

Supplementary Materials

Structural Effect of Fluorophore on Phenylboronic Acid Fluorophore/Cyclodextrin Complex for Selective Glucose Recognition

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1. Characterization data

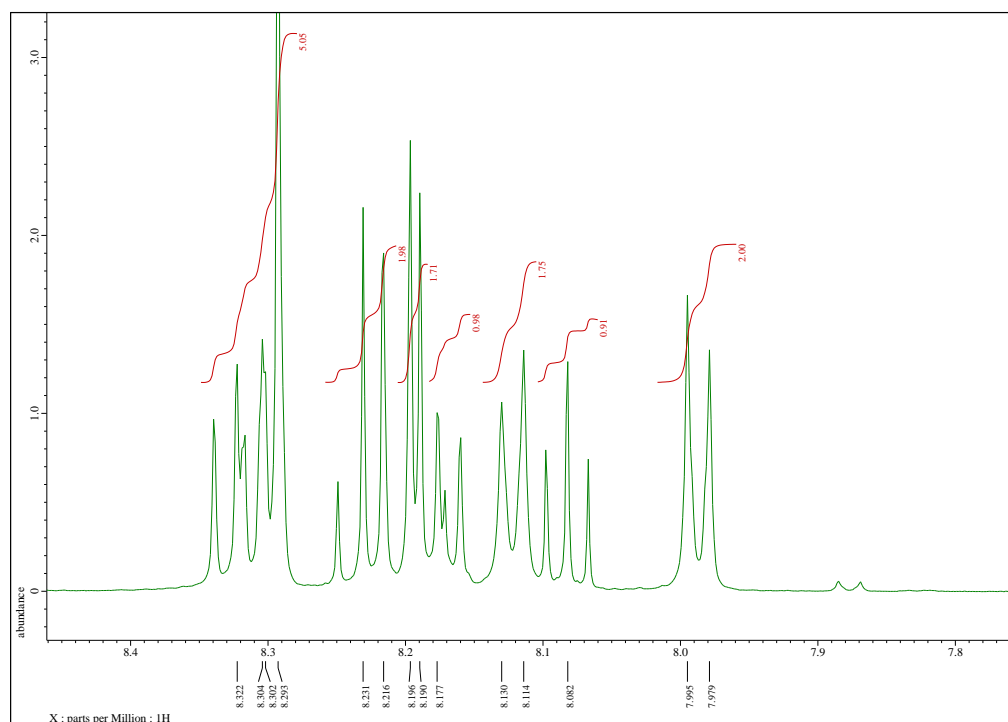
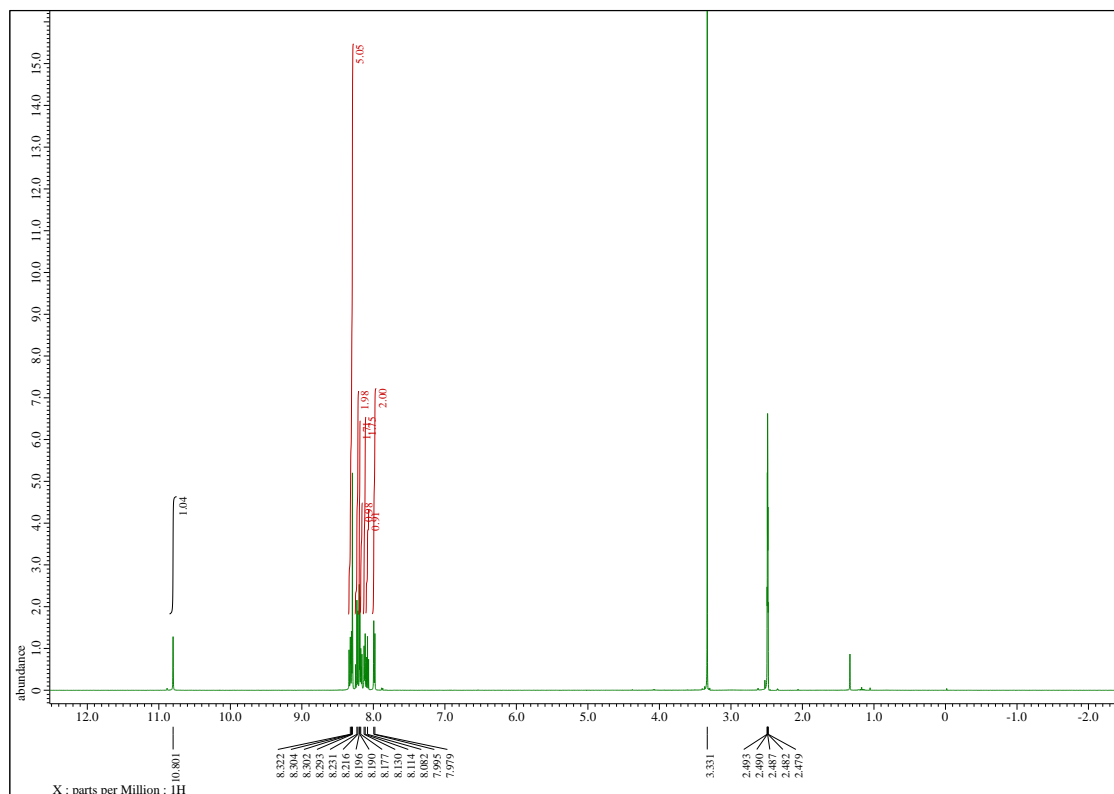


Fig. S1 ^1H NMR spectra for **1** (500 MHz, in $\text{DMSO-}d_6$).

