Supporting information

Maleonitriledithiolate Modified β-Cyclodextrin: Self-Inclusion and Response to Metal Ions

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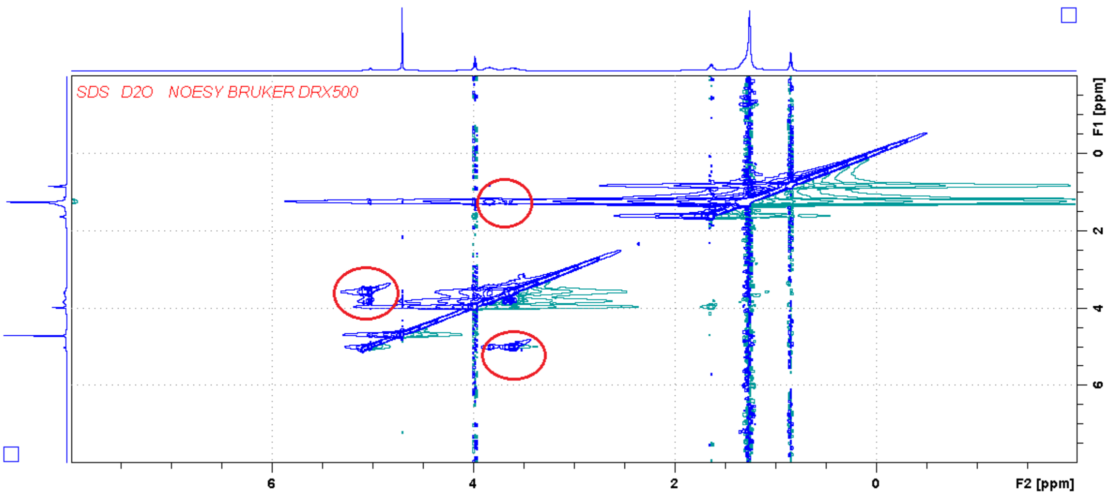


Fig. S1 ^{1}H-NOESY spectrum of a mixture of 6-mnt-β-cyclodextrin (1.0×10^{-4} mol L^{-1}) and SDS (1.0×10^{-3} mol L^{-1}) in D_2O at 298 K. The highlighted two spots evidently showed the interactions between protons from Ada and the interior (H3/H5) of β-cyclodextrin cavity.

