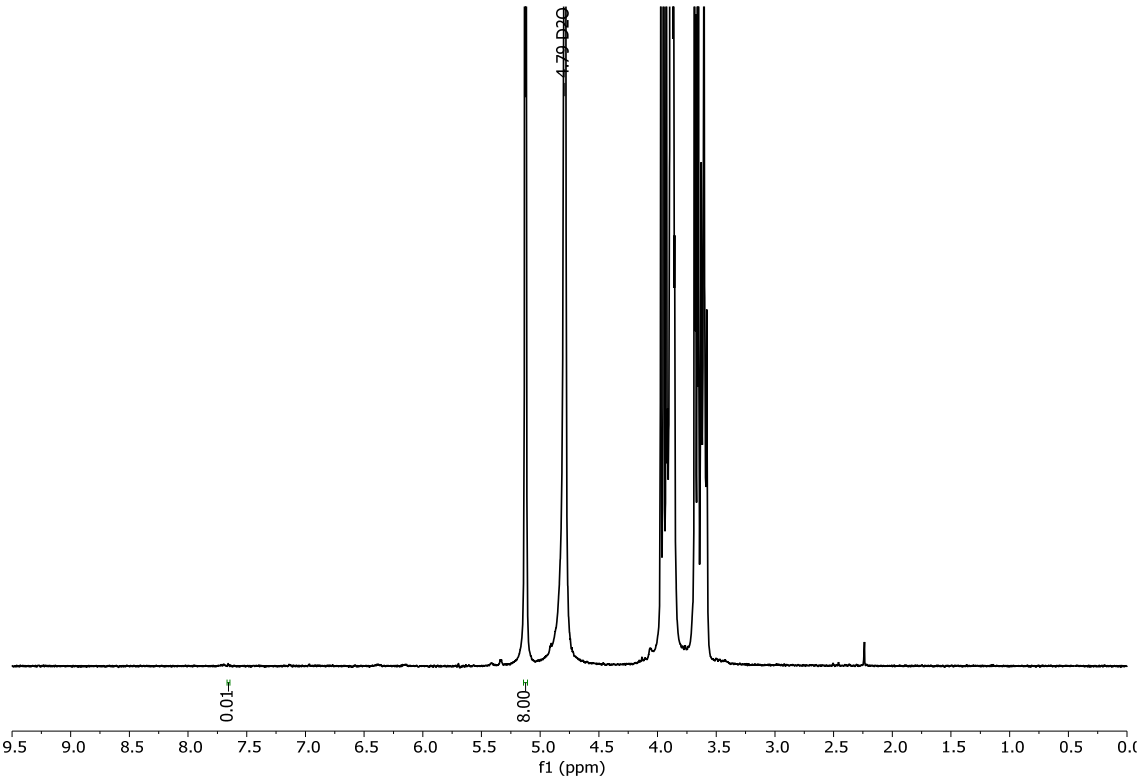


Figure S8. ^{1}H-NMR spectrum of compound **I.4a** and γ-CD.

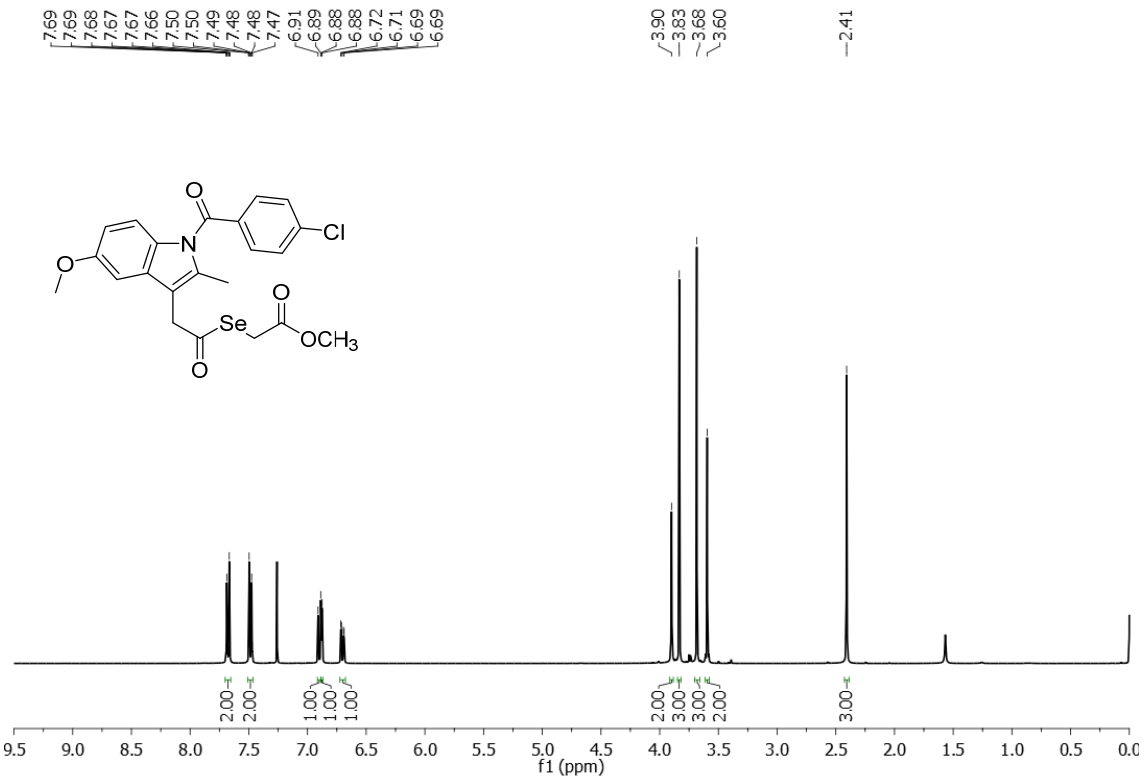


Figure S9. ^{1}H-NMR spectrum of compound **I.4b**.

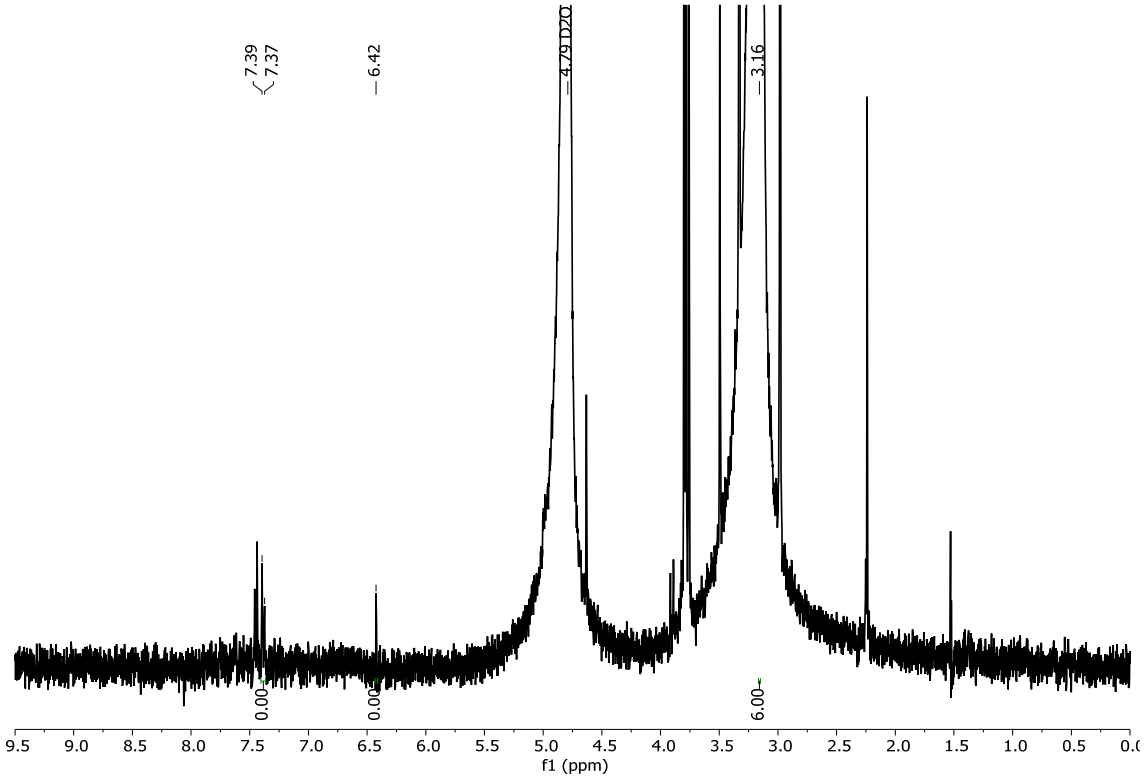


Figure S10. ^{1}H-NMR spectrum of compound **I.4b** and dimethyl sulfone.

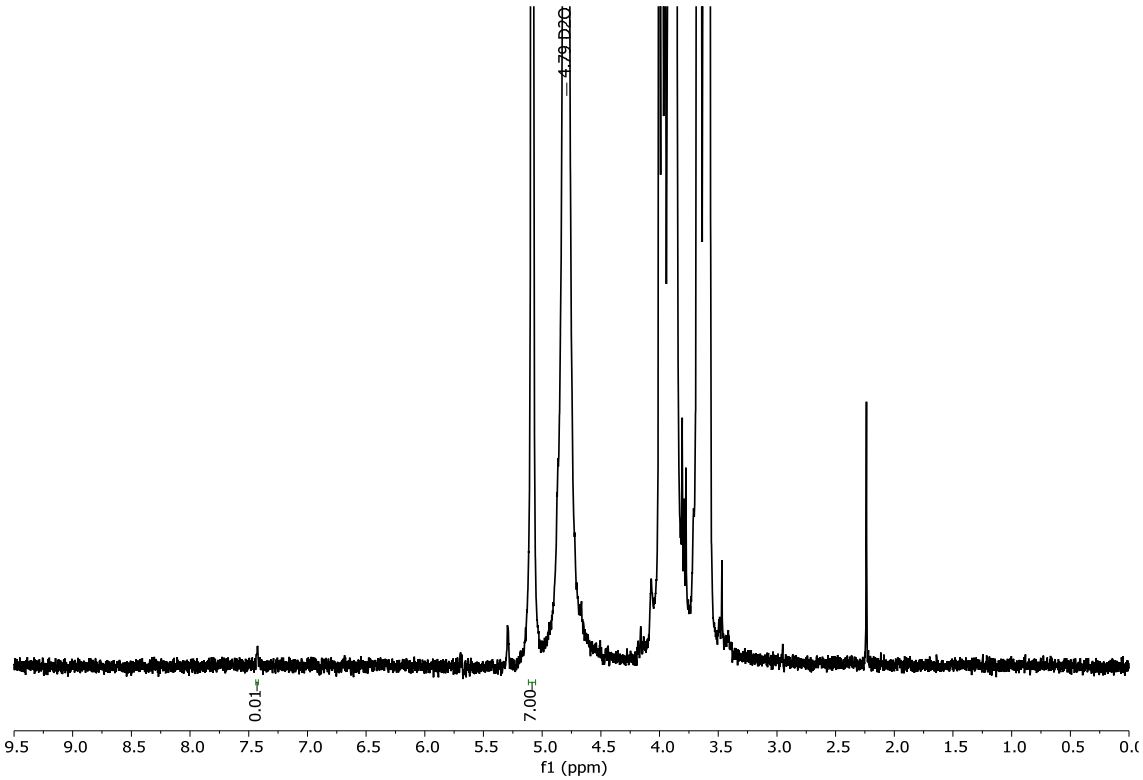


Figure S11. ^{1}H-NMR spectrum of compound **I.4b** and β-CD.

