

Supporting Informaion

Synthesis and fluorescence properties of butadiyne-linked linear and cyclic carbazole oligomers

Kazuya Ogawa,* Shohei Tanaka and Kyosuke Shimura

Graduate Faculty of Interdisciplinary Research, University of Yamanashi, 4-3-11 Takeda, Kofu, Yamanashi
400-8511, Japan

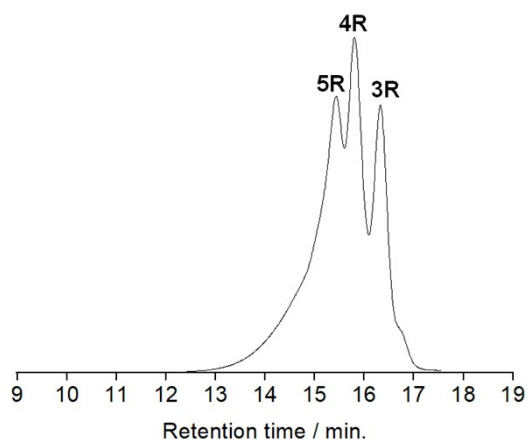


Fig. S1 GPC chart after the reaction of the synthesis of **3R**, **4R**, and **5R**.

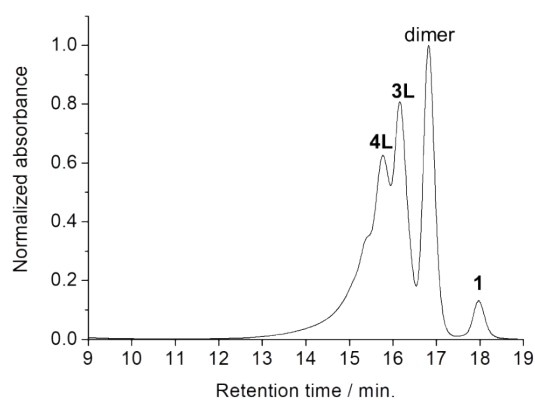


Fig. S2 GPC chart after the reaction of the synthesis of **3L** and **4L**.

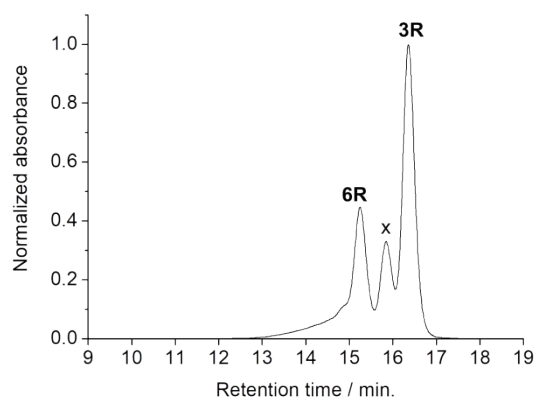


Fig. S3 GPC chart after the reaction of the synthesis of **6R**.

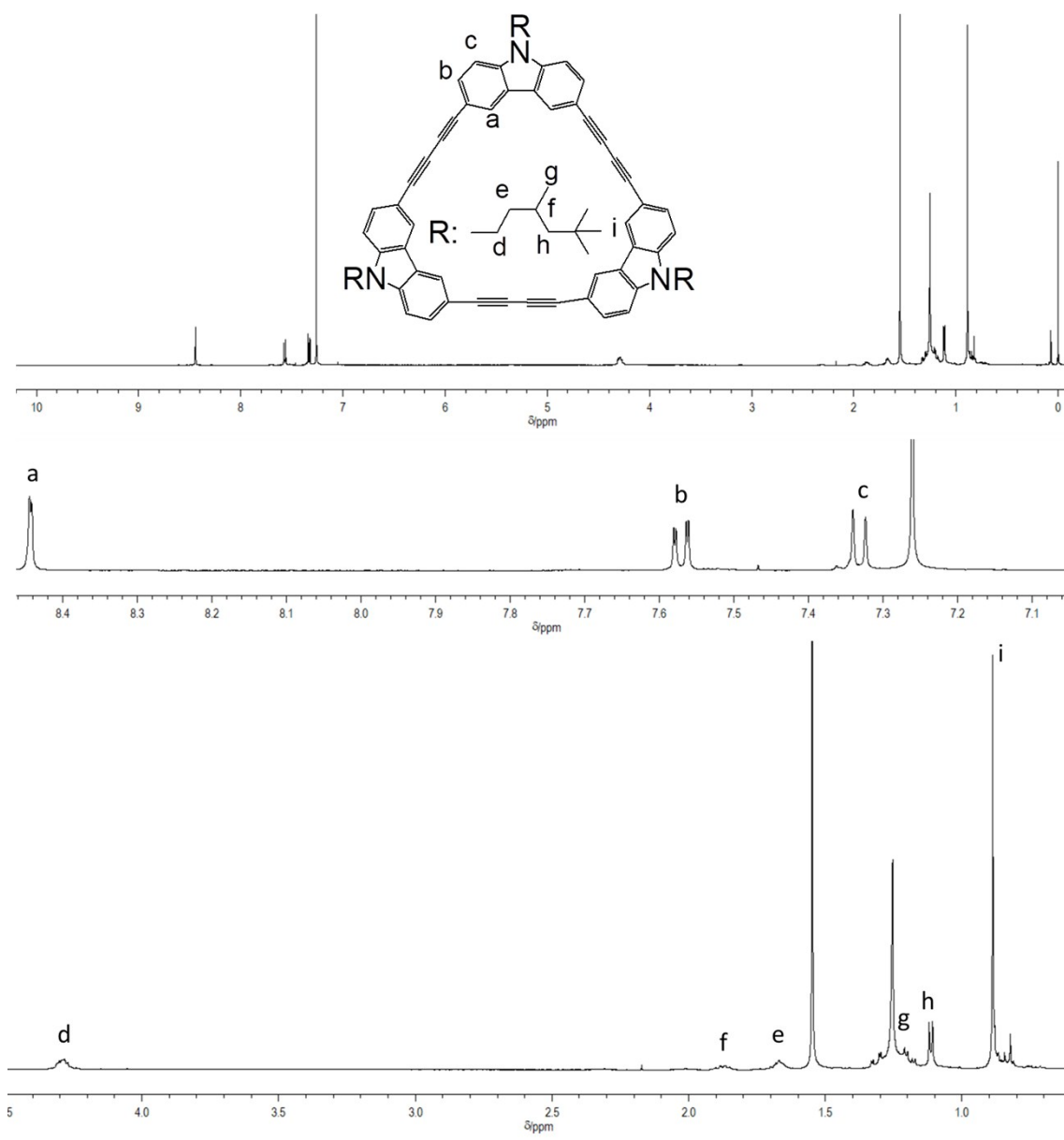


Fig. S4 ^1H NMR spectra of **3R** in CDCl_3 .

