Supporting Information for

Multistep Chirality Transfer in Pillar[5]arene with Halogen-modulated Flipping Kinetics of Ring Units

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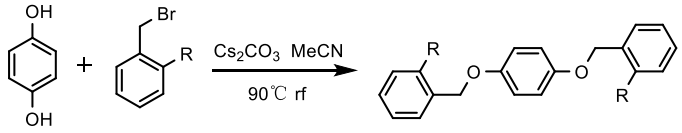
1 General information

Chemicals and instruments: All of the chemicals used for synthesis were analytically pure and were used as received. Solvents were dried and distilled before use for synthesis. ^{1}H NMR and ^{13}C NMR spectra were recorded at room temperature on a Bruker AMX–400 (operating at 400 MHz for ^{1}H NMR and 101 MHz for ^{13}C NMR) in $CDCl_3$ and/or CD3OD with TMS as internal standard. HRMS were measured with a Waters–Q–TOF Premiers (ESI). Single crystal X-ray data sets were collected on a Bruker D8 Venture rotating anode diffractometer. UV-vis spectra were obtained on JASCO V–650. CD spectra and binding constants with CD titration were acquired using J1500 CD spectrometer.

The single crystal structure of P1-P5 can be found at the Cambridge Crystallographic Data Centre, CCDC numbers: 2323526, 2323535, 2323538, 2323573, 2323543. All the chemicals were obtained from suppliers, used without further purification in case of analysis investigation. Solvents were distilled before used for analysis.

2 Synthesis and structure characterization data of the host



M1, R=H
M2, R=F
M3, R=Cl
M4, R=Br

Synthesis of M1-M4

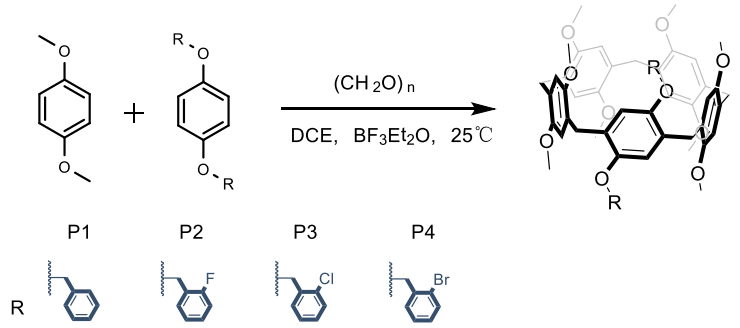
Hydroquinone (30 mmol, 3.32 g), Cs_2CO_3 (75 mmol, 24.44 g), and 2-halogen phenyl bromide (60 mmol) were mixed and refluxed in acetonitrile (300 mL) under a nitrogen atmosphere for 12 h. After cooling, the reaction mixture was filtered and evaporated to give a white solid. The crude product was purified on a silica gel column (PE/DCM= 1/1, v/v), and the eluent was removed under vacuum to give compound **M1-M4** as a white solid (yield: 80%).

M1: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.32 (m, 10H), 6.91 (s, 4H), 5.02 (s, 4H). [1]

M2: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.50 (m, 2H), 7.33 (ddd, J = 7.6, 5.7, 3.6 Hz, 2H), 7.18 (td, J = 7.5, 1.0 Hz, 2H), 7.13 – 7.08 (m, 2H), 6.95 (s, 4H), 5.11 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.80, 159.35, 153.20, 129.86, 129.82, 129.77, 129.69, 124.37, 124.34, 116.01, 115.54, 115.33, 64.52, 64.48.

M3: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, J = 7.3, 1.9 Hz, 2H), 7.42 (dd, J = 7.4, 1.8 Hz, 2H), 7.34 – 7.29 (m, 4H), 6.96 (s, 4H), 5.15 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.18, 135.09, 132.69, 129.47, 129.03, 128.92, 127.07, 116.02, 67.94.

M4: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.56 (m, 1H), 7.36 (td, J = 7.6, 0.9 Hz, 1H), 7.21 (td, J = 7.9, 1.6 Hz, 1H), 6.96 (s, 1H), 5.12 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.15, 136.67, 132.73, 129.31, 129.03, 127.68, 122.42, 116.04, 77.36, 70.22.



Synthesis of Pn

Mn (2.00 g, 6.89 mmol), 1,4-dimethoxybenzene (5.71 g, 6 equiv), and paraformaldehyde (1.54 g, 21 equiv) were mixed in DCE at 25℃, stirring for five minutes and then adding boron trifluoride ether (4 ml). At the end of the reaction, washed with saturated sodium bicarbonate three times, the organic phase was dried over Na_2SO_4, and the solvent was removed under reduced pressure. The crude product was purified on a silica gel column, and the eluent was removed under vacuum to give **Pn** as a white solid**.**

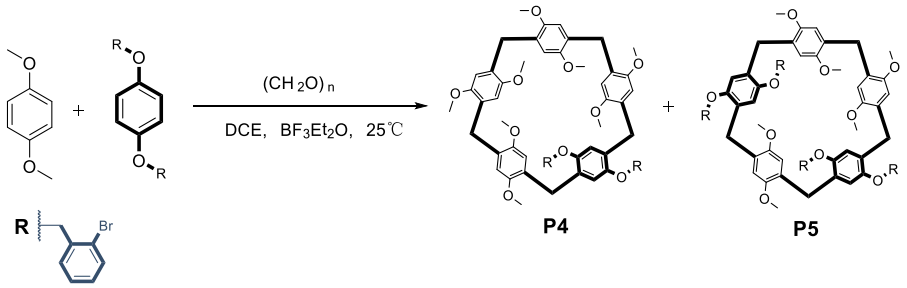
P1: The crude product was purified on a silica gel column (PE/DCM= 2/1, v/v), and the eluent was removed under vacuum to give compound **P1** as a white solid (yield: 30%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.41 (m, 4H), 7.35 (d, J = 6.3 Hz, 6H), 6.93 (s, 2H), 6.81 (s, 2H), 6.76 (s, 2H), 6.75 (s, 2H), 6.71 (s, 2H), 4.95 (s, 4H), 3.92 (d, J = 19.7 Hz, 2H), 3.78 (s, 2H), 3.75 (s, 4H), 3.71 (d, J = 7.1 Hz, 2H), 3.68 (s, 6H), 3.66 (s, 6H), 3.57 (s, 6H), 3.33 (s, 6H). ^{13}C NMR (101 MHz, CDCl3) δ 150.85, 150.78, 150.71, 150.15, 138.19, 128.95, 128.63, 128.54, 128.42, 128.36, 128.26, 128.07, 127.68, 127.31, 115.05, 114.06, 114.04, 113.97, 113.92, 70.39, 55.88, 55.83, 55.70, 55.41, 53.14, 39.62, 29.87, 29.77, 29.48, 27.06, 14.27. ESI -HRMS: m/z called for $[C_{57}H_{59}O_{10}]^+$, $[M+H]^+$: 903.4108, found: 903.4106; $[C_{57}H_{62}NO_{10}]^+$, $[M+NH_4]^+$: 920.4374, found: 920.4348.

P2: The crude product was purified on a silica gel column (PE/DCM= 3/1, v/v), and the eluent was removed under vacuum to give compound **P2** as a white solid (yield: 46%). ^{1}H NMR (400 MHz, CDCl3) δ 7.50 (t, J = 6.9 Hz, 2H), 7.32 (dd, J = 10.6, 4.8 Hz, 2H), 7.14 – 7.06 (m, 4H), 6.98 (s, 2H), 6.84 (s, 2H), 6.77 (d, J = 3.9 Hz, 4H), 6.72 (s, 2H), 5.07 (s, 4H), 3.93 (d, J = 12.6 Hz, 2H), 3.79 (d, J = 11.2 Hz, 8H), 3.71 (s, 6H), 3.68 (s, 6H), 3.61 (s, 6H), 3.40 (s, 6H). ^{13}C NMR (101 MHz, CDCl3) δ 150.88, 150.74, 150.70, 150.62, 150.03, 129.45, 129.40, 129.31, 129.23, 128.75, 128.44, 128.36, 128.26, 127.90, 125.42, 125.28, 124.34, 124.30, 115.28, 115.17, 115.07, 114.16, 113.91, 113.84, 113.79, 77.36, 64.28, 64.23, 55.91, 55.78, 55.50, 55.38, 53.09, 29.79, 29.75, 29.44. ESI-HRMS: m/z called for $[C_{57}H_{57}F_2O_{10}]^+$, $[M+H]^+$: 939.3920, found: 939.3918; $[C_{57}H_{60}NO_{10}]^+$, $[M+NH_4]^+$: 956.4185, found: 956.4172.

P3: The crude product was purified on a silica gel column (PE/DCM= 1/2, v/v), and the eluent was removed under vacuum to give compound **P3** as a white solid (yield: 40%). ^{1}H NMR (400 MHz, CDCl3) δ 7.53 (d, J = 7.6 Hz, 2H), 7.41 (d, J = 8.9 Hz, 2H), 7.24 (d, J = 7.6 Hz, 2H), 7.13 (d, J = 7.6 Hz, 2H), 6.97 (s, 2H), 6.85 (s, 2H), 6.77 – 6.74 (m, 6H), 5.10 (d, J = 12.3 Hz, 4H), 3.95 (d, J = 12.8 Hz, 2H), 3.81 (s, 2H), 3.77 (d, J = 7.4 Hz, 6H), 3.71 (s, 6H), 3.66 (s, 6H), 3.58 (s, 6H), 3.38 (s, 6H).^{13}C NMR (101 MHz, CDCl3) δ δ 150.96, 150.73, 150.55, 149.93, 135.82, 132.06,

129.20, 128.68, 128.63, 128.47, 128.45, 128.35, 128.17, 127.74, 127.03, 115.27, 114.31, 113.89, 113.79, 113.72, 77.36, 67.60, 55.94, 55.77, 55.39, 29.87, 29.34. ESI -HRMS: m/z called for $[C_{57}H_{57}Cl_2O_{10}]^+$, $[M+H]^+$: 971.3328, found: 971.3325; $[C_{57}H_{60}Cl_2NO_{10}]^+$, $[M+NH_4]^+$: 988.3594, found: 988.3577.

Synthesis of P4 and P5



The synthesis route is similar to **P1**. **M4** (2.0 g, 4.46 mmol), 1,4-dimethoxybenzene (3.85 g, 6 equiv). The crude product was purified on a silica gel column (PE/DCM= 1/1, V/V), and the eluent was removed under vacuum to give compounds **P4** and **P5** as white solid.

P4: yield 30%, ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (dd, J = 7.4, 1.8 Hz, 2H), 7.50 (d, J = 6.9 Hz, 2H), 7.17 (dd, J = 8.8, 4.5 Hz, 4H), 6.96 (s, 2H), 6.86 (s, 2H), 6.76 (d, J = 7.5 Hz, 6H), 5.24 (s, 4H), 3.80 (s, 2H), 3.77 (s, 4H), 3.73 (s, 2H), 3.72 (s, 6H), 3.72 (s, 2H), 3.67 (s, 6H), 3.58 (s, 6H), 3.39 (s, 6H). ^{13}CNMR (101 MHz, $CDCl_3$) δ 151.00, 150.74, 150.55, 149.86, 137.33, 132.43, 128.92, 128.66, 128.60, 128.50, 128.35, 128.15, 127.71, 127.63, 121.73, 115.28, 114.37, 113.91, 113.81, 113.73, 77.36, 69.85, 55.99, 55.81, 55.46, 55.43, 29.89, 29.32. ESI-HRMS: m/z called for $[C_{57}H_{57}Br_2O_{10}]^+$, $[M+H]^+$: 1059.2318, found: 1059.2316; $[C_{57}H_{60}Br_2NO_{10}]^+$, $[M+NH_4]^+$: 1076.2584, found: 1076.2568.

P5: yield 15%,^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 7.1 Hz, 2H), 7.49 (d, *J* = 6.8 Hz, 2H), 7.15 (d, *J* = 7.0 Hz, 4H), 6.94 (s, 2H), 6.84 (s, 2H), 6.75 (d, *J* = 7.4 Hz, 6H), 5.11 – 5.00 (m, 4H), 3.95 (d, *J* = 12.8 Hz, 2H), 3.78 (dd, *J* = 12.6, 8.7 Hz, 8H), 3.70 (s, 6H), 3.65 (s, 6H), 3.57 (s, 6H), 3.37 (s, 6H). ^{13}CNMR (101 MHz, CDCl3) δ 150.79, 150.47, 149.92, 149.74, 137.32, 132.52, 128.99, 128.55, 127.76, 127.60, 121.84, 115.45, 115.03, 113.97, 113.59, 77.36, 69.97, 69.77, 55.47, 55.19, 29.96, 29.49. ESI -HRMS: m/z called for m/z $[C_{57}H_{60}Br_2NO_{10}]^+$, $[M+NH_4]^+$: 1384.1420, found: 1384.1451

3 NMR and HRMS spectra

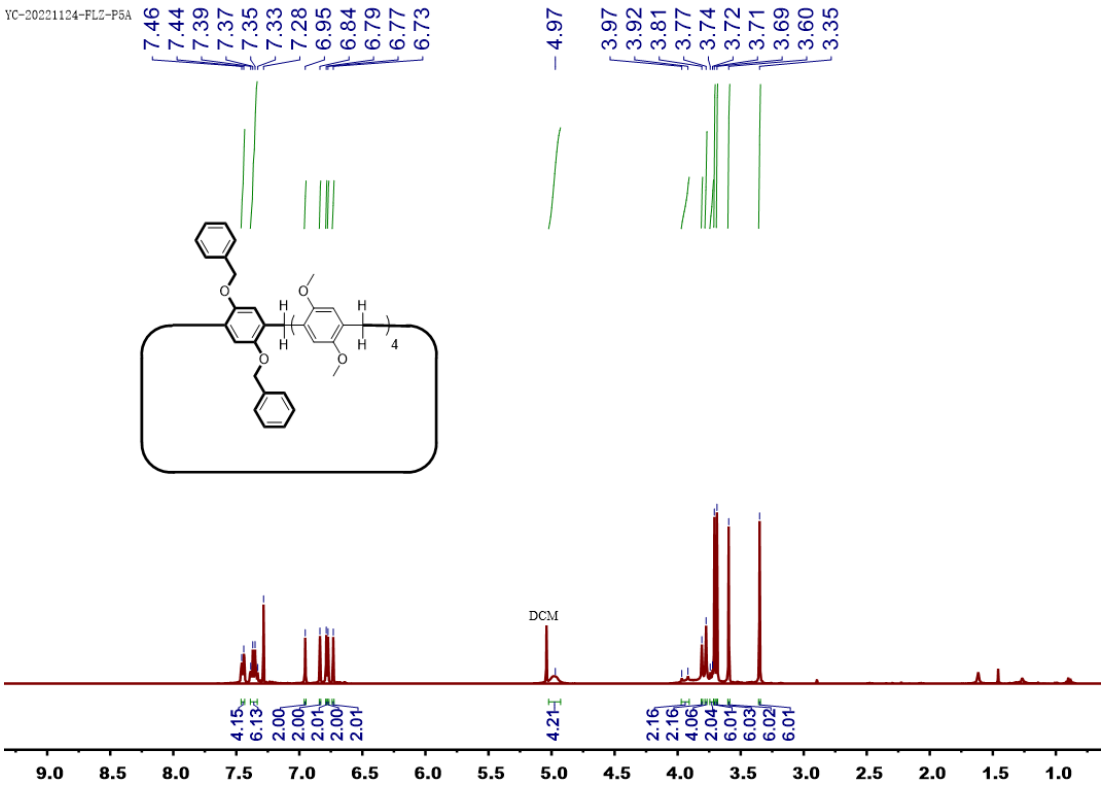


Figure S1. ^{1}H NMR spectrum (400 MHz, chloroform–d, room temperature) of **P1**.

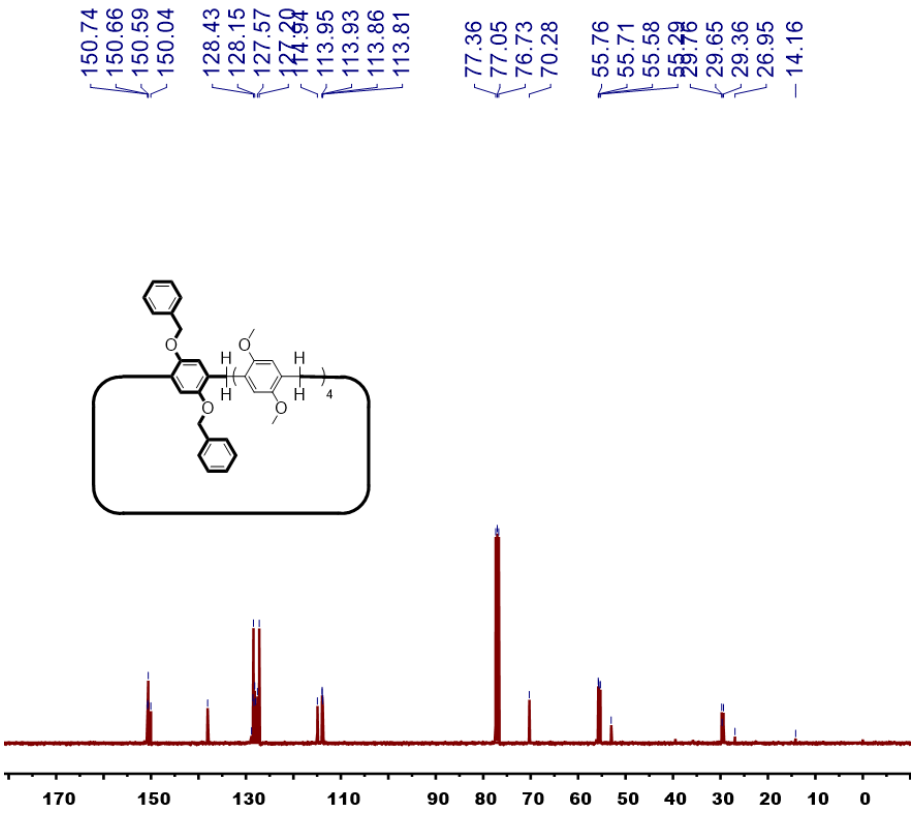


Figure S2. ^{13}C NMR spectrum (101 MHz, chloroform–d, room temperature) of **P1**.

