Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

Effect of different substituents on the water-solubility and stability properties of 1:2 [60]fullerene derivative•gamma-cyclodextrin complexes

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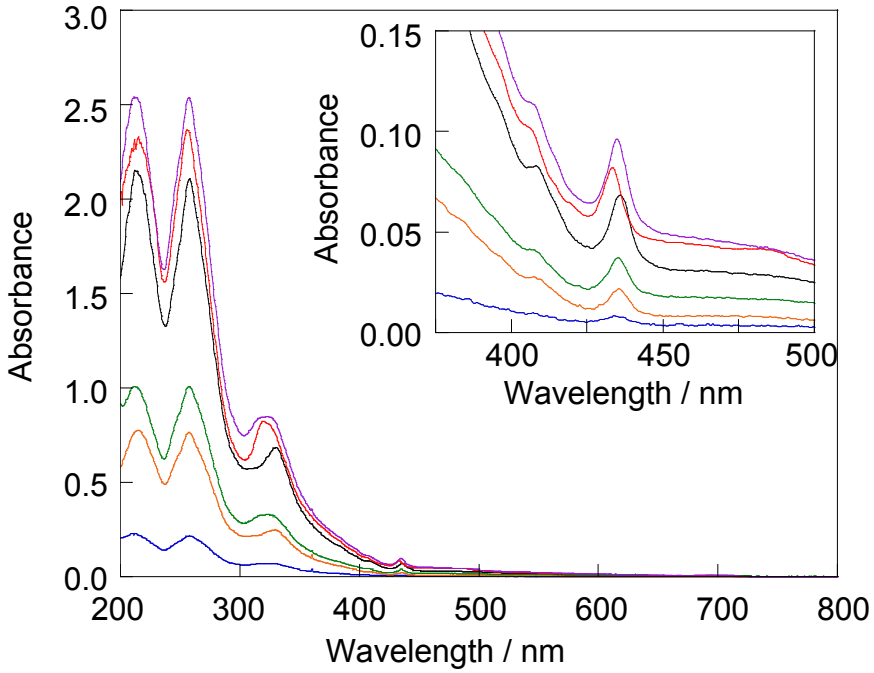

Fig. S1 UV-vis absorption spectra of the γ-CDx-complexes of **1** (black line), **2** (red line), **3** (blue line), **4** (green line), **5** (purple line) and **8** (orange line). The inset shows the region of 375-500 nm. All of the spectra were measured at 25 °C (1 mm cell). All of the solutions were diluted to 1:10.

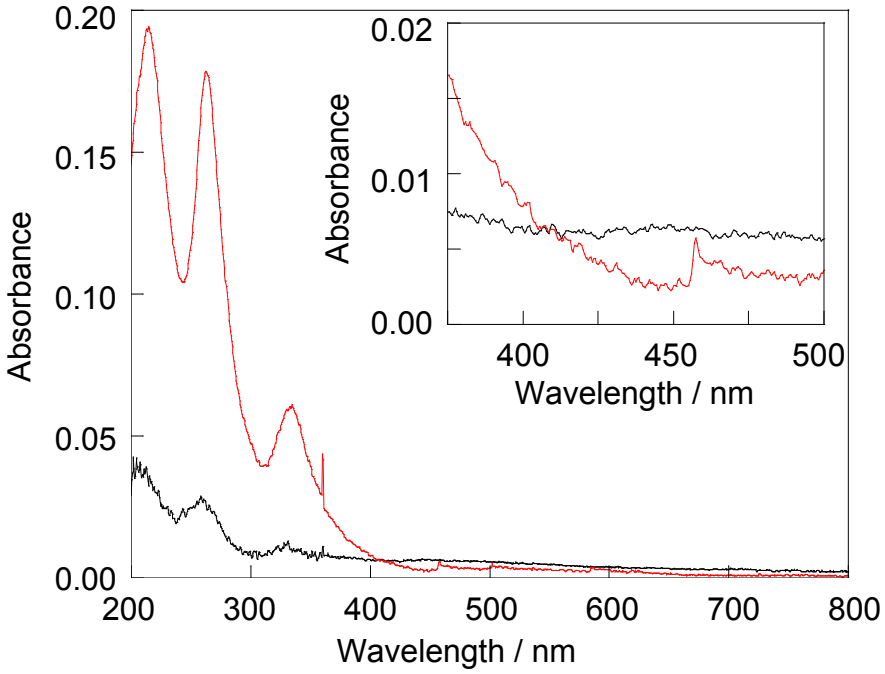

Fig. S2 UV-vis absorption spectra of the *γ*-CDx-complexes of **13** (black line) and **14** (red line). The inset shows the region of 375-500 nm. All of the spectra were measured at 25 °C (1 mm cell). All of the solutions were diluted to 1:10.

