Role of free space and conformational control on photoproduct selectivity of optically pure α-alkyldeoxybenzoins within a water-soluble organic capsule

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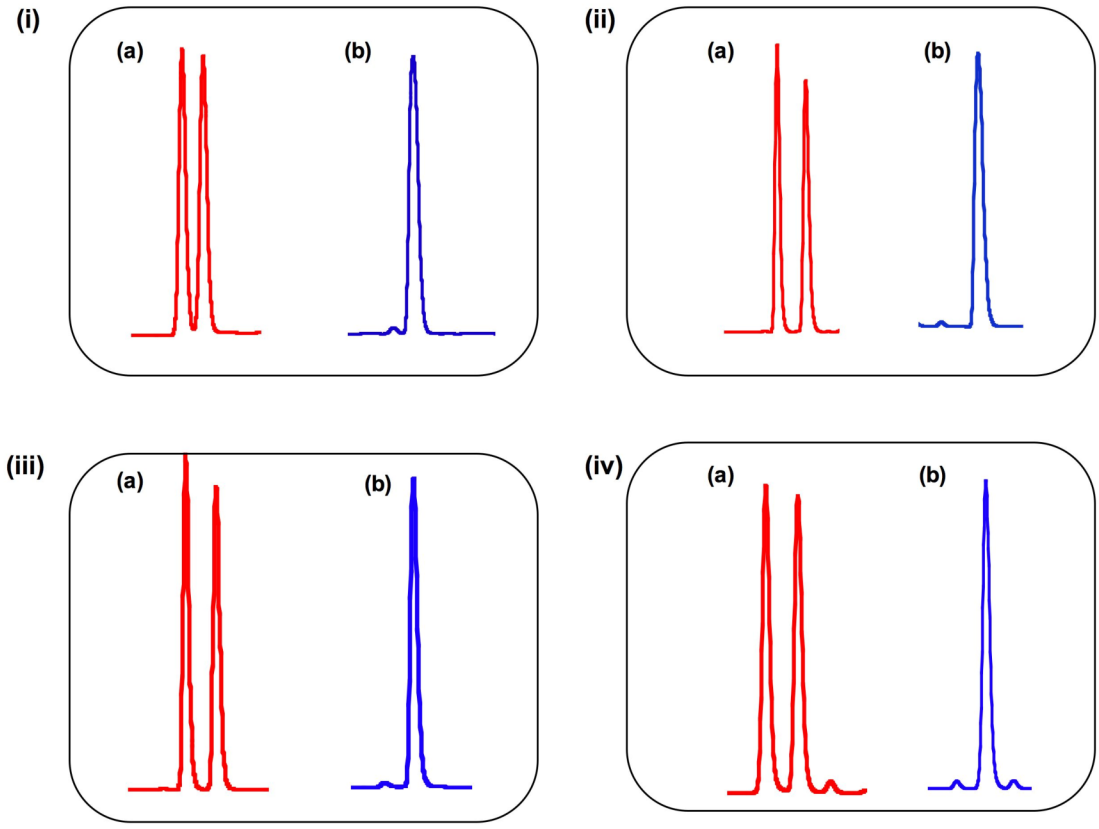

Figure S1: HPLC traces of racemic (red) and chiral (blue) of α-alkyl deoxybenzoin. (i) α-methyl deoxybenzoin (**1a**), (ii) α-propyl deoxybenzoin (**1b**), (iii) α-hexyl deoxybenzoin (**1c**) and (i) α-octyl deoxybenzoin (**1d**).

^{1}H NMR titration spectra of host-guest complexes:

