Supporting Information

Merging Dynamic and Static Chirality in Propeller-Shaped Carbazole Oligomers via Chiral Amine Substitution

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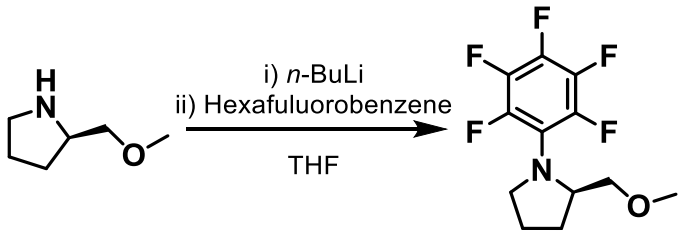
General Information.

All reagents and solvents were of commercial reagent grade and used without further purification unless otherwise specified. Unless noted otherwise, all reactions were performed in dry solvents under a nitrogen atmosphere in dried glassware using standard vacuum-line techniques. Work-up and purification procedures were carried out in air with reagent-grade solvents. TLC analyses were conducted on commercial neutral aluminum oxide plates (Aluminum oxide 60 F254, Merck), and chromatogram were visualized under UV illumination at 254 and 365 nm. Alumina column chromatography was performed on activated alumina (approximately 200 mesh) purchased from FUJIFILM Wako Pure Chemical Corporation.

^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded on a JEOL AL-400 spectrometers (at 400, 100, and 376 MHz, respectively) or a BRUKER AV500 instruments (at 500, 125, and 470 MHz, respectively). Melting points were measured on a Büchi M-565 melting point apparatus and are uncorrected. Mass spectra were recorded on a Shimadzu GCMS QP-2010 (EI, 70 eV) or a JEOL JMS-700 instrument (FAB in 3-nitrobenzyl alcohol). LDI-TOF mass spectra were recorded on a Bruker neofleX or a JEOL JMS-S3000 at the Ehime Institute of Industrial Technology. IR spectra were obtained using a Thermo Scientific Nicolet iS5 FT-IR spectrometer equipped with an iD5 ATR diamond plate. UV-Vis absorption and CD spectra were recorded on JASCO V-770 and JASCO J-820 spectrophotometers, respectively. CPL measurements were performed with a JASCO CPL-200 at N-BARD in Hiroshima University. Elemental analyses were performed with a Yanaco MT-5 elemental analyzer at the Advanced Research Support Center in Ehime University.

Synthetic procedures and characterization data

(*R*)-**4**



(*R*)-**3** (*R*)-**4**

(*R*)-2-(Methoxymethyl)pyrrolidine (0.53 mL, 4.32 mmol) and THF (20 mL) were added to a 100 mL three-necked reaction flask, and the resulting solution was cooled to -70 ºC. After cooling, 1.6 M *n*-BuLi (3.10 mL, 4.96 mmol) was added dropwise, and the reaction was stirred for 20 min. Separately, a solution of hexafluorobenzene (2.20 mL, 19.0 mmol) in THF (10 mL) was prepared in a 20 mL pear-shaped flask. This solution was added dropwise to the reaction mixture at -70 ºC and the resulting mixture was stirred for 4 h. The reaction was quenched with water and extracted with EtOAc. The organic layer was washed with water and saturated brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure to afford (*R*)-**4** as a colorless liquid (872 mg, 3.10 mmol, 72%).

^{1}H NMR ($CDCl_3$): δ 4.00 (m, 1H), 3.52 (m, 1H), 3.33–3.14 (m, 3H), 3.24 (s, 3H), 2.14 (m, 1H), 2.02–1.83 (m, 2H), 1.77 (m, 1H).

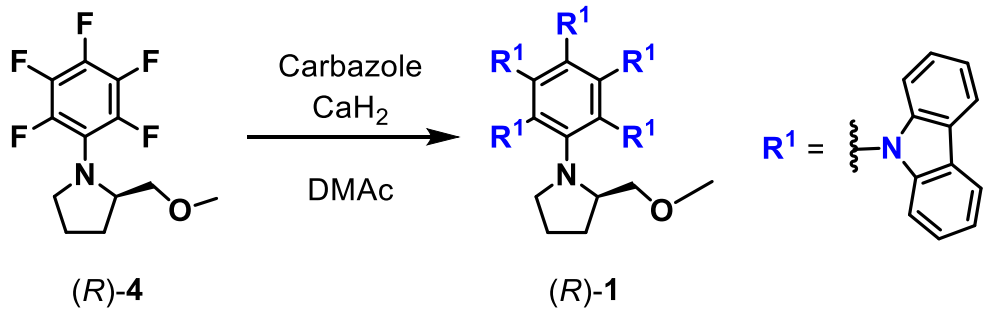
^{13}C NMR ($CDCl_3$): δ 142.93, 138.12, 135.01, 123.67, 75.42, 59.96, 59.08, 52.65, 29.02, 24.84.

^{19}F NMR ($CDCl_3$): δ -152.74 (m, 2F), -166.85 (m, 2F), -168.75 (m, 1F).

MS (EI): *m*/*z* 236.1 $[M–45\ (C_2H_5O)]^+$.

$[\alpha]_D^{20} = –0.17$ (*c* 0.10, CH_2Cl_2)

(*R*)-**1**



(*R*)-**4** (*R*)-**1**

Carbazole (1.610 g, 9.63 mmol) and CaH_2 (1.232 g, 29.3 mmol) were added to a 100 mL three-necked reaction flask. DMAc (60 mL) was then added, and the mixture was stirred at room temperature for 20 min. Separately, a DMAc solution (20 mL) of (*R*)-**4** (270 mg, 0.960 mmol) was prepared in a 50 mL pear-shaped flask and added to the reaction flask. The reaction was stirred at 160 °C for 19 h. After cooling to room temperature, the solvent was removed, and the crude product was purified by silica gel column chromatography (CH_2Cl_2/*n*-hexane) to afford (*R*)-**1** as a white solid (491 mg, 0.483 mmol, 50%).

^{1}H NMR ($C_2D_2Cl_4$, 80 °C): δ 7.85 (d, J = 7.7 Hz, 2H), 7.71 (m, 2H), 7.64–7.56 (m, 4H), 7.37–7.08 (m, 14H), 6.88 (d, J = 8.4 Hz, 2H), 6.84–6.53 (m, 16H), 3.39 (m, 1H), 3.00 (m, 1H), 2.94 (s, 3H), 2.85 (m, 1H), 2.26 (m, 1H), 1.63 (m, 1H), 1.12-0.79 (m, 3H), 0.58 (m, 1H).

^{13}C NMR ($C_2D_2Cl_4$, 80 °C): δ 148.64, 140.11, 139.86, 139.83, 139.16, 139.05, 138.03, 130.36, 125.58, 125.55, 124.62, 124.36, 124.11 124.00, 123.66, 123.61, 123.43, 123.40, 120.69, 120.65, 119.85, 119.69, 119.59, 119.51, 119.34, 119.27, 119.20, 119.12, 119.08, 112.09, 111.79, 111.76, 111.74, 111.20, 111.17, 110.91, 76.37, 58.23, 58.00, 53.44, 29.95, 24.93.

MS (FAB in 3-nitrobenzyl alcohol): *m*/*z* 1018 $[M+H]^+$, 972 $[M–45\ (C_2H_5O)]^+$.

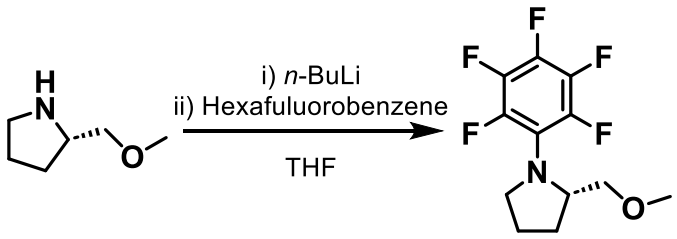
HR-MS (LDI-TOF): *m*/*z* 1016.4143, Calcd. for $C_{72}H_{52}N_6O$: 1016.4203 $[M]^+$; 971.3840, Calcd. for $C_{70}H_{47}N_6$: 971.3857 $[M–45\ (C_2H_5O)]^+$; 850.3529, Calcd. for $C_{60}H_{44}N_5O$: 850.3541 $[M–166\ (C_{12}H_8N)]^+$.

Anal. Calcd. for $C_{72}H_{52}N_6O$: C 85.01, H 5.15, N 8.26; Found: C 85.04, H 5.39, N, 8.30.

Mp: >300 ºC.

$[\alpha]_D^{20}$ = –0.86 (*c* 0.10, CH_2Cl_2)

(S)-**4**



(*S*)-**3** (*S*)-**4**

(*S*)-2-(Methoxymethyl)pyrrolidine (0.21 mL, 1.69 mmol) and THF (5 mL) were added to a 50 mL three-necked reaction flask, and the resulting solution was cooled to -70 ºC. After cooling, 1.6 M *n*-BuLi (1.16 mL, 1.86 mmol) was added dropwise, and the reaction was stirred for 20 min. Separately, a solution of hexafluorobenzene (0.78 mL, 6.76 mmol) in THF (7 mL) was prepared in a 20 mL pear-shaped flask. This solution was added dropwise to the reaction mixture at -70 ºC, and the resulting mixture was stirred for 4 h. The reaction was quenched with water and extracted with EtOAc. The organic layer was washed with water and saturated brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure to afford (*S*)-**4** as a colorless liquid (264 mg, 0.94 mmol, 56%).

^{1}H NMR ($CDCl_3$): δ 4.00 (m, 1H), 3.62 (m, 1H), 3.34–3.12 (m, 3H), 3.25 (s, 3H), 2.14 (m, 1H), 2.01–1.84 (m, 2H), 1.77 (m, 1H).

^{13}C NMR ($CDCl_3$): δ 142.91, 138.22, 135.74, 123.65, 75.40, 59.94, 59.08, 52.64, 29.02, 24.84.

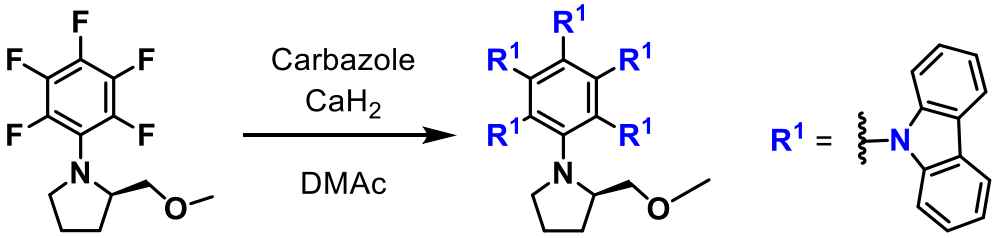
^{19}F NMR ($CDCl_3$): δ -152.74 (m, 2F), -166.85 (m, 2F), -168.74 (m, 1F).

MS (EI): *m*/*z* 236.1 $[M–45\ (C_2H_5O)]^+$.

Anal. Calcd. for $C_{12}H_{12}F_5NO$: C 51.25, H 4.30, N 4.98; Found: C 51.34, H 4.42, N 4.74.

$[\alpha]_D^{20}$ = +0.16 (*c* 0.10, CH_2Cl_2)

(*S*)-**1**



(*S*)-**4** (*S*)-**1**

Carbazole (1.193 g, 7.13 mmol) and CaH_2 (0.934 g, 22.2 mmol) were added to a 100 mL three-necked reaction flask. DMAc (60 mL) was then added, and the mixture was stirred at room temperature for 20 min. Separately, a DMAc solution (20 mL) of (*S*)-**4** (201 mg, 0.72 mmol) was prepared in a 50 mL pear-shaped flask and added to the reaction flask. The reaction was stirred at 160 °C for 19 h. After cooling to room temperature, the solvent was removed, and the crude product was purified by silica gel column chromatography (CH_2Cl_2/*n*-hexane) to afford (*S*)-**1** as a white solid (455 mg, 0.447 mmol, 63%).

^{1}H NMR ($C_2D_2Cl_4$, 80 °C): δ 7.86 (d, J = 7.7 Hz, 2H), 7.73 (d, J = 7.7 Hz, 2H), 7.64–7.57 (m, 4H), 7.36–7.12 (m, 14H), 6.90 (m, 2H), 6.80 (m, 2H), 6.78–6.57 (m, 14H), 3.39 (m, 1H), 3.00 (m, 1H), 2.96 (s, 3H), 2.85 (m, 1H), 2.31 (m, 1H), 1.65 (m, 1H), 1.09–0.85 (m, 3H), 0.60 (m, 1H).

^{13}C NMR ($C_2D_2Cl_4$, 80 °C): δ 148.70, 140.15, 139.89, 139.85, 139.21, 139.08, 138.08, 130.43, 125.52, 124.62, 124.34, 124.09, 124.04, 123.64, 123.46, 123.45, 123.43, 120.65, 120.63, 119.84, 119.68, 119.57, 119.49, 119.28, 119.15, 119.07, 119.04, 112.09, 111.78, 111.19, 110.93, 76.38, 58.19, 58.01, 53.38, 29.85, 24.87.

MS (FAB in 3-nitrobenzyl alcohol): *m*/*z* 1018 $[M+H]^+$, 972 $[M–45\ (C_2H_5O)]^+$.

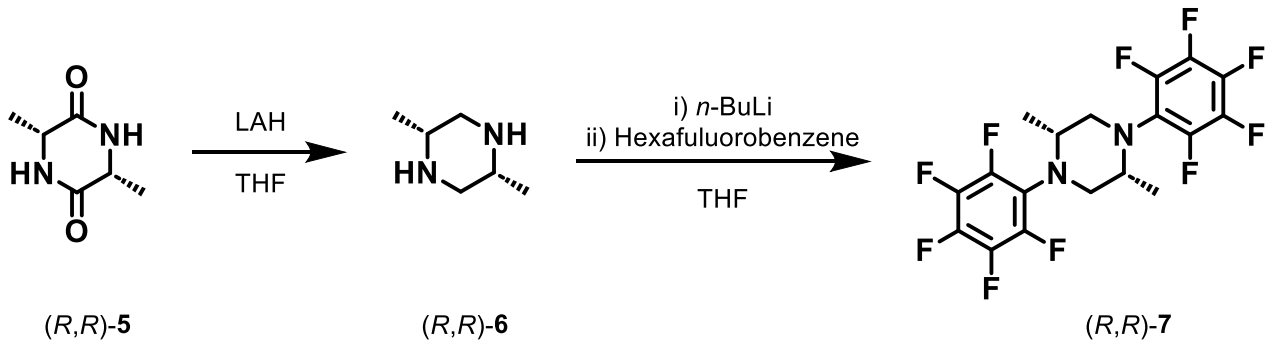
HR-MS (LDI-TOF): *m*/*z* 1016.4175, Calcd. for $C_{72}H_{52}N_6O$: 1016.4203 $[M]^+$; 971.3874, Calcd. for $C_{70}H_{47}N_6$: 971.3857 $[M–45\ (C_2H_5O)]^+$; 850.3560, Calcd. for $C_{60}H_{44}N_5O$: 850.3541 $[M–166\ (C_{12}H_8N)]^+$.

Anal. Calcd. for $C_{72}H_{52}N_6O$: C 85.01, H 5.15, N 8.26; Found: C 85.03, H 5.42, N 8.28.

Mp: >300 ºC.

$[\alpha]_D^{20}$ = +0.87 (*c* 0.10, CH_2Cl_2)

(*R*,*R*)-**7**



(*R*,*R*)-**5** (*R*,*R*)-**6** (*R*,*R*)-**7**

(*R*,*R*)-**6** was synthesized according to the literature procedure[1] To a solution of the diketopiperazine (*R*,*R*)-**5** (900 mg, 6.33 mmol) in THF (63 mL) was added $LiAlH_4$ (1.93 g, 50.6 mmol) over a period of 10 min with stirring at 0 °C. After the addition, the reaction mixture was refluxed overnight, then cooled to 0 °C, and carefully quenched by the addition of water. The mixture was filtered, and the solid residue was washed with dichloromethane. The combined filtrates were dried over Na_2SO_4, filtered through Celite, and concentrated under reduced pressure to give the piperazine (*R*,*R*)-**6** (573 mg, 5.78 mmol, 91%) as a colorless oil.

(*R*,*R*)-**6** (573 mg, 5.78 mmol) and THF (29 mL) were added to a 50 mL three-necked reaction flask, and the resulting solution was cooled to -70 ºC. After cooling, 2.6 M *n*-BuLi (4.25 mL, 11.05 mmol) was added dropwise, and the mixture was stirred for 30 min. Hexafluorobenzene (2.0 mL, 13.4 mmol) was then added to the reaction mixture at -70 ºC, and stirring was continued for 2 h. The reaction was quenched with water and extracted with EtOAc. The organic layer was washed with water and saturated brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure to afford (*R*,*R*)-**7** as a white solid **(**1.93 g, 4.34 mmol, 75%).