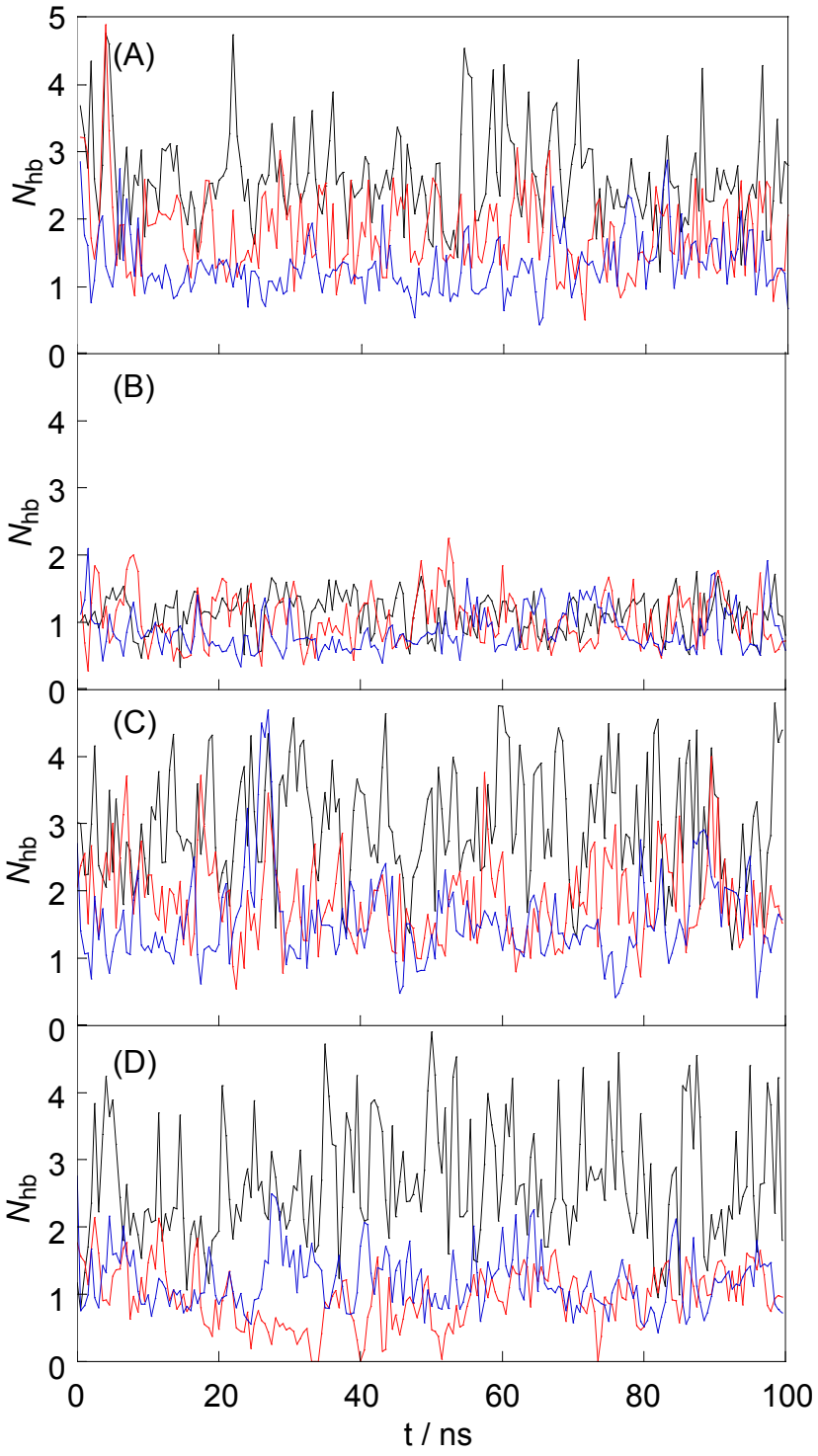

Fig. S3 Time evolutions of the number of hydrogen bonds (N_{hb}) between the two γ-CDxs in the complexes with (A) C_{60}, (B) C_{70}, (C) **1** and (D) **9**. The MD simulations were performed in water (black line) and in DMSO solutions at DMSO volume fractions of 0.33 (red line) and 0.50 (blue line). The block-averaged N_{hb} values over every 0.5 ns were plotted.