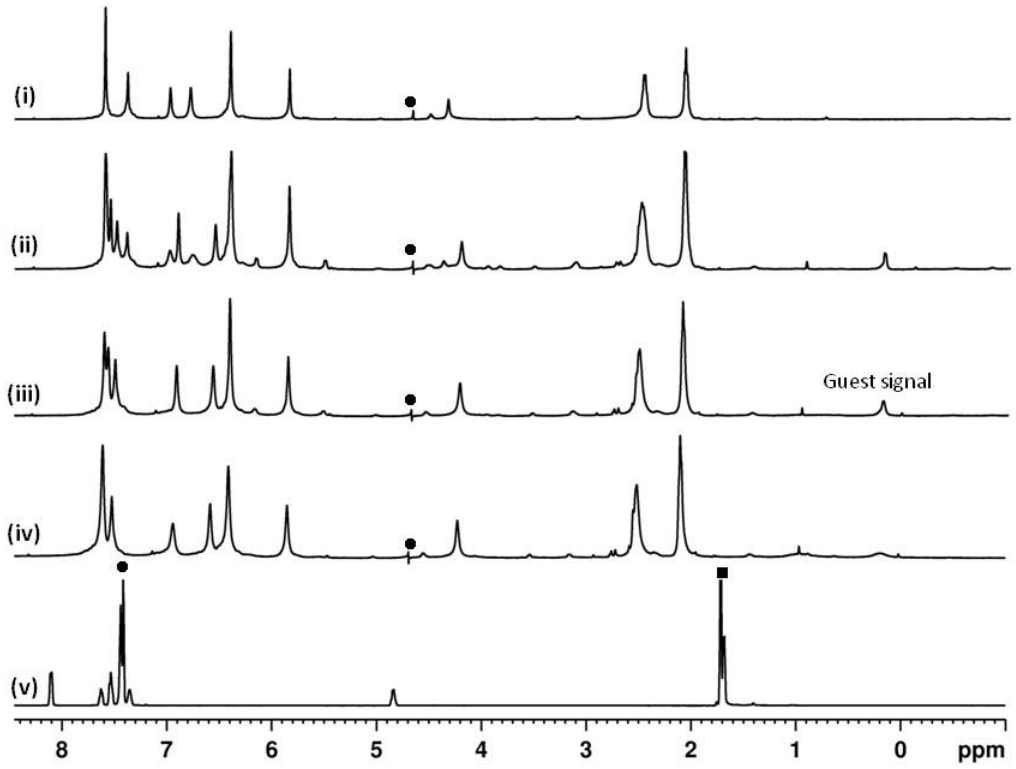

Figure S2: ^{1}H NMR titration spectra (500 MHz) of **1a**@**OA**$_2$ capsular assembly. (i) **OA** (1 mM in 10 mM borate buffer, (ii) **OA**: **1a** (1:0.25), (iii) **OA**: **1a** (1:0.5), (iv) **OA**: **1a** (1:0.75) and (v) **1a** (1mM in $CDCl_3$). Solvent peak is marked as • and residual water peak is marked as■.

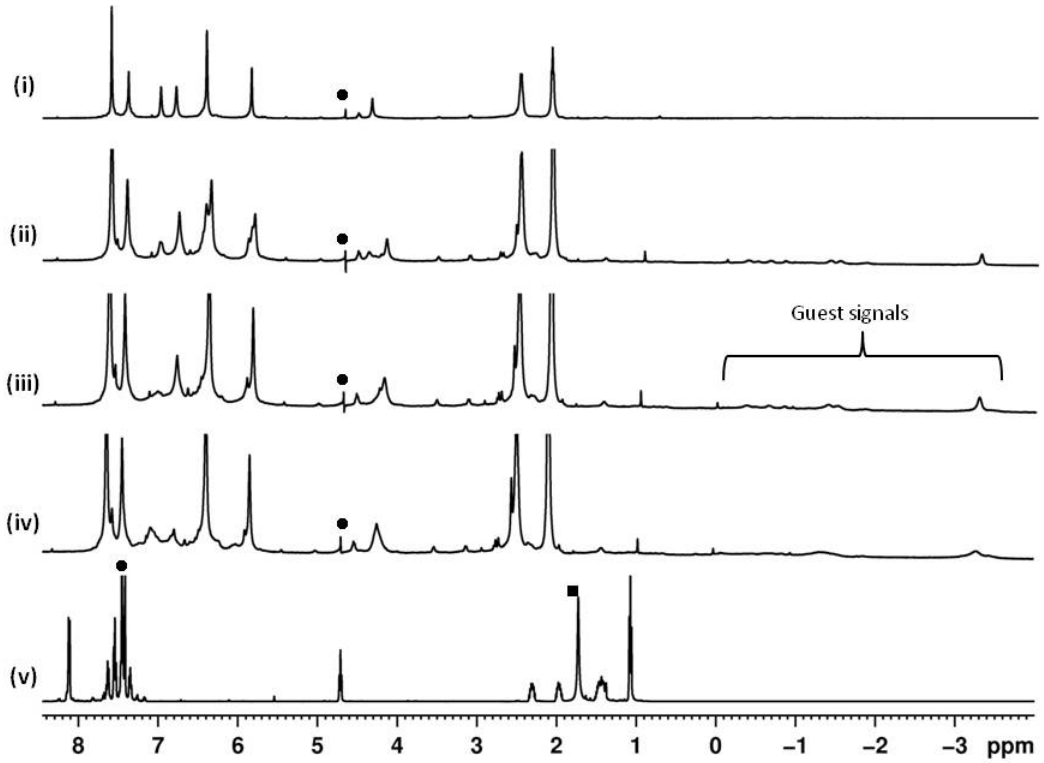

Figure S3: ^{1}H NMR titration spectra (500 MHz) of **1b**@OA_2 capsular assembly. (i) **OA** (1 mM in 10 mM borate buffer, (ii) **OA**: **1b** (1:0.25), (iii) **OA**: **1b** (1:0.5), (iv) **OA**: **1b** (1:0.75) and (v) **1b** (1mM in $CDCl_3$). Solvent peak is marked as • and residual water peak is marked as■.

