Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Chiral Supramolecular Polymerization of Dicyanostilbenes with Emergent Circularly Polarized Luminescence Behavior

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*1. Spectroscopy of (R)-**1** [or (S)-**1**] at the monomeric and self-assembled states*

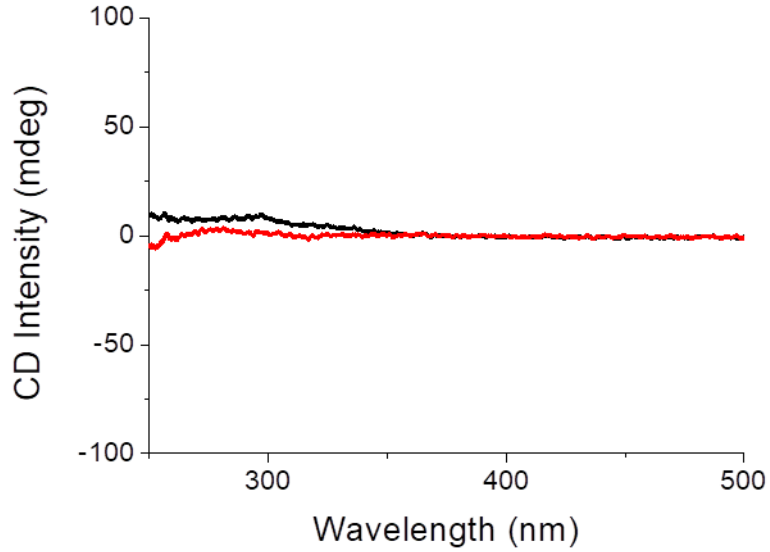


Fig. S1 CD spectra of (*R*)-**1** (black line, 0.01 mM) and (*S*)-**1** (red line, 0.01 mM) in $CHCl_3$. No Cotton effect was observed, suggesting the dominance of molecularly dissolved state.

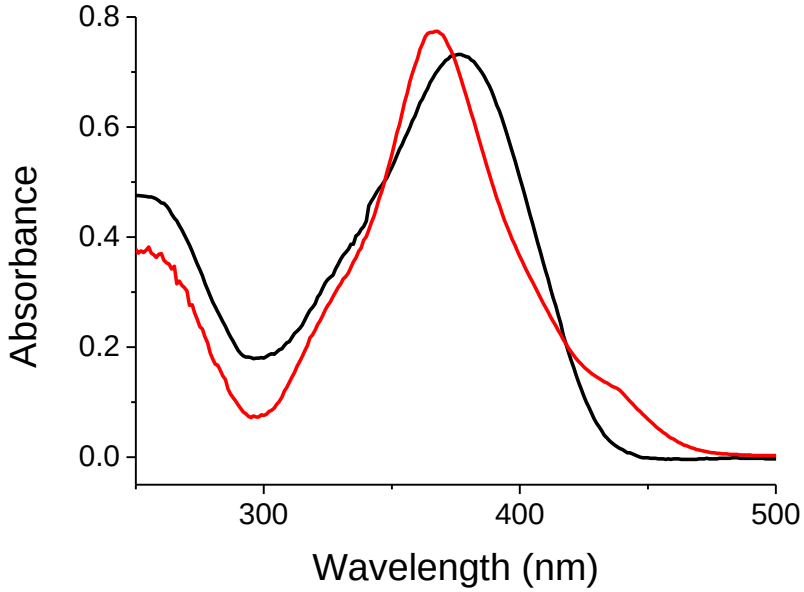


Fig. S2 UV-Vis spectra of (*S*)-**1** (0.01 mM) in $CHCl_3$ (black line) and MCH (red line). As can be seen, (*S*)-**1** exhibited the same absorption signal changes as compared to those of (*R*)-**1**.

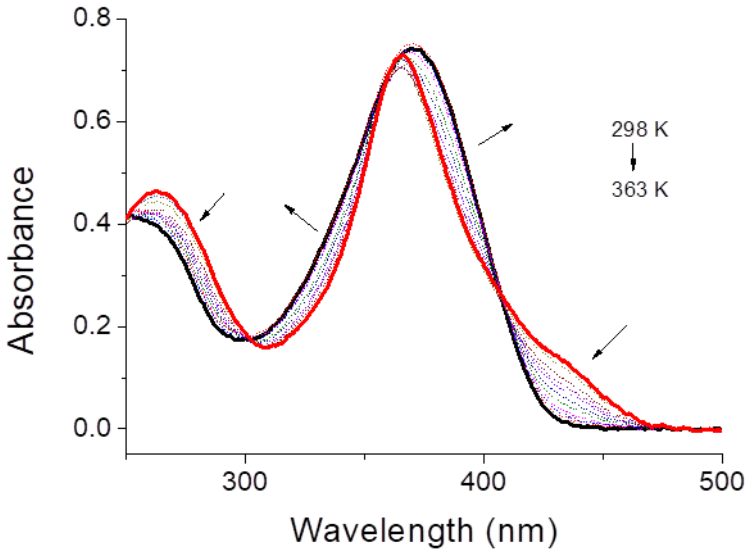


Fig. S3 UV-Vis spectra of (*R*)-**1** in MCH (*c* = 0.01 mM, 10 mm cuvette). The arrows show spectral changes upon heating from 298 to 363 K. By varying the temperature between 298 K and 363 K, two isosbestic points existed in UV–Vis spectra (λ = 301 and 407 nm), suggesting reversible conversion of (*R*)-**1** between the monomeric and supramolecular polymeric states.

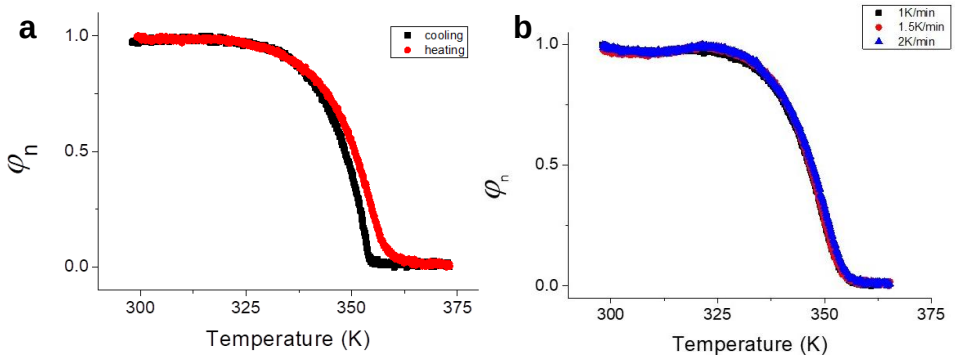


Fig. S4 (a) CD intensities of (*R*)-**1** at 387 nm (*c* = 0.01 mM, 10 mm cuvette) *versus* temperature upon cooling (black dots) and heating (red dots) at the rate of 60 K h^{-1}. (b) Heating curves of (*R*)-**1** at 387 nm (*c* = 0.01 mM, 10 mm cuvette) at three different melting rates. Slight thermal hysteresis was observed between the CD heating and cooling curves of (*R*)-**1**, illustrating the presence of pathway complexity for the supramolecular polymerization processes. The heating process was under thermodynamic control, since no distinct changes occurred upon variation of the heating rate.

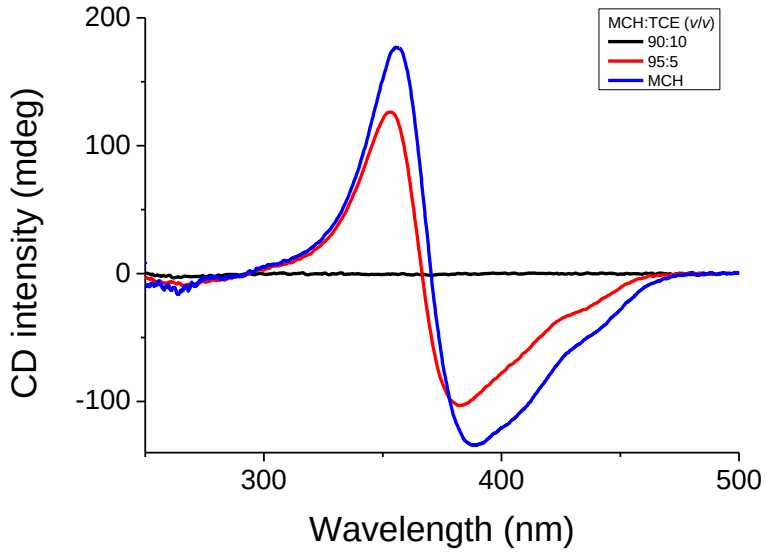


Fig. S5 CD spectra of (*R*)-**1** at different solvent compositions (c = 0.01 mM, 10 mm cuvette). As can be seen, no Cotton effects existed when the volume fraction of polar TCE exceeded 10% in MCH. In MCH/TCE (v/v = 95/5, c = 1.00 × 10^{-5} M), Cotton effects still existed, albeit for the lower CD intensity than that in pure MCH ($\Delta\varepsilon$ at 355 nm: 377 *versus* 521 L cm^{-1} mol^{-1}).

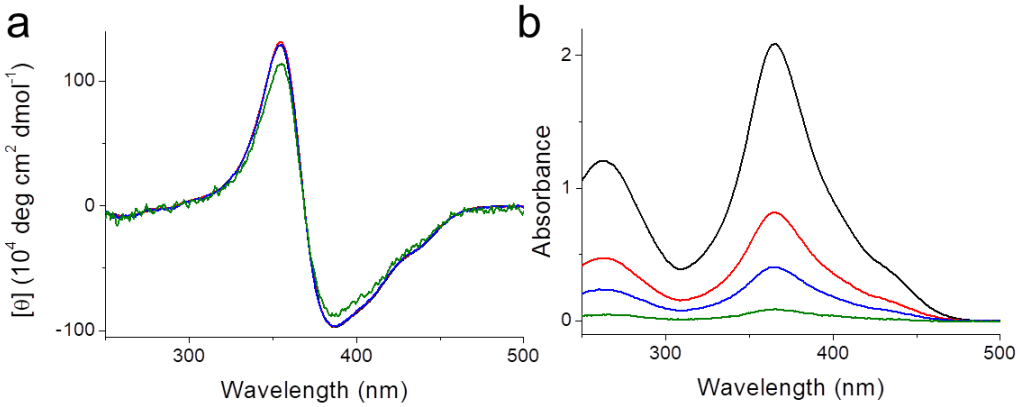


Fig. S6 (a) Molar ellipticity values and (b) UV-Vis spectra of (*R*)-**1** in MCH at four different monomer concentrations (2 mm cuvette): 0.20 mM (black line); 0.08 mM (red line); 0.04 mM (blue line); 0.01 mM (green line). As can be seen, the molar ellipticity values of (*R*)-**1** in MCH at high concentrations were similar to those at 0.01mM.

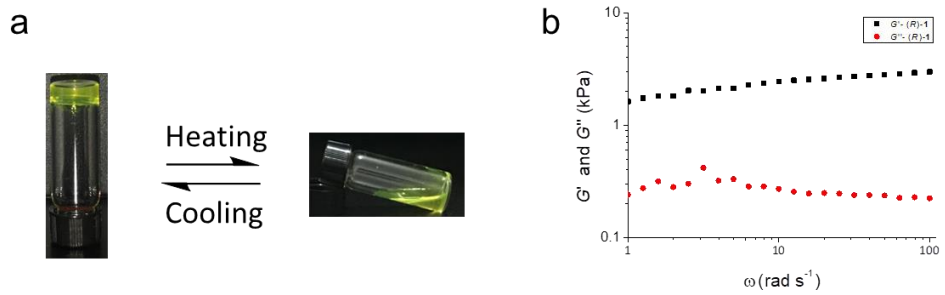


Fig. S7 (a) Organogel of (*R*)-**1** at the concentration of 10.0 mM in MCH. (b) Elastic modulus *G*' (black symbols) and viscous modulus *G*" (red symbols) for the gels [9.85 mM of (*R*)-**1** in MCH] as a function of oscillation frequency at 298 K with a strain of 0.2%.

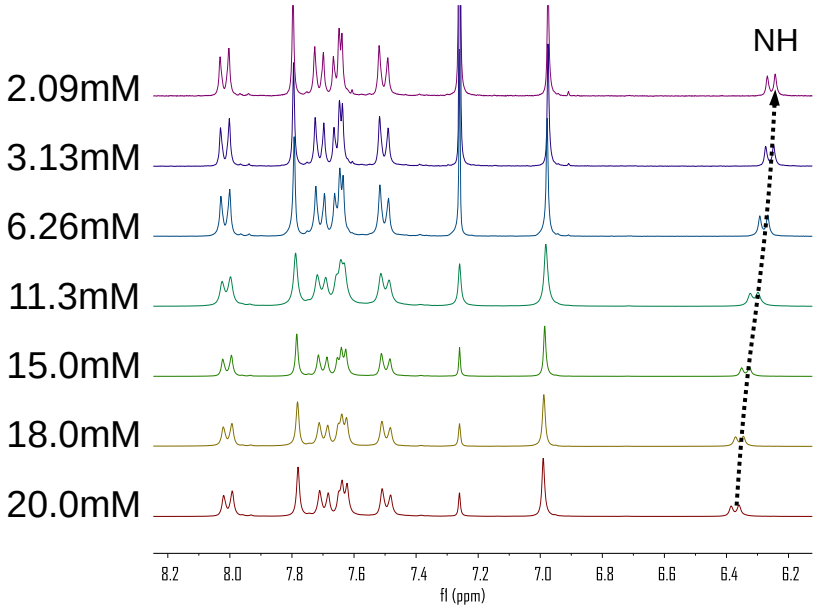


Fig. S8 Concentration-dependent ^{1}H NMR spectra (300 MHz, $CDCl_3$, 298 K) of (*R*)-**1**. The arrow exhibits upfield shifting of the NH protons upon diluting the sample. The phenomenon reveals that intermolecular hydrogen bonds are involved in the (*R*)-**1** self-assembly process.

