

Supplementary Information

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Analysis data of

- Figure S1.** DEPTQ-NMR spectrum of P₃N₃-[O-C₆H₄-O-(CH₂)₃-βCD]₆ (**I**) in D₂O. p2
- Figure S2.** 2D NMR COSY spectrum of P₃N₃-[O-C₆H₄-O-(CH₂)₃-βCD]₆ (**I**) in D₂O. p3
- Figure S3.** ¹H NMR spectrum of P₃N₃-[O-C₆H₄-O-(CH₂)₄-βCD]₆ (**II**) in D₂O. p4
- Figure S4.** DEPTQ-NMR spectrum of P₃N₃-[O-C₆H₄-O-(CH₂)₄-βCD]₆ (**II**) in D₂O. p5
- Figure S5.** 2D NMR HMQC spectrum of P₃N₃-[O-C₆H₄-O-(CH₂)₄-βCD]₆ (**II**) in D₂O. p6
- Figure S6.** 2D NMR NOESY spectrum of P₃N₃-[O-C₆H₄-O-(CH₂)₄-βCD]₆ (**II**) in D₂O. p7
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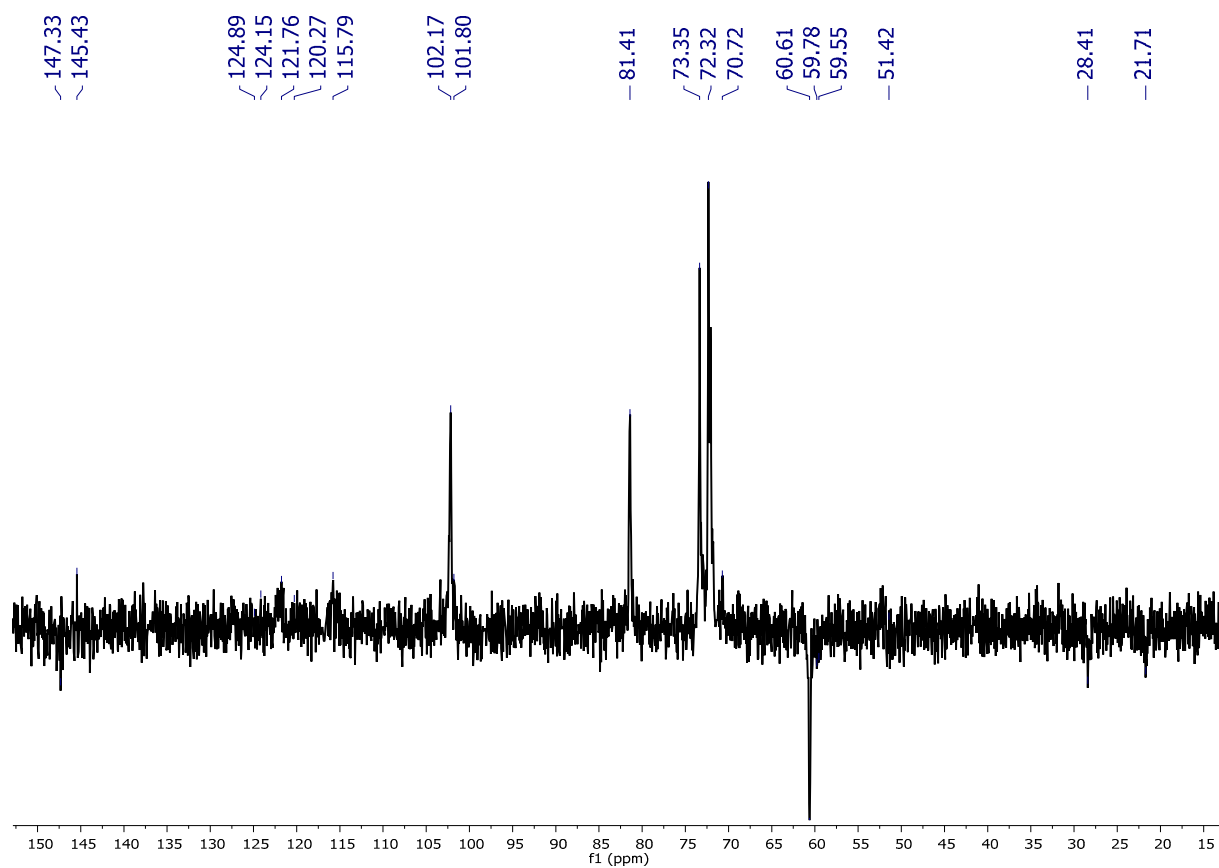


Figure S1. DEPTQ-NMR spectrum of $P_3N_3-[O-C_6H_4-O-(CH_2)_3-\beta CD]_6$ (I) in D_2O .