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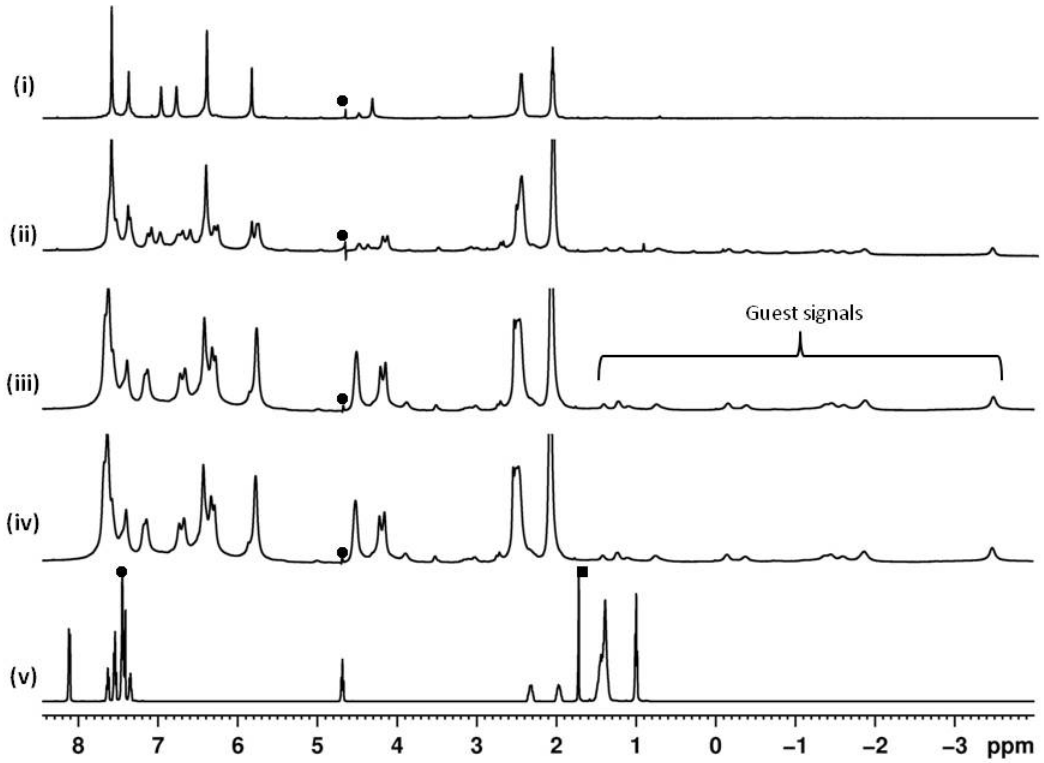

Figure S4: ^{1}H NMR titration spectra (500 MHz) of **1c**@$\mathbf{OA}_2$ capsular assembly. (i) **OA** (1 mM in 10 mM borate buffer, (ii) **OA**: **1c** (1:0.25), (iii) **OA**: **1c** (1:0.5), (iv) **OA**: **1c** (1:0.75) and (v) **1c** (1mM in $CDCl_3$). Solvent peak is marked as • and residual water peak is marked as■.