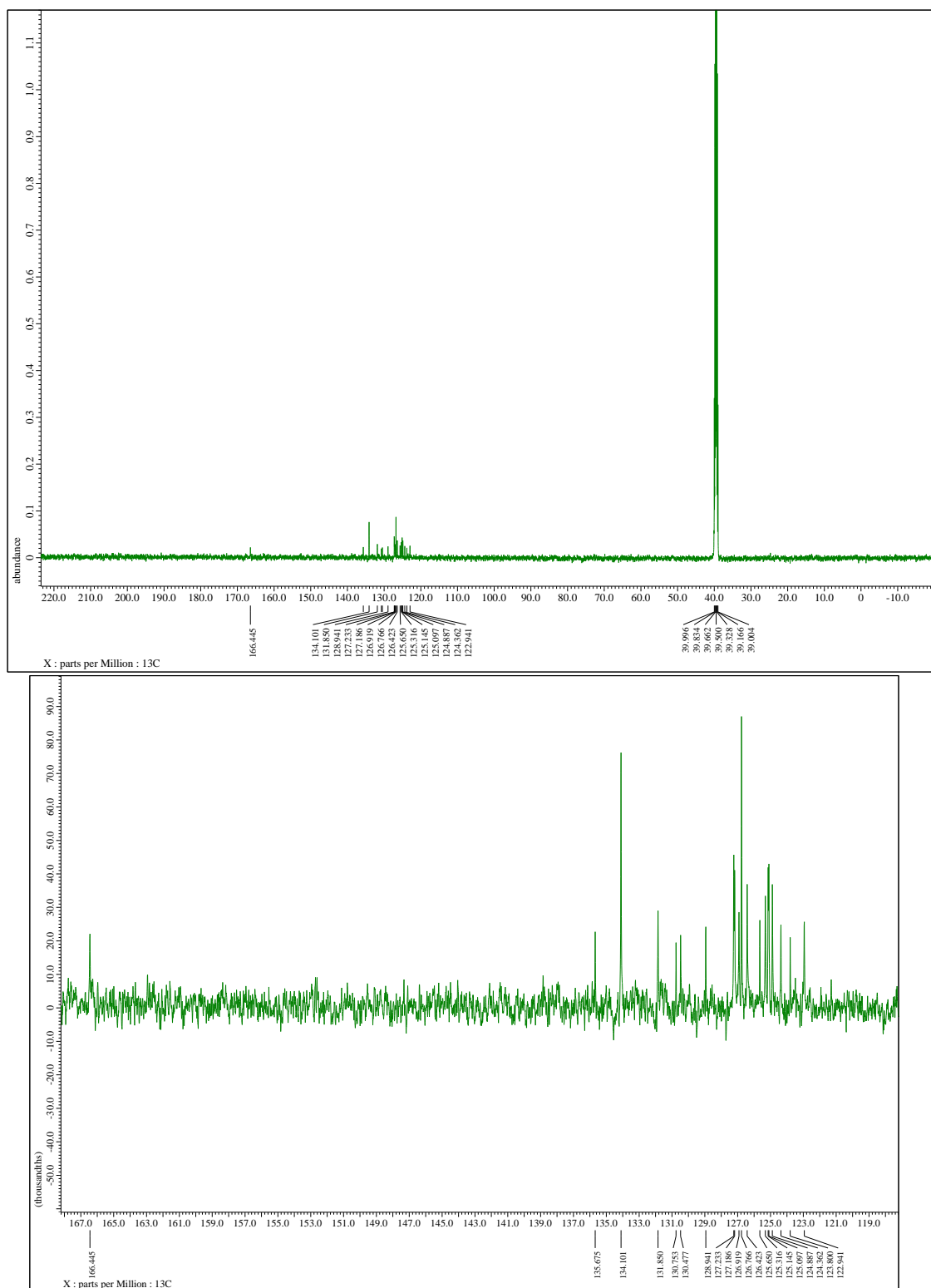


Fig. S2 ^{13}C NMR spectra for **1** (125 MHz, in $\text{DMSO-}d_6$).