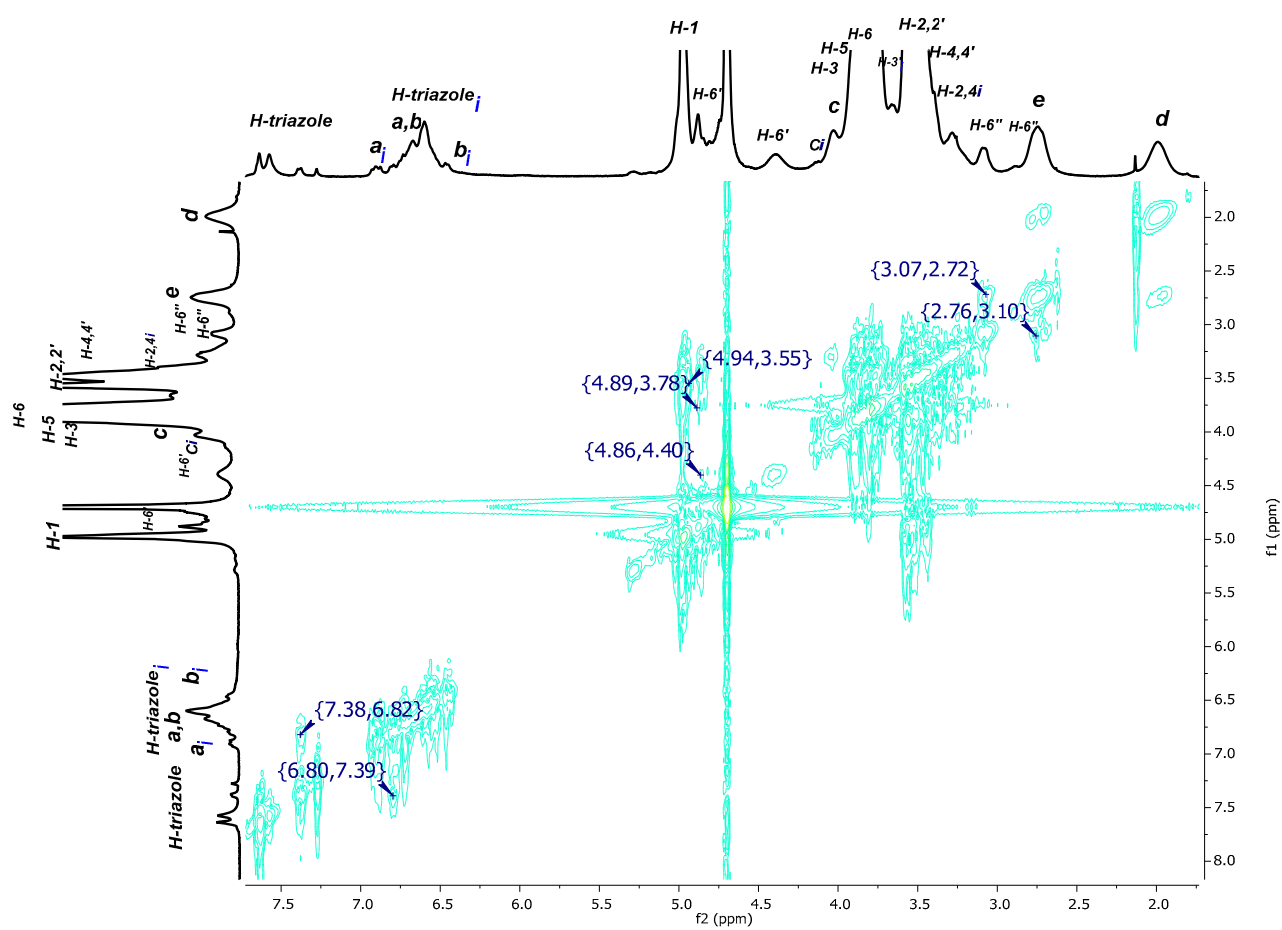


Figure S2. 2D NMR COSY spectrum of $\text{P}_3\text{N}_3\text{-[O-C}_6\text{H}_4\text{-O-(CH}_2\text{)}_3\text{-}\beta\text{CD]}_6$ (**I**) in D_2O .