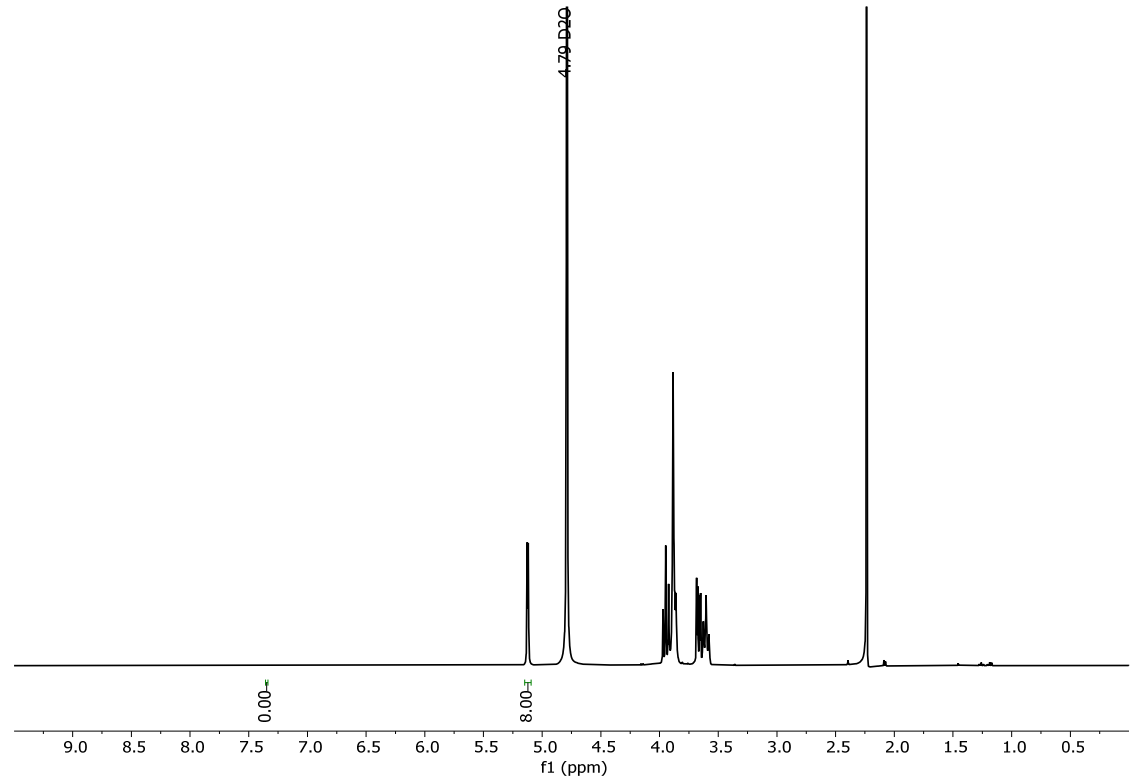


Figure S12. ^{1}H-NMR spectrum of compound **I.4b** and γ-CD.

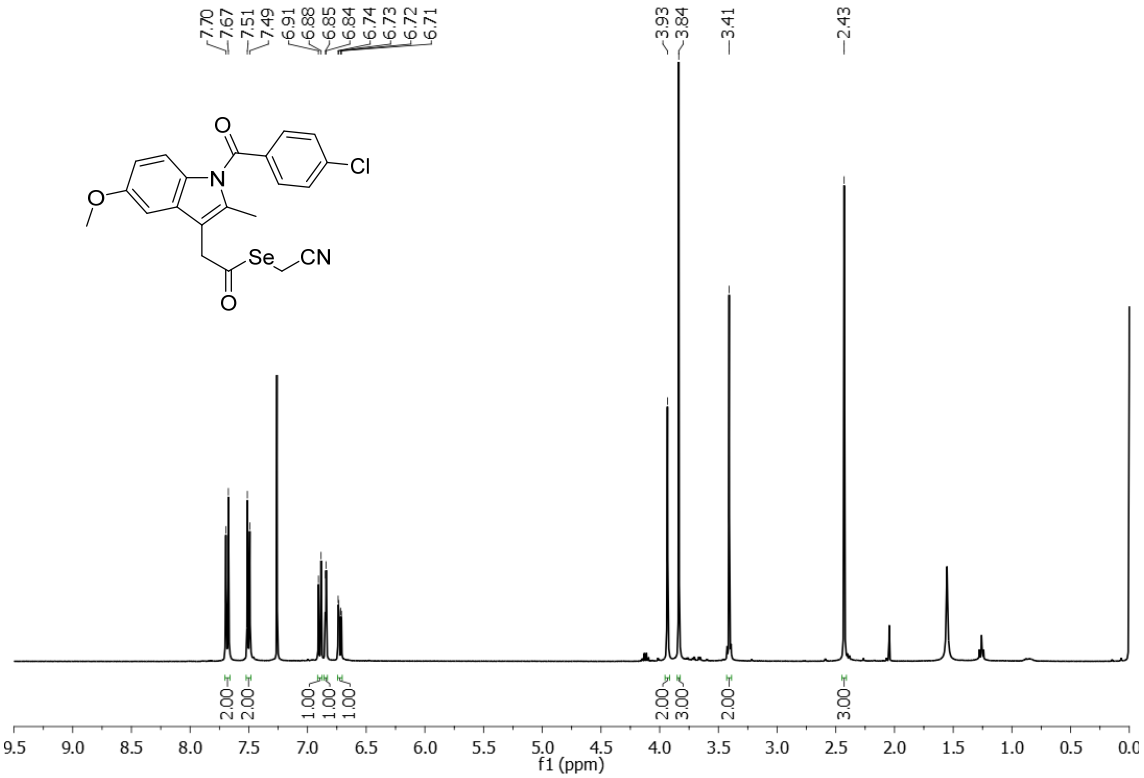


Figure S13. ^{1}H-NMR spectrum of compound **I.4d**.

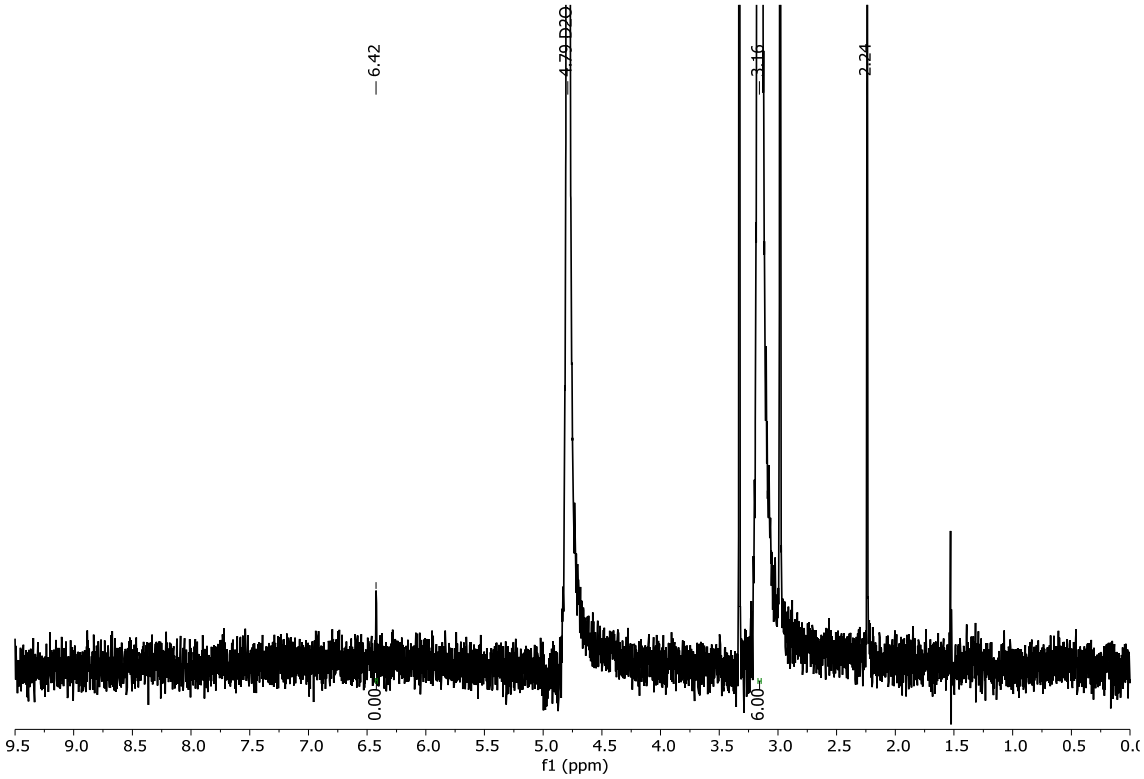


Figure S14. ^{1}H-NMR spectrum of compound **I.4d** and dimethyl sulfone.

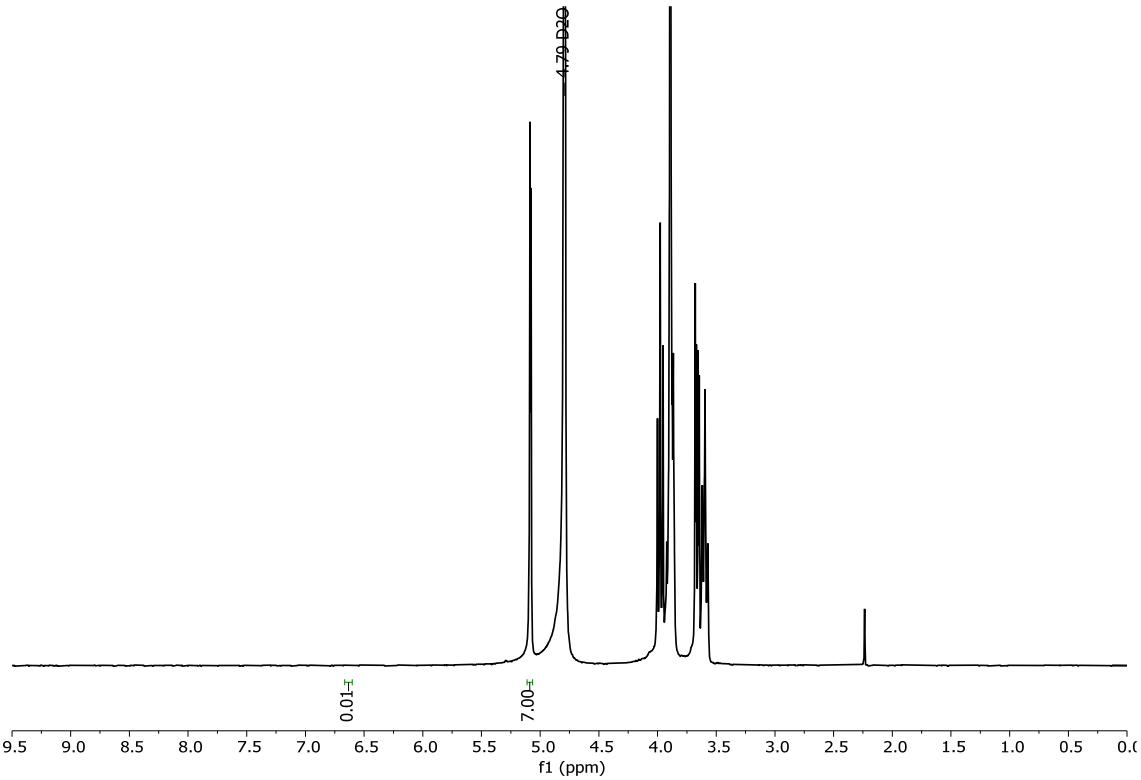


Figure S15. ^{1}H-NMR spectrum of compound **I.4d** and β-CD.