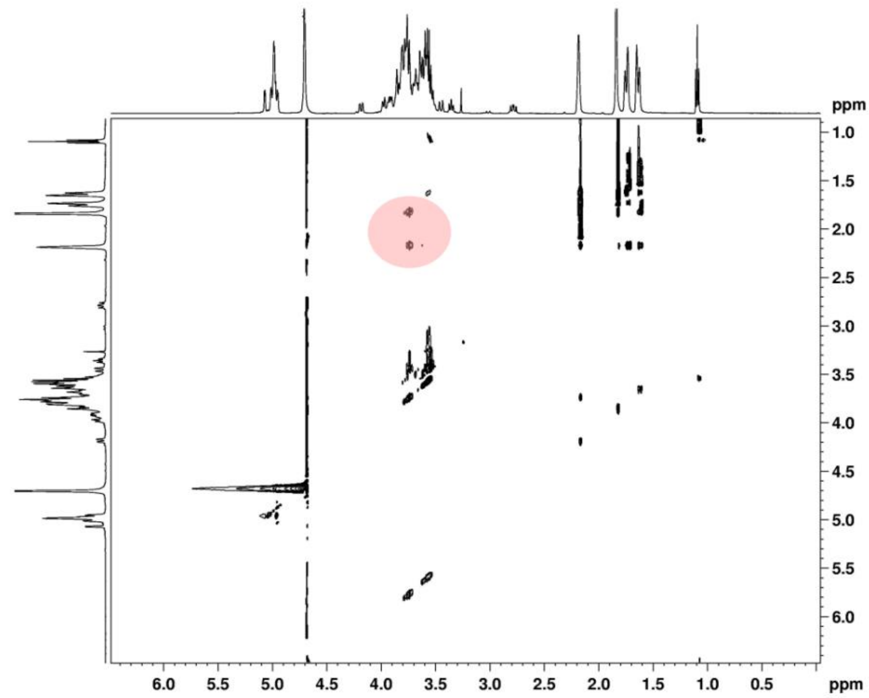


Fig. S2 ^{1}H-NOESY spectrum of a mixture of 6-mnt-β-cyclodextrin (1.0×10^{-4} mol L^{-1}) and Ada (1.0×10^{-4} mol L^{-1}) in D_2O at 298 K. The highlighted two spots evidently showed the interactions between protons from Ada and the interior (H3/H5) of β-cyclodextrin cavity.

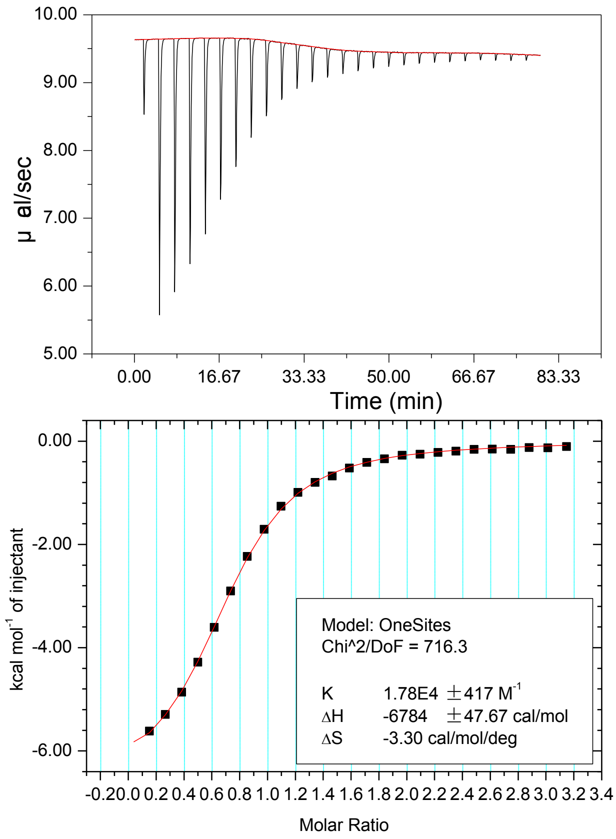


Fig. S3 ITC experiments of Ada (7.65×10^{-3} mol L^{-1}) into 6-mnt-β-cyclodextrin (5.02×10^{-4} mol L^{-1}) in PBS (pH 4.92) at 298 K. The inset gives the best fitting of the titration curve with $K_{binding}$ of $(1.78\pm0.04)\times10^{4}$ M^{-1}.

