Supporting Information

Controlled keto-enol tautomerism of coumarin containing β-ketodithioester by its encapsulation in cucurbit[7]uril.

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Figure S1A. $^1$H NMR spectrum for CAM1 alone in DMSO-$d_6$.

Figure S1B. $^1$H NMR spectrum for CAM1 alone in CD$_3$CN.

Figure S2. $^{13}$C NMR spectrum for CAM1 alone in DMSO-$d_6$.

Figure S3. HRMS of CAM1 (2 mM) in water-DMSO (99:1, v/v) solution.

Figure S4A. $^1$H NMR spectrum for CAM2 alone in DMSO-$d_6$.

Figure S4B. $^1$H NMR spectrum for CAM2 alone in CD$_3$CN.

Figure S5. $^{13}$C NMR spectrum for CAM2 alone in DMSO-$d_6$.

Figure S6. $^{13}$C NMR-DEPT spectrum for CAM2 alone in DMSO-$d_6$.

Figure S7. COSY spectrum of CAM2 alone in DMSO-$d_6$.

Figure S8. $^1$H-HMQC spectrum of CAM2 alone in DMSO-$d_6$.

Figure S9. $^1$H-HMBC spectrum of CAM2 alone in DMSO-$d_6$.

Figure S10. HRMS-ESI of CAM2 (2 mM) in water-DMSO (99:1, v/v) solution.

Figure S11. Normalized UV-vis absorption spectra of: A) coumarin-derivative CAM1 dye (2 µM) and B) coumarin-derivative dye CAM2 (4 µM), in different solvents.

Figure S12. Comparison of partial $^1$H NMR spectra for: A) CAM1 alone in CD$_3$CN/D$_2$O and B) CAM1 and CB7 (3 eq.).

Figure S13. Comparison of partial $^1$H NMR spectra for: A) CAM1 alone in CD$_3$CN/D$_2$O and B) CAM1 and CB7 (3 eq.).

Figure S14. Comparison of partial $^1$H NMR spectra (400 MHz) for: A) Intermediate 2 alone in CD$_3$CN/D$_2$O and B) Intermediate 2 and CB7 (3 eq.).

Figure S15. ESI mass spectra of a 1:10 molar ratio in aqueous solution of coumarin-derivative CAM1 and CB7, respectively.

Figure S16. Normalized excitation and emission spectra of dyes: A) CAM1 and (B) CAM2, in aqueous solutions.

Figure S17. Job plot for the complexes CAM1-CB7 and CAM2-CB7.

Figure S18. HRMS-ESI of a 1:10 molar ratio in aqueous solution of coumarin-derivative A) CAM1 and CB7, and B) CAM2 and CB7, respectively.

Figure S19. Comparison of partial $^1$H NMR spectra (200 MHz) for: A) CAM2 alone in CD$_3$CN/D$_2$O, B) CAM2 and CB7 (3 eq.) and C) CAM2 and β-CD (3 eq.).

Figure S20. A) Fluorescence spectra of CAM1 with increasing concentrations of CB7. Inset shows the fluorescence titration of CAM1 with CB7. B) Determination of the effective binding constant by fitting data to a 1:1 host:guest model.

Table S1. Binding energy from docking studies for CAM1 and CAM2 in CB7 and β-CD.
Figure S1A. $^1$H NMR spectrum (400 MHz) for CAM1 alone in DMSO-$d_6$.

Figure S1B. $^1$H NMR spectrum (400 MHz) for CAM1 alone in CD$_3$CN.
Figure S2. $^{13}$C NMR spectrum (400 MHz) for CAM1 alone in DMSO-$d_6$.

Figure S3. HRMS (ESI, negative mode) of CAM1 (2mM) in water-DMSO (99:1, v/v) solution.
Figure S4A. \(^1\)H NMR spectrum (400 MHz) for CAM2 alone in DMSO-\(d_6\).
**Figure S4B.** $^1$H NMR spectrum (400 MHz) for **CAM2** alone in CD$_3$CN.
Figure S5. $^{13}$C NMR spectrum (400 MHz) for CAM2 alone in DMSO-$d_6$. 
Figure S6. $^{13}$C NMR-DEPT spectrum (101 MHz) for CAM2 alone in DMSO-$d_6$. 
Figure S7. COSY spectrum (400 MHz) of CAM2 alone in DMSO-d$_6$.

Figure S8. $^1$H-HMQC spectrum (400 MHz) of CAM2 alone in DMSO-d$_6$. 
Figure S9. $^1$H-HMBC spectrum (400 MHz) of CAM2 alone in DMSO-$d_6$.

Figure S10. HRMS-ESI (positive mode) of CAM2 (2 mM) in water-DMSO (99:1, v/v) solution.
Figure S11. Normalized UV-vis absorption spectra of: A) coumarin-derivative CAM1 dye (2 µM) and B) coumarin-derivative dye CAM2 (4 µM) in chloroform (a), DMSO (b), ethanol (c), aqueous solution (d) and with CB7 (100 µM) in aqueous solution (e).

Figure S12. Comparison of partial $^1$H NMR spectra (400 MHz) for: A) CAM1 alone in CD$_3$CN/D$_2$O and B) CAM1 and CB7 (3 eq.).
**Figure S13.** Comparison of partial $^1$H NMR spectra (400 MHz) for: A) CAM1 alone in CD$_3$CN/D$_2$O and B) CAM1 and CB7 (3 eq.).

**Figure S14.** Comparison of partial $^1$H NMR spectra (400 MHz) for: A) Intermediate 2 alone in CD$_3$CN/D$_2$O and B) Intermediate 2 and CB7 (3 eq.).
Figure S15. ESI mass spectra of a 1:10 molar ratio in aqueous solution of coumarin-derivative CAM1 and CB7, respectively.

Figure S16. Normalized excitation and emission spectra of coumarin-derivative dyes: A) CAM1 (5 μM) and B) CAM2 (5 μM), excitation and emission slits of 5 nm were used. All spectra were carried out in aqueous solutions.
Figure S17. Job plot for the complexes CAM1-CB7 ($\lambda_{\text{exc}} = 460$ nm; $\lambda_{\text{em}} = 500$ nm) (A) and CAM2-CB7 (B) ($\lambda_{\text{exc}} = 420$ nm; $\lambda_{\text{em}} = 490$ nm).

Figure S18. HRMS-ESI (negative mode) of a 1:10 molar ratio in aqueous solution of coumarin-derivative A) CAM1 and CB7, and B) CAM2 and CB7.
Figure S19. Comparison of partial $^1$H NMR spectra (400 MHz) for: A) CAM2 alone in CD$_3$CN/D$_2$O, B) CAM2 and CB7 (3 eq.) and C) CAM2 and β-CD (3 eq.).

Figure S20. A) Fluorescence spectra of the coumarin-derivative CAM1 (5 μM) with increasing concentrations of CB7 (5-400 μM). Inset shows the fluorescence titration of 5 μM CAM1 with CB7 in aqueous solution. B) The effective binding constant was determined as $K_{\text{CAM1CB7}} = 3.95 \times 10^3$ M$^{-1}$ by fitting data to the 1:1 host:guest model. Excitation and emission slits of 5 nm were used.
Table S1. Binding energy from docking studies for CAM1 and CAM2 in CB7 and β-CD.

<table>
<thead>
<tr>
<th>Guest</th>
<th>Binding Energy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CB7</td>
</tr>
<tr>
<td>CAM1</td>
<td>-1.2</td>
</tr>
<tr>
<td>CAM2</td>
<td>-2.1</td>
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