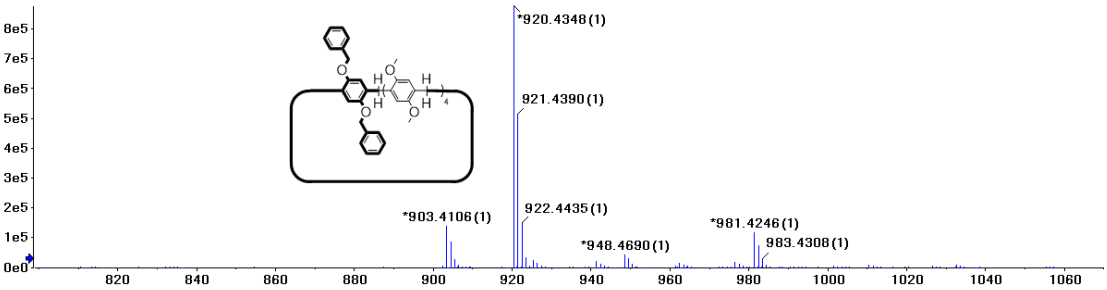


Figure S3. ESI-HRMS spectrum of **P1**. Assignment of main peaks: m/z $[C_{57}H_{59}O_{10}]^+$, $[M+H]^+$: 903.4018, found: 903.4106; $[C_{57}H_{62}NO_{10}]^+$, $[M+NH_4]^+$: 920.4374, found: 920.4348.

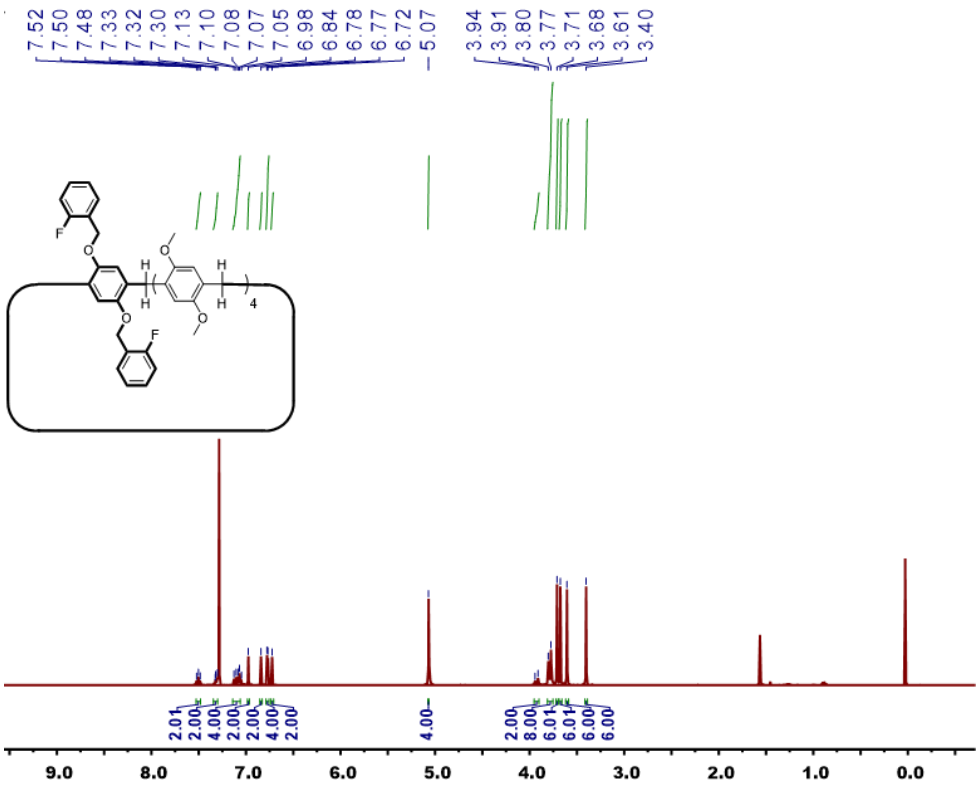


Figure S4. ^{1}H NMR spectrum (400 MHz, chloroform–d, room temperature) of **P2**.

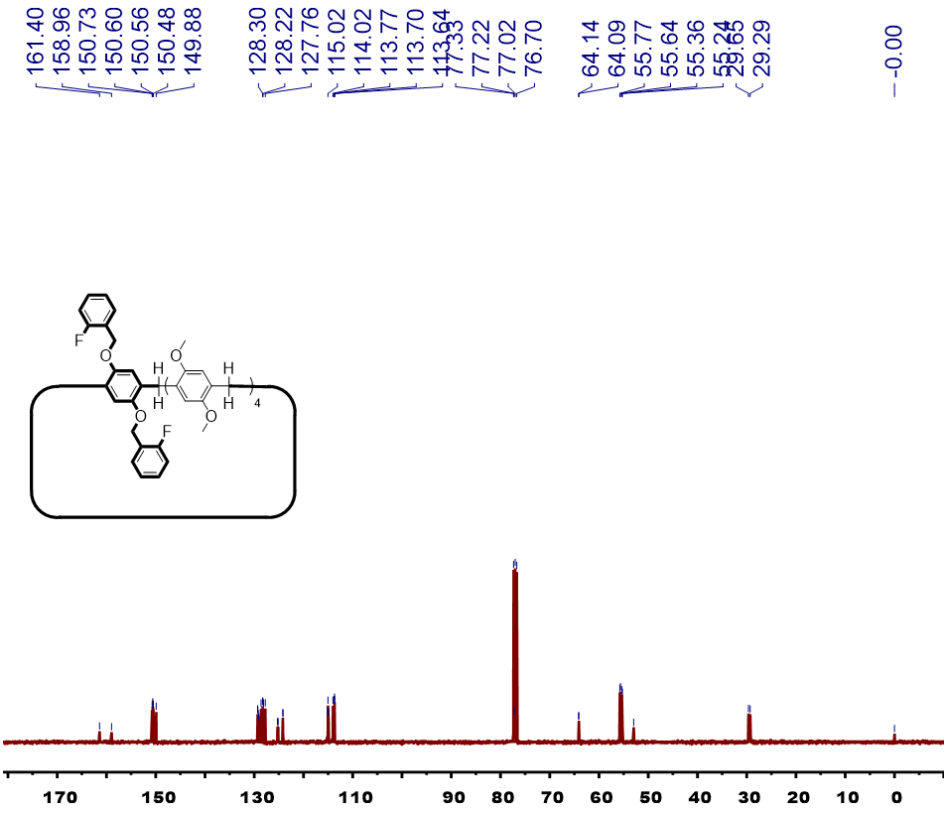


Figure S5. ^{13}C NMR spectrum (101 MHz, chloroform–d, room temperature) of **P2**.

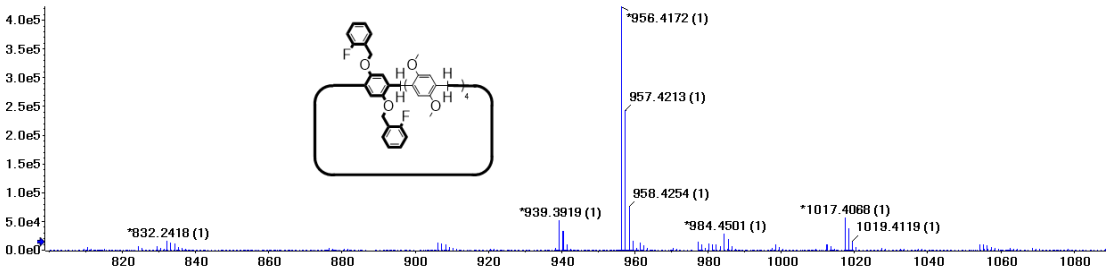


Figure S6. ESI-HRMS spectrum of P2. Assignment of main peaks: m/z $[C_{57}H_{57}F_2O_{10}]^+$, $[M+H]^+$: 939.3920, found: 939.3918; $[C_{57}H_{60}NO_{10}]^+$, $[M+NH_4]^+$: 956.4185, found: 956.4172

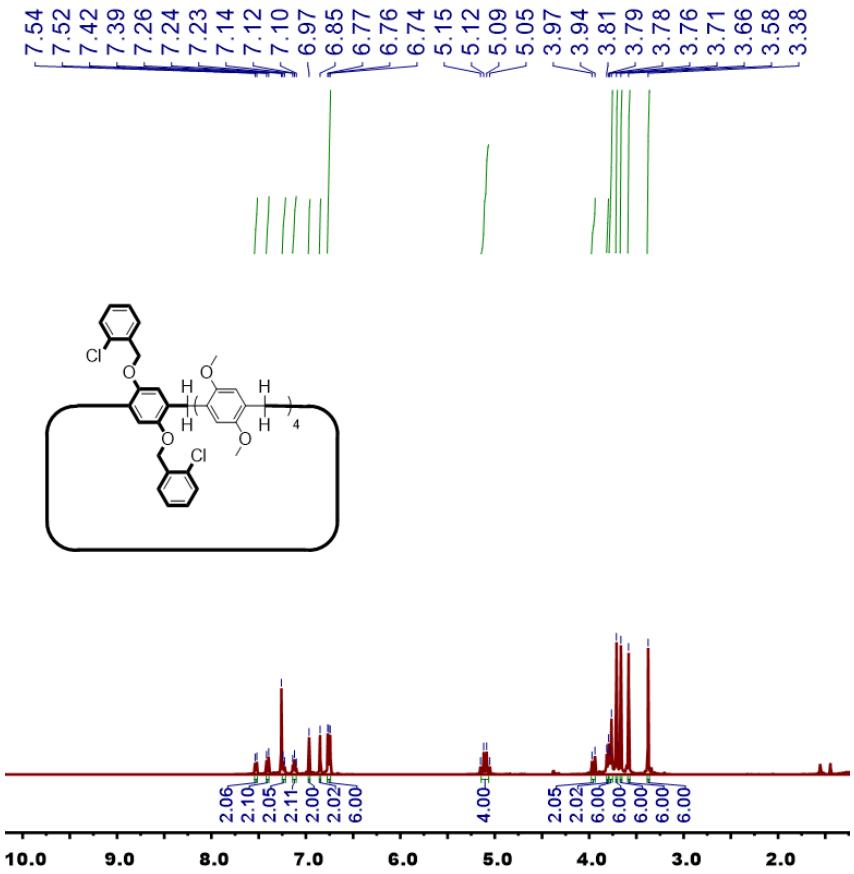


Figure S7. [1]H NMR spectrum (400 MHz, chloroform–d, room temperature) of **P3**.

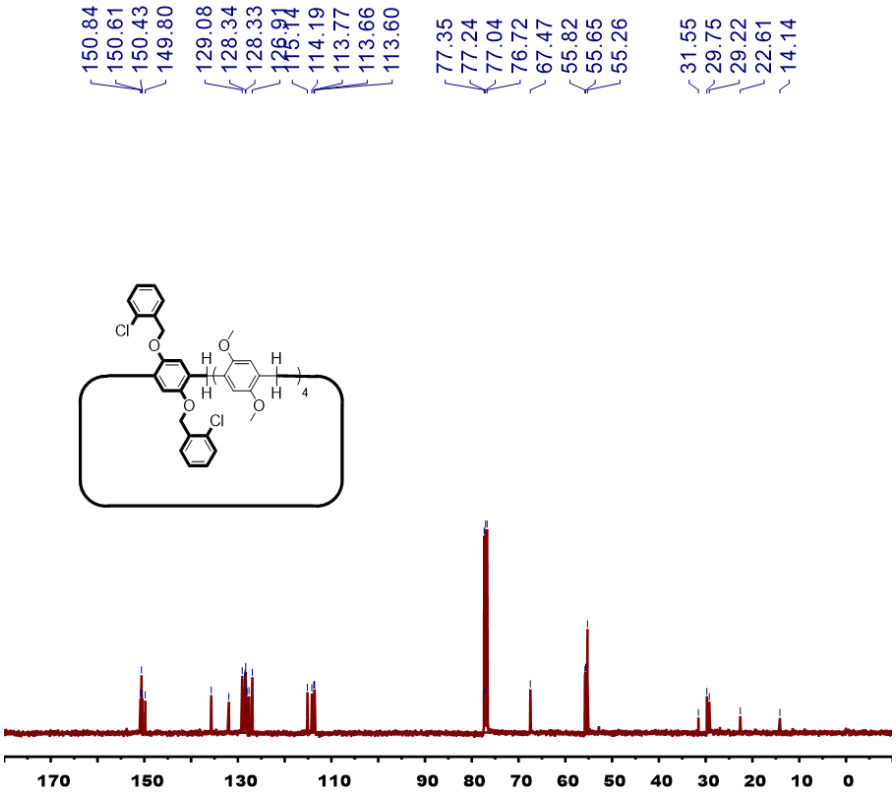


Figure S8. [13]C NMR spectrum (101 MHz, chloroform–d, room temperature) of **P3**.

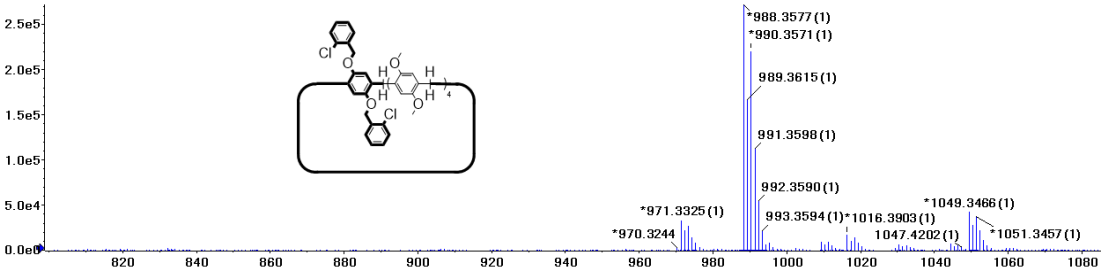


Figure S9. ESI-HRMS spectrum of **P3**. Assignment of main peaks: m/z $[C_{57}H_{57}Cl_2O_{10}]^+$, $[M+H]^+$: 971.3320, found: 971.3325; $[C_{57}H_{60}Cl_2NO_{10}]^+$, $[M+NH_4]^+$: 988.3594, found: 988.3577.

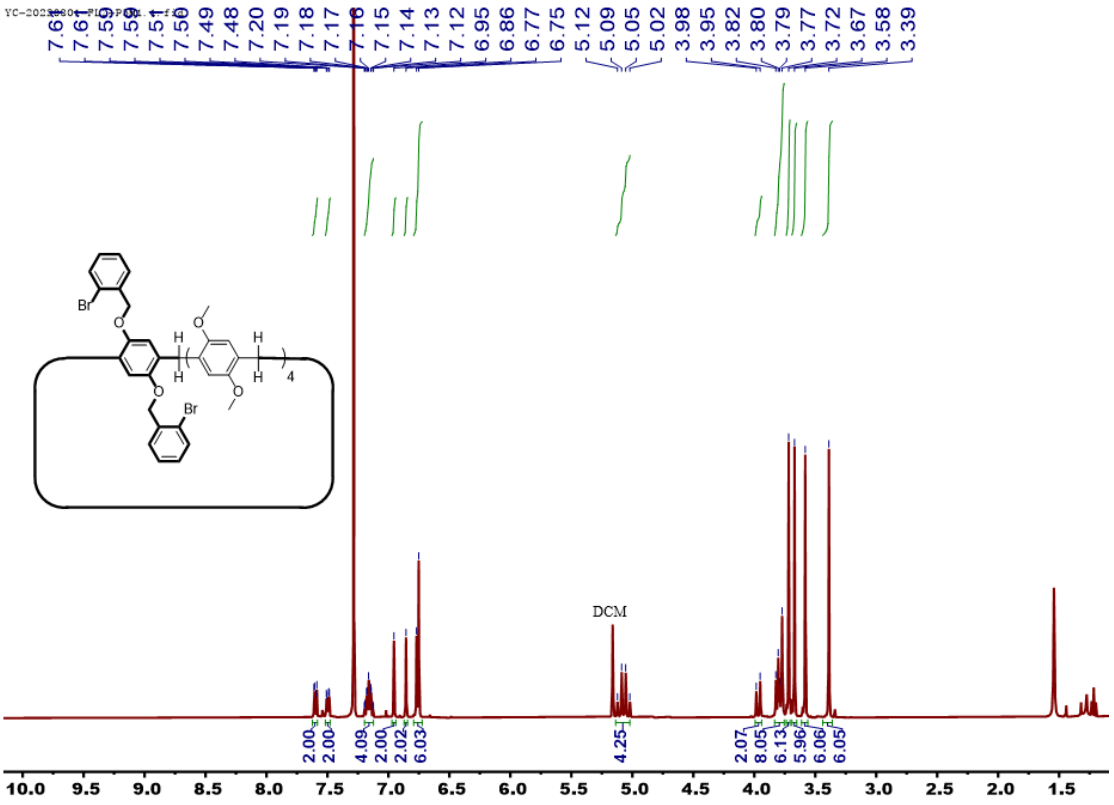


Figure S10. ^{1}H NMR spectrum (400 MHz, chloroform–d, room temperature) of **P4**.

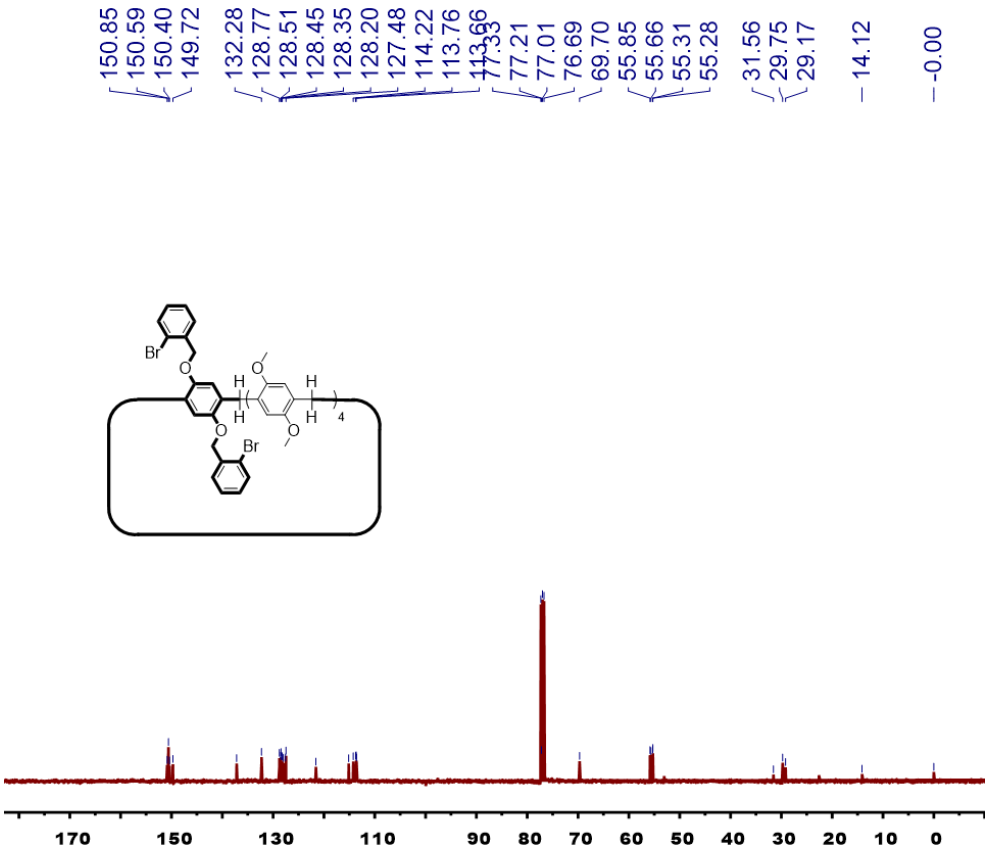


Figure S11. ^{13}C NMR spectrum (101 MHz, chloroform–d, room temperature) of **P4**.