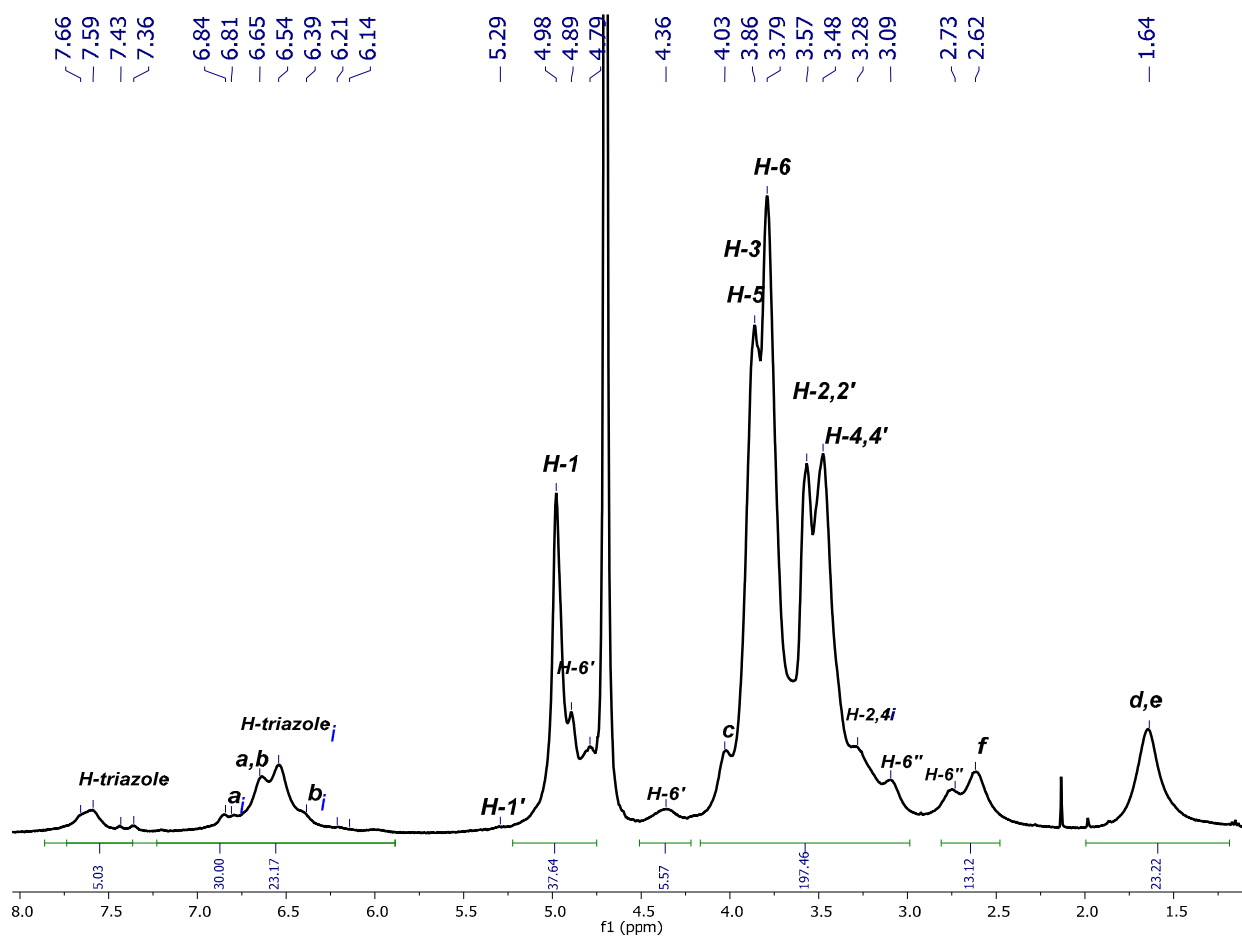


Figure S3. ^1H NMR spectrum of $\text{P}_3\text{N}_3\text{-[O-C}_6\text{H}_4\text{-O-(CH}_2\text{)}_4\text{-}\beta\text{CD]}_6$ (II) in D_2O .

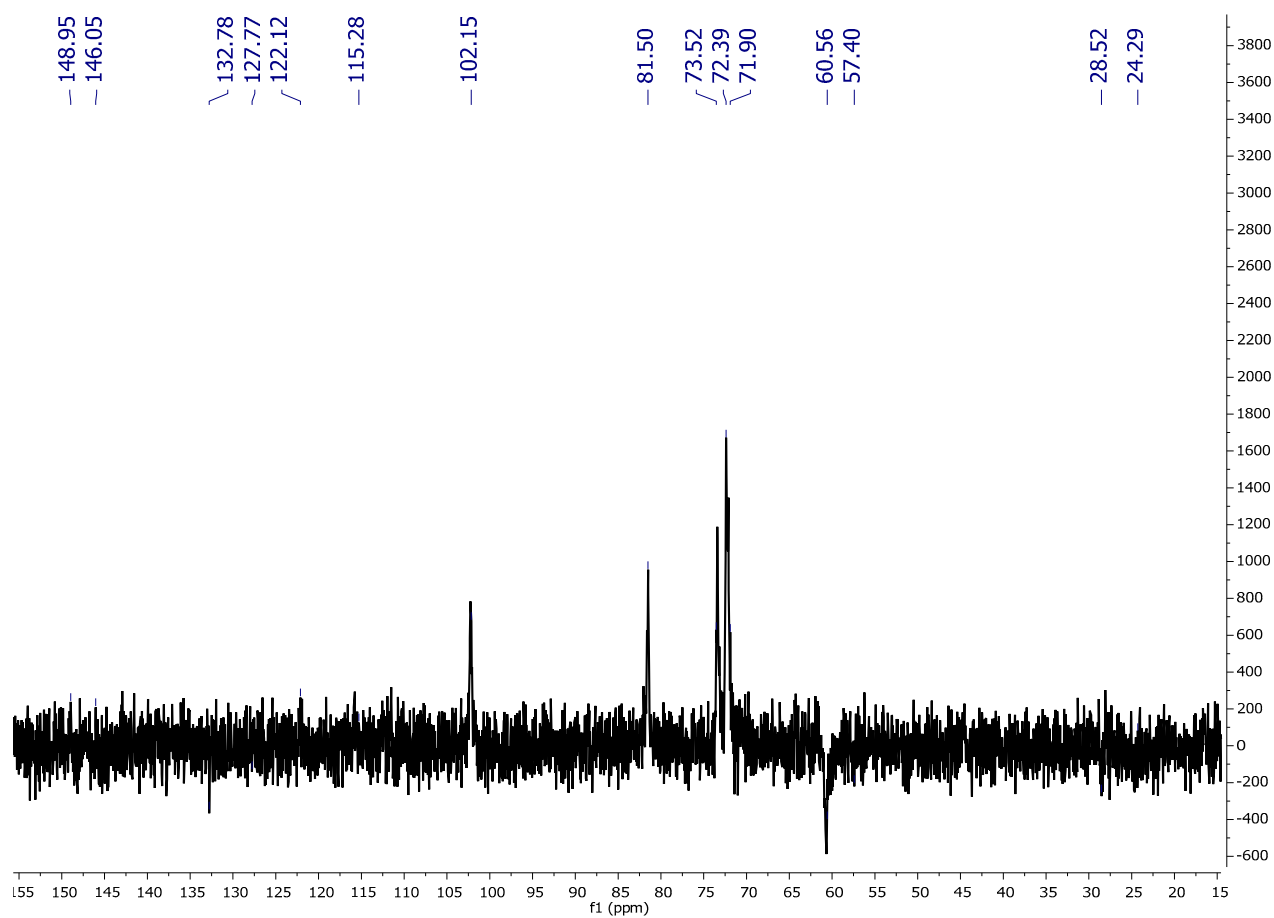


Figure S4. DEPTQ-NMR spectrum of $P_3N_3-[O-C_6H_4-O-(CH_2)_4-\beta CD]_6$ (II) in D_2O .