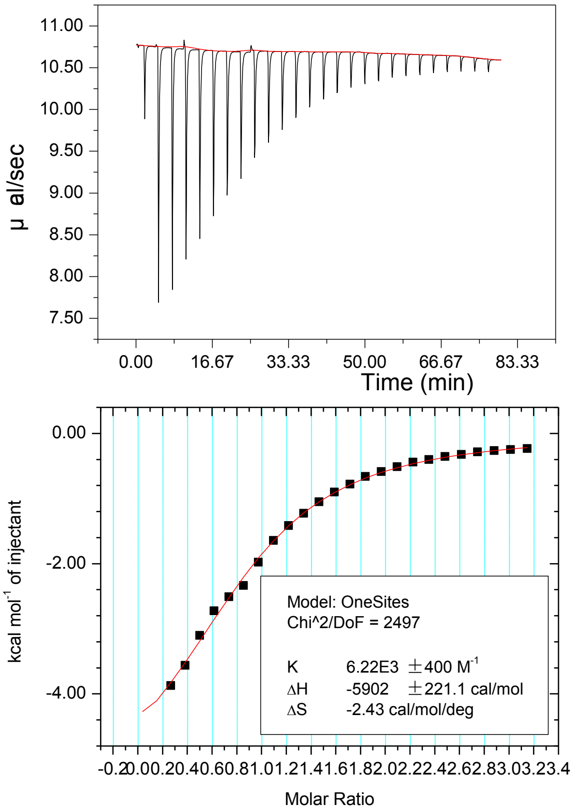
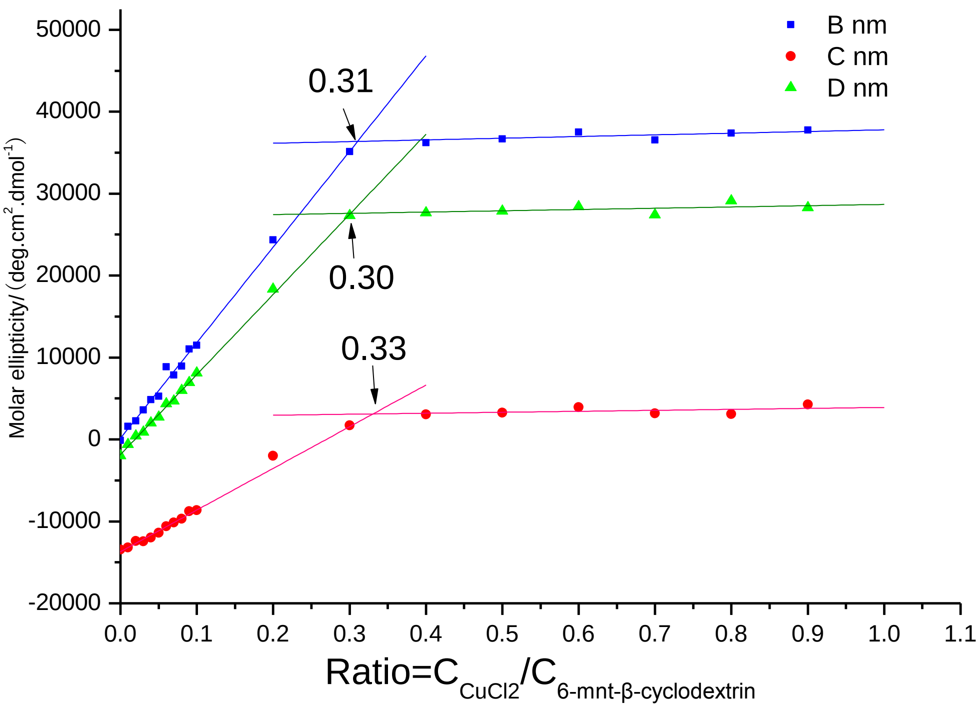


Fig. S4 ITC experiments of Ada (7.65×10^{-3} mol L^{-1}) into β-cyclodextrin (5.02×10^{-4} mol L^{-1}) in PBS (pH 4.92) at 298 K. The inset gives the best fitting of the titration curve with $K_{binding}$ of $(6.22\pm0.40)\times10^{3}$ M^{-1}.



(a)

Fig. S5 Plot of the ellipticity at different nm versus addition of $CuCl_2$ in the presence of 6-mnt-β-cyclodextrin (1.0×10^{-4} mol L^{-1}) in water at 298 K based on Fig. 4 in manuscript.