^{1}H NMR ($CDCl_3$): δ 3.46 (m, 2H), 3.28 (m, 2H), 3.15 (m, 2H), 1.14 (m, 6H).

^{13}C NMR ($CDCl_3$): δ 144.91, 137.99, 124.70, 55.12, 54.49, 15.15.

^{19}F NMR ($CDCl_3$): δ -152.74 (m, 2F), -166.85 (m, 2F), -168.74 (m, 1F).

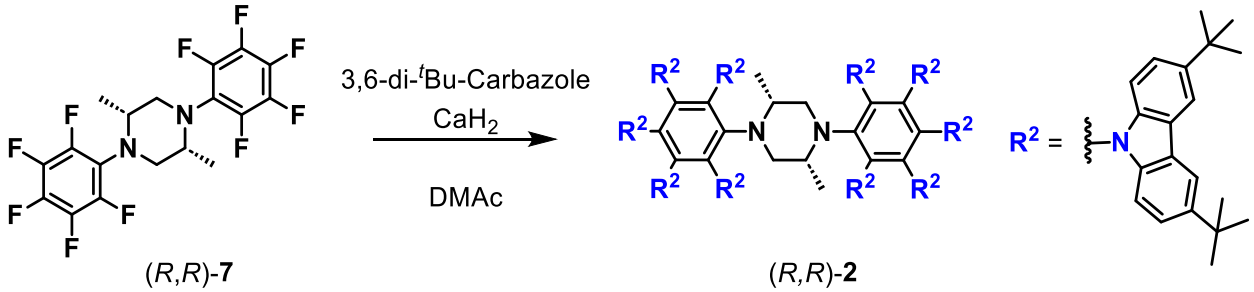
MS (FAB in 3-nitrobenzyl alcohol): *m*/*z* 446 $[M]^+$, 431 $[M–15\ (CH_3)]^+$.

Anal. Calcd. for $C_{18}H_{12}F_{10}N_2$: C 48.44, H 2.71, N 6.28; Found: C 48.30, H 2.82, N 6.17.

Mp: 104–107 °C.

$[\alpha]_D^{20}$ = +0.17 (*c* 0.10, CH_2Cl_2)

(*R*,*R*)-**2**



(*R*,*R*)-**7** (*R*,*R*)-**2**

(*R*,*R*)-**7** (100 mg, 0.22 mmol), CaH_2 (272 mg, 6.48 mmol) and 3,6-di-*t*Bu-Carbazole (936 mg, 3.36 mmol) were added to a 20 mL pressure bottle. Dry DMAc (6.7 mL) was added by a syringe and the mixture was heated 70 ºC with stirring for 1 h. Then, the mixture was heated at 175 ºC with stirring overnight. After cooling to room temperature, the reaction was stopped by pouring into ice/water. The precipitated solid was collected by filtration washed repeatedly with water and MeOH. The residue was purified by silica gel column chromatography ($CHCl_3$/*n*-hexane = 3/1) to afford (*R*,*R*)-**2** as a white solid (470.8 mg, 0.15 mmol, 70%).

^{1}H NMR ($CDCl_3$): δ 7.37 (m, 4H), 7.22–6.77 (m, 32H), 6.77–6.49 (m, 12H), 6.29–5.96 (m, 12H), 3.39 (m, 2H), 2.93 (m, 2H), 2.53 (m, 2H), 1.53 (s, 18H), 1.23–1.07 (m, 128H), 1.01–0.86 (m, 36H), 0.82 (m, 6H).

^{13}C NMR ($CDCl_3$, typical signals): δ 150.26, 144.22, 141.30, 141.21, 141.02, 140.40, 138.31, 137.07, 134.99, 123.61, 123.02, 122.89, 122.80, 122.54, 121.16, 120.47, 114.96, 114.33, 114.04, 113.75, 111.44, 110.09, 58.43, 52.30, 34.64, 34.15 34.03, 34.01, 33.94, 32.45, 31.86, 31.80, 31.62, 31.52, 18.17.

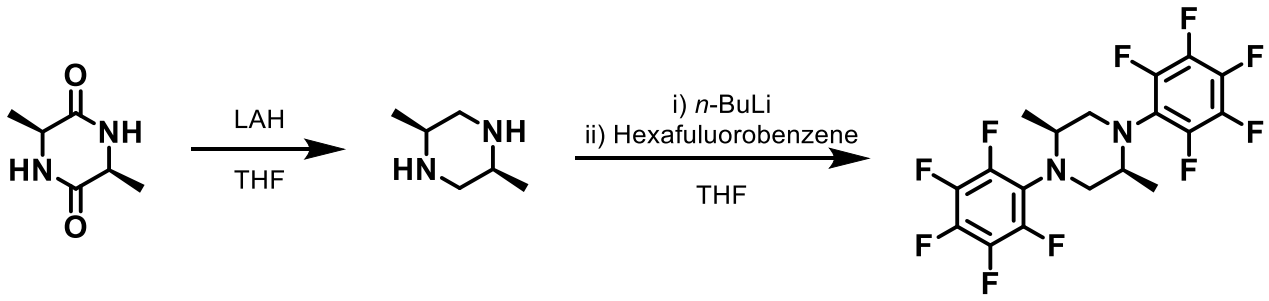
HR-MS (LDI-TOF): *m*/*z* 2761.8432, Calcd. for $C_{198}H_{228}N_{11}$: 2761.8329 [M–279 ($C_{20}H_{24}N$)]$^+$.

Anal. Calcd. for $C_{218}H_{252}N_{12}$: C 86.12, H 8.35, N 5.53; Found: C 85.84, H 8.49, N 5.53.

Mp: >300 ºC.

$[\alpha]_D^{20}$ = +0.41 (*c* 0.10, CH_2Cl_2)

(*S*,*S*)-**7**



(*S*,*S*)-**5** (*S*,*S*)-**6** (*S*,*S*)-**7**

(*S*,*S*)-**6** was synthesized according to the literature procedure.[1] To a solution of the diketopiperazine (*S*,*S*)-**5** (612 mg, 4.31 mmol) in THF (45 mL) was added $LiAlH_4$ (1.31 g, 34.5 mmol) over a period of 10 min with stirring at 0 °C. After the addition, the reaction mixture was refluxed overnight, then cooled to 0 °C, and carefully quenched by the addition of water. The mixture was filtered, and the solid residue was washed with dichloromethane. The combined filtrates were dried over Na_2SO_4, filtered through Celite, and concentrated under reduced pressure to give the piperazine (*S*,*S*)-**6** (440.4 mg, 3.86 mmol, 89%) as a colorless oil.

(*S*,*S*)-**6** (512.9 mg, 4.46 mmol) and THF (22 mL) were added to a 50 mL three-necked reaction flask, and the resulting solution was cooled to -70 ºC. After cooling, 1.6 M *n*-BuLi (6.2 mL, 9.92 mmol) was added dropwise, and the mixture was stirred for 30 min. Hexafluorobenzene (1.55 mL, 13.4 mmol) was then added to the reaction mixture at -70 ºC, and stirring was continued for 2 h. The reaction was quenched with water and extracted with EtOAc. The organic layer was washed with water and saturated brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure to afford (*S*,*S*)-**7** as a white solid **(**1.58 g, 3.53 mmol, 79%).

^{1}H NMR ($CDCl_3$): δ 3.46 (m, 2H), 3.28 (m, 2H), 3.15 (m, 2H), 1.14 (m, 6H).

^{13}C NMR ($CDCl_3$): δ 144.91, 138.02, 124.67, 55.09, 54.46, 15.15.

^{19}F NMR ($CDCl_3$): δ -152.74 (m, 2F), -166.85 (m, 2F), -168.74 (m, 1F).

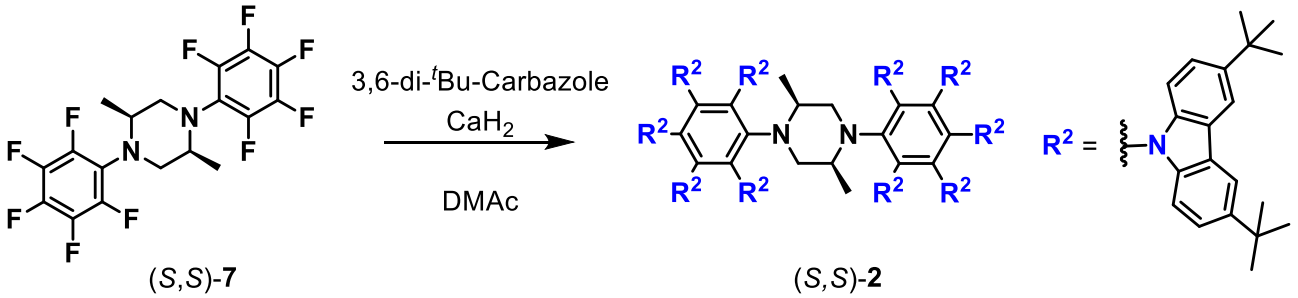
MS (FAB in 3-nitrobenzyl alcohol): *m*/*z* 446 $[M]^+$, 431 $[M–15\ (CH_3)]^+$.

Anal. Calcd. for $C_{18}H_{12}F_{10}N_2$: C 48.44, H 2.71, N 6.28; Found: C 48.35, H 2.72, N 6.28.

Mp: 104–107 °C.

$[\alpha]_D^{20}$ = –0.18 (*c* 0.10, CH_2Cl_2)

(*S*,*S*)-**2**



(*S*,*S*)-**7** (21.2 mg, 0.048 mmol), CaH_2 (56.5 mg, 1.35 mmol) and 3,6-di-*t*Bu-Carbazole (195.4 mg, 0.67 mmol) were added to a 20 mL pressure bottle. Dry DMAc (1.3 mL) was added by a syringe and the mixture was heated 70 ºC with stirring for 1 h. Then, the mixture was heated at 175 ºC with stirring overnight. After cooling to room temperature, the reaction was stopped by pouring into ice/water. The precipitated solid was collected by filtration washed repeatedly with water and MeOH. The residue was purified by silica gel column chromatography ($CHCl_3$/*n*-hexane = 3/1) to afford (*S*,*S*)-**2** as a white solid (98.3 mg, 0.15 mmol, 68%).

^{1}H NMR ($CDCl_3$): δ 7.37 (m, 4H), 7.22–6.77 (m, 32H), 6.77–6.49 (m, 12H), 6.27–6.06 (m, 12H), 3.38 (m, 2H), 2.93 (m, 2H), 2.53 (m, 2H), 1.53 (s, 18H), 1.23-1.07 (m, 128H), 1.01-0.86 (m, 36H), 0.81 (m, 6H).

^{13}C NMR ($CDCl_3$, typical signals): δ 150.26, 144.22, 141.31, 141.20, 141.02, 140.40, 138.31, 137.06, 134.99, 123.02, 122.89, 122.80, 122.51, 121.17, 120.46, 114.97, 114.33, 114.05, 113.76, 111.43, 110.08, 58.43, 52.29, 34.64, 34.15 34.03, 34.01, 33.95, 32.45, 31.86, 31.80, 31.63, 31.52, 18.17.

HR-MS (LDI-TOF): *m*/*z* 2761.8372, Calcd. for $C_{198}H_{228}N_{11}$: 2761.8329 [M–279 ($C_{20}H_{24}N$)]$^+$.

Anal. Calcd. for $C_{218}H_{252}N_{12}$: C 86.12, H 8.35, N 5.53; Found: C 85.74, H 8.46, N 5.49.

Mp: >300 ºC.

$[\alpha]_D^{20}$ = –0.41 (*c* 0.10, CH_2Cl_2)

^{1}H, ^{19}F and ^{13}C NMR spectra

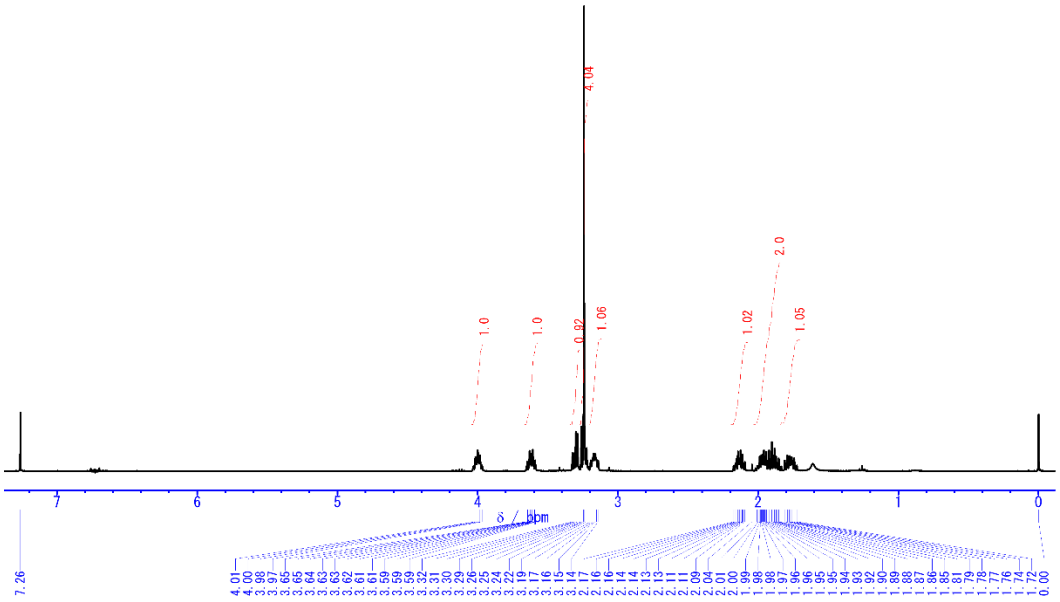


Figure S1a. ^{1}H-NMR spectrum of (*R*)-**4** in $CDCl_3$.

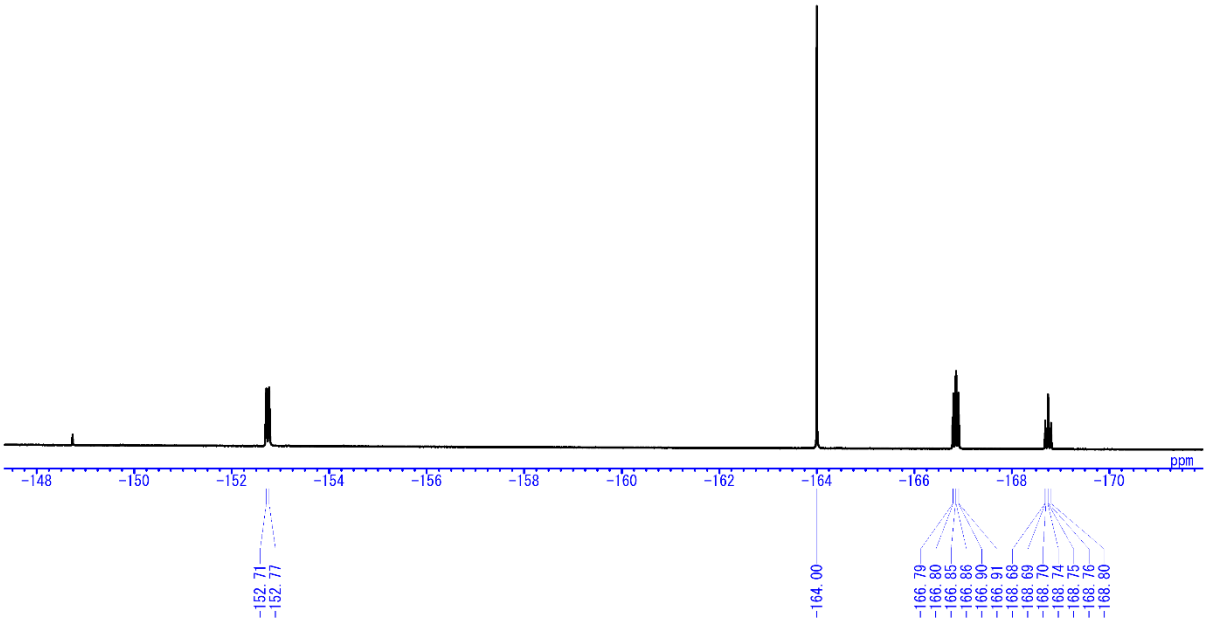


Figure S1b. ^{19}F-NMR spectrum of (*R*)-**4** in $CDCl_3$.