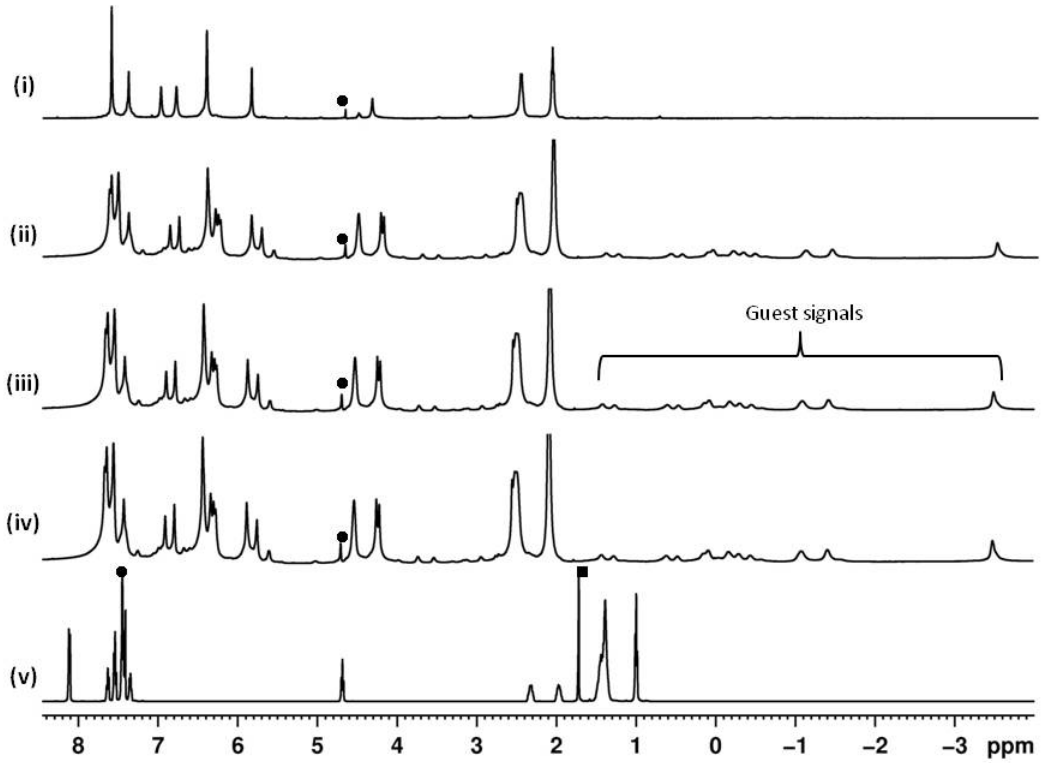

Figure S5: ^{1}H NMR titration spectra (500 MHz) of **1d**@**OA**$_2$ capsular assembly. (i) **OA** (1 mM in 10 mM borate buffer, (ii) **OA**: **1d** (1:0.25), (iii) **OA**: **1d** (1:0.5), (iv) **OA**: **1d** (1:0.75) and (v) **1d** (1mM in $CDCl_3$). Solvent peak is marked as • and residual water peak is marked as■.

Table S1. Diffusion coefficients of complexes of octa acid and guests **1a- d** calculated by DOSY NMR analysis.

Complex	Diffusion Constant ($10^{-10}m^2s^{-1}$)
OA	1.88
1a@OA_2	1.23
1b@OA_2	1.25
1c@OA_2	1.19
1d@OA_2	1.17

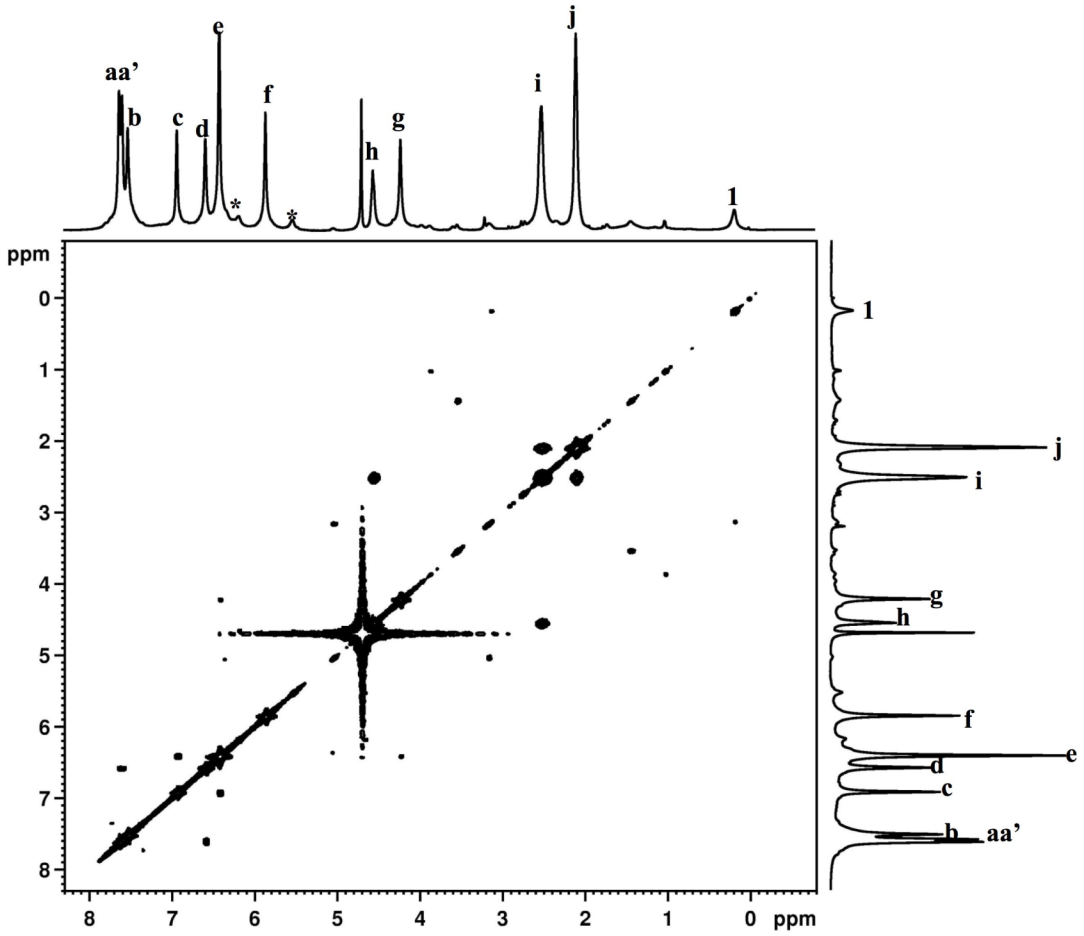

Figure S6. 2D COSY spectrum of **1a@OA$_2$** (5mM of **OA**, 50mM sodium tetraborate in D_2O). Aliphatic signals of the guest are labeled with numbers and host signals are labeled from **a-j** as shown above. Aromatic signals of the guest marked with *.