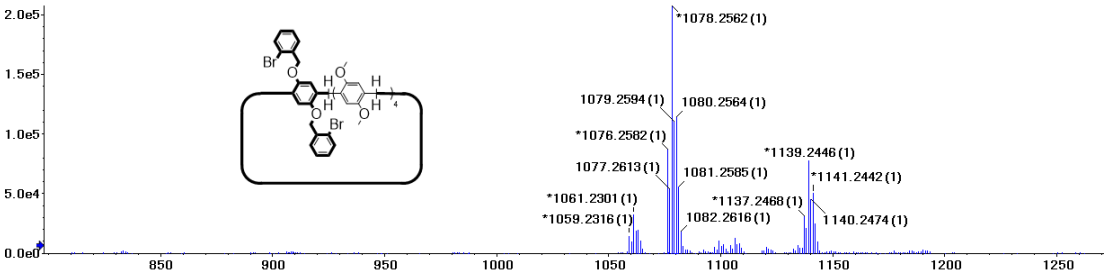


Figure S12. ESI-HRMS spectrum of **P4**. Assignment of main peaks: m/z $[C_{57}H_{57}Br_2O_{10}]^+$, $[M+H]^+$: 1059.2318, found: 1059.2316; $[C_{57}H_{60}Br_2NO_{10}]^+$, $[M+NH_4]^+$: 1076.2584, found: 1076.2568

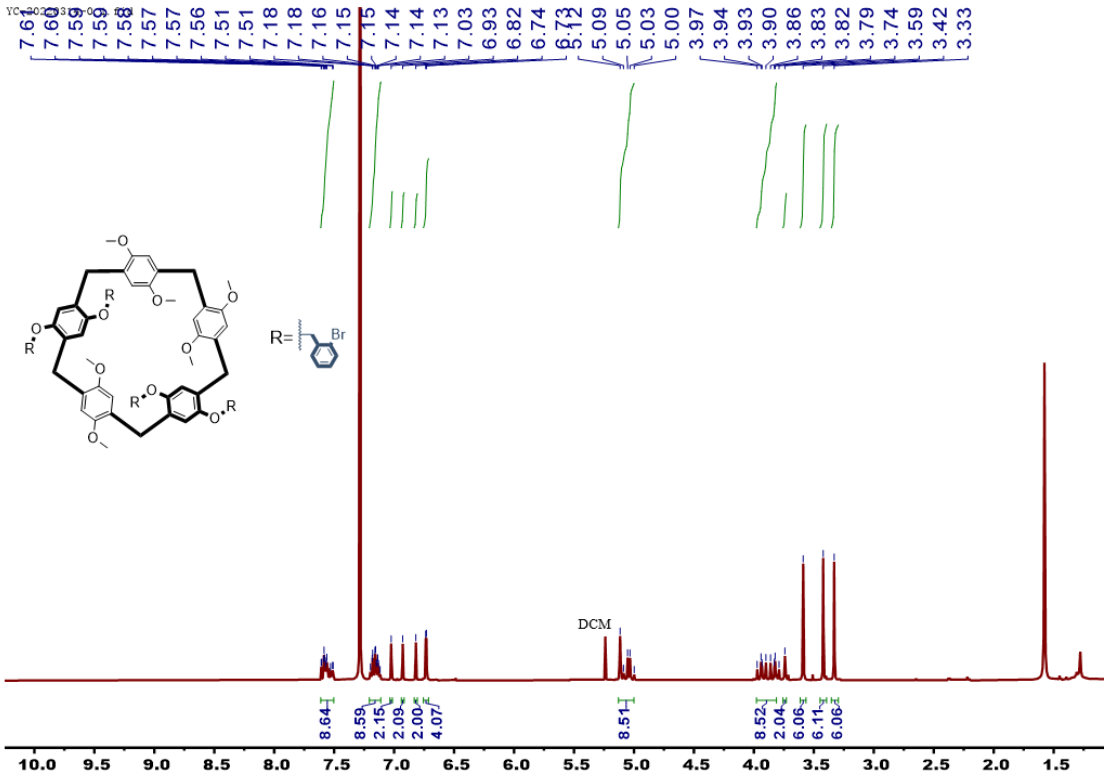


Figure S13. [1]H NMR spectrum (400 MHz, chloroform–d, room temperature) of **P5**.

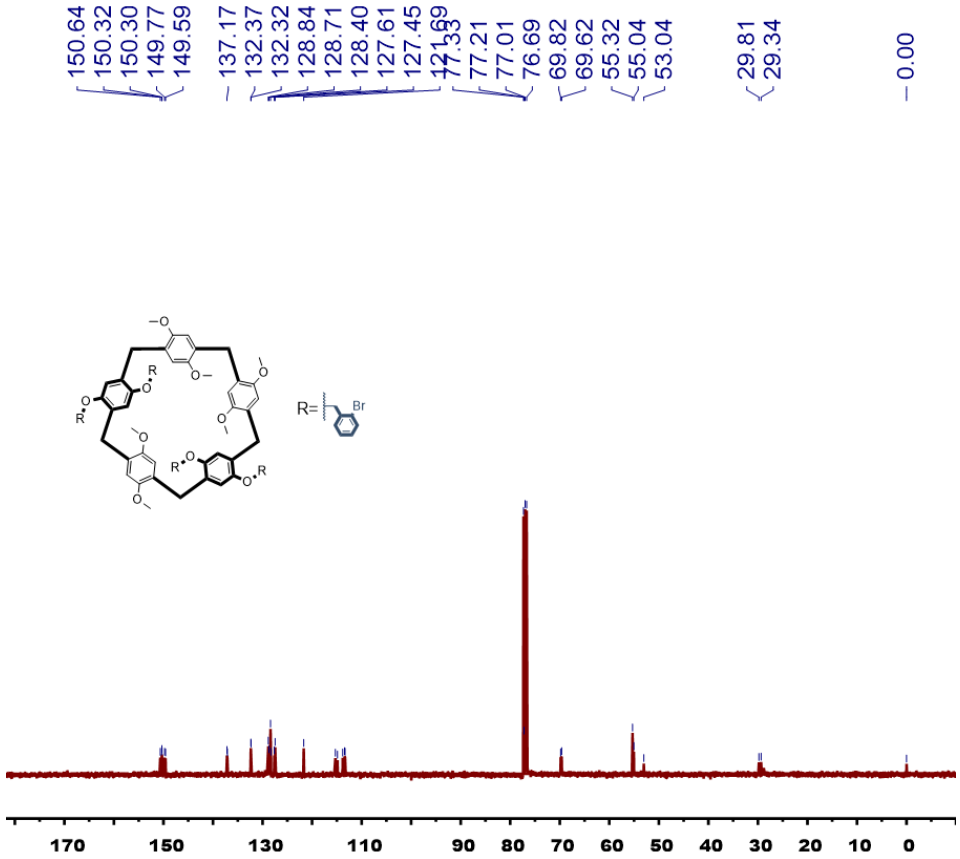


Figure S14. [13]C NMR spectrum (101 MHz, chloroform–d, room temperature) of **P5**.

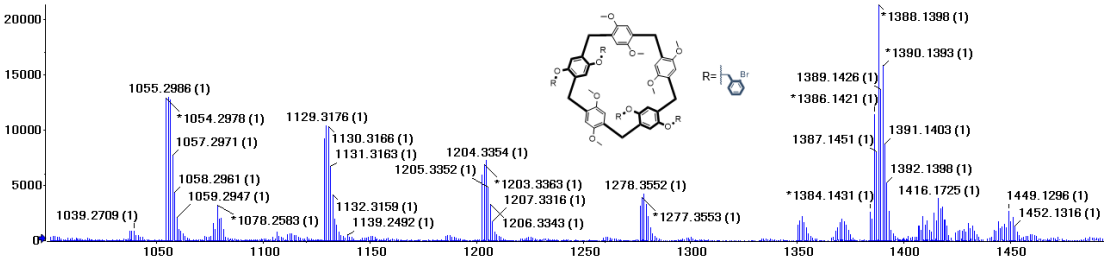


Figure S15. ESI-HRMS spectrum of P5. Assignment of main peaks: m/z $[C_{57}H_{60}Br_2NO_{10}]^+$, $[M+NH_4]^+$: 1388.1379, found: 1388.1398

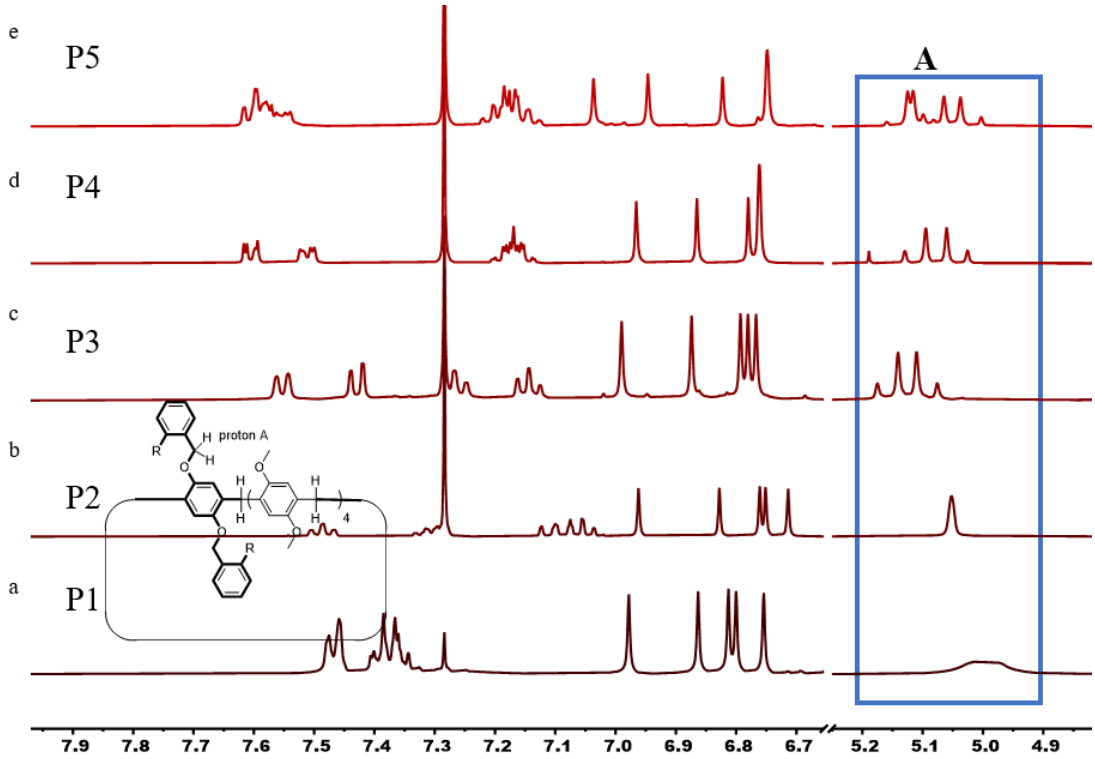


Figure S16. ^{1}H NMR spectrum (400 MHz, chloroform–d, room temperature) of **P1-P5** correspond to a-e, respectively.

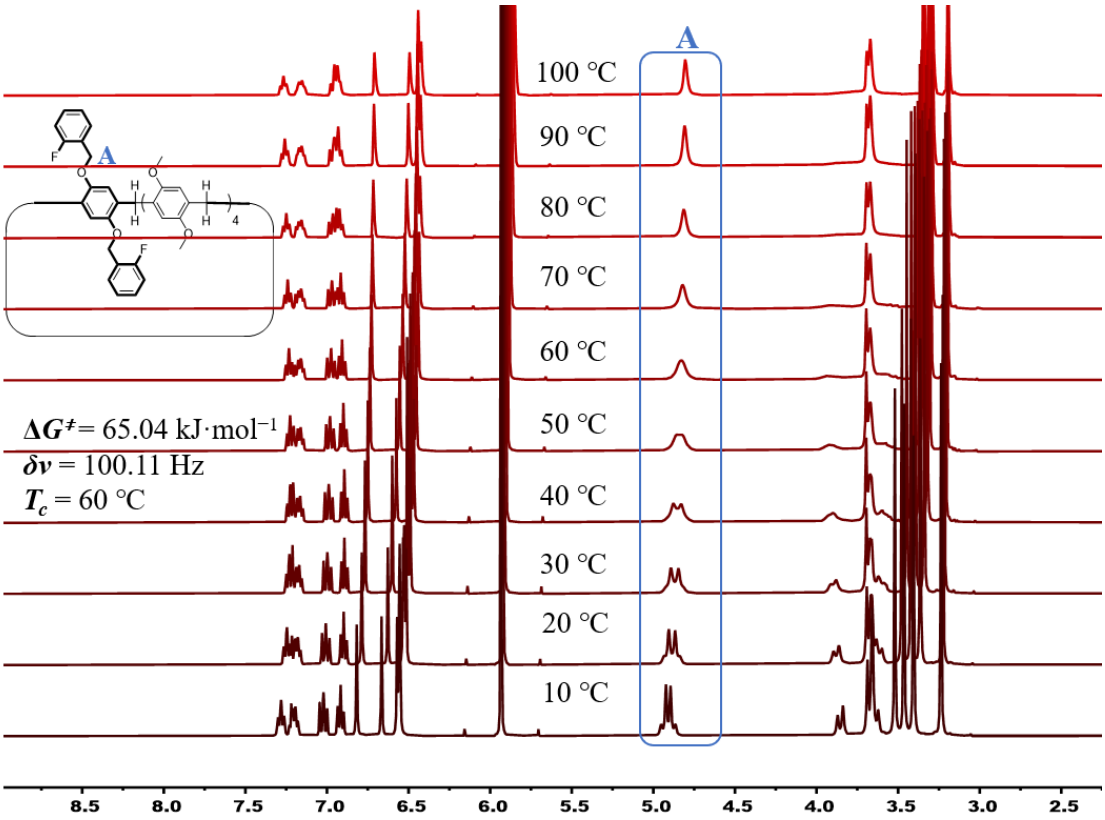


Figure S17. ^{1}H NMR spectrum (400 MHz, 1,1,2,2-Tetrachloroethane-d_2) of **P2** at various temperatures and racemization thermokinetic parameters of **P2** $\Delta G^{\neq} = 8.314T_c[22.96 + \log(T_c / \delta\nu)]$.

4 The racemization kinetics and thermodynamics of P3-P5

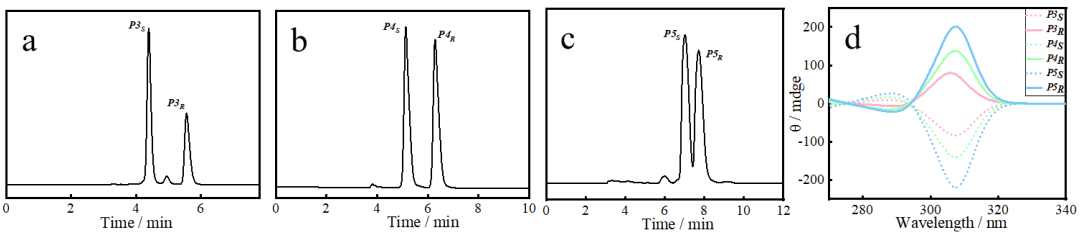


Figure S18. Chiral HPLC traces of (a) **P3** eluted with DCM: hexane, 1:2 (*v* / *v*), (b) **P4** eluted with DCM: hexane, 1:2 (*v* / *v*)) and (c) **P5** eluted with DCM: hexane, 1:3 (*v* / *v*) and (d) CD spectra of **P3**$_{R/S}$, **P4**$_{R/S}$ and **P5**$_{R/S}$ at room temperature ([M] = 0.05 mM) in chloroform.