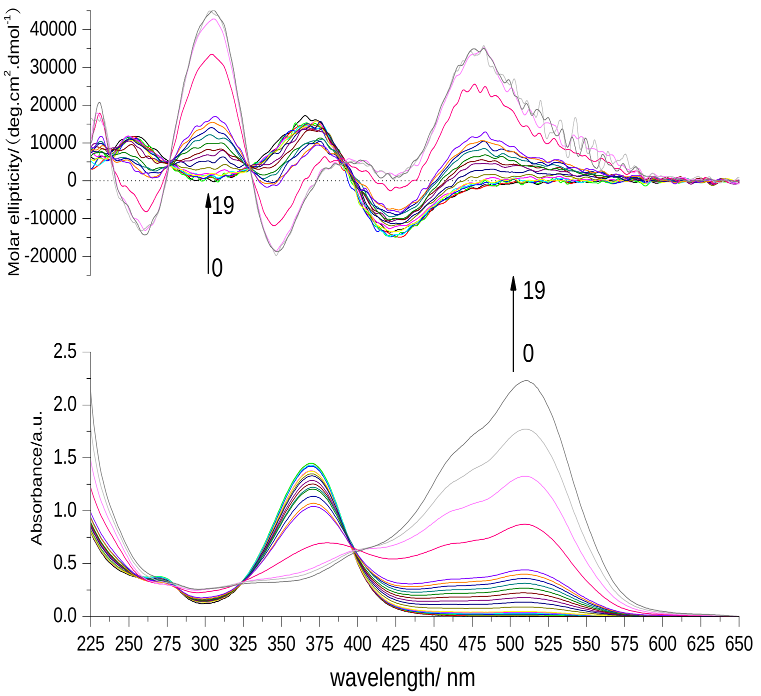


Fig. S6 CD (above) and UV (below) spectra of 6-mnt-β-cyclodextrin (1×10^{-4} mol L^{-1}) in water at 298 K in the presence of increasing concentrations of $CoCl_2$. (C_{CoCl2} = 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 20, 30, 40 $\times10^{-2}$ mol L^{-1} for curves 0 to 19.)

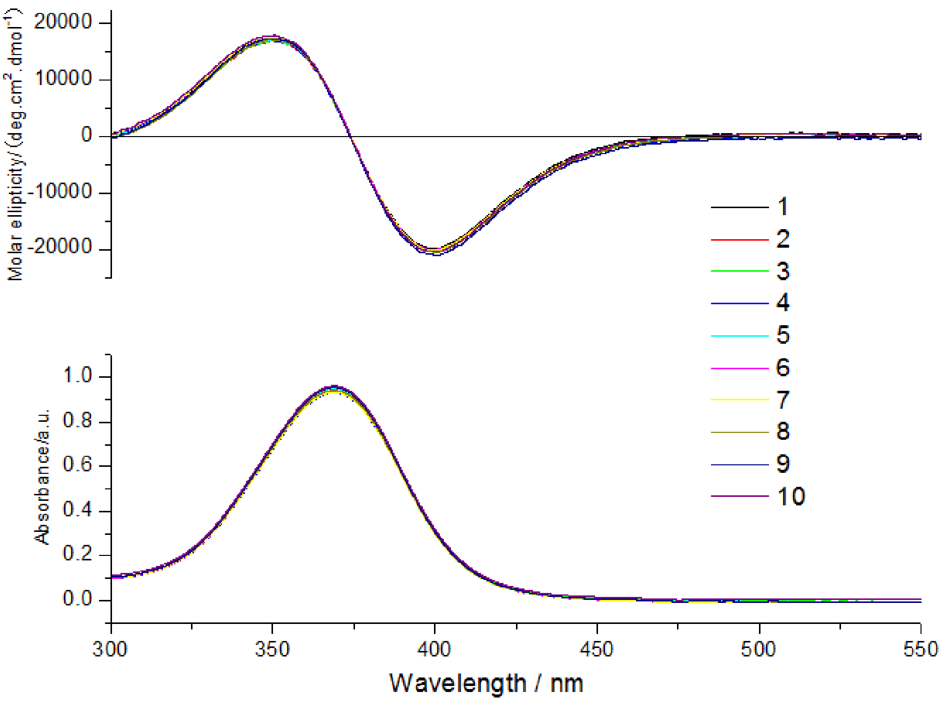


Fig. S7 CD (above) and UV (below) spectra of 6-mnt-β-cyclodextrin (1×10^{-4} mol L^{-1}) in water at 298 K in the presence of increasing concentrations of $ZnCl_2$. C_{ZnCl2} = 0, 2, 4, 6, 8, 10, 30, 50, 70, 90×10^{-3} mol L^{-1} for curves 1 to 10.