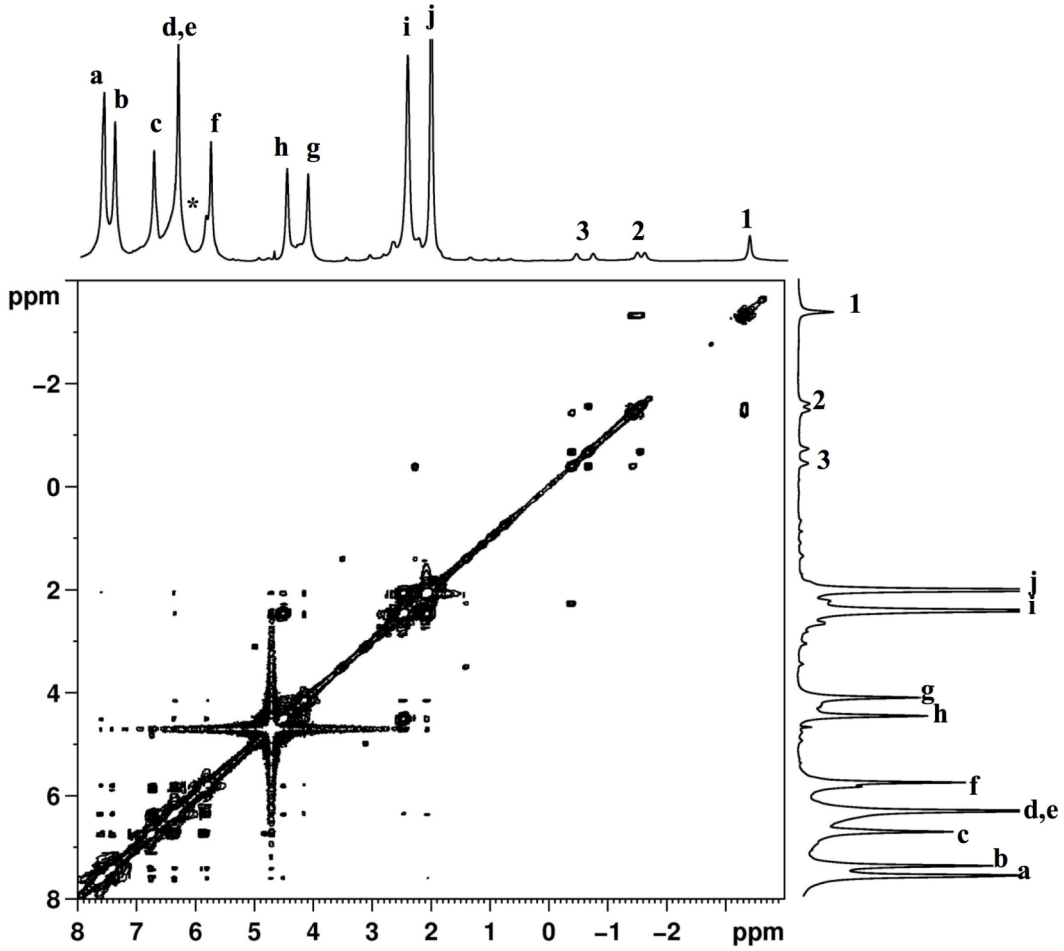

Figure S7. 2D COSY spectrum of **1b@OA$_2$** (5mM of **OA**, 50mM sodium tetraborate in D_2O). Aliphatic signals of the guest are labeled with numbers and host signals are labeled from **a-j** as shown above. Aromatic signals of the guest marked with *.

