Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Unprecedented Phthalocyanine-porphyrin-fused Oligomers with Induced Chirality Nature

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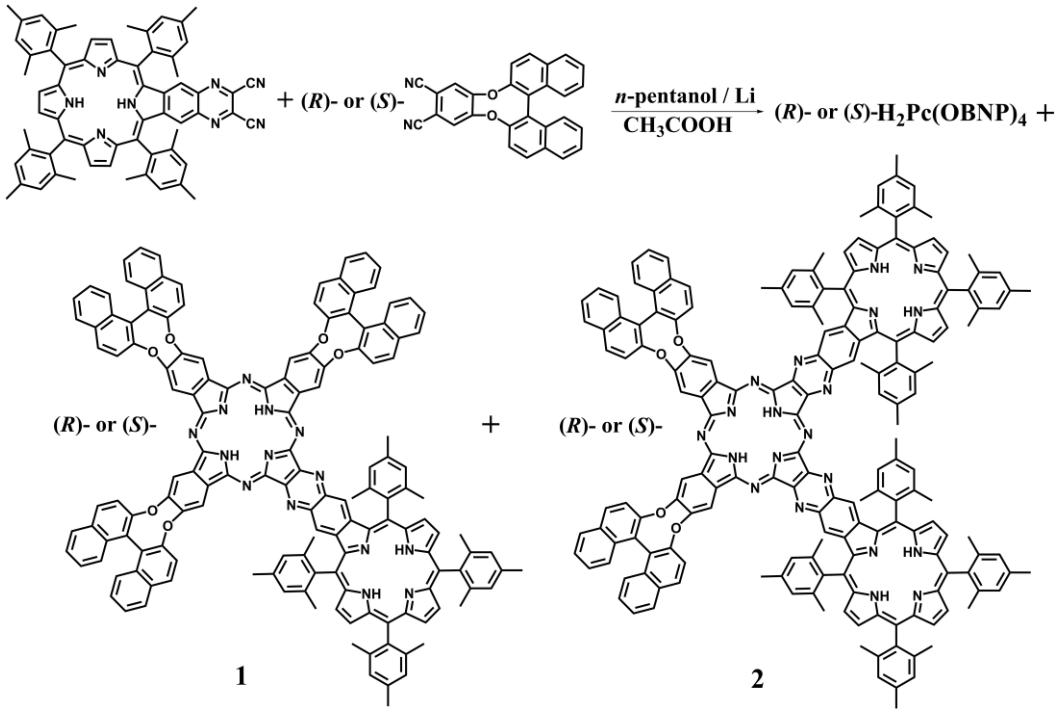
Caption of Content



Scheme S1 Synthesis of dimer **1** and trimer **2**.

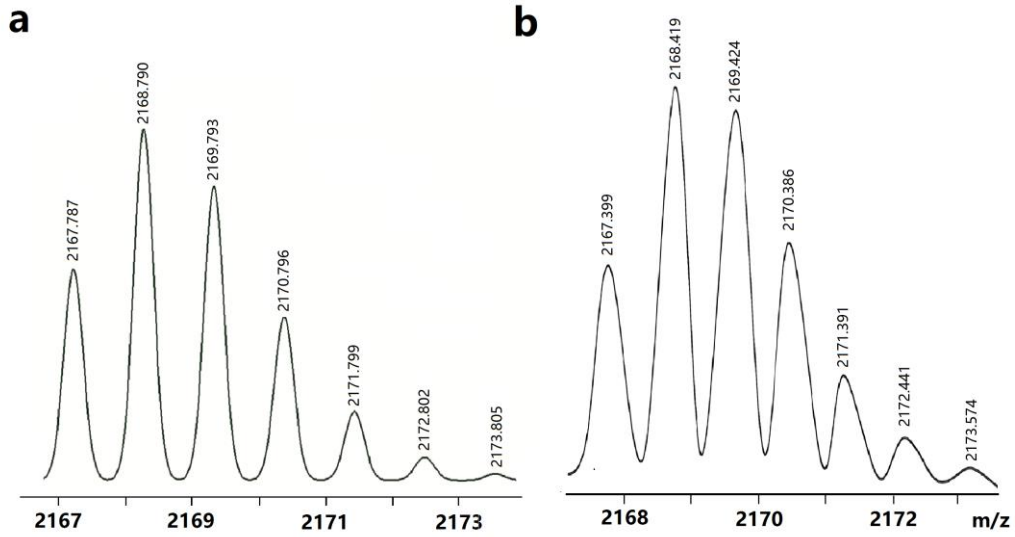


Fig. S1 Simulated (a) and experimental isotopic (b) pattern for the protonated molecular ion of Pc-Por-fused dimer **1**.

