Supplementary Information

to the article

Title: Self-assembly of cucurbiturils and cyclodextrins to supramolecular millstones with naphthalene derivatives capable of translocations in the host cavities

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Table of Contents

<table>
<thead>
<tr>
<th></th>
<th>Fig. S1 1H NMR spectrum of compound 1.</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>Fig. S2 1H NMR spectrum of compound 2.</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>Fig. S3 1H NMR spectrum of compound 3.</td>
<td>5</td>
</tr>
<tr>
<td>4</td>
<td>Fig. S4 1H NMR spectrum of compound 4.</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>Fig. S5 1H NMR spectrum of compound 5.</td>
<td>7</td>
</tr>
<tr>
<td>6</td>
<td>Fig. S6 13C NMR spectrum of compound 1.</td>
<td>8</td>
</tr>
</tbody>
</table>
7. Fig. S7 $^{13}$C NMR spectrum of compound 2.
8. Fig. S8 $^{13}$C NMR spectrum of compound 3.
9. Fig. S9 $^{13}$C NMR spectrum of compound 4.
10. Fig. S10 $^{13}$C NMR spectrum of compound 5.
11. Fig. S11 $^1$H NMR spectrum of complex (1)$_2$@CB[8]·6.5H$_2$O.
12. Fig. S12 $^1$H NMR spectrum of complex 2(5)$_2$@γ-CD-6H$_2$O.
13. Fig. S13 $^1$H NMR spectrum of complex (5)$_2$@CB[8]·5H$_2$O.
14. Fig. S14 $^1$H NMR spectra of compound 4 and its mixture with β-CD.
15. Fig. S15 $^1$H NMR spectra of compound 4 and its mixture with γ-CD.
16. Fig. S16 $^1$H NMR spectra of compound 5 and its mixture with β-CD.
17. Fig. S17 $^1$H NMR spectra of compound 5 and its mixture with γ-CD.
18. Fig. S18 $^1$H NMR spectra of compound 2 and its mixture with γ-CD.
19. Fig. S19 $^1$H NMR spectra of compound 5 and its mixtures with CB[7].
20. Fig. S20 $^1$H NMR spectrum of a mixture of compound 5 and CB[7].
21. Fig. S21 $^1$H NMR spectra of compound 2 and its mixture with CB[7].
22. Fig. S22 NOESY spectrum of a mixture of compound 3 and β-CD.
23. Fig. S23 Absorption spectrum of compound 1.
24. Fig. S24 Fluorescence spectrum of compound 1.
25. Fig. S25 Absorption and fluorescence spectra of compound 2 and complex 2@β-CD.
26. Fig. S26 Absorption and fluorescence spectra of compound 4 and complex 4@β-CD.
27. Fig. S27 Absorption and fluorescence spectra of compound 5 and complex 5@β-CD.
28. Fig. S28 Absorption and fluorescence spectra of compound 2 and complex 2@γ-CD.
29. Fig. S29 Absorption and fluorescence spectra of compound 4 and complex 4@γ-CD.
30. Fig. S30 Absorption and fluorescence spectra of compound 5 and complex 5@γ-CD.
31. Fig. S31 Absorption and fluorescence spectra of compound 2 and complexes 2@CB[7] and 2@(CB[7])$_2$.
32. Fig. S32 Absorption and fluorescence spectra of compound 4 and complexes 4@CB[7] and 4@(CB[7])$_2$.
33. Fig. S33 Absorption and fluorescence spectra of compound 5 and complexes 5@CB[7] and 5@(CB[7])$_2$.
34. Fig. S34 Absorption and fluorescence spectra of compound 5 and complexes 5@CB[8] and (5)$_2$@CB[8].
Fig. S1 $^1$H NMR spectrum of compound 1 (500.13 MHz, DMSO-$d_6$, 25 °C).
**Fig. S2** $^1$H NMR spectrum of compound 2 (500.13 MHz, DMSO-$d_6$, 26 °C).
Fig. S3 $^1$H NMR spectrum of compound 3 (500.13 MHz, DMSO-$d_6$, 26 °C).
Fig. S4 $^1$H NMR spectrum of compound 4 (500.13 MHz, DMSO-$d_6$, 26 °C).
Fig. S5 $^1$H NMR spectrum of compound 5 (500.13 MHz, DMSO-$d_6$, 28 °C).
Fig. S6 $^{13}$C NMR spectrum of compound 1 (125.76 MHz, DMSO-$d_6$, 25 °C).
Fig. S7 $^{13}$C NMR spectrum of compound 2 (125.76 MHz, DMSO-$d_6$, 26 °C).
Fig. S8 $^{13}$C NMR spectrum of compound 3 (125.76 MHz, DMSO-$d_6$, 25 °C).
Fig. S9 $^{13}\text{C}$ NMR spectrum of compound 4 (125.76 MHz, DMSO-$d_6$, 25 °C).
Fig. S10 $^{13}$C NMR spectrum of compound 5 (125.76 MHz, DMSO-$d_6$, 26 °C).
Fig. S11 $^1$H NMR spectrum of complex $(1)_2@CB[8] \cdot 6.5\text{H}_2\text{O}$, which was obtained by crystallization ($C_{\text{complex}} = 3 \times 10^{-4} \text{ M}$), $\text{D}_2\text{O}$, 25 °C.
Complex 2(5)·γ-CD

