Electronic Supplementary Information (ESI)

Guest-Induced Supramolecular chirality transfer in [2Pseudorotaxanes: Experimental and Computational Study

Hui-Juan Wang, ‡,[a] Haoyang Zhang, ‡,[a] Heng-Yi Zhang,* [a] Guoxing Liu,[b] Xianyin Dai,[a] Huang Wu,[a] and Yu Liu*[a,]

[a] College of Chemistry, State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, P. R. China

[b] College of Chemistry and Chemical Engineering, Henan University of Technology, Zhengzhou 450001, (P. R. China)

‡ These authors contributed equally to this work.

E-mail: hyzhang@nankai.edu.cn, yuliu@nankai.edu.cn

1. Experimental Section

Synthesis of (*R*)-**1,** (*S*)-**1:** (*R*)-**1** and (*S*)-**1** were synthesized according a previous method.[1, 2] **Synthesis of 2**, **3**, **4**, **5**: **2**, **3**, **4** and **5** were synthesized according a previous method.[3-5] The specific rotation of (*S*)-**1** and (*R*)-**1** have been tested. The values are [α]26.6 D = -51.6 (1.0, CH_2Cl_2:CH_3CN = 20:1) for (*S*)-**1** and [α]26.6 D = +52.0 (1.0, CH_2Cl_2:CH_3CN = 20:1) for (*R*)-**1**.

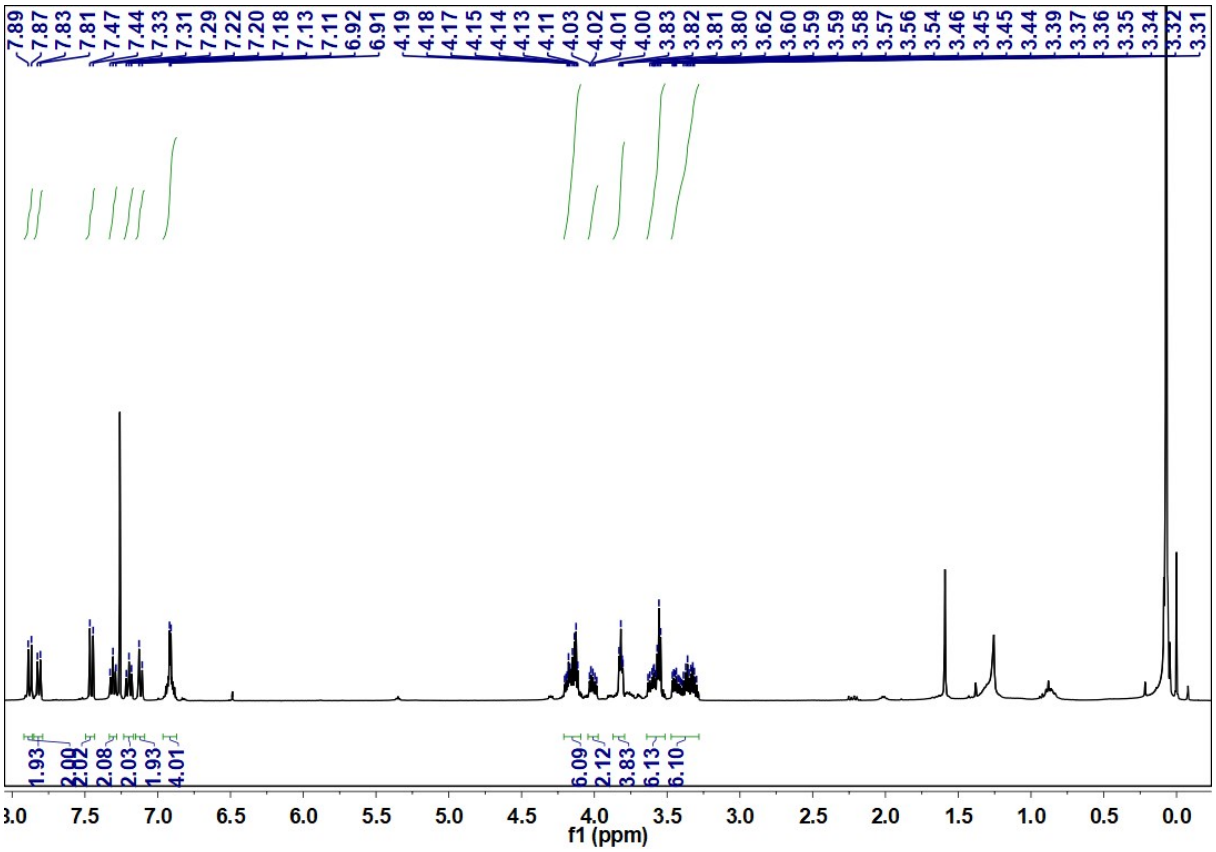

Figure S1. ^1H NMR spectrum of (*S*)-**1** in $CDCl_3$, 400 MHz, 298 K.

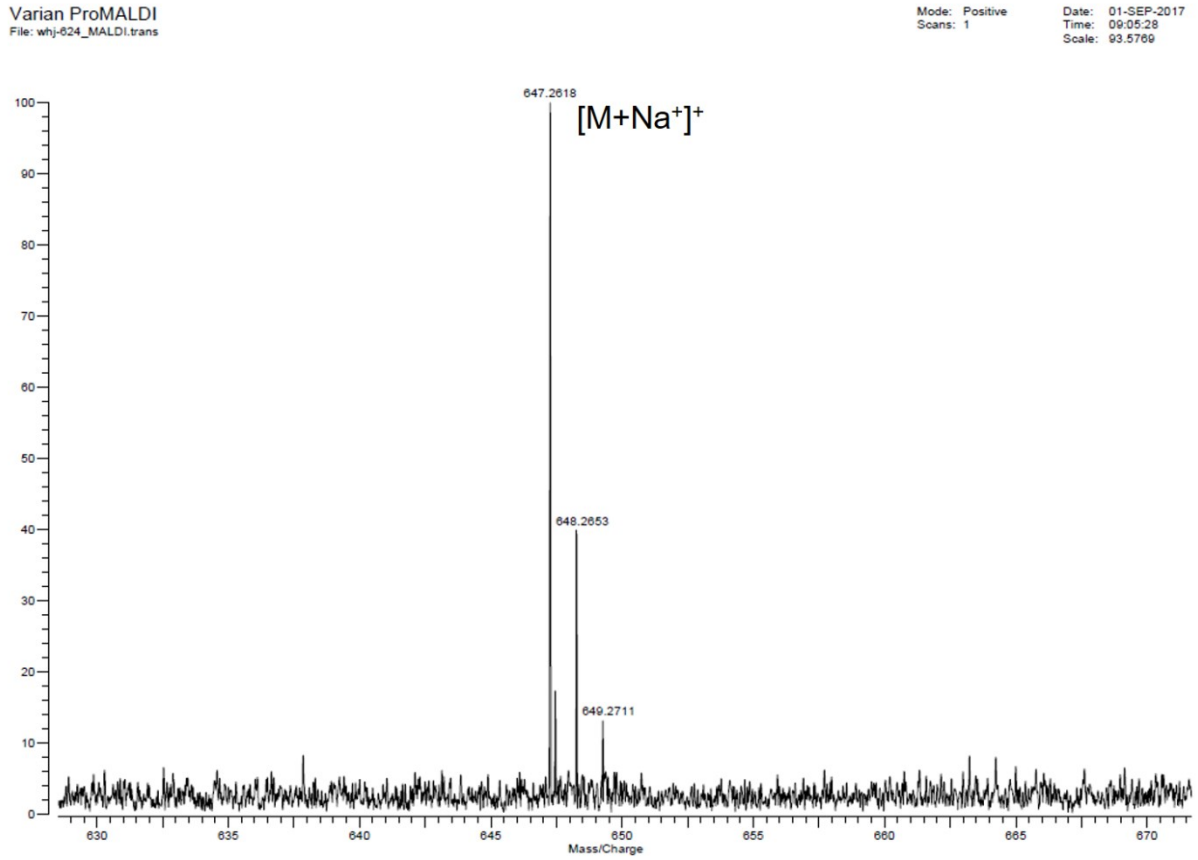

Figure S2. MADILI-TOFMS spectrum of (*S*)-**1** ($C_{38}H_{40}O_8$): calcd. $[M+Na^+]^+$: 647.2615, found: 647.2618.