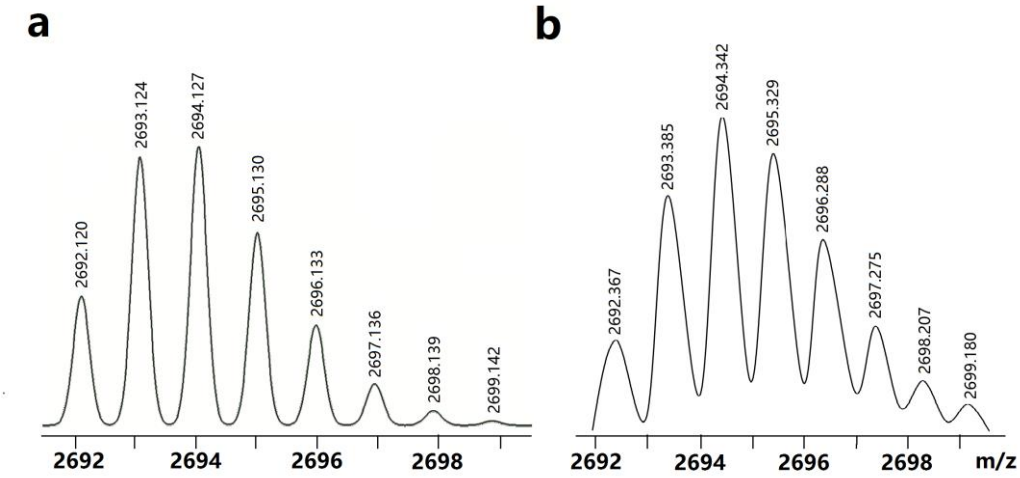


Fig. S2 Simulated (a) and experimental isotopic (b) pattern for the protonated molecular ion of Pc-Por-fused trimer **2**.

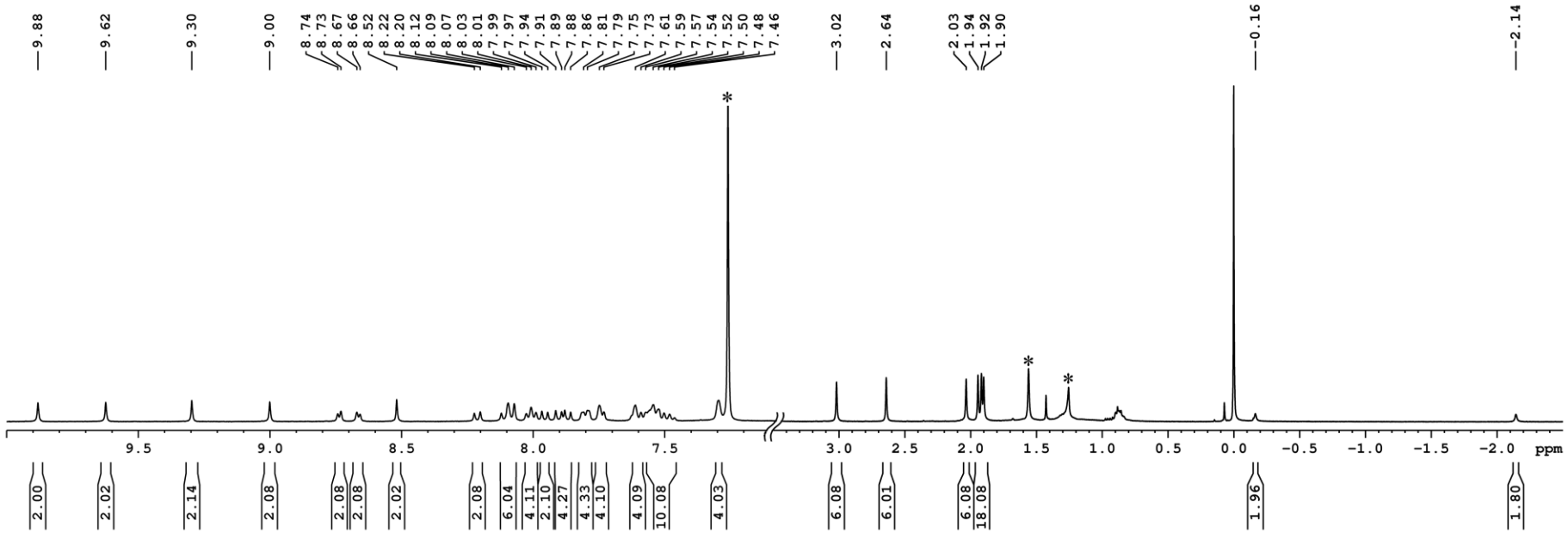


Fig. S3 ^{1}H NMR spectrum of dimer **1** in $CDCl_3$ at 298K; * indicates the signals for residual solvents.