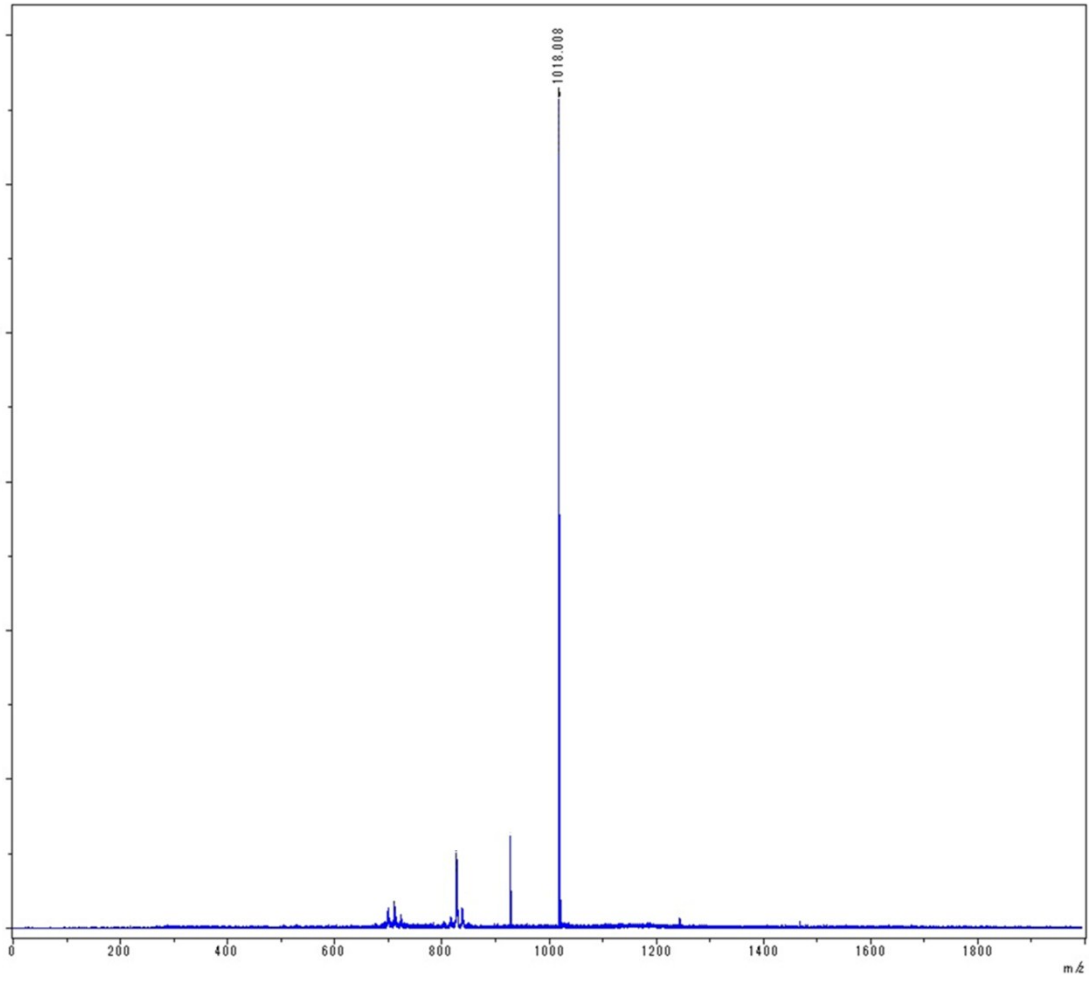


Fig. S5 MALDI-TOF mass chart of **3R**.

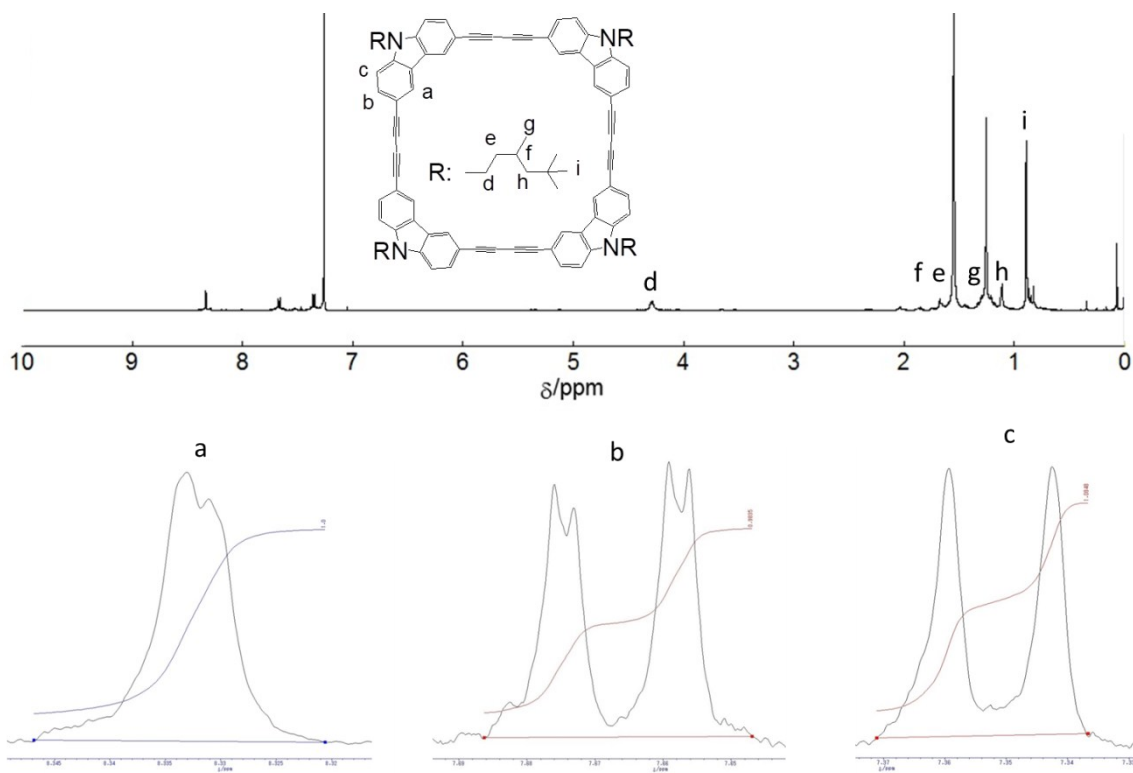


Fig. S6 ^1H NMR spectra of **4R** in CDCl_3 .

