Electronic Supplementary Information for


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1. Synthesis and Characterization of Rotaxanes

Materials and Instruments

γ-Cyclodextrin, dimethyl naphthalene-2, 6-dicarboxylate, 2-(Tert-butylamino) ethanol were purchased from Tokyo Chemical Industry and were vacuum-dried before use. Amino acids and HAS were purchased from Solarbio (Shanghai, China). CB [6] and compound 6 was prepared according to the literature method. \(^1\)H and \(^{13}\)C NMR spectra were recorded at room temperature on Bruker AMX-400 (operating at 400 MHz for \(^1\)H NMR and 101 MHz for \(^{13}\)C NMR) with TMS as the internal standard. HRMS data were measured in waters-Q-TOF Premiers (ESI) and MALDI-TOF-MS spectrometers. UV-vis. spectra were recorded using a JASCO V650 spectrometer. Circular dichroism spectra were measured on a JASCO J-1500 spectrometer. Fluorescence and phosphorescence spectra were taken on a Fluoromax-4 spectrofluorometer or a JASCO FP-8500 spectrofluorometer. The bandwidth for the measurement was not fixed. Fluorescence and phosphorescence lifetime decay were taken on the Fluoromax-4 spectrofluorometer. The phosphorescence spectra were measured by bubbling Ar gas over 10 min in an ice bath to remove dissolved oxygen. Titration calorimetry measurements were performed with a VP-ITC calorimeter.

Synthesis and characterizations of 1, 2, 3, 4, 5, Rot0, Rot1, Rot2, Rot3, Rot4:

\[
\begin{align*}
\text{Naphthalene -2, 6-diyldimethanol:} & \quad \text{Dimethyl naphthalene-2, 6-dicarboxylate (2 g) was dissolved in THF (50 ml), and the resulting solution was cooled with ice-bath. LiAlH}_4\,(2.3 g) \text{ was then added in batches under stirring. The reaction mixture was stirred at room temperature for 30h. Methanol (50 ml) was added to quench the reaction and NaOH (1.0 g) was added. The precipitate was filtered and washed by dichloromethane, and the filtrate was collected. The solvent was removed under reduced pressure, and the resulting white solid (965 mg) were collected.}^{1}\text{H NMR (400 MHz, CD}_3\text{OD):} \delta =7.78 \,(s, 1H), \,7.75 \,(d, J = 6.7 \text{ Hz, 3H}), \,7.44 \,(d, J = 1.3 \text{ Hz, 1H}), \,4.71 \,(s, 4H). \\
\text{2, 6-bis (chloromethyl) naphthalene:} & \quad \text{Naphthalene-2, 6-diyldimethanol (800 mg) was dissolved in SOCl}_2\,(5 ml), \text{ and the mixture was reacted at 40 \text{ ºC} \text{ for 6 h. SOCl}_2 \text{ was removed under reduced pressure, and the crude product was purified by column chromatography to give the product as white solid (320.5 mg).}^{1}\text{H NMR (400 MHz, CD}_3\text{OD) \delta =7.87 \,(d, J = 8.5 \text{ Hz, 4H}), \,7.56 \,(d, J = 1.3 \text{ Hz, 1H}), \,7.54 \,(d, J = 1.5 \text{ Hz, 1H}), \,4.80 \,(s, 4H).} \\
\text{Compound 5:} & \quad \text{2, 6-bis (chloromethyl) naphthalene (160 mg) was dissolved in ethanol (1.0 ml) and 2-propynylamine (2 ml) was added under stirring. The mixture was reacted at 80 \text{ ºC} \text{ for 10 h under nitrogen, then the solvent was removed under reduced pressure. The crude product was} 
\end{align*}
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purified by column chromatography (ethyl acetate: methanol=8:1) to afford the product (102 mg) as white solid. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$=7.80 – 7.76 (m, 3H), 7.48 (dd, $J$ = 8.4, 1.3 Hz, 2H), 7.26 (s, 1H), 4.05 (s, 4H), 3.47 (d, $J$ = 2.4 Hz, 4H), 2.29 (t, $J$ = 2.4 Hz, 2H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 136.67, 132.74, 128.02, 126.97, 126.71, 82.04, 71.70, 52.34, 37.34, 29.71. HRMS (ESI). calcd for [M + H]$^+$ m/z = 263.1543, found m/z = 263.1544.