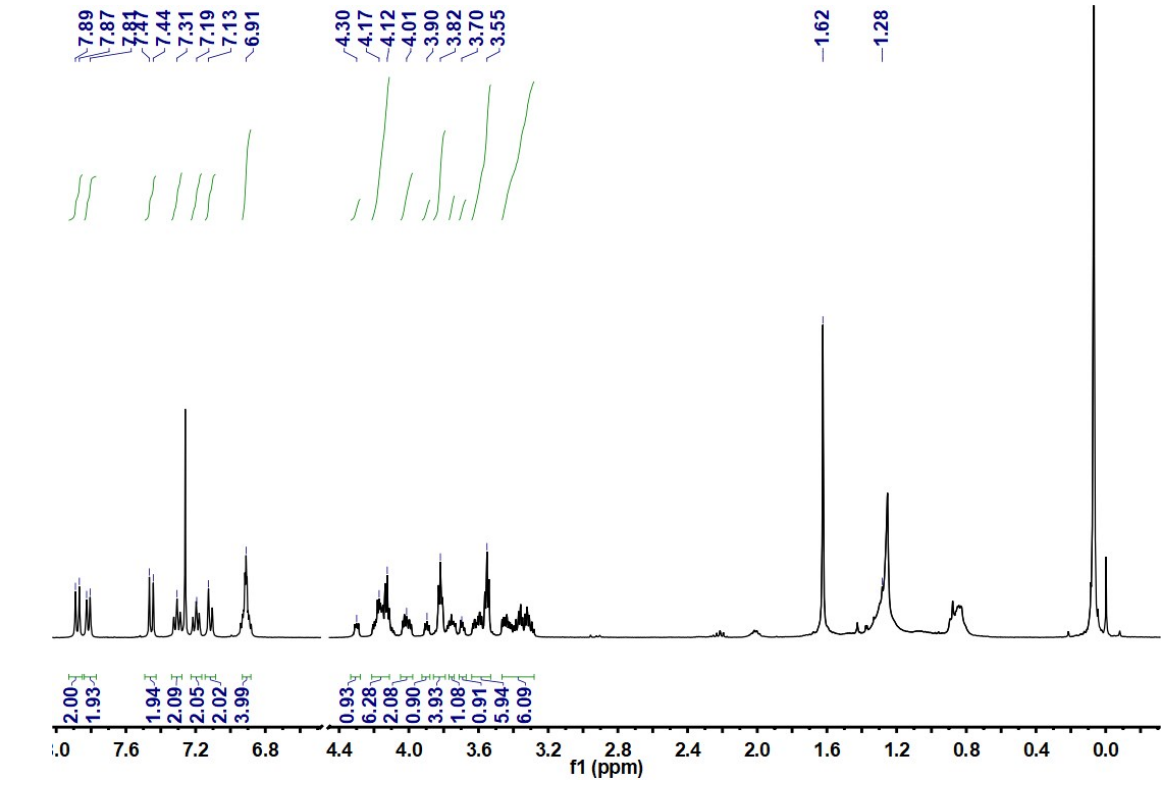

Figure S3. ^1H NMR spectrum of (*R*)-**1** in $CDCl_3$, 400 MHz, 298 K.

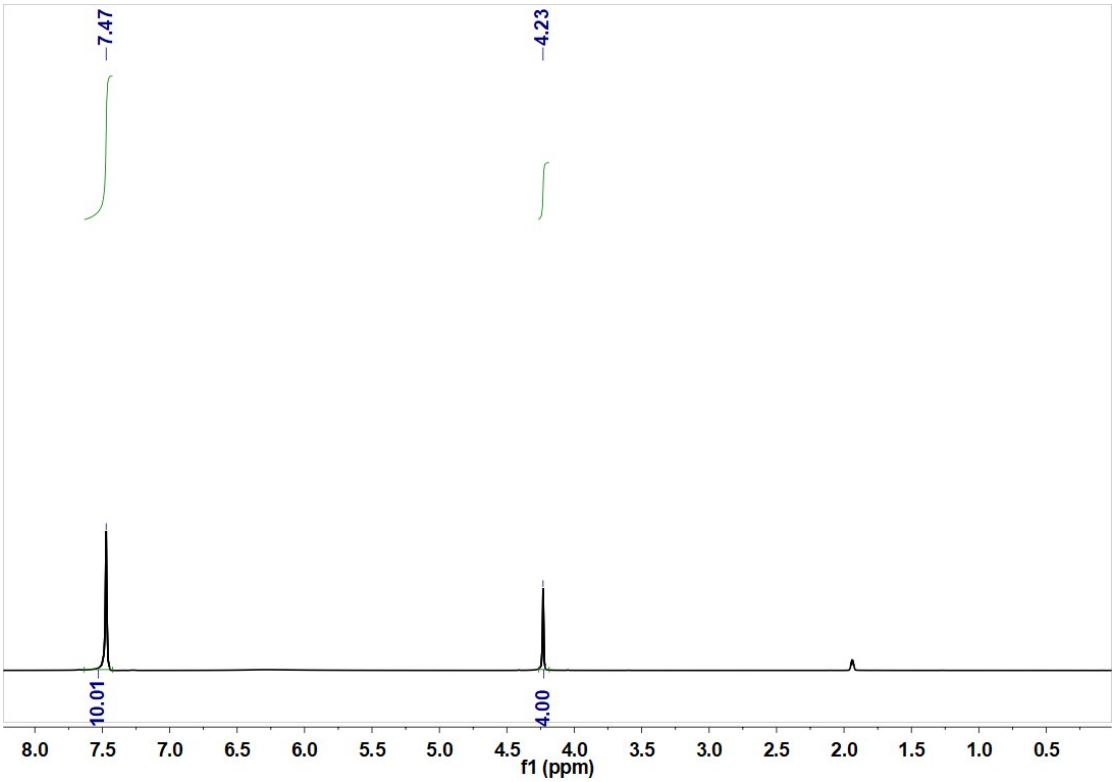

Figure S4. ^{1}H NMR spectrum of **2** in CD_3CN, 400 MHz, 298 K.

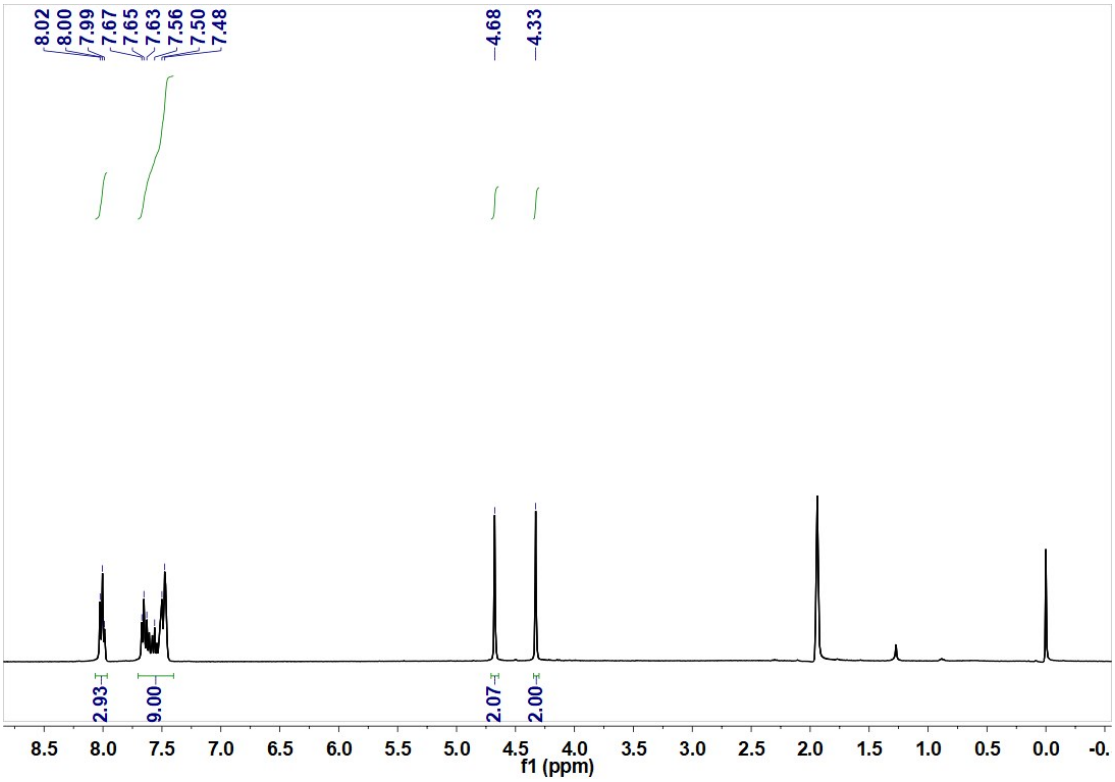

Figure S5. ^{1}H NMR spectrum of **3** in CD_3CN, 400 MHz, 298 K.