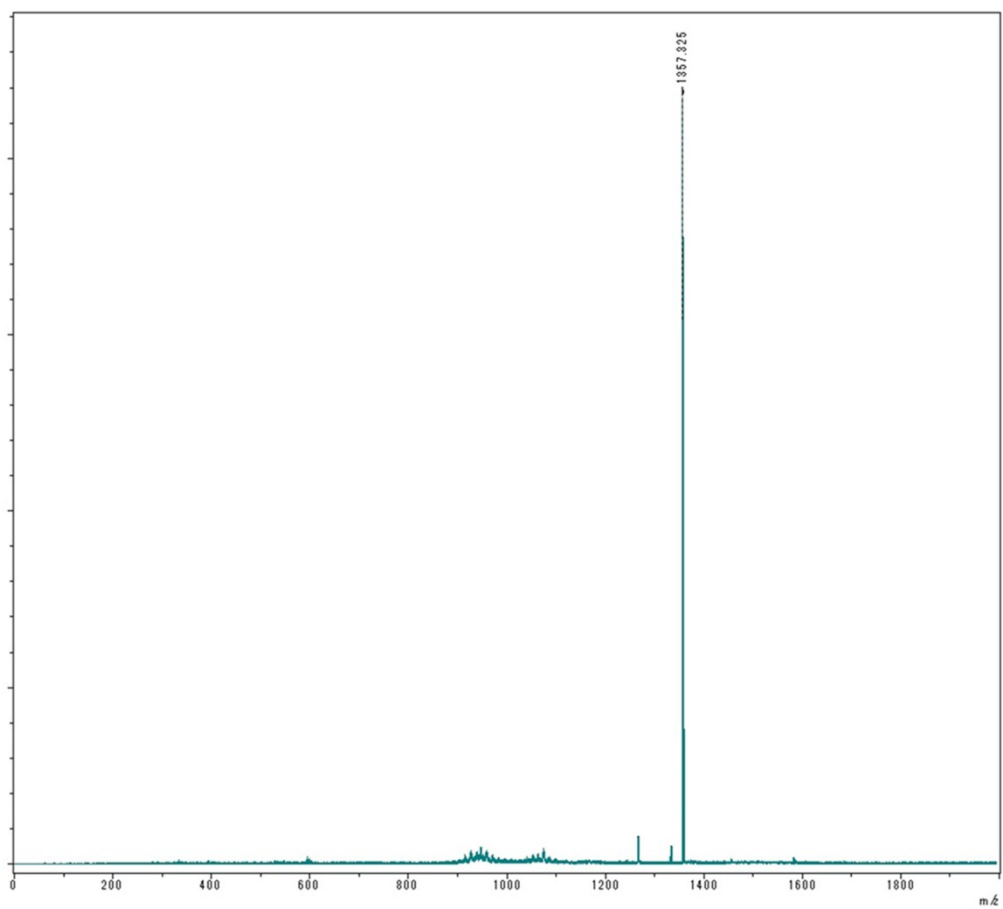


Fig. S7 MALDI-TOF mass chart of **4R**.

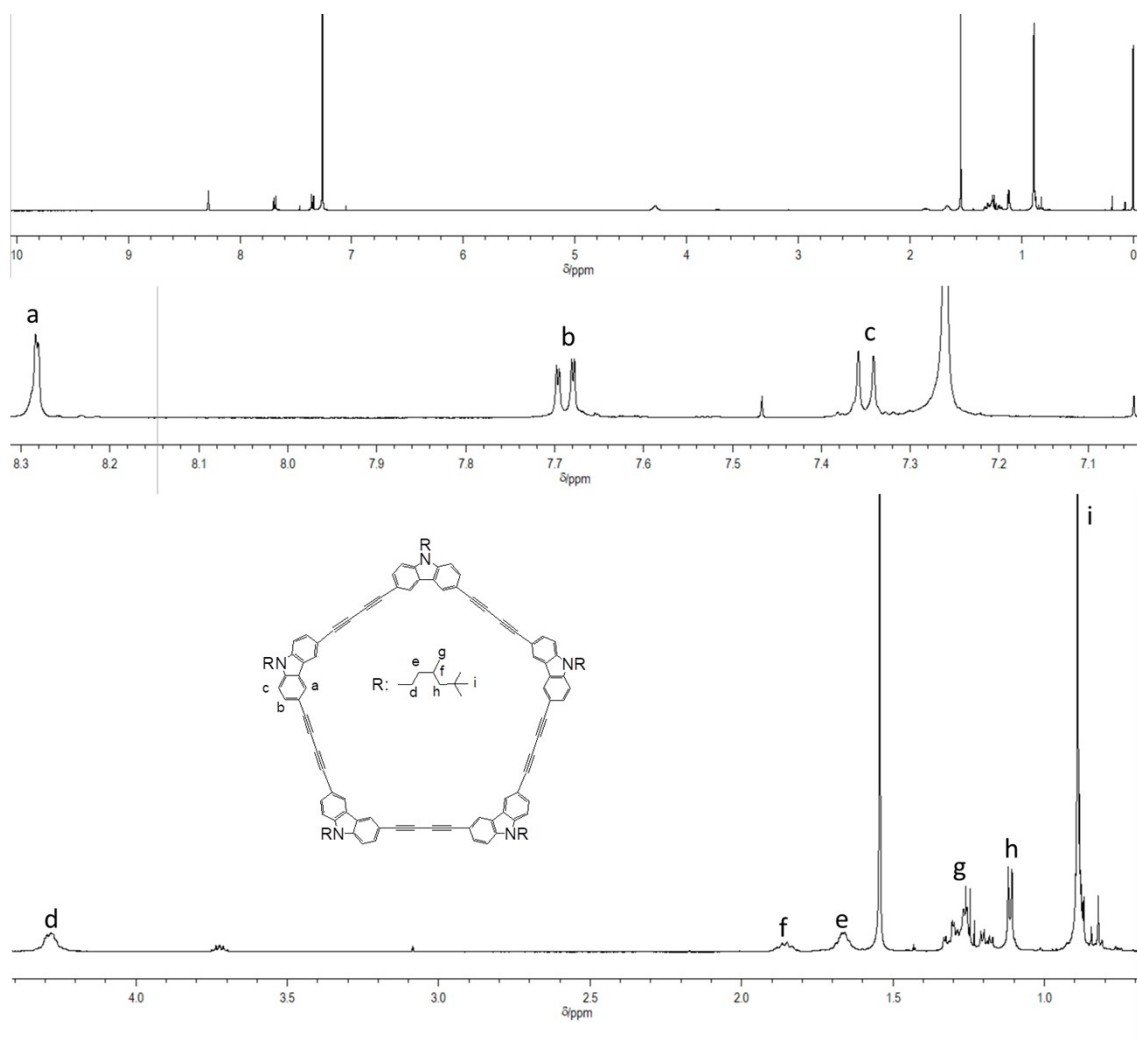


Fig. S8 ^1H NMR spectra of **5R** in CDCl_3 .