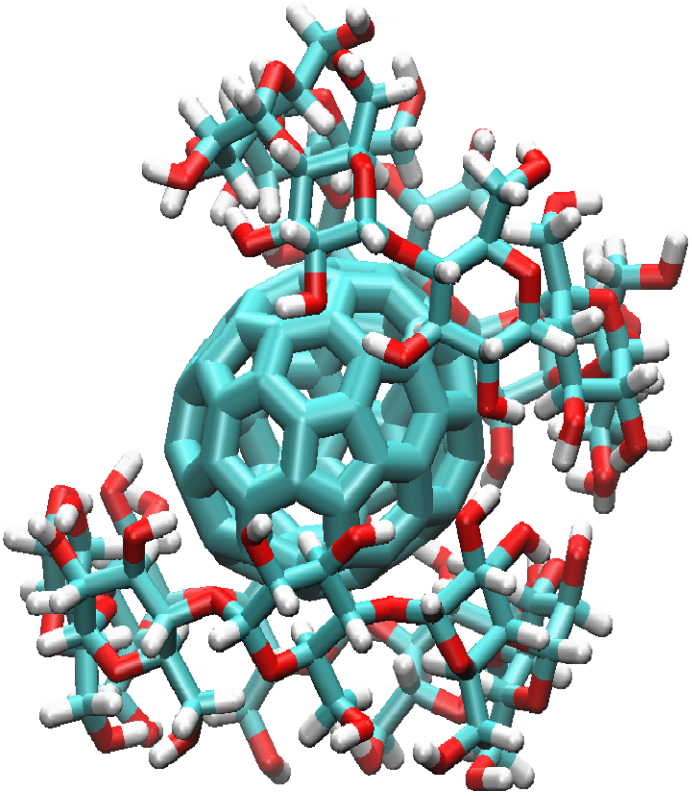

Fig. S4 Snapshot of the **C_{70}•γ-CDx** complex from the MD simulation. The carbon atoms are shown in cyan, oxygen atoms in red and hydrogen atoms in white.