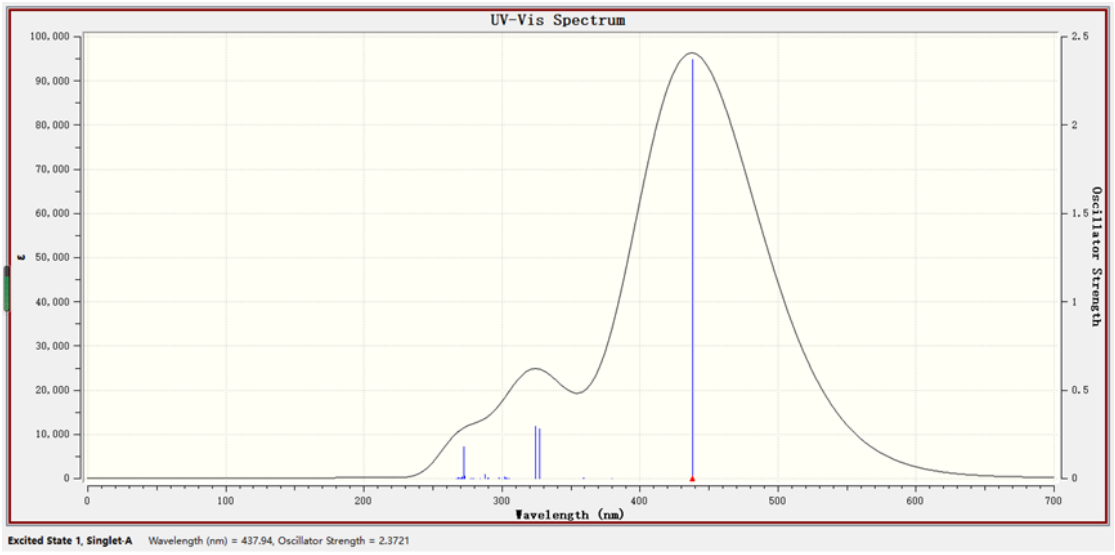


Fig. S9 Simulated UV–Vis spectrum of (*R*)-**1** *via* TD-DFT calculation.

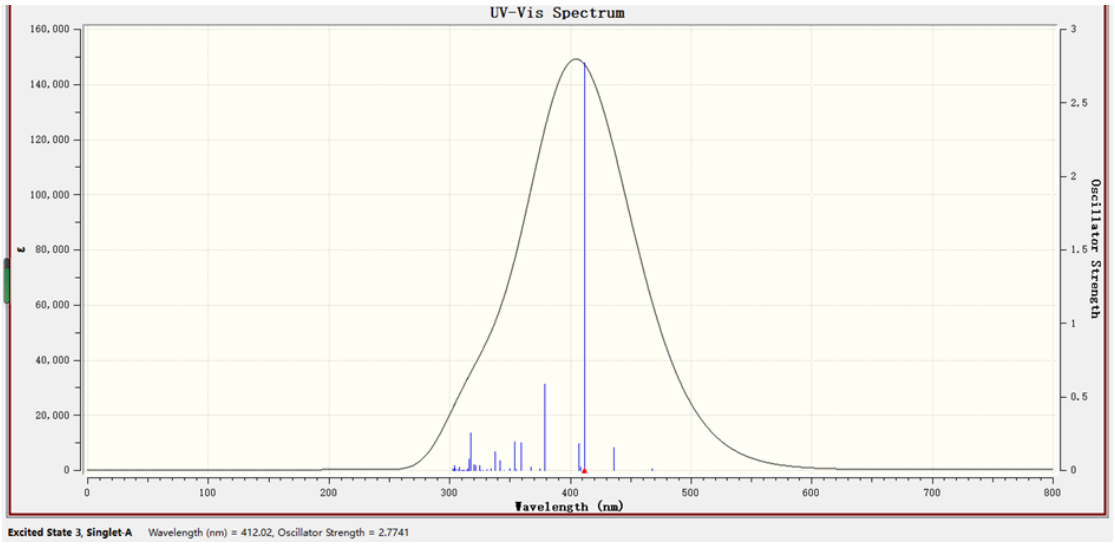


Fig. S10 Simulated UV–Vis spectrum of (*R*)-**1**$_2$ *via* TD-DFT calculation.

*2. Supramolecular polymerization thermodynamics of (R)-**1***

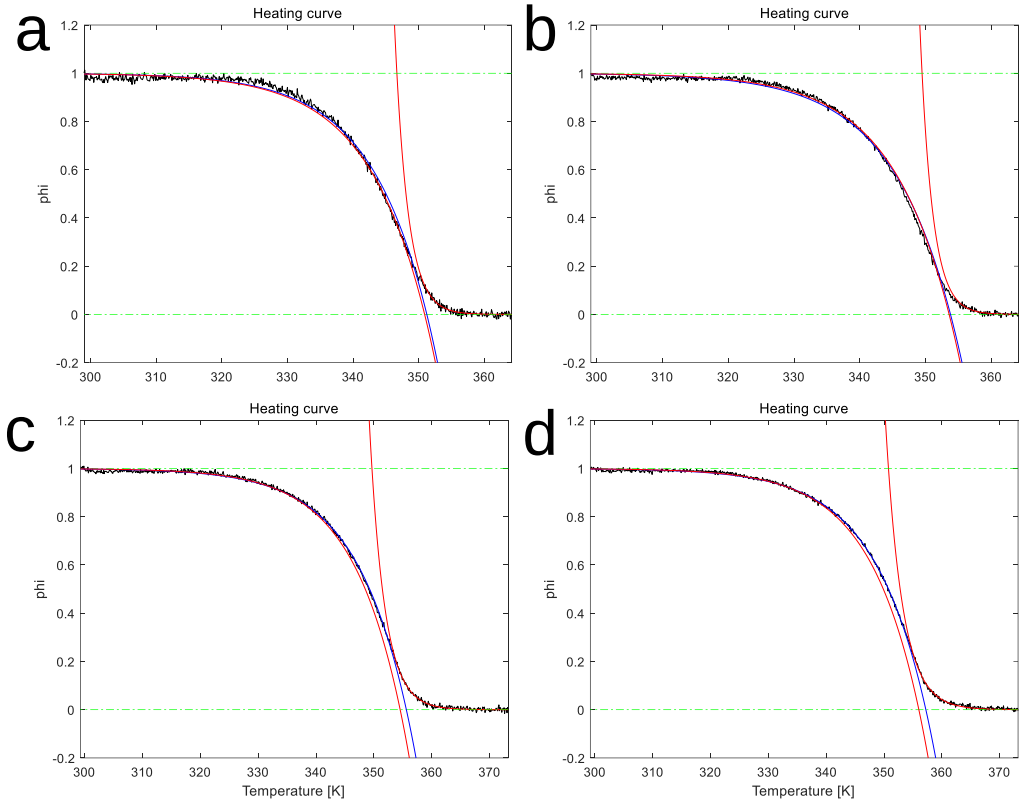


Fig. S11 Normalized CD intensities of (*R*)-**1** *versus* temperature at 387 nm in MCH at different monomer concentrations: (a) 0.004 mM; (b) 0.006 mM; (c) 0.008 mM; (d) 0.01 mM. The red lines denote mathematical fitting of the curves by the Meijer–Schenning–van der Schoot model. The quantitative thermodynamic values are shown in **Table S1**.

Table S1 Thermodynamic parameters of (*R*)-**1** in MCH obtained by fitting temperature-dependent CD data.

(*R*)-**1**	0.004 mM	0.006 mM	0.008 mM	0.01 mM
T_e (K)	351.2	353.8	355.6	357.2
h_e (kJ mol^{-1})	-114.2	-108.2	-114.9	-113.8
K_a	1.75×10^{-3}	1.45×10^{-3}	3.59×10^{-3}	4.49×10^{-3}

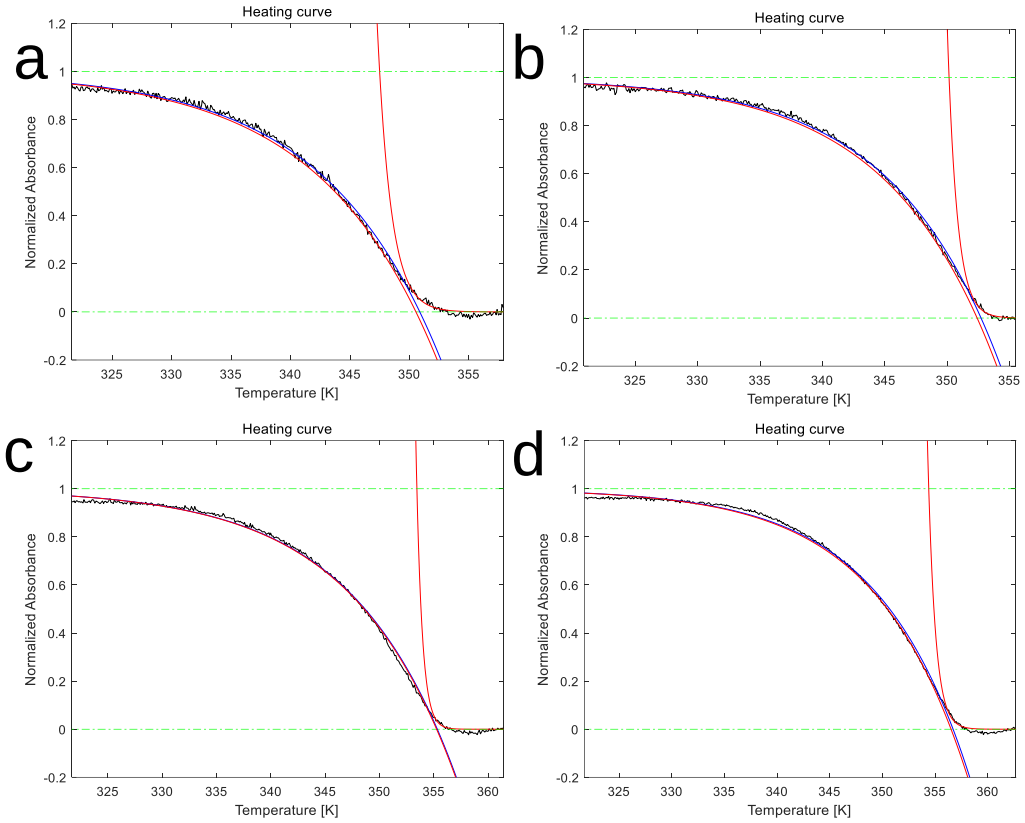


Fig. S12 Normalized UV–Vis absorbance intensities of (*R*)-**1** *versus* temperature at 387 nm in MCH at different monomer concentrations: (a) 0.004 mM; (b) 0.006 mM; (c) 0.008 mM; (d) 0.01 mM. The red lines denote mathematical fitting of the curves by Meijer–Schenning–van der Schoot model. The quantitative thermodynamic values are shown in **Table S2**.

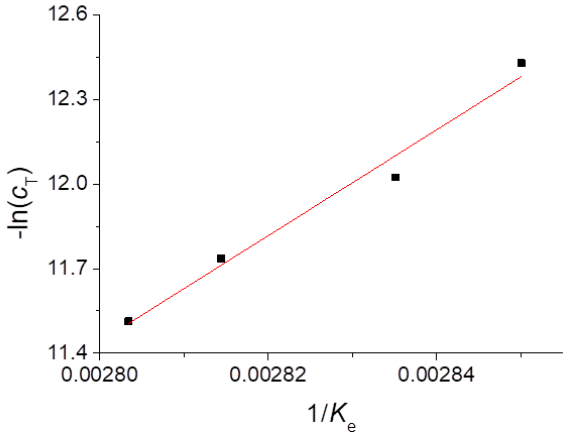


Fig. S13 Van't Hoff plots for (*R*)-**1** in MCH obtained by fitting temperature-dependent UV–Vis data. The red line denotes the linear fitting curve. Depending on the modified van't Hoff plot, the enthalpy (ΔH) and entropy (ΔS) values for the whole supramolecular polymerization process were determined to be –156 kJ mol^{-1} and –342 J mol^{-1}, respectively. Accordingly, the Gibbs free energy value (ΔG) was calculated to be –54.2 kJ mol^{-1} at 298 K.

Table S2 Thermodynamic parameters of (*R*)-1 in MCH obtained by fitting temperature-dependent UV–Vis data.