SOCl$_2$, CHCl$_3$ 75$^\circ$C

H$_2$ O

H$_2$ N

SOCl$_2$, CHCl$_3$ 75$^\circ$C

NaN$_3$, DMF 75$^\circ$C

H$_2$ N

N-(2-Chloroethyl)-2-methylpropan-2-aminium chloride: 2-(Tert-butylamino) ethanol (10.0 g, 85.5 mmol) was dissolved in CHCl$_3$ (150 ml). To the resulting ice-bath cooled solution was added dropwise SOCl$_2$ (15 ml, 197.5 mmol). The mixture was heated to reflux for 24 h, after which excess SOCl$_2$ and solvent were removed under reduced pressure. The resulting crude product was recrystallized from acetone to yield the compound as a white powder (8.5 g, 54.4%). $^1$H NMR (400 MHz, D$_2$O) $\delta$=3.87 (t, $J$ = 5.3 Hz, 2H), 3.45 (t, $J$ = 5.2 Hz, 2H), 1.38 (s, 9H). $^{13}$C NMR (101 MHz, D$_2$O) $\delta$ 57.9, 43.2, 39.9, 24.8. HRMS (ESI): calcd for [M - Cl]$^+$, m/z =136.0888, found m/z =136.0878.

Compound 4: Sodium azide (2 g, 30.8 mmol) was add to a solution of N-(2-chloroethyl)-2-methylpropan-2-aminium chloride (2.0 g, 11.6 mmol) in 80 ml ethanol, and the mixture was stirred at 75$^\circ$C for 15 h. After the removal of solvent under reduced pressure, 10 ml water was added to dissolve the crude product, which was then subjected to a reverse-phase flash column chromatography (cosmosil 75C$_{18}$-PREP) with pure water to afford 4 as a white powder (1.3 g, 63%). $^1$H NMR (400 MHz, D$_2$O) $\delta$ = 5.08 (d, $J$ = 3.9 Hz, 1H), 4.98 (d, $J$ = 3.3 Hz, 7H), 3.87 – 3.68 (m, 30H), 3.61 – 3.32 (m, 20H). $^{13}$C NMR (101 MHz, D$_2$O) $\delta$ 101.51, 84.36, 80.74, 79.99, 72.8, 72.22, 71.92, 71.67, 70.09, 60.52, 60.30, 16.82, 16.62. HRMS (ESI): calcd for [M - Cl]$^+$, m/z =143.1291, found m/z = 143.1295. 