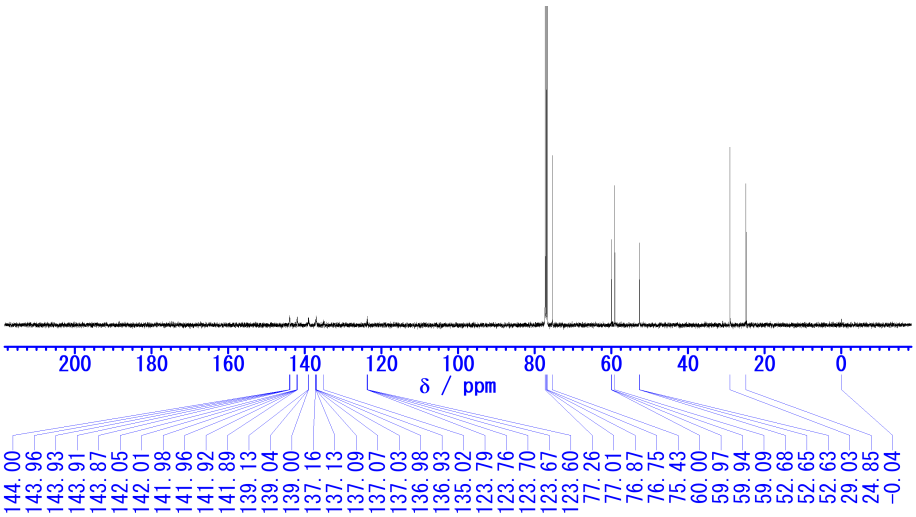


Figure S1c. ^{13}C-NMR spectrum of (*R*)-**4** in $CDCl_3$.

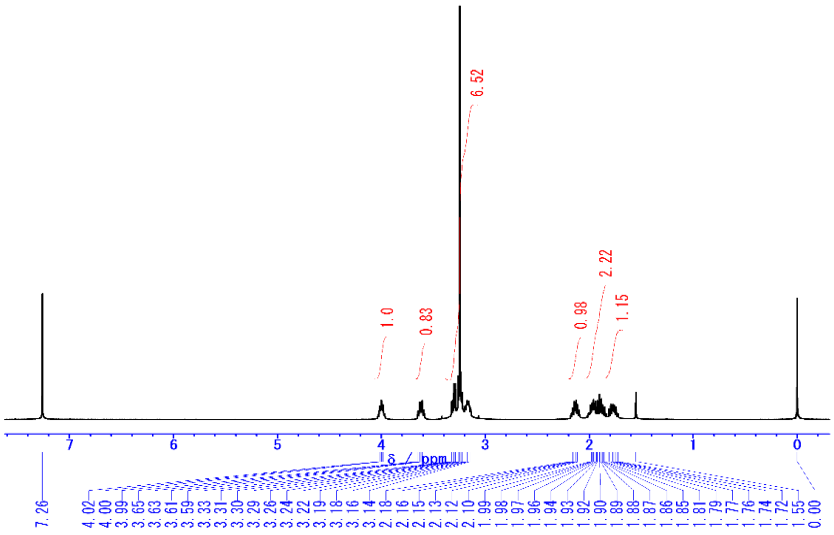


Figure S1d. ^{1}H-NMR spectrum of (*S*)-**4** in $CDCl_3$.

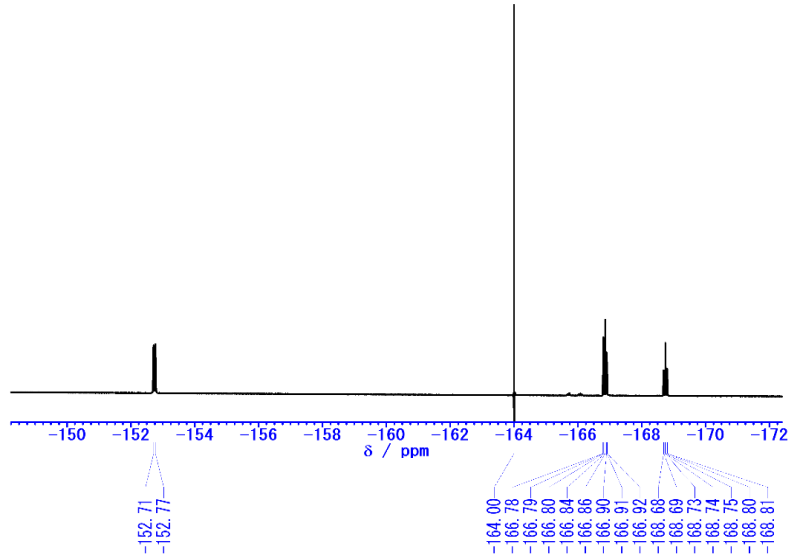


Figure S1e. ^{19}F-NMR spectrum of (*S*)-**4** in $CDCl_3$.

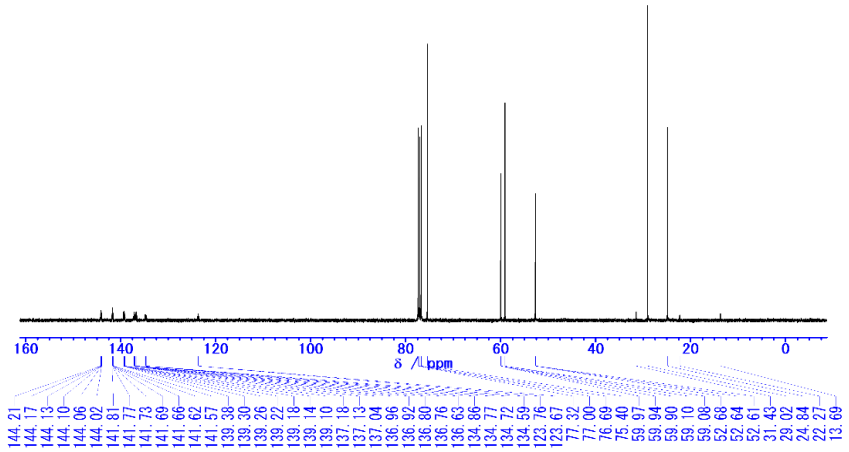


Figure S1f. ^{13}C-NMR spectrum of (*S*)-**4** in $CDCl_3$.

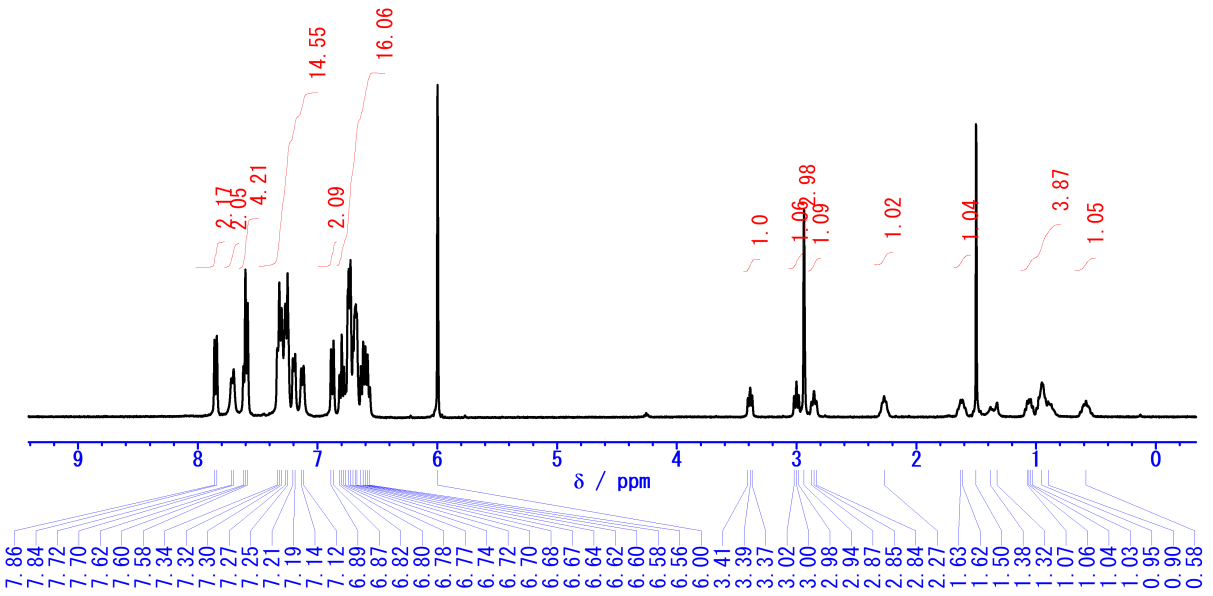


Figure S1g. ^{1}H-NMR spectrum of (*R*)-**1** at 80 °C in $C_2D_2Cl_4$.

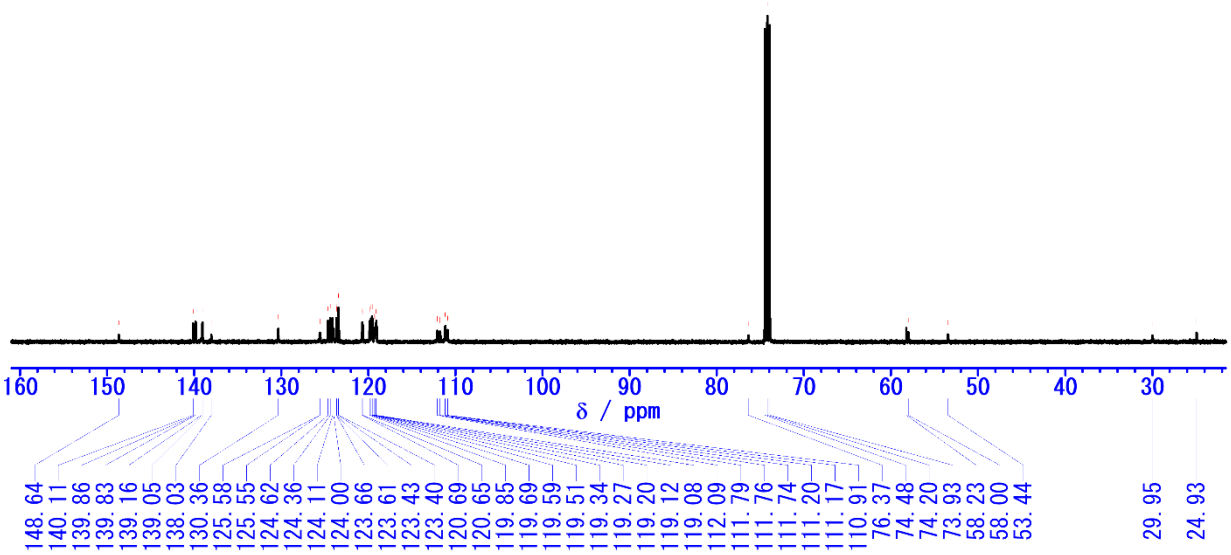


Figure S1h. ^{13}C-NMR spectrum of (*R*)-**1** at 80 °C in $C_2D_2Cl_4$.

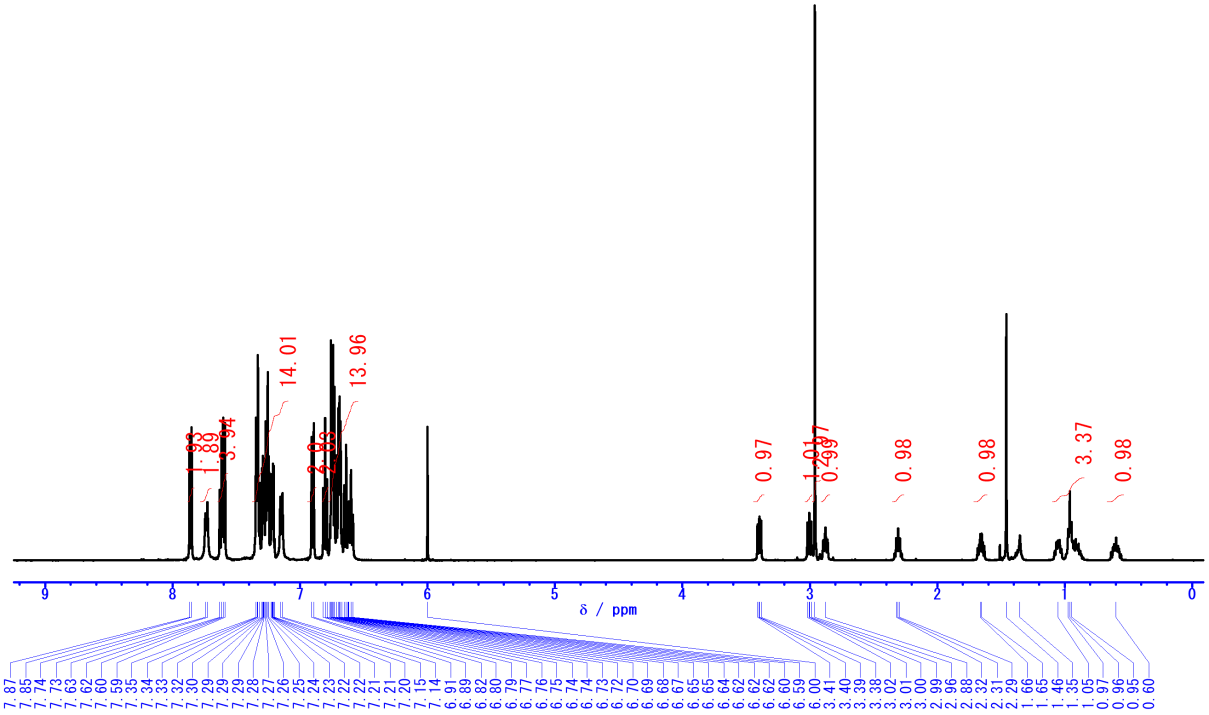


Figure S1i. ^{1}H-NMR spectrum of (*S*)-**1** at 80 °C in $C_2D_2Cl_4$.

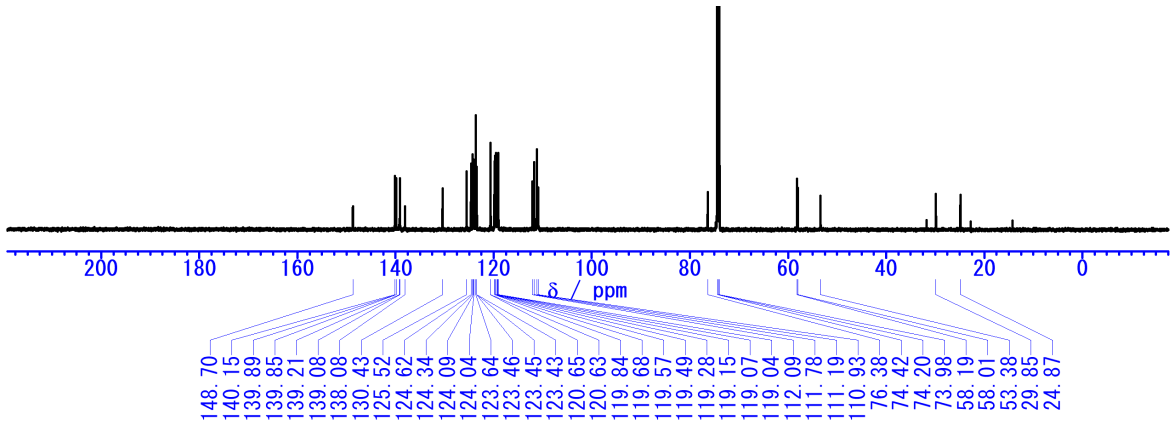


Figure S1j. ^{13}C-NMR spectrum of (*S*)-**1** at 80 °C in $C_2D_2Cl_4$.

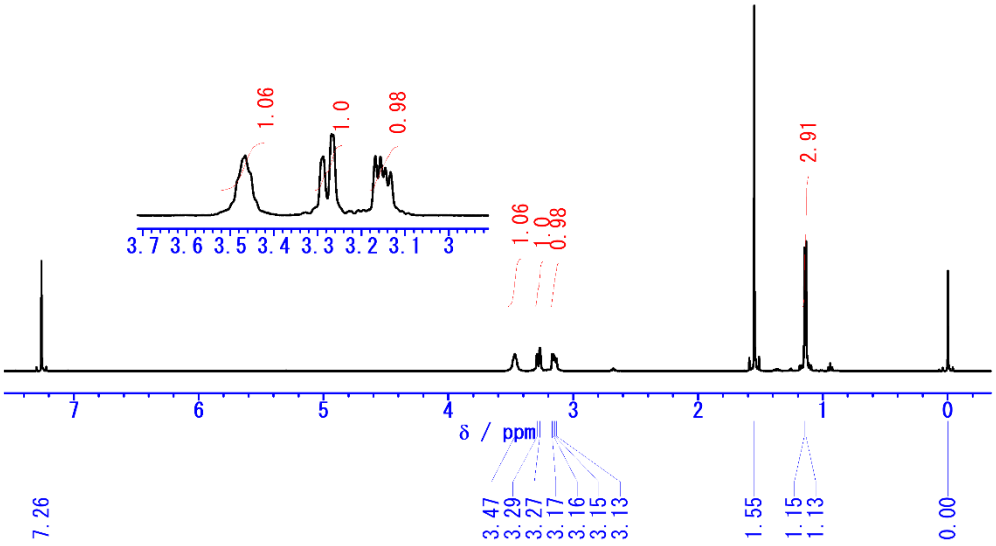


Figure S1k. ^{1}H-NMR spectrum of (*R*,*R*)-**7** in $CDCl_3$.