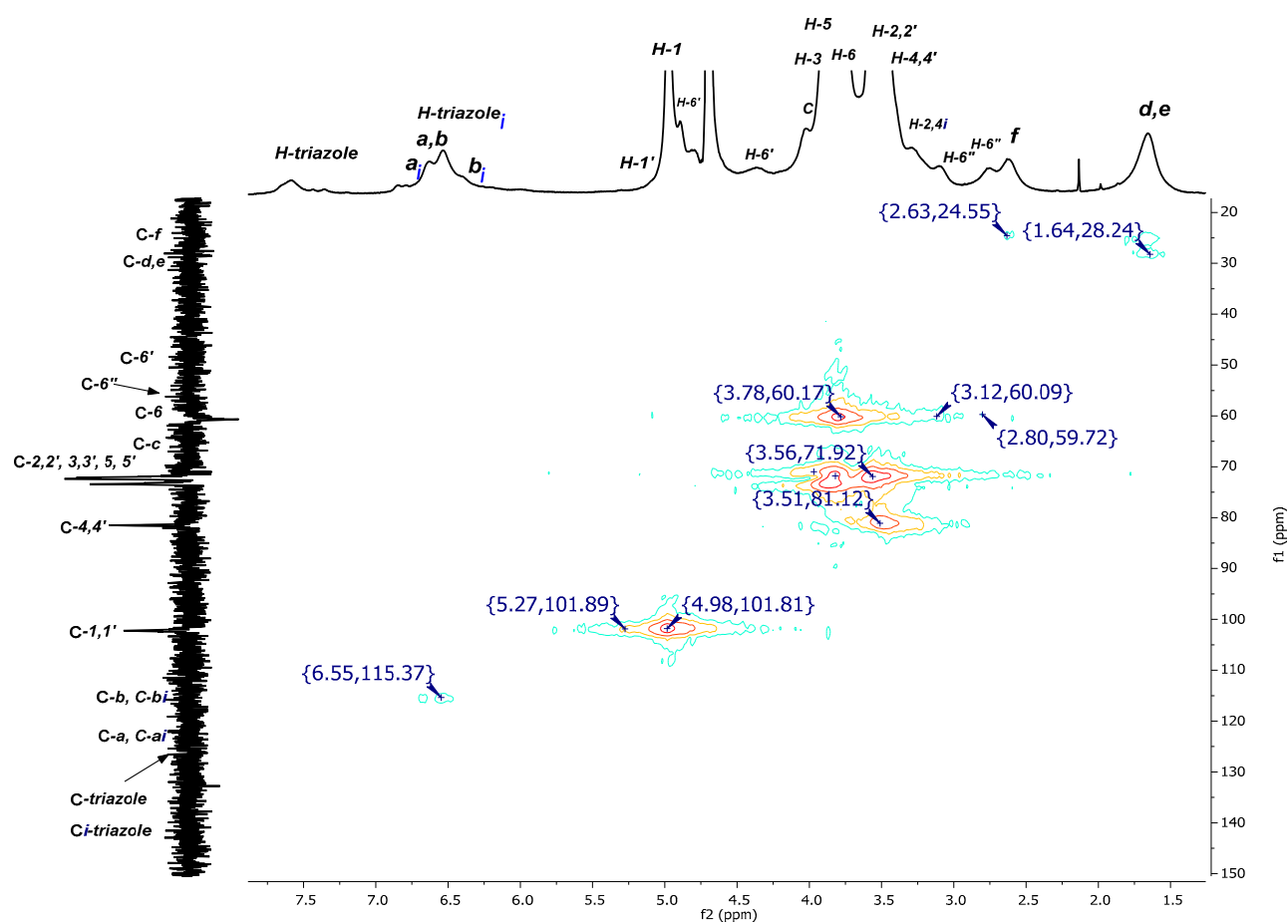


Figure S5. 2D NMR HMQC spectrum of $P_3N_3-[O-C_6H_4-O-(CH_2)_4-\beta CD]_6$ (II) in D_2O .