(*R*)-**1**	0.004 mM	0.006 mM	0.008 mM	0.01 mM
T_e (K)	350.9	352.7	355.3	356.7
h_e (kJ mol^{-1})	-104.7	-120.1	-109.3	-121.8
K_a	2.85×10^{-4}	1.81×10^{-4}	2.88×10^{-4}	1.26×10^{-4}

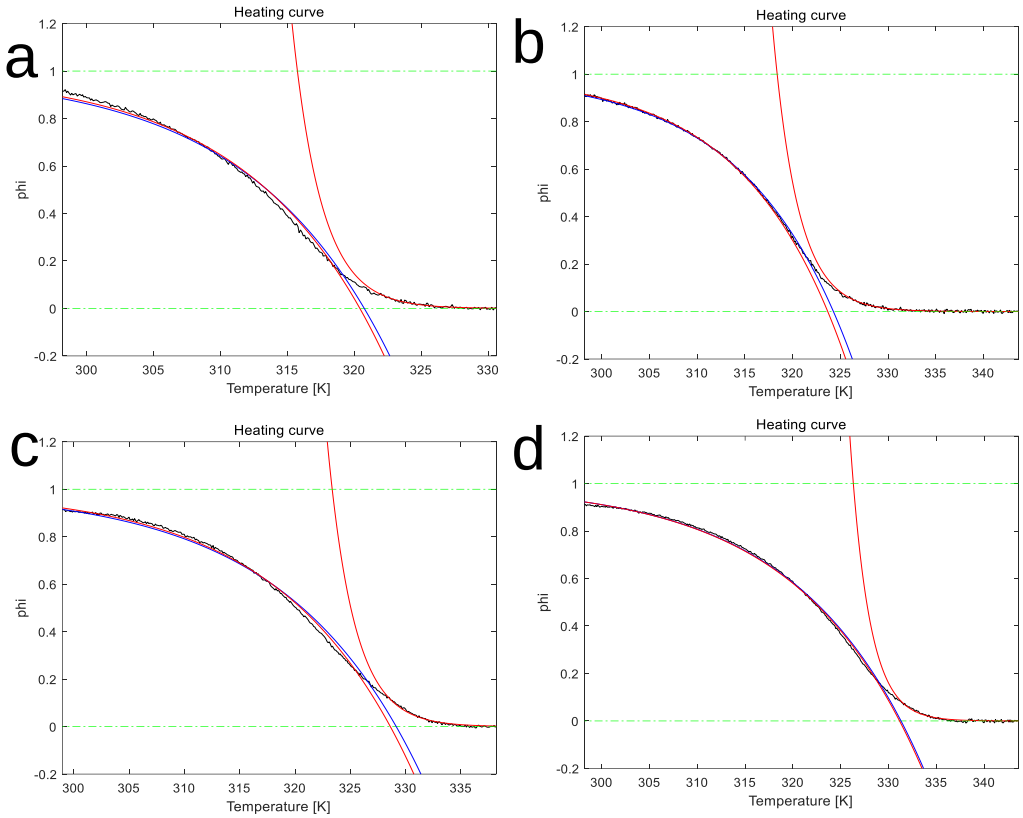


Fig. S14 Normalized CD intensities of (*R*)-**1** *versus* temperature at 381 nm in MCH/TCE (95:5, *v*/*v*) at different monomer concentrations: (a) 0.004 mM; (b) 0.006 mM; (c) 0.008 mM; (d) 0.01 mM. The red lines denote mathematical fitting of the curves by the Meijer–Schenning–van der Schoot model. The quantitative thermodynamic values are shown in **Table S3**.

Table S3 Thermodynamic parameters of (*R*)-**1** in MCH/TCE (95:5, *v*/*v*) obtained by fitting temperature-dependent CD data.

(*R*)-**1**	0.004 mM	0.006 mM	0.008 mM	0.01 mM
T_e (K)	320.7	324.3	329.2	331.3
h_e (kJ mol^{-1})	-81.7	-80.4	-73.6	-70.5
K_a	8.69×10^{-4}	7.20×10^{-5}	6.37×10^{-4}	7.28×10^{-4}

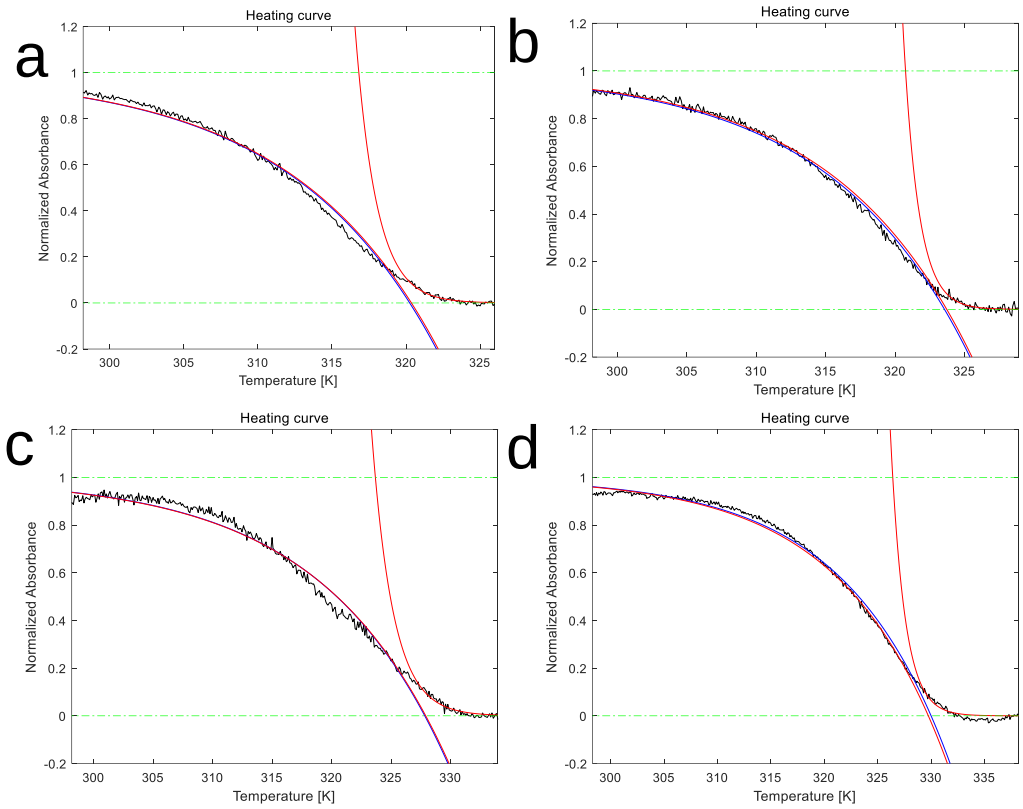


Fig. S15 Normalized UV–Vis absorbance intensities of (*R*)-**1** *versus* temperature at 381 nm in MCH/TCE (95:5, *v*/*v*) at different monomer concentrations: (a) 0.004 mM; (b) 0.006 mM; (c) 0.008 mM; (d) 0.01 mM. The red lines denote mathematical fitting of the curves by the Meijer–Schenning–van der Schoot model. The quantitative thermodynamic values are shown in **Table S4**.

Table S4 Thermodynamic parameters of (*R*)-**1** in MCH/TCE (95:5, *v*/*v*) obtained by fitting temperature-dependent UV–Vis data.

(*R*)-**1**	0.004 mM	0.006 mM	0.008 mM	0.01 mM
T_e (K)	320.3	323.6	327.8	330.0
h_e (kJ mol^{-1})	-86.0	-86.3	-83.7	-92.6
K_a	5.97×10^{-4}	2.83×10^{-4}	8.73×10^{-4}	4.81×10^{-4}

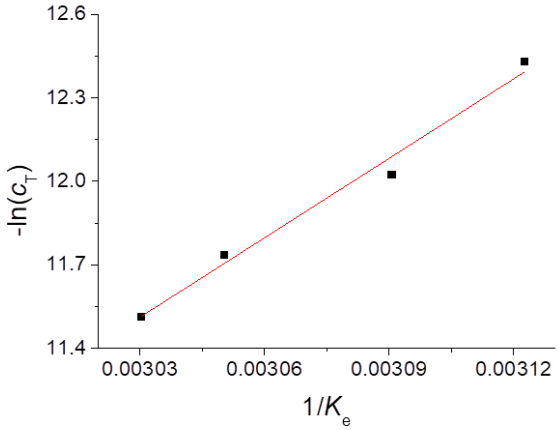


Fig. S16 Van't Hoff plots for (*R*)-**1** in MCH/TCE (95:5, *v*/*v*) obtained by fitting temperature-dependent UV–Vis data. The red line denotes the linear fitting curve. Depending on the modified van't Hoff plot, the enthalpy (Δ*H*) and entropy (Δ*S*) values for the whole supramolecular polymerization process were determined to be –79 kJ mol^{-1} and –144 J mol^{-1}, respectively. Accordingly, the Gibbs free energy value (Δ*G*) was calculated to be –36.2 kJ mol^{-1} at 298 K.

*3. Emission and CPL behaviors of (R)-**1***

Fluorescence quantum yields of (*R*)-**1** were determined by using optically matching solutions of Coumarin 102 (Φ_F=0.764 in ethanol) and Coumarin 153 (Φ_F=0.544 in ethanol) as standards. The quantum yield was calculated according to the following equation,

$$\Phi_F(X) = \Phi_F(S)\,(A_S F_X / A_X F_S)\,(n_X/n_S)^2 \quad \text{.....(Eq. S1)}$$

In this equation, Φ_F is the fluorescence quantum yield. A is the absorbance at the excitation wavelength. F is the area under the corrected emission curve, and n is the refractive index of the solvents used. Subscripts S and X refer to the standard and to the unknown, respectively. Therefore, the values of non-radiative rate k_{nr} and radiative rate k_r values can be calculated according to

$$\Phi_F = k_r \tau_F = k_r / (k_r + k_{nr}) \quad \text{.....(Eq. S2)}$$

with τ_F being the fluorescence lifetime.

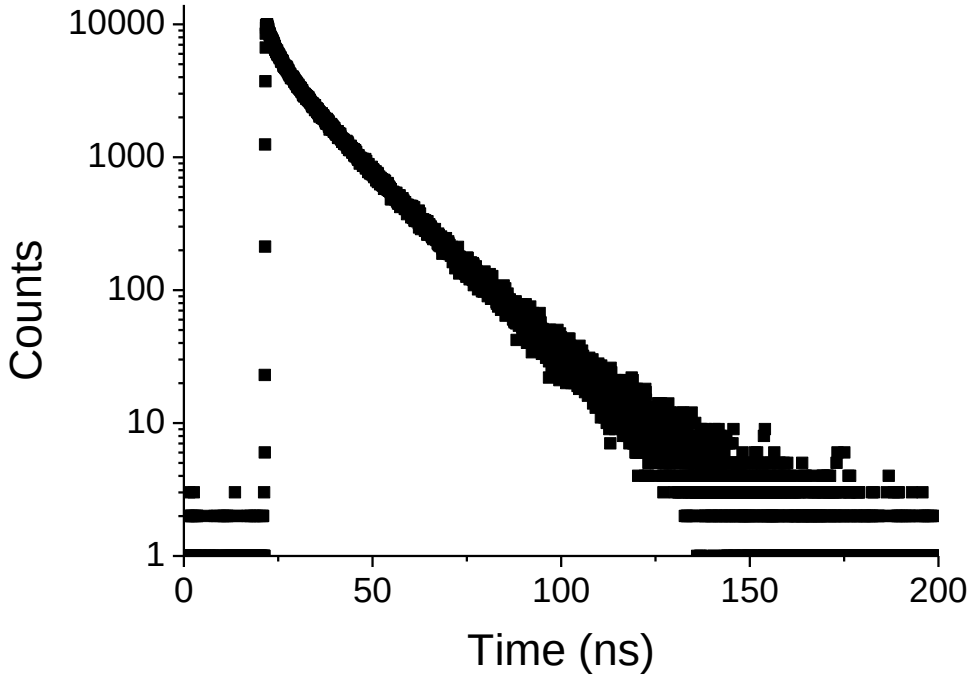


Fig. S17 Fluorescent lifetime measurements of (*R*)-**1** in MCH (c = 0.01 mM).

Table S5 Photophysical data of (*R*)-**1** in $CHCl_3$ and MCH

Solvent	Φ_F (%)	τ_F(ns)	k_r(s^{-1})	k_{nr}(s^{-1})
$CHCl_3$	0.07	$<1.0 \times 10^{-1}$	$>7.00 \times 10^6$	$>9.99 \times 10^9$
MCH	48.4	8.37	5.78×10^7	6.17×10^7

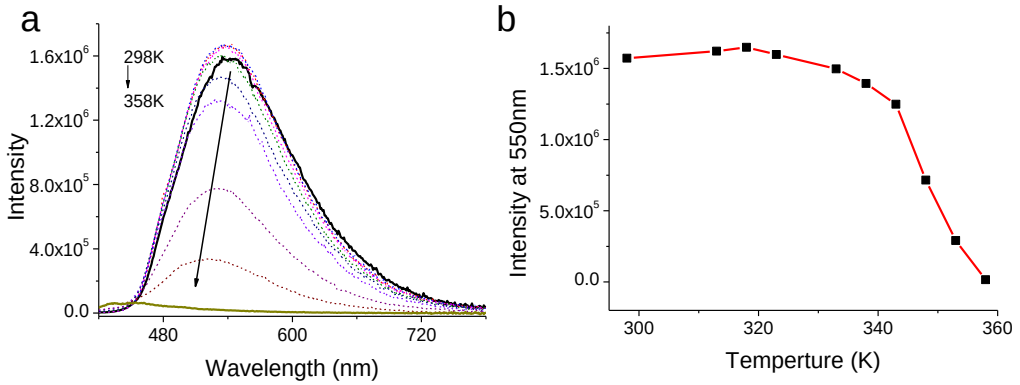


Fig. S18 (a) Fluorescent spectra and (b) emission intensity at 550 nm of (*R*)-**1** in MCH (*c* = 0.01 mM, 10 mm cuvette). The arrow in (a) shows spectral changes upon heating from 298 to 361 K.

