Supplementary Information

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Analysis data of

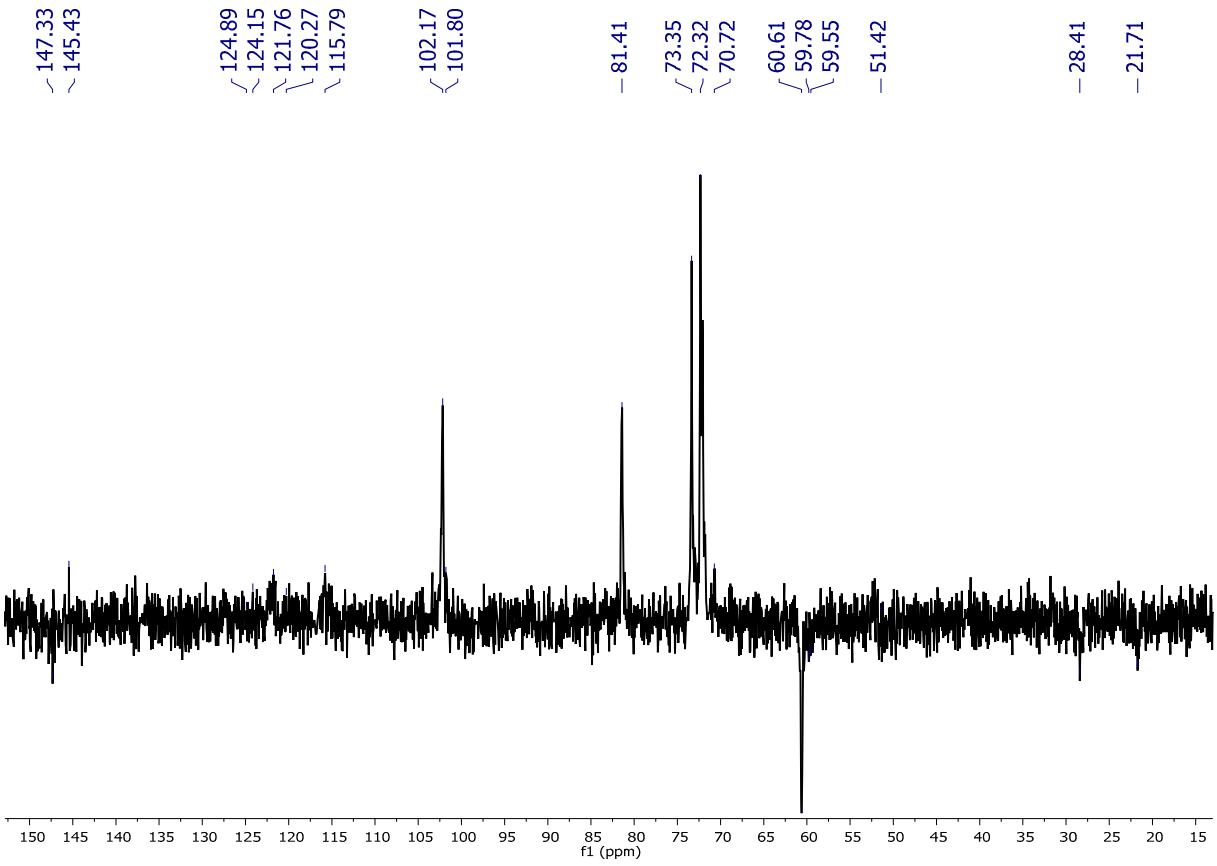

Figure S1. DEPTQ-NMR spectrum of P_3N_3-[O-C_6H_4-O-$(CH_2)_3$-βCD]$_6$ (**I**) in D_2O.