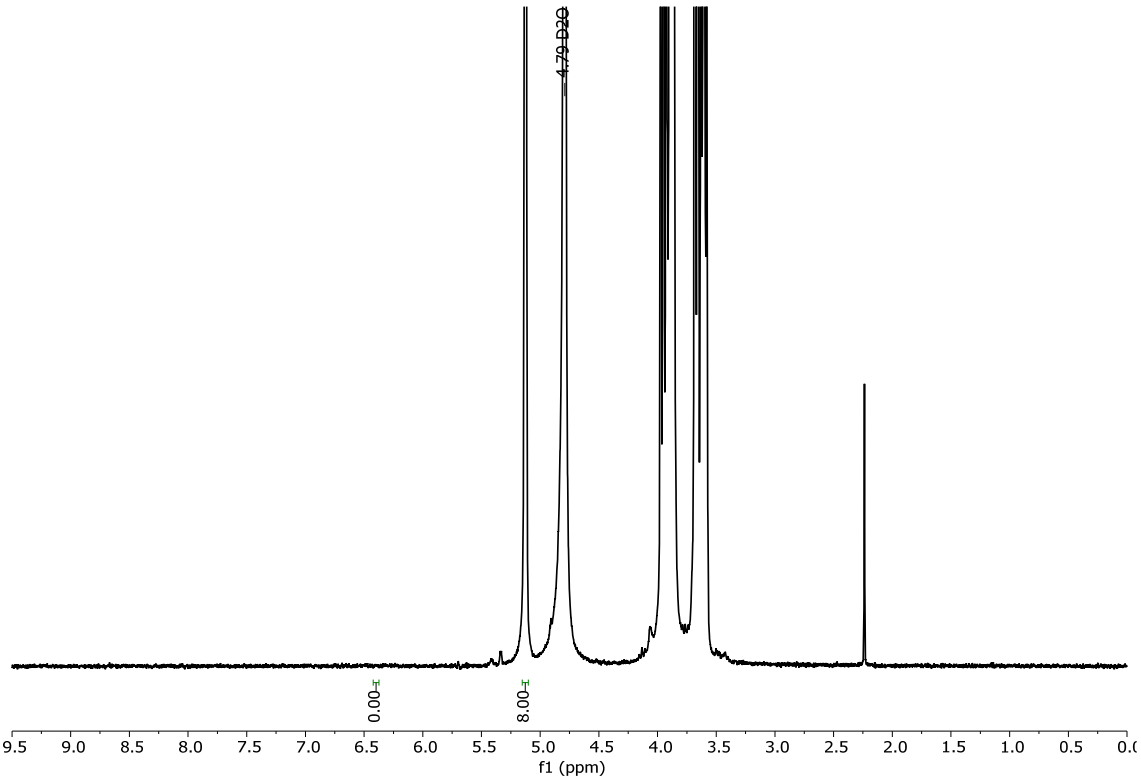
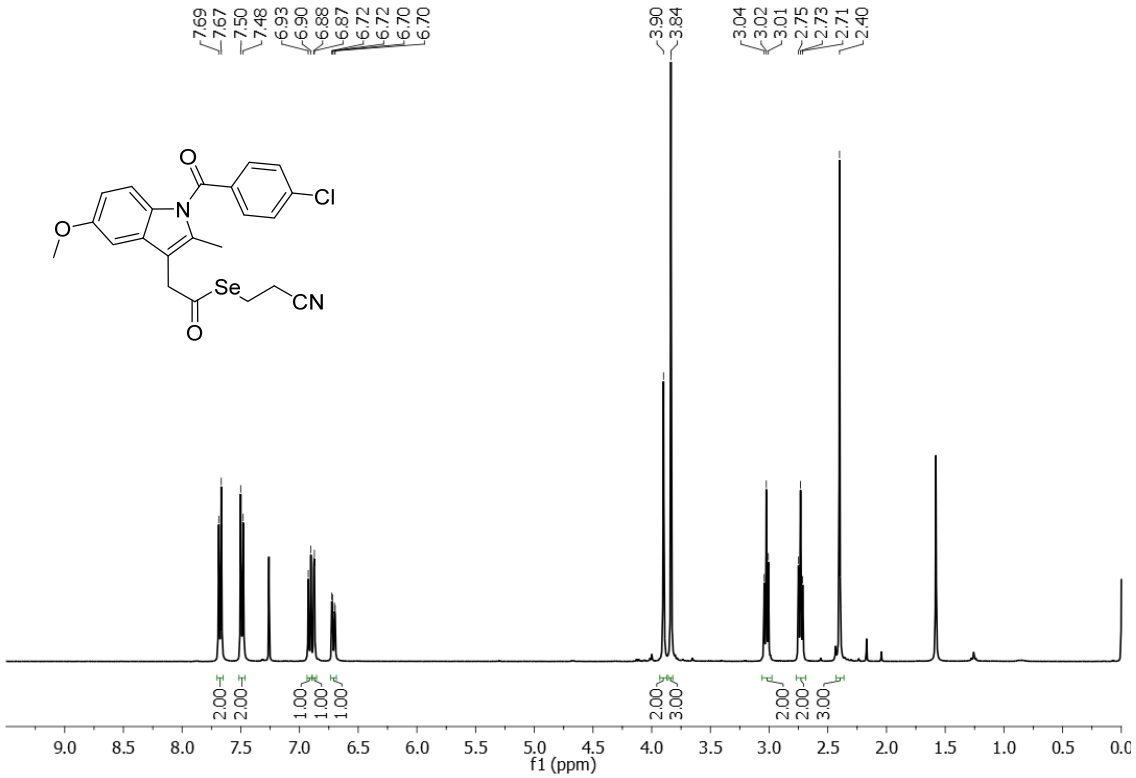


Figure S16. ^{1}H-NMR spectrum of compound **I.4d** and γ-CD.



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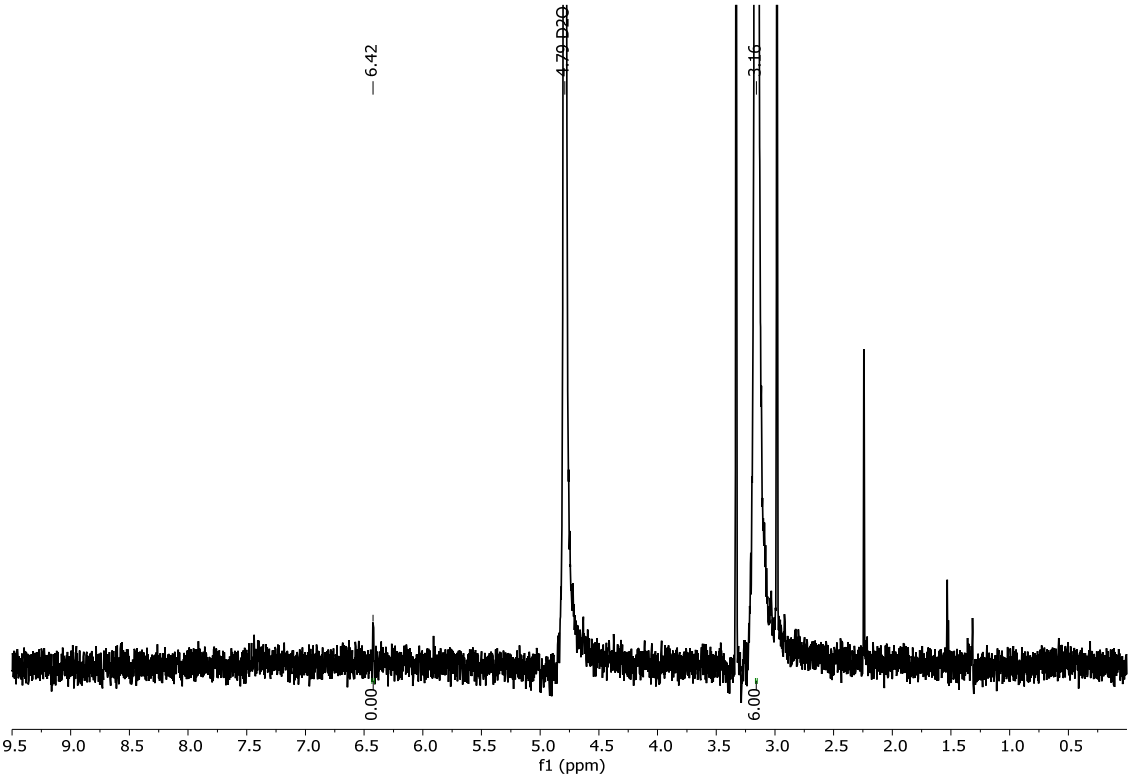

Figure S18. ^{1}H-NMR spectrum of compound **I.4e** and dimethyl sulfone.

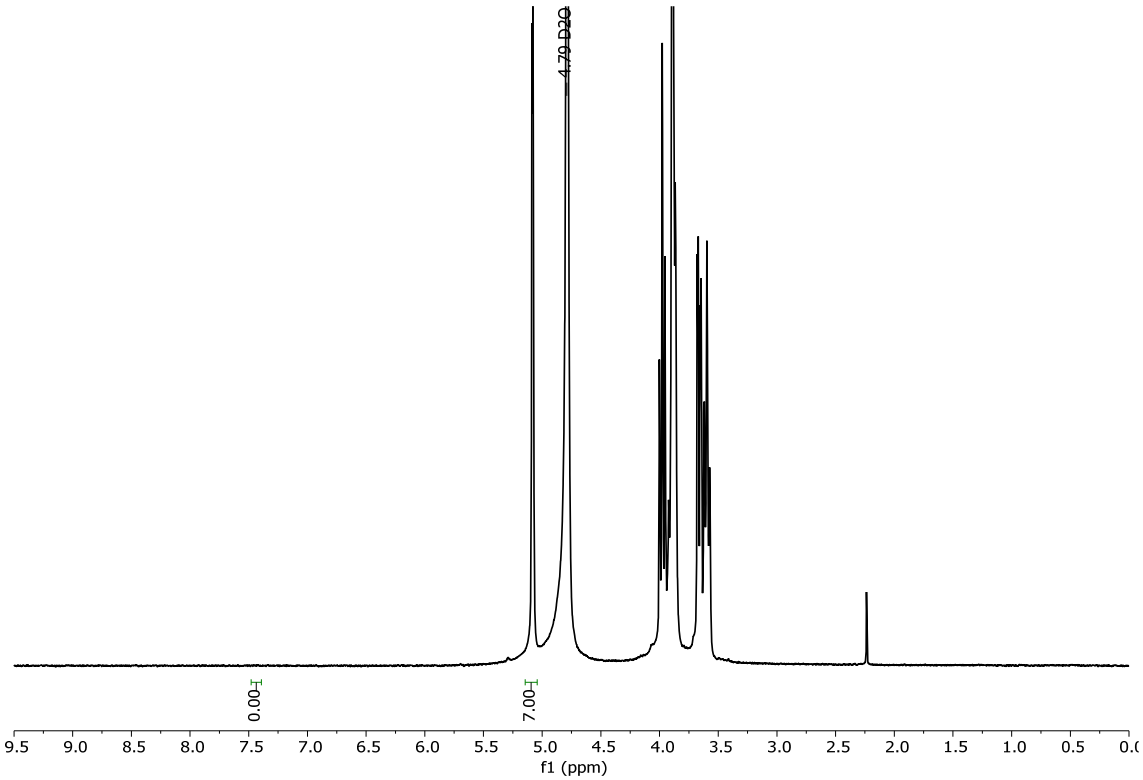

Figure S19. ^{1}H-NMR spectrum of compound **I.4e** and β-CD.

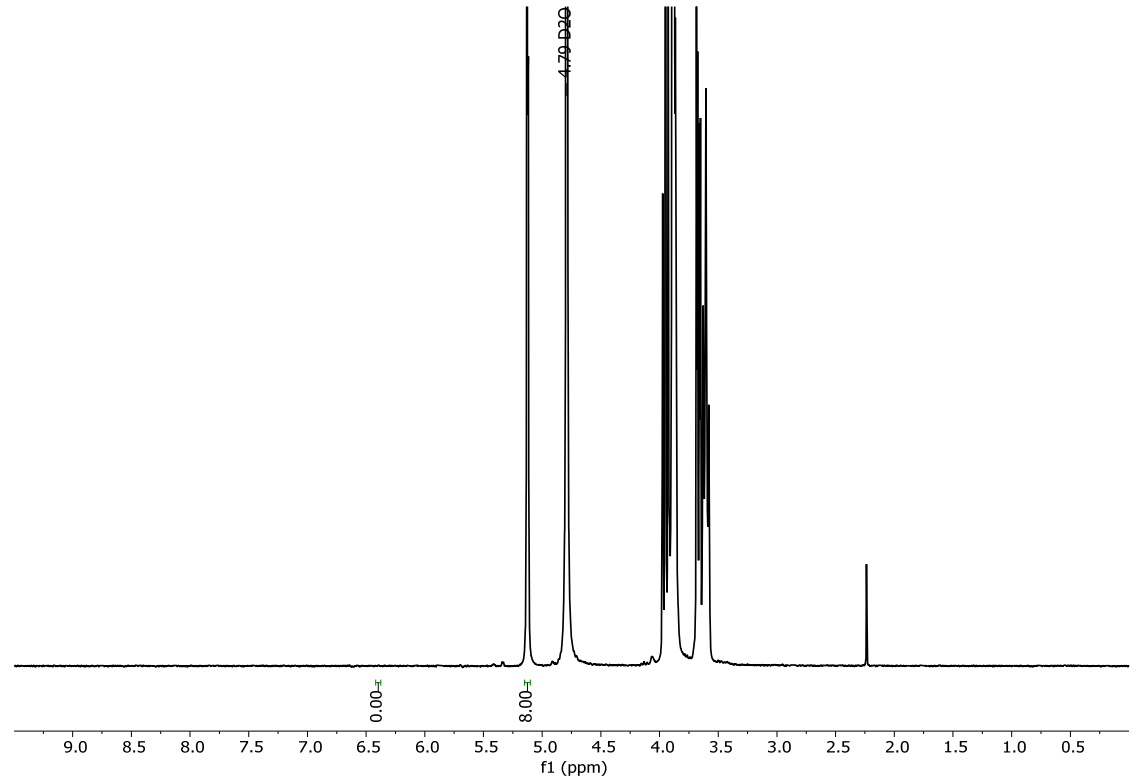

Figure S20. ^{1}H-NMR spectrum of compound **I.4e** and γ-CD.