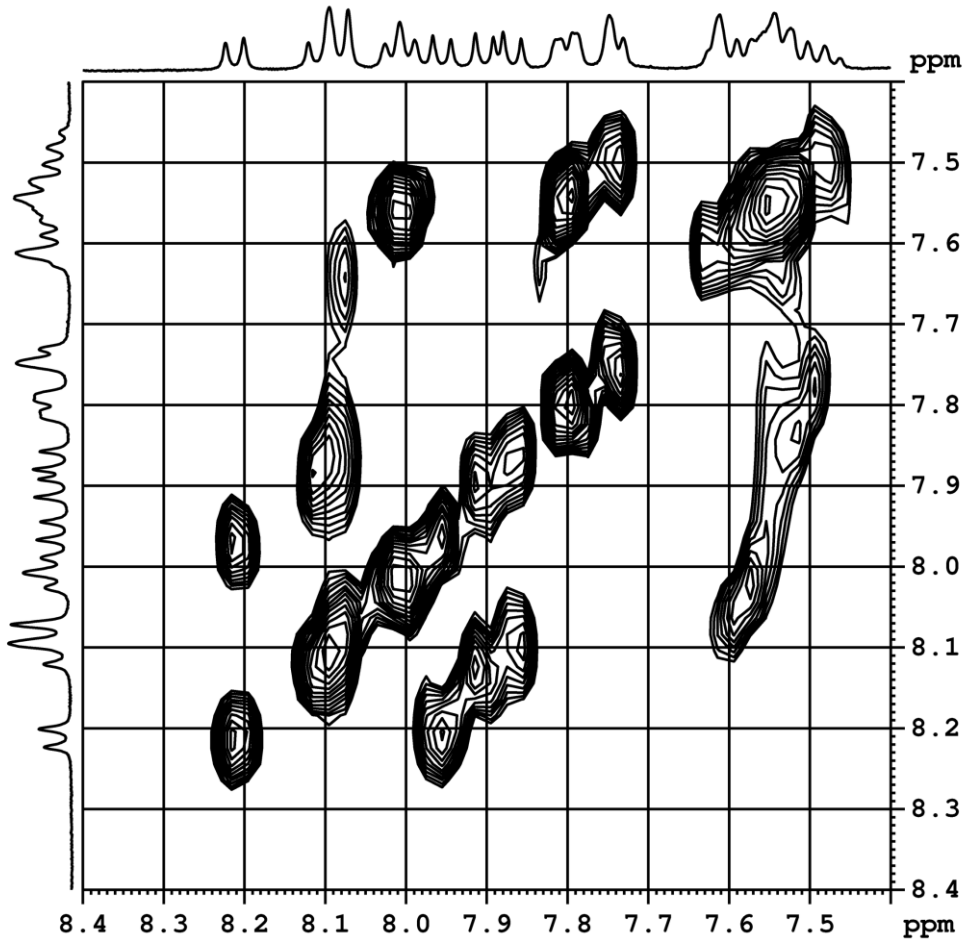


Fig. S4 ^{1}H-^{1}H COSY spectrum of dimer **1** in $CDCl_3$ at 298K with the range from δ = 8.4 to 7.4 ppm.

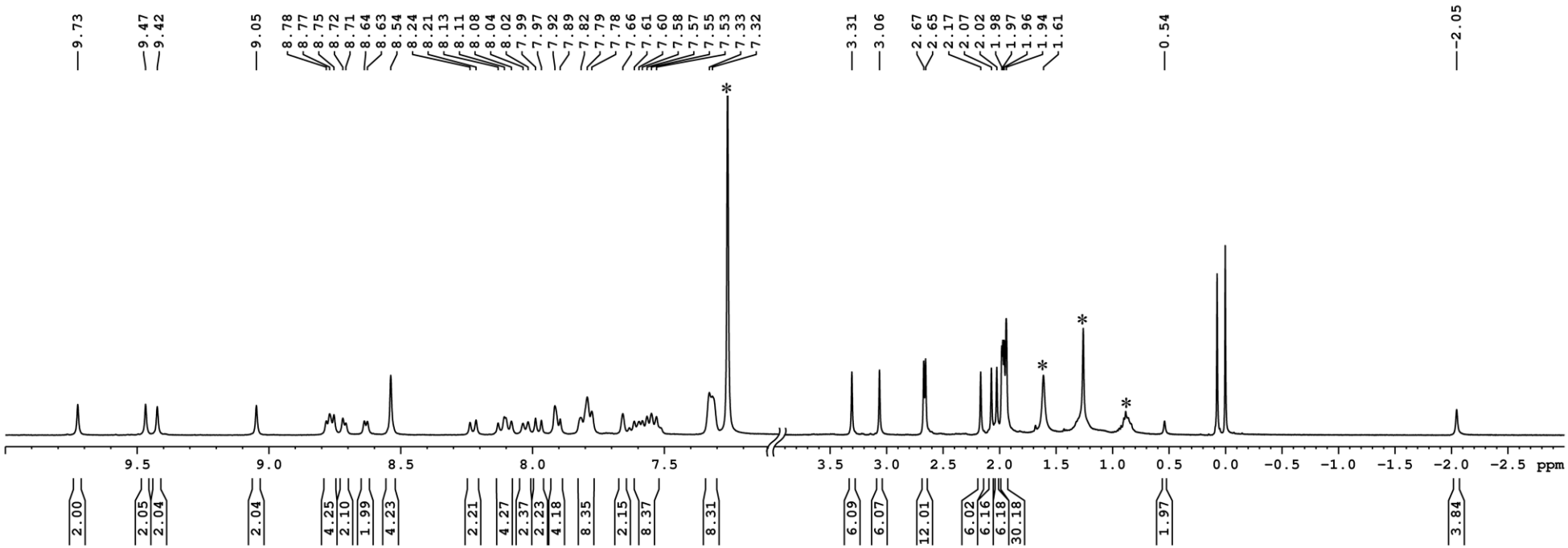


Fig. S5 ^{1}H NMR spectrum of trimer **2** in $CDCl_3$ at 298K; * indicates the signals for residual solvents.