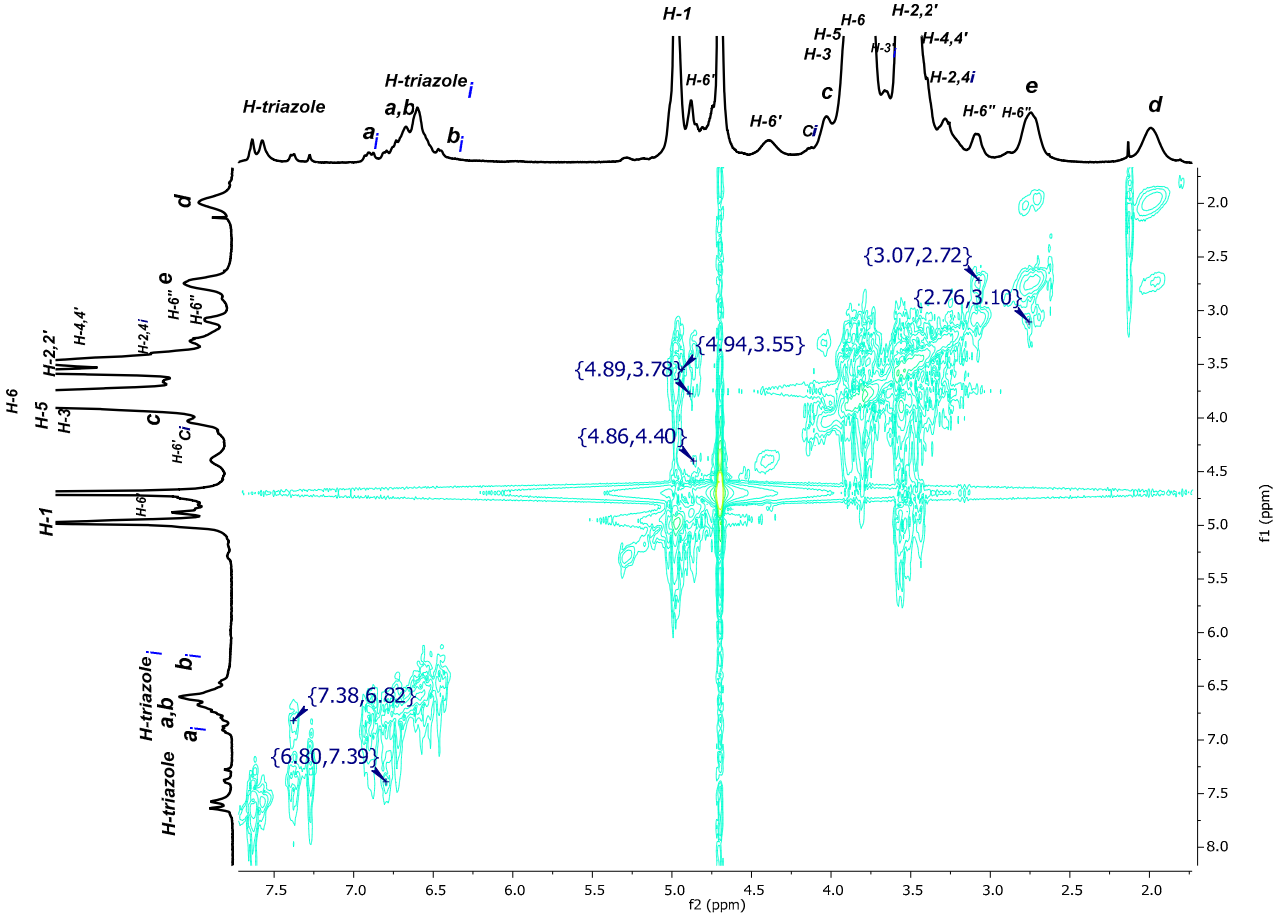

Figure S2. 2D NMR COSY spectrum of P_3N_3-[O-C_6H_4-O-$(CH_2)_3$-βCD]$_6$ (**I**) in D_2O.

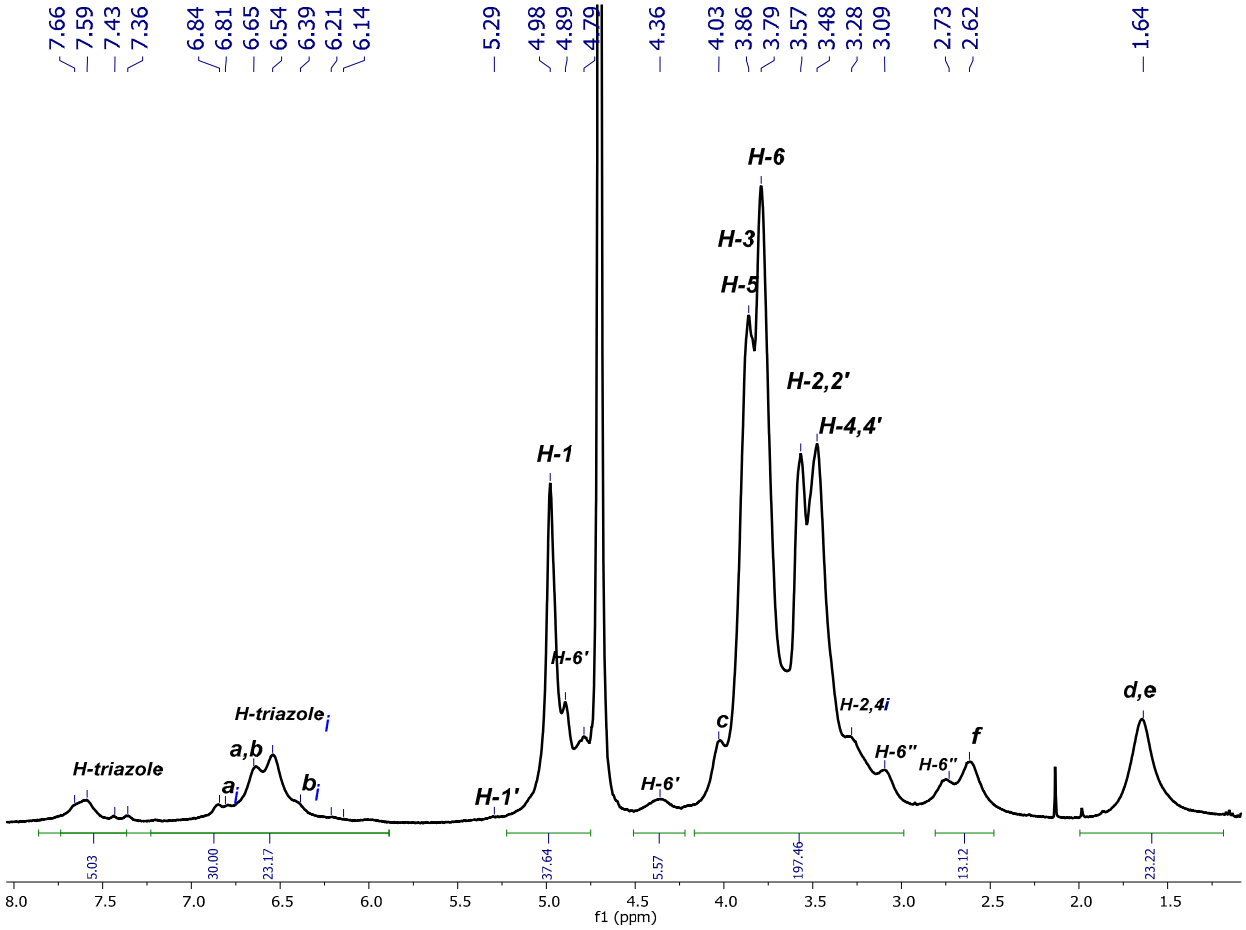

Figure S3. ^{1}H NMR spectrum of P_3N_3-[O-C_6H_4-O-$(CH_2)_4$-βCD]$_6$ (**II**) in D_2O.