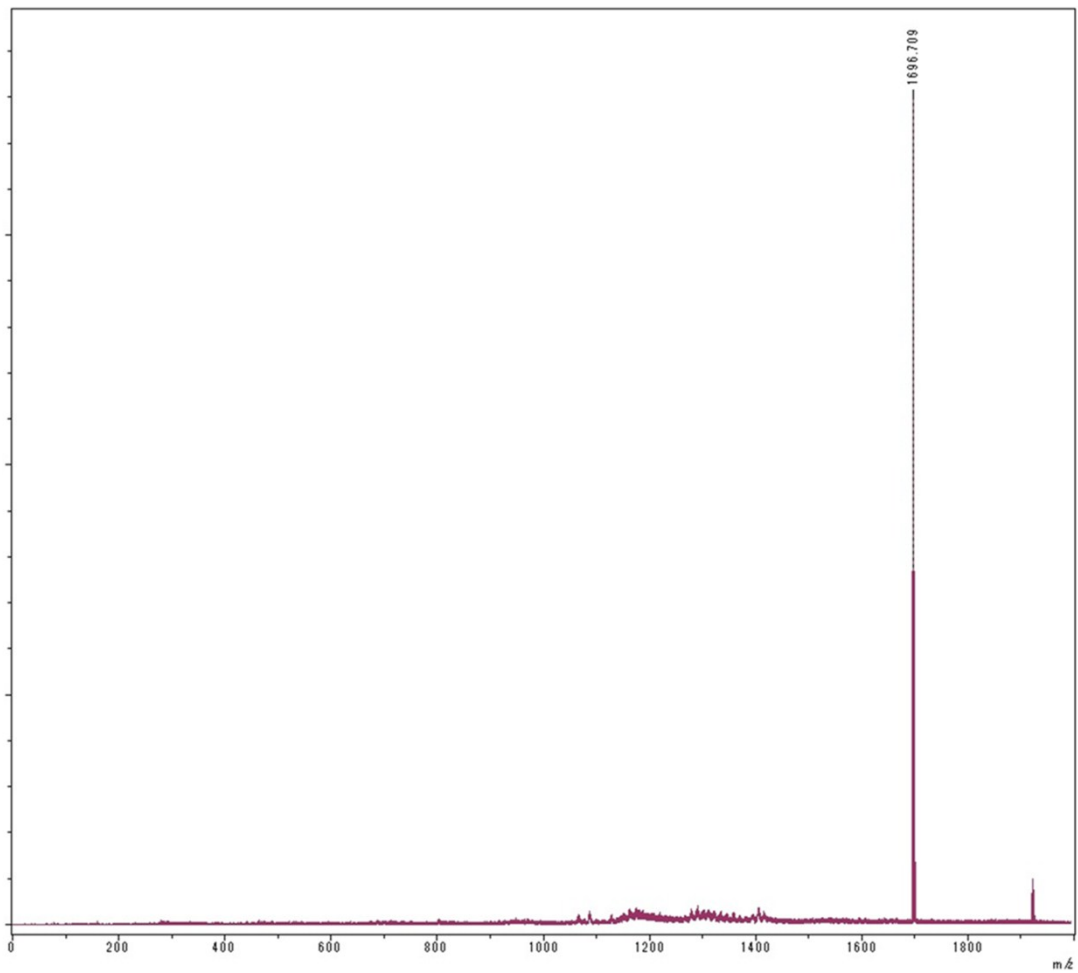


Fig. S9 MALDI-TOF mass chart of **5R**.

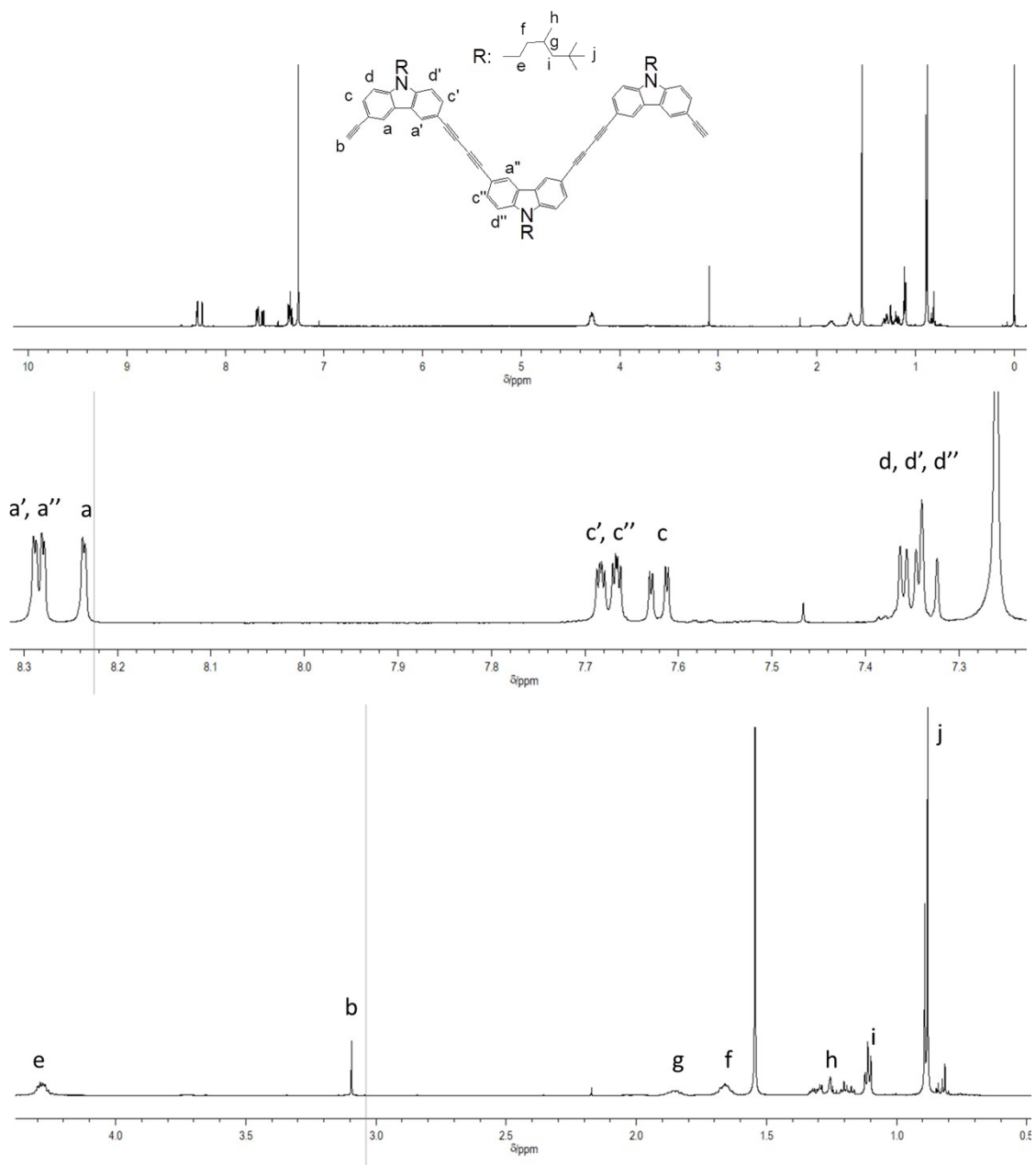


Fig. S10 ^1H NMR spectra of **3L** in CDCl_3 .