Compound 2: 6-mono-sulfonylation-$\gamma$-CD(100 mg) was dissolved in DMF(2 ml). After the mixture was stirred, sodium iodide (600 mg) was added. The mixture was reacted to 80 $^\circ$C and refluxed for 10h. The solvent were removed under reduced pressure. The crude product was subjected to reversed-phase flash column chromatography (cosmosil 75C$_{18}$-PREP) with a gradient elution from 0 % aqueous ethanol to 35 % aqueous ethanol to afford 2 (55.5 mg) as a white solid. $^1$H NMR (400 MHz, D$_2$O) $\delta$ = 5.08 (d, $J$ = 3.9 Hz, 1H), 4.98 (d, $J$ = 3.3 Hz, 7H), 3.87 – 3.68 (m, 30H), 3.61 – 3.32 (m, 20H). $^{13}$C NMR (101 MHz, D$_2$O) $\delta$ 101.51, 84.36, 80.74, 79.99, 72.8, 72.22, 71.92, 71.67, 70.09, 60.52, 60.30, 16.82, 16.62. HRMS (ESI). calcd for [M + Na]$^+$, m/z = 1429.3141, found m/z = 1429.3940. [M+K]$^+$, m/z = 1445.2880, found m/z = 1445.3777.
Compound 3: 6\(^\Delta\), 6\(^\Delta\)-Dideoxy-6\(^\Delta\), 6\(^\Delta\)-disulfonylation-\(\gamma\)-CD (100 mg) was dissolved in DMF (1.5 ml). After the mixture was stirred, sodium iodide (600 mg) was added. The mixture was reacted to 80 \(^\circ\)C and refluxed for 10 h. The solvent were removed under reduced pressure. The crude product was subjected to reversed-phase flash column chromatography (cosmosil 75C18-PREP) with a gradient elution from 0% aqueous ethanol to 35% aqueous ethanol to afford Rot1: Compound 4 (10 mg), compound 5 (10 mg), and CB [6] (100 mg) were mixed in 5 ml water. The reaction mixture was stirred at 50 \(^\circ\)C for 4 h to give a homogenous solution. Then the mixture was subjected to reversed-phase flash column chromatography (cosmosil 75C18-PREP) with pure water to afford the targeted rotaxane. Rot0: Compound 4 (10 mg), compound 5 (10 mg), and CB [6] (100 mg) were mixed in 5 ml water. The reaction mixture was stirred at 50 \(^\circ\)C for 4 h to give a homogenous solution. Then the mixture was subjected to reversed-phase flash column chromatography (cosmosil 75C18-PREP) with pure water to afford the targeted rotaxane.
mixed in 5 ml water. The reaction mixture was stirred at 50 °C for 3 h to give a homogenous solution. Then the mixture was subjected to reversed-phase flash column chromatography (cosmosil 75C₁₈-PREP) with pure water to afford the targeted rotaxane. ¹H NMR (400 MHz, D₂O) δ 8.26 (s, 1H), 8.20 (s, 1H), 7.91 – 7.84 (m, 2H), 7.73 (d, J = 8.3 Hz, 1H), 7.64 (d, J = 8.6 Hz, 1H), 6.47 (d, J = 5.0 Hz, 2H), 5.63 (dt, J = 15.3, 13.2 Hz, 24H), 5.39 (d, J = 7.3 Hz, 24H), 4.94 (d, J = 3.7 Hz, 8H), 4.59 – 4.46 (m, 4H), 4.28 – 4.05 (m, 32H), 3.78 (s, 3H), 3.65 (d, J = 15.3 Hz, 25H), 3.57 (dd, J = 9.8, 3.6 Hz, 8H), 3.47 (d, J = 6.5 Hz, 16H), 1.50 (d, J = 5.1 Hz, 18H). ¹³C NMR (151 MHz, D₂O) δ 156.45,156.13, 138.71, 138.37, 133.25, 132.79, 131.13, 130.64, 129.75, 129.14, 128.79, 128.33, 127.83, 127.17, 120.89, 120.63, 102.50, 81.16, 73.09, 72.21, 71.91, 70.15, 59.72, 58.73, 58.43, 53.60, 52.92, 51.33, 51.07 ,50.88, 47.59, 47.43, 42.76, 39.97, 39.78, 25.19, 24.66. HRMS (ESI) of compound Rot1. calcd for [M - 4Cl]⁺, m/z = 960.1087, found m/z = 960.3503.

