## Supplementary Information Intra- and intermolecular complexation in C(6) monoazacoronand substituted cyclodextrins

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**Fig. S1.** <sup>1</sup>H 600 MHz 2D ROESY NMR spectrum at 298 K of a  $D_2O$  solution in which [**3**]<sub>total</sub> is 0.023 mol dm<sup>-3</sup>. There are no cross-peaks to indicate intramolecular complexation of the substituent.



**Fig. S2.** <sup>1</sup>H 600 MHz 2D ROESY NMR spectrum at 298 K of a D<sub>2</sub>O solution in which [4]<sub>total</sub> is 0.014 mol dm<sup>-3</sup>. There are no cross-peaks to indicate the intramolecular complexation of the substituent.



**Fig. S3.** <sup>1</sup>H 600 MHz 2D ROESY NMR spectrum at 298 K of a D<sub>2</sub>O solution in which [**3**]<sub>total</sub> and  $[\alpha CD]_{total}$  are 0.022 mol dm<sup>-3</sup> and 0.032 mol dm<sup>-3</sup>, respectively. There are no cross-peaks to indicate the intermolecular complexation of the substituent.