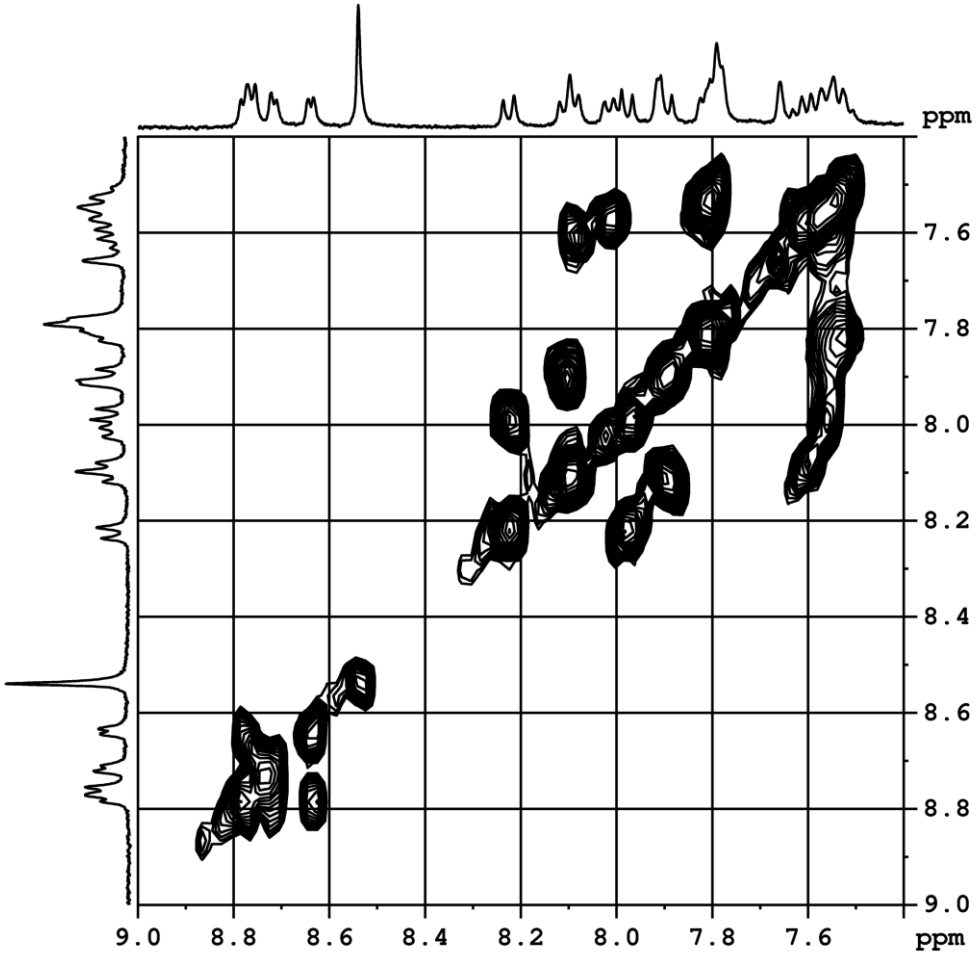


Fig. S6 ^{1}H-^{1}H COSY spectrum of trimer **2** in $CDCl_3$ at 298K with the range from δ = 9.0 to 7.4 ppm.

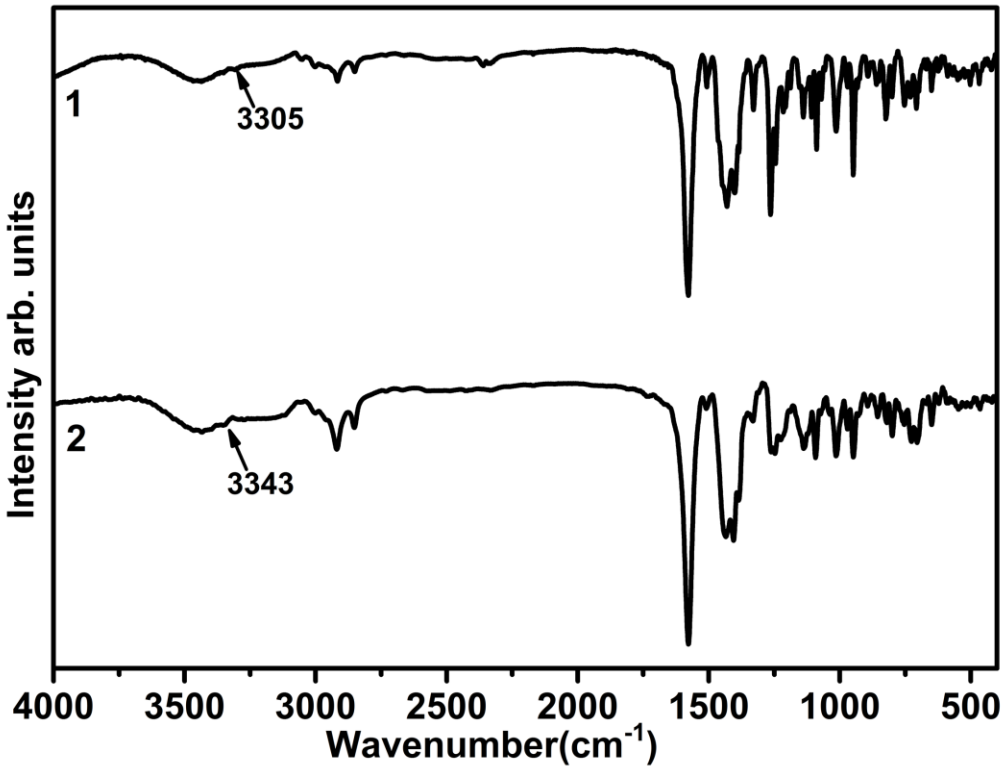


Fig. S7 IR spectra of the dimer **1** and trimer **2** in the region of 400-4000 cm^{-1}.