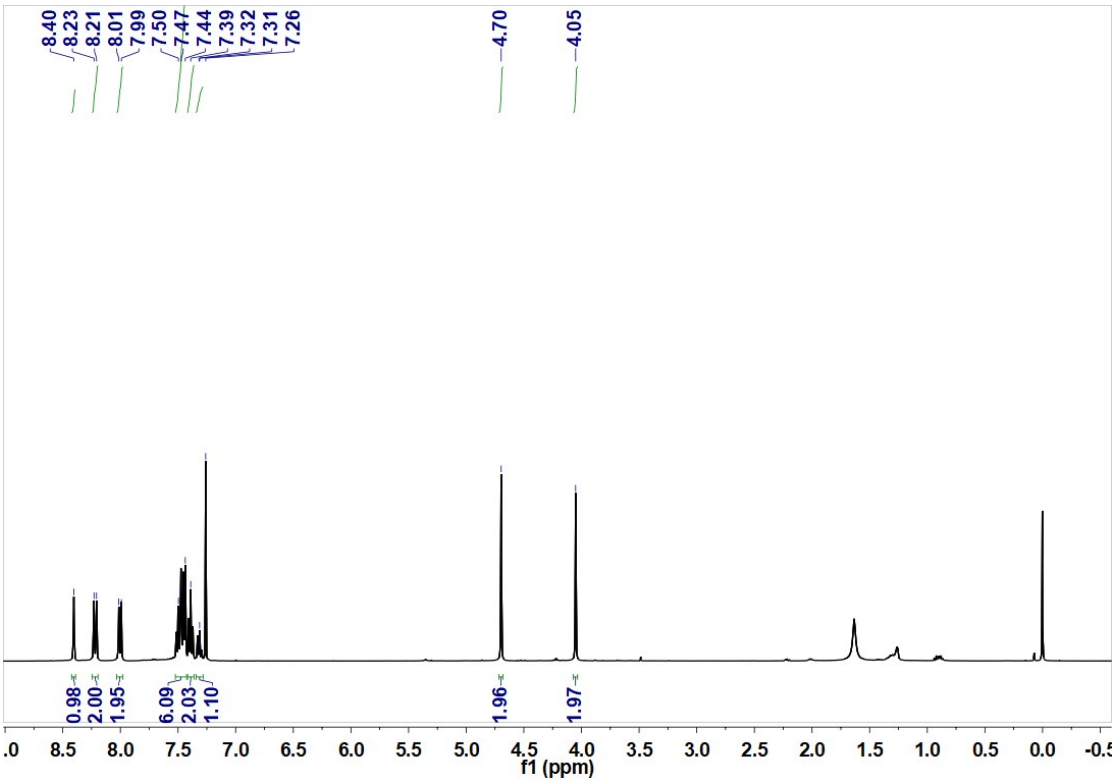

Figure S6. ^{1}H NMR spectrum of **4** in CD_3CN, 400 MHz, 298 K.

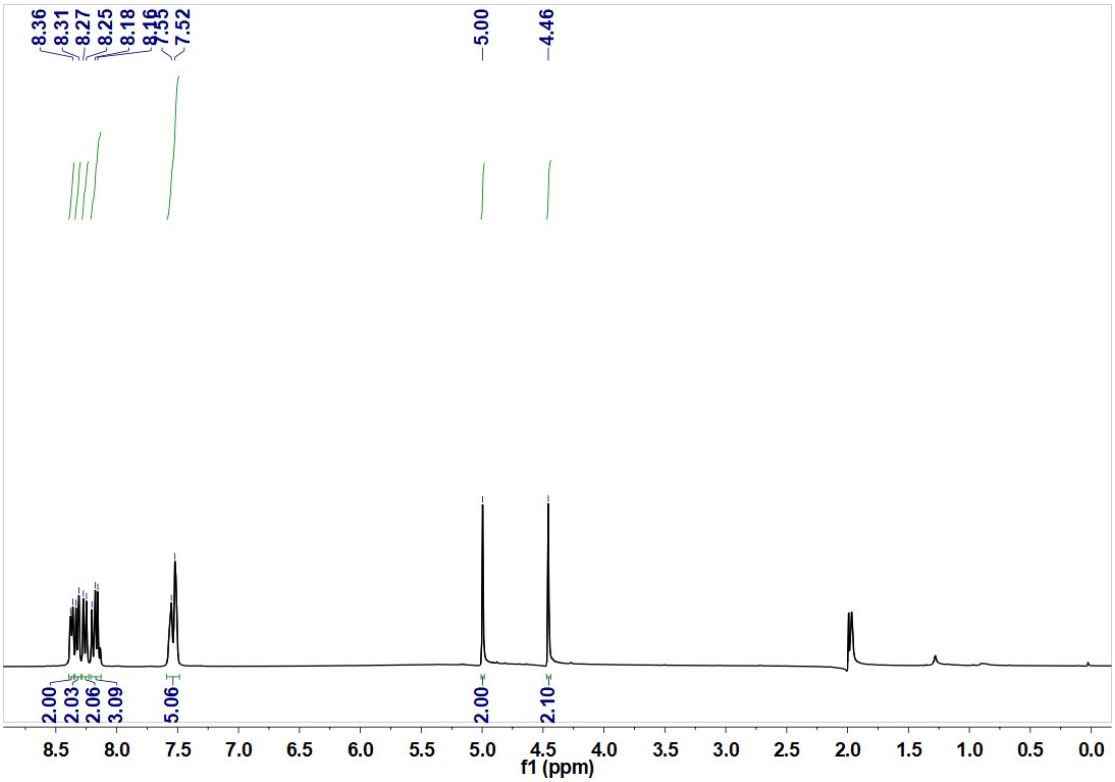

Figure S7. ^{1}H NMR spectrum of **5** in CD_3CN, 400 MHz, 298 K.

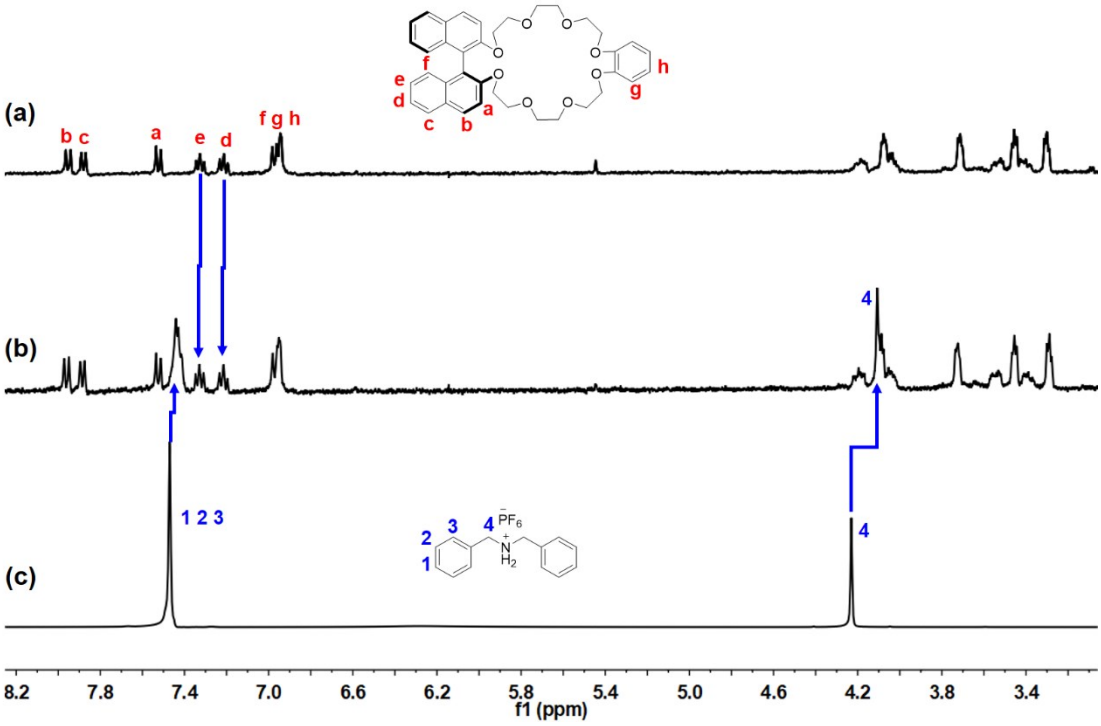

Figure S8. ^{1}H NMR spectrum of a) (*S*)-**1**, b) **2**, c) **2** ⊂ (*S*)-**1** in CD_3CN, 400 MHz, 298 K.