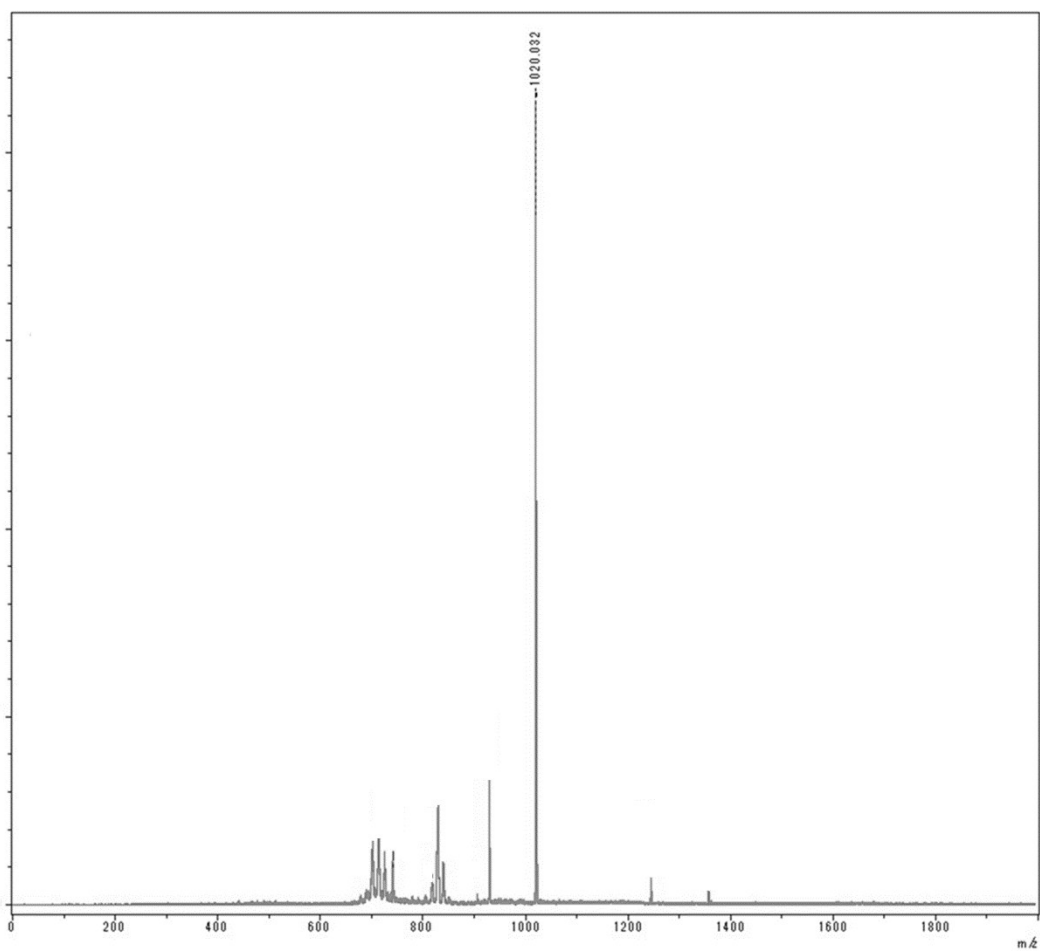


Fig. S11 MALDI-TOF mass chart of **3L**.

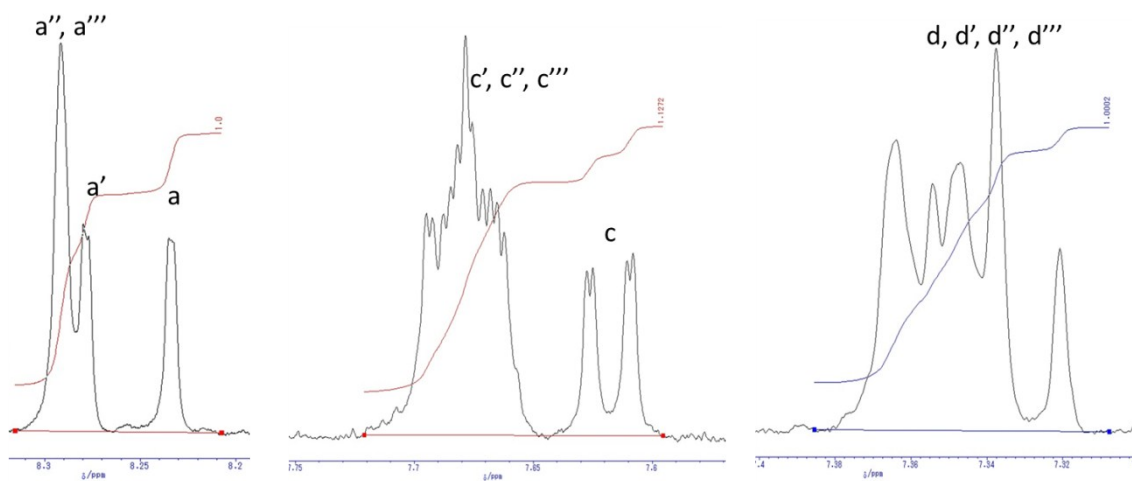
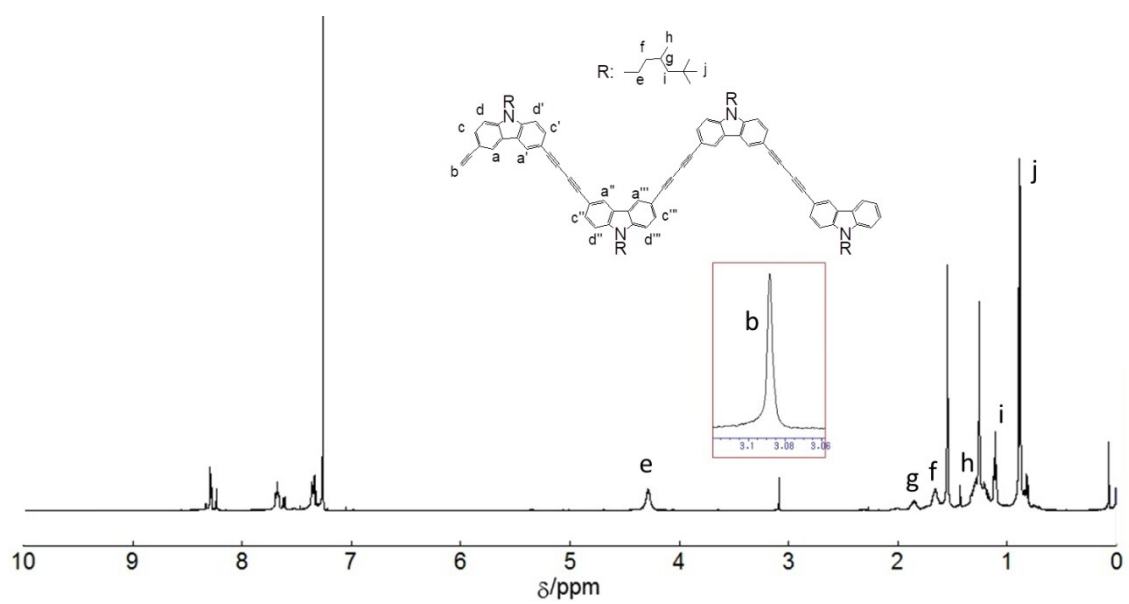


Fig. S12 ^1H NMR spectra of **4L** in CDCl_3 .