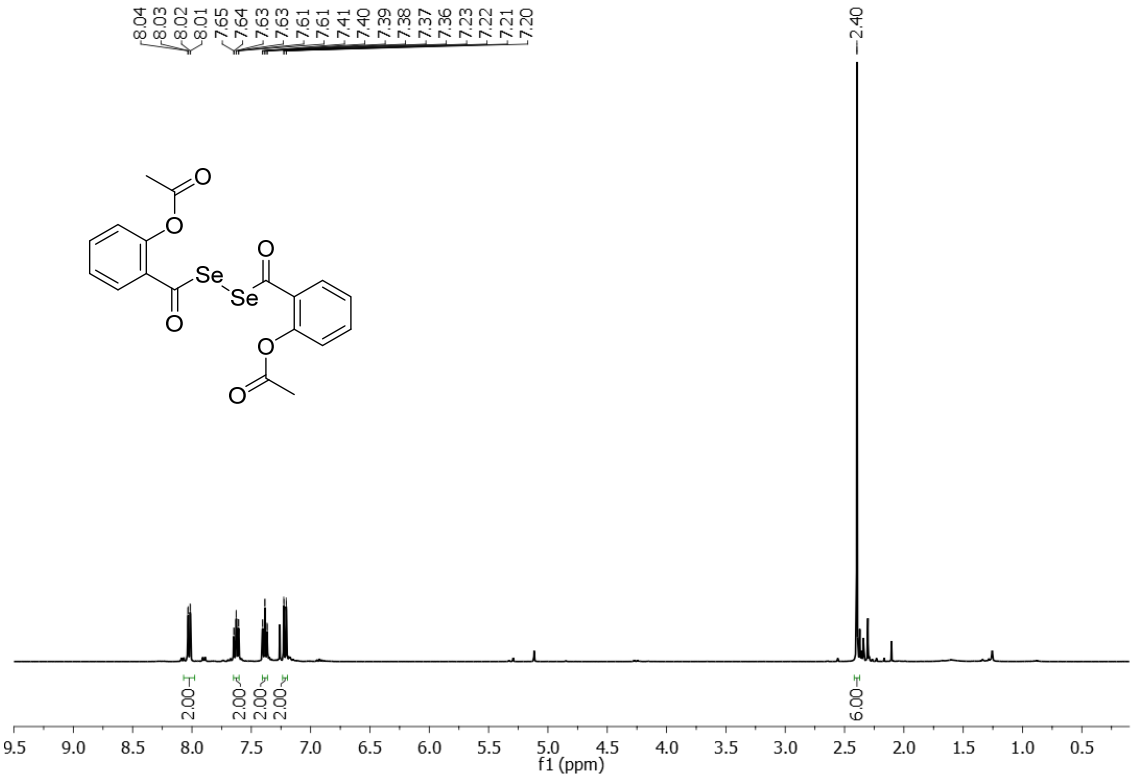

Figure S21. ^{1}H-NMR spectrum of compound **II.1**.

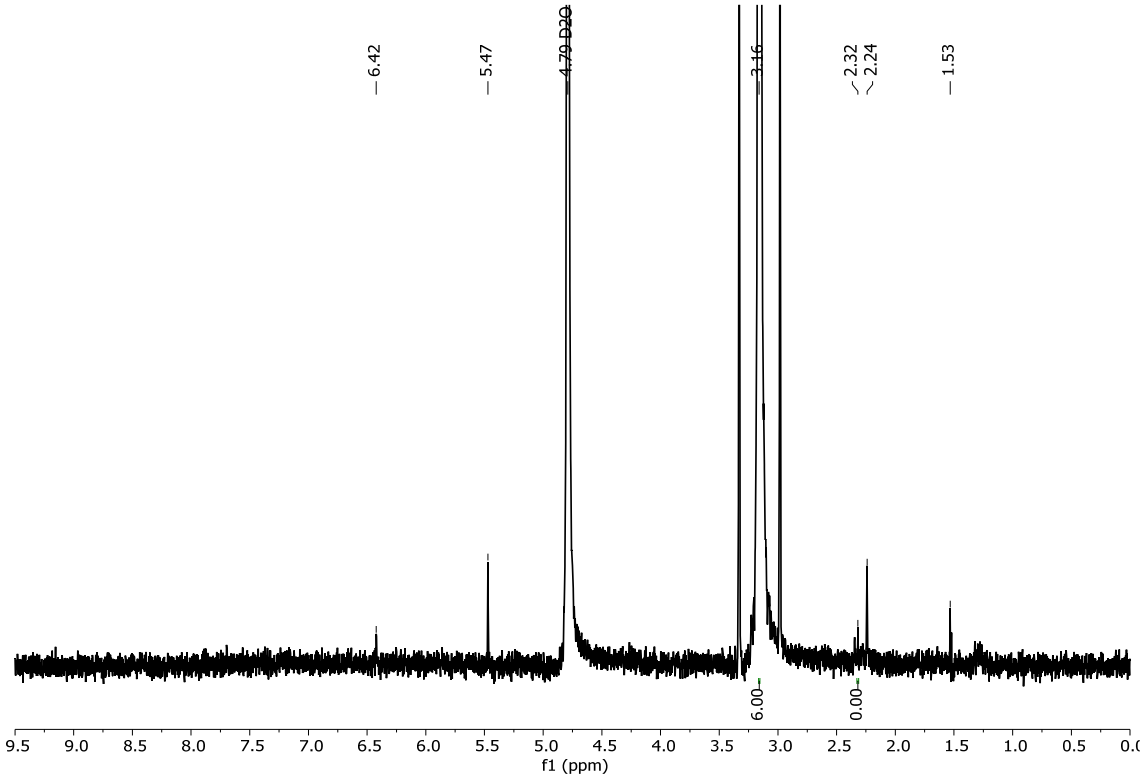

Figure S22. ^{1}H-NMR spectrum of compound **II.1** and dimethyl sulfone.

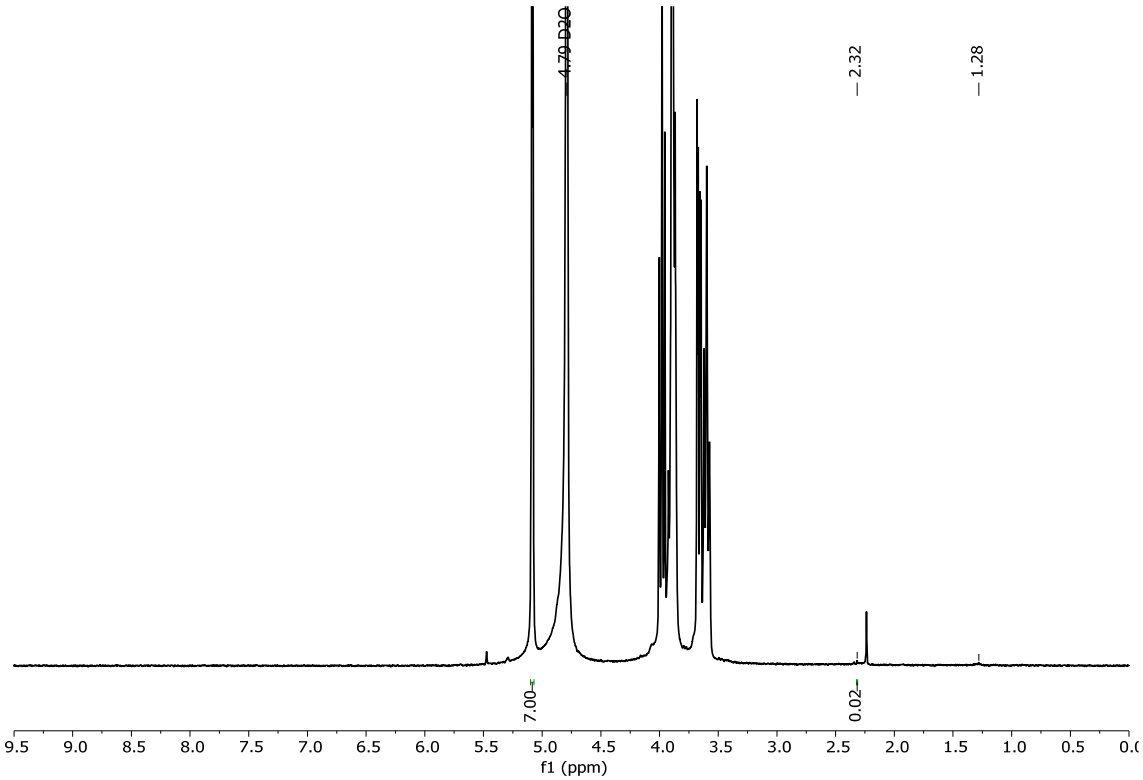

Figure S23. ^{1}H-NMR spectrum of compound **II.1** and β-CD.

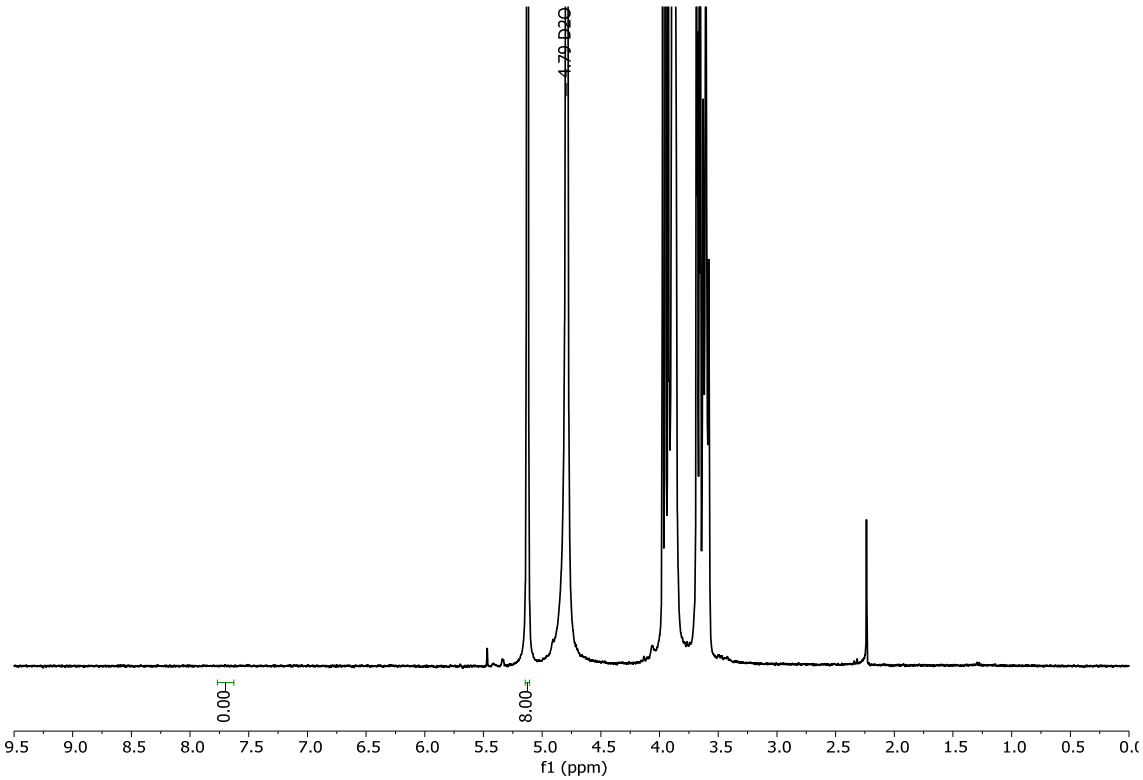

Figure S24. ^{1}H-NMR spectrum of compound **II.1** and γ-CD.

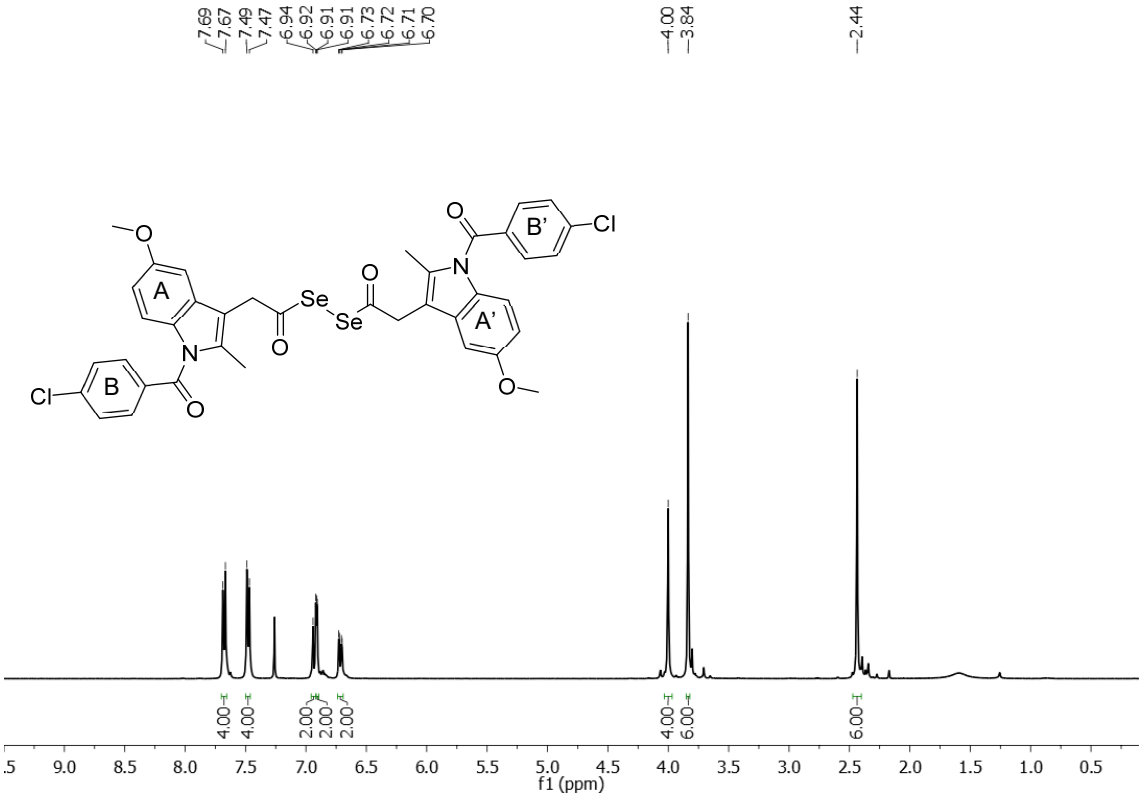

Figure S25. ^{1}H-NMR spectrum of compound **II.2**.