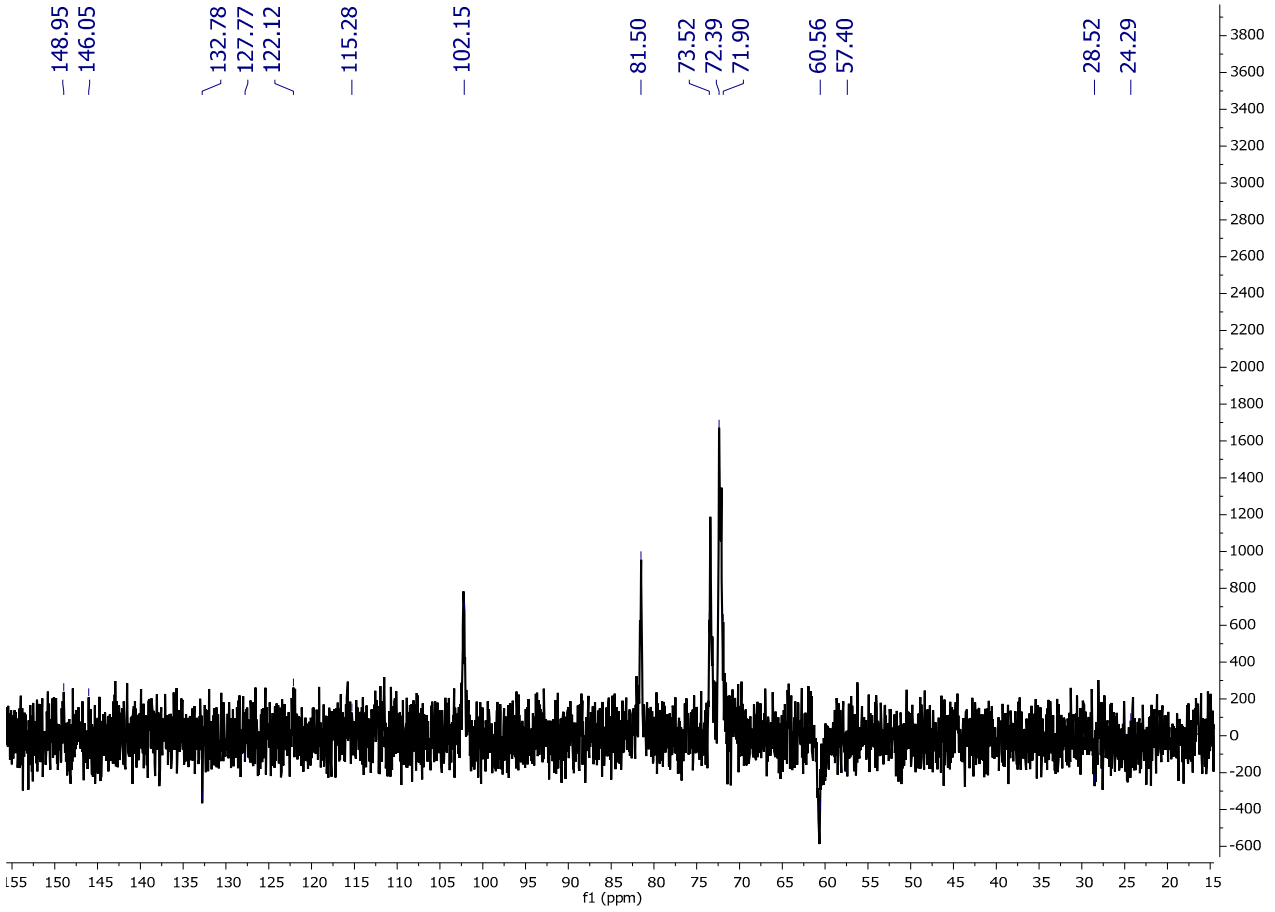

Figure S4. DEPTQ-NMR spectrum of P_3N_3-[O-C_6H_4-O-$(CH_2)_4$-βCD]$_6$ (**II**) in D_2O.