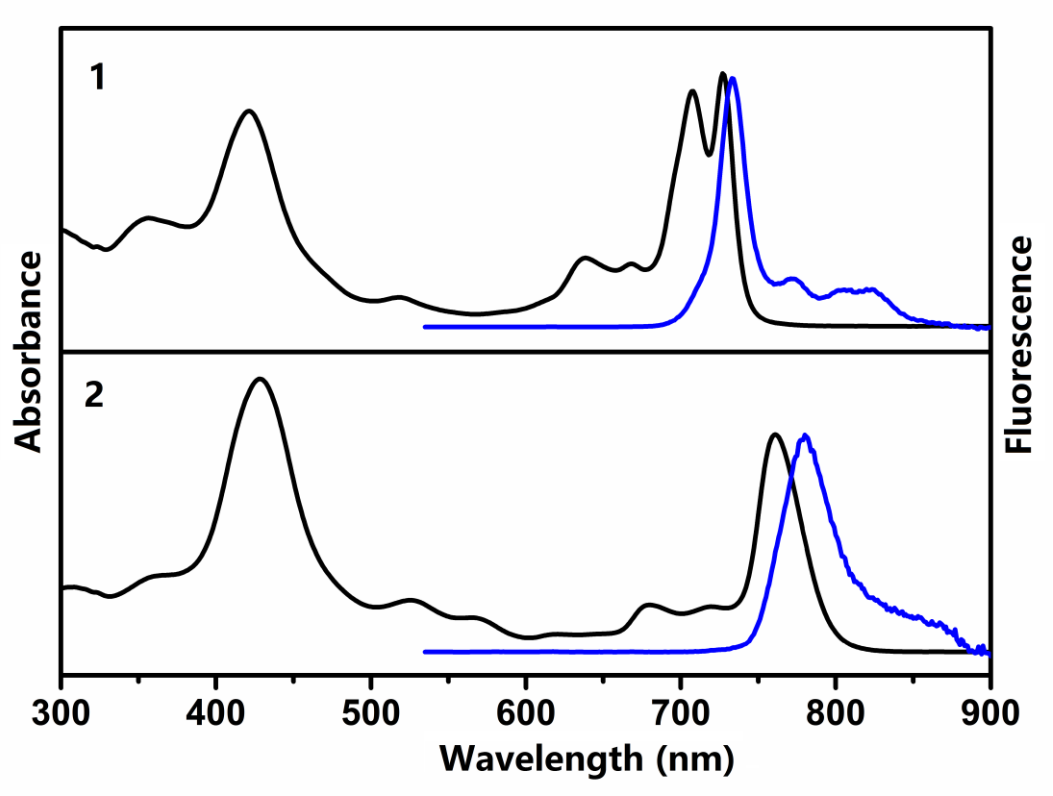


Fig. S8 Electronic absorption (black line) and fluorescence (blue line) spectra for dimer **1** and trimer **2**.

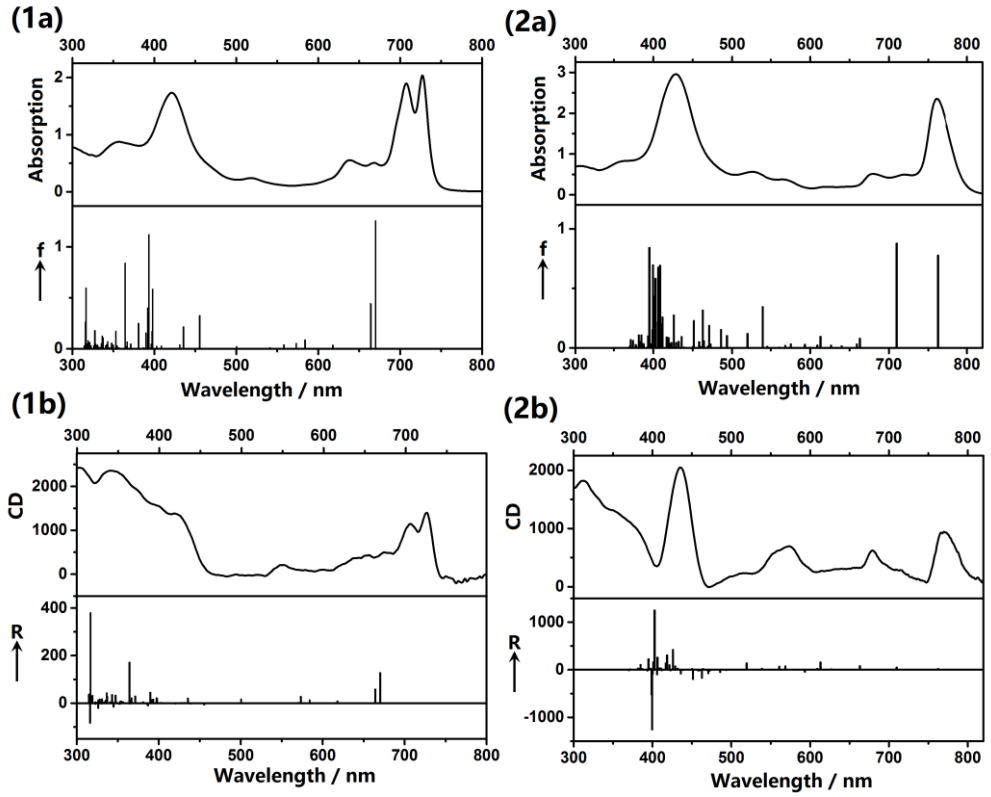


Fig. S9 The experimental and simulated electronic absorption (a) and CD spectra (b) for (*R*)-enantiomers of **1** and **2**. (The unit for R is 10^{-40} erg-esu-cm/Gauss.)