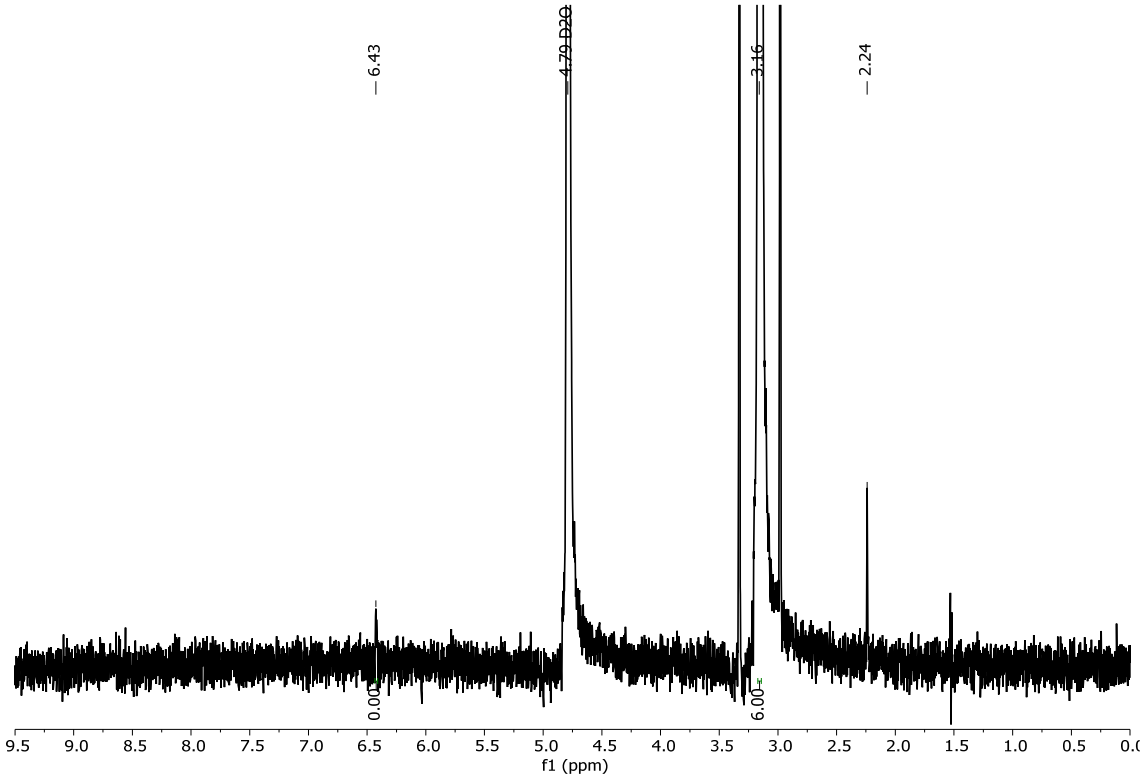

Figure S26. ^{1}H-NMR spectrum of compound **II.2** and dimethyl sulfone.

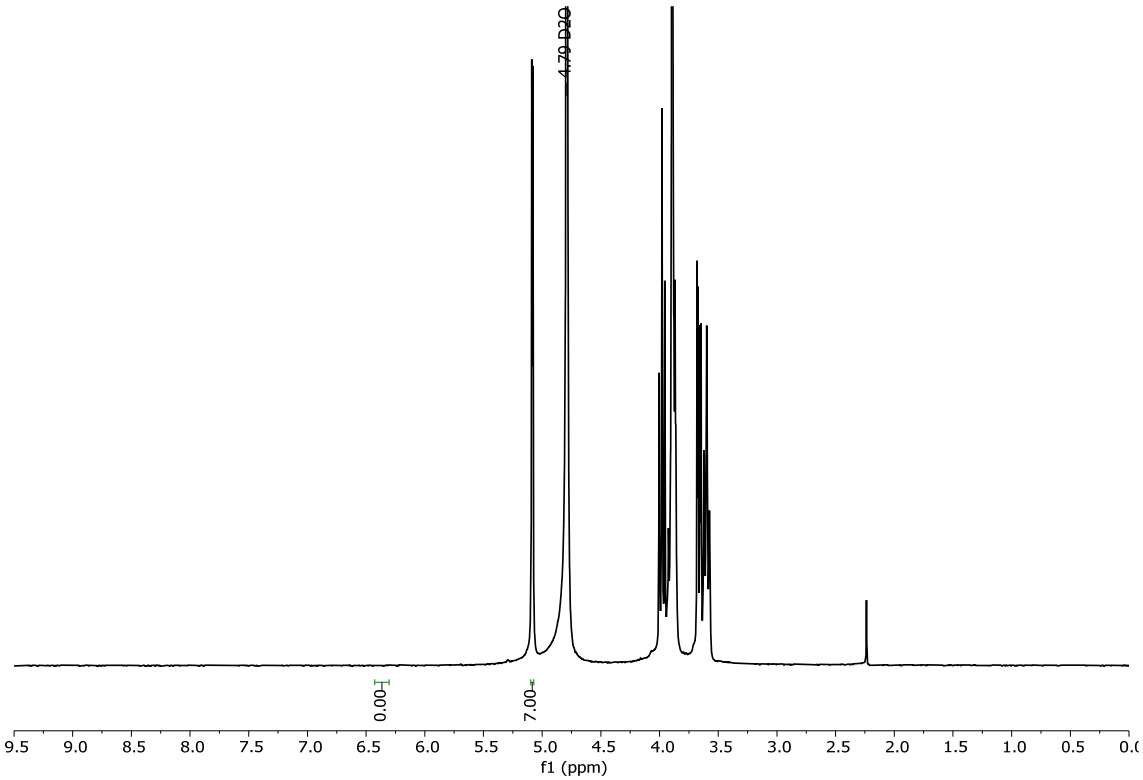

Figure S27. ^{1}H-NMR spectrum of compound **II.2** and β-CD.

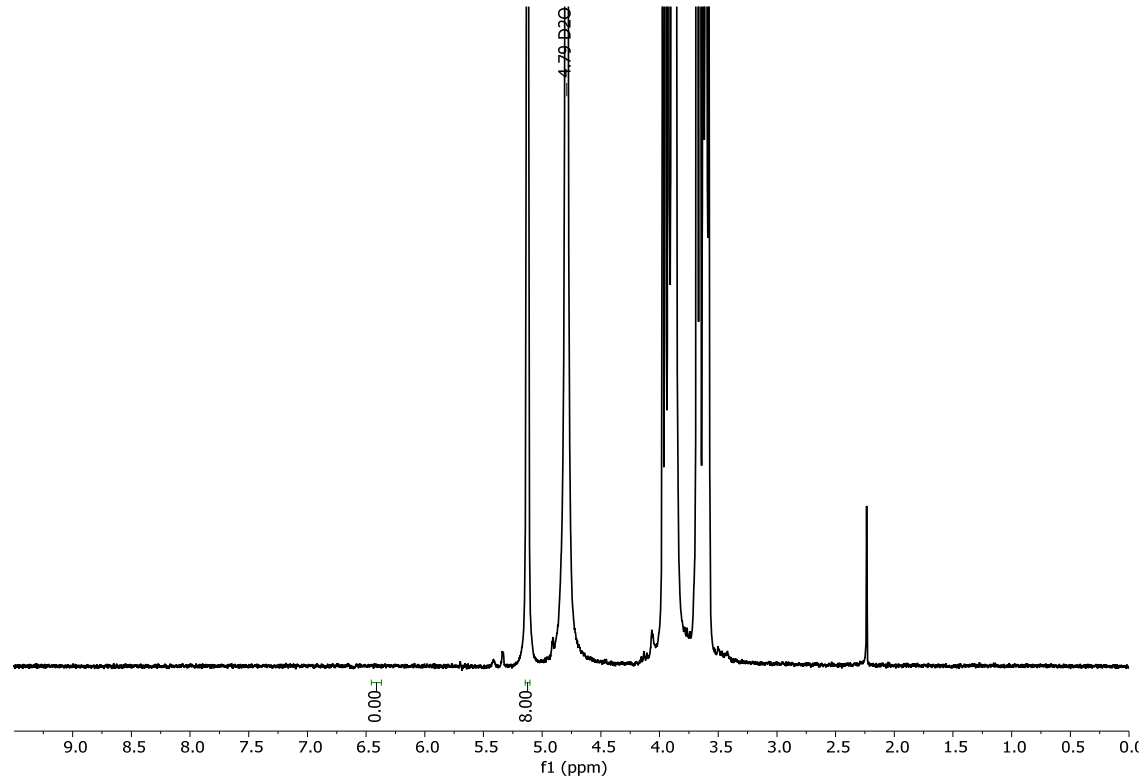

Figure S28. ^{1}H-NMR spectrum of compound **II.2** and γ-CD.

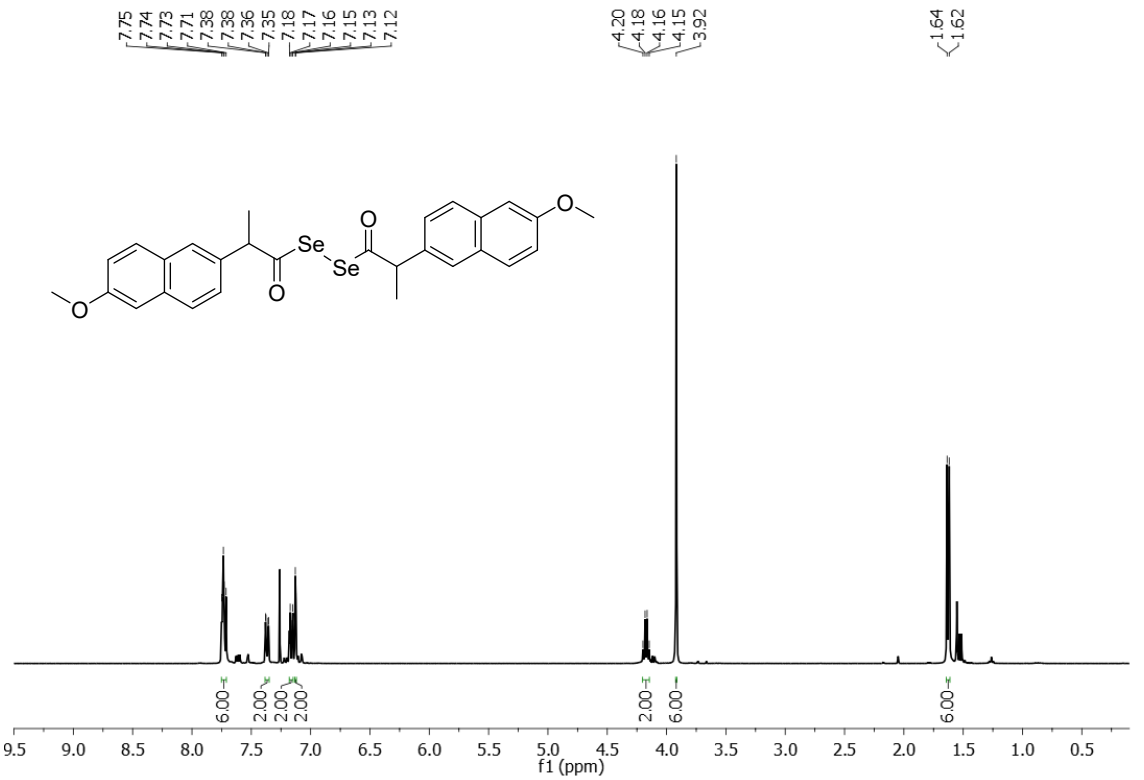

Figure S29. ^{1}H-NMR spectrum of compound **II.3**.