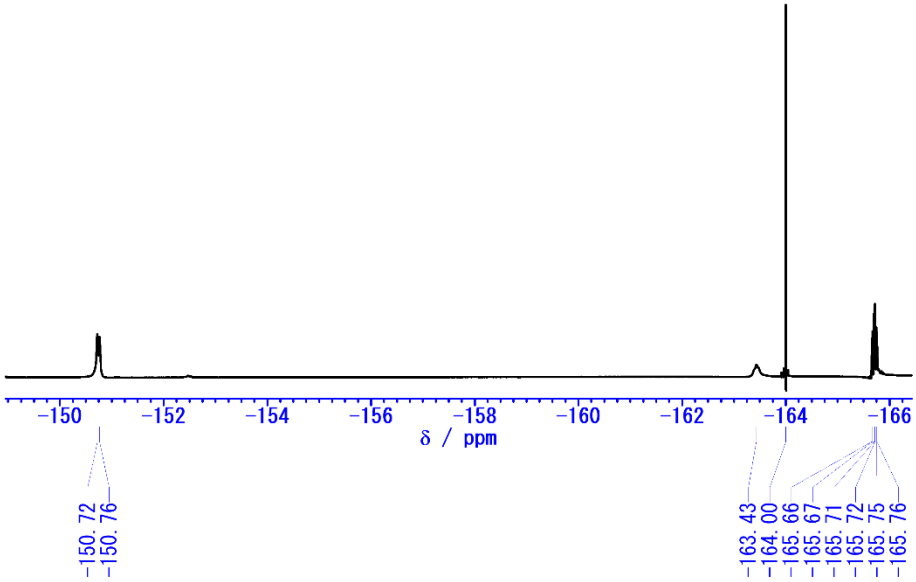


Figure S1l. ^{19}F-NMR spectrum of (*R*,*R*)-**7** in $CDCl_3$.

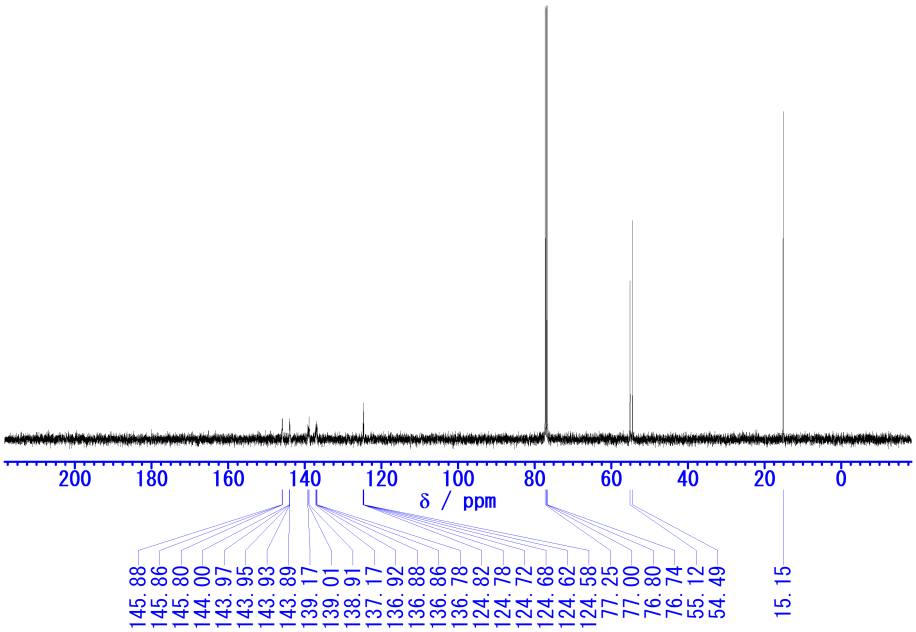


Figure S1m. ^{13}C-NMR spectrum of (*R*,*R*)-**7** in $CDCl_3$.

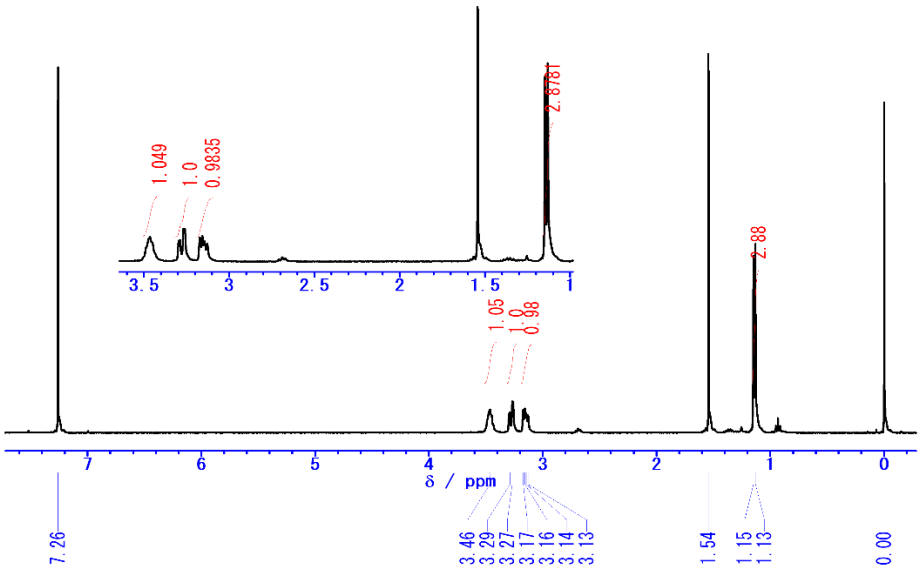


Figure S1n. ^{1}H-NMR spectrum of (*S*,*S*)-**7** in $CDCl_3$.

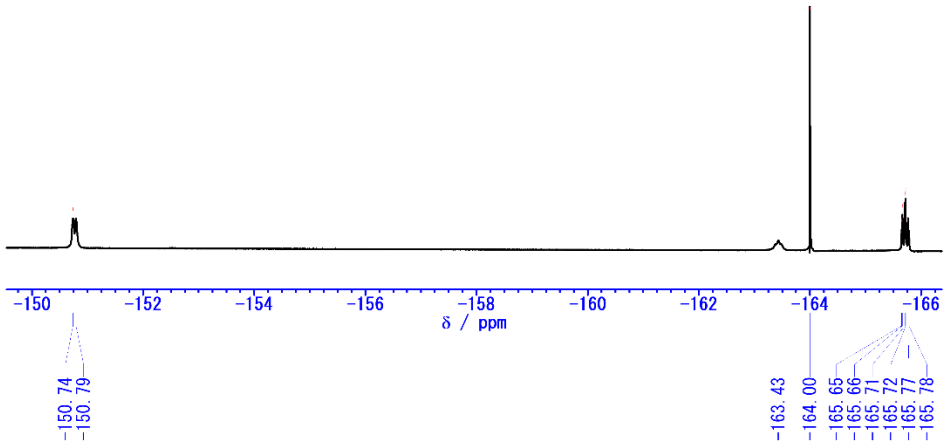


Figure S1o. ^{19}F-NMR spectrum of (*S*,*S*)-**7** in $CDCl_3$.

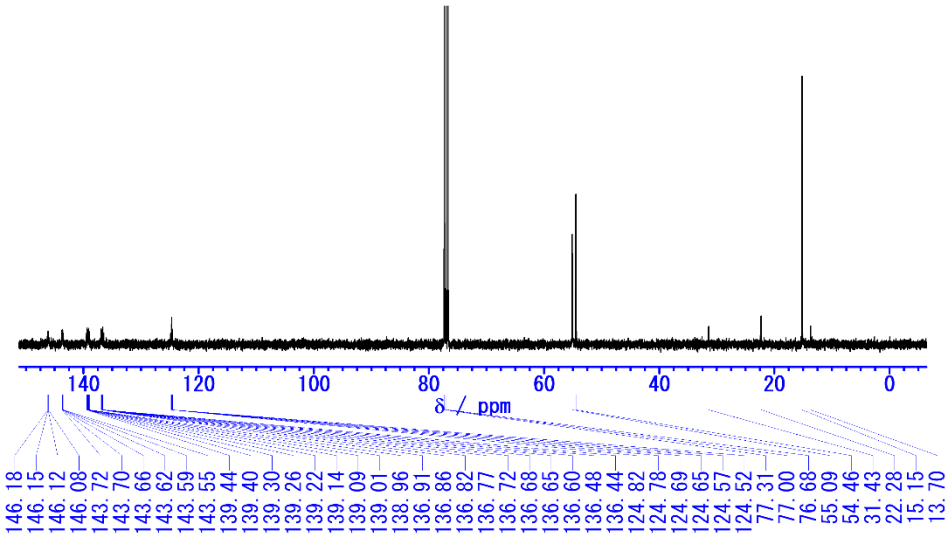


Figure S1p. ^{13}C-NMR spectrum of (*S*,*S*)-**7** in $CDCl_3$.

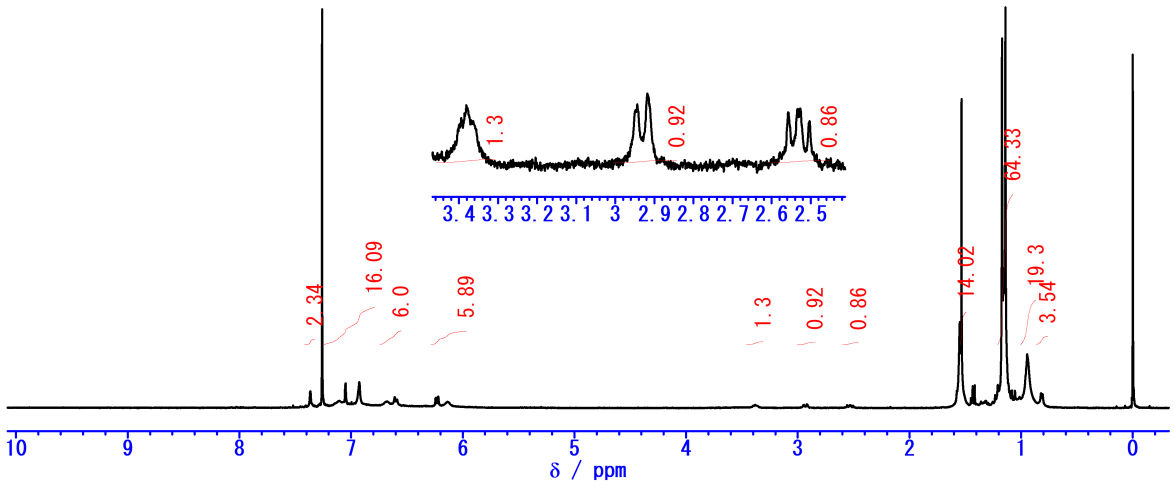


Figure S1q. ^{1}H-NMR spectrum of (*R,R*)-**2** in $CDCl_3$.

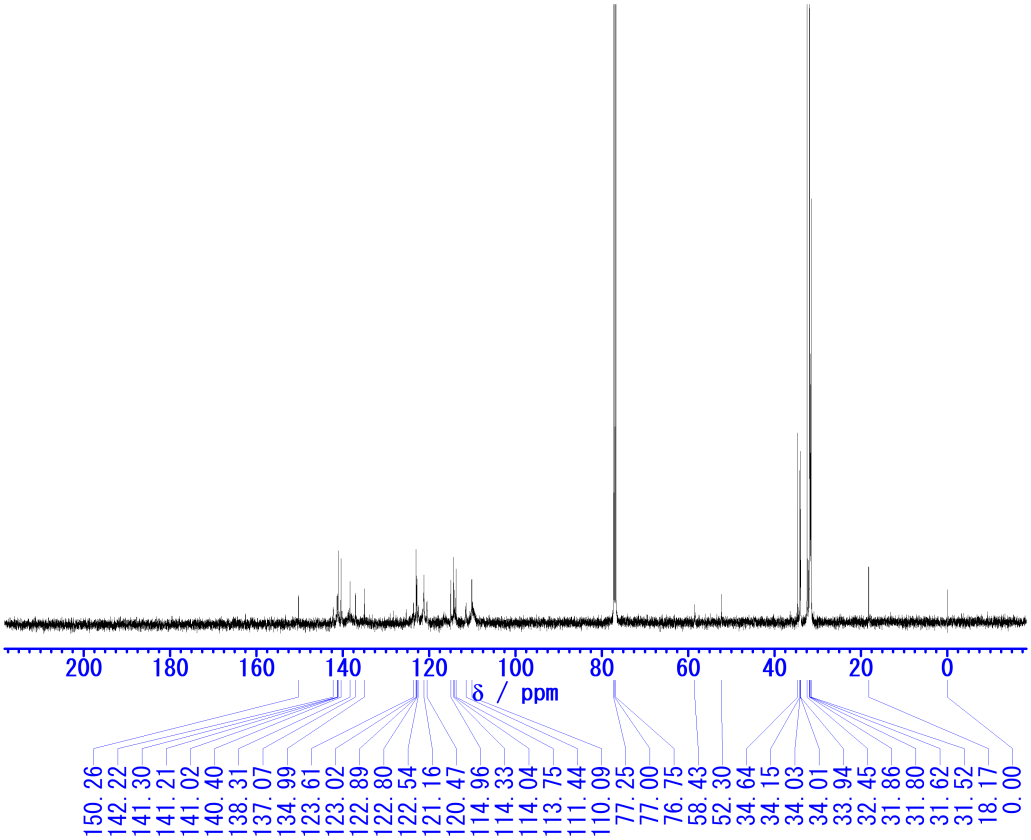


Figure S1r. ^{13}C-NMR spectrum of (*R,R*)-**2** in $CDCl_3$.

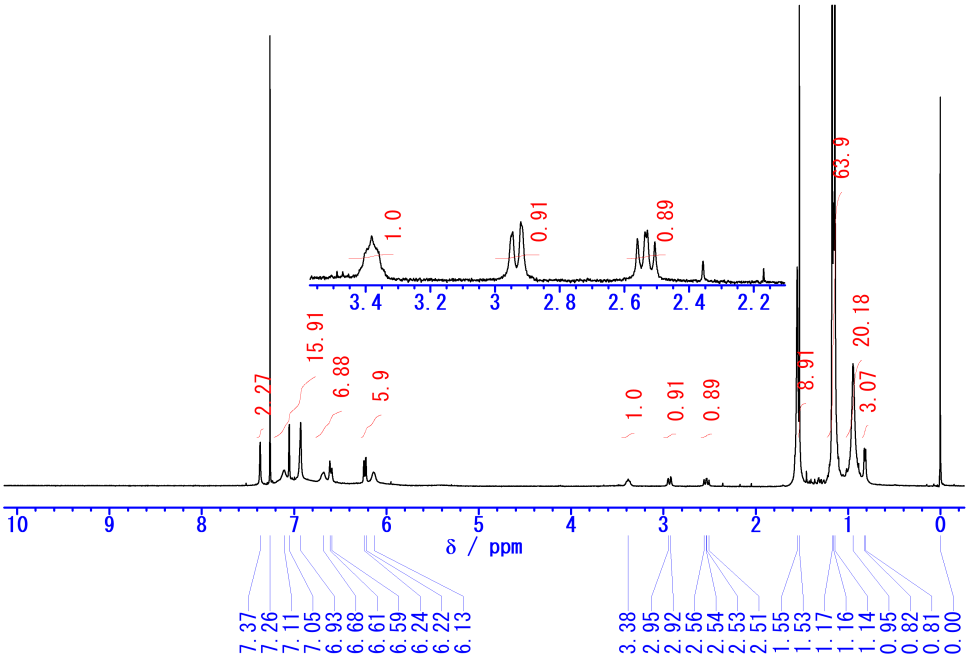


Figure S1s. ^{1}H-NMR spectrum of (*S*,*S*)-**2** in $CDCl_3$.