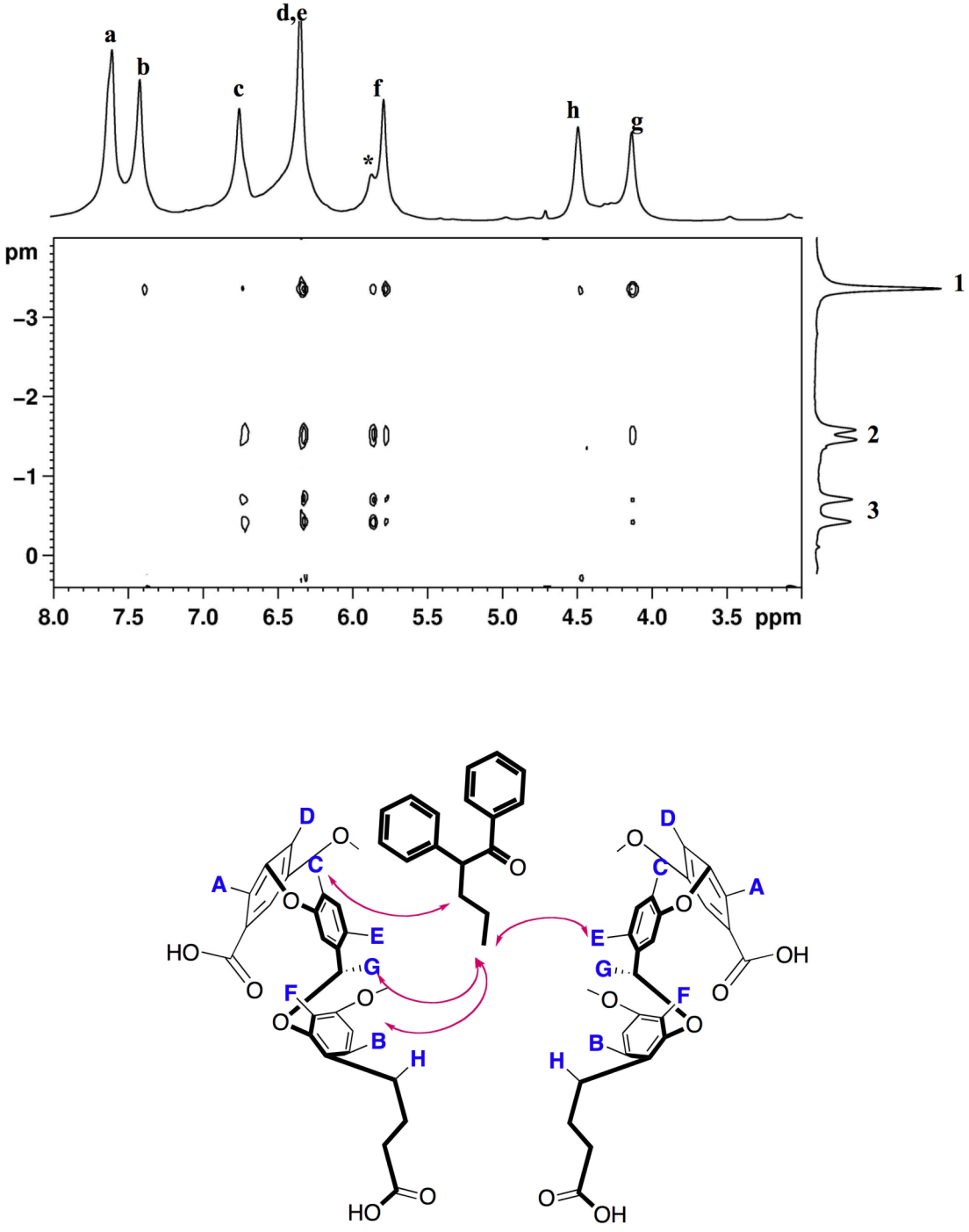

Figure S8. (Top) Partial 2D NOESY spectrum of **1b@OA$_2$** (5mM of **OA**, 50mM sodium tetraborate in D_2O). Aliphatic signals of the guest are labeled with numbers and host signals are labeled from **a-h** as shown above. Aromatic signals of the guest marked with *. (Bottom) NOESY interactions of the host- guest complex.