Fig. S12 $^1$H NMR spectrum of complex 2(5)@γ-CD·6H$_2$O, which was obtained by crystallization ($C_{\text{complex}} = 3 \times 10^{-4}$ M), D$_2$O, 25 °C.
Complex (5)$_2$@CB[8]

Fig. S13 $^1$H NMR spectrum of complex (5)$_2$@CB[8]·5H$_2$O, which was obtained by crystallization (sat., $C_{\text{complex}} < 1\times10^{-4}$ M), D$_2$O, 25 °C.
Fig. S14 $^1$H NMR spectra ((a, b) aromatic and (c, d) aliphatic proton regions) of (a, c) compound 4 and (b, d) a 1:6.0 mixture of compound 4 and $\beta$-CD ($C_4 = 5.0 \times 10^{-3}$ M), D$_2$O–MeCN-$d_3$ (10:1, v/v), 25 °C.

Fig. S15 $^1$H NMR spectra ((a, b) aromatic and (c, d) aliphatic proton regions) of (a, c) compound 4 and (b, d) a 1:7.4 mixture of compound 4 and $\gamma$-CD ($C_4 = 4.3 \times 10^{-4}$ M), D$_2$O–MeCN-$d_3$ (10:1, v/v), 25 °C.
Fig. S16 $^1$H NMR spectra ((a, b) aromatic and (c, d) aliphatic proton regions) of (a, c) compound 5 and (b, d) a 1:5.8 mixture of compound 5 and β-CD ($C_5 = 5.2\times10^{-4}$ M), D$_2$O–MeCN-d$_3$ (10:1, v/v), 25 °C.

Fig. S17 $^1$H NMR spectra ((a, b) aromatic and (c, d) aliphatic proton regions) of (a, c) compound 5 and (b, d) a 1:6.1 mixture of compound 5 and γ-CD ($C_5 = 5.2\times10^{-4}$ M), D$_2$O–MeCN-d$_3$ (10:1, v/v), 25 °C.
**Fig. S18** $^1$H NMR spectra ((a, b) aromatic and (c, d) aliphatic proton regions) of (a, c) compound 2 and (b, d) a 1:6.5 mixture of compound 2 and γ-CD ($C_2 = 4.7 \times 10^{-4}$ M), D$_2$O–MeCN-$d_3$ (10:1, v/v), 25 °C.

**Fig. S19** $^1$H NMR spectra (aromatic proton region) of (a) compound 5 and (b) 1:0.7 and (c) 1:1.9 mixtures of compound 5 and CB[7] ($C_s = 6.4 \times 10^{-4}$ M), D$_2$O–MeCN-$d_3$ (10:1, v/v), 25 °C.
Fig. S20 $^1$H NMR spectrum of a 1:1.9 mixture of compound 5 and CB[7] ($C_5 = 6.4 \times 10^{-4}$ M), D$_2$O–MeCN-$d_3$ (10:1, v/v), 25 °C.
Fig. S21 $^1$H NMR spectra of (a) compound 2 and (b) a 1:1.9 mixture of compound 2 and CB[7] ($C_2 = 5.7 \times 10^{-3}$ M), D$_2$O–MeCN-$d_3$ (10:1, v/v), 25 °C.
Fig. S22 NOESY spectrum of an equimolar mixture of compound 3 and β-CD ($C_3 = C_{CD} = 6 \times 10^{-3}$ M), D$_2$O, 25 °C.
Fig. S23  Absorption spectrum of compound 1 ($C = 2 \times 10^{-5}$ M), water, ambient temperature, 1-cm quartz cell.