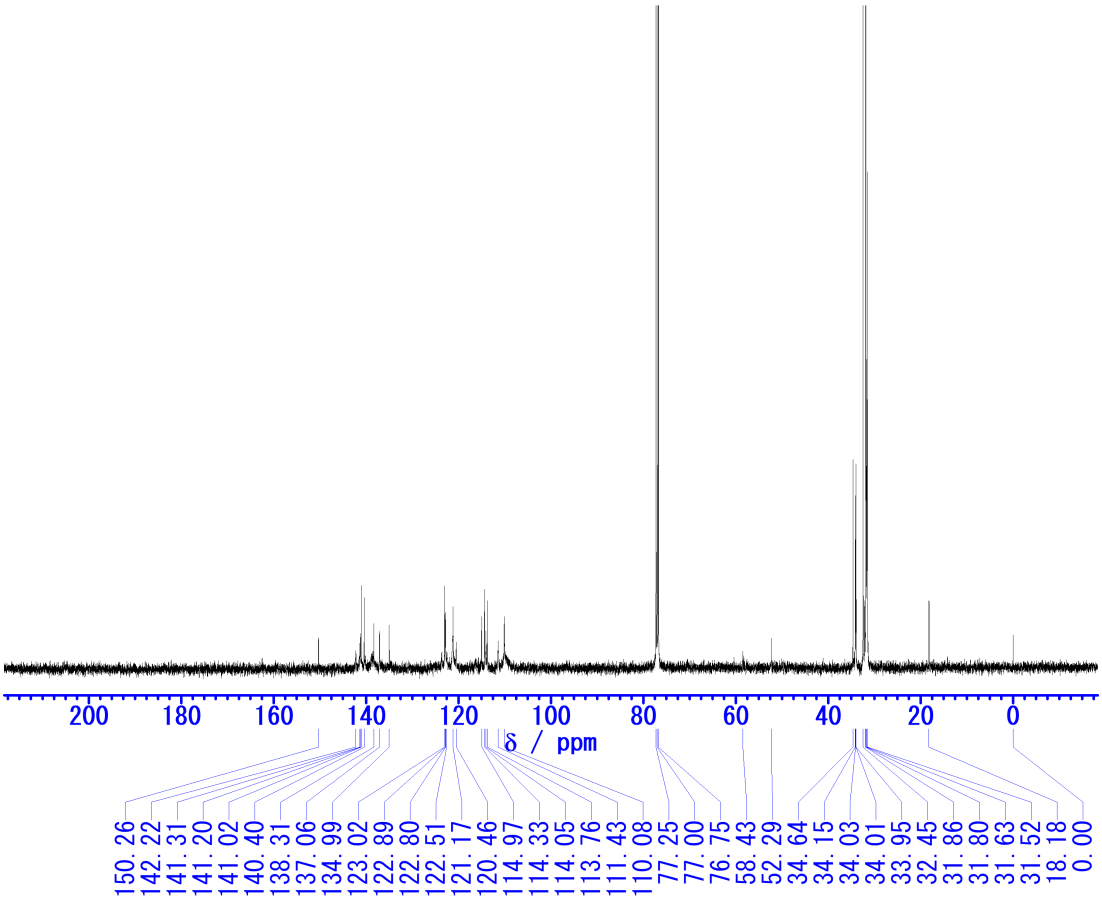


Figure S1t. ^{13}C-NMR spectrum of (*S*,*S*)-**2** in $CDCl_3$.

High–resolution mass spectra

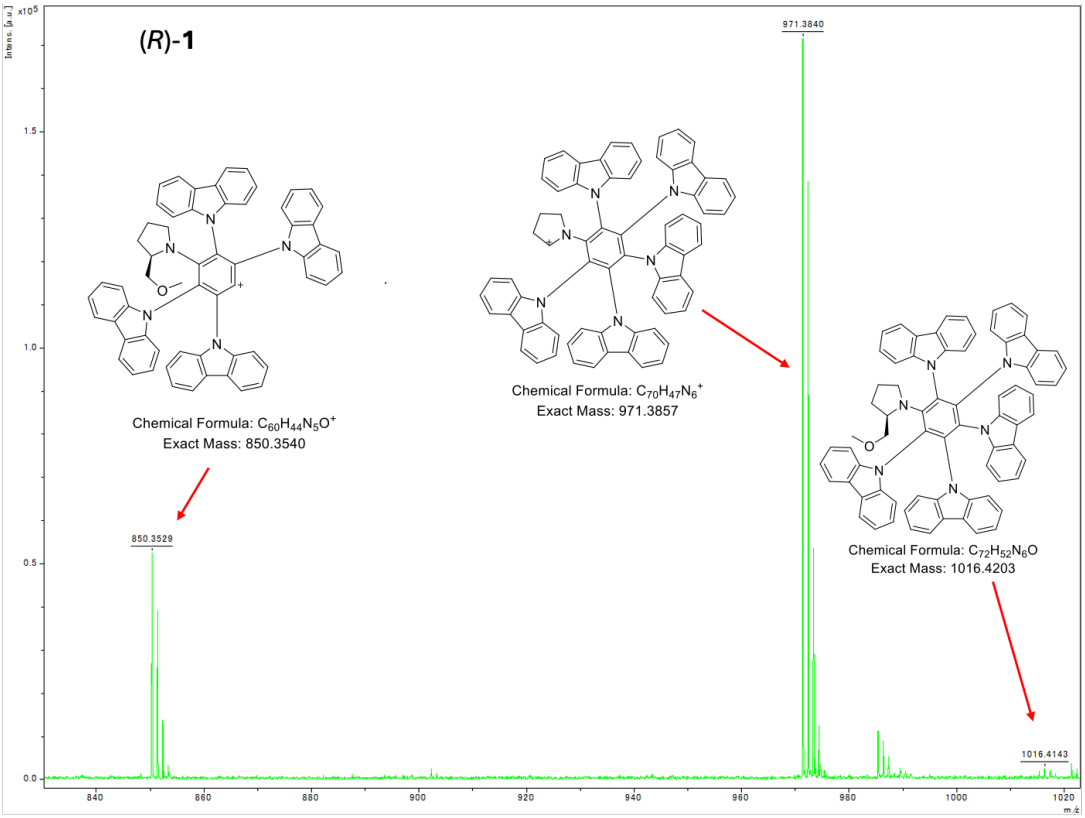


Figure S2a. High–resolution LDI-TOF mass spectrum of (*R*)-**1**.

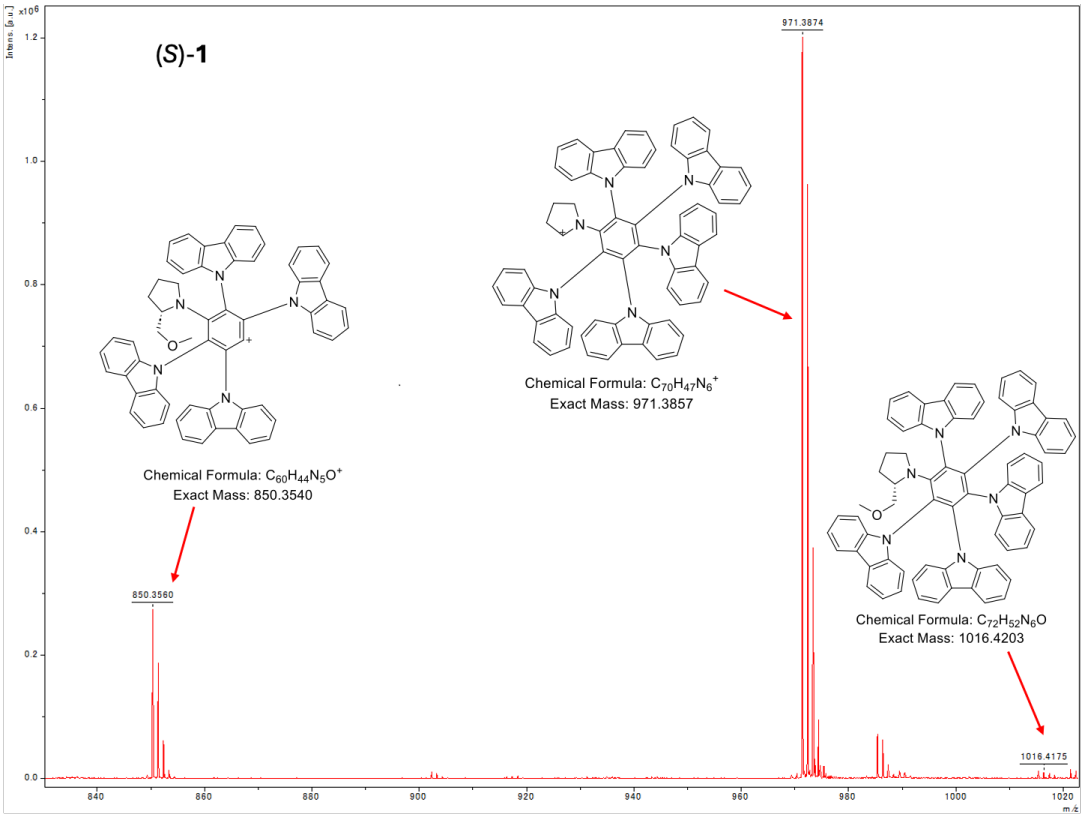


Figure S2b. High–resolution LDI-TOF mass spectrum of (*S*)-**1**.

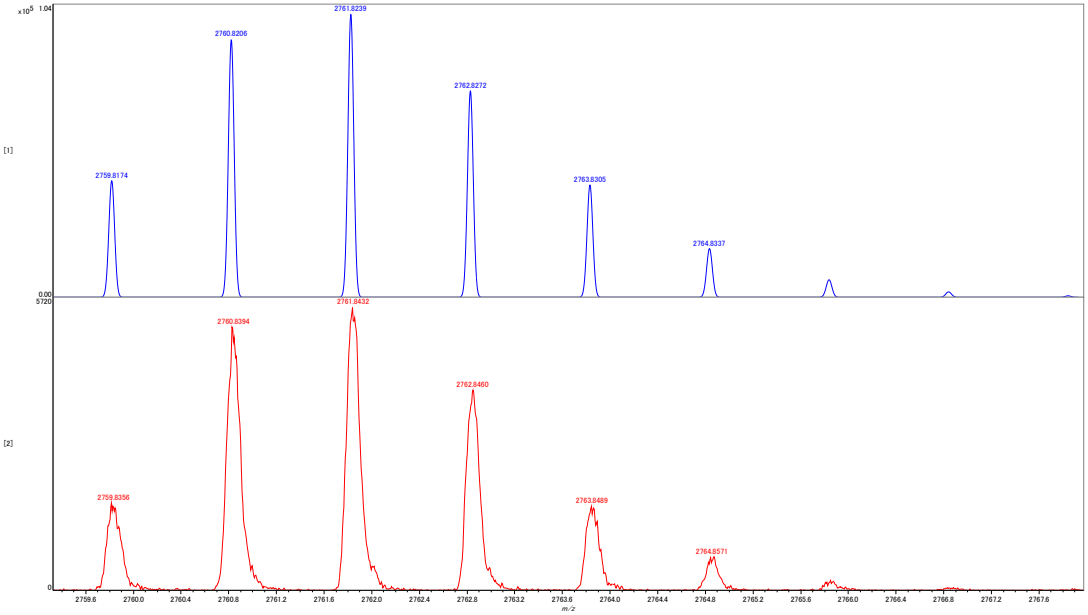


Figure S2c. High–resolution LDI-TOF mass spectrum of (*R,R*)-**2** assigned to the fragment [M–279 ($C_{20}H_{24}N$)]$^+$ (Top: simulated, Bottom: observed).

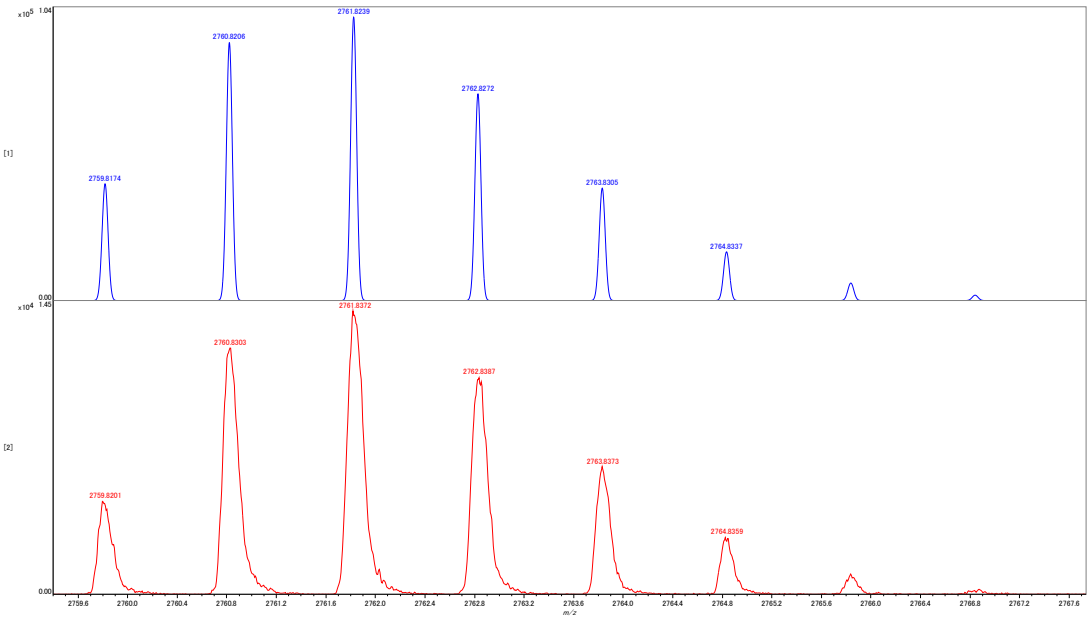


Figure S2d. High–resolution LDI-TOF mass spectrum of (*S,S*)-**2** assigned to the fragment [M–279 ($C_{20}H_{24}N$)]$^+$ (Top: simulated, Bottom: observed).

VT-NMR spectra

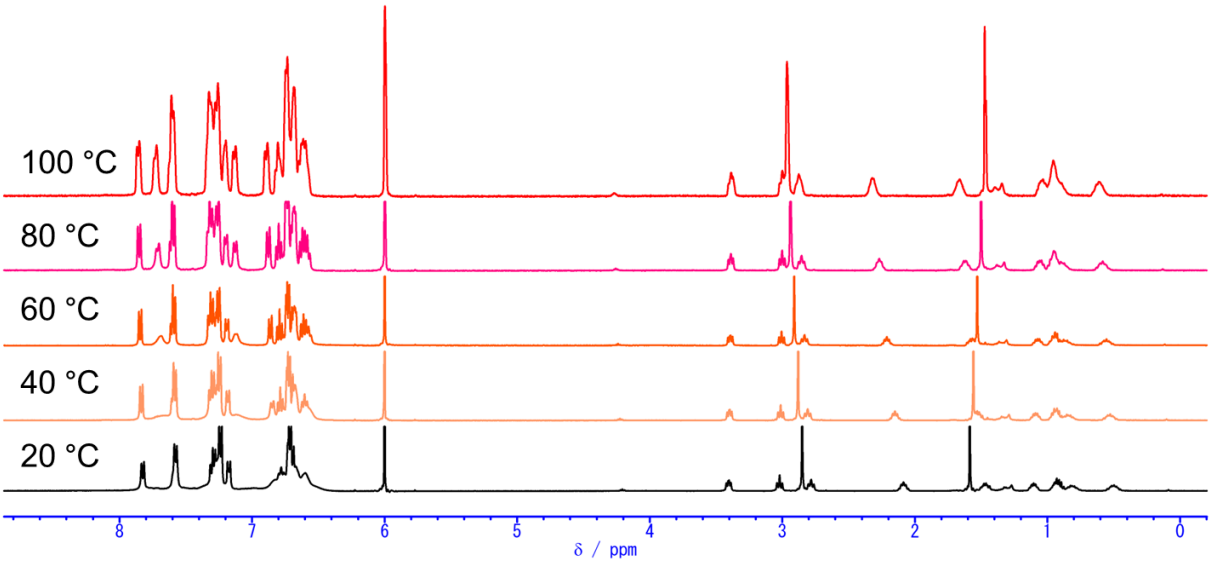


Figure S3a.VT-NMR spectra of (*R*)-**1** in $C_2D_2Cl_4$.