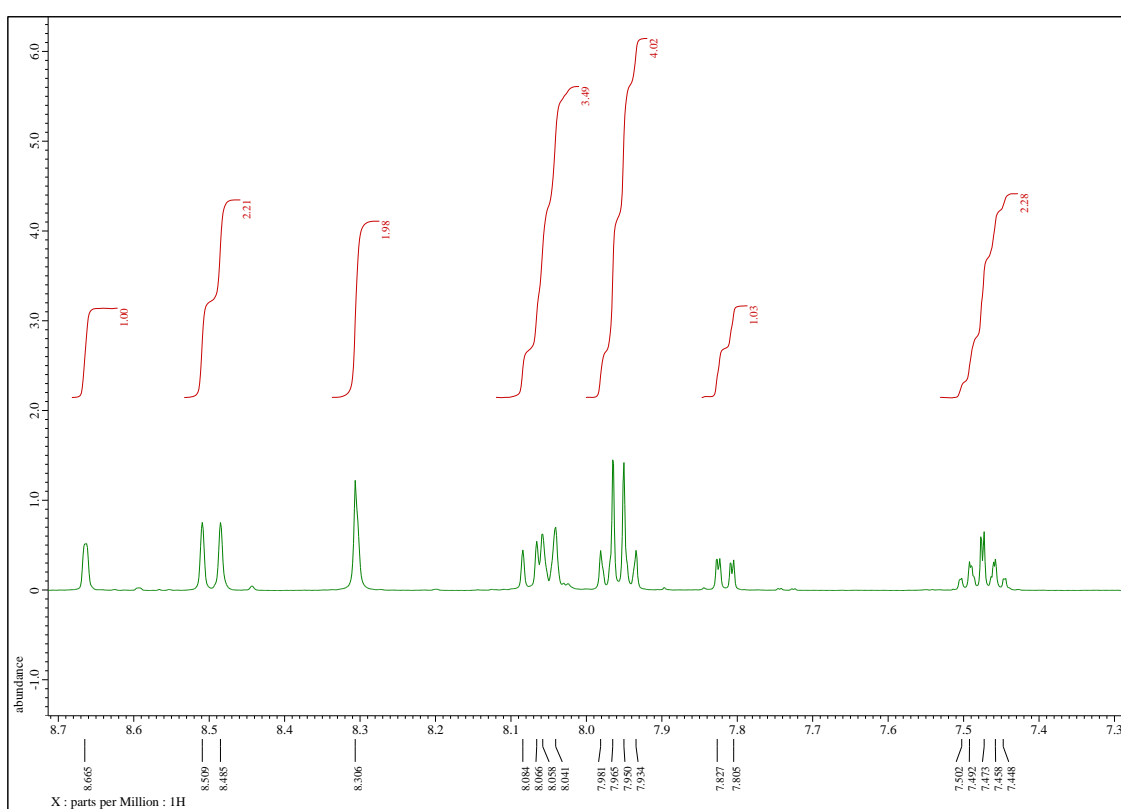
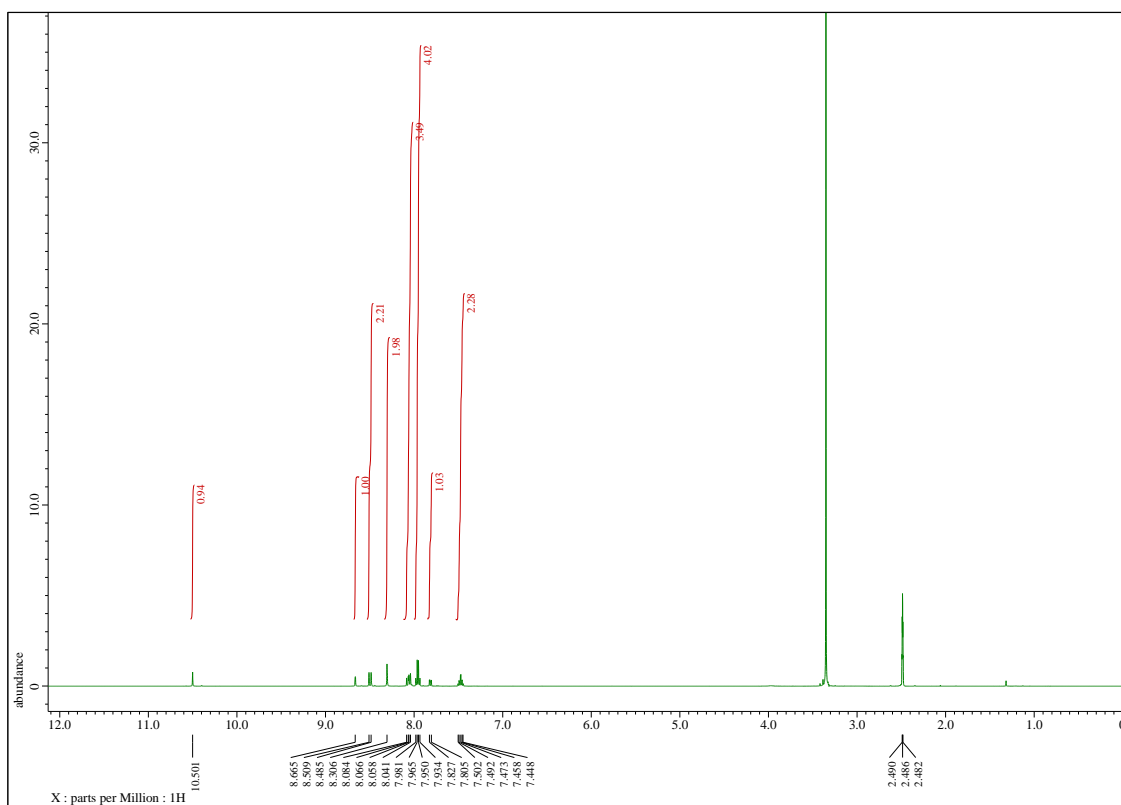


Fig. S3 ^1H NMR spectra for **2** (500 MHz, in $\text{DMSO-}d_6$).