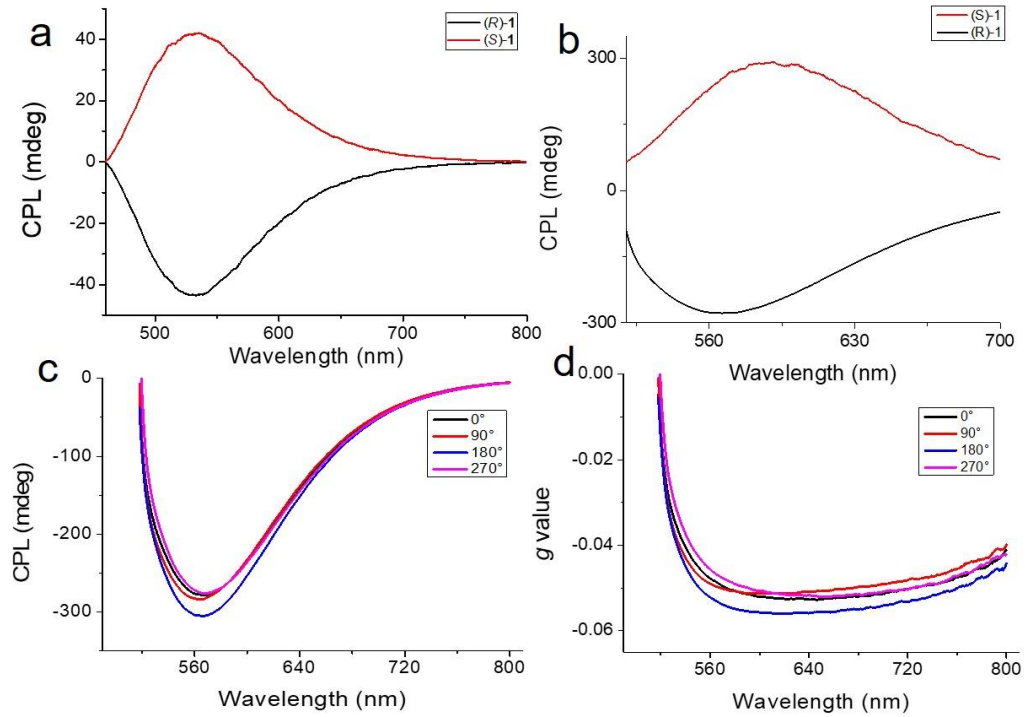
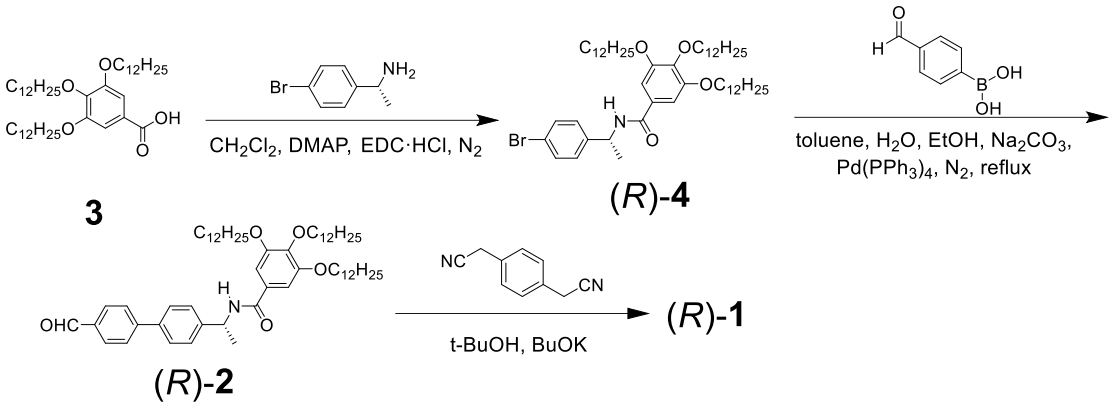


Fig. S19 CPL spectra of (*R*)-**1** (blue lines) and (*S*)-**1** (red lines): (a) in MCH (*c* = 0.01 mM, 10 mm cuvette); (b) for the drop-casting thin films. Angle-dependent (c) CPL and (d) g_{lum} value for the drop-casting thin film of (*R*)-**1**. Unlike the symmetrical CPL signals in dilute MCH (Fig. S19a), the CPL signals of (*S*)-**1** and (*R*)-**1** in the film state are not fully mirror symmetrical to each other (Fig. S19b). When rotating the sample about the optical axis, the CPL intensities and g_{lum} values showed slightly different amplitude. This result suggests that macroscopic aligning of supramolecular polymers might contribute to CPL signal enhancement in the film state.

*4. Synthesis and structural characterization (R)-**1** and (S)-**1***



Scheme S1 Synthetic Route toward (*R*)-**1.**

*4.1 Synthesis of (R)-**4***

Compounds **3** (2.00 g, 2.96 mmol), (*R*)-1-(4-bromophenyl)ethan-1-amine (0.46 g, 2.47 mmol), DMAP (0.50 g, 4.15 mmol) and EDC·HCl (1.14 g, 5.95 mmol) were mixed in CH_2Cl_2 (50 mL) under nitrogen and stirred at room temperature for 12 h. The solution was extracted with H_2O/CH_2Cl_2 for three times. The solvent was evaporated with a rotary evaporator. The residue was purified by flash column chromatography (silica gel, petroleum ether/CH_2Cl_2, 1 : 2 *v*/*v* as the eluent) to provide (*R*)-**4** as a white solid (1.69 g, 80%). ^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ7.47 (d, J = 8.5 Hz, 2H), 7.27 – 7.25(d, 2H), 6.93(s, 2H), 6.16 (d, J = 7.6 Hz, 1H), 5.26 (m, 1H), 4.01 – 3.96(m, 6H), 1.85 – 1.70 (m, 6H), 1.57(s, 3H), 1.50 – 1.40 (m, 6H), 1.37 – 1.23 (m, 48H), 0.88 (t, J = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 166.8, 153.4, 142.7, 141.7, 132.1, 129.5, 128.3, 121.5, 106.1, 73.9, 69.8, 53.8, 49.1, 32.3, 30.6, 30.1, 30.0, 29.9, 29.8, 29.7, 26.4, 23.0, 14.5.

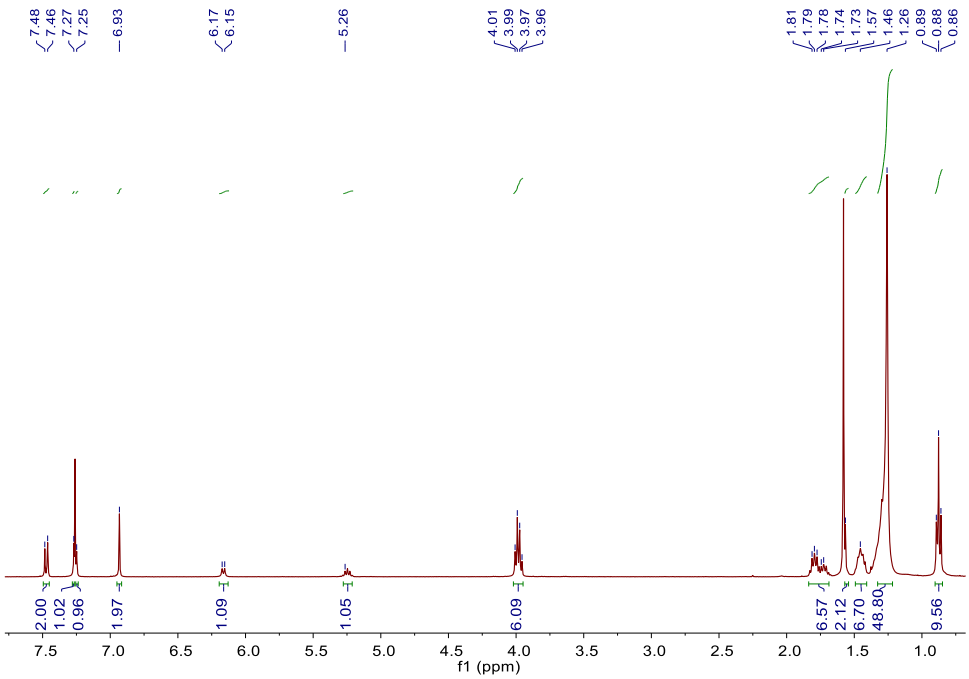


Fig. S20 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of (*R*)-**4**.

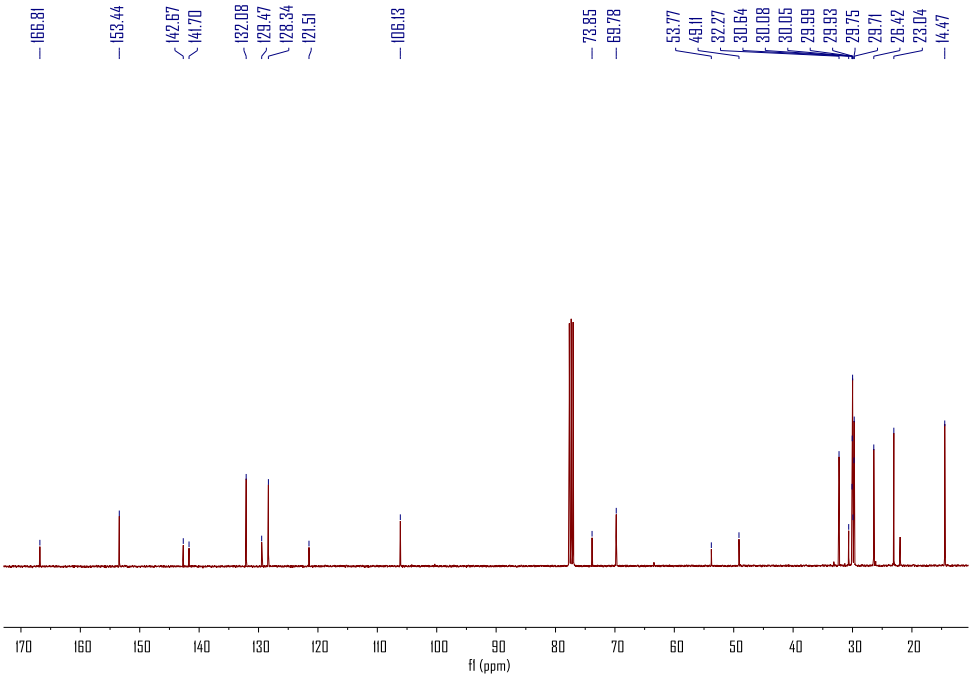


Fig. S21 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of (*R*)-**4**.

*4.2 Synthesis of (R)-**2***

Compounds (*R*)-**4** (808 mg, 0.942 mmol) and (4-formylphenyl)boronic acid (155 mg, 1.04 mmol) and $Pd(PPh_3)_4$ (109 mg, 0.094 mmol) were mixed in toluene (10 mL) and ethanol (8 mL) under nitrogen. Na_2CO_3 (2.12 g, 19.9 mmol) in H_2O (10 mL) was added to the reaction solution, and the whole mixture was refluxed for 24 h. the

solvent was evaporated with a rotary evaporator. The residue was extracted with H_2O/CH_2Cl_2 for three times, the CH_2Cl_2 solvent was evaporated with a rotary evaporator. The residue was purified by flash column chromatography (silica gel, petroleum ether/CH_2Cl_2, 1 : 2 *v*/*v* as the eluent) to provide (*R*)-**2** as a white solid (515 mg, 62%).^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ 10.05 (s, 1H) , 7.95 (d, J = 8.3 Hz, 2H) , 7.74 (d, J = 8.3 Hz, 2H), 7.63 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.3 Hz, 2H), 6.98 (s, 2 H), 6.26 (d, J = 7.7 Hz, 1H), 5.38 (m, 1H), 4.00 (m, 6H),1.85 – 1.70 (m, 6H), 1.65 (d, J = 6.9 Hz, 3H), 1.60 – 1.40 (m, 6H), 1.34 – 1.23 (m, 48H), 0.88 (t, J = 6.8 Hz, 9H). ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 192.2, 166.9, 153.5, 147.0, 144.1, 141.7, 139.1, 135.5, 130.6, 129.6, 128.0, 127.9, 127.3, 106.2, 73.9, 69.8, 49.4, 32.3, 30.7, 30.1, 30.0, 29.8, 29.7, 26.4, 23.0, 22.2, 14.5.