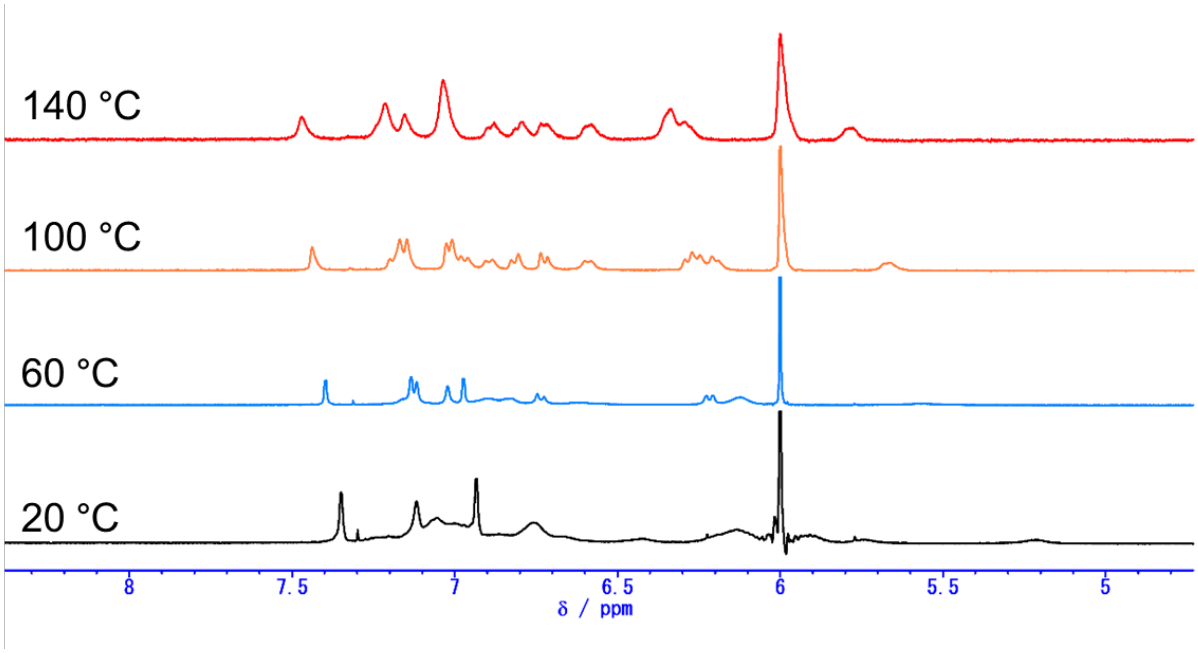


Figure S3b.VT-NMR spectra of (*R,R*)-**2** in $C_2D_2Cl_4$.

Optical Properties

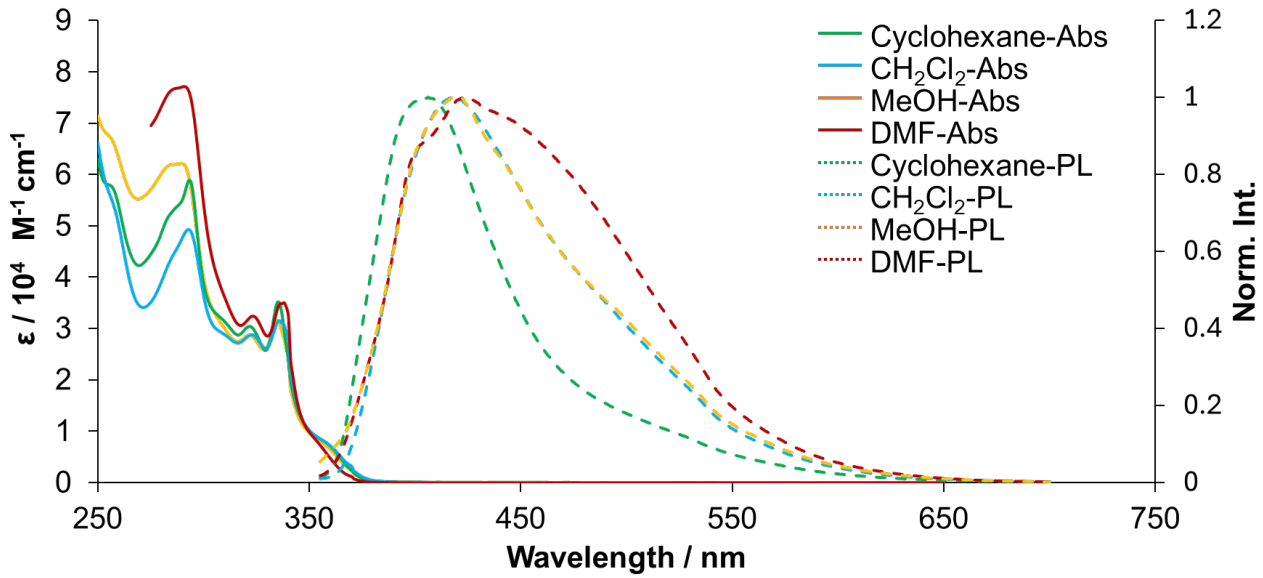


Figure S4a. Absorption and PL spectra of **1** in various solvents.

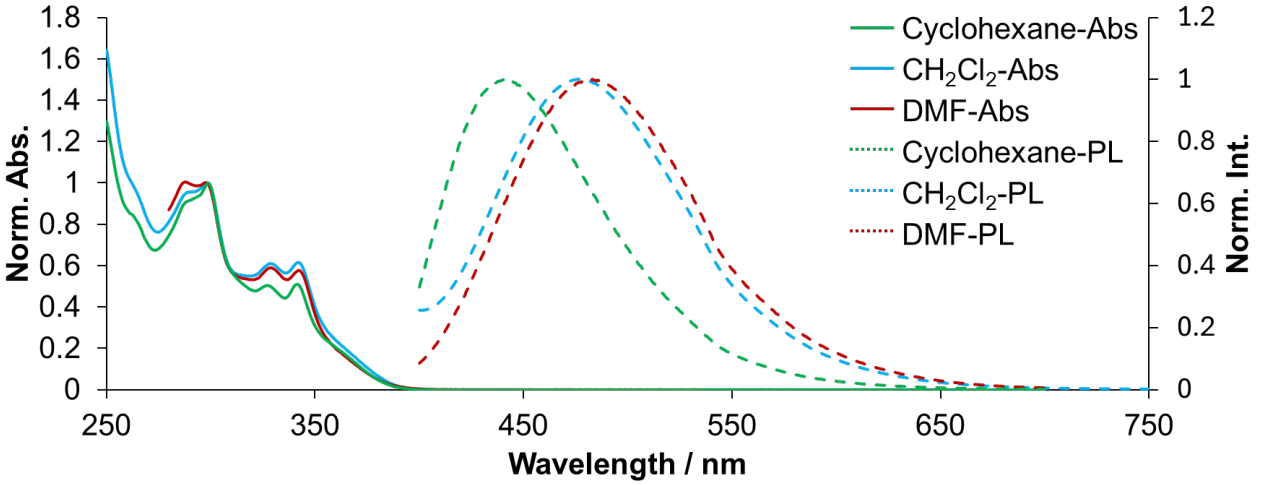


Figure S4b. Absorption and PL spectra of **2** in various solvents.

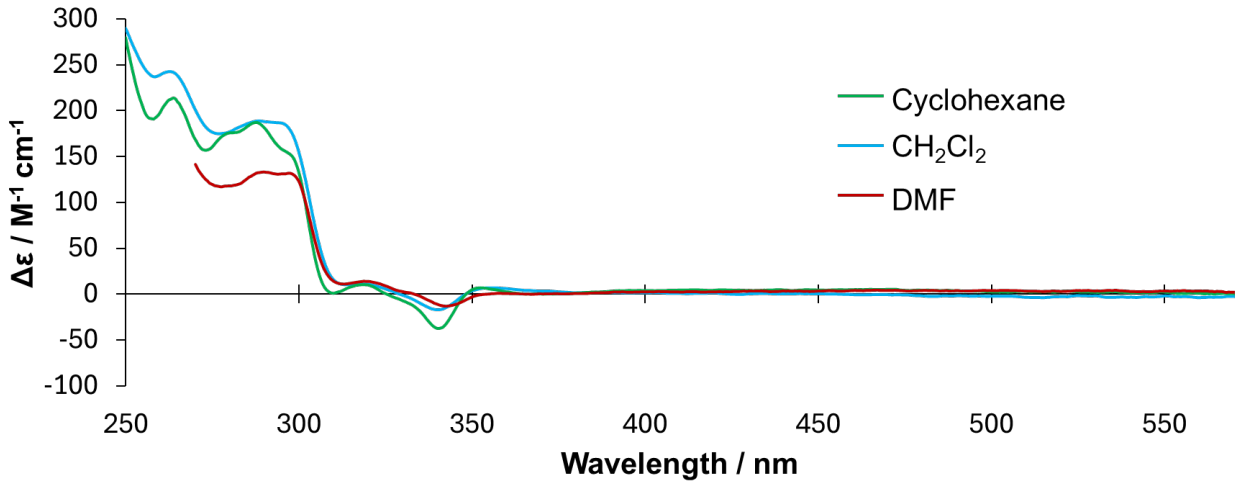


Figure S4c. CD spectra of (*R*,*R*)-**2** in various solvents.

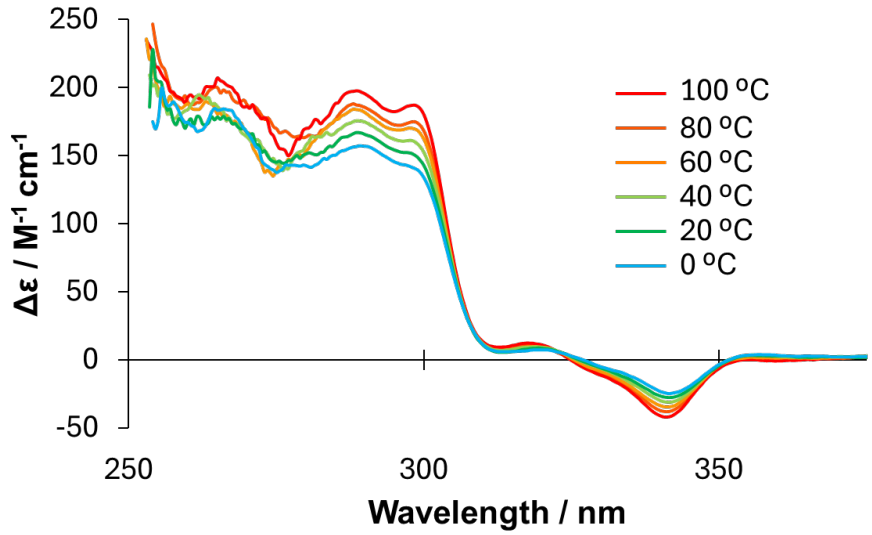


Figure S4d. VT-CD spectra of (*R*,*R*)-**2** in tetrachloroethane.

Table S1. (Chir)optical properties of (*R*)-**1** and (*R*,*R*)-**2** in DCM.

	$\varepsilon_{max}\times 10^4$ (λ / nm)	g_{abs} (λ_{abs} / nm)	PL / nm	Φ_F	g_{lum}	B_{CPL} / $M^{-1}cm^{-1}$
(*R*)-**1**	3.15, 2.87 (335, 323)	1.54×10^{-3} (355)	423	13	$+2.0\times10^{-3}$	4.1
(*R*,*R*)-**2**	5.77, 5.71 (343, 329)	2.55×10^{-4} (357)	476	8	$+1.0\times10^{-3}$	4.6

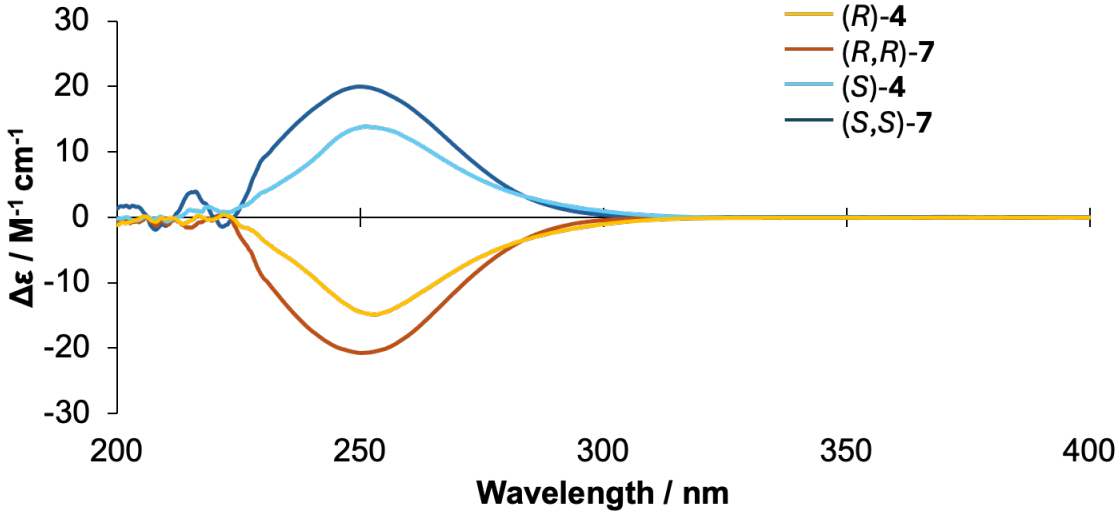


Figure S4e. CD spectra of (*R*)-**4**, (*R*,*R*)-**7**, (*S*)-**4**, and (*S*,*S*)-**7** in CH_2Cl_2.

DFT Calculations[2]

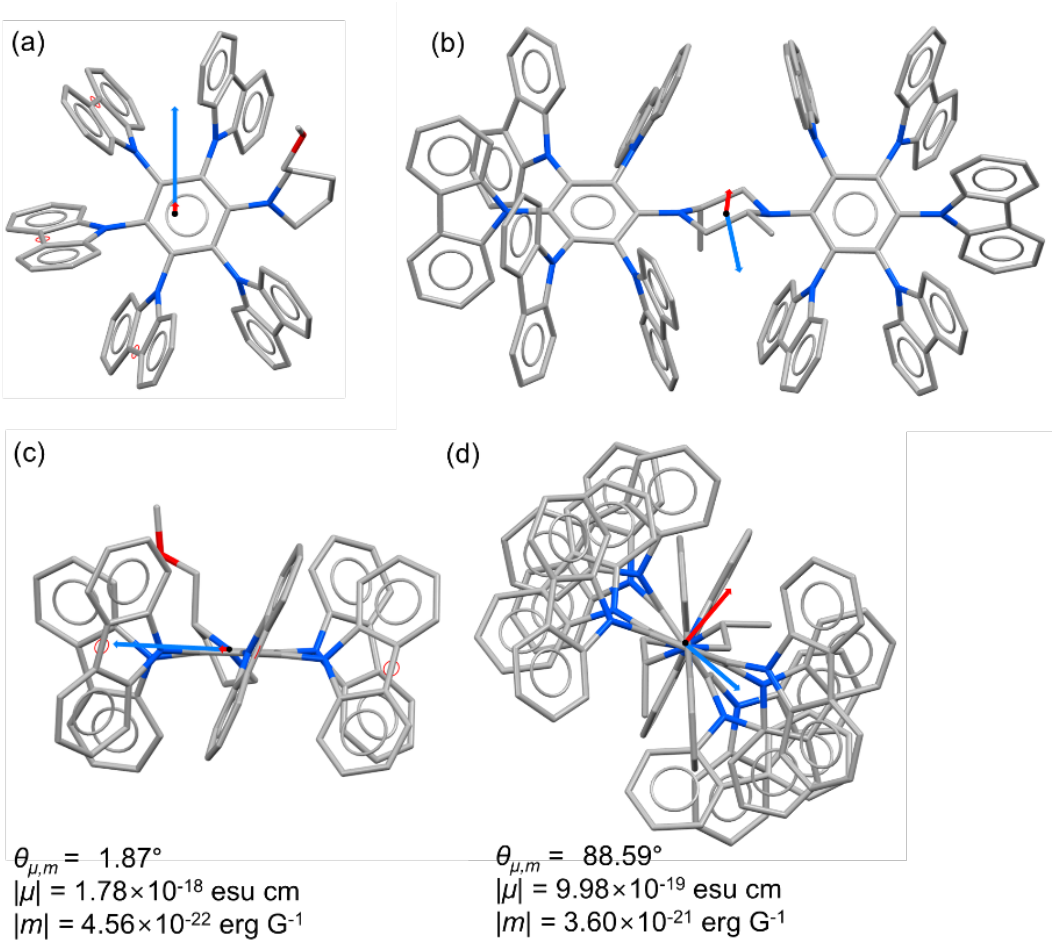


Figure S5a. Calculated transition dipole moments for the S0→S1 electronic transitions in (a, c) (*R*)-**1** and (b, d) (*R*,*R*)-**2**. The electric transition dipole moments (μ) are shown in red, and the magnetic transition dipole moments (m) are shown in blue. Arrows for moments are displayed with 1 a.u.=5.29 Å.