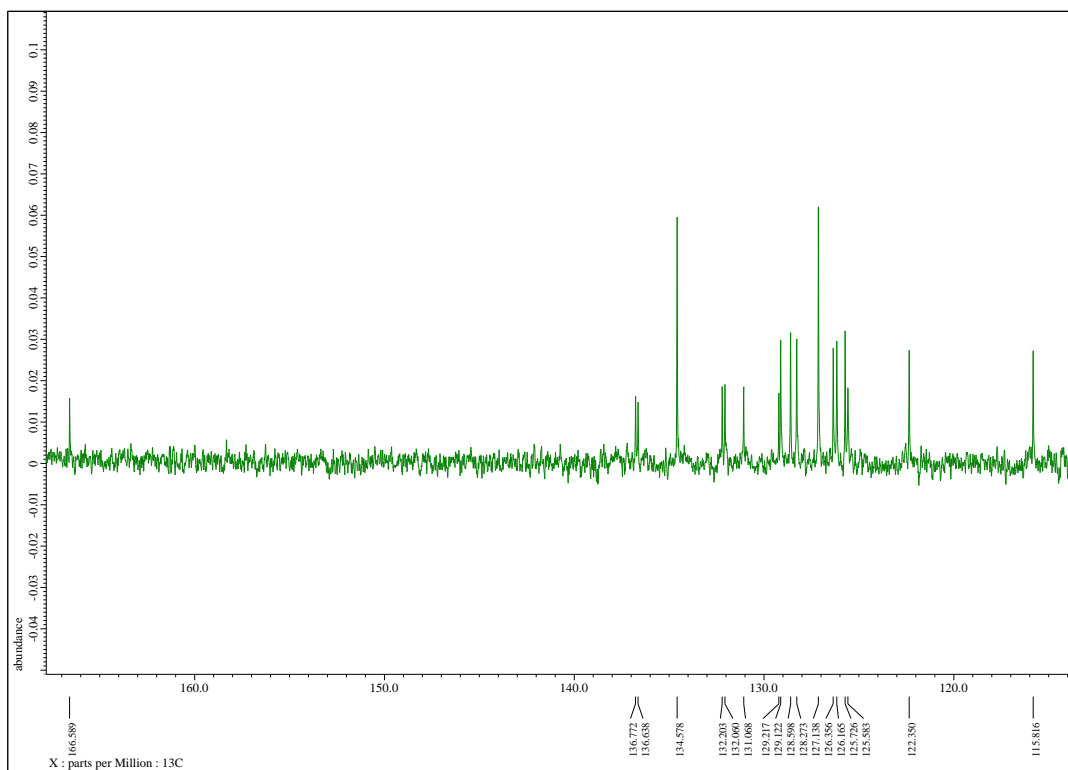
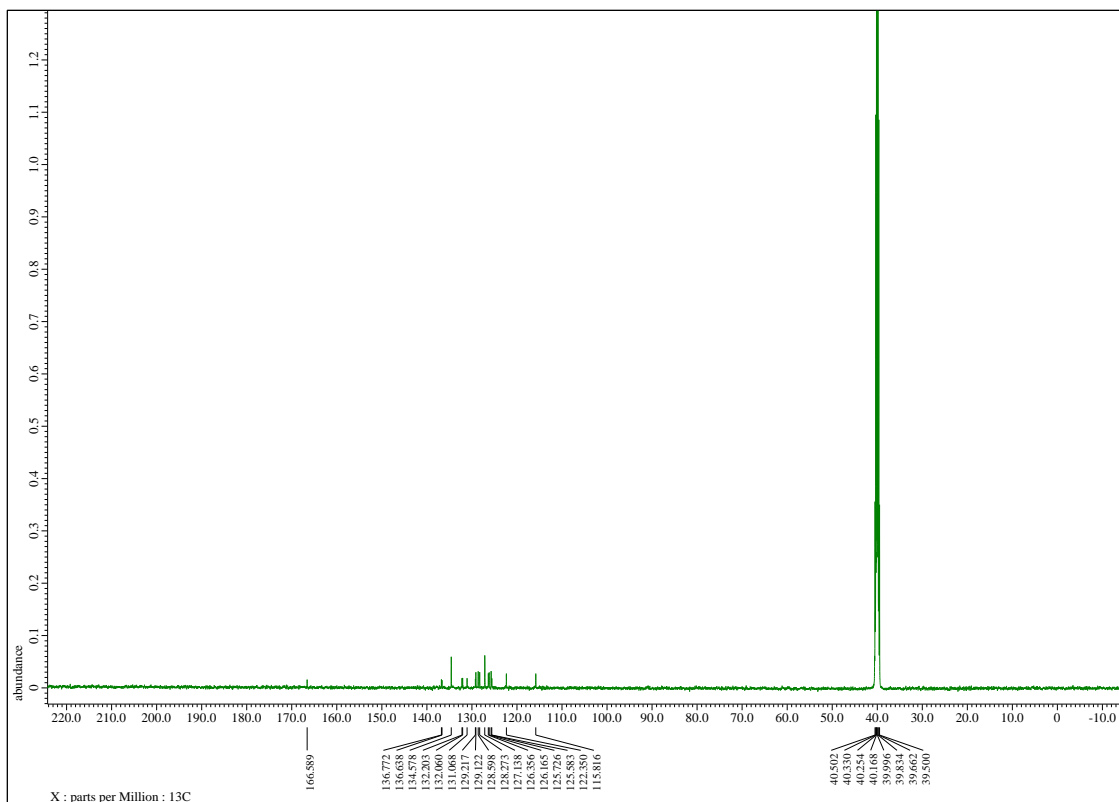


Fig. S4 ^{13}C NMR spectra for **2** (125 MHz, in $\text{DMSO-}d_6$).