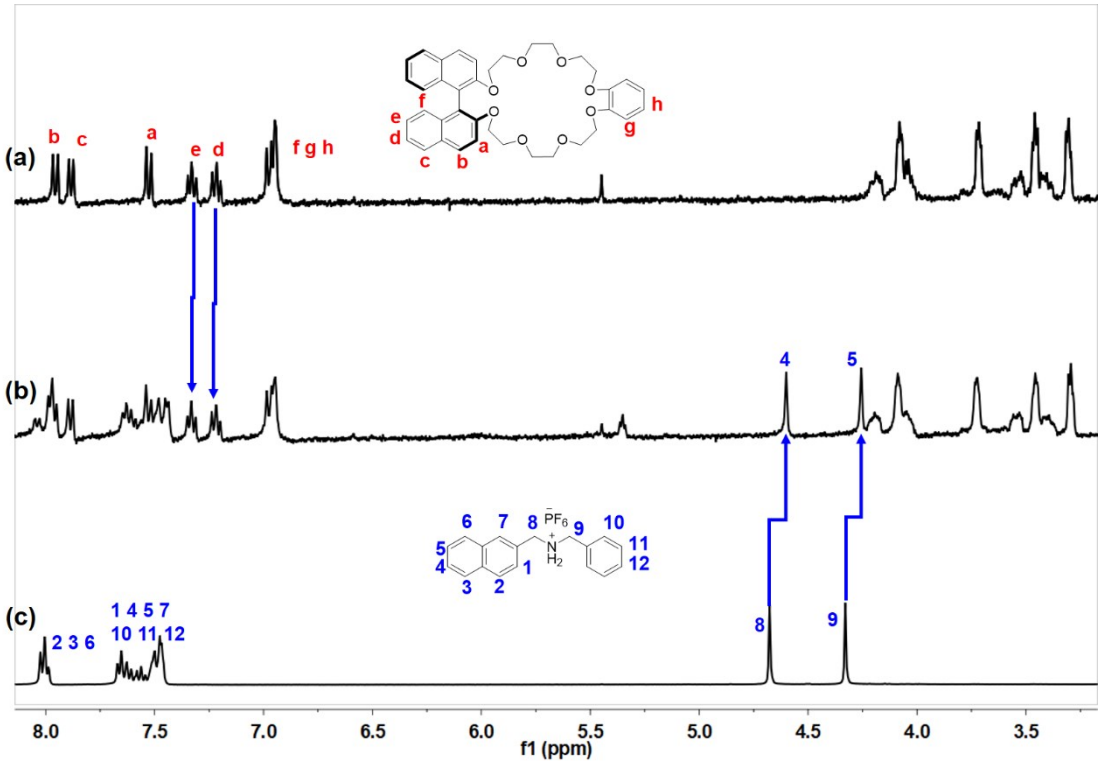

Figure S9. ^{1}H NMR spectrum of a) (*S*)-**1**, b) **3**, c) **3** ⊂ (*S*)-**1** in CD_3CN, 400 MHz, 298 K.

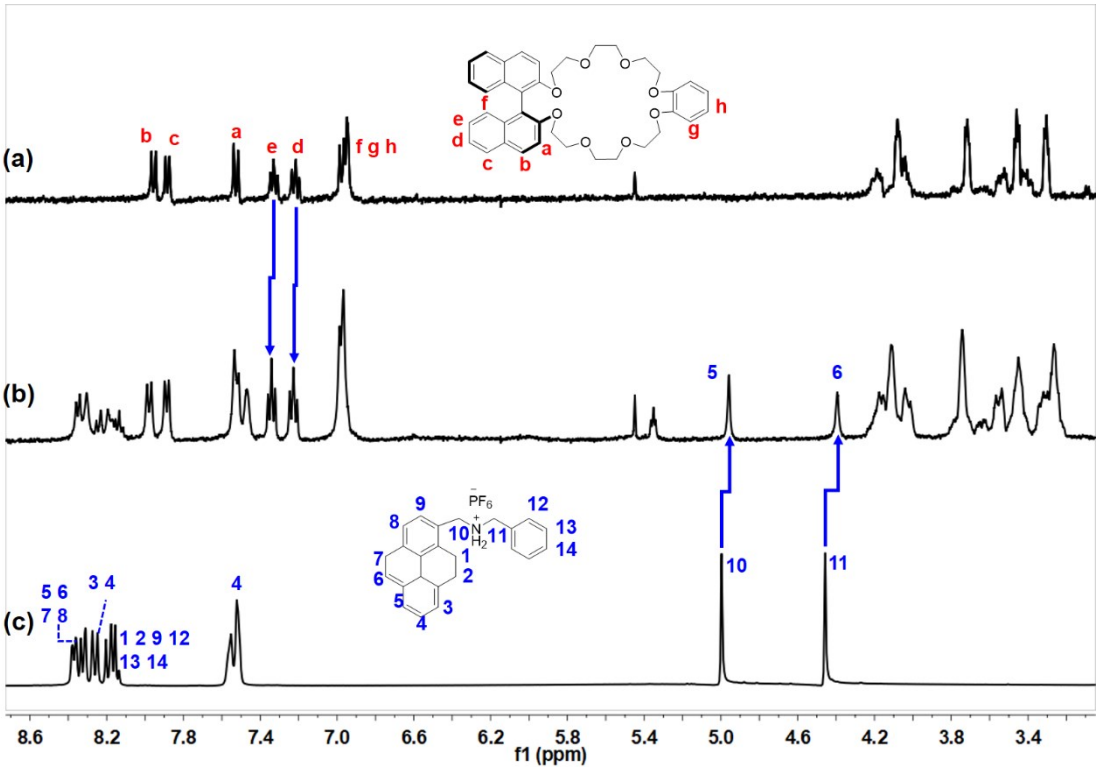

Figure S10. ^{1}H NMR spectrum of a) (*S*)-**1**, b) **5**, c) **5** ⊂ (*S*)-**1** in CD_3CN, 400 MHz, 298 K.

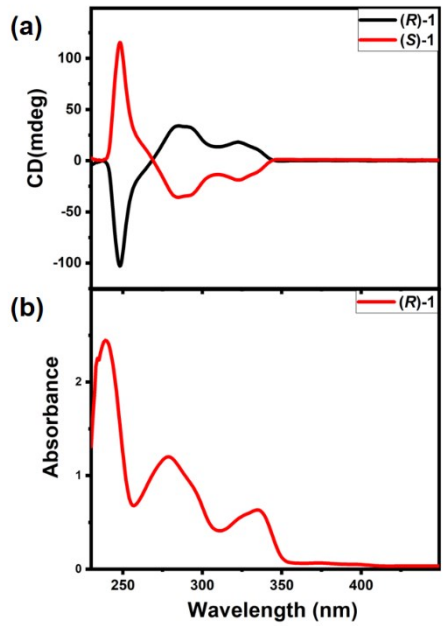

Figure S11. a) Circular dichroism spectra of (*R*)-**1** and (*S*)-**1**, b) UV/Vis spectra of (*R*)-**1** ([(*R*)-**1**] = [(*S*)-**1**] = 1×10^{-4} M) in CH_2Cl_2:CH_3CN = 20:1, at 298 K.

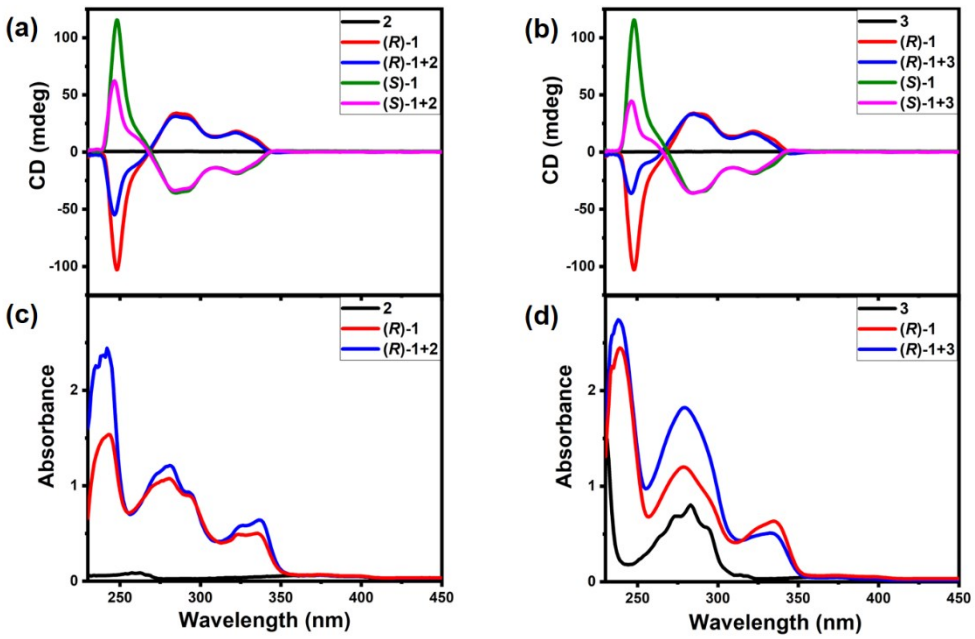

Figure S12. Circular dichroism spectra of a) **2**, (*R*)-**1**, (*S*)-**1**, **2** ⊂ (*R*)-**1** and **2** ⊂ (*S*)-**1**, b) a) **3**, (*R*)-**1**, (*S*)-**1**, **3** ⊂ (*R*)-**1** and **3** ⊂ (*S*)-**1**, UV/Vis spectra of c) 2, (*R*)-**1**, **2** ⊂ (*R*)-**1**, d) **3**, (R)-**1**, **3** ⊂ (*R*)-**1** ([(*R*)-**1**] = [(*S*)-**1**] = [**2**] = [**3**] = 1×10^{-4} M) in CH_2Cl_2:CH_3CN = 20:1, at 298 K.