Table S1 Elemental analytical and mass spectroscopic data for compounds **1** and **2**.

Compound	Yield (%)	$[M+H]^+$ (*m/z*)[a,b]	Analysis (%)[a]		
			C	H	N
1[c]	9.8	2168.4 (2168.8)	80.17 (80.31)	4.78 (4.80)	8.05 (8.04)
2[d]	5.8	2694.3 (2694.1)	78.57 (78.51)	4.86 (5.02)	9.80 (9.86)

[a] Calculated values given in parentheses. [b] By MALDI-TOF mass spectrometry. The value corresponds to the most abundant isotopic peak of the protonated molecular ion $[M+H]^+$ for **1** and **2**. [c] Contain 1equiv. of solvated CH_2Cl_2 and 2 equiv. of solvated C_7H_8. [d] Contain 1.75 equiv. of solvated CH_2Cl_2.

Table S2 ^{1}H NMR data (δ) for the dimer **1** and trimer **2** in $CDCl_3$ at 298K.

Compound	H_{NH}	Pc		$H_{benzo[\alpha]pyrazine}$	Por		
		H_{α}	H_{aryl}		H_{β}	H_{aryl}	H_{methyl}
1	-0.16 (s, 2H), -2.14 (s, 2H)	9.88 (s, 2H), 9.62 (s, 2H), 9.30 (s, 2H)	8.21 (d, 2H, *J*=8.00 Hz), 8.09 (t, 6H, *J*=8.00 Hz), 8.03~7.86 (m, 10H), 7.80(d, 4H, *J*=8.00 Hz), 7.74(d, 4H, *J*=8.00 Hz), 7.59~7.46 (m, 10H)	9.00 (s, 2H)	8.74 (d, 2 H, *J*=4.00 Hz), 8.66 (d, 2H, *J*=4.00 Hz), 8.52 (s, 2 H)	7.61 (s, 4H), 7.29 (s, 4H)	3.02 (s, 6H), 2.64 (s, 6H), 2.03 (s, 6H), 1.94~1.90 (m, 18H)
2	0.54 (s, 2H), -2.05 (s, 4H)	9.73 (s, 2H), 9.47 (s, 2H)	8.22 (d, 2H, *J*=12.00 Hz), 8.11 (t, 4H, *J*=8.00 Hz), 8.03 (d, 2H, *J*=8.00 Hz), 7.98 (d,	9.42 (s, 2H), 9.05 (s, 2H)	8.77(br, 4H), 8.72 (d, 2H, *J*=4.00 Hz), 8.64 (d, 2H, *J*=4.00 Hz), 8.54 (s, 4 H)	7.82~7.78 (m, 8H)[a], 7.66(s, 2H), 7.31(s, 8H)	3.31 (s, 6H), 3.06 (s, 6H), 2.67 (s, 6H), 2.65(s, 6H), 2.17 (s, 6H), 2.07 (s, 6H), 2.02 (s, 6H), 1.98~1.94

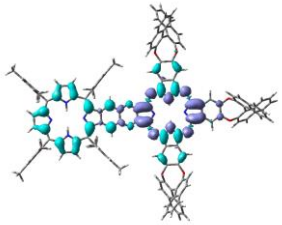
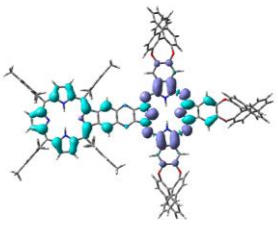
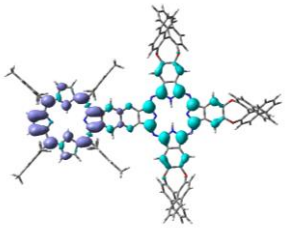
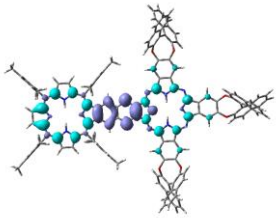
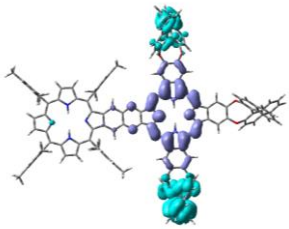
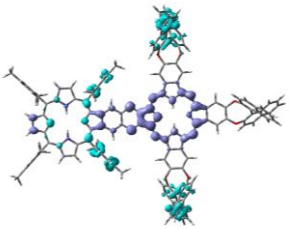
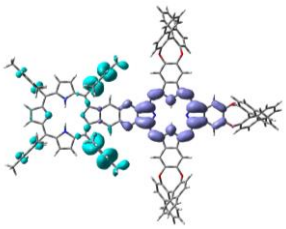
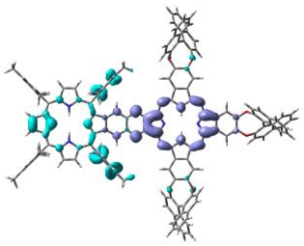
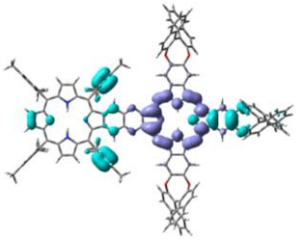
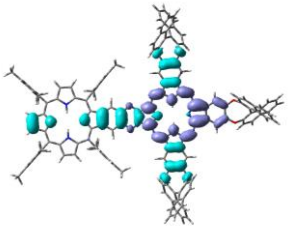
	2H, *J*=8.00 Hz), 7.91 (d, 4H, *J*=12.00 Hz), 7.82~7.78 (m, 8H)[a], 7.61~7.32 (m, 8H)	(m, 30H)

[a] These protons signals were partially overlapped.