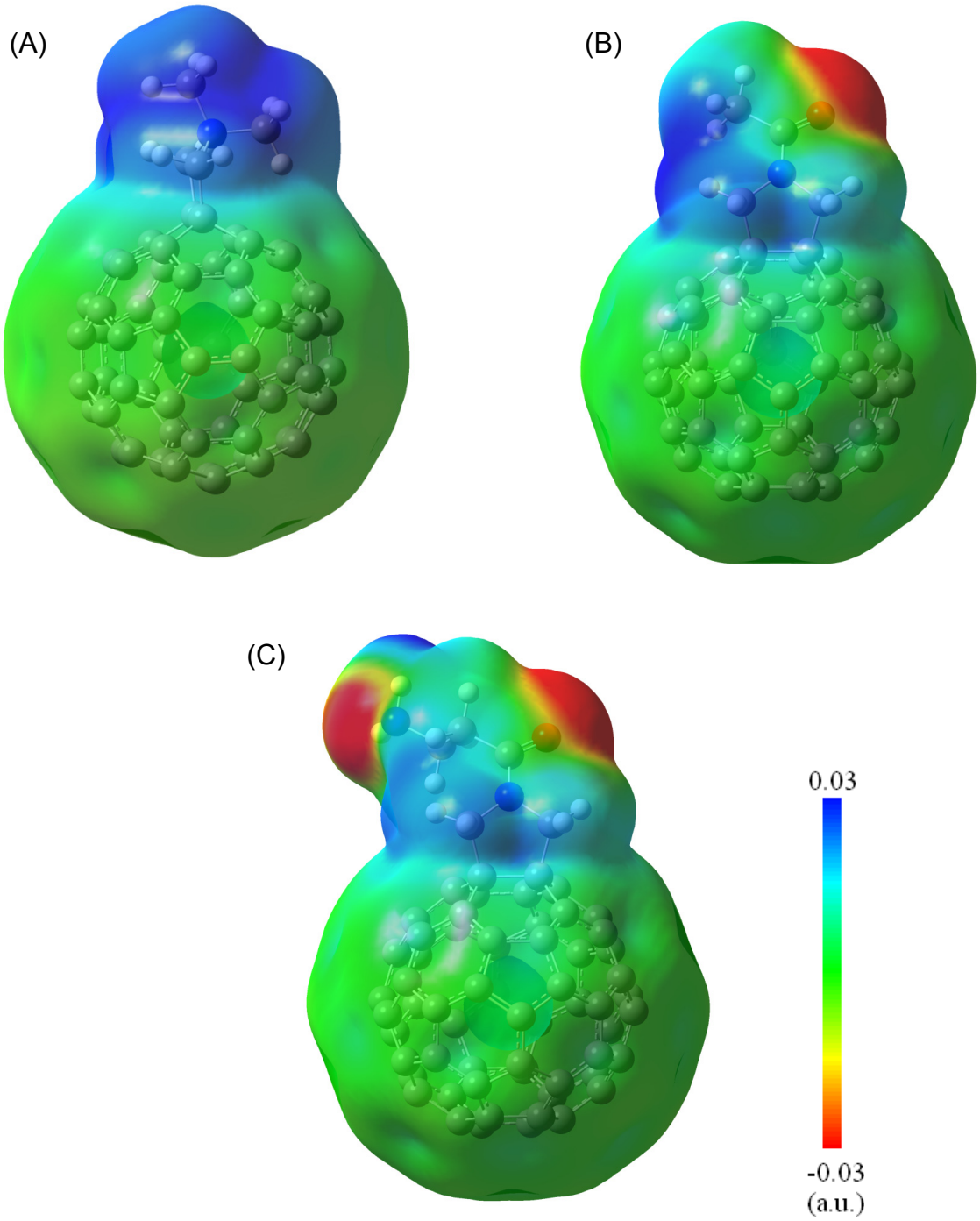

Fig. S5 Electrostatic potential maps of (A) **2**, (B) **3** and (C) **5**. The red and blue surfaces mean negatively- and positively-polar, respectively.

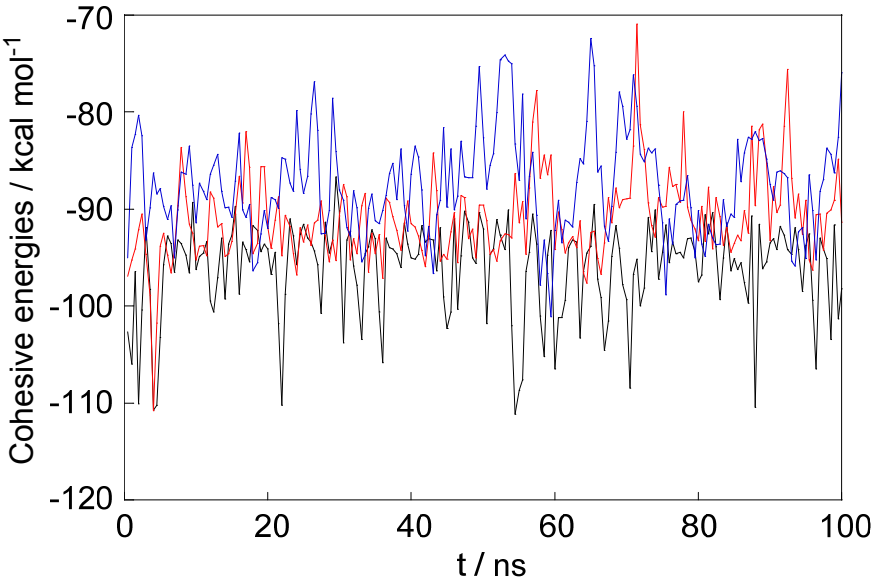

Fig. S6 Time evolutions of the number of cohesive energies (kcal/mol) of the C_{60}•γ-CDx complex [DMSO/(H_2O + DMSO) = 0 (black), 33 (red) and 50 (blue) vol%].

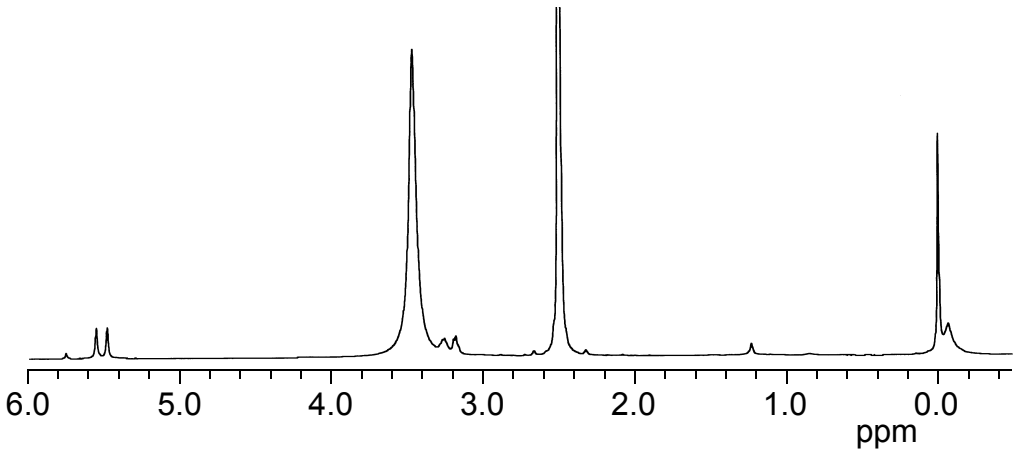

Fig. S7 ^{1}H NMR spectrum of **5** (400 MHz, DMSO-d_6, TMS, 25 °C).