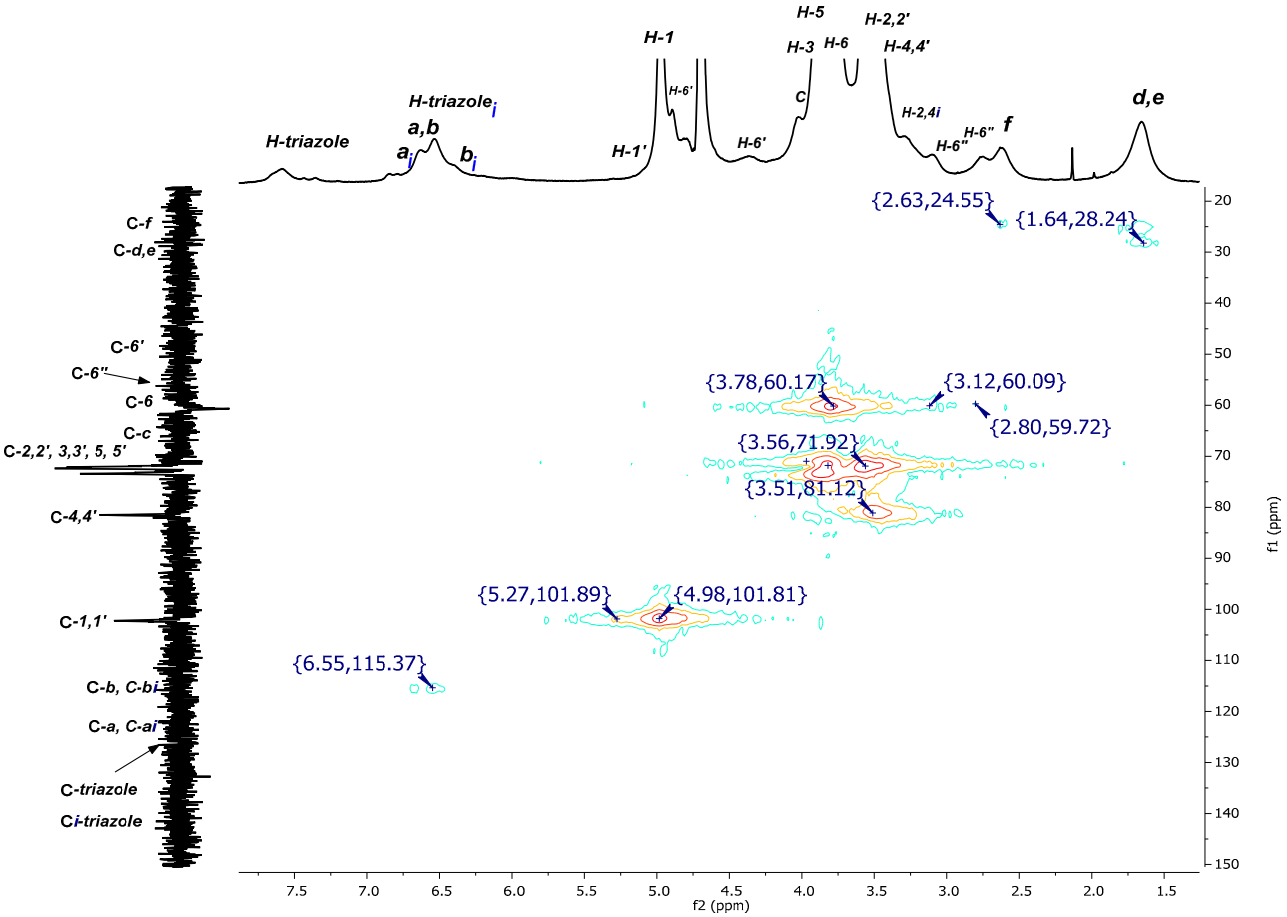

Figure S5. 2D NMR HMQC spectrum of P_3N_3-[O-C_6H_4-O-$(CH_2)_4$-βCD]$_6$ (**II**) in D_2O.