Table S3 Anisotropic factor, *g*, for dimer **1** and trimer **2**.

Compound	Absorption	10^{-6} ε (M^{-1} cm^{-1})	10^{-3} θ (deg M^{-1} cm^{-1})	$10^{-4}g$
1	Q_1	2.04	1.48	2.20
	Q_2	1.91	1.19	1.90
	Soret	1.74	1.21	2.12
2	Q_1	2.34	1.24	1.60
	Soret	2.95	1.51	1.55

Table S4 Electron density difference plots of electron transitions (isovalue: 4.0×10^{-4} *e au*$^{-3}$) for **1**. Electron densities move from the blue area to the purple area. Excited states with less than 30000 cm^{-1} and configurations which contribute more than 5% are shown (assignment: H = HOMO, L = LUMO, L+1 = LUMO+1, H-1 = HOMO-1, etc.). The unit for R is 10^{-40} erg-esu-cm/Gauss.

Q band			
	**670.1 nm_1** (f=1.2549) (R=127.6944) Main Transitions: H→L(95%)		**664.2 nm_2** (f=0.4432) (R=58.2671) Main Transitions: H→L+1(92%)
Soret band			
	**455.5 nm_11** (f=0.3263) (R=-6.7926) Main Transitions: H-2→L+3(68%) H→L+3(15%) H-1→L+2(12%)		**435.6 nm_14** (f=0.2147) (R=19.9292) Main Transitions: H-2→L+4(60%) H-1→L+3(13%) H-2→L (7%) H-2→L+2(6%)
	**397.9 nm_25** (f=0.5853) (R=18.7013) Main Transitions: H-7→L+1 (57%) H-2→L+3 (9%) H-7→L (5%)		**466.4 nm_29** (f=1.1192) (R=15.6385) Main Transitions: H-2→L+3 (27%) H-1→L+2(12%) H-7→L+1(11%) H-1→L+4(10%) H-9→L(11%) H-8→L(9%)
	**392.7 nm_30** (f=0.2509) (R=8.1137) Main Transitions: H-9→L(60%)		**392.1 nm_31** (f=0.4003) (R=14.4233) Main Transitions: H-9→L (20%) H-2→L+4(17%) H-1→L+3(17%) H-2→L+2(11%) H-19→L (10%) H-22→L (7%)
	**380.9 nm_36** (f=0.2503) (R=4.7602) Main Transitions: H-13→L (47%) H-12→L (22%) H-18→L+1(5%)		**364.4 nm_47** (f=0.8395) (R=171.5599) Main Transitions: H-22→L(56%) H-19→L(30%)

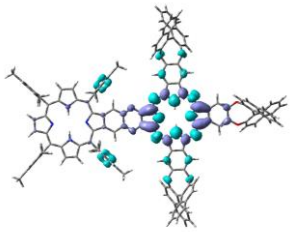
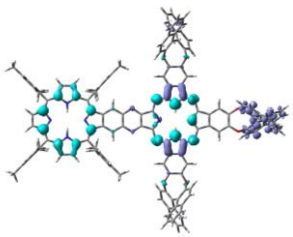
	**316.7 nm_120** (f=0.5969) (R=379.4471) Main Transitions: H-32→L(53%) H-37→L+1(19%) H-15→L+3(8%)
	**316.1 nm_121** (f=0.2625) (R=-83.8487) Main Transitions: H-32→L+1(34%) H-2→L+8(10%) H-2→L+10(7%) H-2→L+7(7%) H-2→L+11(6%)

Table S5 Electron density difference plots of electron transitions (isovalue: 4.0×10^{-4} *e au*$^{-3}$) for compound **2**. Electron densities move from the green area to the blue area. Excited states with less than 30000 cm^{-1} and configurations which contribute more than 5% are shown (assignment: H = HOMO, L = LUMO, L+1 = LUMO+1, H-1 = HOMO-1, etc.). The unit for R is 10^{-40} erg-esu-cm/Gauss.