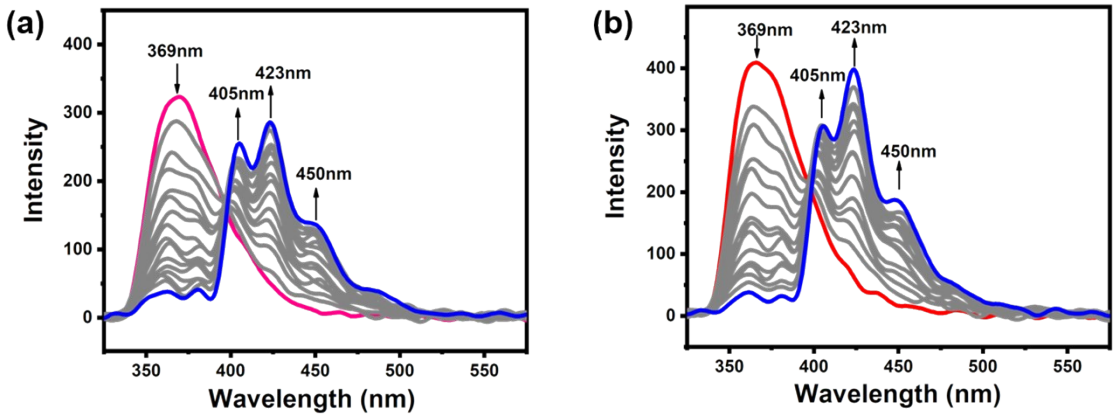

Figure S13. a) Fluorescence titration spectra (λ_{ex} = 295 nm) of (*S*)-**1** (1×10^{-4} M) upon addition of **4** ((0-30) × 10^{-5} M) in CH_2Cl_2:CH_3CN = 20:1. b) Fluorescence titration spectra (λ_{ex} = 295 nm) of (*R*)-**1**（1 × 10^{-4} M）upon addition of **4** ((0-30) × 10^{-5} M) in CH_2Cl_2:CH_3CN = 20:1. The silt width was 2.5 and 2.5 nm for emission, respectively.

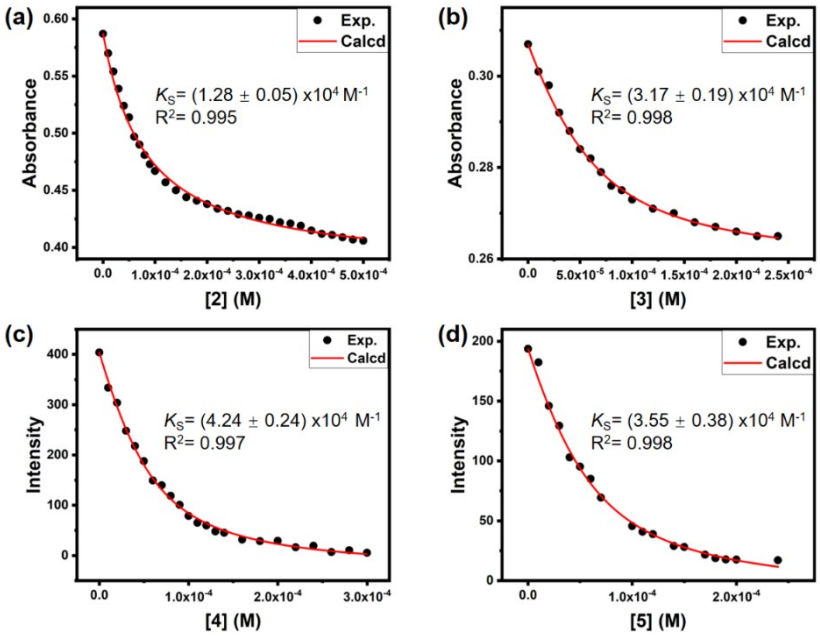

Figure S14. a) Nonlinear least squares fit of the absorption changes at 337 nm of (*R*)-**1** (1×10^{-4} M) upon addition of **2** ((0-50) $\times 10^{-5}$ M) to determine the complex stability constant (K_s) as $(1.28 \pm 0.05) \times 10^4$ M^{-1}. b) Nonlinear least squares fit of the absorption changes at 330 nm of (*R*)-**1**(1×10^{-4} M) upon addition of **3** ((0-25) $\times 10^{-5}$ M) to determine the complex stability constant (K_s) as $(3.17 \pm 0.19) \times 10^4$ M^{-1}. c) Nonlinear least squares fit of the fluorescence changes at 369 nm of (*R*)-**1** (1×10^{-4} M) upon addition of **4** ((0-30) $\times 10^{-5}$ M) to determine the complex stability constant (K_s) as $(4.24 \pm 0.24) \times 10^4$ M^{-1}. d) Nonlinear least squares fit of the fluorescence changes at 350 nm of (*R*)-**1** (1×10^{-4} M) upon addition of **5** ((0-20) $\times 10^{-5}$ M) to determine the complex stability constant (K_s) as $(3.55 \pm 0.38) \times 10^4$ M^{-1}.

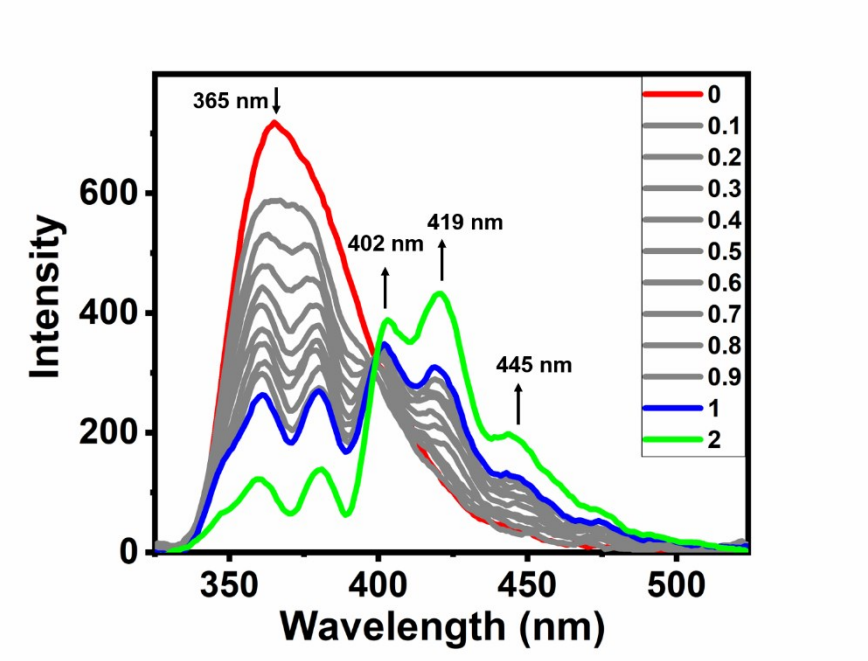

Figure S15. Fluorescence titration spectra (λ_{ex} = 295 nm) of (*S*)-**1** (1×10^{-4} M) upon addition of **4** ((0-20) × 10^{-5} M) in CH_2Cl_2: CH_3CN: CH_3OH = 20:1:1. The silt width was 10 (Ex) and 1.5 (Em) nm for emission.

Theoretical calculational section

The forming mechanism of the triple peak

To further understand the triple peak phenomenon of such host-guest complexation, density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were carried out. The NTOs calculations and the MOs participated in the transition are shown in Table S1 and Figure S15.