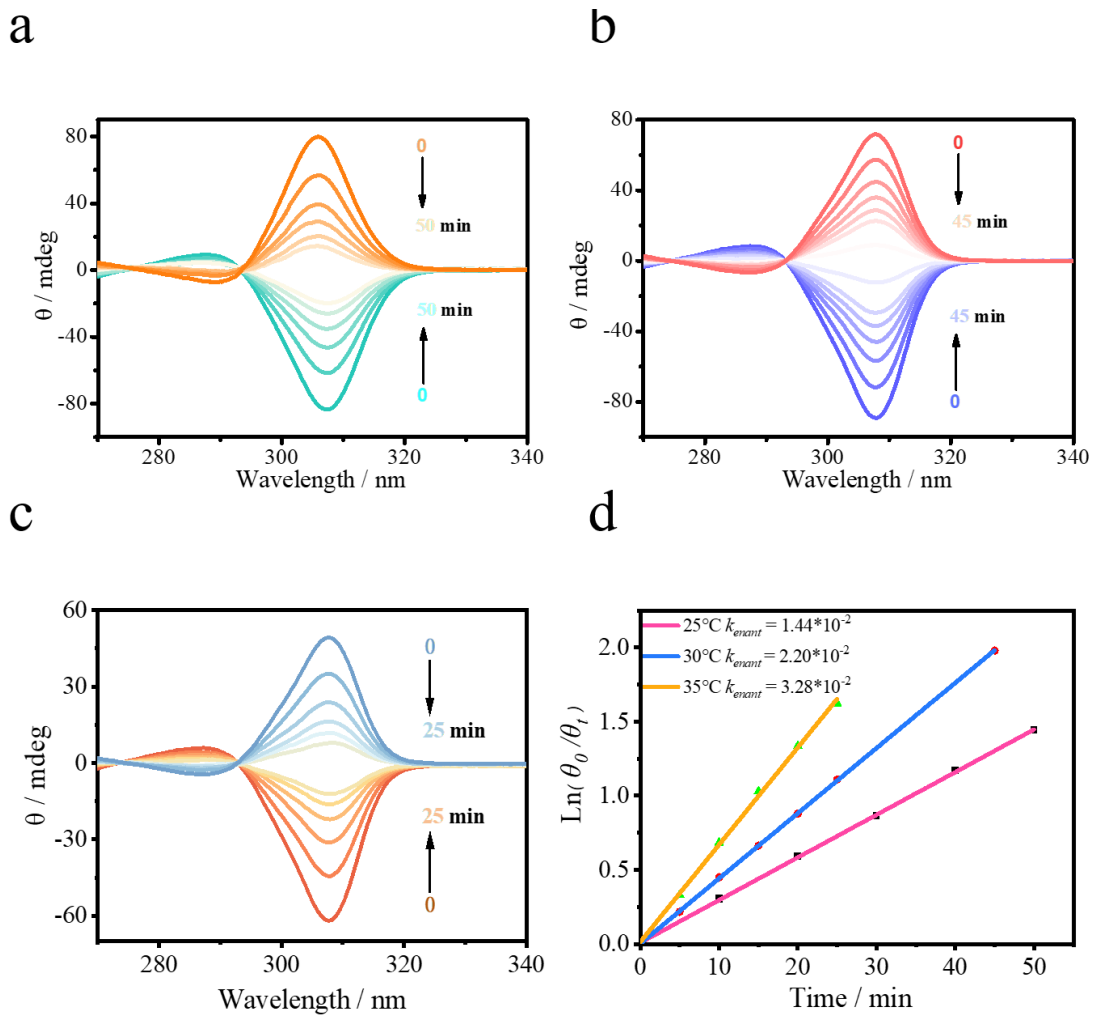


Figure S19. Time-dependent CD spectral changes of **P3** in chloroform ([**P3**] = 0.05 mM) (a) at 25 ℃, (b) at 30 ℃, (c) at 35 ℃. (d) Kinetic fittings of **P3** at various temperatures (308.8 nm). All the measurements were carried out in chloroform.

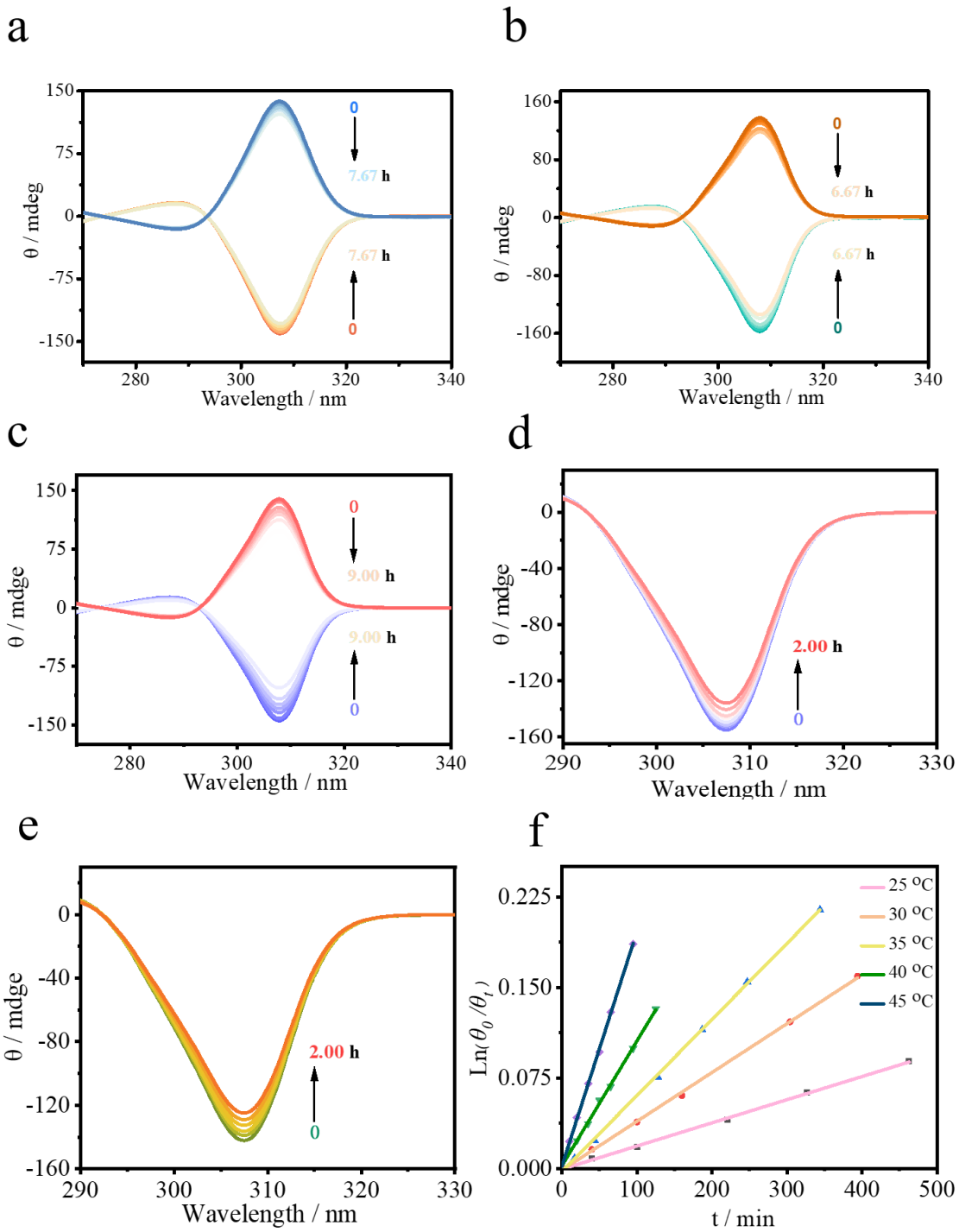


Figure S20. Time-dependent CD spectral changes of **P4** in chloroform ([**P4**] = 0.05 mM) (a) at 25 ℃, (b) at 30 ℃, (c) at 35 ℃, (d) at 40 ℃, (e) at 45 ℃. (f) Kinetic fittings of **P4*S*** at various temperatures (307.5 nm). All the measurements were carried out in chloroform.

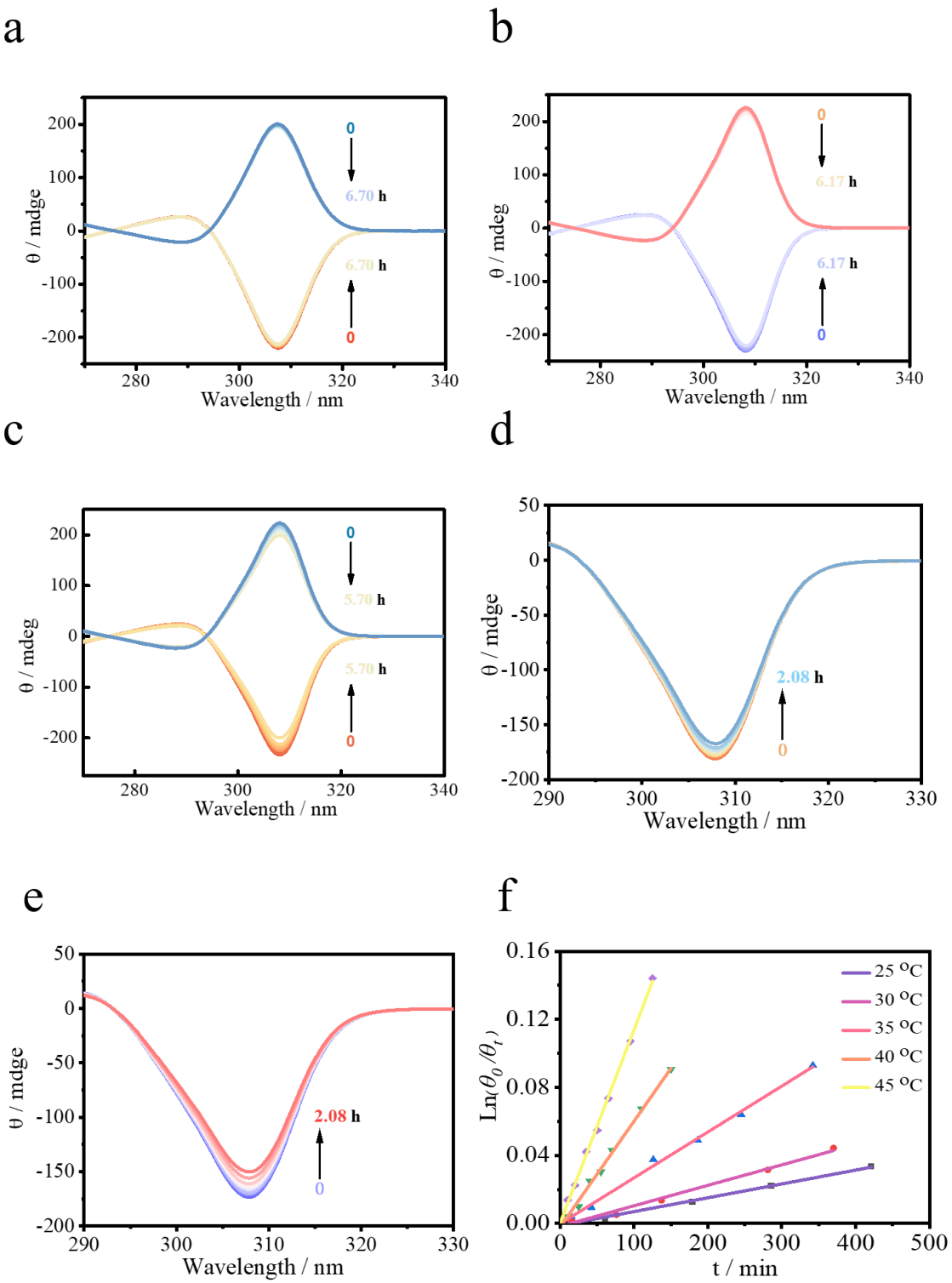


Figure S21. Time-dependent CD spectral changes of **P5** in chloroform ([**P5**] = 0.05 mM) a) at 25 ℃, (b) at 30 ℃, (c) at 35 ℃, (d) at 40 ℃, (e) at 45 ℃. (f) Kinetic fittings of **P5*s*** at various temperatures (308.8 nm). All the measurements were carried out in chloroform.

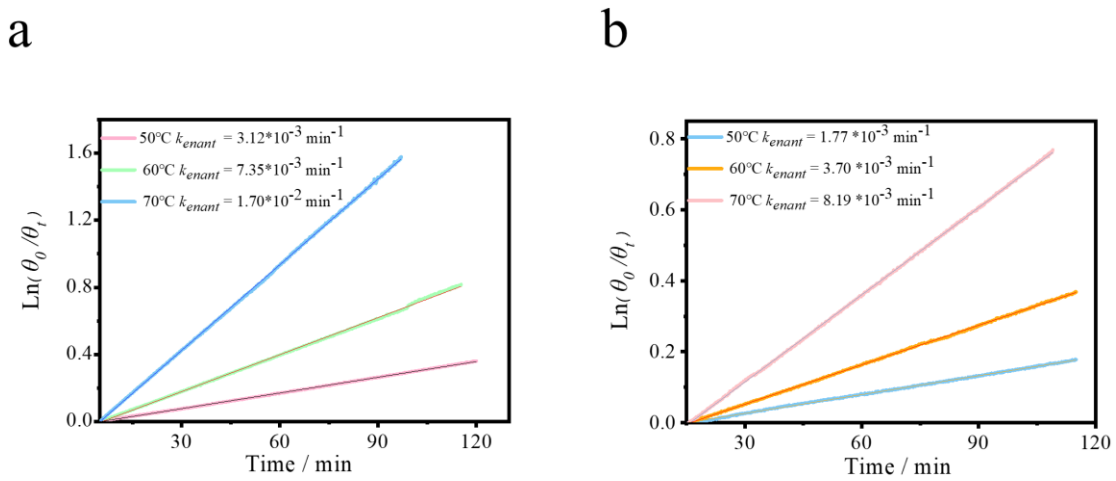


Figure S22. Kinetic fittings of **P5$_S$** at various temperatures (308.8 nm) in 1,4-dioxane (a) and toluene (b) at different temperatures.

Table S1. The kinetic parameters of **P3*s*-P5*s*** in chloroform at different temperatures.

	k_{enant}·min^{-1}[a]			$t_{1/2}$·h[b]		
	P3	**P4**	**P5**	**P3**	**P4**	**P5**
25 ℃	1.44×10^{-2}	9.60×10^{-5}	4.06×10^{-5}	0.40	60.23	142.30
30 ℃	2.20×10^{-2}	2.02×10^{-4}	6.01×10^{-5}	0.26	28.60	96.27
35 ℃	3.28×10^{-2}	3.15×10^{-4}	1.35×10^{-4}	0.18	18.05	42.79
40 ℃	/	5.15×10^{-4}	3.11×10^{-4}	/	11.18	18.57
45 ℃	/	9.70×10^{-4}	5.70×10^{-4}	/	5.92	10.17

[a] *Ln (θ_0 / θ_t) = 2k_{enant}t.* [b] *$t_{1/2}$ = ln 2/(2k_{enant})*

Table S2. Thermodynamic data of racemic reaction of **P3$_S$-P5$_S$** series derivative

	Δ*G*$^{\neq}$/ kJ·mol^{-1}	**Δ*H*$^{\neq}$ / kJ·mol^{-1}**	**Δ*S*$^{\neq}$/ J·mol^{-1}**	**Δ*Ea* / kJ·mol^{-1}[b]**
P1	62.40 [c]	/	/	/
P2	65.04 [d]	/	/	/
P3	93.68 [a]	60.61	-110.94	63.11
P4	95.82 [a]	85.46	-34.75	88.02
P5	98.23 [a]	103.36	17.13	109.02

[a] *Δ$G^{\neq}$ = Δ$H^{\neq}$ − Δ$S^{\neq}$T. ln(k/T) = Δ$S^{\neq}$/R − ln(h/k_b) − Δ$H^{\neq}$/(RT). @at 298.15k*

[b] *Lnk=LnA-ΔE/RT*

[c] *Data from previously reported literature* [1]

[d] *Data from the coalescence temperature (T) of NMR signals see Figure S17.*

Table S3. The kinetic parameters **P5*S*** at different temperatures in 1,4-dioxane and toluene.

Solvent	**1,4-dioxane**			**toluene**		
T / ℃	50 ℃	60 ℃	70 ℃	50 ℃	60 ℃	70 ℃
k_{enant}·**min**$^{-1a}$	1.56×10^{-3}	3.68×10^{-3}	8.51×10^{-3}	8.85×10^{-4}	1.85×10^{-3}	4.10×10^{-3}
$t_{1/2}$·**h**^{b}	3.70	1.57	0.68	6.53	3.12	1.41

[a] *Ln* $(\theta_0 / \theta_t) = 2k_{enant}t$. [b] $t_{1/2} = ln2/(2k_{enant})$.

Table S4. Thermodynamic data of racemic reaction of **P5*S*** in toluene and 1,4-dioxane

P5*S*	**$\Delta G^{\neq}$/ kJ·mol^{-1a}**	**$\Delta H^{\neq}$ / kJ·mol^{-1}**	**$\Delta S^{\neq}$/ J·mol^{-1}**	**ΔEa / kJ·mol^{-1b}**
Toluene	113.700	67.80	-128.391	70.57
1,4-dioxane	97.620	75.42	-100.017	80.40

[a] $\Delta G^{\neq} = \Delta H^{\neq} - \Delta S^{\neq}T$. $ln(k/T) = \Delta S^{\neq}/R - ln(h/k_b) - \Delta H^{\neq}/(RT)$. @at 298.15k

[b] *Lnk=LnA-ΔE/RT*

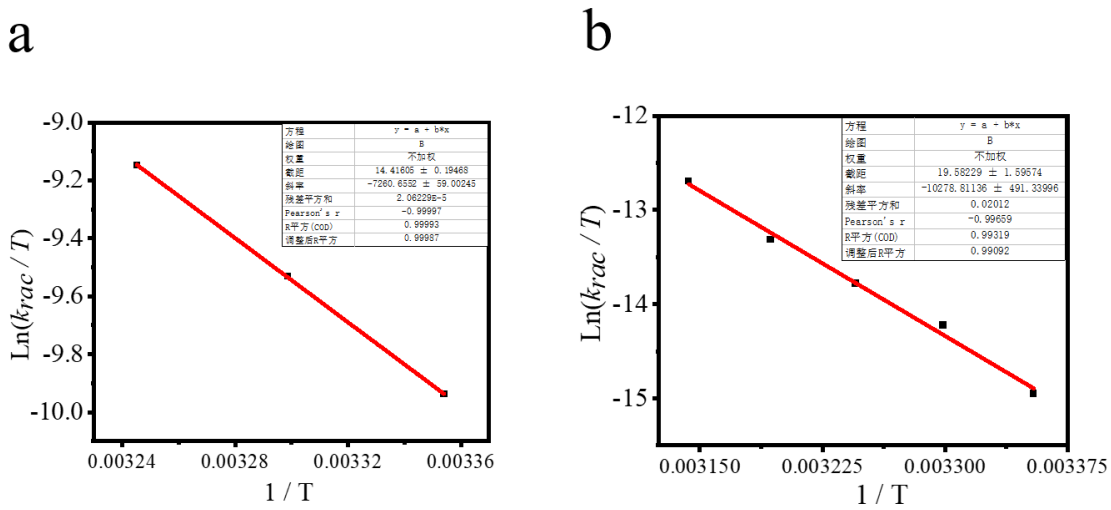


Figure S23. Eyring plots for the racemization of **P3*s*** (a), **P4*s*** (b) in $CHCl_3$.