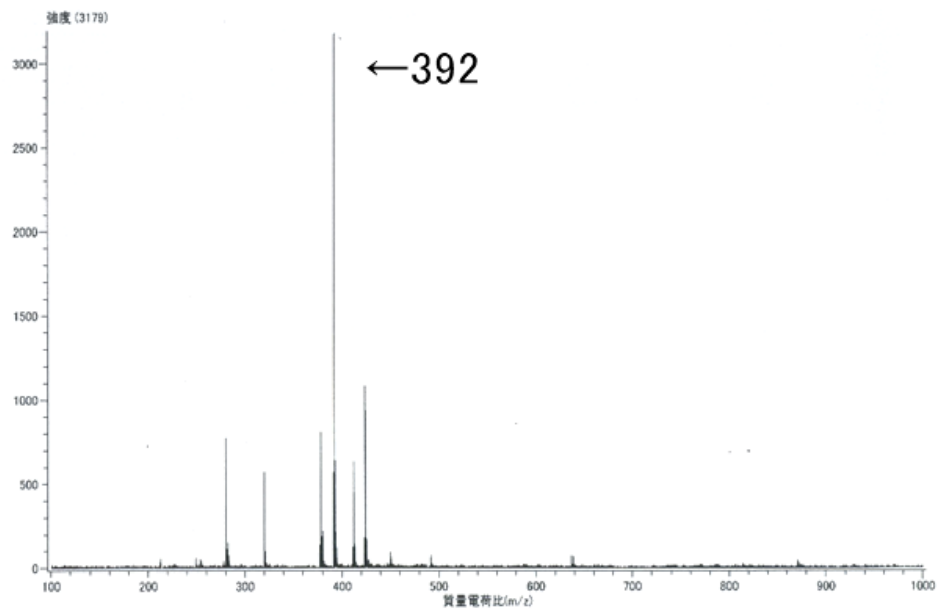


Fig. S5 The ESI-TOF-MS spectra for **1**.

2. The pH dependence of UV-vis spectra for probe/ β -CyD complex.

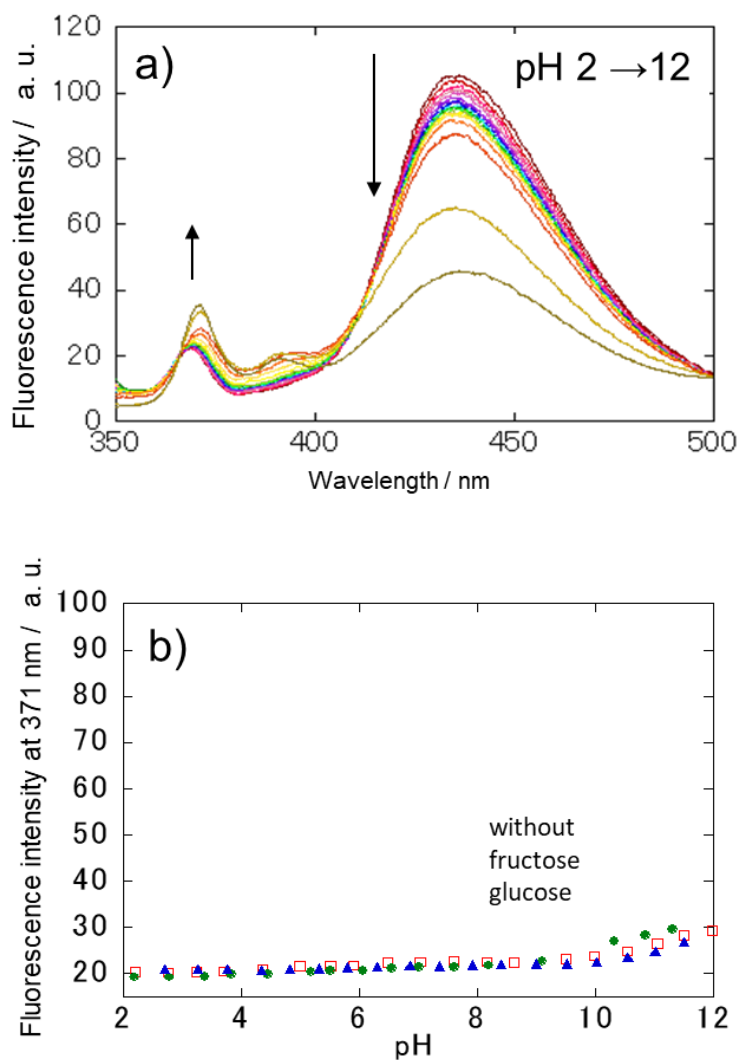


Fig. S6 pH dependence of fluorescence spectra (a) and fluorescence intensity at 371 nm (b) for 1/ β -CyD in 2% DMSO–98% water (v/v). [1] = 1.0×10^{-5} M (M = mol dm⁻³), [β -CyD] = 5 mM, pH adjusted with 0.01 M phosphate buffer, at 25 °C, $I = 0.1$ M with NaCl, [fructose], [glucose] = 0 or 30 mM, $\lambda_{\text{ex}} = 328$ nm.