Table S1. Important electronic excited states and their NTOs analysis for **4,** (*S*)-**1** and **4** ⊂ (*S*)-**1**

Complex	Electronic transition	λ	Energy	R_{vel}	Assignment (H = HOMO, L = LUMO)
4_{nosymm}	$S_0\rightarrow S_1$	358.95nm[a]	3.4541eV	0.1602[b]	(0.70)H→L
	$S_0\rightarrow S_2$	306.75nm	4.0419eV	-0.0387	(0.54)H-1→L
					(-0.44)H→L+1

4_{Cs}	$S_0 \rightarrow S_1$	358.96nm	3.4539eV	0	(0.70)H→L
	$S_0 \rightarrow S_2$	306.77nm	4.0417eV	0	(0.54)H-1→L
					(-0.44)H→L+1
(*S*)-1	$S_0 \rightarrow S_1$	304.11 nm	4.0769 eV	37.1272	(0.21)H-2→L+1
					(0.64)H→L
					(-0.11)H→L+2
4⊂ (*S*)-1	$S_0 \rightarrow S_1$	359.49nm	3.4489eV	-15.7091	(0.18)H-1→L
					(0.68)H→L
	$S_0 \rightarrow S_2$	306.87nm	4.0402eV	-0.7871	(0.52)H-7→L
					(0.12)H-1→L+3
					(0.45)H→L+3
	$S_0 \rightarrow S_3$	300.21nm	4.1300eV	-55.4426	(0.10)H-4→L+7
					(-0.17)H-3→L+2
					(0.61)H-1→L+1
					(-0.15)H-1→L+2
					(-0.18)H→L+1

a. The system error is 0.57eV between theoretical and experimental spectra.

b. The unit of R_{vel} is $10^{-40}esu^2cm^2$.

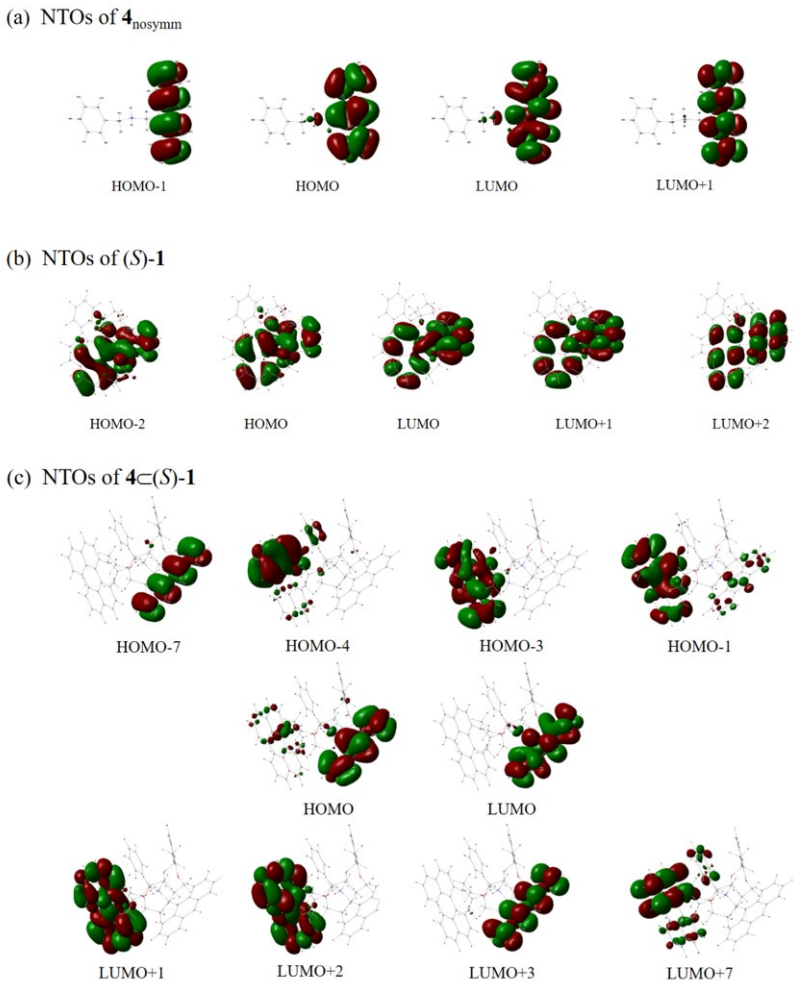

Figure S16. The MOs participated in the transition of (a) the guest **4**, (b) the host (*S*)-**1** and (c) the complexation **4** ⊂ (*S*)-**1**.

The continuous electron-hole distributions

To reveal the effect of the assembly on molecular excitation visually and easily, continuous electron–hole (C_{ele}-C_{hole}) distributions was calculated and drawn by Multiwfn program (version 3.6) and VMD 1.9.3. For the independent guest **4**, the C_{ele}-C_{hole} distribution was contracted symmetrically due to the LE in anthracene, which causes that the CD signal cannot be observed. After the assembly of the **4** ⊂ (*S*)-**1**, the C_{ele}-C_{hole} distribution produce a very weak shift towards the direction of binaphthalene for the LE in anthracene. In addition, we also found that the C_{ele}-C_{hole} distribution have a more obvious shift towards the direction

of anthracene for the LE in binaphthalene of the **4** ⊂ (*S*)-**1** compared to the independent host (*S*)-**1**. To sum up, the intermolecular induction between binaphthalene and anthracene make the LE produce weak directional shifts, which change the directions of the three peaks into the same and enhance the strength of the CD signal. As a result, the triple peak could be observed due to the assembly.

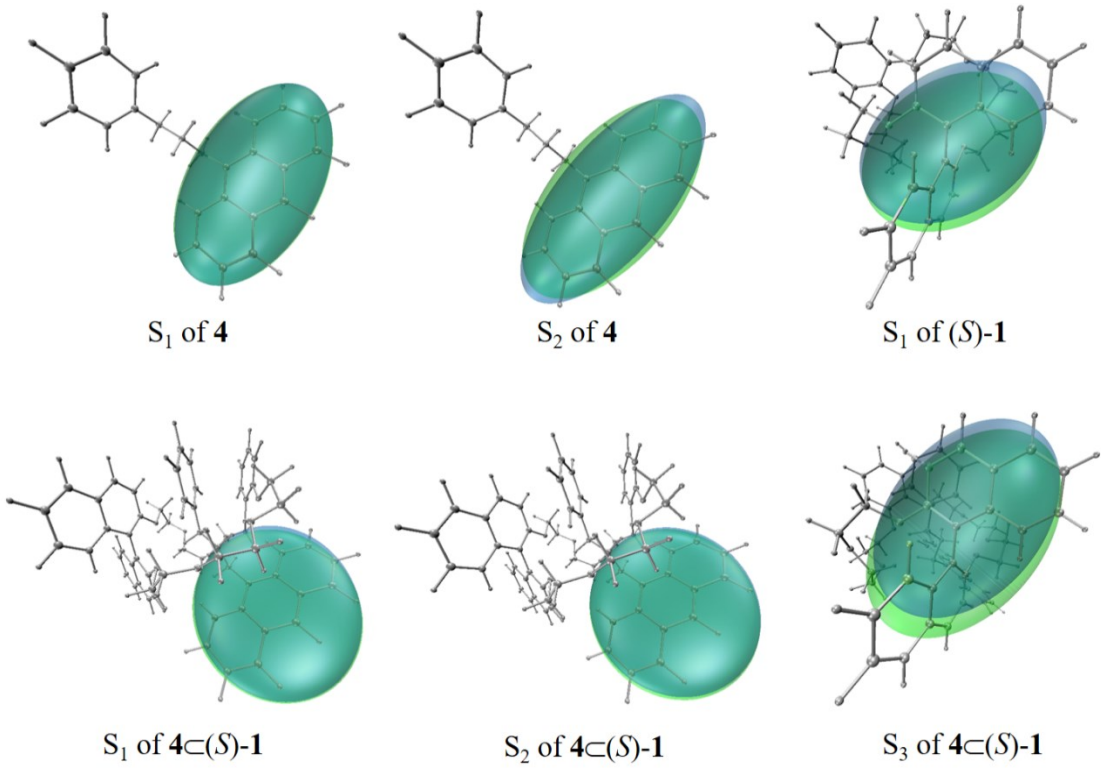

Figure S17. The C_{ele}-C_{hole} distributions which is equivalently described by Gauss function (green = electron, blue = hole).