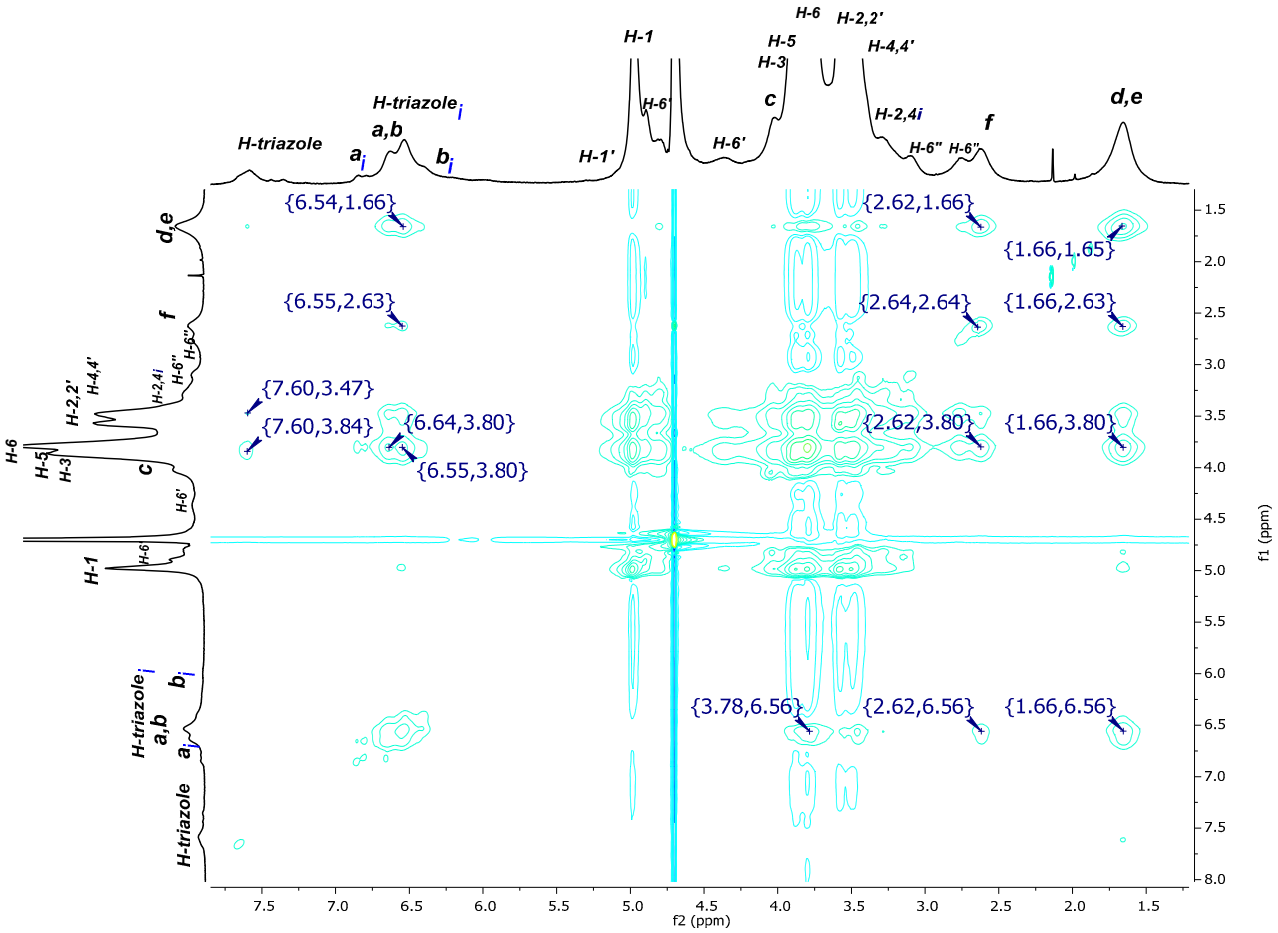

Figure S6. 2D NMR NOESY spectrum of P_3N_3-[O-C_6H_4-O-$(CH_2)_4$-βCD]$_6$ (**II**) in D_2O.

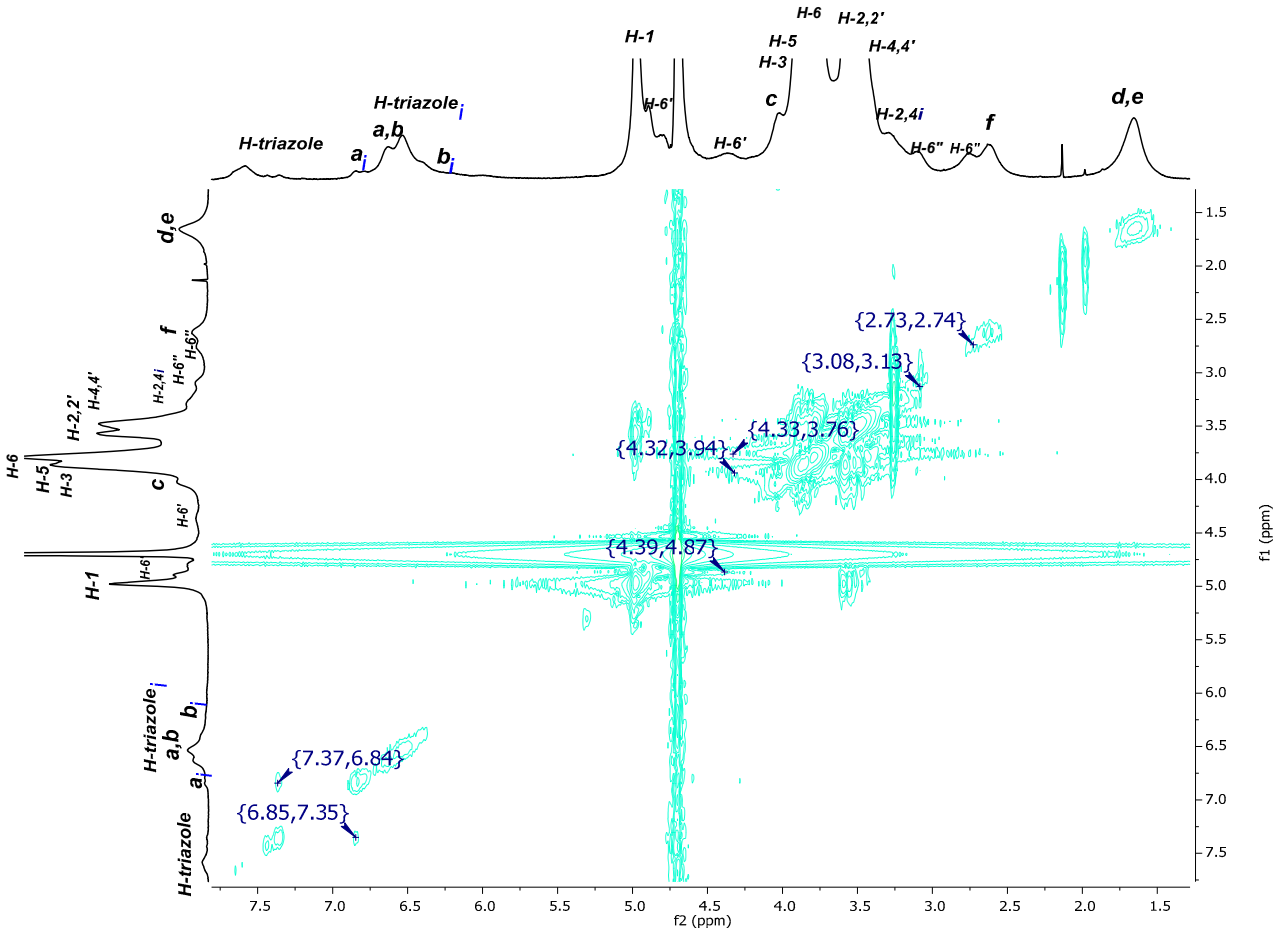

Figure S7. 2D NMR COSY spectrum of P_3N_3-[O-C_6H_4-O-$(CH_2)_4$-βCD]$_6$ (**II**) in D_2O.