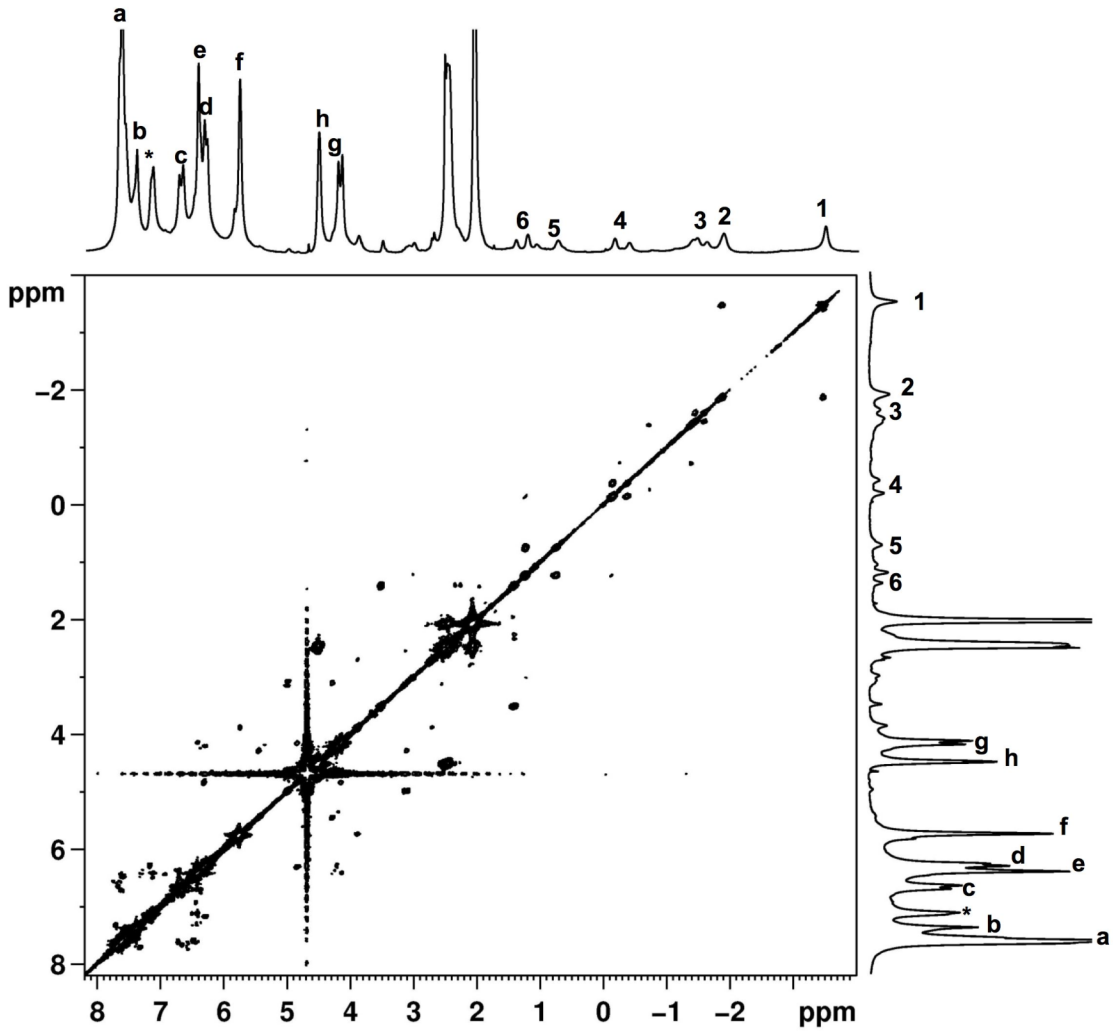

Figure S9. 2D COSY spectrum of **1c@OA$_2$** (5mM of **OA**, 50mM sodium tetraborate in D_2O). Aliphatic signals of the guest are labeled with numbers and host signals are labeled from **a-j** as shown above. Aromatic signals of the guest marked with *.