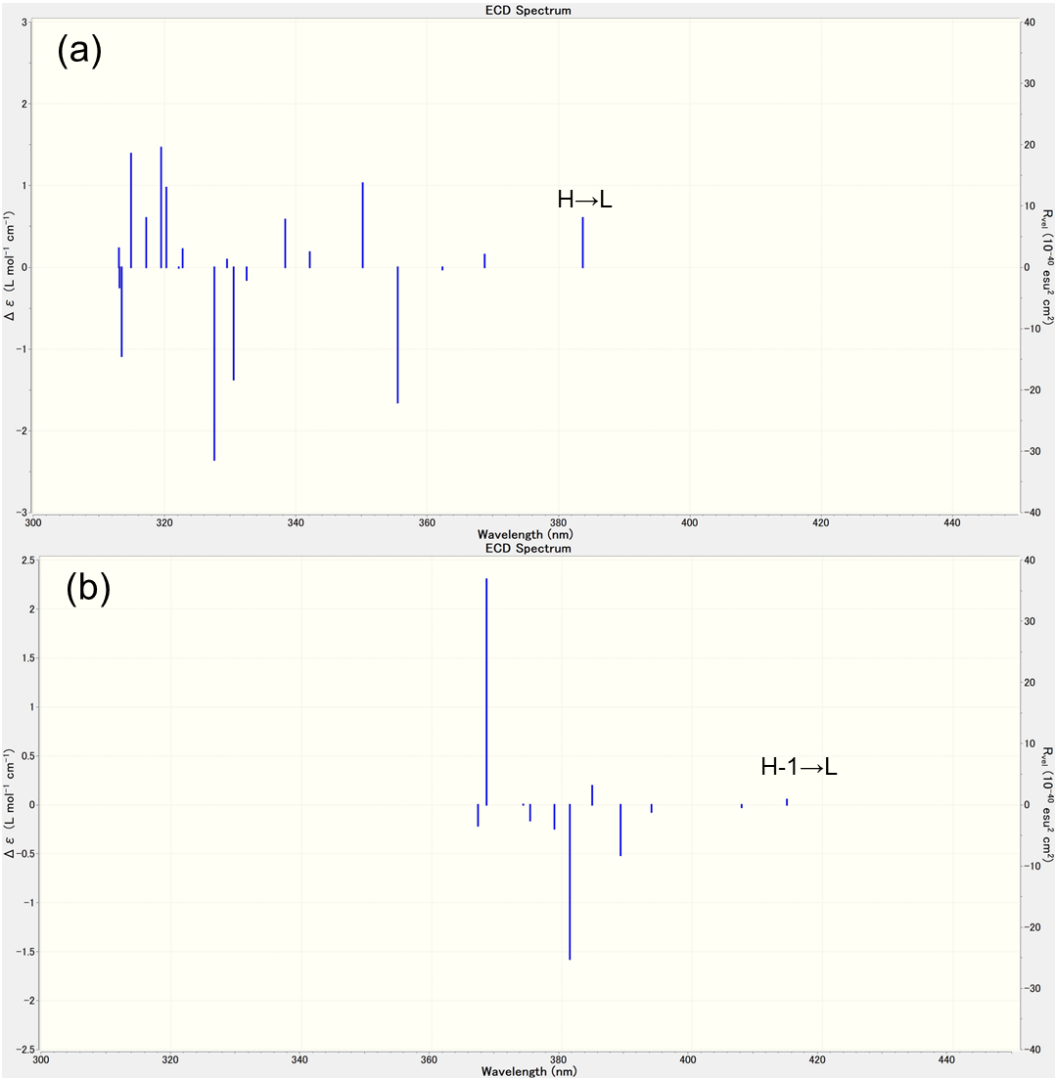


Figure S5b. Calculated CD spectra of (a) (*R*)-**1** at the B3LYP/6-31+G(d)//B3LYP/6-31G(d) level and (b) (*R,R*)-**2** at the B3LYP/6-31+G(d)//B3LYP/6-31G level.

(*R*)-1

Excited State 1: Singlet-A 3.2311 eV 383.72 nm f=0.0387 <S**2>=0.000
267 -> 268 0.69866
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3178.75113893
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3620 eV 368.78 nm f=0.0320 <S**2>=0.000
266 -> 268 0.68629
267 -> 269 -0.12364

Excited State 3: Singlet-A 3.4216 eV 362.35 nm f=0.0009 <S**2>=0.000
265 -> 268 0.66999
266 -> 269 0.12981

Excited State 4:	Singlet-A	3.4872 eV	355.54 nm	f=0.0722	<S**2>=0.000
264 -> 268	0.69235				
Excited State 5:	Singlet-A	3.5402 eV	350.21 nm	f=0.0658	<S**2>=0.000
266 -> 268	0.12802				
267 -> 269	0.66257				
267 -> 271	0.13298				
Excited State 6:	Singlet-A	3.6238 eV	342.14 nm	f=0.0008	<S**2>=0.000
260 -> 268	-0.26305				
262 -> 268	0.20333				
263 -> 268	0.60719				
Excited State 7:	Singlet-A	3.6640 eV	338.39 nm	f=0.0062	<S**2>=0.000
257 -> 268	0.21091				
261 -> 268	-0.30997				
262 -> 268	0.20985				
263 -> 268	-0.11068				
265 -> 268	-0.17256				
266 -> 269	0.49487				
Excited State 8:	Singlet-A	3.7286 eV	332.52 nm	f=0.0498	<S**2>=0.000
261 -> 268	-0.19013				
262 -> 268	0.52148				
263 -> 268	-0.15111				
266 -> 269	-0.38363				
Excited State 9:	Singlet-A	3.7511 eV	330.53 nm	f=0.0263	<S**2>=0.000
261 -> 268	0.55544				
262 -> 268	0.33700				
266 -> 269	0.20893				
Excited State 10:	Singlet-A	3.7624 eV	329.54 nm	f=0.0310	<S**2>=0.000
260 -> 268	-0.28176				
263 -> 268	-0.15092				
264 -> 269	0.16900				
265 -> 269	0.57947				
Excited State 11:	Singlet-A	3.7847 eV	327.60 nm	f=0.0134	<S**2>=0.000
260 -> 268	0.56739				
263 -> 268	0.22946				
264 -> 269	0.19841				
265 -> 269	0.25932				
Excited State 12:	Singlet-A	3.8412 eV	322.77 nm	f=0.0007	<S**2>=0.000
264 -> 269	0.10517				
266 -> 270	-0.17036				
266 -> 271	-0.12149				

267 -> 269 -0.10885
267 -> 270 0.43579
267 -> 271 0.26569
267 -> 272 -0.35258

Excited State 13: Singlet-A 3.8482 eV 322.19 nm f=0.0003 <S**2>=0.000
257 -> 268 0.19492
260 -> 268 -0.10981
264 -> 269 0.57954
265 -> 269 -0.22014

Excited State 14: Singlet-A 3.8710 eV 320.29 nm f=0.0103 <S**2>=0.000
257 -> 268 0.55357
259 -> 268 0.15999
261 -> 268 0.19274
263 -> 269 -0.20074
264 -> 269 -0.18626
266 -> 269 -0.10491
267 -> 272 -0.10419

Excited State 15: Singlet-A 3.8807 eV 319.49 nm f=0.0127 <S**2>=0.000
265 -> 270 -0.11237
266 -> 270 -0.17691
266 -> 271 -0.15382
267 -> 270 0.27996
267 -> 272 0.54818

Excited State 16: Singlet-A 3.9085 eV 317.21 nm f=0.0031 <S**2>=0.000
265 -> 271 -0.18405
266 -> 270 -0.28391
266 -> 271 0.25631
267 -> 270 -0.27972
267 -> 271 0.45793

Excited State 17: Singlet-A 3.9372 eV 314.90 nm f=0.0354 <S**2>=0.000
259 -> 268 0.33072
260 -> 269 -0.14866
263 -> 269 0.39867
264 -> 270 -0.17558
265 -> 270 0.17344
266 -> 271 0.16290
266 -> 272 0.16002
267 -> 273 0.22937

Excited State 18: Singlet-A 3.9552 eV 313.47 nm f=0.0366 <S**2>=0.000
257 -> 268 -0.13173
258 -> 268 0.26790
259 -> 268 0.48525
266 -> 272 -0.18875

267 -> 273 -0.30958

Excited State 19: Singlet-A 3.9591 eV 313.16 nm f=0.0018 <S**2>=0.000
257 -> 268 -0.17338
258 -> 268 -0.15922
259 -> 268 0.31969
263 -> 269 -0.23154
264 -> 270 0.13797
265 -> 270 -0.12934
265 -> 271 0.10003
266 -> 271 -0.15189
266 -> 272 0.19152
267 -> 270 -0.15458
267 -> 273 0.32255

Excited State 20: Singlet-A 3.9602 eV 313.07 nm f=0.0025 <S**2>=0.000
258 -> 268 0.59012
259 -> 268 -0.12139
266 -> 272 0.14620
267 -> 271 -0.10474
267 -> 273 0.25132
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 20 LETran= 370.

(*R*,*R*)-2

Excited State 1: Singlet-A 2.9910 eV 414.52 nm f=0.0113 <S**2>=0.000
501 -> 503 0.69795
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -5971.30360431
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0420 eV 407.57 nm f=0.0108 <S**2>=0.000
502 -> 504 0.67336
502 -> 505 -0.18107

Excited State 3: Singlet-A 3.1490 eV 393.72 nm f=0.0044 <S**2>=0.000
498 -> 503 0.52370
501 -> 504 -0.12047
501 -> 505 -0.43729

Excited State 4: Singlet-A 3.1874 eV 388.98 nm f=0.0542 <S**2>=0.000
498 -> 503 0.44193
501 -> 504 0.14187
501 -> 505 0.50909

Excited State 5: Singlet-A 3.2234 eV 384.64 nm f=0.0210 <S**2>=0.000
500 -> 504 0.66261
500 -> 505 -0.17392

Excited State 6:	Singlet-A	3.2525 eV	381.20 nm	f=0.0297	<S**2>=0.000
493 -> 503	0.40096				
494 -> 503	0.28361				
495 -> 503	0.27605				
496 -> 503	-0.27320				
497 -> 503	0.17691				
499 -> 503	0.15156				
502 -> 503	-0.11646				
Excited State 7:	Singlet-A	3.2727 eV	378.84 nm	f=0.0008	<S**2>=0.000
488 -> 503	0.11337				
493 -> 503	0.23772				
494 -> 503	0.25068				
495 -> 503	-0.48127				
496 -> 503	0.17264				
498 -> 505	-0.18906				
502 -> 503	-0.13643				
Excited State 8:	Singlet-A	3.3055 eV	375.09 nm	f=0.0033	<S**2>=0.000
493 -> 503	-0.14873				
494 -> 503	-0.10395				
502 -> 503	-0.66745				
Excited State 9:	Singlet-A	3.3148 eV	374.03 nm	f=0.0012	<S**2>=0.000
497 -> 504	0.27797				
499 -> 504	-0.59341				
499 -> 505	0.15704				
Excited State 10:	Singlet-A	3.3653 eV	368.42 nm	f=0.0342	<S**2>=0.000
493 -> 504	0.12567				
495 -> 504	0.16018				
496 -> 504	0.23518				
497 -> 504	-0.52521				
497 -> 505	0.13471				
499 -> 504	-0.25440				
Excited State 11:	Singlet-A	3.3775 eV	367.09 nm	f=0.0245	<S**2>=0.000
493 -> 503	-0.11372				
494 -> 503	-0.11681				
495 -> 503	0.15513				
498 -> 504	-0.17416				
498 -> 505	-0.61654				
Excited State 12:	Singlet-A	3.3788 eV	366.95 nm	f=0.0028	<S**2>=0.000
485 -> 503	0.14228				
486 -> 503	0.13706				
489 -> 503	0.13115				
490 -> 503	-0.53991				
494 -> 503	0.17616				

497 -> 503 -0.11654
498 -> 505 -0.10347
500 -> 503 0.22901

Excited State 13: Singlet-A 3.4340 eV 361.05 nm f=0.0156 <S**2>=0.000
494 -> 504 -0.15085
502 -> 505 0.31993
502 -> 506 -0.55896

Excited State 14: Singlet-A 3.4521 eV 359.15 nm f=0.0640 <S**2>=0.000
488 -> 505 -0.12555
493 -> 505 -0.20982
494 -> 505 -0.25377
495 -> 504 0.13959
495 -> 505 0.47469
496 -> 505 -0.18644
502 -> 506 0.10745

Excited State 15: Singlet-A 3.4570 eV 358.64 nm f=0.0006 <S**2>=0.000
489 -> 503 0.10460
490 -> 503 -0.24681
491 -> 503 0.27664
492 -> 503 -0.14056
494 -> 503 -0.10387
495 -> 503 -0.12538
499 -> 503 0.12988
500 -> 503 -0.49845

Excited State 16: Singlet-A 3.4647 eV 357.85 nm f=0.0053 <S**2>=0.000
491 -> 503 0.36978
493 -> 504 -0.15387
493 -> 505 -0.25971
494 -> 505 -0.23717
495 -> 505 -0.11773
496 -> 505 0.13919
497 -> 505 -0.11907
500 -> 503 0.29491
502 -> 505 0.12432

Excited State 17: Singlet-A 3.4744 eV 356.85 nm f=0.0067 <S**2>=0.000
489 -> 504 -0.18075
491 -> 503 -0.20500
493 -> 504 -0.28428
493 -> 505 0.11951
494 -> 504 0.43543
496 -> 504 0.14329
502 -> 505 0.22644

Excited State 18: Singlet-A 3.4842 eV 355.85 nm f=0.0022 <S**2>=0.000

488 -> 503 0.12831
491 -> 503 -0.30871
493 -> 505 -0.26590
494 -> 504 -0.15909
494 -> 505 -0.13653
495 -> 503 0.11272
495 -> 505 -0.20011
496 -> 505 0.19968
497 -> 505 -0.12185
499 -> 505 -0.11454
500 -> 503 -0.21732
502 -> 505 0.11776
502 -> 506 0.15457

Excited State 19: Singlet-A 3.4981 eV 354.44 nm f=0.0013 <S**2>=0.000
493 -> 504 0.13855
493 -> 505 0.18453
494 -> 505 0.17277
502 -> 504 0.13208
502 -> 505 0.51271
502 -> 506 0.31811
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 19 LETran= 352.
Hyperfine terms turned off by default for NAtoms > 100.