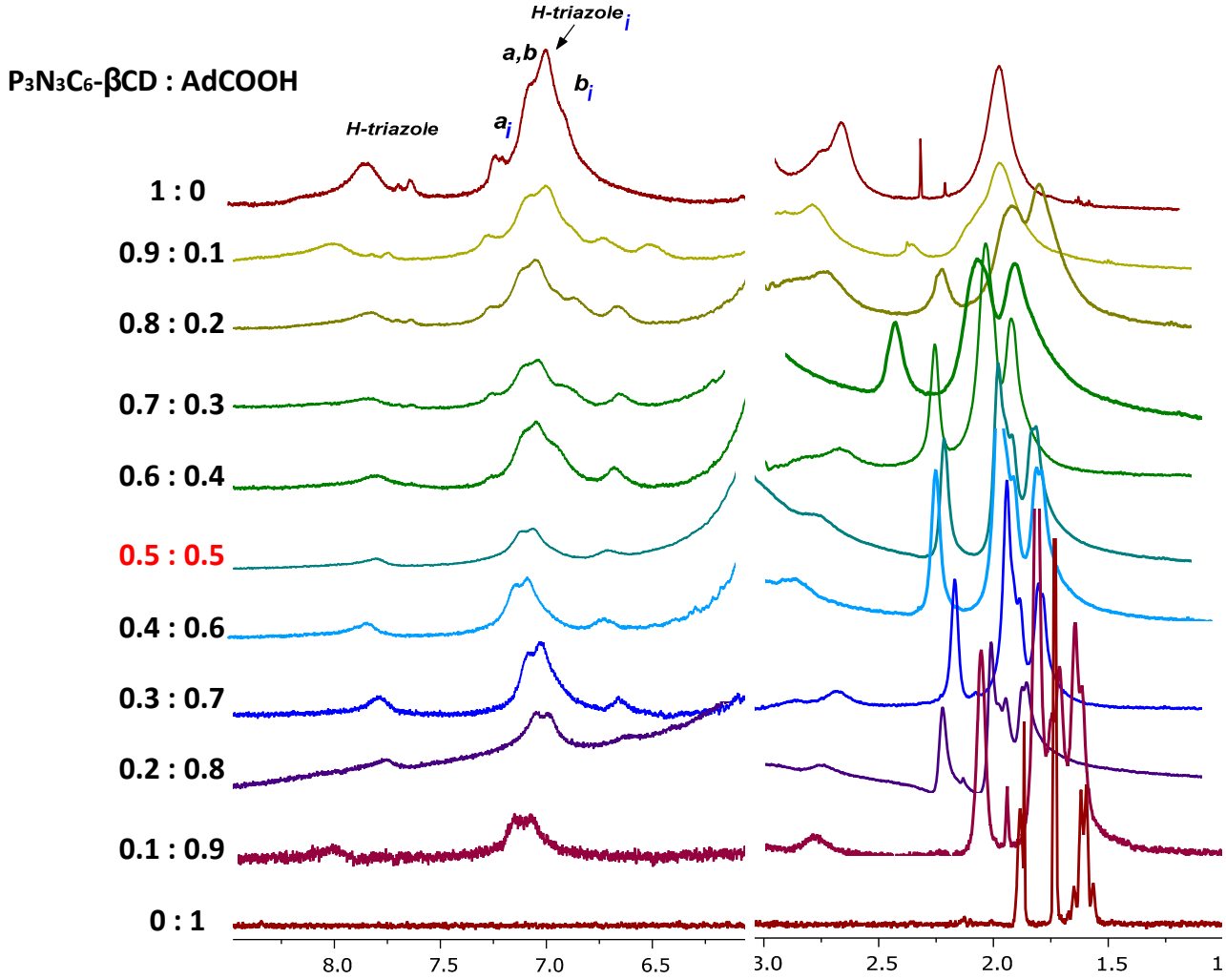

Figure S8. ^{1}H-NMR titration experiment of dendritic compound (**II**).