Rot2: Compound 4 (10 mg), compound 5 (10 mg), CB [6] (100 mg), and compound 2 (120 mg) were mixed in 5 ml water. The reaction mixture was stirred at 55 °C for 5 h to give a homogenous solution. The crude product was subjected to reversed-phase flash column chromatography (cosmosil 75C₁₈-PREP) with a gradient elution from 0% aqueous ethanol to 50% aqueous ethanol to afford Rot2 (56 mg) as a white solid. ¹H NMR (400 MHz, D₂O) δ 8.34 (s, 1H), 7.92 (dd, J = 15.2, 8.0 Hz, 2H), 7.81 (d, J = 8.5 Hz, 1H), 7.70 (d, J = 8.5 Hz, 1H), 6.51 (d, J = 6.6 Hz, 2H), 5.67 (dt, J = 15.4, 12.0 Hz, 21H), 5.42 (dd, J = 7.1, 4.0 Hz, 20H), 5.07 (d, J = 4.1 Hz, 1H), 5.04 – 4.92 (m, 6H), 4.62 – 4.48 (m, 6H), 4.32 – 4.07 (m, 28H), 3.91 – 3.45 (m, 40H), 3.92 (dd, J = 16.0, 9.6 Hz, 4H), 3.17 – 3.03 (m, 2H), 1.54 (d, J = 5.0 Hz, 15H). ¹³C NMR (101 MHz, D₂O) δ 170.96, 156.58, 156.55, 155.95, 138.71, 120.87, 120.65, 102.69, 102.39, 81.49, 80.95, 73.15, 72.48, 72.14, 71.95, 70.55, 69.66, 59.80, 51.52, 51.20, 47.80, 47.61, 47.44, 42.78, 39.96, 25.18. HRMS (ESI) of compound Rot2. calcd for [M - Cl]⁺, m/z = 4055.2446, found m/z = 4055.2655.
Rot3: Compound 4 (10 mg), compound 5 (10 mg), CB [6] (100 mg), and compound 3 (130 mg) were mixed in 5ml water. The reaction mixture was stirred at 55 °C for 5 h to give a homogenous solution. The crude product was subjected to reversed-phase flash column chromatography (cosmosil 75C18-PREP) with a gradient elution from 0% aqueous ethanol to 50% aqueous ethanol to afford Rot3 (50 mg) as a white solid. 1H NMR (400 MHz, D2O) δ 8.38 – 8.20 (m, 4H), 8.08 – 7.61 (m, 4H), 6.48 (d, J = 8.5 Hz, 2H), 5.79 – 5.53 (m, 24H), 5.42 (d, J = 4.4 Hz, 24H), 5.11 – 4.88 (m, 7H), 4.33 – 4.02 (m, 32H), 3.96 – 2.99 (m, 46H), 1.52 (d, J = 4.7 Hz, 18H). 13C NMR (101 MHz, D2O) δ 156.35, 141.69, 141.02, 138.72, 138.20, 131.89, 131.64, 130.72, 130.06, 126.70, 102.60, 81.27, 73.12, 72.31, 72.00, 70.18, 59.80, 58.73, 58.41, 51.93 – 50.85, 47.60, 42.62, 40.01, 39.77, 25.23. HRMS (ESI) of Rot3. calcd for [M-3Cl]+, m/z = 1365.0692, found m/z = 1365.0407.

Rot4: Compound 6 (10 mg), compound 4 (10 mg), CB [6] (100 mg), and compound 3 (130 mg) were mixed in 5 ml water. The reaction mixture was stirred at 55 °C for 5 h to give a homogenous solution. The crude product was subjected to reversed-phase flash column chromatography (cosmosil 75C18-PREP) with a gradient elution from 0% aqueous ethanol to 50% aqueous ethanol to afford Rot4 (50 mg) as a white solid. 1H NMR (400 MHz, D2O) δ 7.88 (t, J = 7.2 Hz, 4H), 7.64 – 7.56 (m, 4H), 6.48 (d, J = 9.0 Hz, 2H), 5.66 (dt, J = 15.4, 10.5 Hz, 24H), 5.43 (d, J = 8.4 Hz, 24H), 4.99 (dd, J = 34.3, 6.4 Hz, 9H), 4.46 (s, 4H), 4.33 (t, J = 6.0 Hz, 2H), 4.25 – 4.06 (m, 29H), 3.86 – 3.43 (m, 58H), 3.12 – 3.06 (m, 4H), 1.52 (d, J = 6.2 Hz, 17H). 13C NMR (101 MHz, D2O) δ 156.35, 141.64, 141.02, 138.72, 138.20, 131.89, 131.64, 130.72, 130.06, 126.79, 102.60, 81.27, 73.12, 72.31, 72.00, 70.18, 59.80, 58.73, 58.41, 51.93 – 50.85, 47.60, 42.62, 40.01, 39.77, 25.23. HRMS (ESI) of Rot4. calcd for [M–3Cl]+, m/z = 1373.7411, found m/z = 1373.3156.
**Fig. S1.** $^1$H NMR spectrum of naphthalene-2,6-diylmethanol measured in CD$_3$OD at 25 °C.

**Fig. S2.** $^1$H NMR spectrum of 2,6-bis(chloromethyl)naphthalene measured in CD$_3$OD at 25 °C.
Fig. S3. $^1$H NMR spectrum of compound 5 measured in CDCl$_3$ at 25 °C.

Fig. S4. $^{13}$C NMR spectrum of compound 5 measured in CDCl$_3$ at 25 °C.
**Fig. S5.** HRMS spectrum of compound 5.

**Fig. S6.** $^1$H NMR spectrum of $N$-(2-Chloroethyl)-2-methylpropan-2-aminium chloride measured in D$_2$O at 25 °C.
Fig. S7. $^1$H NMR spectrum of compound 4 measured in D$_2$O at 25 °C.