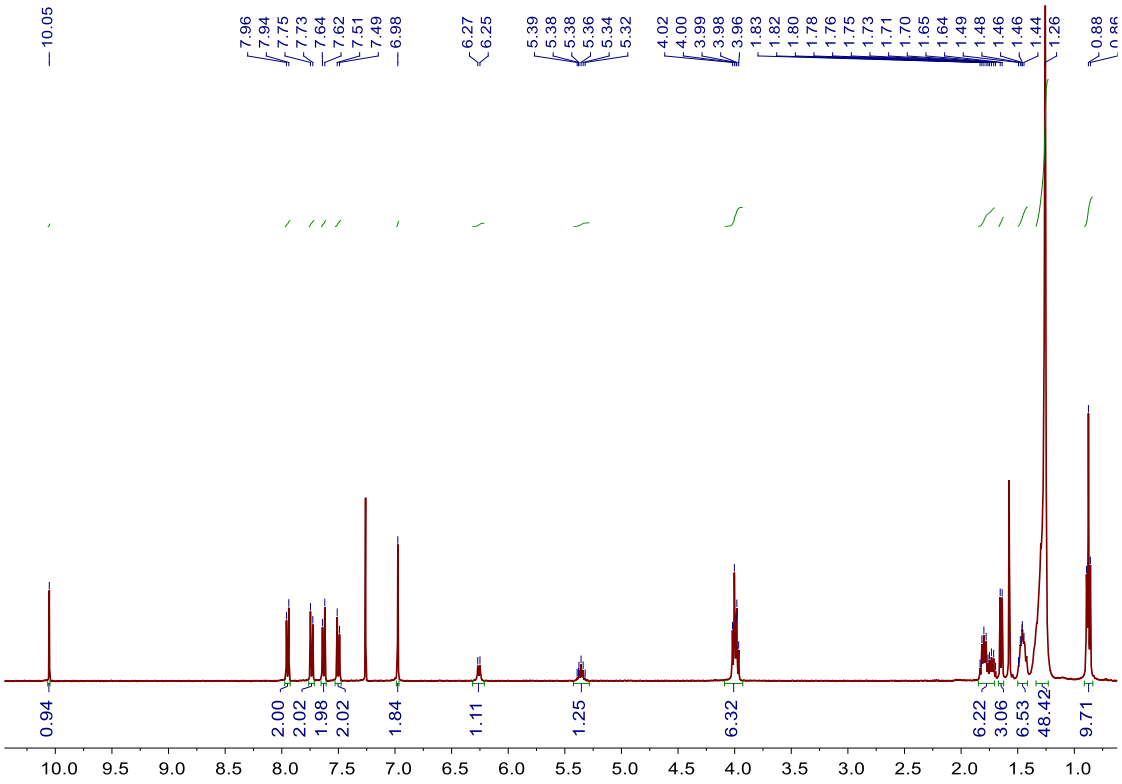


Fig. S22 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of (*R*)-**2**.

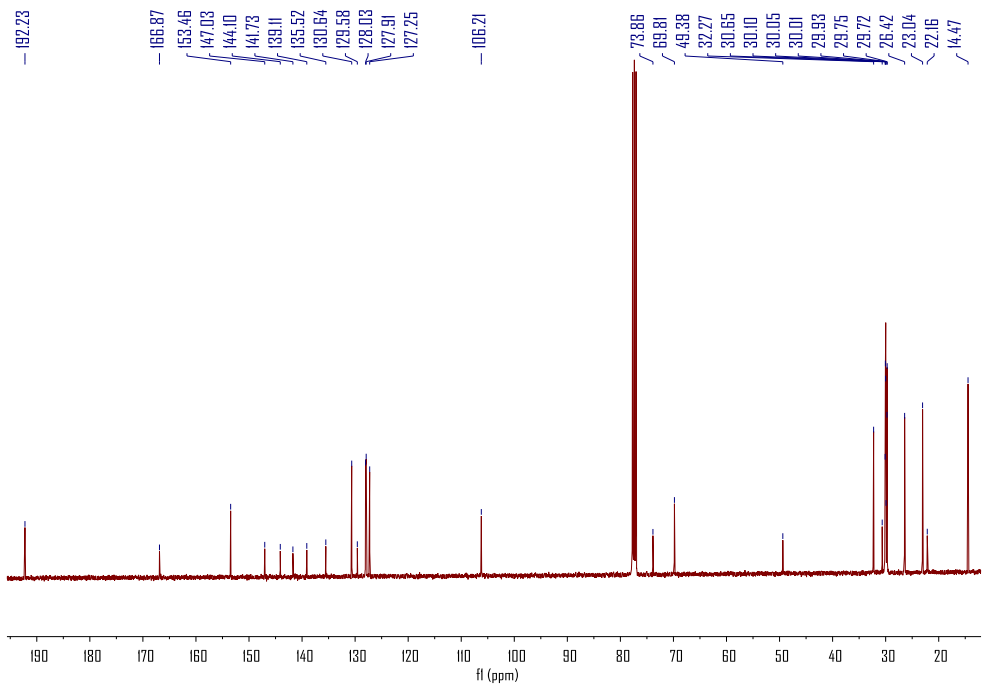


Fig. S23 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of (*R*)-**2**.

*4.3 Spectroscopy of (R)-**1***

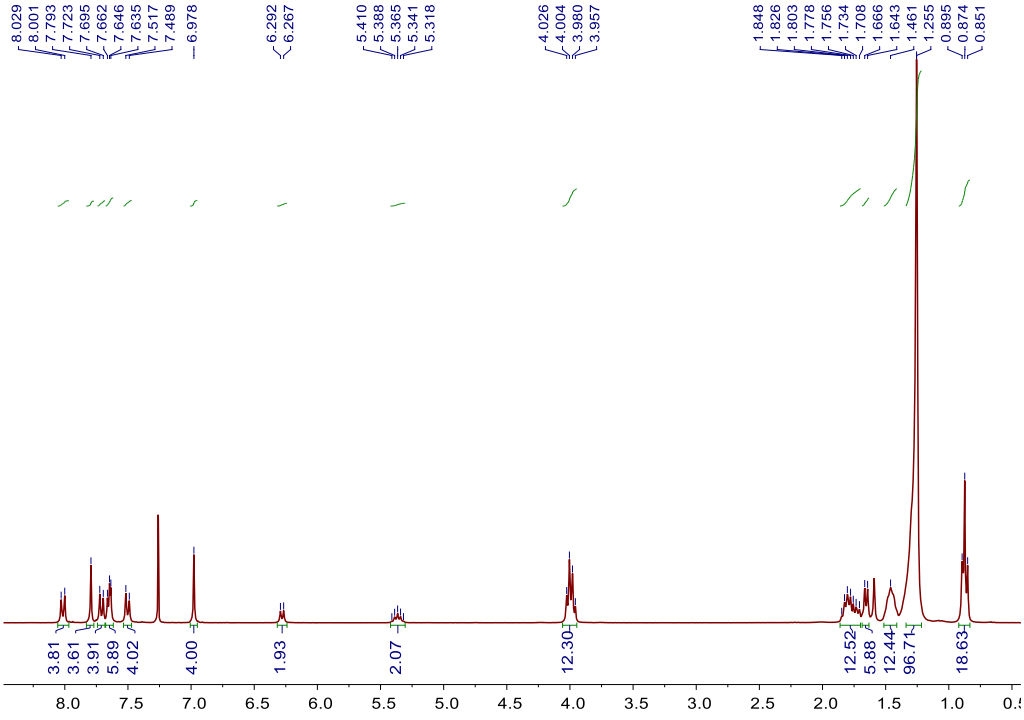


Fig. S24 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of (*R*)-**1**.

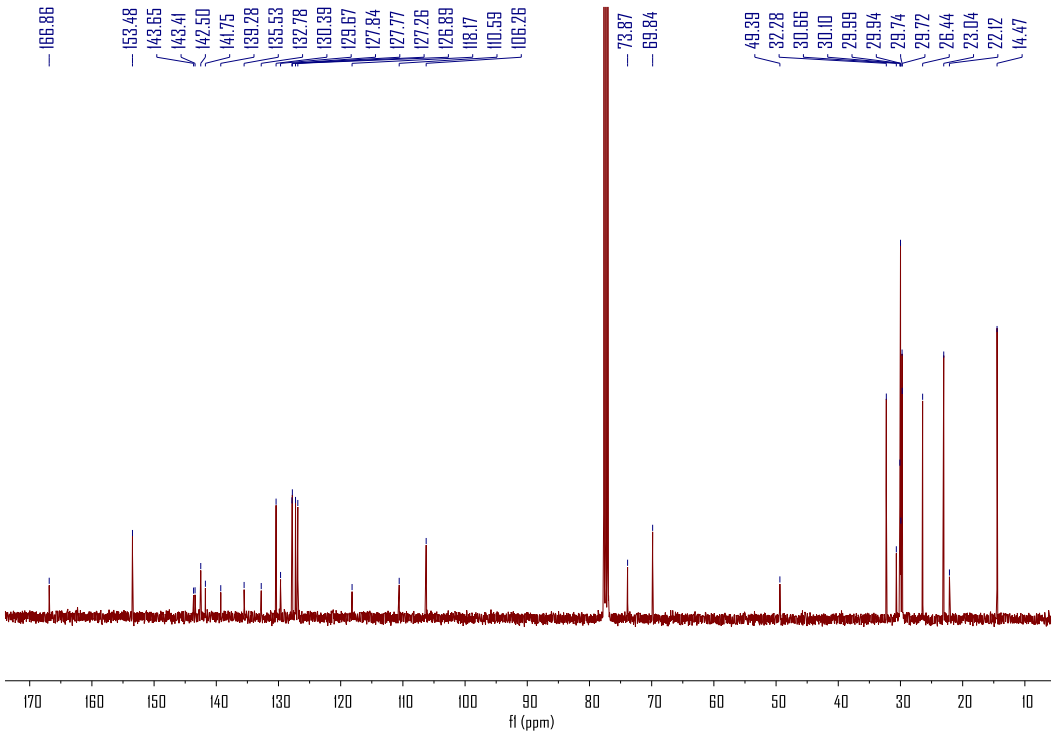


Fig. S25 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of (*R*)-**1**.

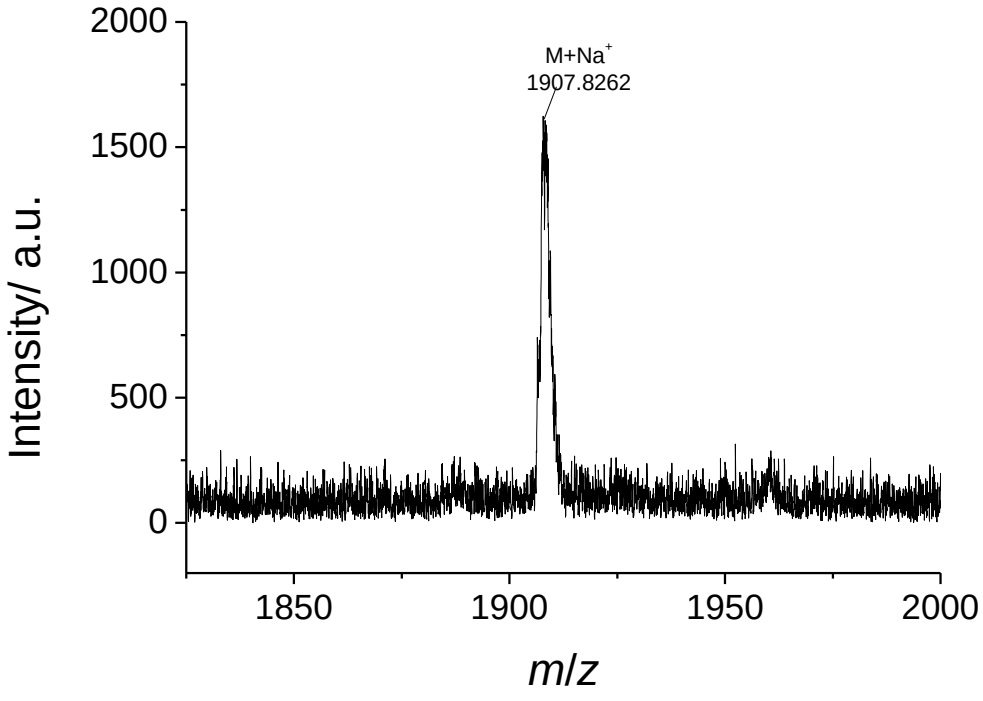
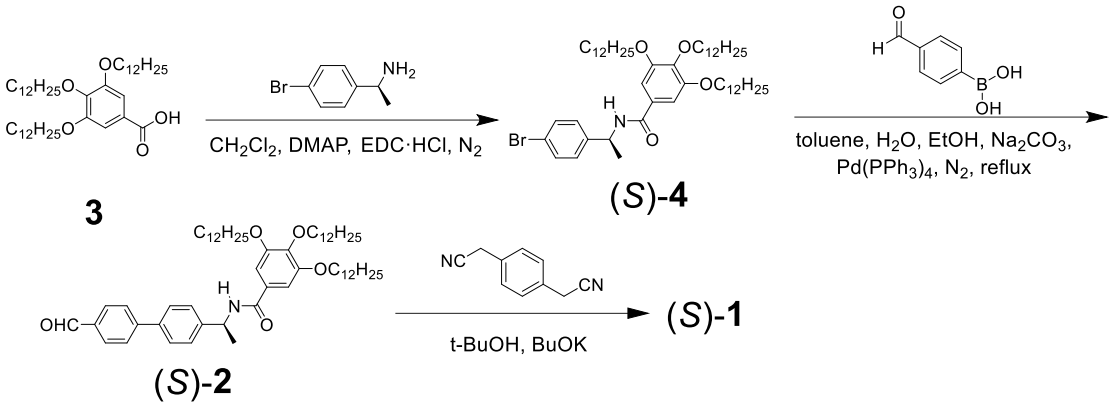


Fig S26 MALDI-TOF mass spectrum of (*R*)-**1**.