Table S2. The Mulliken charges of 4 ⊂ (*S*)-1

Number	Element	Mulliken charge
1	O	-0.55726
2	C	0.04568
3	C	0.03049
4	O	-0.51137
5	C	0.05917
6	C	0.02954
7	O	-0.51145
8	C	0.06127

9	C	0.00944
10	O	-0.55425
11	C	0.31340
12	C	-0.14825
13	C	-0.12719
14	C	-0.12740
15	C	-0.14888
16	C	0.33703
17	O	-0.55934
18	C	0.03027
19	C	0.03888
20	O	-0.52778
21	C	0.03017
22	C	0.05904
23	O	-0.53089
24	C	0.04673
25	C	0.03194
26	O	-0.57931
27	C	0.31462
28	C	-0.13242
29	C	-0.16873
30	C	0.08490
31	C	-0.15329
32	C	-0.11440
33	C	-0.11959
34	C	-0.14258
35	C	0.09233
36	C	-0.04532
37	C	-0.06804
38	C	0.34710
39	C	-0.12787
40	C	-0.16155
41	C	0.08007
42	C	0.09489
43	C	-0.15370
44	C	-0.12159
45	C	-0.11961
46	C	-0.15311
47	H	0.11981
48	H	0.12144
49	H	0.11091
50	H	0.11882
51	H	0.09992
52	H	0.11823

53	H	0.11599
54	H	0.10589
55	H	0.12256
56	H	0.10982
57	H	0.13168
58	H	0.13616
59	H	0.12441
60	H	0.10987
61	H	0.10942
62	H	0.12474
63	H	0.13485
64	H	0.13221
65	H	0.12413
66	H	0.11942
67	H	0.12273
68	H	0.12555
69	H	0.12219
70	H	0.11764
71	H	0.12534
72	H	0.12401
73	H	0.12277
74	H	0.12758
75	H	0.12629
76	H	0.11905
77	H	0.11257
78	H	0.11179
79	H	0.11159
80	H	0.10920
81	H	0.12175
82	H	0.11418
83	H	0.10686
84	H	0.10802
85	H	0.10785
86	H	0.10982
87	C	-0.14281
88	N	-0.54810
89	C	-0.13431
90	C	0.08262
91	C	-0.13134
92	C	-0.10762
93	C	-0.10836
94	C	-0.11752
95	C	-0.10481
96	H	0.18312

97	H	0.16701
98	H	0.36919
99	H	0.37998
100	H	0.18018
101	H	0.17429
102	H	0.11474
103	H	0.11005
104	H	0.10968
105	H	0.10630
106	C	-0.04980
107	C	0.07412
108	C	0.08055
109	C	0.09910
110	C	-0.14581
111	C	0.09826
112	C	-0.13508
113	C	-0.14102
114	C	-0.22022
115	C	-0.12770
116	H	0.13512
117	C	-0.13880
118	C	-0.11745
119	H	0.10505
120	C	-0.11613
121	H	0.11621
122	H	0.12213
123	H	0.11219
124	H	0.11778
125	C	-0.12000
126	H	0.11736
127	H	0.11585
128	H	0.11720
129	H	0.10994

a. The numbers are consistent with these of coordinates

References

1. E. Ishow, A. Credi, V. Balzani, F. Spadola and L. Mandolini, *Chem*. *Eur*. *J*., 2015, **5**, 984-989.
2. I. Fumitaka, F. Kei-Ichiro, S. Takashi, N. Kazuko, K. Yasuhito and T. Toshikazu, *Chem*. *Eur*. *J*., 2011, **17**, 12067-12075.
3. P. R. Ashton, P. J. Campbell, E. J. T. Chrystal, P. T. Glink, S. Menzer, D. Philp, N. Spencer, J. F. Stoddart, P. A. Tasker and D. J. Williams, *Angew*. *Chem*. *Int*. *Ed*., 2010, **107**, 1997-2001.
4. C. Xu, Y. Chen, H. Y. Zhang and Y. Liu, *J*. *Photochem*. *Photobiol*. *A*., 2016, **331**, 240-246.

5. M. Suresh, A. K. Mandal, E. Suresh and A. Das, *Chem*. *Sci*., 2013, **4**, 2380-2386.

Coordinates of molecular structure

4_{nosymm}

Total SCF energy (B3LYP-D3/6-31G(d, p)): -905.111113 a.u.

Gibbs free energy at 298K (B3LYP-D3/6-31G(d, p)): -904.791979 a.u.

	Cartesian coordinates		
ATOM	X	Y	Z
N	-1.24422200	0.07867600	-0.68544400
C	-0.01170800	0.05589900	-1.56911800
H	-1.17898000	0.87516900	-0.04052500
H	-1.24085200	-0.75946600	-0.09204300
H	-0.11901800	-0.81017400	-2.22022200
H	-0.06831700	0.94293400	-2.19759700
C	1.24074900	0.00917800	-0.73523000
C	1.77399300	-1.24329900	-0.34135200
C	1.85436000	1.21862200	-0.32469400
C	2.99357300	-1.27807000	0.43592200
C	1.16141600	-2.50089500	-0.65720800
C	3.07262600	1.16325600	0.45359000
C	1.32571400	2.51754700	-0.62426000
C	3.54507100	-2.53753000	0.83009600
C	3.61203300	-0.07873500	0.80056500
C	1.71652900	-3.68771600	-0.25060000
H	0.23437800	-2.53074800	-1.21961600
C	3.70378900	2.37859400	0.86654800
C	1.95597500	3.65994600	-0.20013000
H	0.40370000	2.61519000	-1.18738300
C	2.92684800	-3.71296000	0.49849000
H	4.46580000	-2.53649900	1.40692100
H	4.52946500	-0.11241300	1.38280700
H	1.22637300	-4.62349900	-0.50277300
H	4.62143500	2.30966500	1.44419100
C	3.16346300	3.59615600	0.55133000
H	1.52821200	4.62908400	-0.43952100
H	3.35010400	-4.66450000	0.80495500
H	3.64660200	4.51378800	0.87239200
C	-2.55907100	0.14765100	-1.43349300
H	-2.55694500	-0.69679100	-2.12540100
H	-2.53846800	1.07870300	-2.00202300
C	-3.70776100	0.08812200	-0.46462700
C	-4.20440200	-1.15244600	-0.04208000
C	-4.25494500	1.26644000	0.05927800

C	-5.23820200	-1.21360000	0.89265100
H	-3.78449300	-2.06756200	-0.45185400
C	-5.29008400	1.20464400	0.99319600
H	-3.87411800	2.22967300	-0.27023700
C	-5.78132100	-0.03489200	1.41091300
H	-5.62281100	-2.17764000	1.21149600
H	-5.71495500	2.12126200	1.39094500
H	-6.58943600	-0.08238100	2.13486100

(*S*)-**1**

Total SCF energy (B3LYP-D3/6-31G(d, p)): -2074.057521 a.u.
Gibbs free energy at 298K (B3LYP-D3/6-31G(d, p)): -2073.416221 a.u.

	Cartesian coordinates		
ATOM	X	Y	Z
O	0.64945500	-1.46688800	1.50739200
C	-0.59663100	-2.10406600	1.82247900
C	-0.59832900	-3.45055100	1.11585100
O	-0.96596300	-3.40203700	-0.25412100
C	-0.12663800	-2.61719500	-1.10326300
C	-0.58756000	-2.77940100	-2.54216600
O	-1.81544300	-2.11335700	-2.82074300
C	-2.97766600	-2.84536700	-2.44444900
C	-4.13032600	-1.87291600	-2.25853900
O	-3.90201800	-0.88192400	-1.25179200
C	-3.98846700	-1.20238200	0.06860000
C	-4.25749000	-2.46825200	0.58854100
C	-4.31507500	-2.67375000	1.97480700
C	-4.11316900	-1.61089800	2.84668800
C	-3.86220400	-0.32775400	2.33902500
C	-3.79930300	-0.11200700	0.96137600
O	-3.58008400	1.09291600	0.37028300
C	-3.45288600	2.24797000	1.20107400
C	-3.26875900	3.44188000	0.29268900
O	-1.97651900	3.38472600	-0.28114300
C	-1.80603600	4.29890100	-1.35024500
C	-0.37764100	4.22595400	-1.83972200
O	-0.14278200	2.94542000	-2.40262000
C	1.17456800	2.80285900	-2.90055300
C	1.50301800	1.33206800	-3.04654600
O	1.49217200	0.75712300	-1.73503700
C	2.39559700	-0.19722600	-1.38385600

C	3.04709000	-1.02493400	-2.33521300
C	3.92430200	-1.99809500	-1.91551600
C	4.19674100	-2.19438700	-0.53758600
C	5.10495700	-3.19309700	-0.08989300
C	5.35375300	-3.37287200	1.25169800
C	4.70061200	-2.55141500	2.20518000
C	3.81368600	-1.57767400	1.80461500
C	3.52809400	-1.36532200	0.42524100
C	2.61293100	-0.36303100	-0.01702100
C	1.82901100	0.47070000	0.94181500
C	0.79429900	-0.12169600	1.66186900
C	-0.03923300	0.64203400	2.51809100
C	0.16355900	1.99649500	2.64246000
C	1.20661100	2.64940000	1.93758900
C	2.05981900	1.87202500	1.08515300
C	3.10928500	2.54388600	0.39601100
C	3.29474700	3.90199100	0.53113300
C	2.44012800	4.66938200	1.36248800
C	1.42151600	4.05019700	2.05153100
H	-1.44213600	-1.49969300	1.47993400
H	-0.68021300	-2.25228500	2.90731400
H	0.39386100	-3.91420400	1.24013900
H	-1.34286800	-4.09443100	1.59377800
H	0.92147600	-2.94287900	-1.01652700
H	-0.17315900	-1.55506700	-0.83804900
H	0.16518000	-2.31564800	-3.18991800
H	-0.64641300	-3.84781000	-2.80161400
H	-2.79494800	-3.41320400	-1.53119600
H	-3.26364800	-3.55730400	-3.23835000
H	-4.26940000	-1.29344900	-3.17545700
H	-5.05675200	-2.42934900	-2.06129200
H	-4.41713100	-3.30567800	-0.07842400
H	-4.51789300	-3.67024900	2.35567900
H	-4.15175600	-1.76161100	3.92134200
H	-3.71466100	0.49832800	3.02398500
H	-2.58680800	2.14935000	1.86677600
H	-4.35750500	2.38477800	1.80969400
H	-4.05097400	3.42849800	-0.48266900
H	-3.39929500	4.36554700	0.88204400
H	-2.01377700	5.33294600	-1.02595400
H	-2.49617000	4.06244000	-2.17644900
H	-0.22020900	5.02328100	-2.58622700
H	0.30943300	4.41054000	-0.99955100
H	1.90397400	3.25483000	-2.21265900