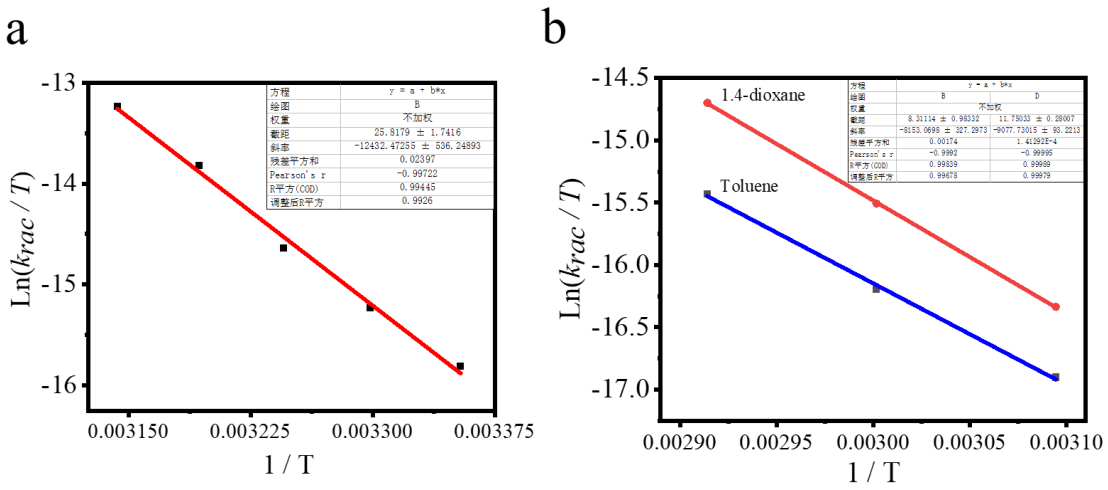


Figure S24. Eyring plots for the racemization of **P5*s*** in chloroform (a) and other solvents (b).

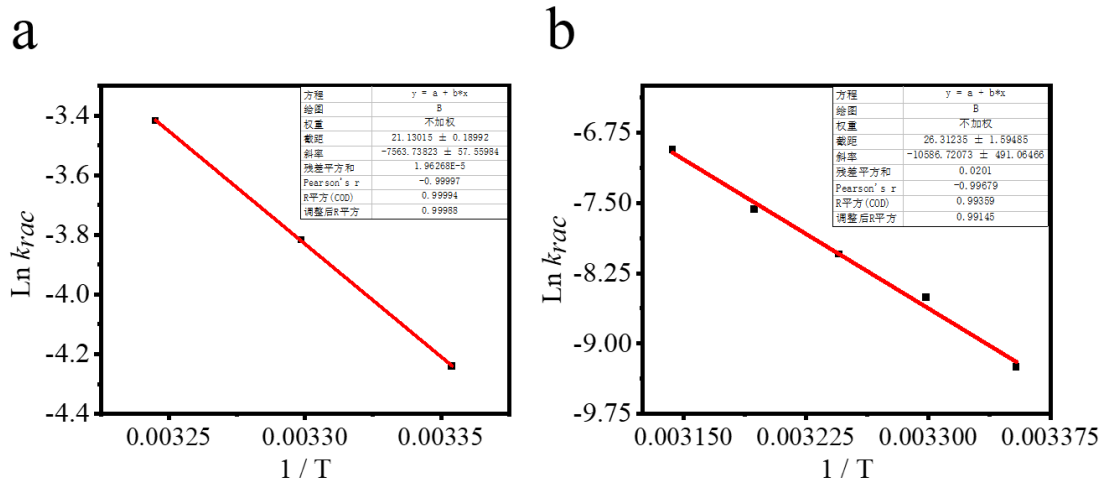


Figure S25. Arrhenius plots for the racemization of **P3s** (a) and **P4*s*** (b) in chloroform.

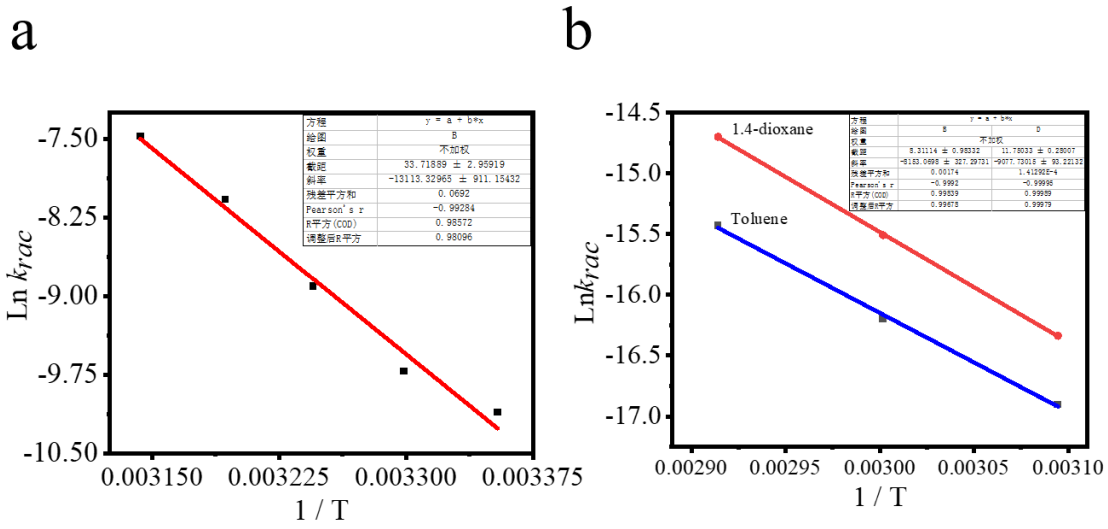


Figure S26. Arrhenius plots for the racemization of **P5*s*** in chloroform (a) and other solvents (b).

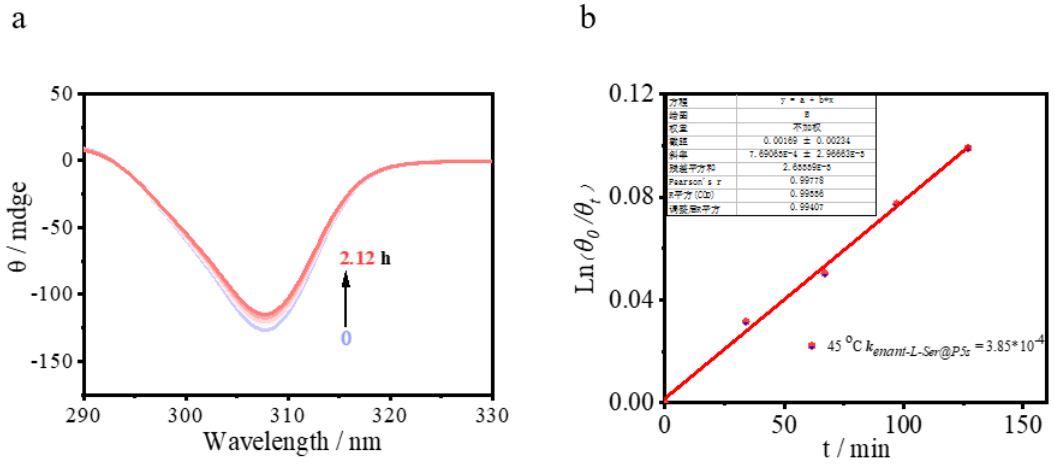


Figure S27. (a) Time-dependent CD spectral changes of ***L***-Ser@**P5*s*** in chloroform ([***L***-Ser] = [**P5s**] = 0.05 mM) at 45 ℃. (b) Kinetic fittings of **P5*s*** at 45 ℃ (308.8 nm) and the $k_{enant\text{-}L\text{-}Ser@P5s}$ = $3.85*10^{-4}$ with $t_{1/2}$ = 15.0 h.

5 The Chiral recognition of P5

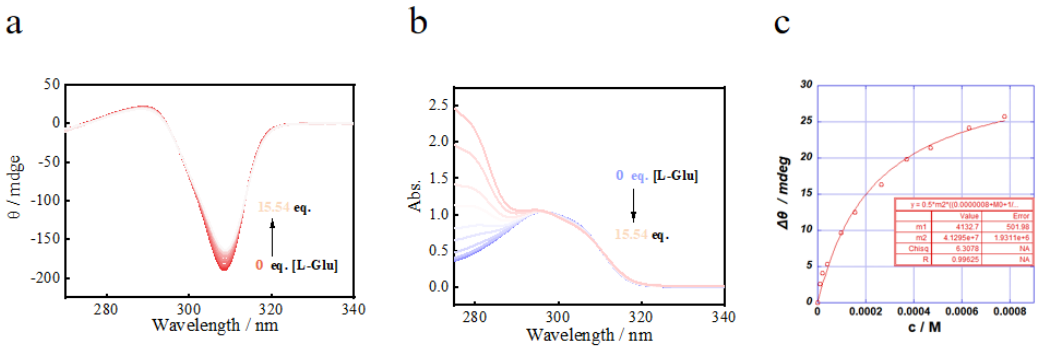


Figure S28. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L***-Glu and **P5*S*** (308.6 nm) (b). Abs spectral changes of **P5s** (0.05 M) upon titration with ***L***-Glu (c). Curve fitting based on the CD intensity changes. The host-guest association constant ($K_{L\text{-}Glu@P5s}$) was estimated to be 4.13 × 10^3 M^{-1}. All the measurements were carried out in chloroform at 25 ℃.

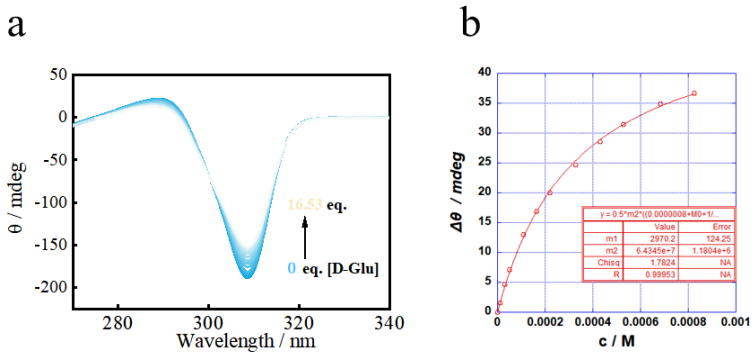


Figure S29. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***D***-Glu and **P5*S*** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The association constant ($K_{D\text{-}Glu@P5s}$) was estimated at 2.97 × 10^3 M^{-1}. All the measurements were carried out in chloroform at 25 ℃.

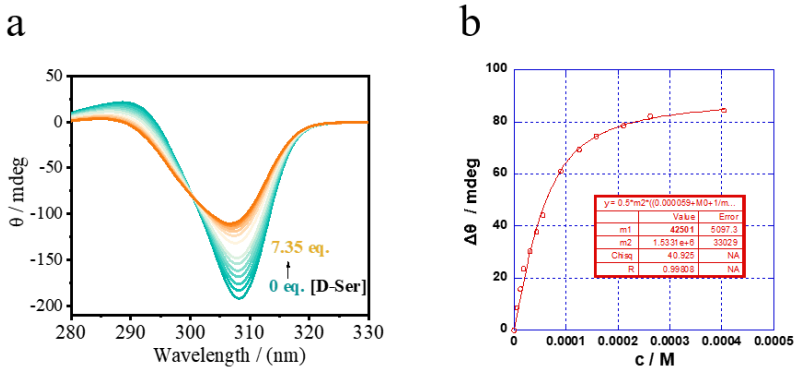


Figure S30. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***D***-Ser and **P5*S*** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The association constant ($K_{D\text{-}Ser@P5s}$) was estimated to be 4.25 × 10^4 M^{-1}. All the measurements were carried out in chloroform at 25 ℃.

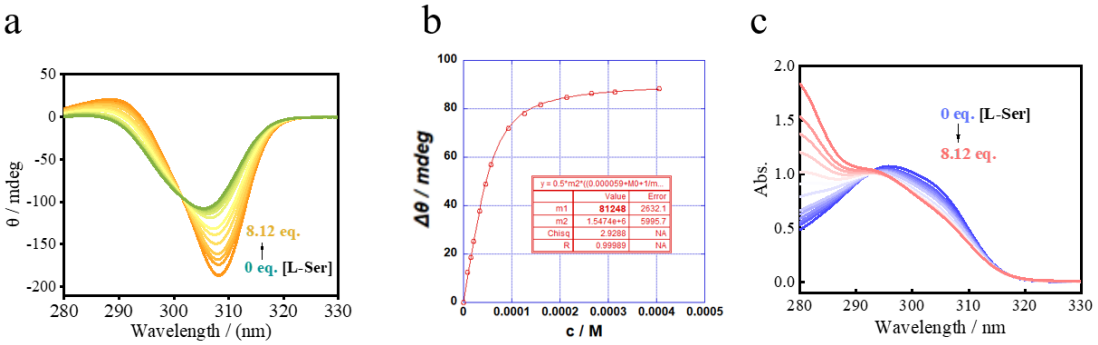


Figure S31. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L***-Ser and **P5*S*** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The association constant ($K_{L\text{-}Ser@P5s}$) was estimated to be 8.12 × 10^4 M^{-1} (c). UV-vis spectral changes of P5*s* (0.05 M) upon titration with ***L*-Ser** All the measurements were carried out in chloroform at 25 ℃.

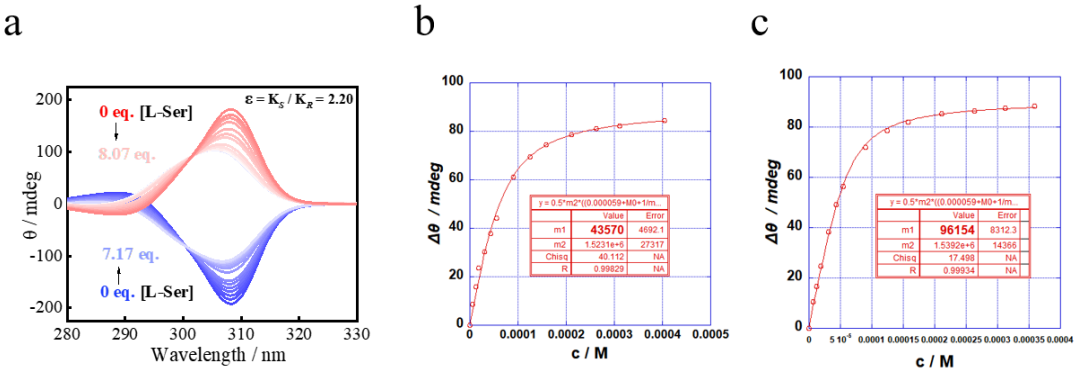


Figure S32. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L***-Ser and **P5*R/S*** (308.6 nm) (b) and (c). Curve fitting based on the CD intensity changes. The association constants ($K_{L\text{-}Ser@P5s}$ and $K_{L\text{-}Ser@P5R}$) were estimated to be 9.62 × 10^4 M^{-1} and 4.36 ×10^4 M^{-1}. All the measurements were carried out in chloroform at 25 ℃.

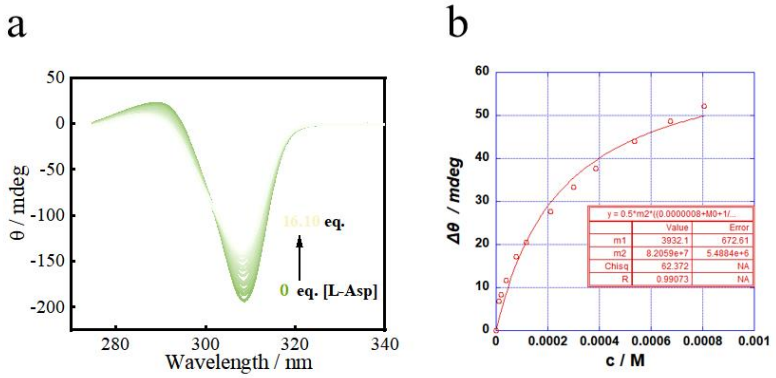


Figure S33. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L***-Asp and **P5S** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The association constant ($K_{L\text{-}Asp@P5s}$) was estimated to be 3.93 × 10^3 M^{-1}. All the measurements were carried out in chloroform at 25 ℃.

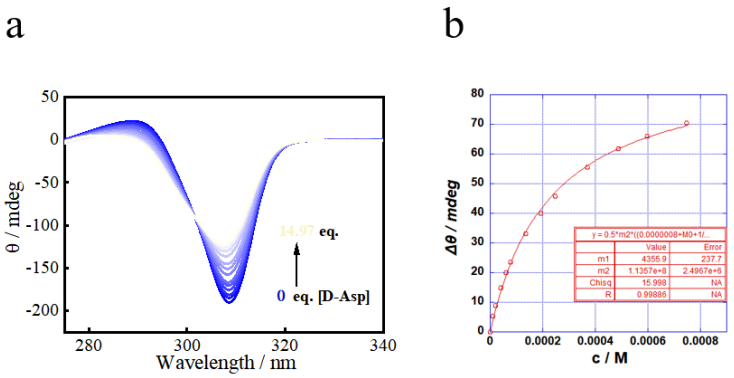


Figure S34. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***D***-Asp and **P5$_S$** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The host-guest association constant ($K_{D\text{-}Asp@P5s}$) was estimated to be 4.36 × 10^3 M^{-1}. All the measurements were carried out in chloroform at 25 °C.

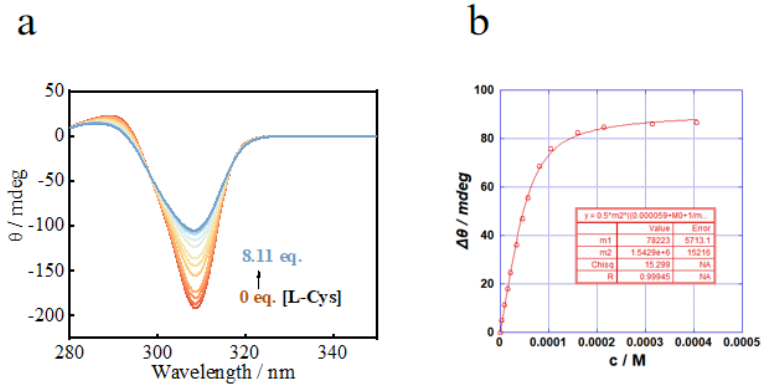


Figure S35. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L*** -Cys and **P5$_S$** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The host-guest association constant ($K_{L\text{-}Cys@P5s}$) was estimated to be 7.82 × 10^4 M^{-1}. All the measurements were carried out in chloroform at 25 °C.