Scheme S2. Synthetic route toward (*S*)-**1**.

4.4 Synthesis of (S)-4

Compounds **3** (1.80 g, 2.66 mmol), (*S*)-1-(4-bromophenyl)ethan-1-amine (0.41 g, 2.22 mmol), DMAP (0.45 g, 3.73 mmol) and EDC·HCl (1.03 g, 5.35 mmol) were mixed in CH_2Cl_2 (50 mL) under nitrogen and stirred at room temperature for 12 h. The solution was extracted with H_2O/CH_2Cl_2 for three times. The solvent was evaporated with a rotary evaporator. The residue was purified by flash column chromatography (silica gel, petroleum ether/CH_2Cl_2, 1 : 2 *v*/*v* as the eluent) to provide (*S*)-**4** as a white solid (1.61 g, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.4 Hz, 2H), 7.27 (s, 1H), 7.25 (s, 1H), 6.93(s, 2H), 6.16 (d, J = 8.1 Hz, 1H), 5.28 – 5.22 (m, 1H), 4.01 – 3.96 (m, 6H), 1.83 – 1.71(m, 6H), 1.58 – 1.56 (m, 3H), 1.50 – 1.40 (m, 6H), 1.34 – 1.22 (m, 48H), 0.88 (t, J = 6.8 Hz, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ 166.8, 153.4, 142.7, 141.7, 132.0, 129.4, 128.3, 121.5, 106.1, 73.8, 69.7, 63.4, 49.1, 32.3, 30.1, 30.0, 29.7, 26.4, 23.0, 22.0, 14.5.

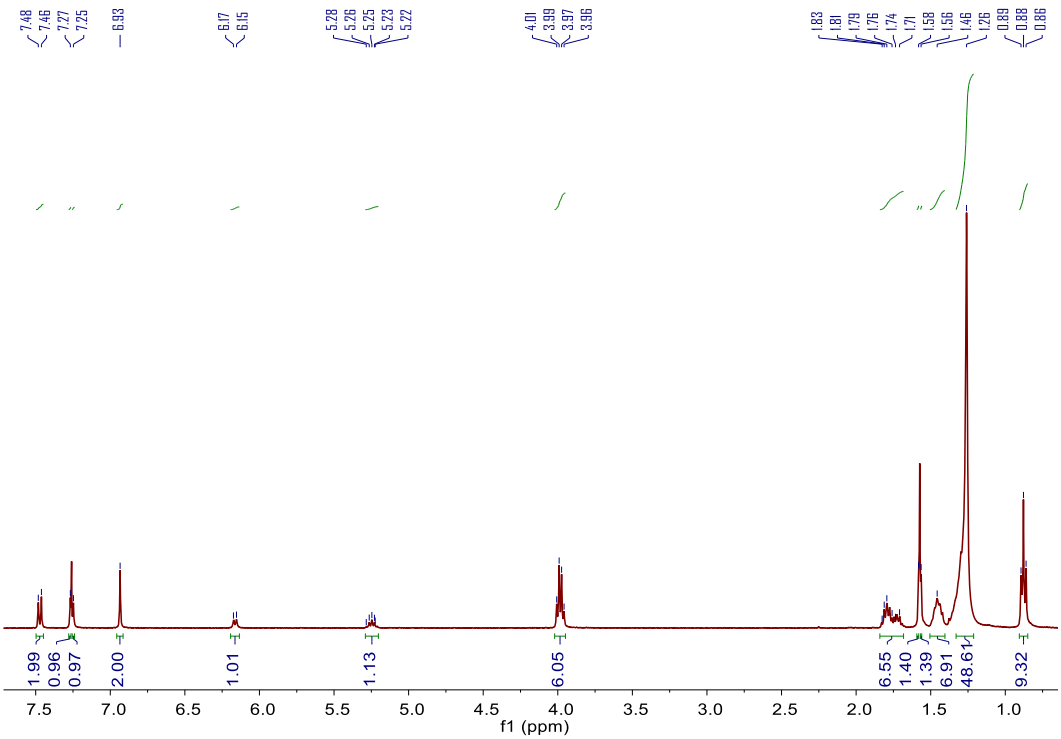


Fig. S27 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of (*S*)-**4**.

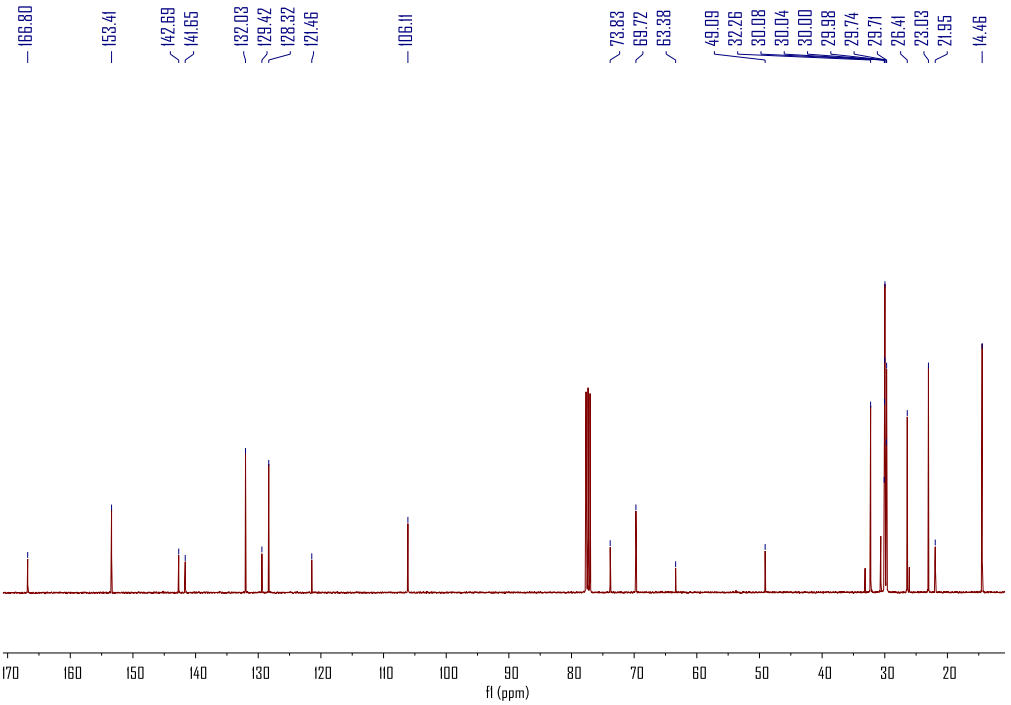


Fig. S28 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of (*S*)-**4**.

*4.5 Synthesis of (S)-**2***

Compounds (*S*)-**4** (888 mg, 1.04 mmol) and (4-formylphenyl)boronic acid (171 mg, 1.14 mmol) and $Pd(PPh_3)_4$ (119 mg, 0.103 mmol) were mixed in toluene (10 mL) and ethanol (8 mL) under nitrogen. Na_2CO_3 (2.12 g, 19.9 mmol) in H_2O (10 mL) was

added to the reaction solution, and the whole was refluxed for 24 h. The solvent was then evaporated with a rotary evaporator. The residue was extracted with H_2O/CH_2Cl_2 for three times. The CH_2Cl_2 solvent was evaporated with a rotary evaporator. The residue was purified by flash column chromatography (silica gel, petroleum ether/CH_2Cl_2, 1 : 2 *v*/*v* as the eluent) to provide (*S*)-**2** as a white solid (680 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ 10.05 (s, 1H) , 7.95 (d, *J* = 8.3 Hz, 2H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.50 (d, *J* = 8.3 Hz, 2H), 6.98 (s, 2 H), 6.26 (d, *J* = 7.7 Hz, 1H), 5.38 (m, 1H), 4.00 (m, 6H), 1.85 – 1.70 (m, 6H), 1.65 (d, *J* = 6.9 Hz, 3H), 1.60 – 1.40 (m, 6H), 1.34 – 1.23 (m, 48H), 0.88 (t, *J* = 6.8 Hz, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, 298K) δ 192.2, 166.9, 153.5, 147.0, 144.1, 141.7, 139.1, 135.5, 130.6, 129.6, 128.0, 127.9, 127.3, 106.2, 73.9, 69.8, 49.4, 32.3, 30.7, 30.1, 30.0, 29.9, 29.8, 29.7, 26.4, 23.0, 22.2, 14.5.

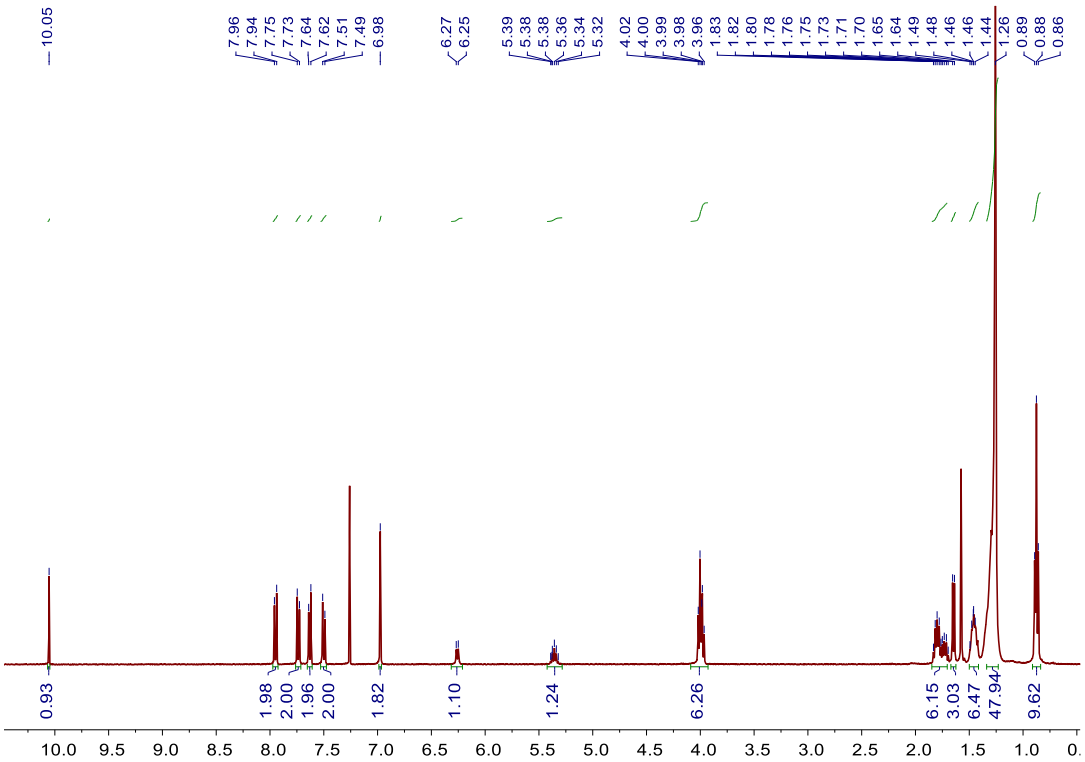


Fig. S29 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of (*S*)-**2**.

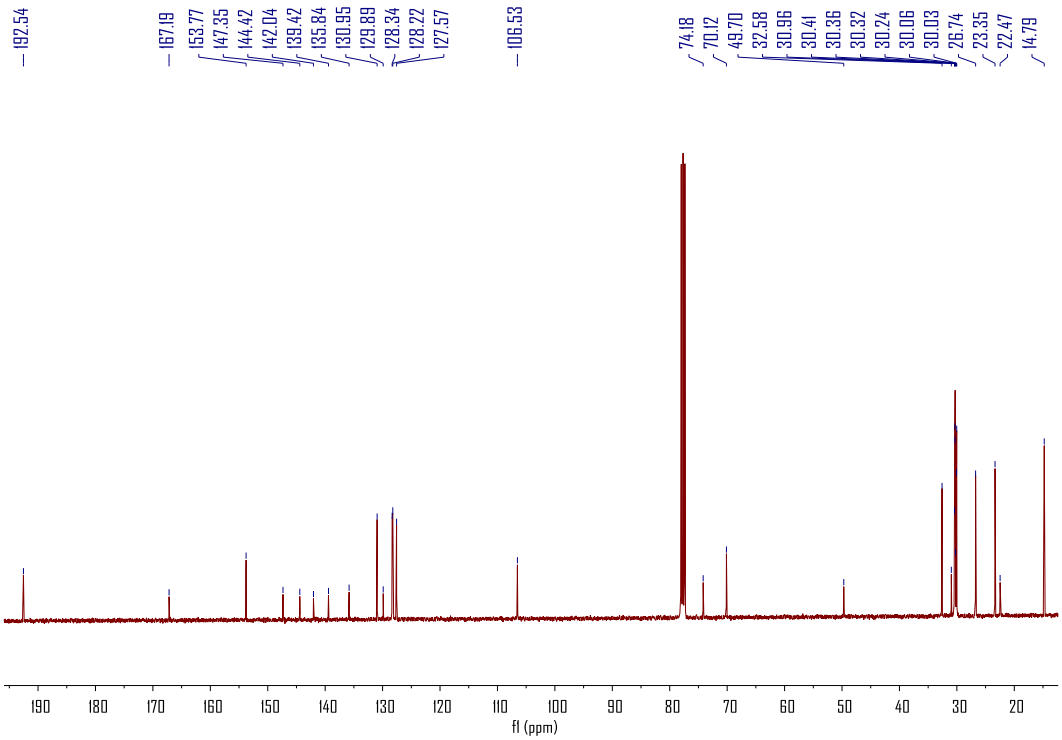


Fig. S30 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of (*S*)-**2**.