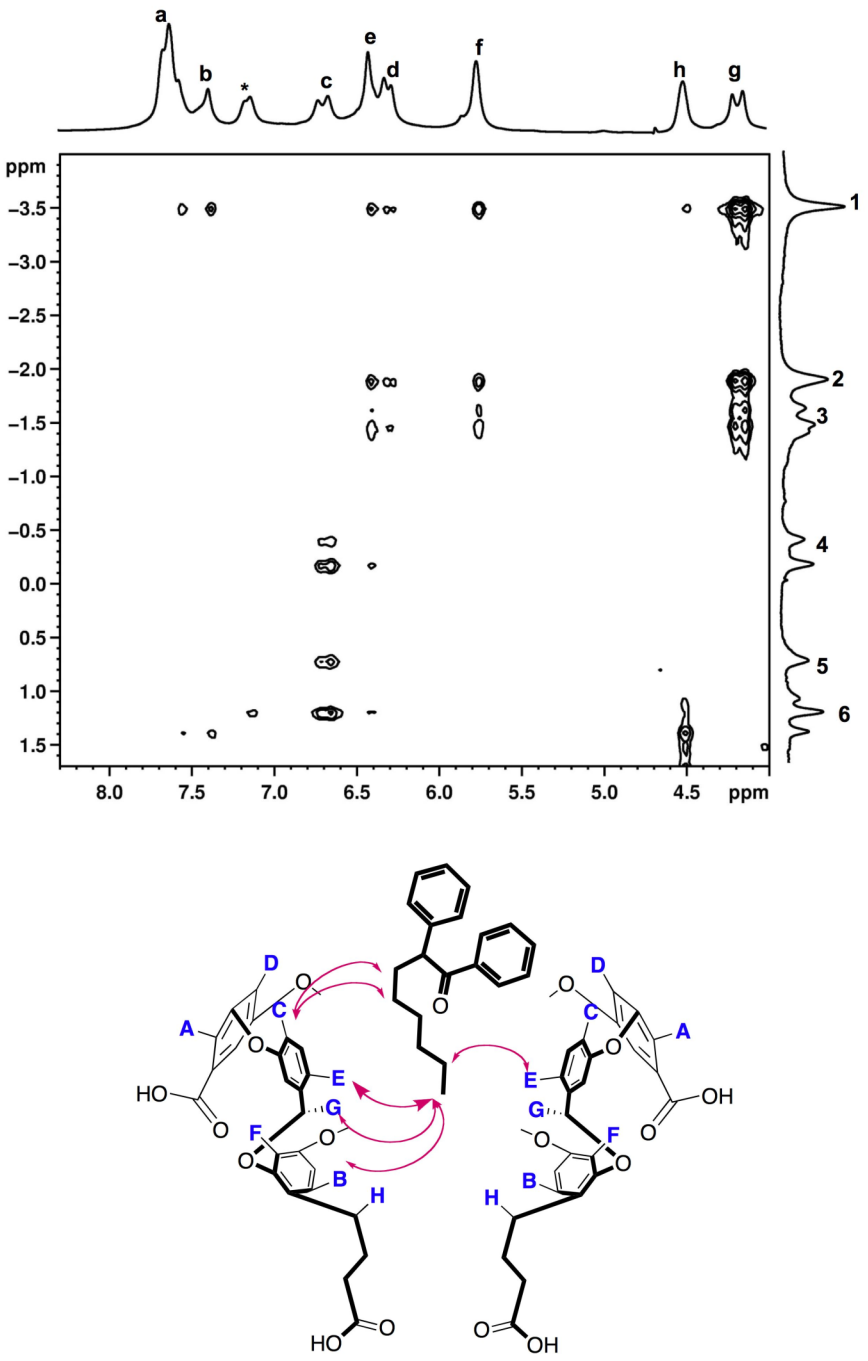

Figure S10. (Top) Partial 2D NOESY spectrum of **1c@OA$_2$** (5mM of **OA**, 50mM sodium tetraborate in D_2O). Aliphatic signals of the guest are labeled with numbers and host signals are labeled from **a-h** as shown above. Aromatic signals of the guest marked with *. (Bottom) NOESY interactions of the host- guest complex.

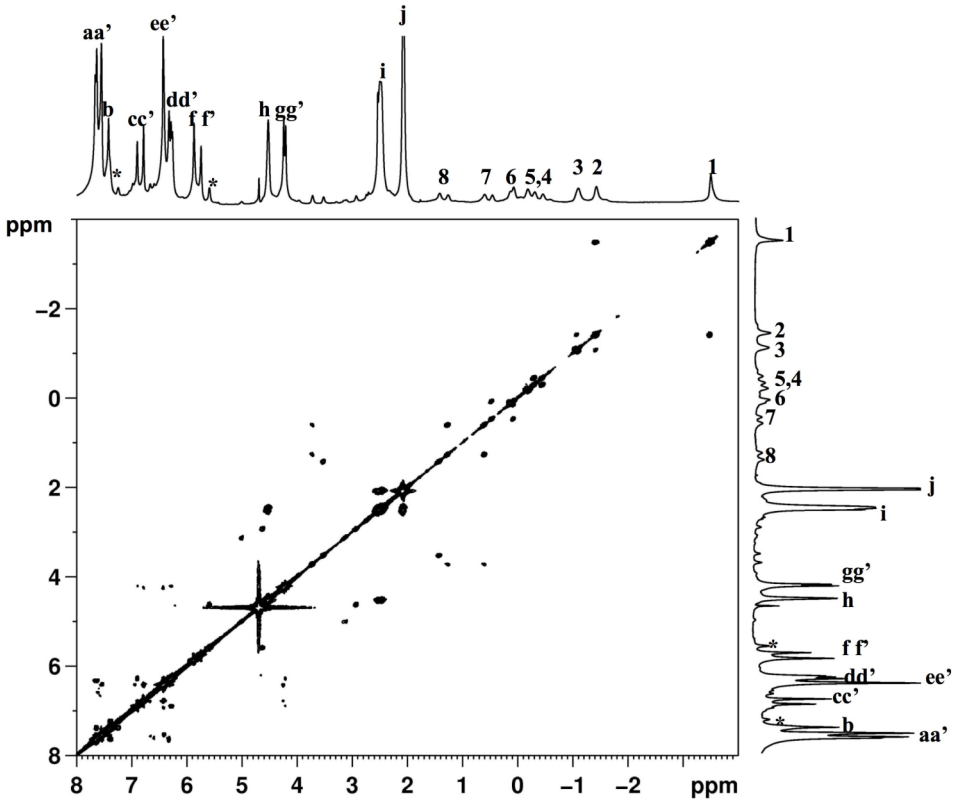

Figure S11. 2D COSY spectrum of $\mathbf{1d@OA_2}$ (5mM of **OA**, 50mM sodium tetraborate in D_2O). Aliphatic signals of the guest are labeled with numbers and host signals are labeled from **a-j** as shown above. Aromatic signals of the guest marked with *.