Fig. S24  Fluorescence spectrum of compound 1 ($C = 1 \times 10^{-6}$ M), water, ambient temperature. The fluorescence was excited by light at 356 nm.
Fig. S25 (a) Absorption and (b) fluorescence spectra of compound 2 \((C_2 = 2 \times 10^{-5} \text{ M for absorption and } C_2 = 1 \times 10^{-5} \text{ M for fluorescence})\) and respective evaluated spectra of complex 2@β-CD, water, ambient temperature. The fluorescence was excited by light at 313 nm.
Fig. S26 (a) Absorption and (b) fluorescence spectra of compound 4 (C₄ = 2×10⁻⁵ M for absorption and C₄ = 1×10⁻⁵ M for fluorescence) and respective evaluated spectra of complex 4@β-CD, water, ambient temperature. The fluorescence was excited by light at 319 nm.
Fig. S27 (a) Absorption and (b) fluorescence spectra of compound 5 ($C_5 = 2 \times 10^{-5}$ M for absorption and $C_5 = 1 \times 10^{-5}$ M for fluorescence) and respective evaluated spectra of complex 5@β-CD, water, ambient temperature. The fluorescence was excited by light at 311 nm.
**Fig. S28** (a) Absorption and (b) fluorescence spectra of compound 2 ($C_2 = 2 \times 10^{-5}$ M for absorption and $C_2 = 1 \times 10^{-5}$ M for fluorescence) and respective evaluated spectra of complex $2@\gamma$-CD, water, ambient temperature. The fluorescence was excited by light at 332 nm.
**Fig. S29** (a) Absorption and (b) fluorescence spectra of compound 4 ($C_4 = 2 \times 10^{-5}$ M for absorption and $C_4 = 1 \times 10^{-5}$ M for fluorescence) and respective evaluated spectra of complex 4@γ-CD, water, ambient temperature. The fluorescence was excited by light at 319 nm.
Fig. S30 (a) Absorption and (b) fluorescence spectra of compound 5 ($C_5 = 2 \times 10^{-5}$ M for absorption and $C_5 = 1 \times 10^{-5}$ M for fluorescence) and respective evaluated spectra of complex 5@γ-CD, water, ambient temperature. The fluorescence was excited by light at 321 nm.
Fig. S31 (a) Absorption and (b) fluorescence spectra of compound 2 ($C_2 = 2 \times 10^{-5}$ M for absorption and $C_2 = 1 \times 10^{-6}$ M for fluorescence) and respective evaluated spectra of complexes $2@CB[7]$ and $2@(CB[7])_2$, water, ambient temperature. The fluorescence was excited by light at 356 nm.
Fig. S32 (a) Absorption and (b) fluorescence spectra of compound 4 ($C_4 = 2 \times 10^{-5}$ M for absorption and $C_4 = 1 \times 10^{-6}$ M for fluorescence) and respective evaluated spectra of complexes 4@CB[7] and 4@(CB[7])$_2$, water, ambient temperature. The fluorescence was excited by light at 356 nm.
Fig. S33 (a) Absorption and (b) fluorescence spectra of compound 5 (C₅ = 2×10⁻⁵ M for absorption and C₅ = 1×10⁻⁶ M for fluorescence) and respective evaluated spectra of complexes 5@CB[7] and 5@(CB[7])₂, water, ambient temperature. The fluorescence was excited by light at 359 nm.
Fig. S34 (a) Absorption and (b) fluorescence spectra of compound 5 \((C_5 = 2 \times 10^{-5} \text{ M for absorption and } C_5 = 1 \times 10^{-6} \text{ M for fluorescence})\) and respective evaluated spectra of complexes 5@CB[8] and \((5)_2@CB[8]\) (per molecule of naphthylpyridine derivative), water, ambient temperature. The fluorescence was excited by light at 333 nm.