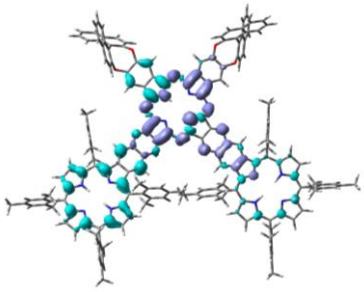
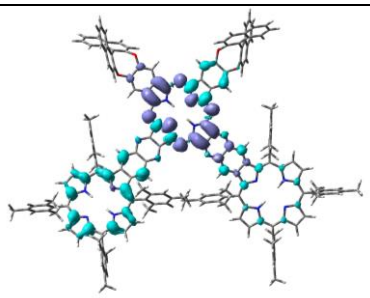
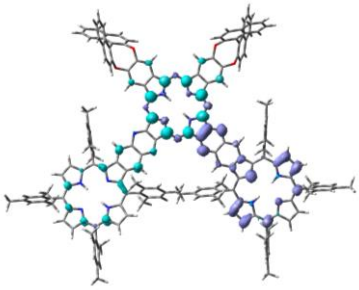
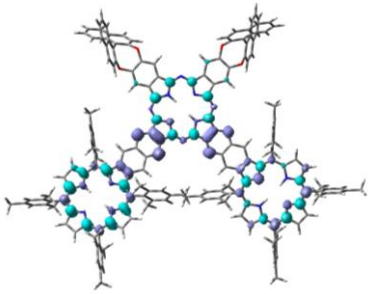
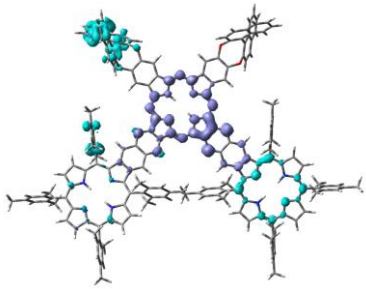
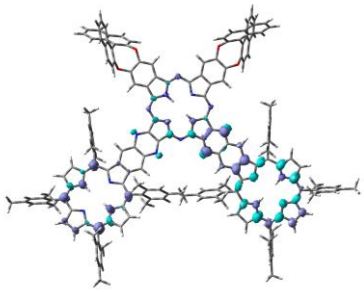
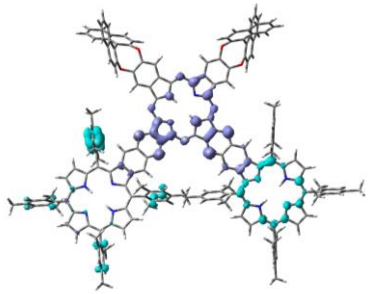
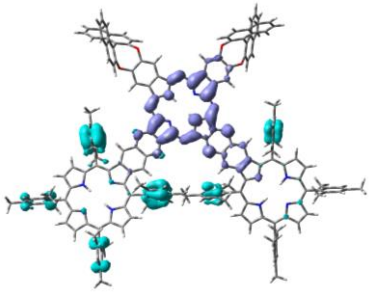
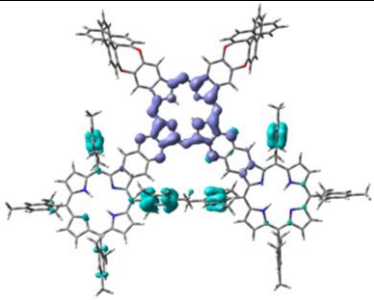
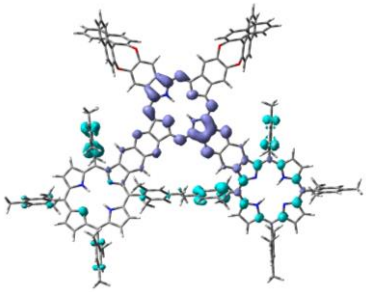
Q band			
	**762.3 nm_1** (f=0.7775) (R=21.3021) Main Transitions: H→L(96%)		**709.8 nm_2** (f=0.8781) (R=49.8480) Main Transitions: H→L+1(93%)
Soret band			
	**538.74 nm_15** (f=0.3435) (R=27.0682) Main Transitions: H→L+2(28%) H→L+6(15%) H-4→L+2(13%) H-3→L+4(10%) H-3→L+1(8%) H-1→L+3(7%)		**462.82 nm_25** (f=0.3167) (R=-173.0440) Main Transitions: H-2→L+2(23%) H→L+7(18%) H-4→L+5(9%) H-4→L+6(7%) H-2→L+6(7%)
	**408.56 nm_50** (f=0.6916) (R=35.0784) Main Transitions: H-8→L+1(15%) H-3→L+6(12%) H-2→L+6(9%) H-4→L+4(7%) H-10→L(6%)		**406.28 nm_51** (f=0.6760) (R=261.2758) Main Transitions: H-4→L+4(25%) H-4→L+5(13%) H-3→L+6(6%) H-2→L+5(6%)
	**402.6 nm_53** (f=0.5824) (R=1250.0466) Main Transitions: H-17→L(12%) H-4→L+5(10%) H-2→L+7(9%) H-3→L+4(8%)		**401.16 nm_54** (f=0.4313) (R=161.9930) Main Transitions: H-17→L(27%) H-22→L(22%) H-15→L(9%) H-2→L+7(6%)
	**399.63 nm_56** (f=0.6953) (R=-1258.9044) Main Transitions: H-22→L(15%) H-9→L+1(11%) H-17→L(8%) H-2→L+7(6%) H-1→L+6(6%)		**395.03 nm_62** (f=0.8416) (R=225.7584) Main Transitions: H-4→L+6(17%) H-4→L+5(12%) H-10→L+1(8%) H-12→L+1(5%)

Table S6 Electronic absorption data for dimer **1** and trimer **2** in toluene.

Compound	λ_{max}/nm (log ε)						
1	357 (4.94)	421 (5.24)	518 (4.39)	639 (4.75)	668 (4.72)	708 (5.28)	727 (5.31)
2	--	428 (5.47)	526 (4.75)	565 (4.58)	680 (4.71)	719 (4.69)	761 (5.37)