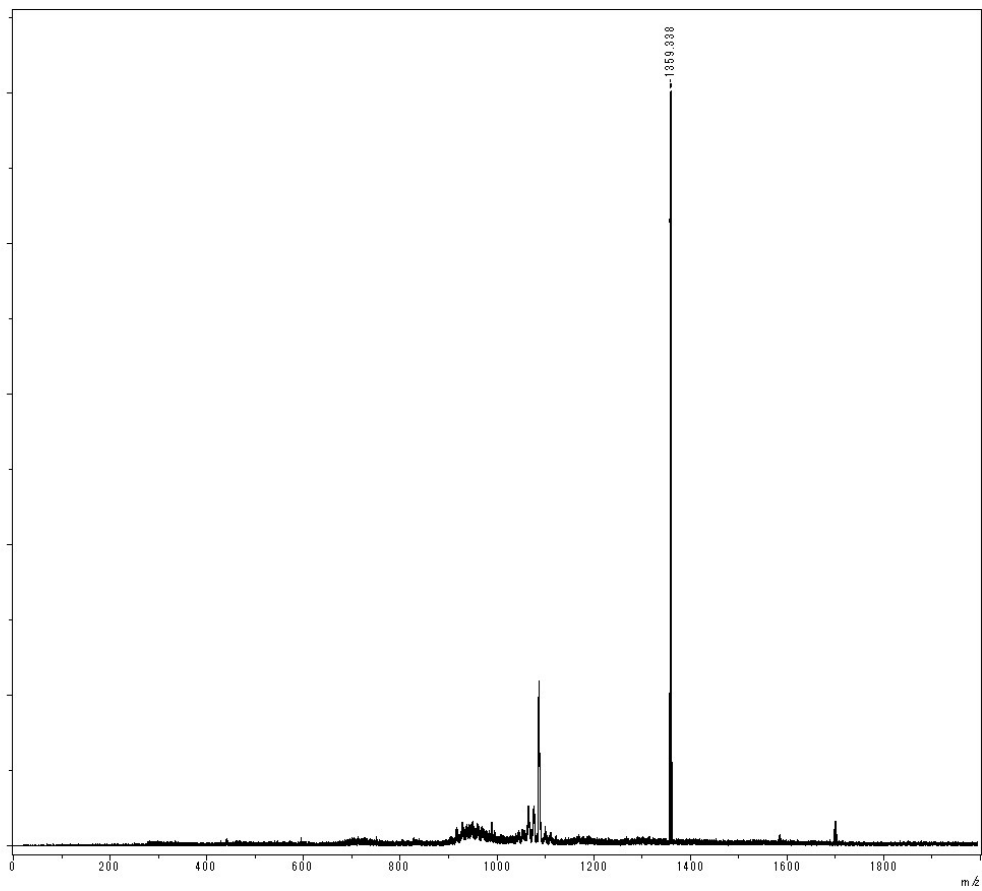


Fig. S13 MALDI-TOF mass chart of **4L**.

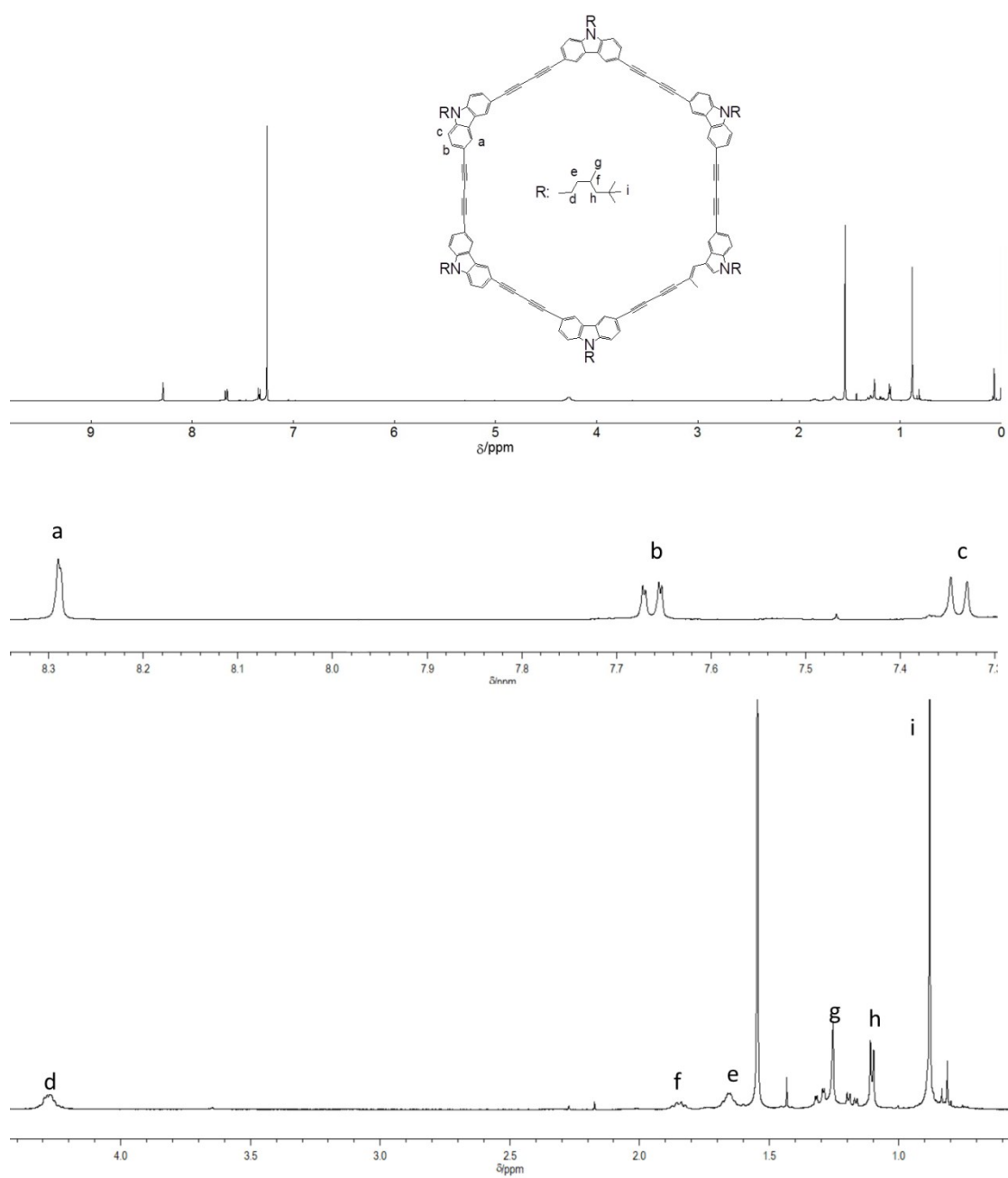


Fig. S14 ^1H NMR spectra of **6R** in CDCl_3 .