*4.6 Spectroscopy of (S)-**1***

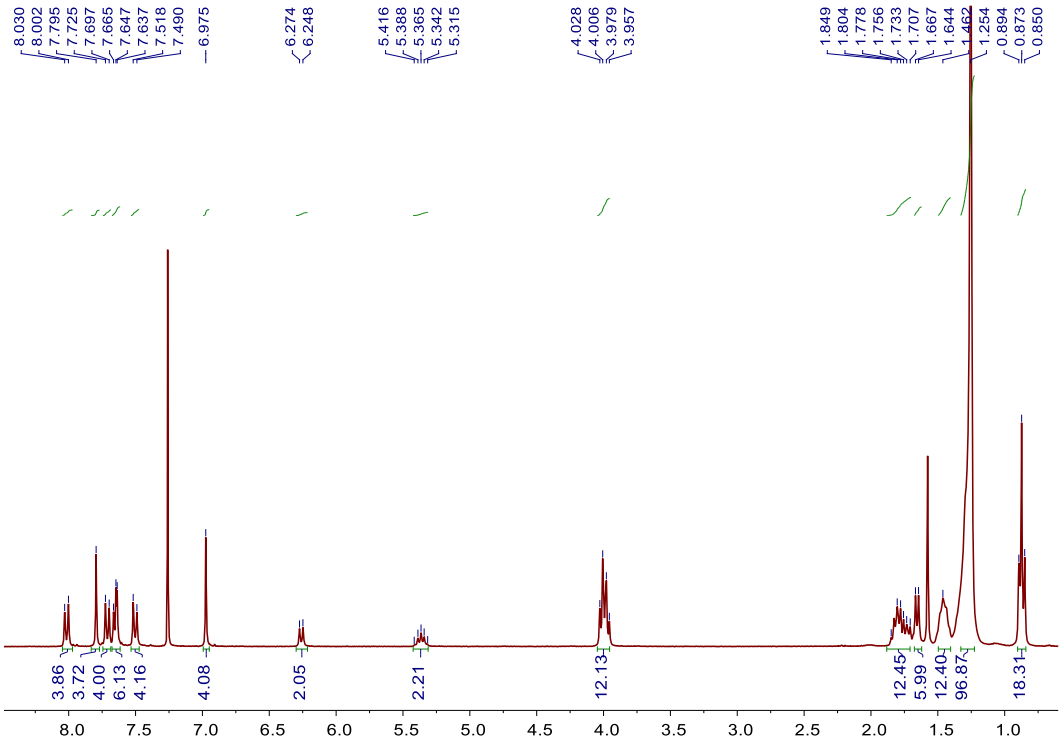


Fig. S31 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of (*S*)-**1**.

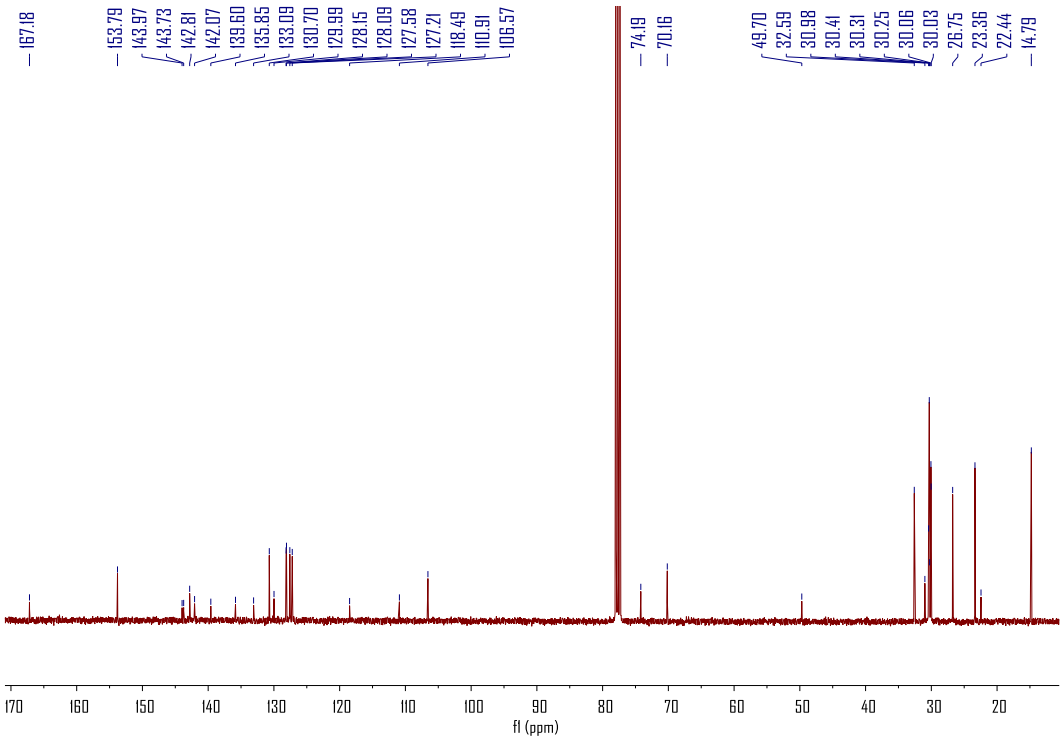


Fig. S32 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of (*S*)-**1**.

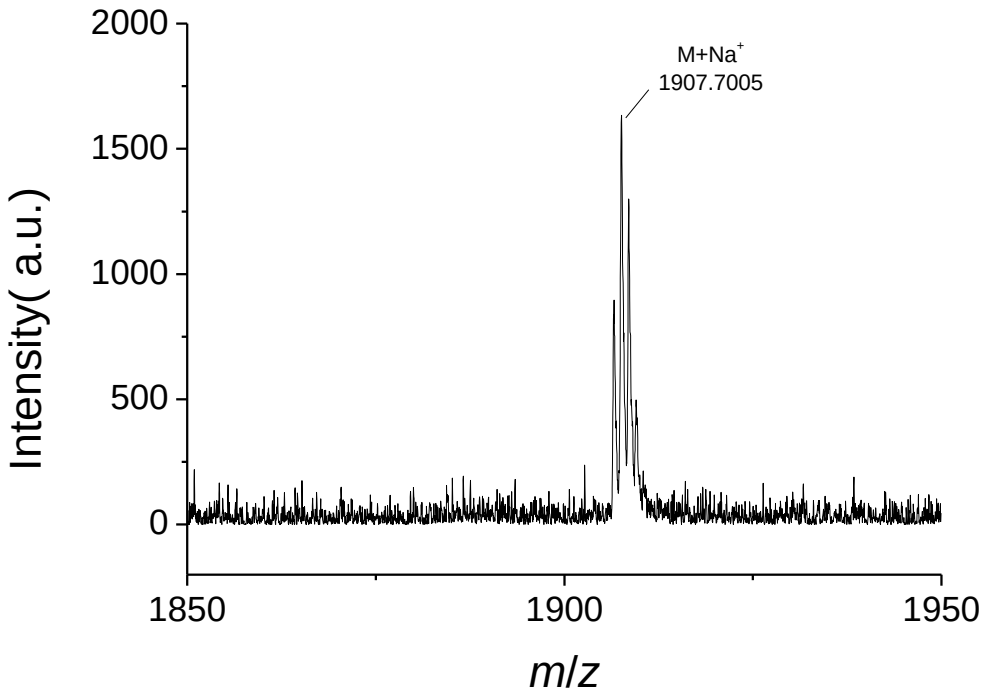
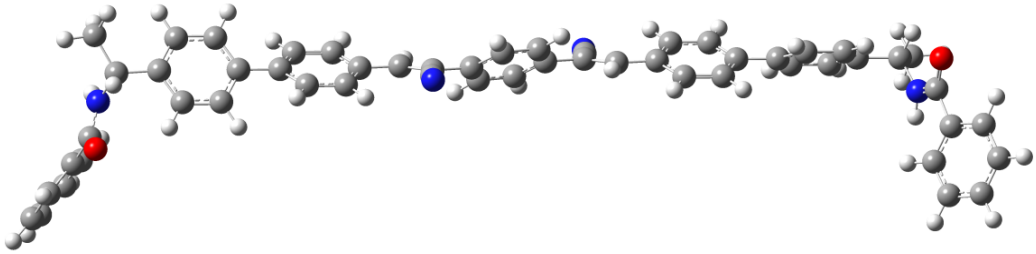


Fig. S33 MALDI-TOF mass spectrum of (*S*)-**1**.

*5. Appendix S1. Standard orientations of (R)-**1** and (R)-**1**$_2$*

(*R*)-**1** calculated *via* B3LYP



E(B3LYP) = -2452.525946 a.u. (ground state)
Stoichiometry C54H42N4O2
Framework group C1[X(C54H42N4O2)]
Deg. of freedom 300
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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6	6	0	-11.639326	0.504700	-1.300572
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8	1	0	-12.280336	-2.812624	-0.955958
9	6	0	-10.254745	0.471198	-1.183991
10	1	0	-12.147411	1.453755	-1.452088
11	6	0	-9.572794	-0.741905	-0.974336
12	1	0	-9.842200	-2.872038	-0.761469
13	1	0	-9.694278	1.400480	-1.232876
14	6	0	-8.096956	-0.780759	-0.851092
15	6	0	-7.278538	0.087051	-1.598502
16	6	0	-7.461160	-1.683920	0.018975

17	6	0	-5.894691	0.059355	-1.492691
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19	6	0	-6.078486	-1.714209	0.129726
20	1	0	-8.059944	-2.348062	0.635239
21	6	0	-5.254498	-0.850047	-0.623438
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23	1	0	-5.616023	-2.416321	0.819636
24	6	0	-3.816342	-0.971006	-0.426156
25	6	0	-2.751416	-0.384355	-1.045824
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37	6	0	6.080412	-0.100670	-0.646002
38	6	0	5.892012	-1.896357	0.951476
39	6	0	7.462742	-0.130742	-0.529976
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41	6	0	7.275414	-1.925348	1.060839
42	1	0	5.309738	-2.605339	1.526231
43	6	0	8.095932	-1.045309	0.330013
44	1	0	8.060380	0.579505	-1.093540
45	1	0	7.734142	-2.667896	1.707010
46	6	0	9.571140	-1.083079	0.459903
47	6	0	10.406342	-0.828940	-0.643981
48	6	0	10.184336	-1.374894	1.687848
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50	1	0	9.964623	-0.633364	-1.617067
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54	1	0	12.417341	-0.674358	-1.387291
55	1	0	12.005445	-1.638129	2.780204
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67	1	0	15.607881	-1.879630	1.936371
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75	6	0	16.421058	2.555023	-1.322281
76	6	0	15.411179	4.415291	0.495657
77	1	0	14.143059	2.835760	1.198058
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79	1	0	16.785321	1.819259	-2.031545
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81	1	0	15.002160	5.141659	1.192631
82	1	0	17.662569	4.156979	-2.042328
83	1	0	16.768066	5.817466	-0.420855
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86	6	0	-16.277687	2.975357	1.195887
87	6	0	-15.598677	1.832291	3.648974
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90	1	0	-16.512528	3.414715	0.232096
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92	1	0	-15.317141	1.396492	4.603703
93	1	0	-17.482017	4.344021	2.337086
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95	1	0	-0.513180	-0.219810	-2.584673
96	1	0	0.513156	-1.600715	2.055673
97	1	0	3.552317	-0.139045	-0.882908
98	6	0	2.911464	-2.320621	1.633343
99	7	0	2.986825	-3.036259	2.549481
100	1	0	-3.551251	-1.682101	0.352922
101	6	0	-2.910843	0.504505	-2.159183
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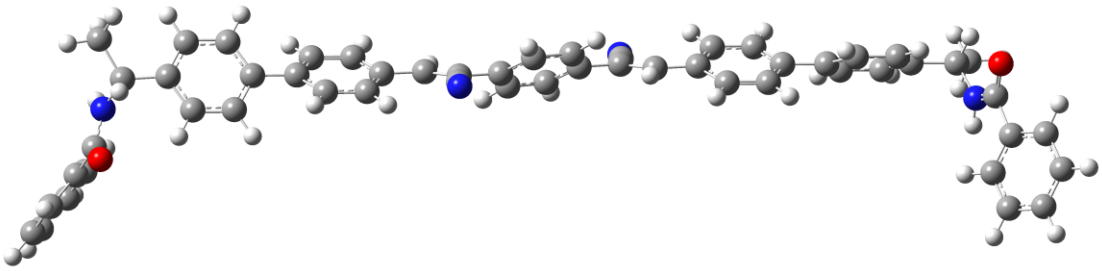
(*R*)-**1** calculated *via* ωb97xd