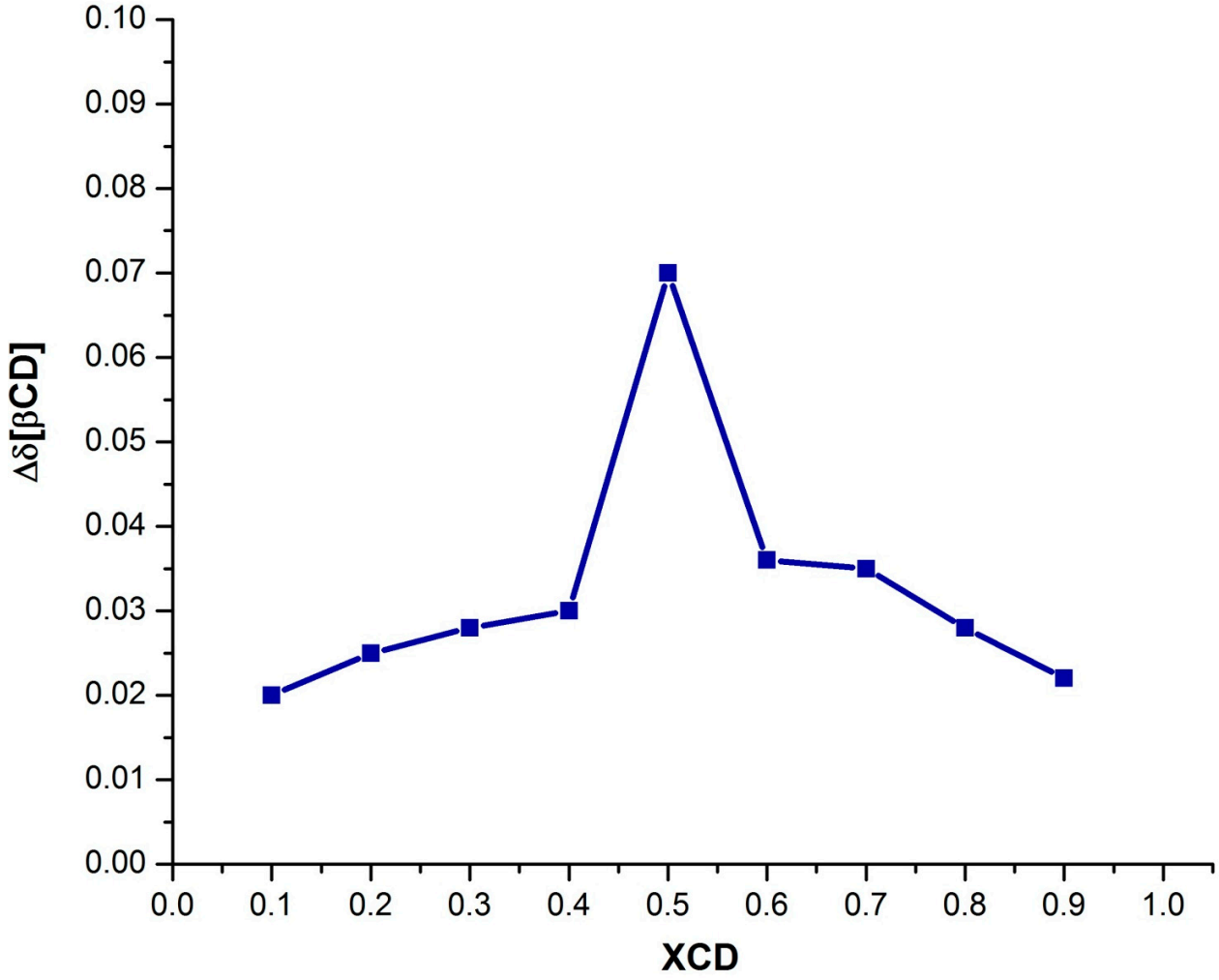

Figure S9. Job plot for the inclusion complex of AdCOOH with βCD cavities in the dendritic compound (**II**), [βCD]+[AdCOOH] = 3 mM at 298 K, in D_2O. (The inflection point was found to be at 0.5, which confirms the stoichiometry 1:1).