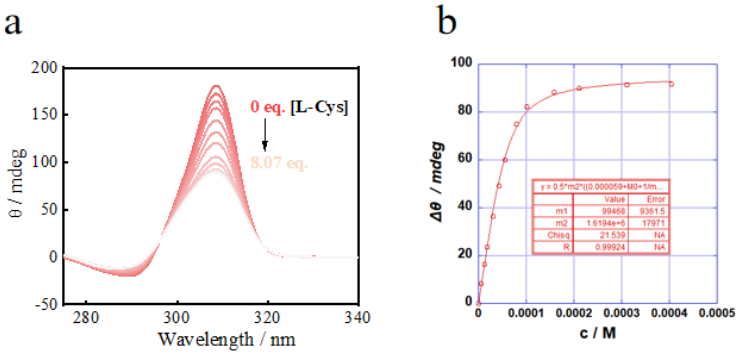


Figure S36. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L*** -Cys and **P5$_R$** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The host-guest association constant ($K_{L\text{-}Cys@P5R}$) was estimated to be 9.95 × 10^4 M^{-1}. All the measurements were carried out in chloroform at 25 °C.

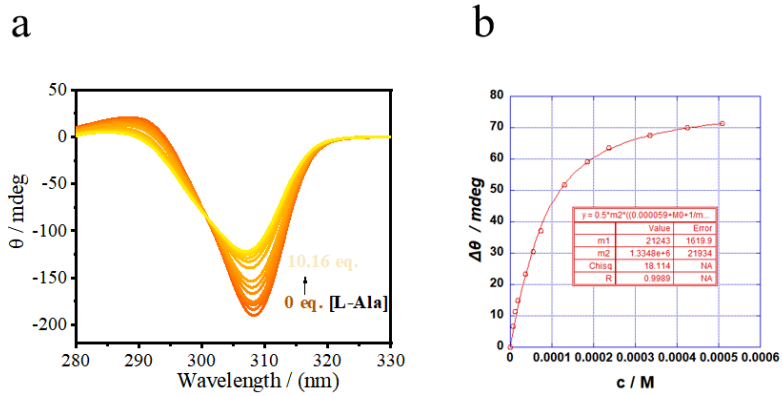


Figure S37. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L*** -Ala and **P5$_S$** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The host-guest association constant ($K_{L\text{-}Ala@P5s}$) was estimated to be 2.12 × 10^4 M^{-1}. All the measurements were carried out in chloroform at 25 ℃.

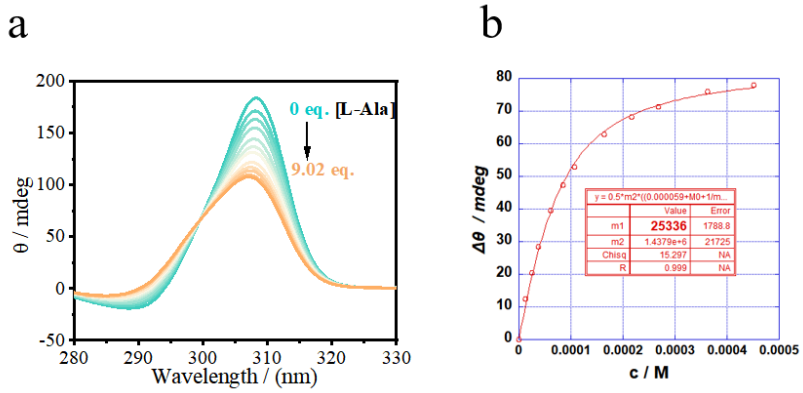


Figure S38. (a). The non-linear curve-fitting (CD titrations) for the complexation of ***L***-Ala and **P5$_R$** (308.6 nm) (b). Curve fitting based on the CD intensity changes. The host-guest association constant ($K_{L\text{-}Ala@P5R}$) was estimated to be 2.53 × 10^4 M^{-1}. All the measurements were carried out in chloroform at 25 ℃.

Table S5. The association constants of **P5$_{R/S}$** with different chiral amino acids and enantioselective recognition.

	$K_{L@P5R}$	$K_{L@P5S}$	ε
***L*-Ala**	2.53 × 10^4	2.21 × 10^4	1.14
***L*-Cys**	9.95 × 10^4	7.82 × 10^4	1.27
***L*-Ser**	4.36× 10^4	9.62 × 10^4	2.20

= $K_{L@P5s}$ / $K_{L@P5R}$ or $K_{L@P5R}$ / $K_{L@P5s}$

Table S6. The association constants of **P5$_S$** with different chiral amino acids and enantioselective recognition ε.

	$K_{L@P5s}$	$K_{D@P5s}$	ε
Glu	4.13× 10^3	2.97× 10^3	1.39
Asp	3.93× 10^3	4.36× 10^3	1.11
Ser	8.12× 10^4	4.25× 10^4	1.92

ε = $K_{L@P5s}$ / $K_{D@P5s}$ or $K_{D@P5s}$ / $K_{L@P5s}$

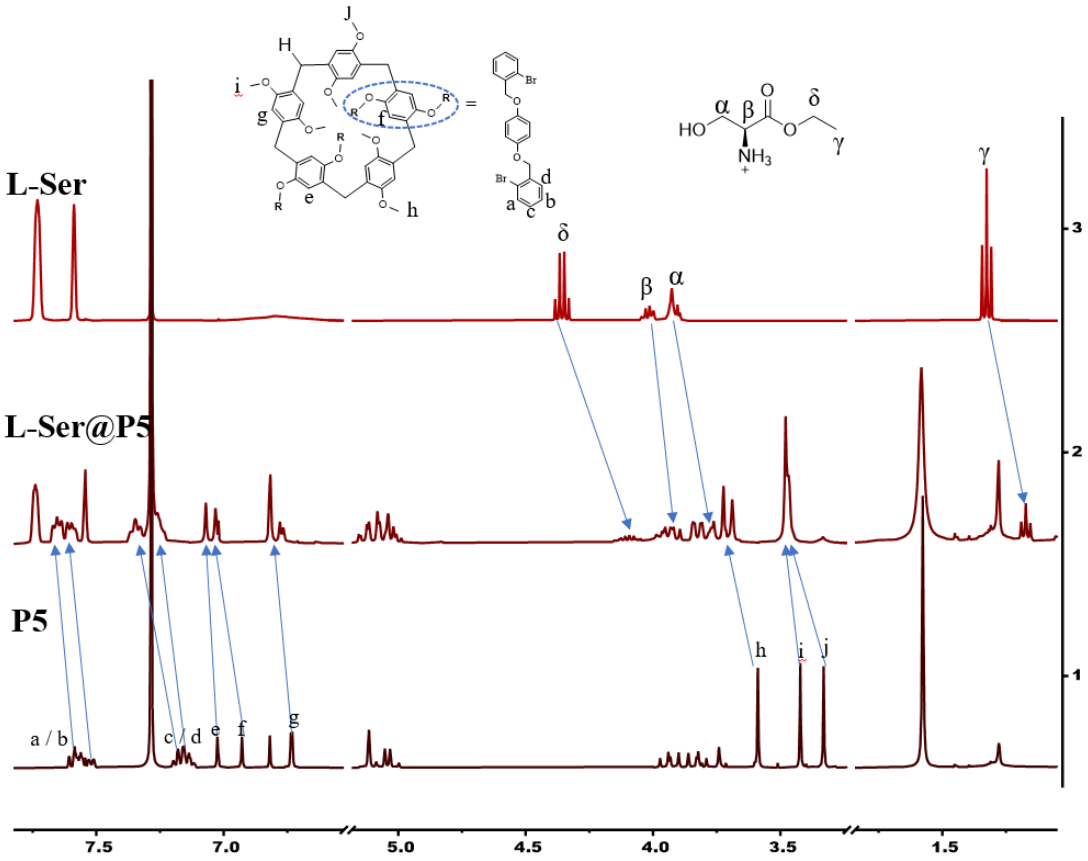


Figure S39. The ^{1}H NMR spectra of ***L***-Ser, **P5** and **P5**@***L***-Ser (H/G = 1:1) in chloroform–d.

6 The X-ray single crystal analyses of P1-P5

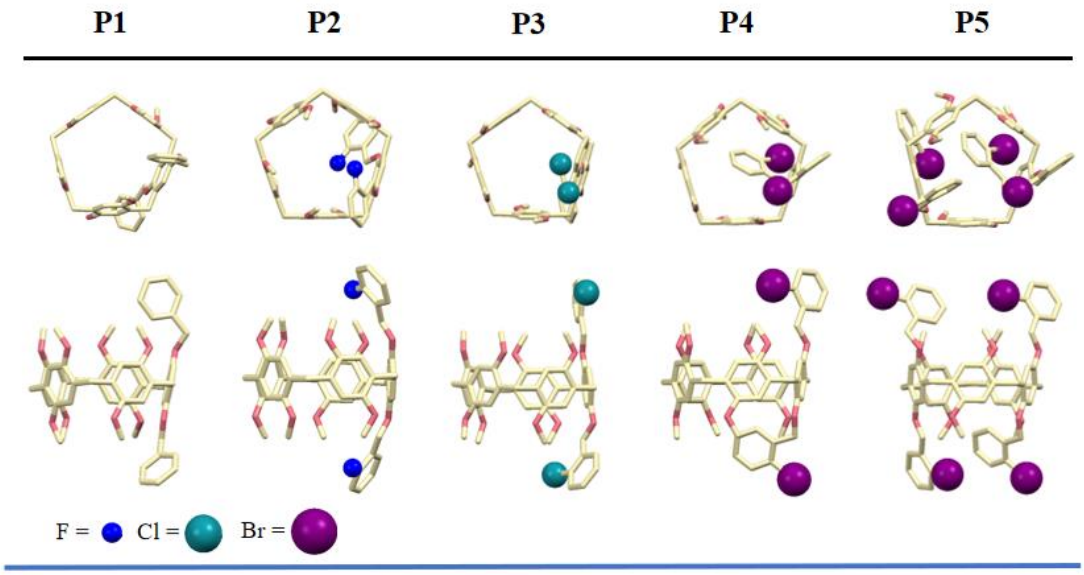


Figure S40. The top and front view of the X-ray structure of **P1-P5** from left to right.

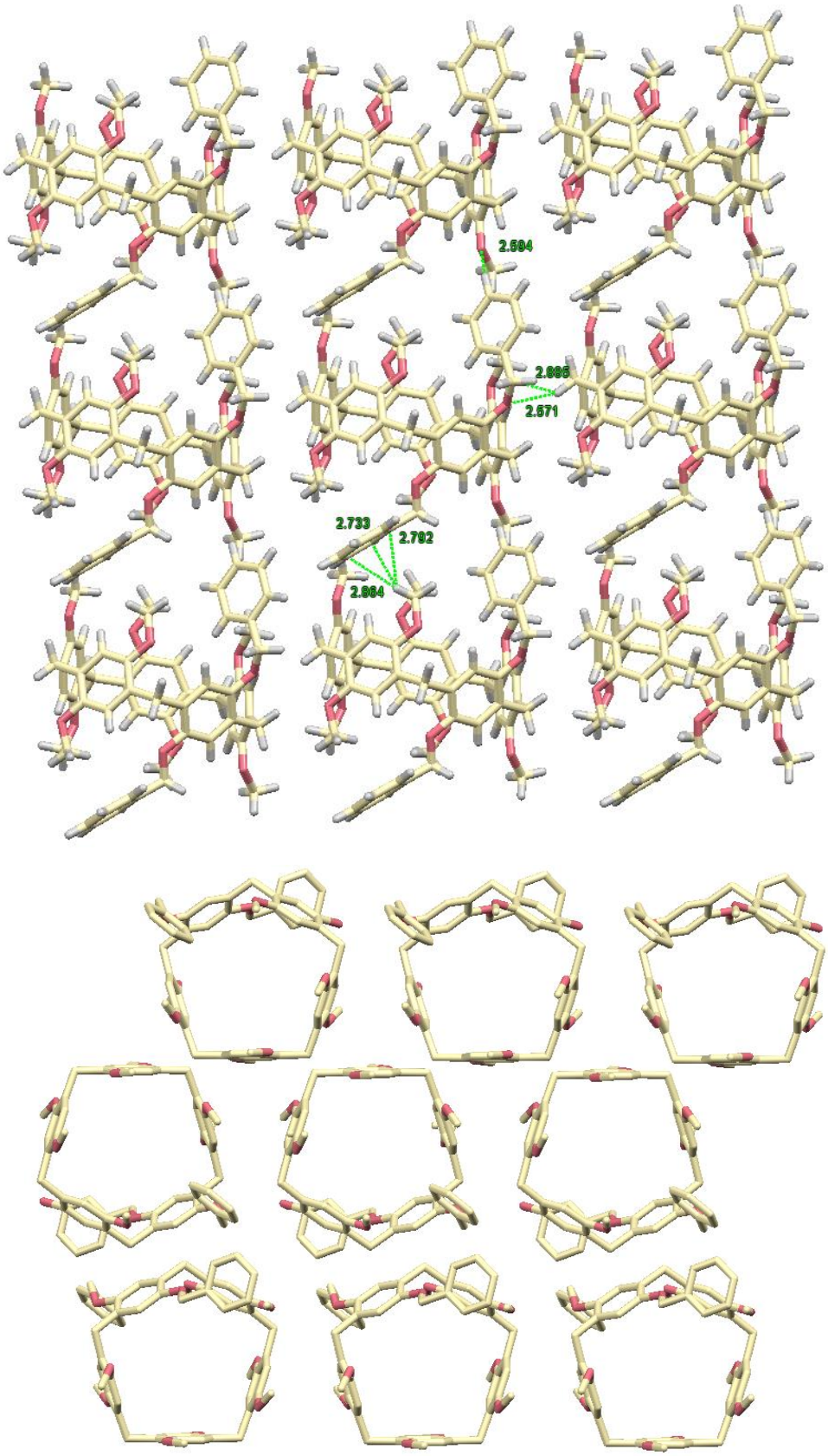


Figure S41. The front view (top) and top view (bottom) of the X-ray structure of **P1**

CCDC	2323526
Empirical formula	$C_{57}H_{58}O_{10}$
Formula weight	903.03
Temperature/K	200.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.1526(6)
b/Å	11.4788(6)
c/Å	39.259(2)
α/°	90
β/°	98.258(2)
γ/°	90
Volume/Å^3	5419.7(5)
Z	4
ρ_{calc}g/cm^3	1.107
μ/mm^{-1}	0.075
F(000)	1920.0
Crystal size/mm^3	0.5 × 0.3 × 0.1
Radiation	MoKα (λ = 0.710)
2Θ range for data collection/°	4.118 to 55.128
Index ranges	$-15 \leq h \leq 15$, $-14 \leq k \leq 14$, $-42 \leq l \leq 51$
Reflections collected	37646
Independent reflections	12291 [R_{int} = 0.0597, R_{sigma} = 0.0727]
Data/restraints/parameters	12291/24/634
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0813, wR_2 = 0.1993
Final R indexes [all data]	R_1 = 0.1192, wR_2 = 0.2192
Largest diff. peak/hole / e Å^3	0.26/-0.23

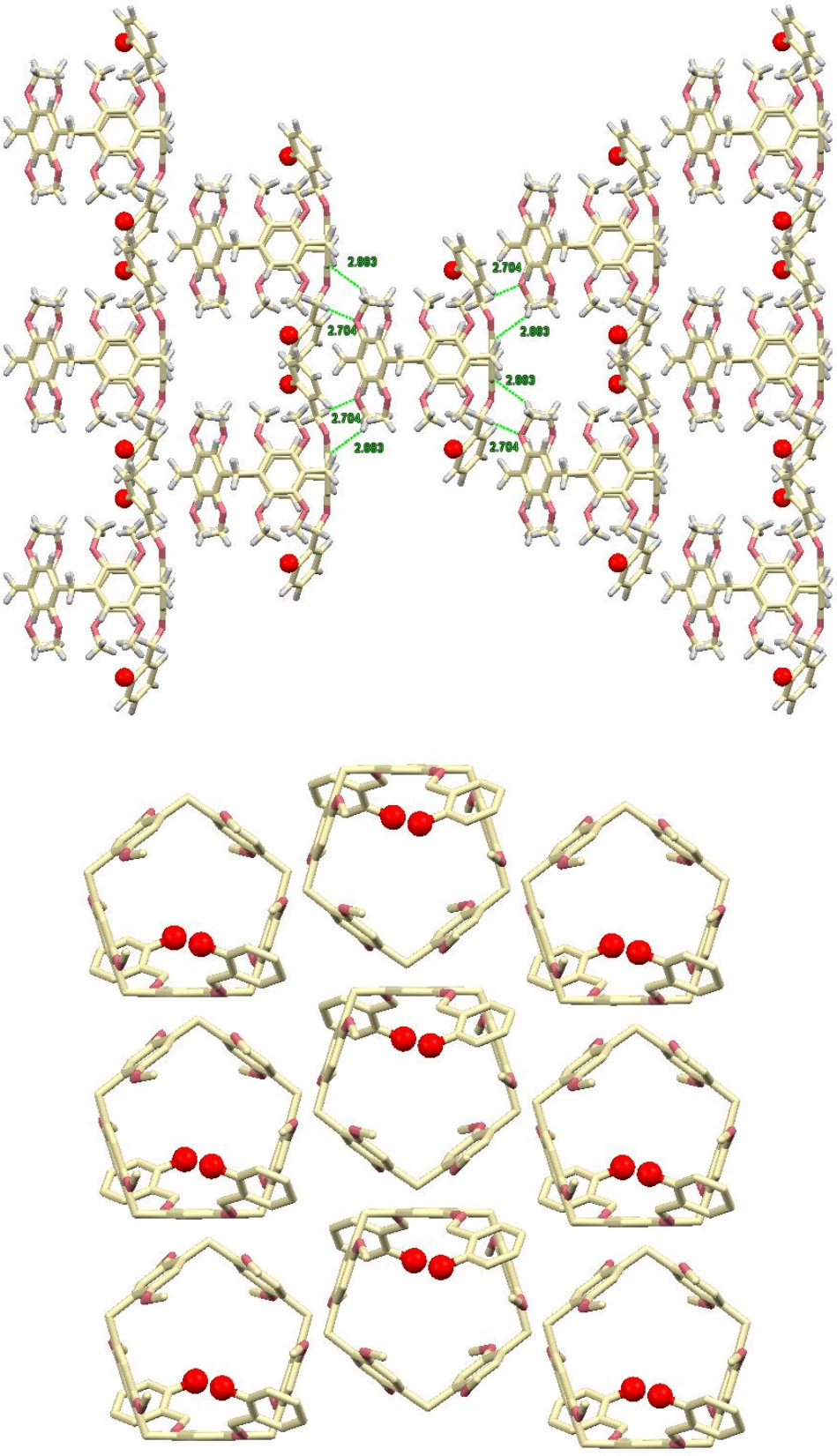


Figure S42. The front view (top) and top view (bottom) of the X-ray structure of **P2**