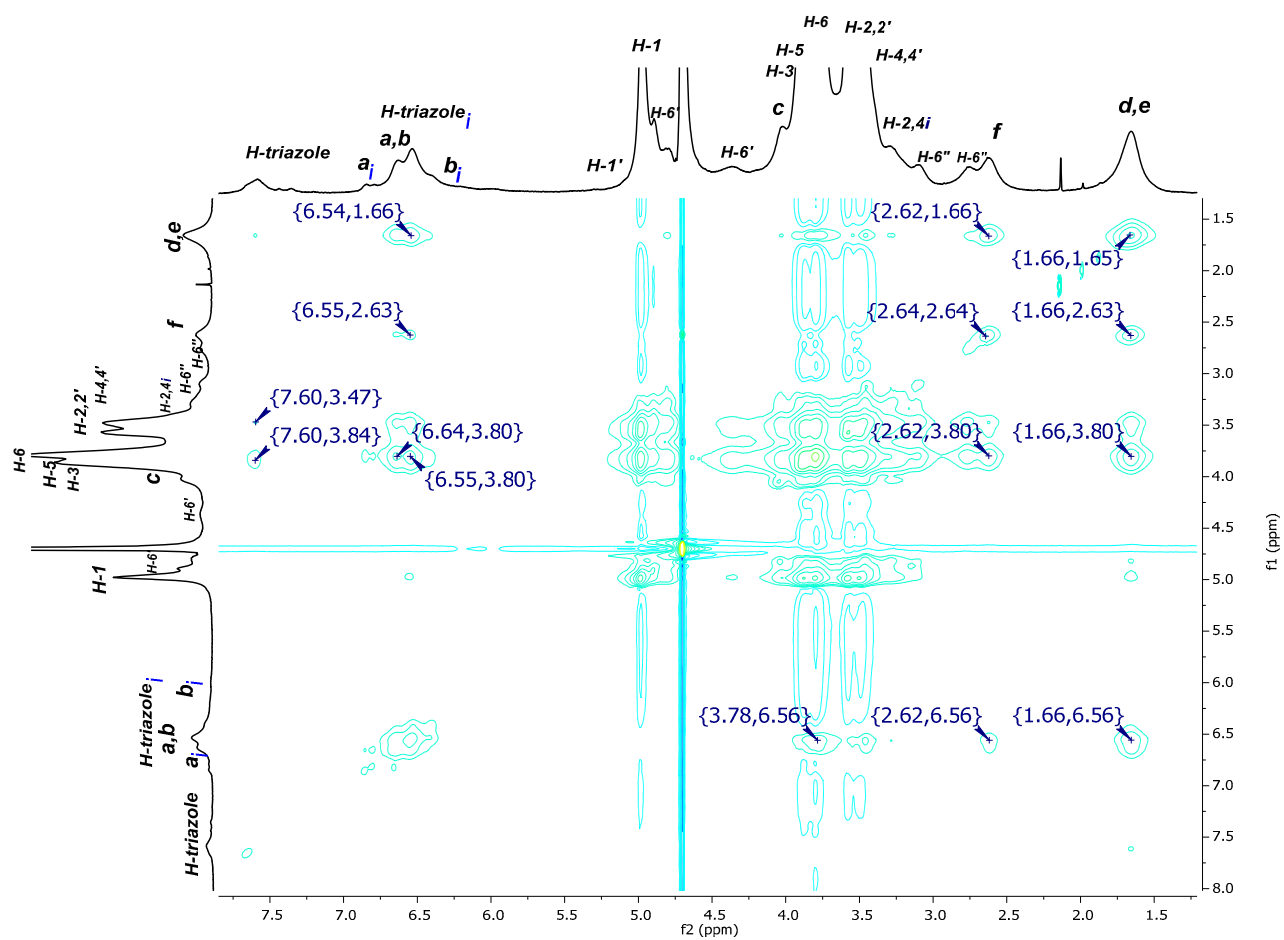


Figure S6. 2D NMR NOESY spectrum of $\text{P}_3\text{N}_3\text{-[O-C}_6\text{H}_4\text{-O-(CH}_2\text{)}_4\text{-}\beta\text{CD]}_6$ (**II**) in D_2O .