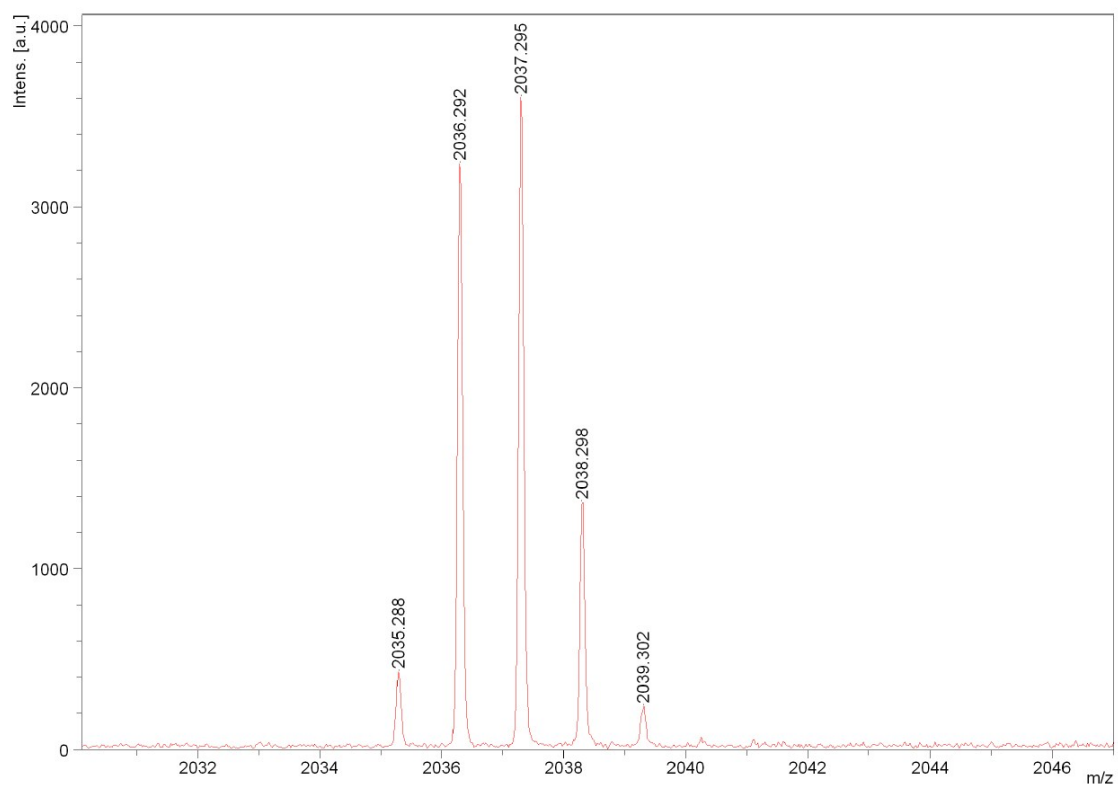


Fig. S15 MALDI-TOF mass chart of **6R**.

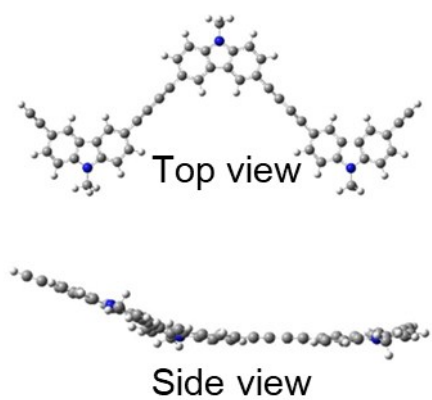


Fig. S16 Optimized structure of **3L**. Note that this structure is one of the conformations in solution.

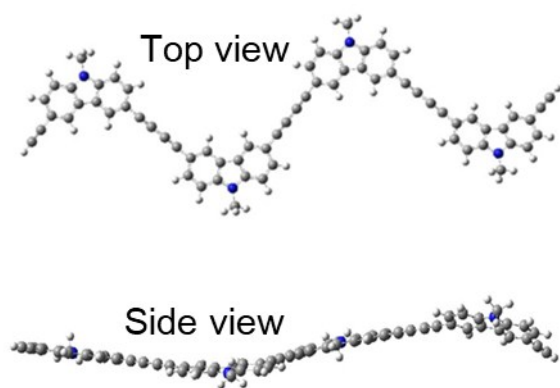


Fig. S17 Optimized structure of **4L**. Note that this structure is one of the conformations in solution.

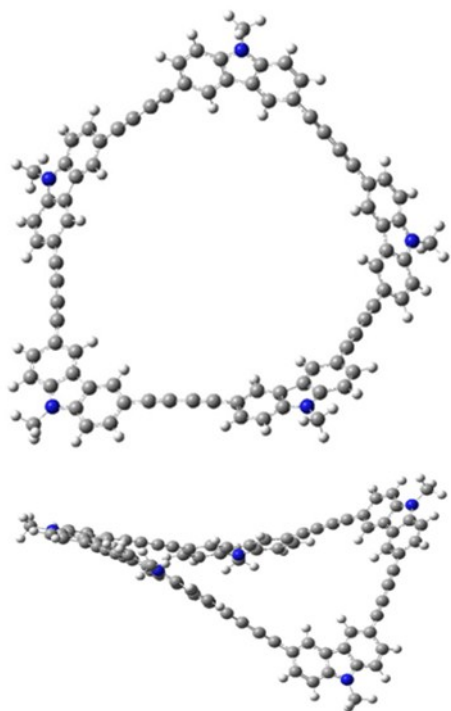


Fig. S18 Optimized structure of **5R** . Two views from different angles. Note that this structure is one of the conformations in solution.

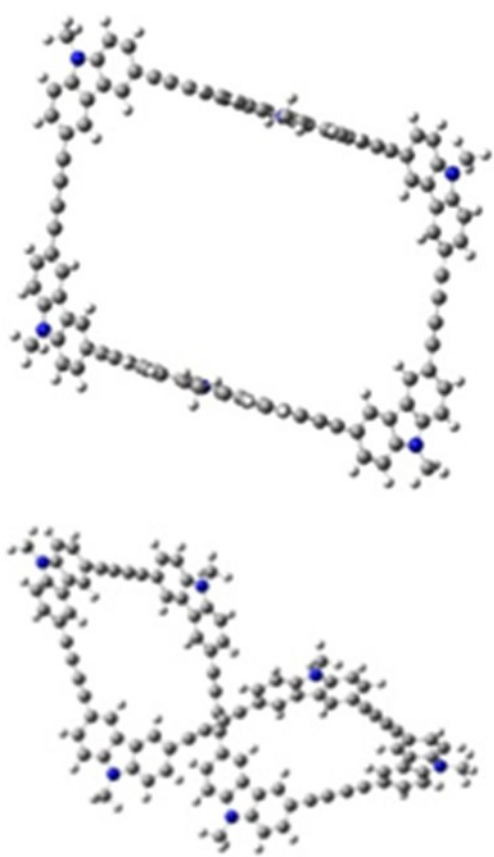


Fig. S19 Optimized structure of **6R**. Two views from different angles. Note that this structure is one of the conformations in solution.

Table S1 Calculated Absorption Wavelengths, Major Transitions, and Oscillator Strengths. .

Entry	Wavelength / nm	Contributions to transition	Oscillator strength
3L	342	HOMO→LUMO (0.56) HOMO-1→LUMO+1 (0.32)	2.76
3R	356	HOMO-1→LUMO (0.45) HOMO→LUMO+1 (0.45)	0.00
4L	346	HOMO→LUMO (0.51) HOMO-1→LUMO+1 (0.30)	3.87
4R	356	HOMO→LUMO (0.47) HOMO-1→LUMO+1 (-0.32) HOMO-2→LUMO+2 (-0.32)	0.00
5R	343	HOMO→LUMO (0.52) HOMO-1→LUMO+1 (-0.23)	1.13
6R	340	HOMO-1→LUMO+1 (0.43) HOMO→LUMO (0.41)	0.03
	337	HOMO→LUMO+1 (0.43) HOMO-1→LUMO (0.42)	3.41

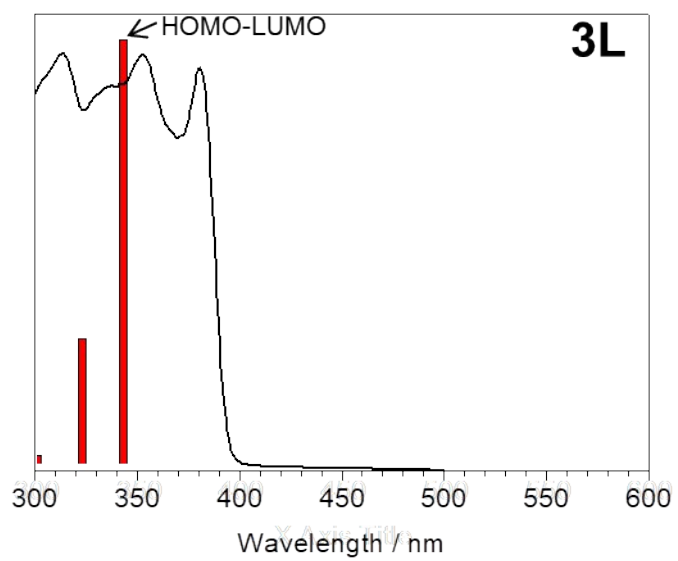


Fig. S20 UV/Vis absorption spectra with the calculated oscillator strengths of **3L**.