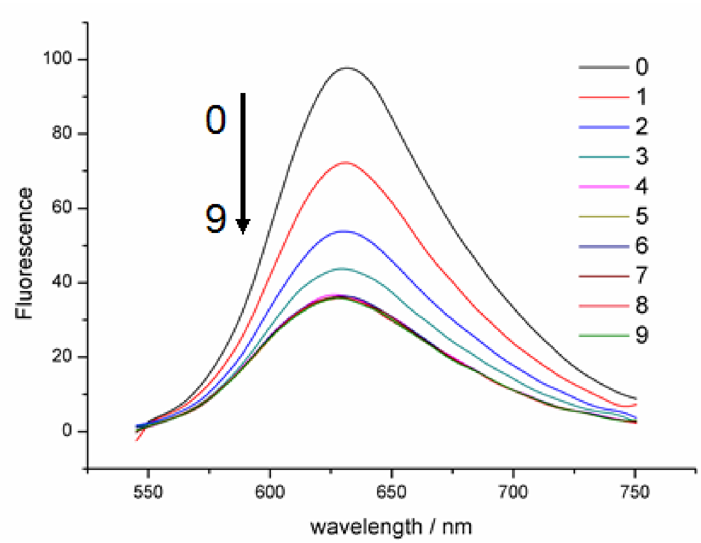


Fig. S8 Fluorescence spectra (λ_{ex} = 453 nm) of NR (1×10^{-5} mol L^{-1}) in buffer (pH = 8.5) at 298 K in the presence of increasing concentrations of Na_2mnt. C_{Na2mnt} = 0, 2, 4, 6, 8, 10, 20, 30, 40, 50×10^{-5} mol L^{-1} for curves 0 to 9.

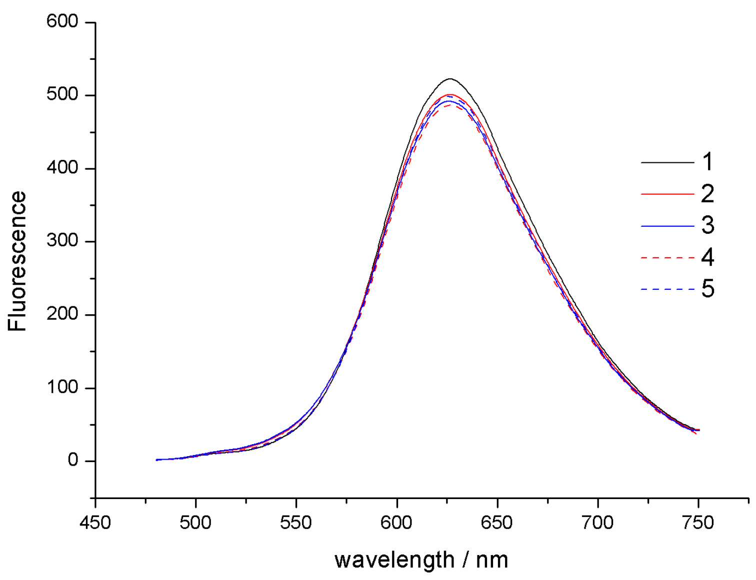


Fig. S9 Fluorescence spectra (λ_{ex} = 453 nm) of NR (1×10^{-5} mol L^{-1}) in buffer (pH = 8.5) at 298 K. C_{Cu2+} = 0, 7, 10, 7, 10×10^{-5} mol L^{-1}, and C_{EDTA} = 0, 0, 0, 1.4, 2×10^{-4} mol L^{-1} for curves 1 to 5.