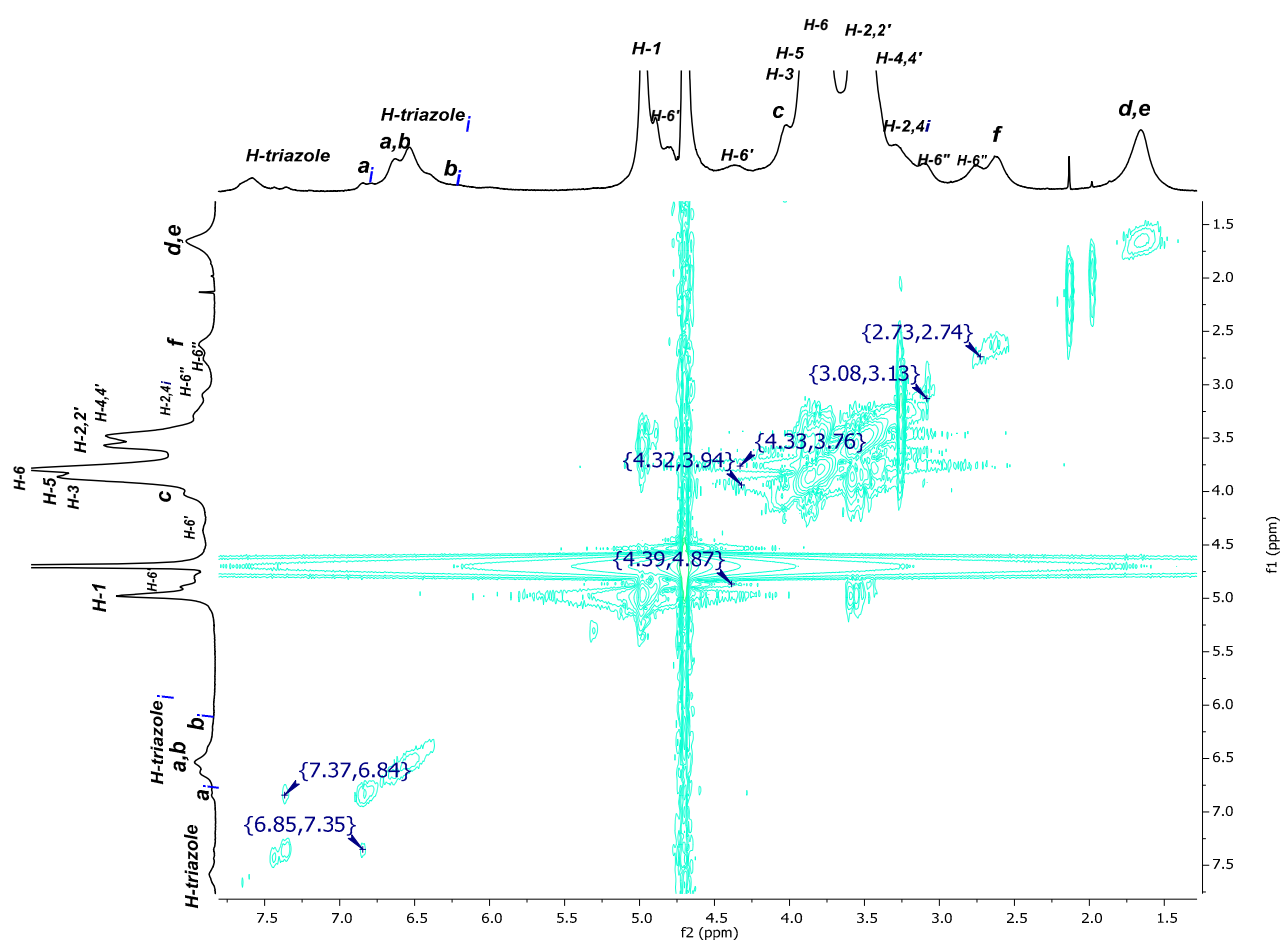


Figure S7. 2D NMR COSY spectrum of P_3N_3 -[O-C₆H₄-O-(CH₂)₄-βCD]₆ (II) in D₂O.

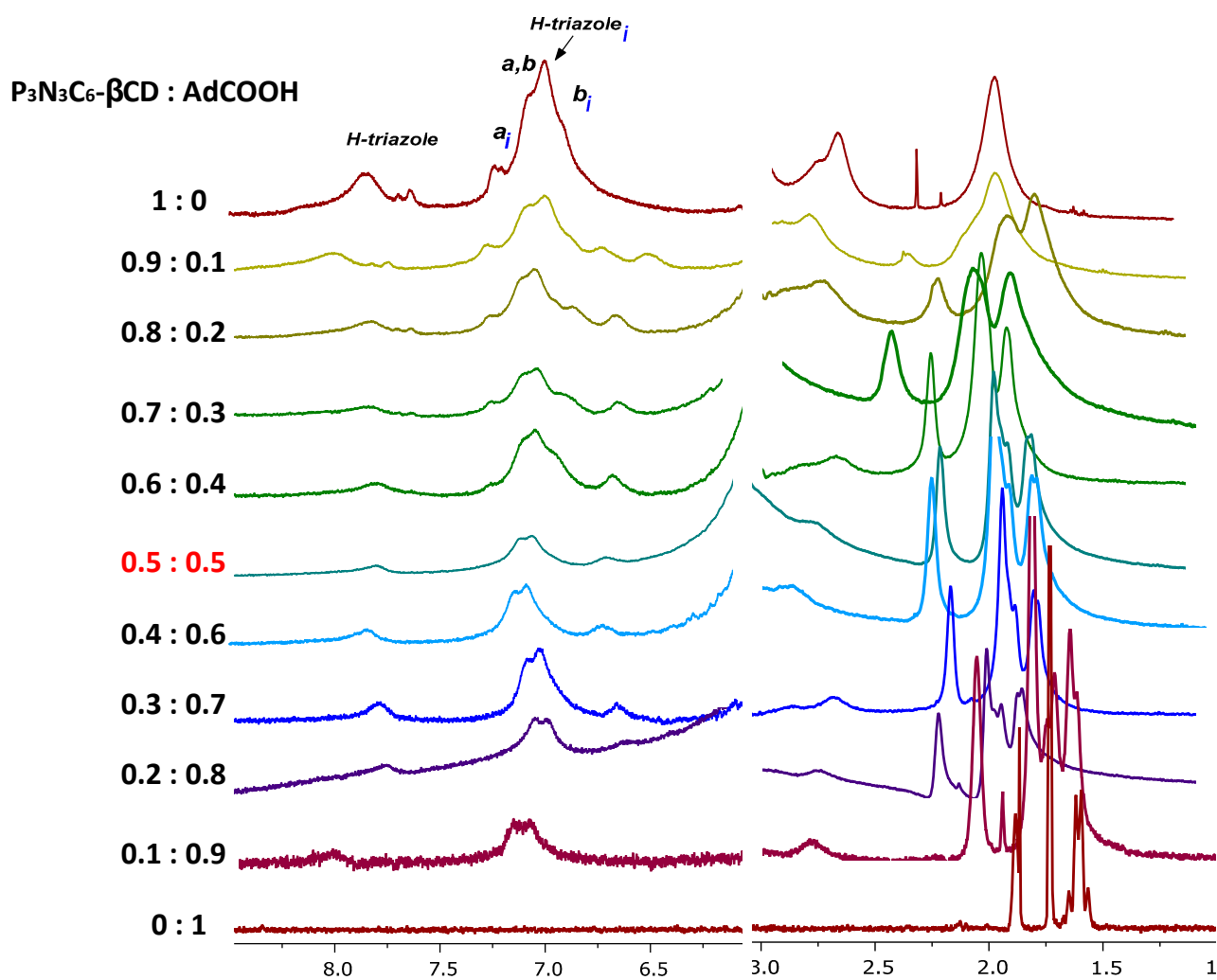


Figure S8. ^1H -NMR titration experiment of dendritic compound (II).