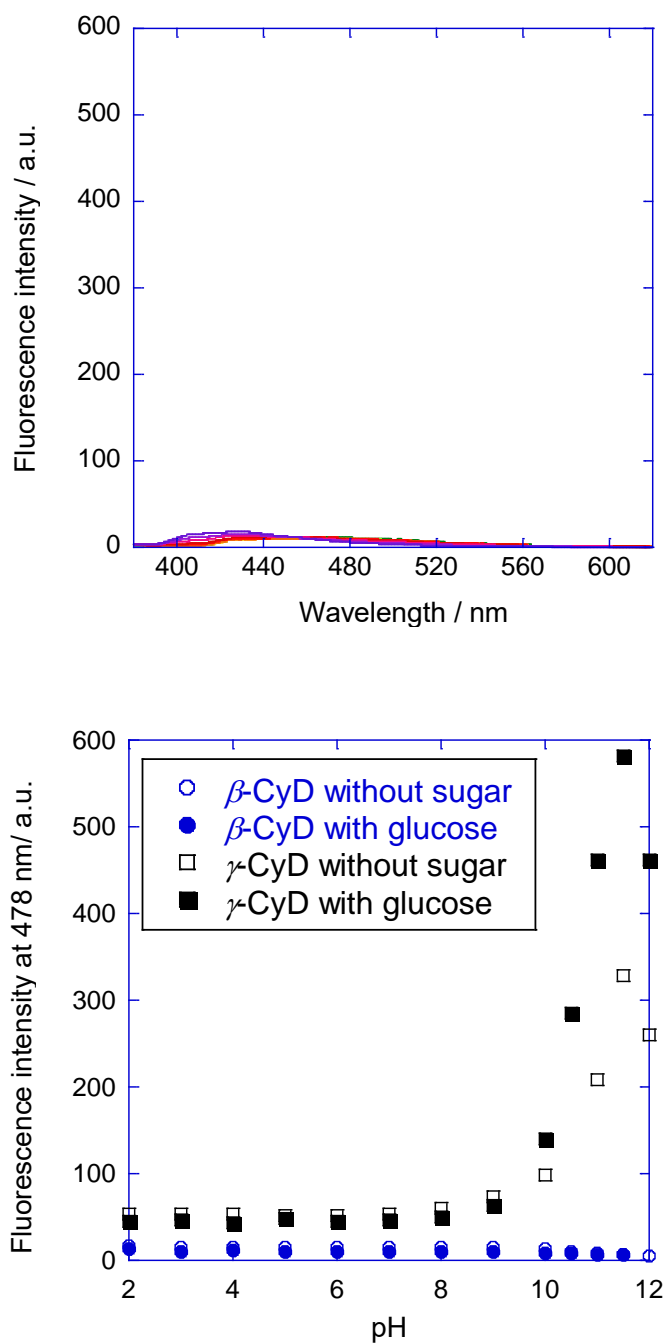


Fig. S7 pH dependence of fluorescence spectra for **2**/ β -CyD (a) and fluorescence intensity at 478 nm (b) for **2**/ β -CyD and **2**/ γ -CyD in 2% DMSO–98% water (v/v). [**2**] = 5.0×10^{-6} M, [β -CyD] = 5 mM, [glucose] = 0 or 6 mM, pH adjusted to 11.0 with 0.01 M Na_2CO_3 buffer, $I = 0.1$ M with NaCl, , at 25 °C. $\lambda_{\text{ex}} = 325$ nm.