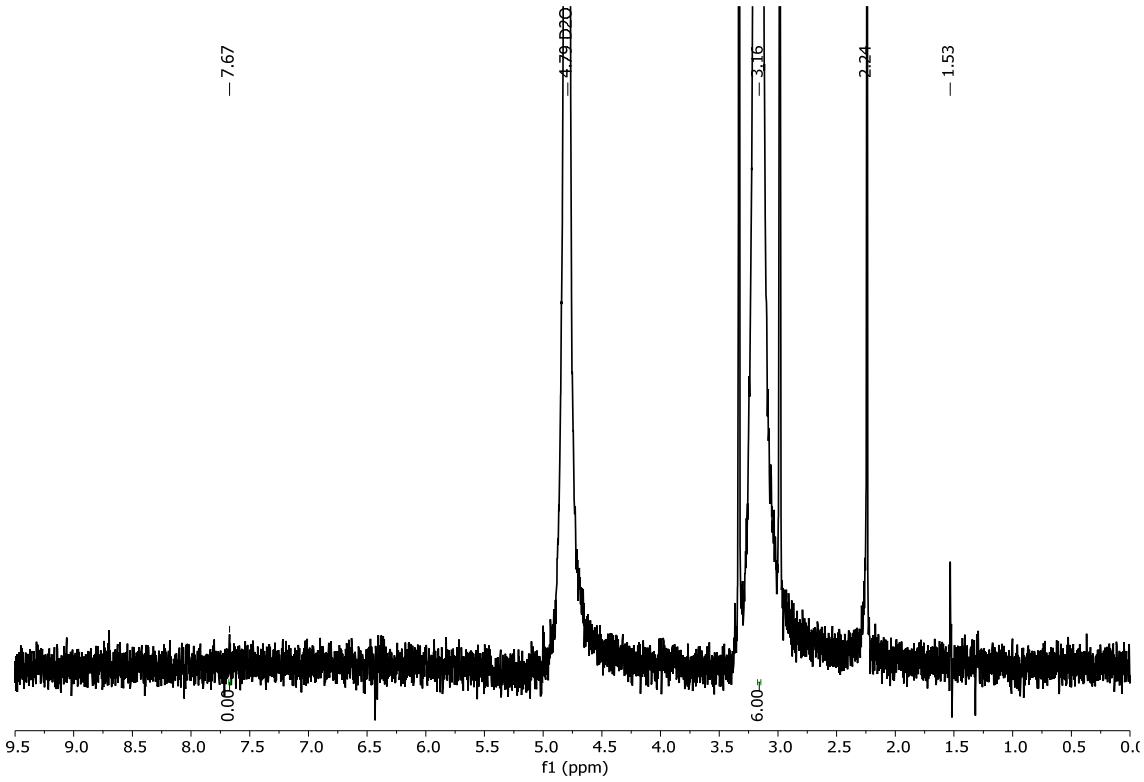

Figure S30. ^{1}H-NMR spectrum of compound **II.3** and dimethyl sulfone.

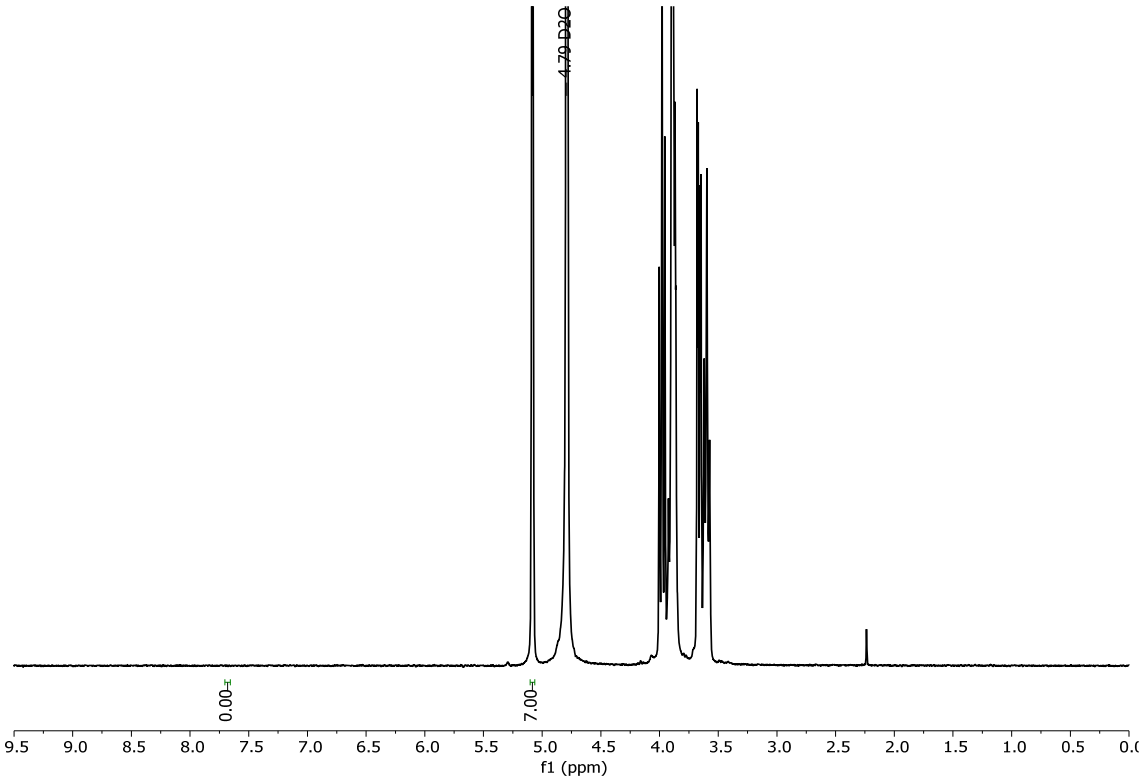

Figure S31. ^{1}H-NMR spectrum of compound **II.3** and β-CD.

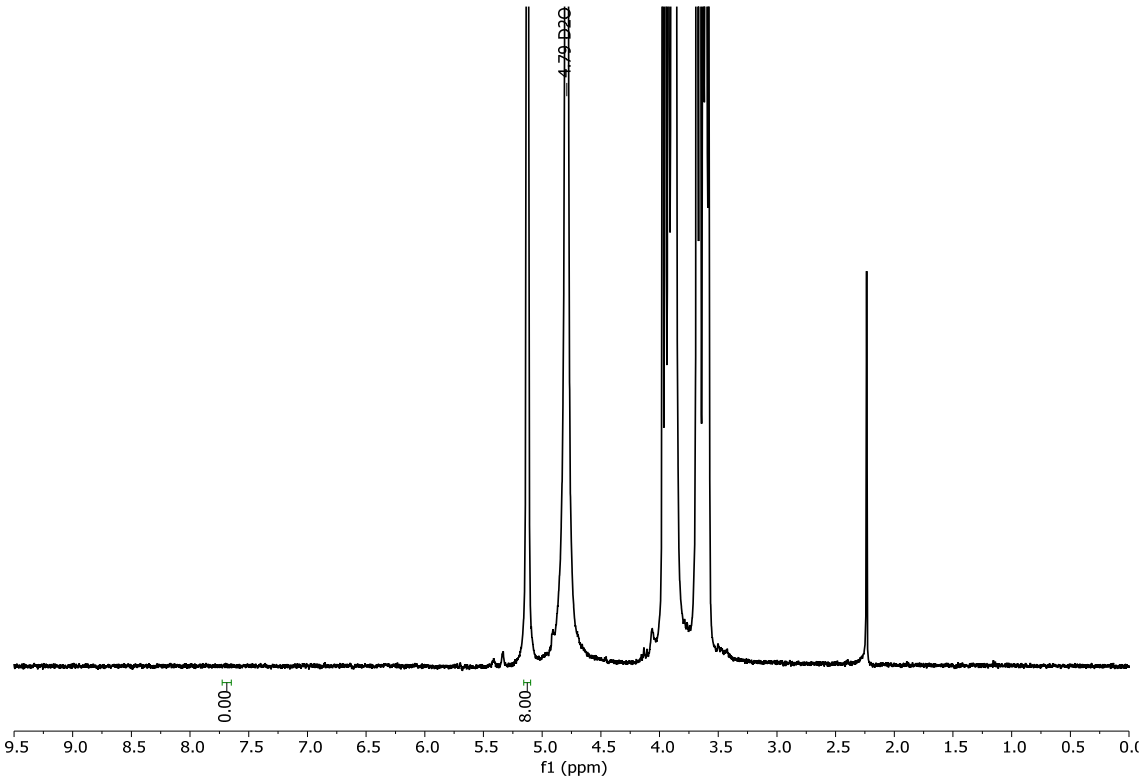

Figure S32. ^{1}H-NMR spectrum of compound **II.3** and γ-CD.

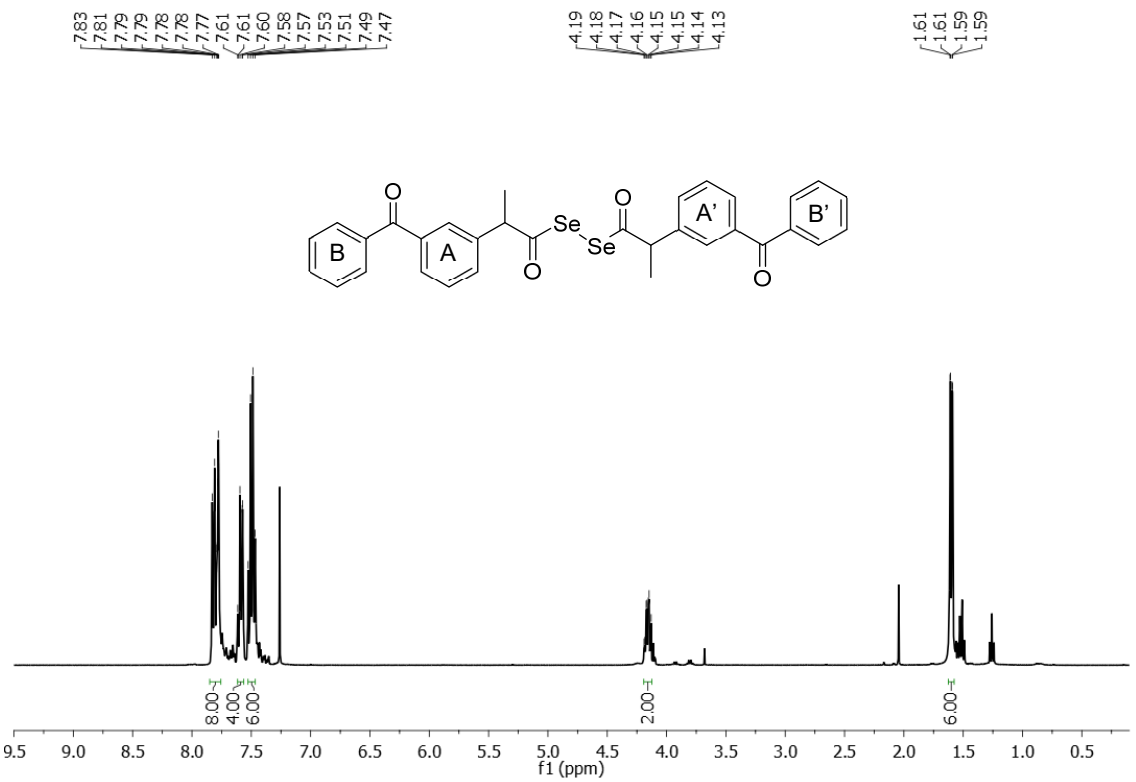

Figure S33. ^{1}H-NMR spectrum of compound **II.4**.