H	1.28449000	3.29593400	-3.88211200
H	0.76415500	0.82152000	-3.67599500
H	2.49007100	1.24341600	-3.51434700
H	2.83482500	-0.90448300	-3.39139300
H	4.41523000	-2.63611600	-2.64564900
H	5.60036800	-3.81391300	-0.83239500
H	6.04853700	-4.13887300	1.58368000
H	4.90326100	-2.69350300	3.26319300
H	3.32151200	-0.95305300	2.54222700
H	-0.84356400	0.15844300	3.05968500
H	-0.48110500	2.58432000	3.29049900
H	3.77043400	1.96535000	-0.24049000
H	4.10432400	4.39160300	-0.00317600
H	2.59587100	5.74014100	1.45703400
H	0.76138300	4.62499100	2.69651500

4 ⊂ (*S*)-**1**

Total SCF energy (B3LYP-D3/6-31G(d, p)): -2979.244812 a.u.
Gibbs free energy at 298K (B3LYP-D3/6-31G(d, p)): -2978.253276 a.u.

	Cartesian coordinates		
ATOM	X	Y	Z
O	3.03138200	-1.65354000	-0.56873400
C	3.17249400	-3.03303800	-0.92675900
C	3.13001300	-3.12915400	-2.44181700
O	1.88890700	-2.72811200	-3.00907300
C	1.78803200	-1.33395000	-3.30268200
C	0.53636600	-1.08616400	-4.12083000
O	-0.67476000	-1.33598400	-3.40829300
C	-1.15700200	-2.67496800	-3.49475100
C	-2.54462700	-2.70917000	-2.88728400
O	-2.52994000	-2.51606400	-1.46178600
C	-2.53068500	-3.60891300	-0.63441400
C	-2.16467900	-4.89593700	-1.02759100
C	-2.19209400	-5.95362300	-0.11011800
C	-2.58171300	-5.72112500	1.20355600
C	-2.93719300	-4.42986100	1.61199600
C	-2.90871900	-3.36737500	0.70832200
O	-3.21344400	-2.07086300	1.02800200
C	-3.67259100	-1.81051500	2.36155800
C	-4.04993300	-0.35337000	2.47288400
O	-2.86628200	0.43231100	2.35513600

C	-3.08511200	1.83233600	2.53454700
C	-1.79862500	2.48776900	2.98084700
O	-0.83378000	2.48890700	1.92355100
C	0.41347200	3.05326100	2.34178600
C	1.29557200	3.28061900	1.14107700
O	1.60921900	2.00011100	0.56918900
C	2.51330200	1.97562300	-0.47268200
C	2.36039100	2.84266300	-1.58553800
C	3.19334300	2.72452200	-2.67080800
C	4.22841800	1.75334700	-2.69144400
C	5.08688100	1.61034900	-3.81580500
C	6.09908000	0.67768300	-3.81745300
C	6.30074300	-0.14284200	-2.68056500
C	5.48185500	-0.03116500	-1.57814100
C	4.41125400	0.90583600	-1.54912800
C	3.52581200	1.02604100	-0.42567800
C	3.67953300	0.14949400	0.77191900
C	3.44266300	-1.21709600	0.65675500
C	3.59363400	-2.08934000	1.76288300
C	3.94868700	-1.58330400	2.98949500
C	4.19278200	-0.19769300	3.16887900
C	4.07420800	0.68048500	2.03980400
C	4.37627200	2.05860900	2.23393200
C	4.72701100	2.54411400	3.47470400
C	4.80706000	1.67920300	4.59401800
C	4.55329500	0.33546600	4.43633900
H	2.36391700	-3.62162200	-0.47938000
H	4.13429200	-3.42795700	-0.57415000
H	3.95777800	-2.54472300	-2.86749800
H	3.27799800	-4.18116900	-2.71311900
H	2.65938800	-1.00116400	-3.88958800
H	1.76066200	-0.73988300	-2.38439400
H	0.51963100	-0.02561400	-4.39863600
H	0.56521800	-1.68126900	-5.04475500
H	-0.47886500	-3.36815400	-2.98537800
H	-1.23486600	-2.98616900	-4.54862500
H	-3.13058900	-1.87428600	-3.28329200
H	-3.05926900	-3.64042600	-3.14402100
H	-1.85055300	-5.08129400	-2.04747300
H	-1.90549400	-6.94895800	-0.43507800
H	-2.60735100	-6.53254600	1.92428700
H	-3.21927600	-4.25979000	2.64300400
H	-2.88086300	-2.04539100	3.08307300
H	-4.55482800	-2.42332200	2.58515600

H	-4.78014500	-0.08373400	1.70047900
H	-4.51283600	-0.19665300	3.45860300
H	-3.83245200	2.00051100	3.32242700
H	-3.45793200	2.28934900	1.60899600
H	-2.01450700	3.52420500	3.27779100
H	-1.39992500	1.95276400	3.85438600
H	0.90997700	2.38835600	3.06225000
H	0.24016600	4.02311100	2.82906600
H	0.77527100	3.91693100	0.42198500
H	2.21478700	3.78175600	1.46422400
H	1.57752300	3.59176600	-1.58160500
H	3.06489000	3.37737200	-3.52968600
H	4.92818500	2.25700300	-4.67488400
H	6.74920600	0.57472500	-4.68115600
H	7.11153500	-0.86580600	-2.67778800
H	5.65392300	-0.66045500	-0.71261800
H	3.38448300	-3.14519100	1.65029000
H	4.03562700	-2.24831900	3.84417000
H	4.34077700	2.72987100	1.38319200
H	4.95191500	3.60023600	3.59512200
H	5.08035300	2.07661700	5.56703400
H	4.62717200	-0.34455400	5.28137000
C	-1.77473800	0.81098400	-1.29873000
N	-1.23509700	0.32916000	0.02981000
C	-0.10766300	-0.66595600	-0.09601800
C	0.10896400	-1.43108800	1.18633400
C	0.23517300	-2.82307900	1.14158200
C	0.44474200	-3.55710800	2.31077600
C	0.52253600	-2.90367000	3.54128900
C	0.40572700	-1.51145400	3.59283900
C	0.20775800	-0.77926800	2.42257600
H	-2.07899000	-0.07562200	-1.84503700
H	-0.92750300	1.22971400	-1.83788400
H	-1.99878700	-0.08608300	0.58456900
H	-0.92856600	1.14235700	0.59535000
H	0.77635700	-0.09495700	-0.37801400
H	-0.36632000	-1.33414300	-0.91529600
H	0.14980500	-3.33655000	0.19007900
H	0.52775000	-4.63828100	2.25701800
H	0.47753600	-0.99242100	4.54415000
H	0.11853900	0.29840200	2.47386900
C	-2.90338000	1.80045200	-1.11819100
C	-4.23497600	1.33348700	-0.97383800
C	-2.63061500	3.18954600	-1.07954500

C	-5.30430500	2.28433900	-0.75700400
C	-4.59104300	-0.05290600	-1.02647000
C	-3.71008400	4.12745800	-0.86125200
C	-1.31981100	3.73489600	-1.25476500
C	-6.64779700	1.81532600	-0.60907900
C	-5.01240600	3.65002600	-0.69554200
C	-5.89316600	-0.46167100	-0.88777300
H	-3.82656700	-0.80776800	-1.14046400
C	-3.43015500	5.53050900	-0.82328800
C	-1.09080700	5.08587300	-1.22556000
H	-0.48564800	3.06577700	-1.41386300
C	-6.94016600	0.47915000	-0.67674900
H	-7.43228300	2.54952800	-0.44661000
H	-5.82001100	4.35848200	-0.52780800
H	-6.12451000	-1.52229500	-0.92667600
H	-4.25774300	6.21417800	-0.65463900
C	-2.15774500	6.00236300	-1.00223500
H	-0.08233000	5.46332800	-1.37013900
H	-7.96360000	0.13292700	-0.56766000
H	-1.95606500	7.06890900	-0.97812400
H	0.67780700	-3.47202300	4.45376500