3. The pH dependence of UV-vis spectra for 2/ γ -CyD complex.

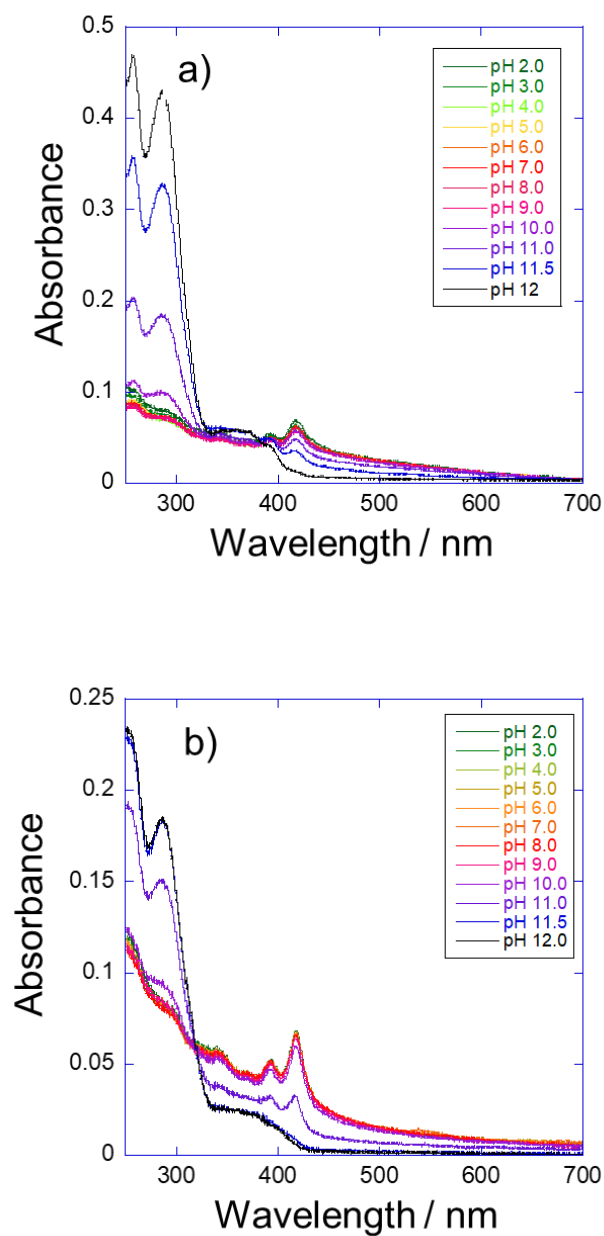


Fig. S8 pH dependence of UV-vis spectra for 2/ γ -CyD in 2% DMSO–98% water (v/v), without sugar (a), in 30 mM glucose (b). [2] = 1.0×10^{-5} M, [γ -CyD] = 5 mM, pH adjusted with 0.01 M phosphate buffer, at 25°C, $I = 0.1$ M with NaCl.

4. The thermal dependence for **2**/ γ -CyD complex.

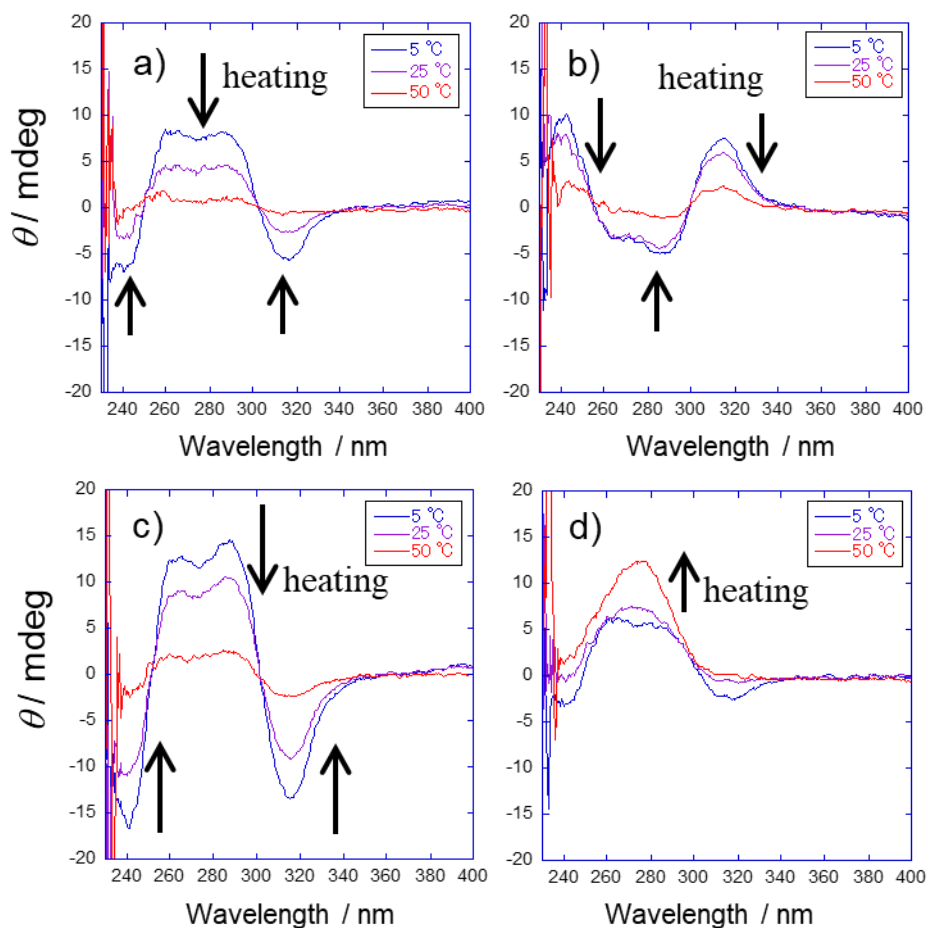


Fig. S9 The thermal-dependence of ICD spectra for **2**/ γ -CyD in 4% DMSO–96% water (v/v), without sugar (a), in 30 mM glucose (b), in 30 mM galactose (c), in 30 mM fructose. [**2**] = 1.0×10^{-5} M, [γ -CyD] = 5 mM, pH adjusted to 11.0 by 0.01 M Na_2CO_3 phosphate buffer, at 25 °C, $I = 0.1$ M with NaCl.