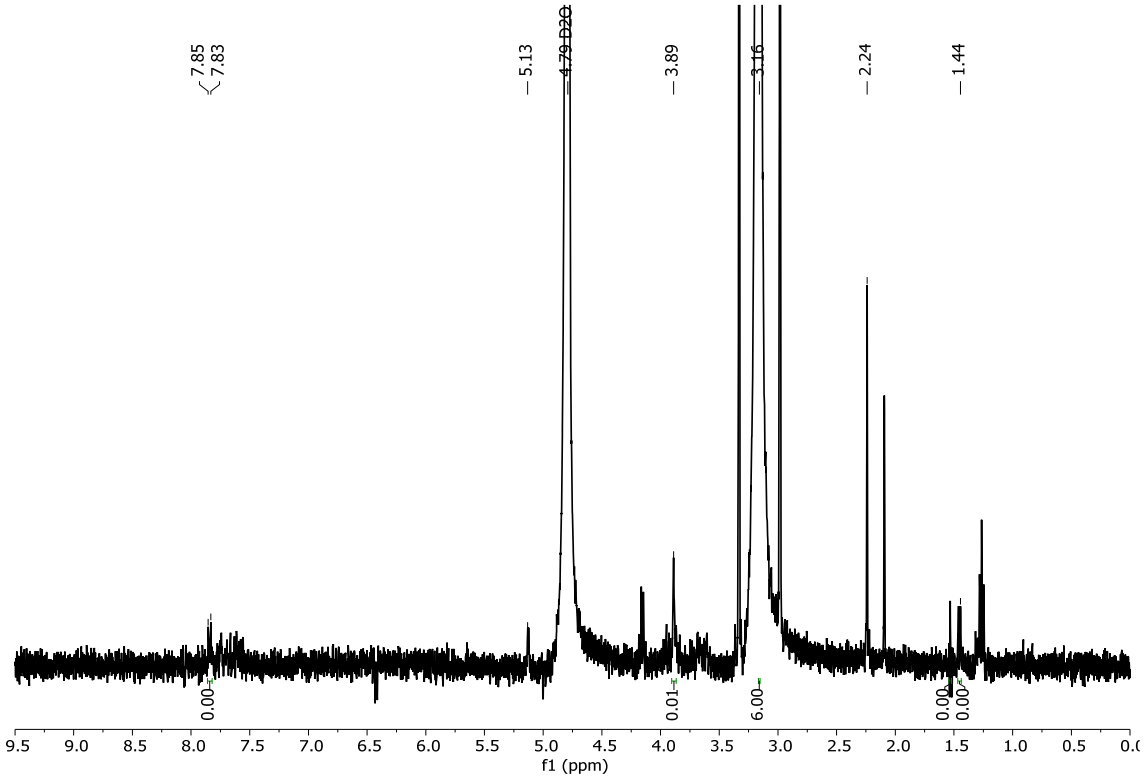

Figure S34. ^{1}H-NMR spectrum of compound **II.4** and dimethyl sulfone.

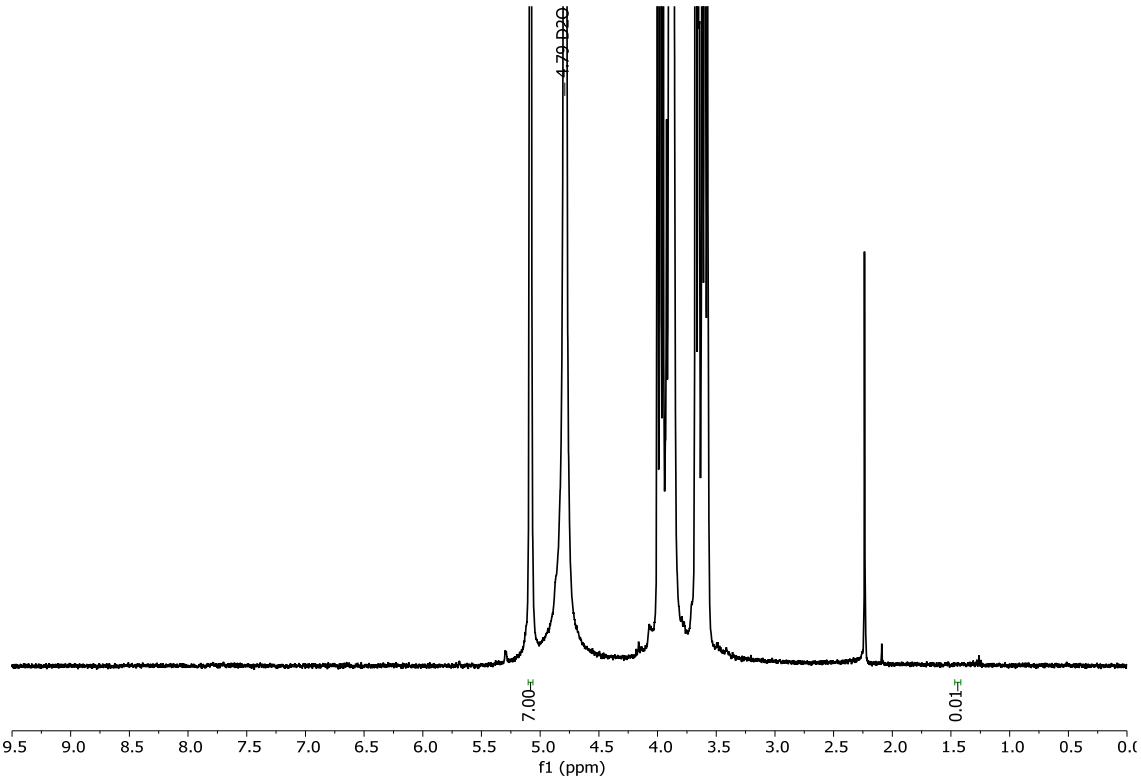

Figure S35. ^{1}H-NMR spectrum of compound **II.4** and β-CD.

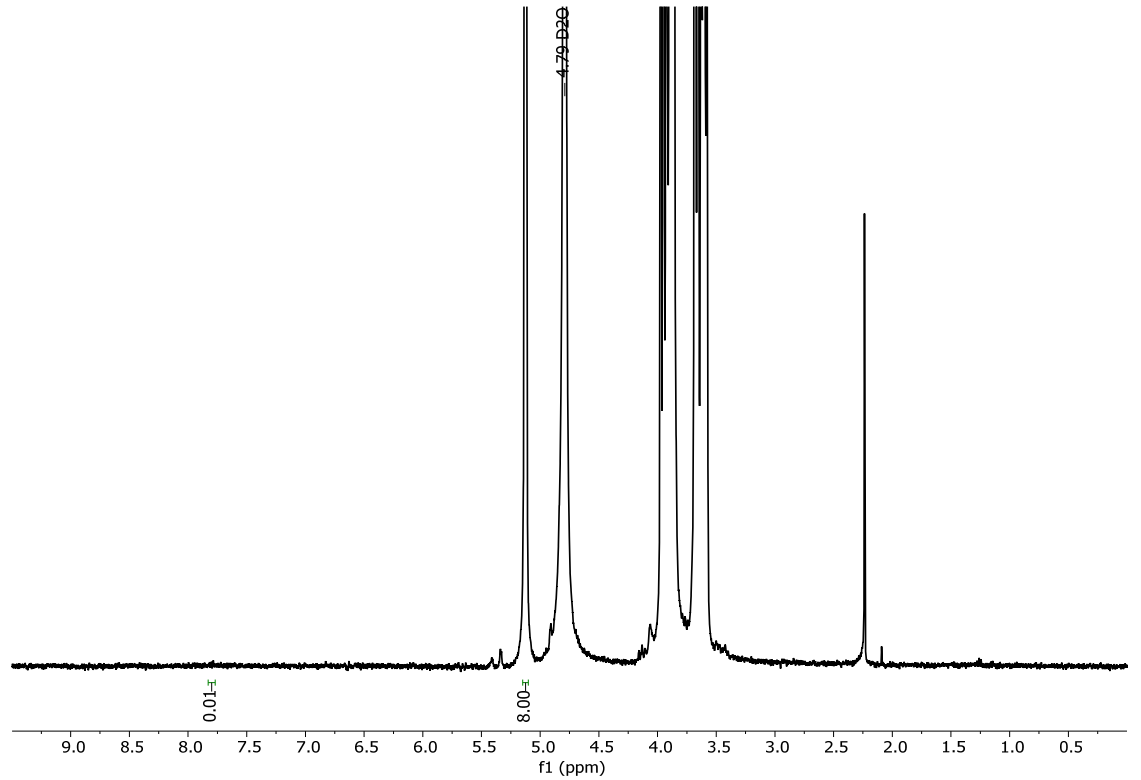

Figure S36. ^{1}H-NMR spectrum of compound **II.4** and γ-CD.

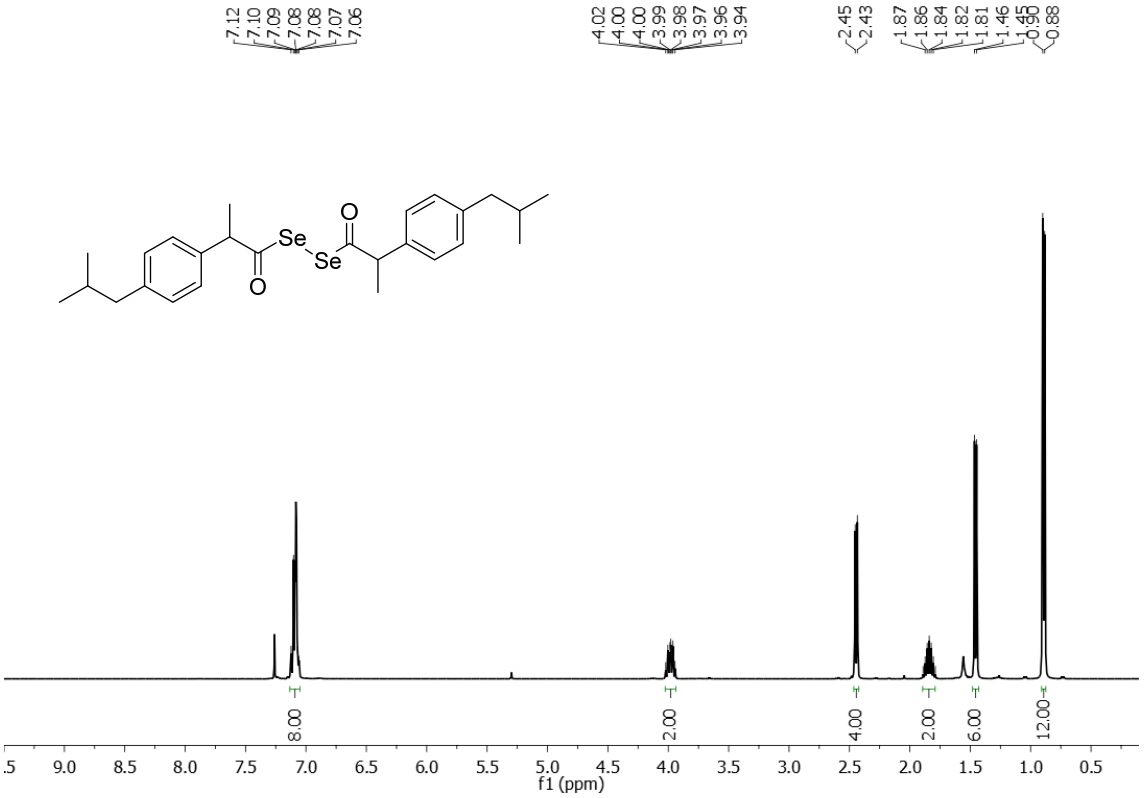

Figure S37. ^{1}H-NMR spectrum of compound **II.5**.

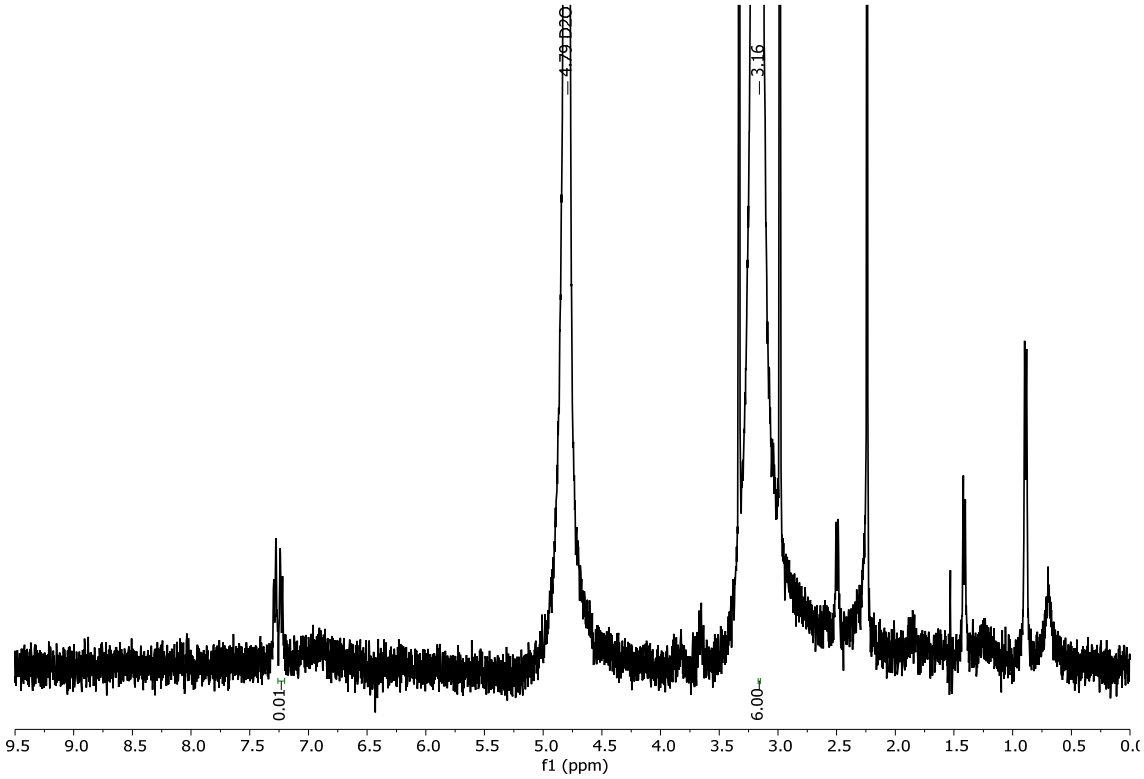

Figure S38. ^{1}H-NMR spectrum of compound **II.5** and dimethyl sulfone.