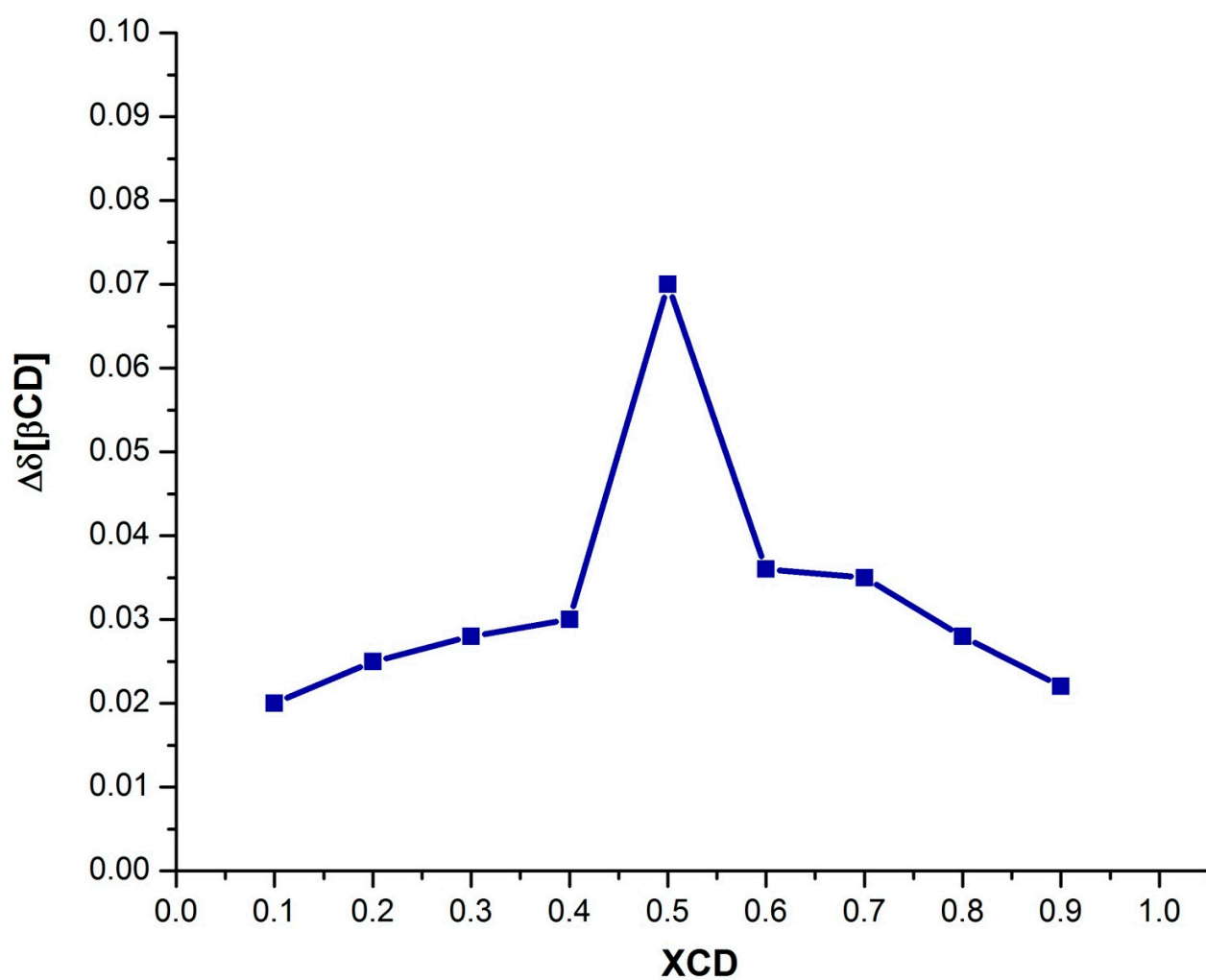


Figure S9. Job plot for the inclusion complex of AdCOOH with β CD cavities in the dendritic compound (**II**), $[\beta\text{CD}] + [\text{AdCOOH}] = 3 \text{ mM}$ at 298 K, in D_2O . (The inflection point was found to be at 0.5, which confirms the stoichiometry 1:1).