CCDC	2323535
Empirical formula	$C_{57}H_{54}F_2O_{10}$
Formula weight	937.00
Temperature/K	200.0
Crystal system	monoclinic
Space group	C2/c
a/Å	14.0735(17)
b/Å	20.2388(17)
c/Å	19.436(2)
α/°	90
β/°	91.622(5)
γ/°	90
Volume/Å^3	5533.9(10)
Z	4
ρ_{calc}g/cm^3	1.125
μ/mm^{-1}	0.081
F(000)	1976.0
Crystal size/mm^3	0.31 × 0.17 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.06 to 49.998
Index ranges	$-16 \le h \le 16$, $-24 \le k \le 24$, $-23 \le l \le 23$
Reflections collected	39022
Independent reflections	4862 [R_{int} = 0.0608, R_{sigma} = 0.0294]
Data/restraints/parameters	4862/0/317
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0491, wR_2 = 0.1324
Final R indexes [all data]	R_1 = 0.0673, wR_2 = 0.1497
Largest diff. peak/hole / e Å^{-3}	0.53/-0.20

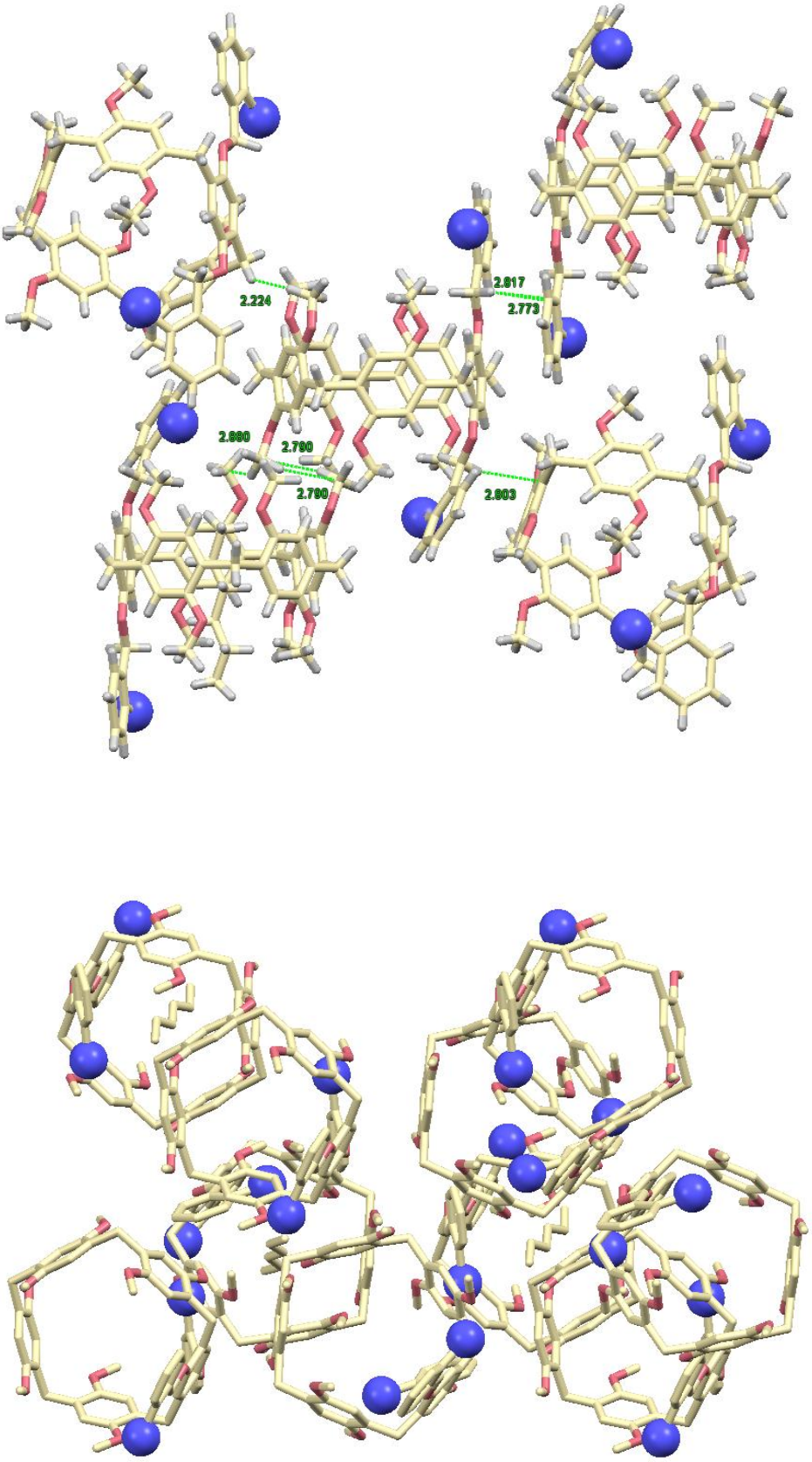


Figure S43. The front view (top) and top view (bottom) of the X-ray structure of **P3**

CCDC	2323538
Empirical formula	$C_{63}H_{70}Cl_2O_{10}$
Formula weight	1058.09
Temperature/K	194.0
Crystal system	monoclinic
Space group	P21/c
a/Å	24.0650(16)
b/Å	12.0314(6)
c/Å	21.5310(15)
α/°	90
β/°	108.464(2)
γ/°	90
Volume/Å^3	5913.1(6)
Z	4
ρcalcg/cm^3	1.189
μ/mm-1	0.166
F(000)	2248.0
Crystal size/mm^3	0.35 × 0.27 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.82 to 55.09
Index ranges	-31 ≤ h ≤ 31, -15 ≤ k ≤ 15, -27 ≤ l ≤ 28
Reflections collected	134969
Independent reflections	13616 [Rint = 0.0830, Rsigma = 0.0371]
Data/restraints/parameters	13616/0/686
Goodness-of-fit on F2	1.020
Final R indexes [I>=2σ (I)]	R1 = 0.0516, wR2 = 0.1242
Final R indexes [all data]	R1 = 0.0870, wR2 = 0.1463
Largest diff. peak/hole / e Å^{-3}	0.51/-0.42

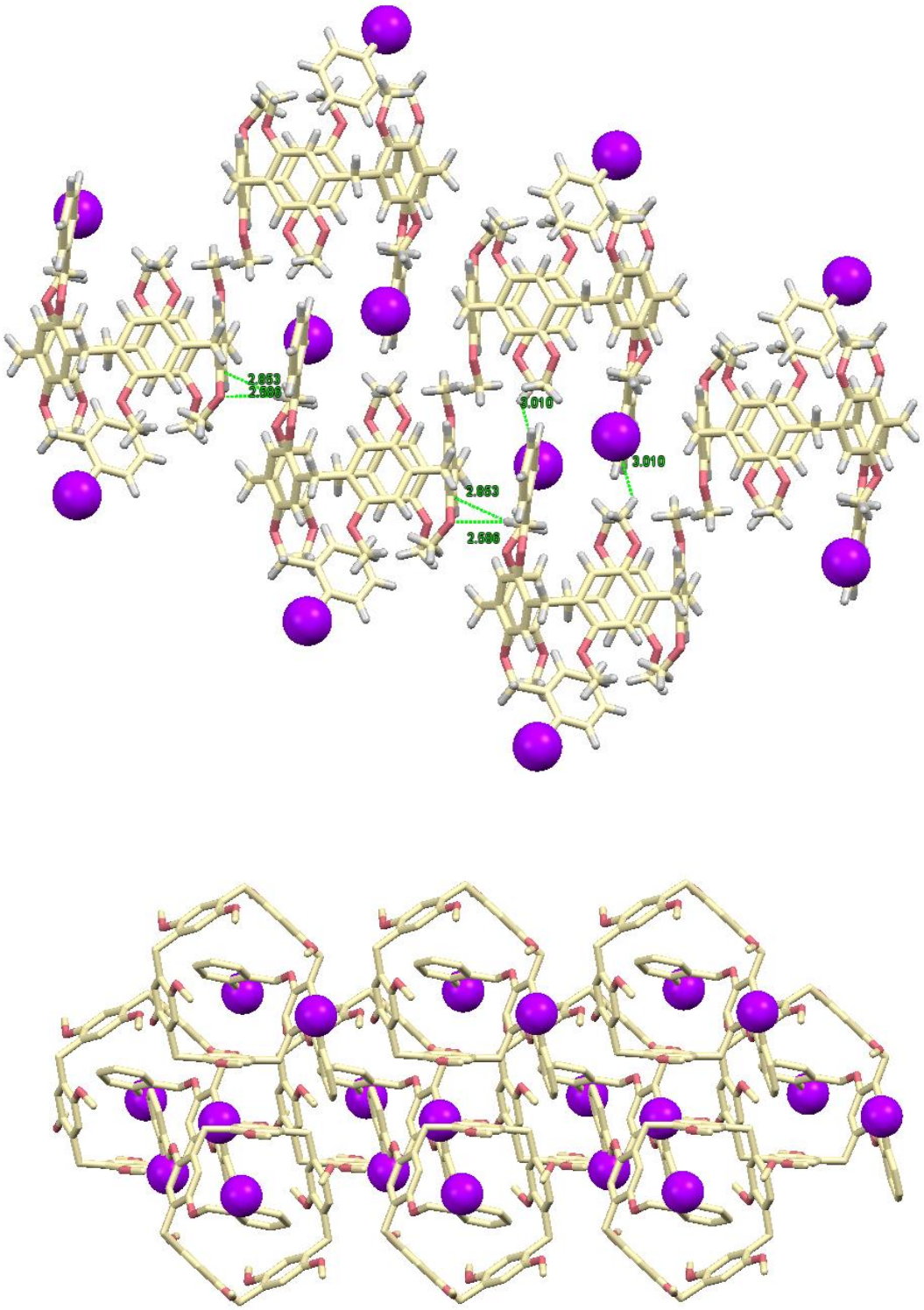


Figure S44. The front view (top) and top view (bottom) of the X-ray structure of **P4**

CCDC	2323573
Empirical formula	$C_{59}H_{59}Br_2NO_{10}$
Formula weight	1101.89
Temperature/K	293.15
Crystal system	triclinic
Space group	P-1
a/Å	11.7611(8)
b/Å	12.0573(7)
c/Å	22.3244(15)
α/°	83.405(5)
β/°	86.013(6)
γ/°	66.593(6)
Volume/Å^3	2885.0(3)
Z	2
ρ_{calc}g/cm^3	1.268
μ/mm^{-1}	1.460
F(000)	1140.0
Crystal size/mm^3	0.35 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.238 to 52.74
Index ranges	$-13 \leq h \leq 14$, $-15 \leq k \leq 15$, $-27 \leq l \leq 27$
Reflections collected	24139
Independent reflections	11778 [R_{int} = 0.0382, R_{sigma} = 0.1050]
Data/restraints/parameters	11778/0/658
Goodness-of-fit on F^2	0.999
Final R indexes [I>=2σ (I)]	R_1 = 0.0696, wR_2 = 0.1636
Final R indexes [all data]	R_1 = 0.1529, wR_2 = 0.1985
Largest diff. peak/hole / e Å^{-3}	0.49/-0.55

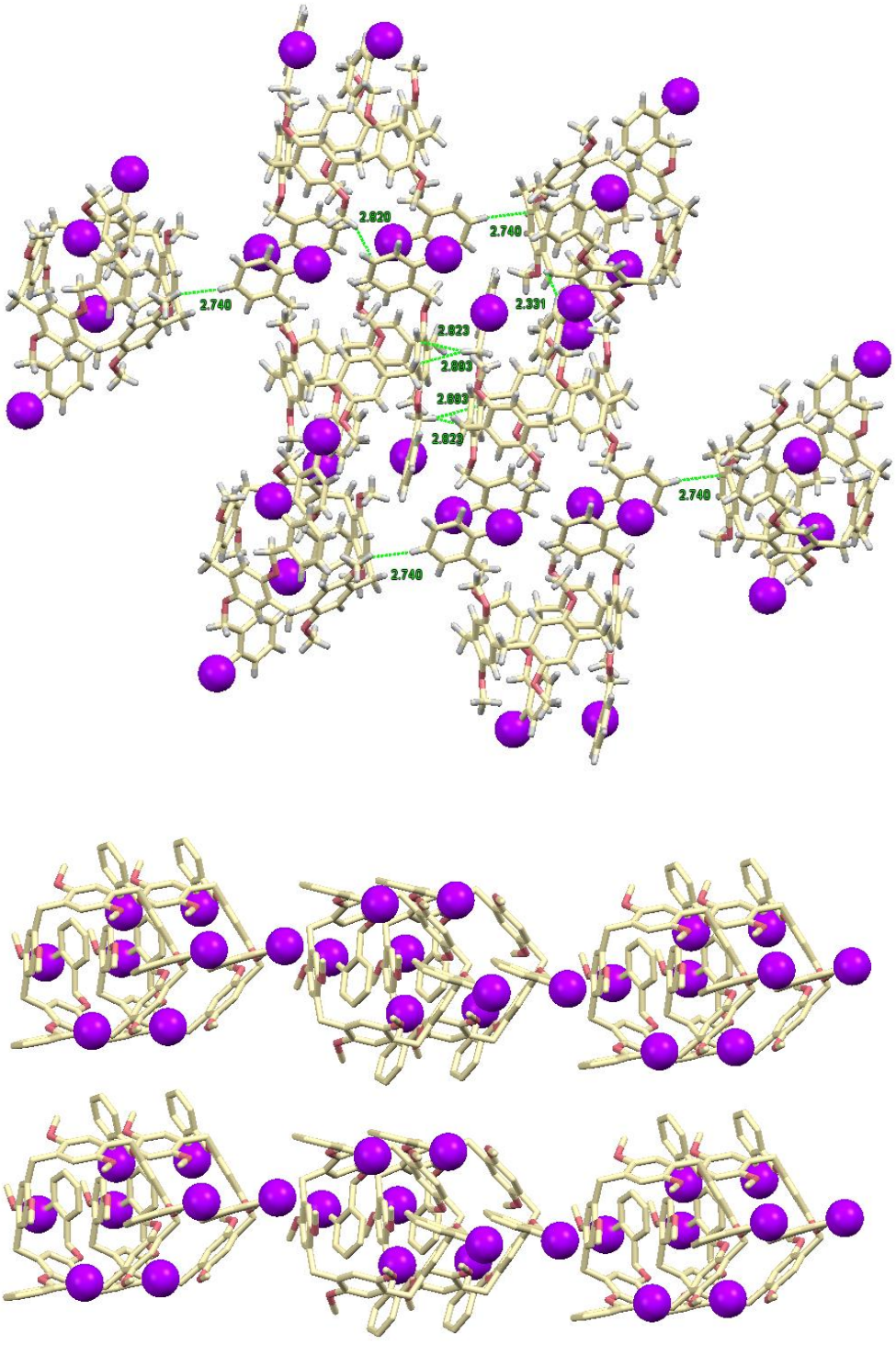


Figure S45. The front view (top) and top view (bottom) of the X-ray structure of **P5**

CCDC	2323543
Empirical formula	$C_{69}H_{62}Br_4O_{10}$
Formula weight	1370.869
Temperature/K	103
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.77605(6)
b/Å	14.68348(8)
c/Å	33.83251(18)
α/°	90
β/°	98.6321(4)
γ/°	90
Volume/Å^3	6274.98(6)
Z	4
ρ_{calc}g/cm^3	1.451
μ/mm^{-1}	3.600
F(000)	2780.7
Crystal size/mm^3	0.362 × 0.348 × 0.147
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.28 to 151.62
Index ranges	-15 ≤ h ≤ 16, -17 ≤ k ≤ 17, -42 ≤ l ≤ 42
Reflections collected	95130
Independent reflections	12878 [R_{int} = 0.0212, R_{sigma} = 0.0112]
Data/restraints/parameters	12878/0/754
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0350, wR_2 = 0.0875
Final R indexes [all data]	R_1 = 0.0352, wR_2 = 0.0876
Largest diff. peak/hole / e Å^{-3}	1.20/-1.29

7 Chiral guest induces P4-P5.

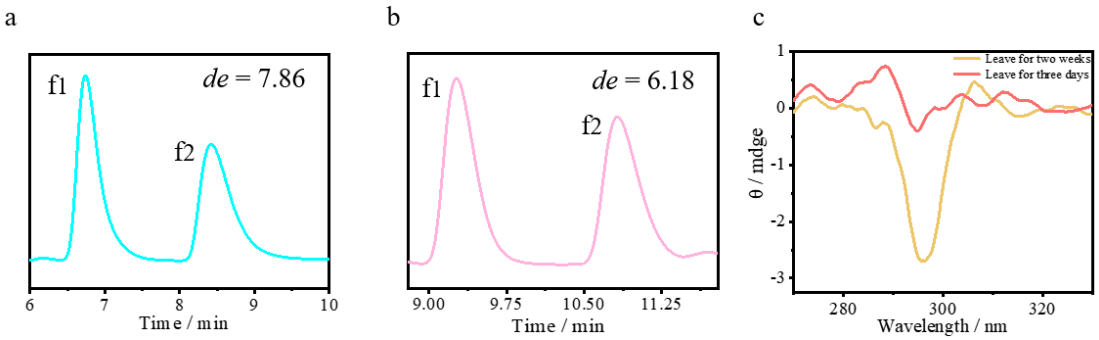


Figure S46. The Chiral HPLC traces of **P5** in (S)-1-chloro-2-methylbutane for two weeks (a) and (b) after removing the (S)-1-chloro-2-methylbutane (DCM: hexane, 1:3 (*v/v*)), (c) the CD spectral of 100 μl a saturated of **P5** in (S)-1-chloro-2-methylbutane to 2 ml chloroform.