E((ωb97xd) = -2451.710949 a.u. (ground state)
Stoichiometry C54H42N4O2
Framework group C1[X(C54H42N4O2)]
Deg. of freedom 300
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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6	6	0	-11.588178	0.621971	-1.203525
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25	6	0	-2.745244	-0.367199	-1.075644
26	6	0	-1.333064	-0.595451	-0.671634
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66	1	0	14.028019	-2.821745	2.336549
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74	6	0	14.690949	3.050988	0.372725
75	6	0	16.338634	2.436670	-1.277770
76	6	0	15.119212	4.373348	0.307111
77	1	0	13.847040	2.798498	1.009726
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79	1	0	16.785320	1.670060	-1.902202
80	6	0	16.166381	4.725105	-0.539564
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83	1	0	16.502455	5.756603	-0.587735
84	6	0	-15.284924	1.711723	1.337780
85	6	0	-14.859407	1.068405	2.502132
86	6	0	-16.194888	2.766172	1.429636
87	6	0	-15.356398	1.460981	3.741152
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89	6	0	-16.699600	3.149917	2.665780
90	1	0	-16.491625	3.275367	0.518720
91	6	0	-16.283398	2.495845	3.823550
92	1	0	-15.011902	0.963907	4.642897
93	1	0	-17.414969	3.964326	2.728254
94	1	0	-16.673438	2.799648	4.790418
95	1	0	-0.571649	-0.594032	-2.688004
96	1	0	0.580883	-1.083525	2.097103
97	1	0	3.534944	-0.184400	-1.058692
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101	6	0	-2.923273	0.383976	-2.286631
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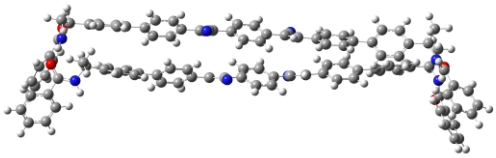
(*R*)-**1**$_2$ calculated *via* ωb97xd



E(ωb97xd) = −4903.527545 a.u. (ground state)

Stoichiometry C108H84N8O4

Framework group C1[X(C108H84N8O4)]

Deg. of freedom 606

Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	14.687802	-2.072737	-1.465436
2	6	0	13.808026	-1.911978	-2.653444
3	1	0	13.984451	-2.793800	-3.335792
4	6	0	12.349950	-1.884398	-2.216436
5	6	0	11.895944	-0.951821	-1.273704
6	6	0	11.444009	-2.798380	-2.773484
7	6	0	10.552917	-0.926479	-0.895583
8	1	0	12.599197	-0.240826	-0.828132
9	6	0	10.096839	-2.767462	-2.407590
10	1	0	11.790061	-3.542914	-3.491035
11	6	0	9.643376	-1.829111	-1.467574
12	1	0	10.210434	-0.197286	-0.162514
13	1	0	9.398056	-3.480184	-2.844526
14	6	0	8.215885	-1.788535	-1.084011
15	6	0	7.230763	-1.568957	-2.059619
16	6	0	7.835203	-1.970005	0.256065
17	6	0	5.881978	-1.540479	-1.704204
18	1	0	7.519901	-1.423134	-3.100971
19	6	0	6.487379	-1.942729	0.613407
20	1	0	8.597293	-2.147551	1.014457
21	6	0	5.500866	-1.736810	-0.366546
22	1	0	5.122115	-1.357130	-2.469704
23	1	0	6.200973	-2.096840	1.652624
24	6	0	4.085527	-1.700706	0.026257

25	6	0	3.084506	-2.352699	-0.594788
26	6	0	1.668523	-2.199172	-0.179789
27	6	0	0.738751	-1.681865	-1.096255
28	6	0	1.257764	-2.555743	1.112939
29	6	0	-0.595013	-1.521693	-0.720968
30	6	0	-0.077392	-2.394520	1.489328
31	1	0	1.977053	-2.966390	1.821010
32	6	0	-1.005274	-1.881513	0.571845
33	1	0	-1.315025	-1.113971	-1.429819
34	6	0	-2.431344	-1.726958	0.957534
35	6	0	-3.388795	-2.532873	0.462184
36	6	0	-4.821820	-2.469687	0.780560
37	6	0	-5.755969	-2.542131	-0.268558
38	6	0	-5.274353	-2.368089	2.105554
39	6	0	-7.122699	-2.496438	0.004380
40	1	0	-5.413825	-2.625161	-1.299475
41	6	0	-6.642654	-2.336329	2.378719
42	1	0	-4.559181	-2.316841	2.926666
43	6	0	-7.573940	-2.395903	1.330613
44	1	0	-7.843860	-2.542296	-0.811427
45	1	0	-6.989150	-2.252875	3.409054
46	6	0	-9.022594	-2.344232	1.625559
47	6	0	-9.815182	-1.320163	1.083234
48	6	0	-9.610101	-3.307890	2.458775
49	6	0	-11.173683	-1.250881	1.392747
50	1	0	-9.366298	-0.566832	0.432761
51	6	0	-10.971381	-3.235904	2.764149
52	1	0	-9.002748	-4.114299	2.867957
53	6	0	-11.757403	-2.196946	2.250106
54	1	0	-11.780330	-0.446681	0.967279
55	1	0	-11.412554	-3.990820	3.413462
56	6	0	-13.231402	-2.051915	2.589290
57	1	0	-13.511499	-0.956156	2.550753
58	7	0	-14.024521	-2.759446	1.542414
59	6	0	-14.920347	-2.078567	0.730423
60	8	0	-15.107326	-0.873079	0.861643
61	1	0	-13.867138	-3.757171	1.441310
62	6	0	15.329873	-3.275794	-1.199828
63	8	0	15.239187	-4.231919	-1.957724
64	1	0	14.780604	-1.253956	-0.853185
65	6	0	-13.601569	-2.592347	3.972027
66	1	0	-12.987560	-2.121560	4.750642
67	1	0	-14.652183	-2.378910	4.209434
68	1	0	-13.465848	-3.676095	4.058240

69	6	0	14.176221	-0.615857	-3.384923
70	1	0	14.167427	0.248468	-2.704067
71	1	0	15.182835	-0.678473	-3.814818
72	1	0	13.473793	-0.410763	-4.199290
73	6	0	-15.639203	-2.919276	-0.279376
74	6	0	-14.930538	-3.576949	-1.292529
75	6	0	-17.036343	-3.004633	-0.216463
76	6	0	-15.626005	-4.329719	-2.243134
77	1	0	-13.844859	-3.492906	-1.349001
78	6	0	-17.724478	-3.763929	-1.166770
79	1	0	-17.581227	-2.474524	0.566478
80	6	0	-17.020210	-4.425861	-2.178445
81	1	0	-15.080436	-4.839443	-3.036675
82	1	0	-18.810775	-3.836529	-1.120635
83	1	0	-17.559516	-5.015932	-2.919565
84	6	0	16.161257	-3.296664	0.050717
85	6	0	15.670819	-2.804056	1.266112
86	6	0	17.442124	-3.862772	-0.017209
87	6	0	16.470384	-2.865919	2.411668
88	1	0	14.666759	-2.381925	1.325360
89	6	0	18.238208	-3.918364	1.129732
90	1	0	17.802911	-4.268373	-0.964824
91	6	0	17.752918	-3.419335	2.343400
92	1	0	16.089568	-2.484048	3.357344
93	1	0	19.232723	-4.358044	1.078868
94	1	0	18.372283	-3.469490	3.237212
95	6	0	-1.700919	2.709899	0.059622
96	6	0	-1.219499	2.756014	-1.257424
97	6	0	-0.813855	2.492736	1.125168
98	6	0	-3.145443	2.913767	0.334363
99	6	0	0.145672	2.607038	-1.506832
100	1	0	-1.909509	2.923156	-2.084267
101	6	0	0.550932	2.344422	0.875855
102	6	0	-4.087814	2.050150	-0.088279
103	6	0	1.037070	2.415023	-0.439676
104	1	0	1.237391	2.172150	1.704365
105	6	0	-5.534199	2.184173	0.135946
106	6	0	2.495037	2.310181	-0.694312
107	6	0	-6.412538	1.983601	-0.943813
108	6	0	-6.054801	2.494860	1.402353
109	6	0	3.382280	3.113324	-0.075680
110	6	0	-7.787931	2.119448	-0.763458
111	1	0	-6.019155	1.733746	-1.927759
112	6	0	-7.432734	2.629921	1.581043

113	1	0	-5.382355	2.626919	2.252365
114	6	0	4.840981	3.097880	-0.252532
115	6	0	-8.309946	2.450380	0.499657
116	1	0	-8.462861	1.968745	-1.605554
117	1	0	-7.826857	2.891442	2.563325
118	6	0	5.518440	4.318753	-0.426829
119	6	0	5.572271	1.900841	-0.216313
120	6	0	-9.769683	2.604591	0.677773
121	6	0	6.905507	4.337597	-0.558708
122	1	0	4.956863	5.251581	-0.468248
123	6	0	6.963056	1.920854	-0.341164
124	1	0	5.059876	0.946856	-0.088565
125	6	0	-10.515012	3.376278	-0.231898
126	6	0	-10.427533	1.976189	1.744399
127	6	0	7.639095	3.138797	-0.507363
128	1	0	7.425156	5.283794	-0.708273
129	1	0	7.520158	0.981353	-0.307662
130	6	0	-11.894736	3.494218	-0.084336
131	1	0	-10.011510	3.889075	-1.050766
132	6	0	-11.814138	2.094277	1.887647
133	1	0	-9.861078	1.381822	2.460408
134	6	0	9.113473	3.168513	-0.620869
135	6	0	-12.557909	2.847006	0.973539
136	1	0	-12.477673	4.082634	-0.803817
137	1	0	-12.305233	1.591903	2.719214
138	6	0	9.868167	4.016101	0.206180
139	6	0	9.770277	2.348990	-1.552407
140	6	0	-14.072512	2.986029	1.049875
141	6	0	11.260241	4.042173	0.102465
142	1	0	9.366124	4.650646	0.935464
143	6	0	11.162473	2.375144	-1.651393
144	1	0	9.192449	1.689101	-2.201524
145	1	0	-14.342574	4.052044	0.782224
146	7	0	-14.682892	2.089116	0.026572
147	6	0	-14.666456	2.660352	2.420855
148	6	0	11.916014	3.220601	-0.824806
149	1	0	11.832336	4.707034	0.746139
150	1	0	11.659854	1.722345	-2.371585
151	6	0	-14.959693	2.569349	-1.248271
152	1	0	-14.816321	1.109283	0.295610
153	1	0	-14.193559	3.262510	3.205425
154	1	0	-15.742429	2.879310	2.440828
155	1	0	-14.552517	1.602929	2.689970
156	6	0	13.431302	3.224024	-0.952069

157	8	0	-14.707852	3.739497	-1.530363
158	6	0	-15.558001	1.624847	-2.244510
159	7	0	14.047251	2.832383	0.348589
160	1	0	13.747588	2.454887	-1.717101
161	6	0	13.953038	4.597227	-1.379560
162	6	0	-16.045569	0.354772	-1.914070
163	6	0	-15.627222	2.073594	-3.574896
164	6	0	14.497782	1.536983	0.572834
165	1	0	14.078297	3.536771	1.077939
166	1	0	13.702432	5.389826	-0.665730
167	1	0	15.043567	4.592609	-1.501437
168	1	0	13.516908	4.890015	-2.344526
169	6	0	-16.585963	-0.465877	-2.908765
170	1	0	-16.010203	-0.007976	-0.879347
171	6	0	-16.170235	1.252919	-4.564868
172	1	0	-15.254221	3.073575	-3.818791
173	8	0	14.446919	0.691826	-0.315052
174	6	0	15.059373	1.271094	1.934329
175	6	0	-16.648420	-0.019327	-4.232077
176	1	0	-16.956717	-1.456464	-2.647046
177	1	0	-16.223058	1.604907	-5.593290
178	6	0	14.315527	1.550298	3.088616
179	6	0	16.334147	0.697942	2.032979
180	1	0	-17.070924	-0.660133	-5.004115
181	6	0	14.858208	1.268377	4.344859
182	1	0	13.313092	1.970780	3.010499
183	6	0	16.872744	0.422317	3.293232
184	1	0	16.897360	0.459582	1.127990
185	6	0	16.137148	0.709186	4.447413
186	1	0	14.283374	1.481394	5.245322
187	1	0	17.864325	-0.023323	3.371967
188	1	0	16.558528	0.493455	5.429204
189	1	0	0.519994	2.651726	-2.529874
190	1	0	-1.195500	2.437183	2.148203
191	1	0	1.062573	-1.404402	-2.102542
192	1	0	-0.398331	-2.671974	2.493094
193	1	0	3.020918	3.875976	0.627794
194	6	0	2.872602	1.312550	-1.653700
195	7	0	3.152435	0.500035	-2.427979
196	1	0	-3.793087	1.162788	-0.661800
197	6	0	-3.440179	4.107734	1.074050
198	7	0	-3.656228	5.077447	1.665778
199	1	0	-3.113866	-3.321717	-0.252767
200	6	0	-2.685946	-0.653987	1.874639

201	7	0	-2.866794	0.219981	2.610452
202	1	0	3.865969	-1.074340	0.899800
203	6	0	3.290019	-3.232525	-1.710137
204	7	0	3.436760	-3.953285	-2.602229