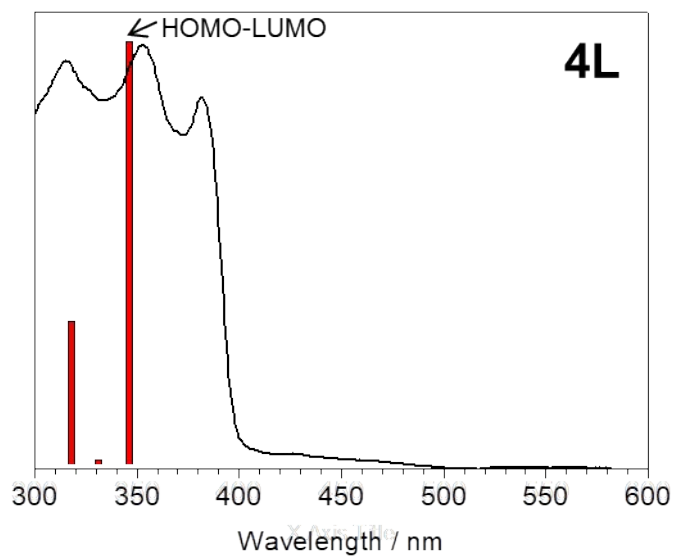


Fig. S21 UV/Vis absorption spectra with the calculated oscillator strengths of **4L**.

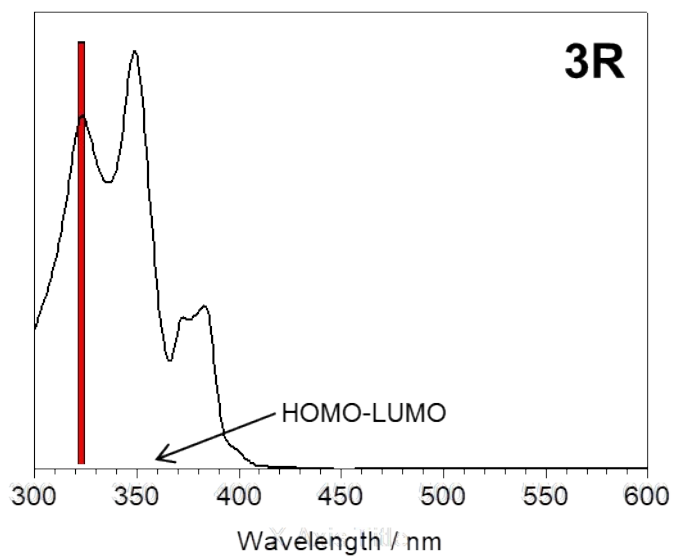


Fig. S22 UV/Vis absorption spectra with the calculated oscillator strengths of **3R**.

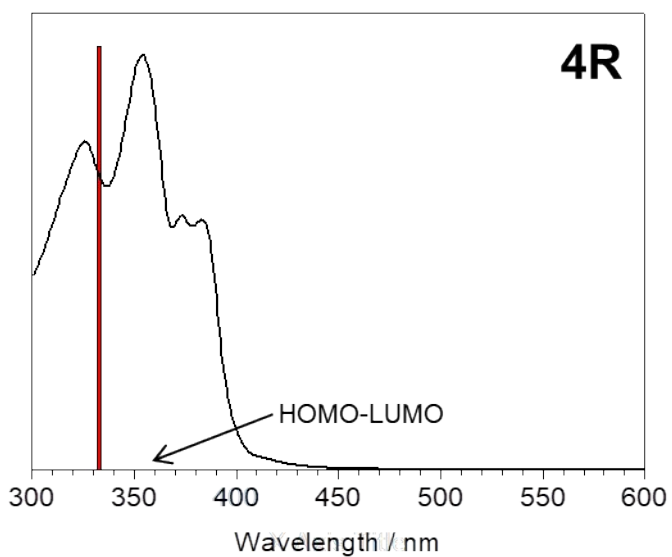


Fig. S23 UV/Vis absorption spectra with the calculated oscillator strengths of **4R**.

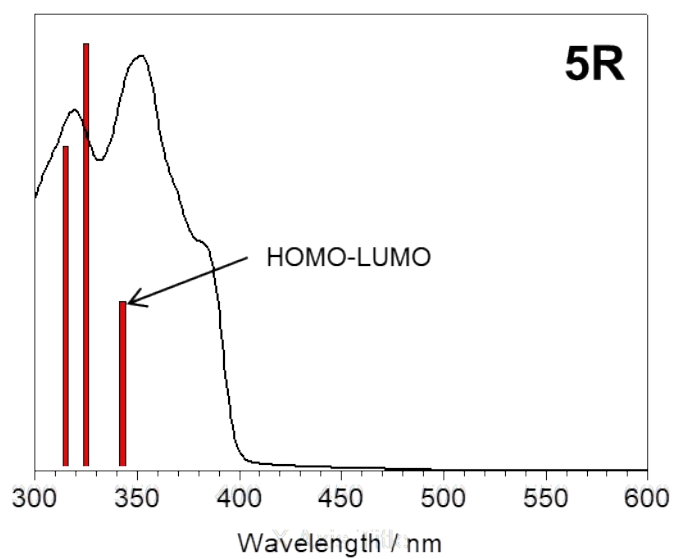


Fig. S24 UV/Vis absorption spectra with the calculated oscillator strengths of **5R**.

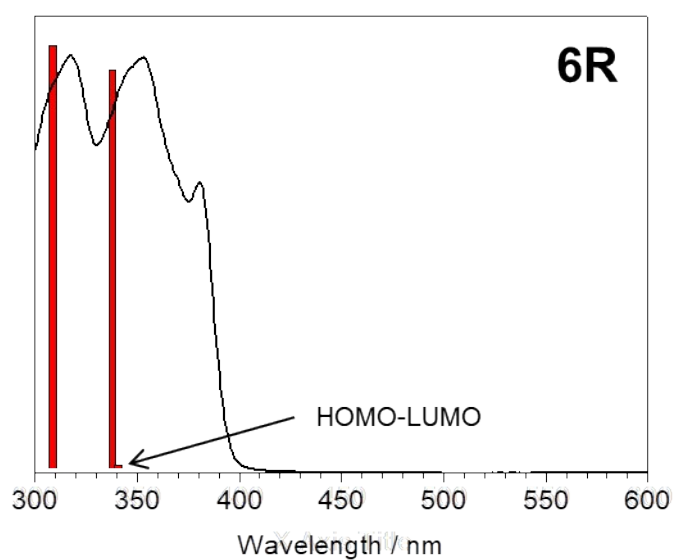


Fig. S25 UV/Vis absorption spectra with the calculated oscillator strengths of **6R**.