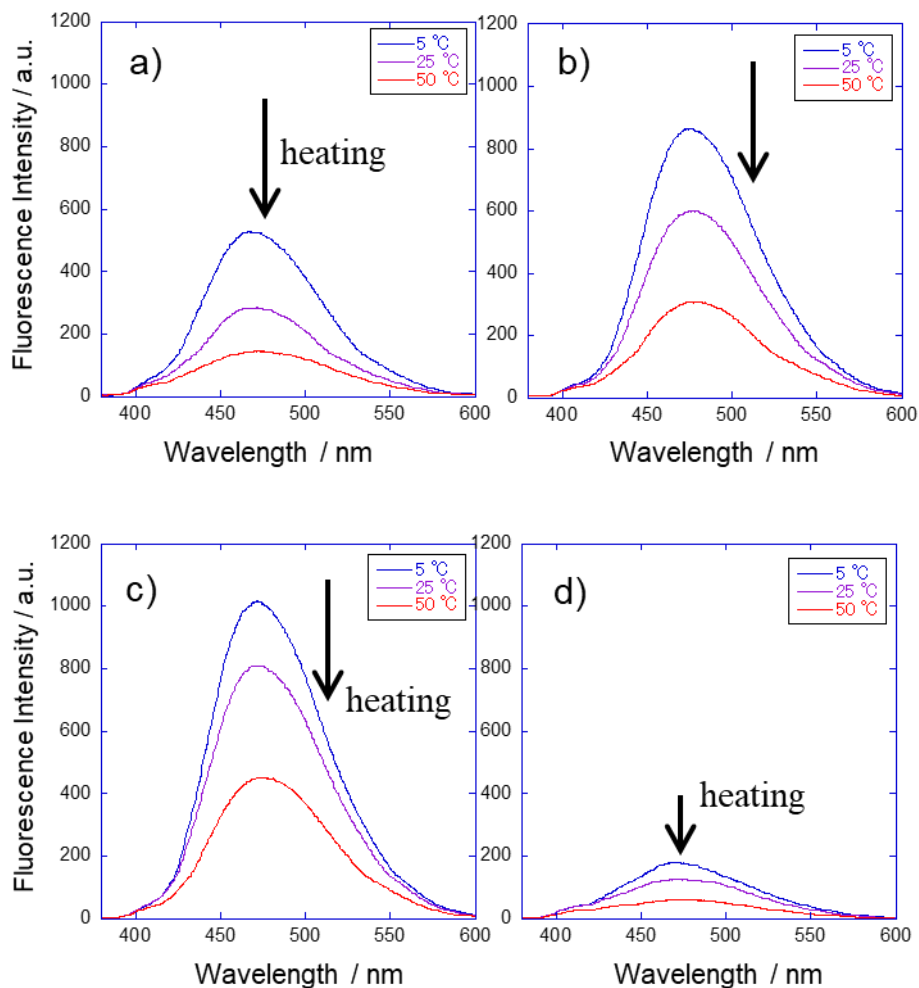


Fig. S10 The thermal-dependence of fluorescence spectra for **2**/ γ -CyD in 2% DMSO–98% water (v/v), without sugar (a), in 6.0 mM glucose (b), in 6.0 mM galactose (c), in 6.0 mM fructose. $[\mathbf{2}] = 5.0 \times 10^{-6}$ M, $[\gamma\text{-CyD}] = 5$ mM, pH adjusted to 11.0 by 0.01 M Na_2CO_3 phosphate buffer, at 25°C,

5. The CD spectra in the presence of sugar only

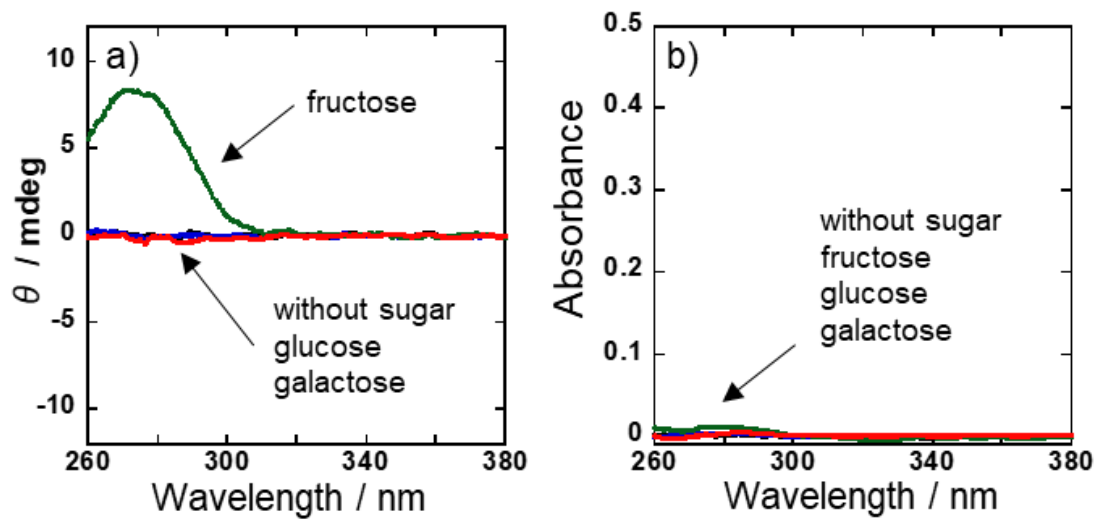


Fig. S11 The ICD (a) and UV-vis (b) spectra for sugars in water. [sugar] = 30 mM, $I = 0.1$ M with NaCl, at 25°C.