Fig. S8. $^{13}$C NMR spectrum of compound 4 measured in D$_2$O at 25 °C.
Fig. S9. HRMS spectrum of compound 4.

Fig. S10. $^1$H NMR spectrum of compound 2 measured in D$_2$O at 25 °C.
Fig. S11. $^{13}$C NMR spectrum of compound 2 measured in D$_2$O at 25 ºC.

Fig. S12. HRMS spectrum of compound 2.
Fig. S13. $^1$H NMR spectrum of compound 3 measured in D$_2$O at 25 °C.

Fig. S14. $^{13}$C NMR spectrum of compound 3 measured in D$_2$O at 25 °C.
Fig. S15. HRMS spectrum of compound 3.

Fig. S16. $^1$H NMR spectrum of Rot0 measured in D$_2$O at 25 °C.
Fig. S17. $^{13}$C NMR spectrum of Rot0 measured in D$_2$O at 25 °C.

Fig. S18. HRMS spectrum of Rot0.
Fig. S19. $^1$H NMR spectrum of Rot1 measured in D$_2$O at 25 °C.

Fig. S20. $^{13}$C NMR spectrum of Rot1 measured in D$_2$O at 25 °C.
Fig. S21. HRMS spectrum of Rot1.

Fig. S22. $^1$H NMR spectrum of Rot2 measured in D$_2$O at 25 °C.
Fig. S23. $^{13}$C NMR spectrum of Rot2 measured in D$_2$O at 25 °C.

Fig. S24. HRMS spectrum of Rot2.
Fig. S25. $^1$H NMR spectrum of Rot3 measured in D$_2$O at 25 °C.

Fig. S26. $^{13}$C NMR spectrum of Rot3 measured in D$_2$O at 25 °C.
**Fig. S27.** HRMS spectrum of Rot3.

**Fig. S28.** $^1$H NMR spectrum of Rot4 measured in D$_2$O at 25 °C.
Fig. S29. $^{13}$C NMR spectrum of Rot4 measured in D$_2$O at 25 °C.

Fig. S30. HRMS spectrum of Rot4.

2. UV-vis, fluorescence, and RTP spectra of rotaxanes
Fig. S31. UV-vis spectra of Rot0 (10 μM), Rot1 (10 μM), Rot2 (10 μM) and Rot3 (10 μM) in water at 25°C.

Fig. S32. Left: Fluorescence spectra of Rot3 (10 μM) upon addition of L-His from 0-0.0222 M at λ<sub>ex</sub> = 280 nm in water at 25°C. Excitation and emission bandwidths are 2.5 nm. Right: Fluorescence spectra of Rot3 (10 μM) upon addition of L-Met from 0-0.0237 M at λ<sub>ex</sub> = 280 nm in water at 25°C. Excitation and emission bandwidths are 2.5 nm and 2.0 nm, respectively. All spectra were measured with the Fluoromax-4 spectrofluorometer.

Fig. S33. Left: Fluorescence spectra of Rot3 (10 μM) upon addition of L-Lys from 0-0.0237 M at λ<sub>ex</sub> = 280 nm in water at 25°C. Excitation and emission bandwidths are 3.0 nm and 3.0 nm, respectively. Right: Fluorescence spectra of Rot3 (10 μM) upon addition of L-Leu from 0-0.0222M at λ<sub>ex</sub> = 280 nm in water at 25°C, Excitation and emission bandwidths are 2.5 nm and 1.0 nm.
respectively. All spectra were measured with the Fluoromax-4 spectrofluorometer.

**Fig. S34.** Phosphorescence spectra of Rot3 5 μM and Rot3 5 μM mixed HSA (0.5, 1.0, 1.5, 2.0 mg/ml) in deaerated water at λ<sub>ex</sub> = 280 nm at 25 °C.

**Fig. S35.** Phosphorescence spectra of Rot3 (20 μM) in the simulated human blood serum solution upon addition of Trp (0-200 μM) at 25 °C. λ<sub>ex</sub> = 280 nm. Inset: Phosphorescence intensity change at 530 nm as a function of the reciprocal of Trp concentration.
Fig. S36 UV-vis spectra of 6 mM Rot3 (black) upon addition of L-Trp (0 eq, 0.25 eq, 0.5 eq, 1.0 eq, 1.5 eq, 2.5 eq and 3.5 eq) and 6 mM Trp (red) in water at 25°C. Inset: partial UV-vis spectra in the wavelength range from 320 nm to 355 nm.
Fig. S37. Fluorescence spectra of Rot3 (5 μM) upon increasing the concentration of L-Trp in water (5 μM–10 μM) at λex = 280 nm at 25 °C, measured with the JASCO FP-8500 spectrofluorometer.