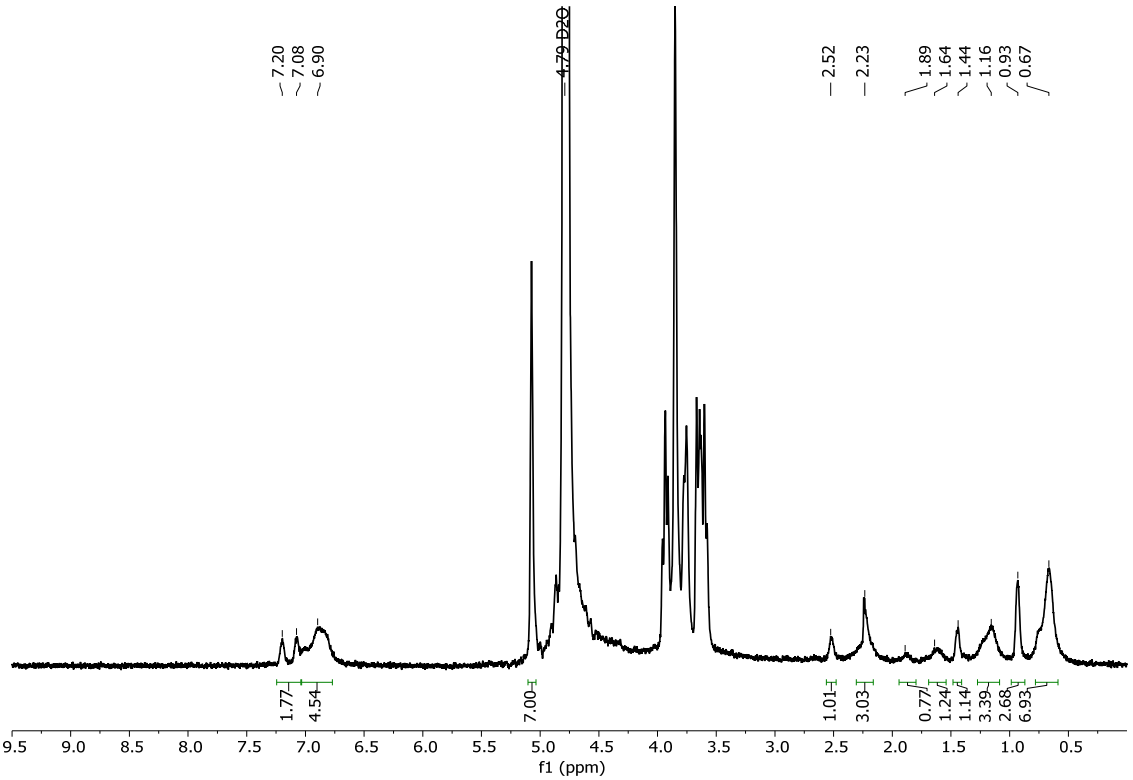

Figure S39. ^{1}H-NMR spectrum of compound **II.5** and β-CD.

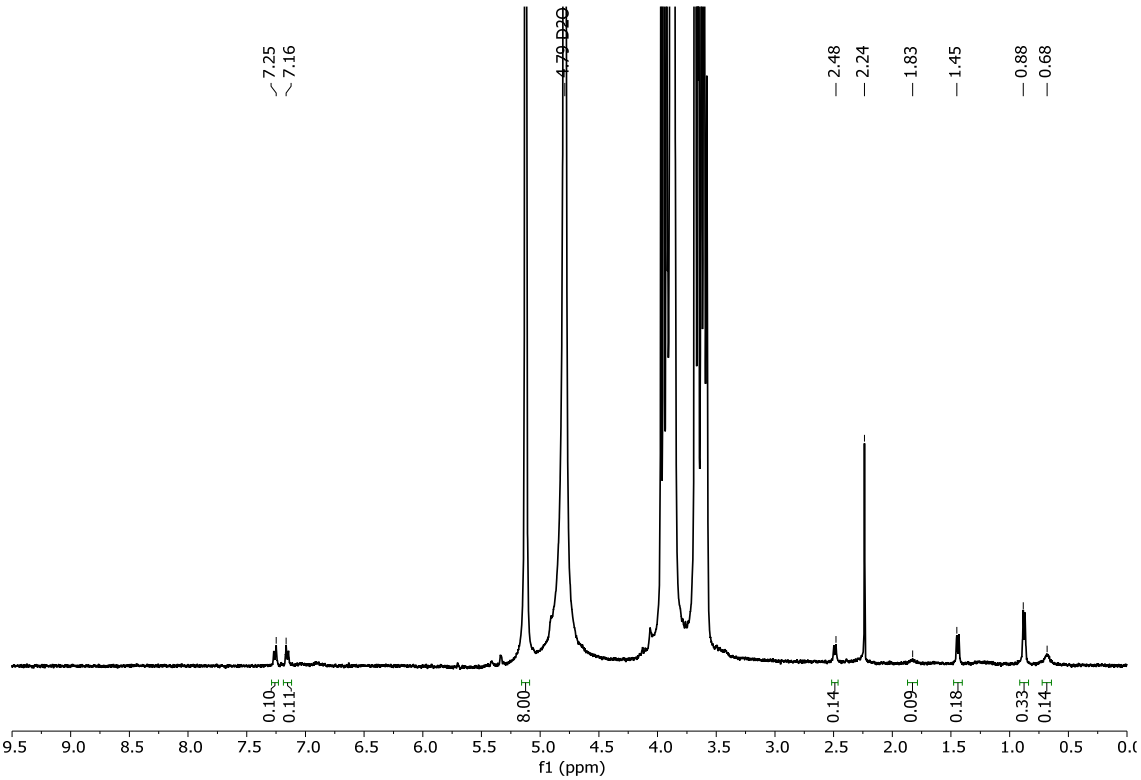

Figure S40. ^{1}H-NMR spectrum of compound **II.5** and γ-CD.

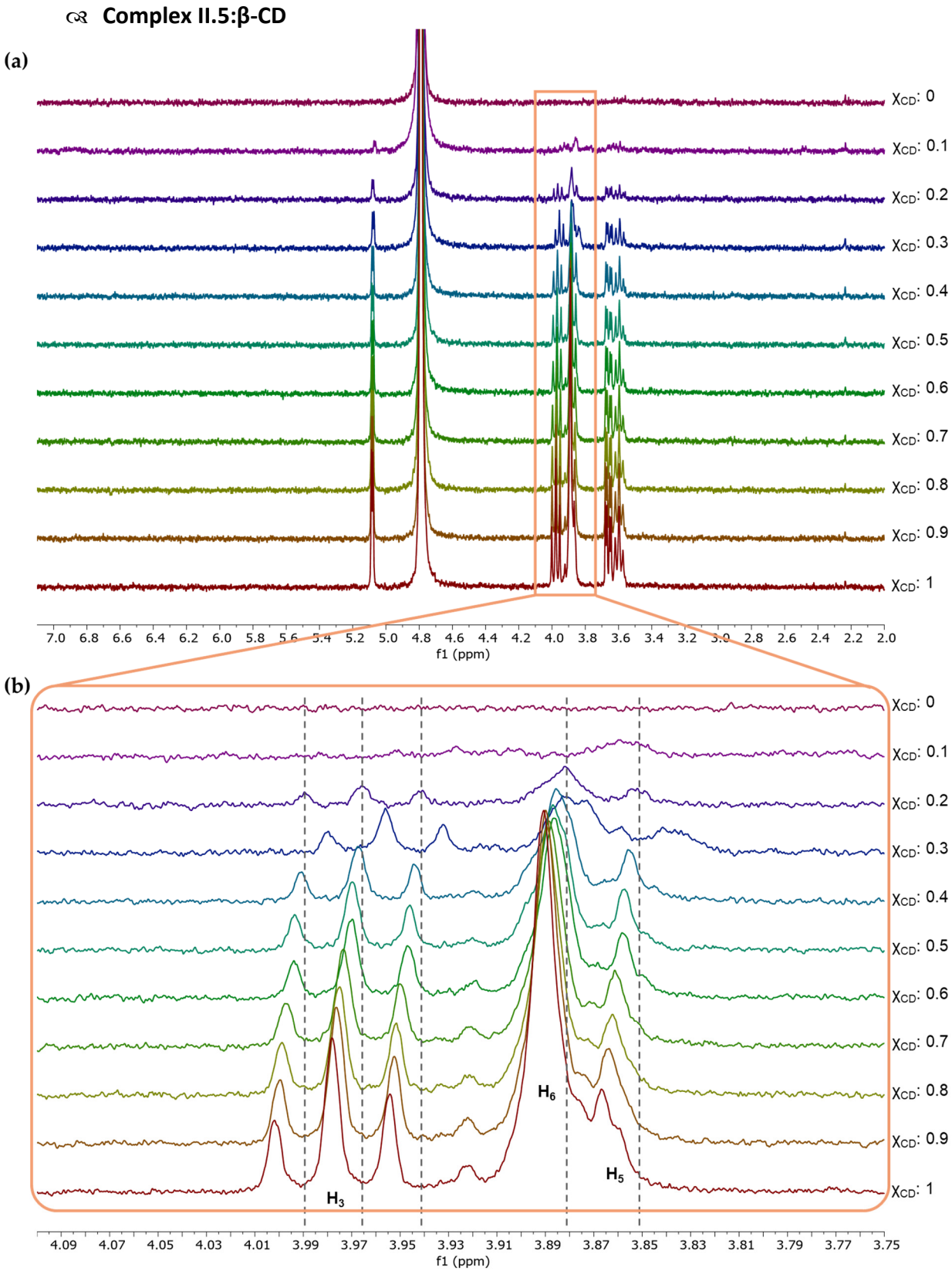

Figure S41. (**a**) ^{1}H-NMR spectra for different molar fractions of the complex **II.5**:β-CD and (**b**) expansion of the region including protons H_3, H_5 and H_6 of the β-CD.

☙ Computational data

Table S1. Scores for best poses with β-CD (London GBVI, explicit solvent).

Ref.	S	rmsd_refine	E_score1	E_refine	E_score2
I.3e	-5.7072	0.9549	-9.1928	-28.8446	-5.7072
I.4a	-6.5707	1.3715	-11.1362	-35.2667	-6.5707
I.4b	-6.6023	2.5629	-9.1989	-37.9295	-6.6023
I.4d	-6.3956	2.1327	-13.9270	-32.9405	-6.3956
I.4e	-6.6008	2.0304	-9.4502	-36.2130	-6.6008
II.1	-6.3968	2.1026	-8.5649	-30.1874	-6.3968
II.2	-7.5321	3.3643	-7.8035	-42.4309	-7.5321
II.3	-6.5140	2.3443	-7.5844	-39.5321	-6.5140
II.4	-6.6059	1.4075	-7.6007	-41.1813	-6.6059
II.5	-6.5295	2.3124	-7.6958	-37.8857	-6.5295

Table S2. Scores for best poses with γ-CD (London GBVI, explicit solvent).

Ref.	S	rmsd_refine	E_score1	E_refine	E_score2
I.3e	-8.0412	1.9909	-3.1866	-33.4640	-8.0412
I.4a	-9.6127	2.2584	-1.8757	-34.6887	-9.6127
I.4b	-8.8817	1.9890	-1.9153	-32.3470	-8.8817
I.4d	-8.8520	4.6771	-2.2712	-35.2892	-8.8520
I.4e	-9.1430	4.9243	-2.1714	-36.6787	-9.1430
II.1	-8.1714	1.2808	-3.8911	-35.5261	-8.1714
II.2	-10.1487	1.6912	1.8735	-42.3182	-10.1487
II.3	-8.9557	2.0750	0.2874	-38.5811	-8.9557
II.4	-9.1211	2.6151	-0.5199	-42.0503	-9.1211
II.5	-7.9440	2.0826	2.5007	-34.7207	-7.9440

Table S3. Energy values for best poses of selected compounds (London GBVI, explicit solvent).

Ref. complex	E all
β-CD	
I3e_best_solvent	-257.77
II5_01_best_solvent	-465.87
II5_02_best_solvent	-463.43
γ-CD	
I3e_best_solvent	-293.76
II5_01_best_solvent	-508.33
II5_02_best_solvent	-507.18