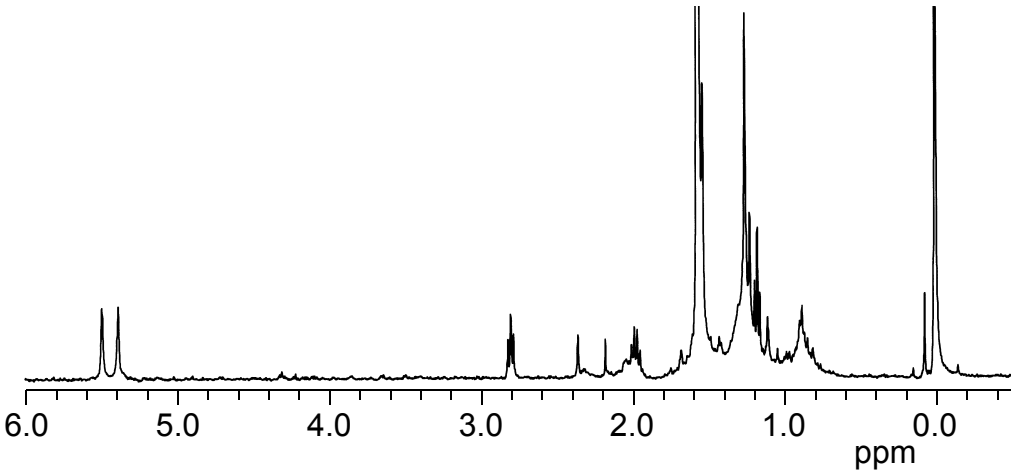

Fig. S8 ^{1}H NMR spectrum of **6** (400 MHz, $CDCl_3$, TMS, 25 °C).

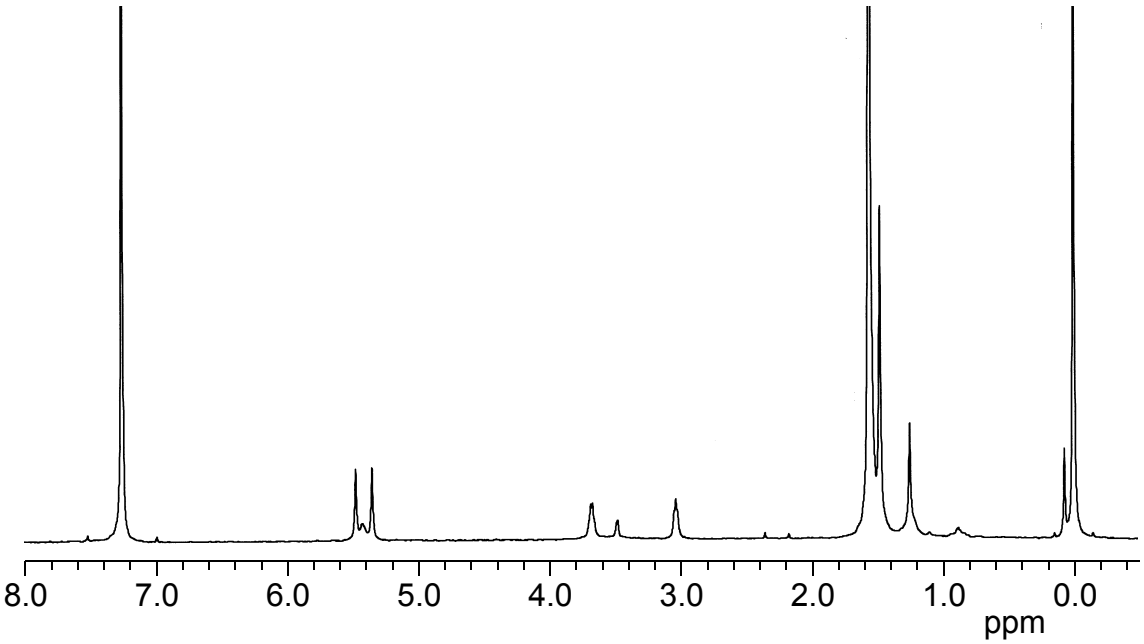

Fig. S9 ^{1}H NMR spectrum of **7** (400 MHz, $CDCl_3$, TMS, 25 °C).