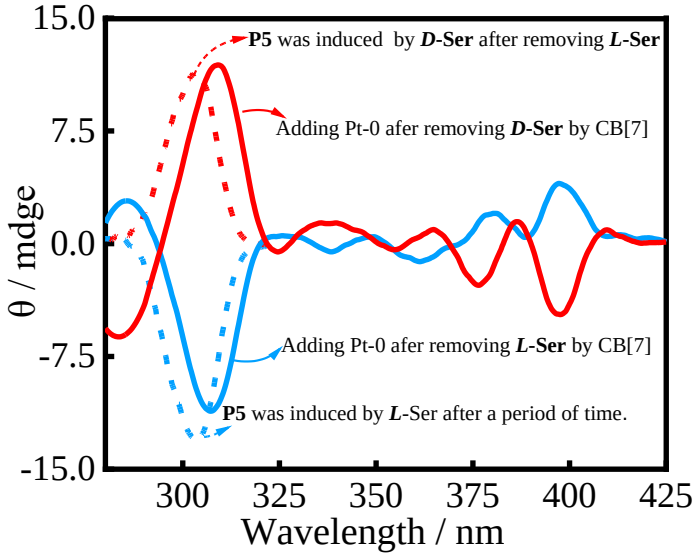


Figure S47. CD spectra of 1 equiv *L*-**Ser** induced **P5** (0.05 mM) (blue dotted line) and then removing *L*-**Ser** by CB[7] and adding **Pt-0** (blue solid line); CD spectra of **P5** was induced by *D*-**Ser** after removing *L*-**Ser** (red dotted line) and then removing *D*-**Ser** by CB[7] and adding **Pt-0** (red solid line), All the measurements were carried out in chloroform at 25 ℃.

8 Calculations for Complexation Between the P5$_{R/S}$ and *L*-Ser.

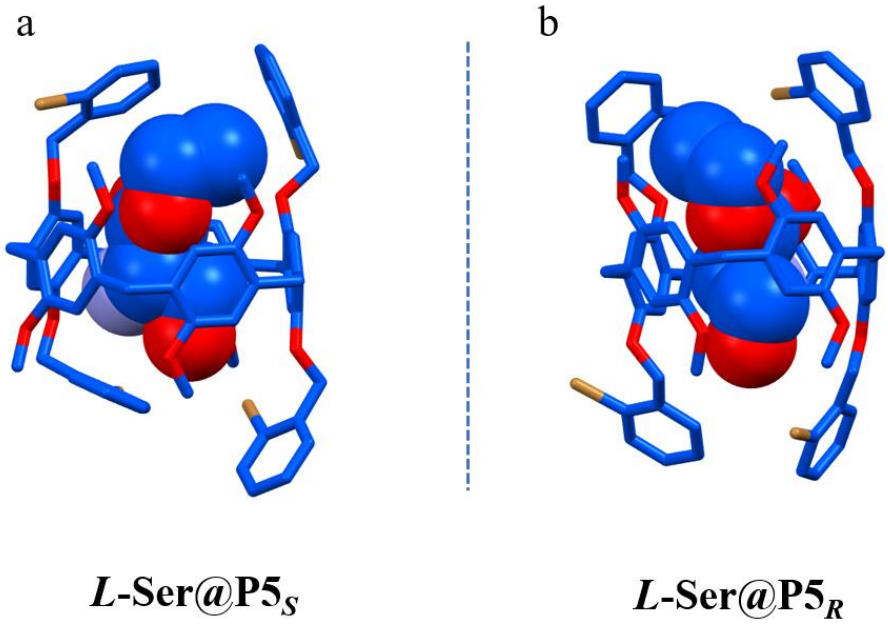


Fig. S48 The calculated optimal structure of enantiomeric complexes of (a) ***L*-Ser@P5$_S$**, (b) ***L*-Ser@P5$_R$.** Color code: blue for carbon, red for oxygen, purple for nitrogen, and yellow for bromine atoms. Hydrogen atoms were omitted for clarity. Calculated structure of complex ***L*-Ser@P5$_S$** and ***L*-Ser@P5$_R$** at B3LYP/6-31G(d) level.

The atomic coordinates of ***L*-Ser@P5$_S$.**

C	-2.8194	0.88933	1.58716
C	-1.63904	1.53776	0.8892
O	-0.5358	0.92733	1.26023
C	0.68414	1.13459	0.47583
O	-1.77522	2.42239	0.06299
C	0.93676	-0.13733	-0.29737
H	-2.66936	0.83631	2.667
H	0.53344	1.99796	-0.1661
H	1.45846	1.34527	1.20979
H	1.03675	-0.98885	0.37921
H	0.11856	-0.33641	-0.98874
H	1.85037	-0.04457	-0.88694
C	0.23141	2.45713	4.00802
C	1.03206	1.45507	4.56026
C	2.40439	1.46379	4.27445
C	2.9327	2.41139	3.3921
C	2.12685	3.39274	2.81132
C	0.76771	3.4337	3.16641
O	0.02318	4.47278	2.65588
O	3.16115	0.498	4.89186
C	-1.18278	4.79101	3.3354
C	4.56339	0.71617	4.97588
C	1.3193	4.7383	-0.2672
C	2.36444	4.07275	0.38005
C	3.06661	3.08246	-0.3303
C	2.70822	2.77802	-1.64414
C	1.65016	3.43025	-2.2832
C	0.96609	4.43686	-1.58714
O	0.00151	5.09224	-2.31594
O	4.07215	2.42553	0.3463
C	-0.84354	6.07497	-1.73308
C	5.15032	1.9308	-0.45105
C	2.70543	4.39095	1.82571
C	-0.65419	1.345	-3.30637
C	0.6776	1.57791	-3.65206
C	1.5051	0.47724	-3.91576
C	0.99496	-0.82111	-3.82974
C	-0.33363	-1.05607	-3.46504
C	-1.16314	0.04787	-3.20706
O	-2.46638	-0.22233	-2.85396
O	2.80723	0.76691	-4.24786
C	-3.33821	0.89313	-2.71265
C	3.71425	-0.32149	-4.35973
C	1.21718	2.99557	-3.6737
C	-2.25379	-3.07082	-1.29759
C	-1.00436	-2.93981	-1.89166
C	0.12755	-3.24492	-1.10852
C	-0.01317	-3.70379	0.19782
C	-1.27654	-3.83611	0.79396
C	-2.3932	-3.50474	0.02616

O	-3.65542	-3.50751	0.62791
O	1.33829	-3.02148	-1.69709
C	-4.65078	-4.37797	0.04314
C	2.50401	-3.47624	-1.01339
C	-0.85068	-2.47543	-3.32763
C	-1.80914	-2.1172	3.58515
C	-0.90205	-3.07964	3.14562
C	0.4566	-2.91601	3.47766
C	0.87261	-1.79743	4.20403
C	-0.04157	-0.82612	4.63454
C	-1.39277	-0.99609	4.30939
O	-2.27197	-0.00085	4.69842
O	1.305	-3.91038	3.06048
C	-3.61864	-0.3973	4.97705
C	2.65919	-3.86964	3.503
C	0.42817	0.37521	5.43488
C	-1.37184	-4.22131	2.26037
C	-2.11202	5.50252	-1.14185
C	6.12424	1.18177	0.41243
C	6.88577	0.13851	-0.12931
C	7.74294	-0.62483	0.66253
C	7.84788	-0.35637	2.02765
C	7.10561	0.6792	2.59535
C	6.26684	1.43726	1.78181
C	-2.43608	5.73456	0.19769
C	-3.64841	5.30958	0.74053
C	-4.56622	4.63158	-0.06374
C	-4.25851	4.36308	-1.39986
C	-3.04262	4.80157	-1.91826
C	-5.99815	-3.90236	0.50713
C	3.71933	-3.16489	-1.84349
C	-6.58522	-2.72818	0.01548
C	-7.81292	-2.2647	0.47734
C	-8.48752	-2.99261	1.45867
C	-7.92988	-4.16504	1.9686
C	-6.6948	-4.6069	1.49609
C	4.74058	-2.38614	-1.28605
C	5.91585	-2.11164	-1.98301
C	6.08575	-2.61864	-3.27154
C	5.077	-3.38447	-3.85905
C	3.91111	-3.64771	-3.14297
Br	-2.69641	4.47442	-3.76966
Br	5.27166	2.85311	2.60336
Br	-5.68171	-1.69533	-1.32888
Br	2.54566	-4.67405	-4.00542
H	-0.8249	2.45731	4.25205
H	3.98124	2.38835	3.12337
H	-1.47545	5.78494	2.99537
H	-1.98427	4.08217	3.09447
H	-1.03314	4.80786	4.4211
H	4.95327	-0.08148	5.61072

H	5.041	0.65591	3.99531
H	4.78281	1.69116	5.42783
H	0.76937	5.47793	0.30047
H	3.22398	2.00878	-2.20344
H	-1.1045	6.73428	-2.56642
H	-0.31145	6.67223	-0.98756
H	5.66246	2.7645	-0.94487
H	4.75939	1.26515	-1.22835
H	2.32685	5.3908	2.05914
H	3.7927	4.41072	1.9455
H	-1.28359	2.2049	-3.12281
H	1.6279	-1.67892	-4.01632
H	-4.31567	0.47886	-2.46354
H	-3.00528	1.55757	-1.90793
H	-3.40717	1.47554	-3.63845
H	4.69231	0.11895	-4.55788
H	3.75168	-0.89393	-3.42962
H	3.44353	-0.9904	-5.1856
H	0.43861	3.66925	-4.03385
H	2.06466	3.05612	-4.36209
H	-3.13342	-2.77888	-1.85802
H	0.8533	-3.93527	0.80214
H	-4.57444	-4.34127	-1.0469
H	-4.4631	-5.40406	0.37487
H	2.59341	-2.97071	-0.04562
H	2.42202	-4.55743	-0.83566
H	-1.8226	-2.5623	-3.82373
H	-0.15208	-3.14714	-3.83685
H	-2.85419	-2.23543	3.32317
H	1.91648	-1.65679	4.45552
H	-4.0808	0.45115	5.48543
H	-4.17007	-0.61857	4.05715
H	-3.63452	-1.2748	5.6332
H	3.12241	-4.78122	3.12259
H	3.17775	-2.99695	3.09613
H	2.7172	-3.85606	4.59801
H	1.17511	0.04712	6.16236
H	-0.42158	0.78725	5.98337
H	-2.40687	-4.46962	2.50481
H	-0.7569	-5.10679	2.44409
H	6.7911	-0.07648	-1.18991
H	8.3198	-1.42886	0.21709
H	8.50285	-0.95117	2.65657
H	7.17793	0.89623	3.6549
H	-1.72753	6.28005	0.81272
H	-3.88403	5.52466	1.77806
H	-5.53306	4.33259	0.33247
H	-4.96497	3.84774	-2.04097
H	-8.23714	-1.35268	0.07308
H	-9.44801	-2.63804	1.8195
H	-8.45179	-4.73154	2.73301

H	-6.25305	-5.51534	1.89555
H	4.58365	-1.97664	-0.29651
H	6.68461	-1.49918	-1.52256
H	6.99385	-2.41427	-3.83019
H	5.18962	-3.77172	-4.86528
N	-4.04771	1.70732	1.30443
H	-4.84092	1.07089	1.13997
H	-4.2919	2.32658	2.08144
H	-3.87343	2.30647	0.4786
C	-3.03223	-0.50745	1.01377
H	-3.08674	-0.47677	-0.08328
H	-2.17027	-1.11321	1.29775
O	-4.24235	-0.98499	1.57048
H	-4.31528	-1.91675	1.27125

The atomic coordinates of ***L*-Ser@P5$_R$.**

C	1.6393	1.5671	-2.3512
C	0.4594	1.4816	-3.0042
C	-0.6466	1.9595	-2.4016
C	-0.6705	2.4704	-1.1538
C	0.4931	2.4451	-0.4662
C	1.6047	2.0031	-1.0781
C	1.4517	1.191	2.5737
C	0.3936	1.8131	2.0097
C	-0.8474	1.455	2.3865
C	-1.1281	0.4897	3.2848
C	-0.0689	-0.1093	3.8717
C	1.1722	0.2638	3.5113
C	0.577	2.9241	0.9779
C	0.8476	-3.2892	4.0625
C	-0.2823	-2.5741	4.2559
C	-1.457	-3.0516	3.8074
C	-1.5824	-4.1736	3.072
C	-0.4421	-4.8505	2.8123
C	0.7209	-4.4101	3.3249
C	-0.2485	-1.2058	4.9231
C	0.8246	-5.6293	-0.205
C	-0.3587	-5.7259	0.4405
C	-1.4976	-5.5038	-0.2402
C	-1.5535	-5.1555	-1.5397
C	-0.3763	-5.1062	-2.1968
C	0.7607	-5.3417	-1.5204
C	-0.4376	-6.0857	1.9216
C	1.1337	-2.7775	-3.99
C	-0.1078	-3.307	-3.946
C	-1.1813	-2.5155	-4.124
C	-1.1118	-1.1803	-4.2936
C	0.1282	-0.6437	-4.2898
C	1.2007	-1.4483	-4.1842
C	0.3439	0.8598	-4.3956
C	-0.3126	-4.7907	-3.6879

O	2.2342	-3.5939	-3.8698
C	3.5003	-3.1125	-4.255
O	-2.2043	-0.3557	-4.4288
C	-3.4834	-0.9189	-4.5953
O	2.0021	-5.8152	0.4843
C	3.2285	-5.5389	-0.1678
O	-2.7053	-4.8578	-2.2231
C	-3.9601	-4.8571	-1.5727
O	2.0479	-2.8005	4.5211
C	3.2467	-3.372	4.0515
O	-2.7781	-4.6318	2.5736
C	-3.9822	-4.0795	3.052
O	2.7257	1.5626	2.2146
C	3.8132	1.1577	3.0129
O	2.7948	1.0397	-2.864
C	3.533	1.8758	-3.7311
O	-1.794	2.9428	-0.5169
C	-3.0787	2.7546	-1.0691
O	-2.4019	0.1203	3.6487
C	-3.5012	0.8638	3.1765
C	4.4243	-5.5216	0.7726
C	-4.9976	-4.1507	-2.4353
C	5.6006	-4.9557	0.429
C	6.6386	-4.9401	1.2836
C	6.5222	-5.493	2.4989
C	5.3642	-6.0675	2.853
C	4.3336	-6.0797	1.9952
C	-5.9499	-3.3254	-1.9503
C	-6.8217	-2.7199	-2.776
C	-6.763	-2.9252	-4.0999
C	-5.8283	-3.7463	-4.5959
C	-4.9621	-4.3484	-3.7678
C	4.5103	2.7707	-2.9904
C	-3.7128	3.8999	-1.8577
C	4.2492	4.0896	-2.908
C	5.0953	4.9373	-2.3098
C	6.2336	4.4719	-1.7715
C	6.5109	3.1635	-1.8354
C	5.6566	2.3194	-2.4443
C	-5.0582	3.8456	-1.9537
C	-5.7837	4.7826	-2.5812
C	-5.1637	5.8234	-3.1486
C	-3.8271	5.9003	-3.0788
C	-3.1055	4.9587	-2.4409
Br	5.8782	-4.1522	-1.2706
Br	-6.1351	-2.9458	-0.0966
Br	6.1406	0.4825	-2.4923
Br	-1.2331	5.2758	-2.4853
H	-1.5783	1.9146	-2.9848
H	2.5433	1.9908	-0.5029
H	-1.6756	1.9965	1.9094

H	2.002	-0.2448	4.0211
H	-0.1714	3.7282	1.1641
H	1.5433	3.4562	1.1317
H	-2.348	-2.4423	4.0148
H	1.6161	-5.001	3.0849
H	-1.1732	-1.0387	5.5202
H	0.5636	-1.1537	5.6826
H	-2.4345	-5.6107	0.3219
H	1.6872	-5.2884	-2.1075
H	-1.3397	-6.7072	2.1227
H	0.4004	-6.7666	2.1948
H	-2.167	-3.0018	-4.089
H	2.1912	-0.9779	-4.2375
H	1.2427	1.0659	-5.0159
H	-0.4733	1.3458	-4.9744
H	-1.2281	-5.1526	-4.2078
H	0.4911	-5.3904	-4.172
H	4.2111	-3.9679	-4.2128
H	3.4714	-2.733	-5.3004
H	3.8573	-2.336	-3.5434
H	-4.2023	-0.0837	-4.7499
H	-3.5038	-1.574	-5.4942
H	-3.7909	-1.4648	-3.6761
H	3.4064	-6.3148	-0.9482
H	3.1449	-4.5265	-0.6225
H	-4.2736	-5.9076	-1.3781
H	-3.8475	-4.3112	-0.6148
H	4.0913	-2.7715	4.4578
H	3.3525	-4.4127	4.4297
H	3.2922	-3.3234	2.9406
H	-4.8199	-4.6618	2.6067
H	-4.0396	-4.1768	4.159
H	-4.0873	-3.0228	2.72
H	4.7303	1.6397	2.6063
H	3.6706	1.5032	4.0611
H	3.9552	0.0559	2.9519
H	4.0905	1.2202	-4.4385
H	2.8389	2.4646	-4.3703
H	-3.7244	2.6256	-0.1649
H	-3.1617	1.778	-1.5912
H	-4.4216	0.4186	3.6169
H	-3.4273	1.921	3.5153
H	-3.5827	0.785	2.0693
H	7.6017	-4.4778	1.0071
H	7.372	-5.4812	3.2015
H	5.2614	-6.528	3.8498
H	3.3998	-6.5638	2.3231
H	-7.6017	-2.0425	-2.3885
H	-7.477	-2.4273	-4.7775
H	-5.7735	-3.9242	-5.6826
H	-4.2061	-5.0187	-4.2103

H	3.3255	4.495	-3.3522
H	4.8572	6.0132	-2.267
H	6.9352	5.1659	-1.2805
H	7.4529	2.8019	-1.3865
H	-5.607	3.0042	-1.497
H	-6.882	4.7003	-2.6285
H	-5.7454	6.603	-3.6679
H	-3.3455	6.7666	-3.565
O	-3.2516	-1.4798	-0.9991
C	-2.3962	-1.7273	0.0921
C	-1.1226	-0.9183	-0.1474
C	0.0924	-1.4282	0.5852
O	1.2251	-0.9617	0.0074
C	2.4119	-1.5913	0.4147
O	0.0525	-2.2161	1.499
N	-0.8483	-1.0607	-1.6186
C	3.5845	-1.0586	-0.3909
H	-3.9238	-2.1558	-1.1249
H	-2.9174	-1.4396	1.0308
H	-2.1917	-2.819	0.1058
H	-1.2855	0.1564	0.0818
H	2.582	-1.3965	1.4977
H	2.3121	-2.6874	0.244
H	0.0662	-0.6147	-1.8529
H	-0.8137	-2.0767	-1.8604
H	-1.6065	-0.5929	-2.1597
H	3.4421	-1.2847	-1.4708
H	3.6973	0.039	-0.2631
H	4.5388	-1.5211	-0.0537

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