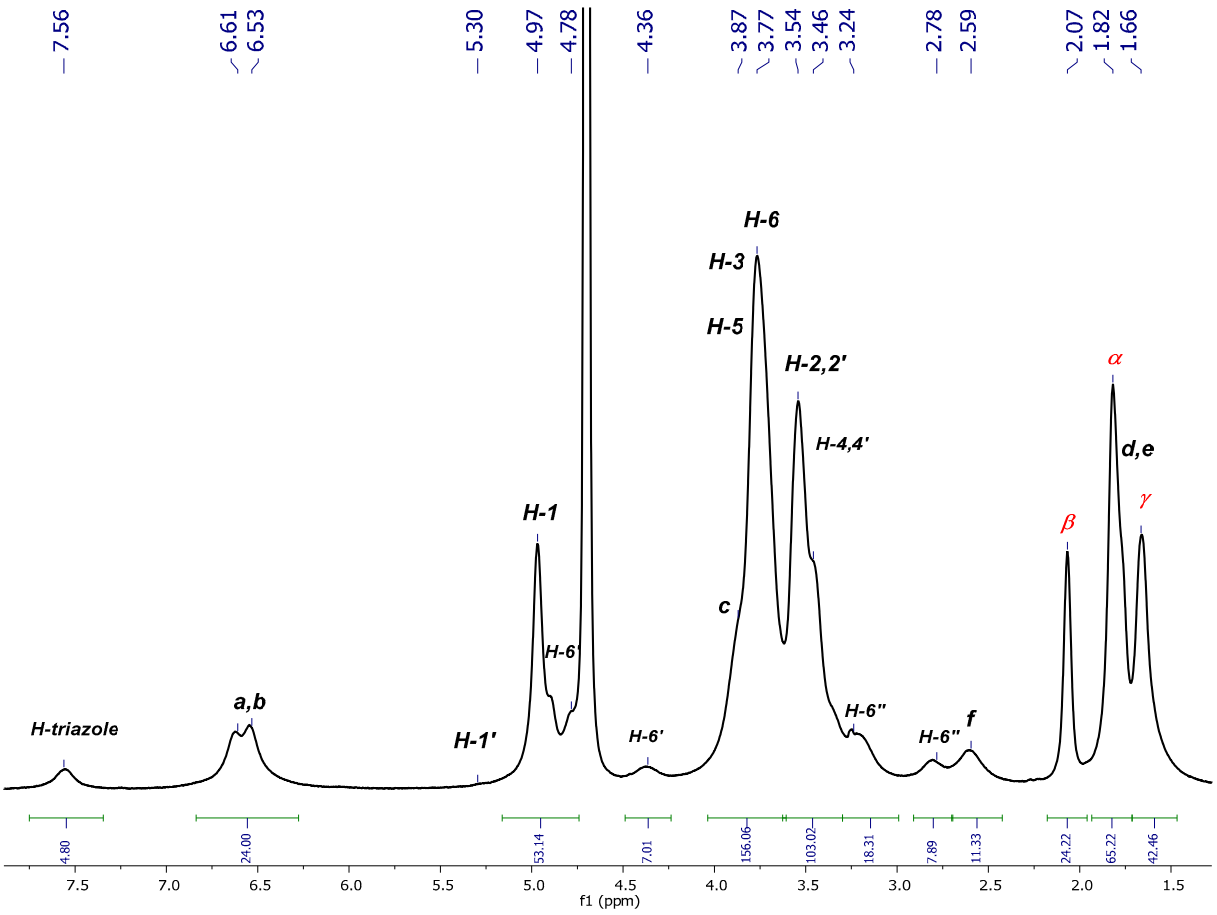

Figure S10. ^{1}H NMR spectrum of inclusion complex P_3N_3-[O-C_6H_4-O-$(CH_2)_4$-βCD]$_6$ (**II**)/AdCOOH in D_2O.

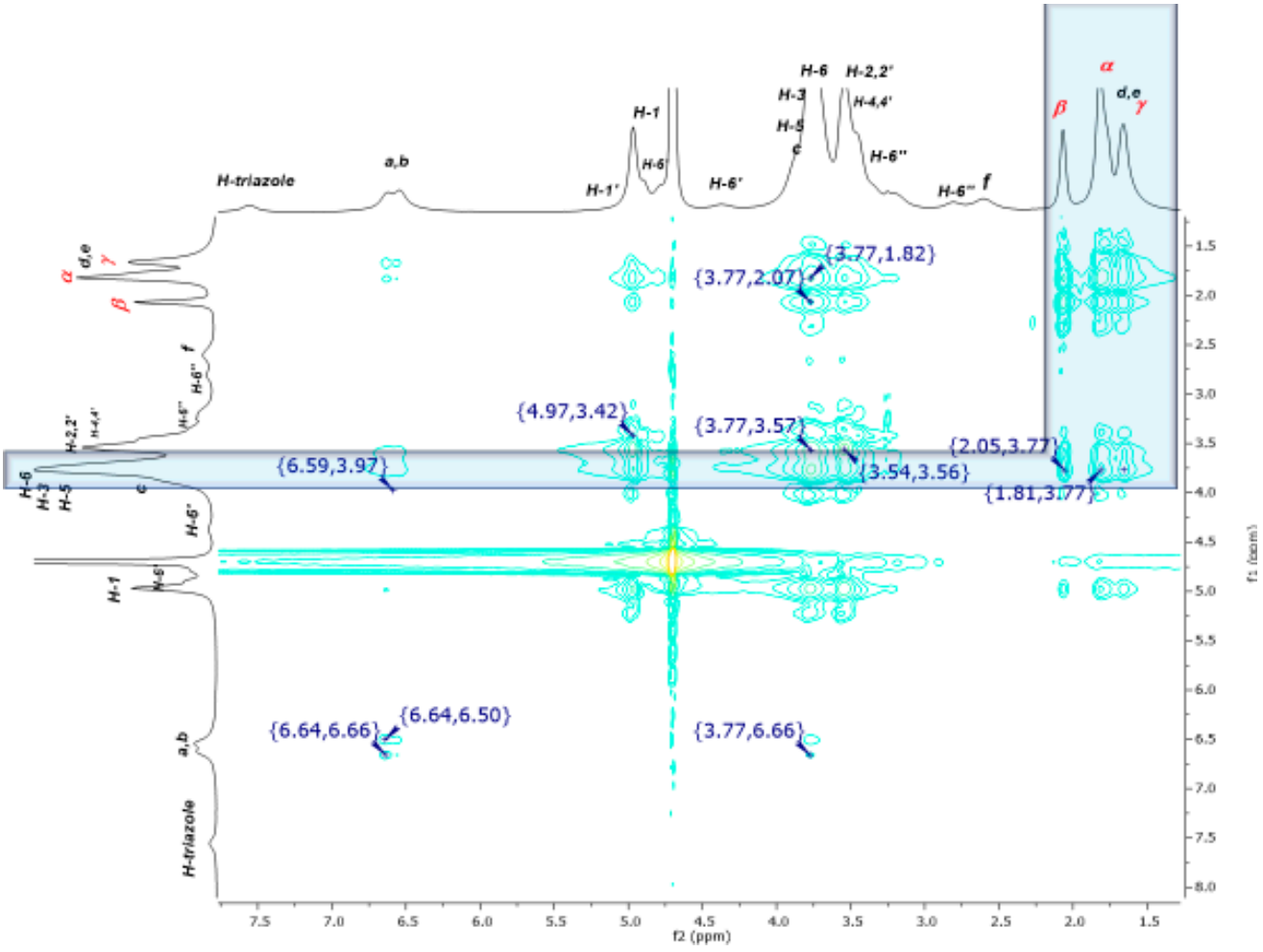

Figure S11. 2D NMR NOESY spectrum of inclusion complex P_3N_3-[O-C_6H_4-O-$(CH_2)_4$-βCD]$_6$ (**II**)/AdCOOH in D_2O.