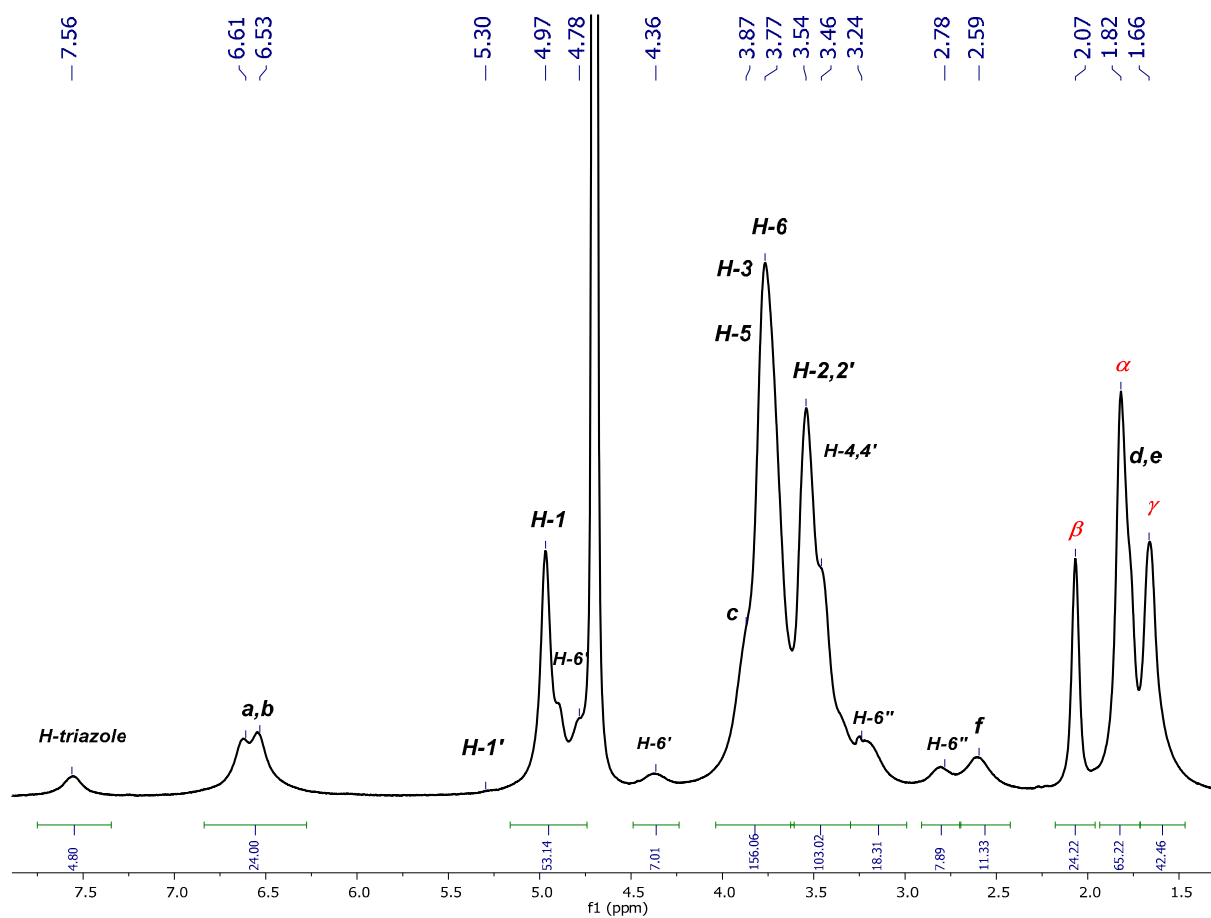


Figure S10. ^1H NMR spectrum of inclusion complex $\text{P}_3\text{N}_3\text{-[O-C}_6\text{H}_4\text{-O-(CH}_2\text{)}_4\text{-}\beta\text{CD]}_6$ (II)/AdCOOH in D_2O .

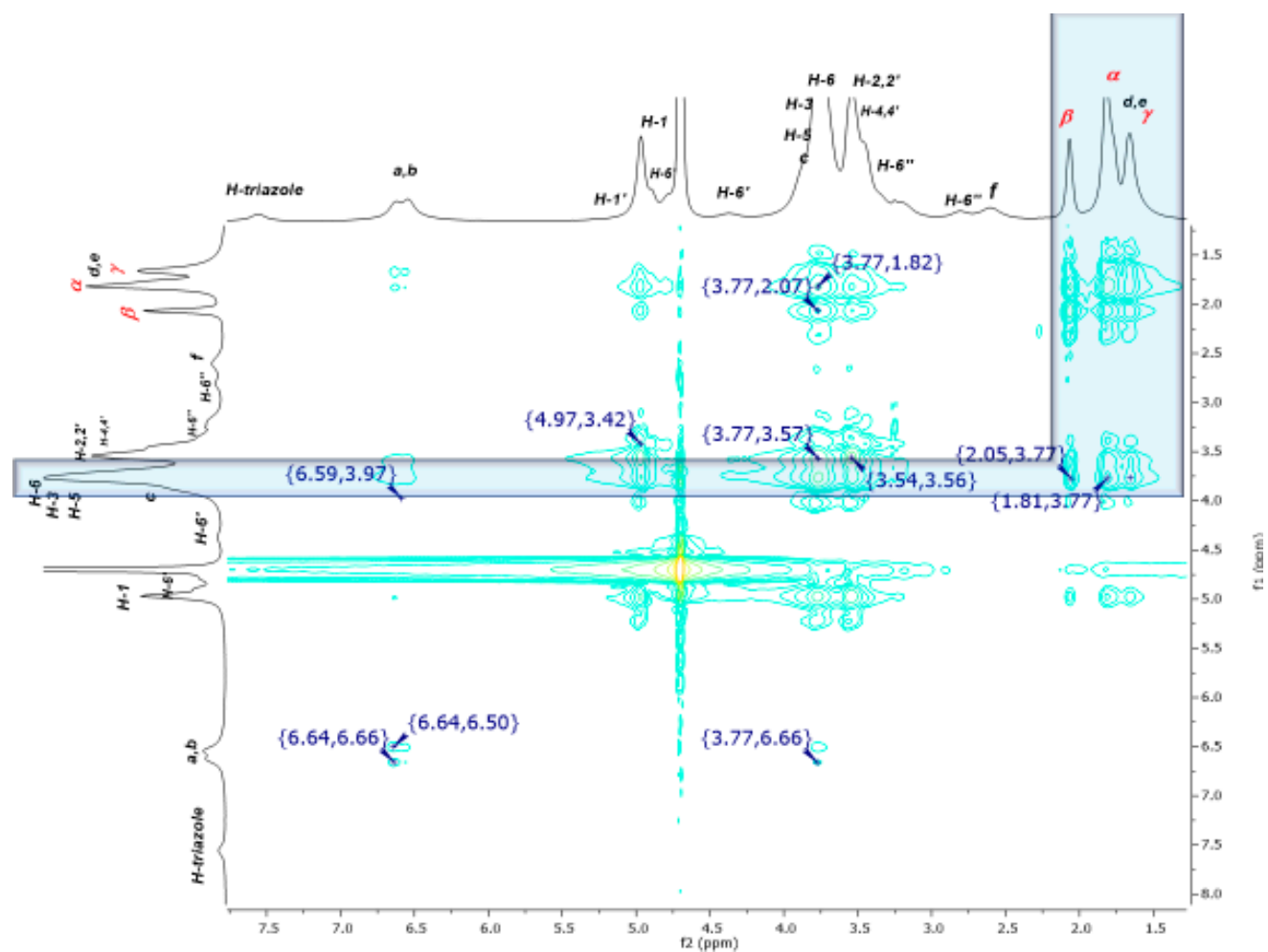


Figure S11. 2D NMR NOESY spectrum of inclusion complex P_3N_3 -[O-C₆H₄-O-(CH₂)₄- β CD]₆ (II)/AdCOOH in D₂O.