Fig. S38 Fluorescence spectra of 10 μM Rot3 (black) upon addition of L-Trp (5 μM–160 μM) at λex = 322 nm in water at 25°C, measured with the JASCO FP-8500 spectrofluorometer.
**Fig. S39.** Fluorescence spectra of Rot3 (5 μM) mixed amino acid that mimic of the human bloodstream without L-Tryptophan in water with the addition of Tryptophan (0–0.5 mM) at λ<sub>ex</sub> = 280 nm at 25 °C, measured with the JASCO FP-8500 spectrofluorometer.

**Fig. S40.** Lifetime decay curves of Compound 5 in water, excited at 280 nm and monitoring at 340 nm. CHISQ=1.06, $\tau$ =38.7 ns.
**Fig. S41.** Lifetime decay curves of Rot0 in water, excited at 280 nm and monitoring at 340 nm. 
CHISQ=1.13, $\tau$ =39.0 ns

**Fig. S42.** Lifetime decay curves of Rot1 in water, excited at 280 nm and monitoring at 340 nm. 
CHISQ=1.10, $\tau$=50.9 ns.

**Fig. S43.** Lifetime decay curves of Rot2 in water, excited at 280 nm and monitoring at 340 nm. 
CHISQ=1.05. $\tau_1$=5.7 ns, $\tau_2$=40.6 ns, $A_1$=35.31%, $A_2$=64.69%
**Fig. S44.** Lifetime decay curves of Rot3 in water, excited at 280 nm and monitoring at 340 nm. CHISQ=1.11. $\tau_1=4.7$ ns, $\tau_2=39.7$ ns, $A_1=21.02\%$, $A_2=78.98\%$.

**Fig. S45.** Lifetime decay curves of Rot4 in water, excited at 280 nm and monitoring at 315 nm. CHISQ=1.01. $\tau_1=5.0$ ns, $\tau_2=8.2$ ns, $A_1=27.23\%$, $A_2=72.77\%$.

**Fig. S46.** Phosphorescence lifetime decay curves of Rot2 (10 µM) in deaerated water, excited at 280 nm and monitoring at 530 nm. CHISQ=1.09. Average lifetime=2.0 ms.
Fig. S47. Phosphorescence lifetime decay curves of Rot3 (10 μM) in deaerated water, excited at 280 nm and monitoring at 530 nm. CHISQ=1.10. Average lifetime=2.5 ms.

3. Complexation Studies of Rotaxanes with Amino Acids

Calculation of the Gibbs free energy change of photoinduced electron transfer.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>$E_{1/2}(X^+/X)$</th>
<th>$E_{1/2}(X/X^-)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>L-Tryptophan</td>
<td>+0.97V</td>
<td>-</td>
</tr>
<tr>
<td>Naphthalene,2,7-dimethyl</td>
<td>-</td>
<td>-2.49V</td>
</tr>
</tbody>
</table>

$\Delta G = 23.05 [(E_{1/2} (D^+/D) - E_{1/2} (A/A^-)) - \frac{e^2}{\varepsilon \alpha} + \Delta E_{0,0}]$

Where $e^2/\varepsilon \alpha$ is Coulomb energy released by ion entering collision distance, the value is probably 0.06V. $\Delta E_{0,0}$ is the excited state energy of the electron donor or acceptor. It is estimated from its fluorescence emission and UV spectra, the value is probably 4.19V (404.2 kJ·mol$^{-1}$). Hence, the value of $\Delta G$ is -76.2 kJ·mol$^{-1}$. 


**Fig. S48.** ITC titration data for the complexation of host Rot3 (1 mM) with for L-Phe (20 mM) in aqueous solution at 25 °C.

**Fig. S49.** ITC titration data for the complexation of host Rot3 (1 mM) with for L-His (20 mM) in aqueous solution at 25 °C.
**Fig. S50.** ITC titration date for the complexation of host Rot3 (5 mM) with for L-Trp (15 mM) in aqueous solution at 25 °C.

**Reference**