Atomic coordinates of optimized structures

The optimized structures of (*R*)-**1** at the B3LYP/6-31G(d) level and (*R,R*)-**2** at the B3LYP/6-31G level

(*R*)-1

C	1.07443600	0.60276300	0.00998600	C	0.29486400	5.84697900	-2.25229500
C	-0.23310400	1.14386400	0.03931100	C	-0.28131400	5.95830300	-0.99080200
C	-1.34028700	0.26903800	-0.08619200	C	-0.48910500	4.80190400	-0.23095400
C	-1.14403700	-1.12713900	-0.16622600	C	-0.11222600	3.54050300	-0.75201700
C	0.16866300	-1.69659000	-0.19193300	C	-1.05755200	4.56756500	1.07829500
N	-2.28045900	-1.98428000	-0.18795100	C	-1.57697700	5.41394900	2.06408400
N	-2.65605900	0.80747800	-0.15113800	C	-2.03673900	4.86473500	3.25716500
N	-0.43619700	2.54270000	0.18599500	C	-1.97438700	3.47852300	3.47178700
N	2.19617500	1.47063600	0.12800200	C	-1.45951200	2.61801000	2.50443200
N	2.58817000	-1.28107300	-0.36480200	C	-1.01148100	3.17127000	1.30496500
C	-0.41703300	-3.89509300	-1.26641200	C	-2.54992800	1.86532900	-2.45152300
C	1.39042400	-3.87780400	0.37987400	C	-3.16396100	1.53266300	-1.24363600
N	0.33723000	-3.07174400	-0.29246900	C	-4.50871600	1.88546600	-0.97861900
C	1.12530300	-5.30689700	-0.12753400	C	-5.23849200	2.59928400	-1.93551900
C	1.33994700	-3.76895200	1.90371200	C	-4.62664900	2.94549400	-3.13657100
C	1.27289200	-0.78887500	-0.14713900	C	-3.29515700	2.57785800	-3.38892500
C	3.65752800	-1.32304500	0.54563500	C	-4.83428900	1.35563200	0.32729900
C	3.70190700	-0.93106700	1.88414100	C	-3.67833400	0.69315500	0.80779700
C	4.90093500	-1.10427000	2.57253800	C	-3.66360100	0.08679800	2.06410600
C	5.97455500	-2.06643400	0.61941000	C	-4.82630200	0.13540400	2.82999900
C	4.78165800	-1.90145200	-0.09368000	C	-5.98219600	0.78231700	2.36407700
C	4.37877500	-2.22678600	-1.44604500	C	-5.98988400	1.39600900	1.11548700
C	5.03883700	-2.80167700	-2.53815900	C	-4.11890200	-2.02742700	-3.44469000
C	4.34747300	-2.98115300	-3.73315500	C	-5.10156300	-2.96580900	-3.08761400
C	3.00286400	-2.58897500	-3.84587000	C	-5.10966200	-3.53183500	-1.81629000
C	2.32325700	-2.01415900	-2.77226600	C	-4.12911000	-3.14838800	-0.89384900
C	3.02316500	-1.83694600	-1.57636100	C	-3.15702600	-2.18653800	-1.26499900
C	2.56037700	2.15479900	1.30063800	C	-3.13282500	-1.62931700	-2.54416900
C	1.96860900	2.12907300	2.56404000	C	-3.82565300	-3.55138400	0.46357500
C	2.55427500	2.88931500	3.57477100	C	-4.41901000	-4.44700000	1.36106200
C	3.70920000	3.65247500	3.33912500	C	-2.67795900	-2.82173800	0.86150700
C	4.30350300	3.66242900	2.08054500	C	-2.12015100	-2.97557900	2.13214300
C	3.73237700	2.90786300	1.05000200	C	-2.72770600	-3.87451100	3.00751200
C	4.09606400	2.67562100	-0.33084600	C	-3.86625800	-4.60573100	2.62863500
C	3.13680300	1.78372400	-0.86936600	C	6.02913600	-1.66344400	1.94981000
C	3.19570300	1.37608100	-2.20284500	C	0.50683900	-5.09026400	-1.51140700
C	4.23807800	1.86092700	-2.99037200	H	-1.37233000	-4.24184900	-0.85793100
C	5.20135700	2.73911700	-2.46839300	H	-0.62684200	-3.31607400	-2.17064400
C	5.13277900	3.15119500	-1.14122500	H	2.39155100	-3.57758500	0.06558000
C	0.45797300	3.42428400	-2.01982800	H	0.40858000	-5.81153400	0.53295600
C	0.65933700	4.58870500	-2.75774500	H	2.04353000	-5.89830800	-0.13887900

H 1.41019700	-2.71578100	2.22366400
H 2.84313800	-0.48695500	2.37353800
H 4.96155000	-0.79072400	3.61099900
H 6.84429000	-2.50703100	0.13926700
H 6.07988500	-3.10185500	-2.45337300
H 4.84985800	-3.42692300	-4.58679200
H 2.47912000	-2.73446800	-4.78683100
H 1.28599200	-1.70923300	-2.86878600
H 1.07482700	1.54826700	2.75927100
H 2.09980200	2.89307900	4.56160600
H 4.14107900	4.23728500	4.14625900
H 5.20270400	4.24531600	1.89920800
H 2.46304900	0.69657700	-2.62189500
H 4.30374200	1.54577000	-4.02807300
H 6.00306200	3.09953200	-3.10665200
H 5.87310600	3.83659200	-0.73698000
H 0.75217200	2.46309600	-2.42286900
H 1.11270000	4.51592800	-3.74245900
H 0.46499100	6.73726500	-2.85103100
H -0.56893500	6.93016500	-0.59832400
H -1.61638400	6.48743800	1.89874800
H -2.44512800	5.51077300	4.02908200
H -2.33856000	3.06268000	4.40716000
H -1.42058700	1.55015000	2.68341600
H -1.52203800	1.59106200	-2.65751300
H -6.27181300	2.87545300	-1.74257400
H -5.18163700	3.50272000	-3.88589100
H -2.82988600	2.85719300	-4.33012200
H -2.78280500	-0.42033400	2.43817700
H -4.83383600	-0.34191900	3.80601900
H -6.87391000	0.80403100	2.98407300
H -6.88085500	1.90304100	0.75446200
H -4.12668500	-1.59635200	-4.44188000
H -5.85842500	-3.25246200	-3.81207200
H -5.86314900	-4.26593900	-1.54313300
H -2.38531600	-0.89792500	-2.82873800
H -5.30328600	-5.00844900	1.07121400
H -1.24613500	-2.40732600	2.43215500
H -2.31147200	-4.00847900	4.00239800
H -4.31860000	-5.29789900	3.33297600
H 6.94988500	-1.78254600	2.51363500
H 1.28031000	-4.83265000	-2.24319700
H -0.04245100	-5.96210000	-1.88053200
O 2.43623500	-4.50888000	2.40195300
H 0.38769500	-4.17303300	2.28211900
C 2.55862100	-4.43441800	3.80568000
H 3.42406000	-5.04056500	4.08584500
H 2.72481000	-3.39894300	4.14219800
H 1.66491800	-4.82948700	4.31599900

(*R*,*R*)-2

C	-0.67402200	0.40070000	1.18461500
C	0.68996800	0.98011200	0.76306900
N	1.49292400	0.01773200	-0.03961500
C	0.72565400	-0.55970600	-1.20605300
C	-0.66513200	-1.05852400	-0.73683900
N	-1.43297200	0.02771500	-0.06276900
C	0.66164600	0.44197600	-2.36694400
C	-1.37407400	1.44309100	2.06457100
C	-5.02229500	-1.18748700	0.24642200
C	-3.60630400	-1.19066200	0.26724200
C	-2.85902500	-0.02142500	-0.02696900
C	-3.59515200	1.16226600	-0.33014200
C	-5.00126700	1.20722400	-0.21238400
C	-5.72397100	0.02704300	0.08032400
C	-8.09424600	0.36999800	-0.78189600
C	-9.39022000	0.27554300	-0.20914200
C	-9.22159700	-0.09113800	1.18605800
C	-7.82869200	-0.22353400	1.41861700
N	-7.13643500	0.05467700	0.21442900
C	-10.12412900	-0.28681700	2.23423900
C	-9.63407200	-0.60396400	3.49964100
C	-8.25218800	-0.71884900	3.72033100
C	-7.33734700	-0.52571100	2.68576300
C	-7.92947600	0.70104400	-2.12402800
C	-9.06850200	0.94761000	-2.88930800
C	-10.35457600	0.85855000	-2.33309700
C	-10.52081700	0.52108900	-0.99198300
C	-5.88544400	3.19020300	-1.55468300
C	-6.66516300	4.33645900	-1.24410800
C	-6.95083000	4.29303300	0.17932100
C	-6.35309500	3.11200800	0.69003000
N	-5.70355000	2.43607800	-0.37003700
C	-7.63248400	5.15545500	1.04131800
C	-7.70642300	4.83902200	2.39664900
C	-7.10185000	3.67174800	2.89102100
C	-6.41701400	2.79815100	2.04594400
C	-5.46219500	2.94366900	-2.85908300
C	-5.82223500	3.85430400	-3.85259000
C	-6.59246900	4.99049600	-3.55737600
C	-7.01597400	5.23634900	-2.25315300
C	-2.40597400	2.31014500	-2.17148200
C	-1.91761900	3.61101900	-2.45960600
C	-2.14914700	4.42252500	-1.27633300
C	-2.79330600	3.59422700	-0.31656500
N	-2.91618400	2.29594700	-0.85746300
C	-1.89886800	5.76489000	-0.98132900
C	-2.28822300	6.26999100	0.25697800
C	-2.92792400	5.44300400	1.19521200
C	-3.18780300	4.10075700	0.92168100
C	-2.43561200	1.31313000	-3.14608100
C	-1.95202000	1.62312300	-4.41711900
C	-1.43698900	2.89828700	-4.70801700
C	-1.41676000	3.89503400	-3.73324200
C	-2.87794400	-3.57673500	-0.16639600
C	-2.41433400	-4.64609700	0.64465500
C	-2.22075200	-4.11443000	1.98350400
C	-2.54006000	-2.73171900	1.93451600
N	-2.94515400	-2.40651700	0.62181200
C	-1.86300700	-4.69740700	3.20120400
C	-1.80678100	-3.90399400	4.34631200
C	-2.10837700	-2.53312000	4.28059500
C	-2.48281800	-1.93336500	3.07727300
C	-3.16351300	-3.75966600	-1.51734800
C	-2.98513000	-5.03316400	-2.05641600
C	-2.52774800	-6.10162800	-1.26645400
C	-2.24159200	-5.91484600	0.08446000
C	-6.41662000	-2.90575000	-0.87022000
C	-7.05672900	-4.12715400	-0.54207700
C	-6.78417700	-4.38795400	0.85959900
C	-5.97432500	-3.32358400	1.34226100
N	-5.75877500	-2.40837600	0.28132500
C	-7.16321900	-5.42541000	1.71505500
C	-6.73422200	-5.40149900	3.03959000
C	-5.93135200	-4.34832400	3.50563100
C	-5.54674500	-3.30245900	2.66769600
C	-6.45655700	-2.39582300	-2.16617700
C	-7.16100300	-3.11154500	-3.13385600
C	-7.80851600	-4.31752700	-2.81903100
C	-7.75758900	-4.83112600	-1.52462400
C	5.06904200	1.14603000	0.44483700
C	3.66005000	1.19232700	0.36224400
C	2.88797800	0.04848200	-0.03476500
C	3.64730200	-1.11598200	-0.39789500
C	5.05490900	-1.10954400	-0.44408800
C	5.78498400	0.02086700	-0.01255400
C	7.98400900	0.87528500	-0.87214600
C	9.35749600	0.60959500	-0.63411600
C	9.42286900	-0.43004400	0.37771400
C	8.08673100	-0.77292400	0.71686000
N	7.20539800	0.03303600	-0.04420100
C	10.49121400	-1.07600000	1.00500900

C	10.22390600	-2.05507500	1.95899000		
C	8.89895000	-2.38608400	2.28634500		
C	7.82096700	-1.74834900	1.67434500		
C	7.58818200	1.80905900	-1.82643400		
C	8.57750800	2.49139000	-2.53332300		
C	9.94015500	2.24437400	-2.29954500		
C	10.33557900	1.30211400	-1.35220500		
C	5.87613200	-3.51926200	-0.30303300		
C	6.69509100	-4.34662900	-1.11747400		
C	7.07718900	-3.56549000	-2.28060400		
C	6.49366700	-2.28050500	-2.13146500		
N	5.75998200	-2.25228600	-0.92267200		
C	7.83799300	-3.85619800	-3.41549800		
C	8.00632400	-2.87219900	-4.38791200		
C	7.41729800	-1.60665200	-4.23178100		
C	6.65349800	-1.29812500	-3.10632700		
C	5.36330800	-3.98675200	0.90544300		
C	5.67303100	-5.29010500	1.29340800		
C	6.48119100	-6.11700700	0.49635800		
C	6.99469100	-5.64911000	-0.71122800		
C	2.91298300	-3.07121900	-1.85347300		
C	2.26449300	-4.31096100	-1.60566100		
C	1.95210200	-4.35483200	-0.18578400		
C	2.37266700	-3.11984600	0.37189000		
N	2.97700200	-2.34800300	-0.64078600		
C	1.40974200	-5.33804200	0.64570500		
C	1.28544900	-5.07547700	2.00774200		
C	1.66580700	-3.83077200	2.53911900		
C	2.20898000	-2.83550400	1.72788200		
C	3.31376700	-2.70398000	-3.13609400		
C	3.07826000	-3.60351400	-4.17573400		
C	2.44618700	-4.83709600	-3.94481800		
C	2.03564400	-5.19635000	-2.66229400		
C	2.82212700	3.01509100	1.92060800		
C	2.22237900	4.29248200	1.75302800		
C	2.10440100	4.52335800	0.32199000		
C	2.60541400	3.36399800	-0.32871100		
N	3.03693100	2.44632500	0.64924500		
C	1.66065600	5.60648300	-0.44020100		
C	1.71934200	5.52512500	-1.83068600		
C	2.20329300	4.36660400	-2.46180800		
C	2.64947600	3.27317400	-1.71942900		
C	3.05642600	2.48212900	3.18701000		
C	2.69276600	3.24836700	4.29473100		
C	2.10278200	4.51497700	4.14460500		
C	1.86604700	5.04318400	2.87651300		
C	6.03205000	3.53225200	0.65311900		
C	6.79505500	4.19441900	1.65446600		
C	7.00270000	3.25079000	2.73744000		
C	6.37346700	2.03787200	2.35799200		
N	5.78624400	2.20541800	1.08172100		
C	7.63656500	3.34663600	3.97895100		
C	7.63181300	2.24215200	4.82866800		
C	6.99604300	1.04967800	4.44531400		
C	6.35883800	0.93532800	3.21004900		
C	5.66838800	4.19690300	-0.51610400		
C	6.06968000	5.52204700	-0.67856800		
C	6.82687700	6.18254600	0.30215300		
C	7.19149200	5.52151300	1.47216600		
H	-0.50156700	-0.51698100	1.76605000		
H	0.50047100	1.90512300	0.20979400		
H	1.23475500	1.21558900	1.67495700		
H	1.25200500	-1.44639900	-1.54183700		
H	-1.21549700	-1.40223700	-1.61558500		
H	-0.50754600	-1.90901000	-0.06360100		
H	0.15338700	1.36204100	-2.08088600		
H	0.11811900	-0.00046600	-3.20635500		
H	1.67461900	0.67849200	-2.70570400		
H	-2.37446100	1.11443700	2.35992300		
H	-1.46205000	2.39748400	1.54404600		
H	-0.78156900	1.59510400	2.97302100		
H	-11.18975900	-0.18691200	2.06378200		
H	-10.32195700	-0.76205300	4.32148500		
H	-7.88640300	-0.96971500	4.70890700		
H	-6.27590500	-0.61998000	2.86595700		
H	-6.94942000	0.79272800	-2.56664100		
H	-8.95216000	1.22258500	-3.93084100		
H	-11.22090800	1.05643000	-2.95274500		
H	-11.51152200	0.44819800	-0.55851500		
H	-8.09215700	6.05977200	0.65976800		
H	-8.23444400	5.49659100	3.07669600		
H	-7.17486300	3.43598600	3.94607400		
H	-5.97026300	1.89417000	2.43491400		
H	-4.84515400	2.09173100	-3.10361100		
H	-5.48729400	3.68147900	-4.86852000		
H	-6.85591000	5.68009100	-4.35037200		
H	-7.61322200	6.11068200	-2.02173500		
H	-1.41231300	6.40162300	-1.70997200		
H	-2.10839900	7.31113900	0.49716100		
H	-3.24121700	5.85527200	2.14692700		
H	-3.71086500	3.48739100	1.64112100		
H	-2.81899900	0.32621500	-2.92016700		

H	-1.96787800	0.86402600	-5.19090500		
H	-1.06291600	3.10833500	-5.70289000		
H	-1.03865600	4.88392300	-3.96303900		
H	-1.64721000	-5.75764700	3.25522900		
H	-1.53585100	-4.34647200	5.29755300		
H	-2.05989700	-1.93044900	5.18026200		
H	-2.73908500	-0.88352800	3.03817300		
H	-3.53825700	-2.94830600	-2.12669100		
H	-3.21227600	-5.20059800	-3.10238200		
H	-2.40398600	-7.08048700	-1.71397900		
H	-1.89533800	-6.74072500	0.69480200		
H	-7.78352100	-6.23520500	1.34865900		
H	-7.01800200	-6.19943000	3.71531100		
H	-5.59057200	-4.34684200	4.53415600		
H	-4.90550000	-2.52008100	3.04163900		
H	-5.96676800	-1.46464900	-2.41554900		
H	-7.21394600	-2.72365000	-4.14427800		
H	-8.35112500	-4.85007300	-3.59079000		
H	-8.25020500	-5.76539200	-1.28147400		
H	11.51230500	-0.81645300	0.75028000		
H	11.04128700	-2.56839400	2.45113600		
H	8.70480000	-3.15848100	3.02106200		
H	6.80945600	-2.02968400	1.92559000		
H	6.54225700	2.01153700	-2.00829500		
H	8.28606000	3.23141900	-3.26928900		
H	10.68704800	2.79199000	-2.86171500		
H	11.38643600	1.10388700	-1.17571600		
H	8.28729000	-4.83506400	-3.53682500		
H	8.59722500	-3.08151000	-5.27154700		
H	7.56593200	-0.84894000	-4.99201500		
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H	4.71793700	-3.37650700	1.51980200		
H	5.26869200	-5.67023300	2.22413400		
H	6.70395400	-7.12533700	0.82427900		
H	7.62243200	-6.28243200	-1.32739400		
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H	3.39567200	-3.34455900	-5.17881300		
H	2.27736200	-5.51335000	-4.77423900		
H	1.53770200	-6.14237300	-2.48535100		
H	1.28019500	6.49714000	0.04477000		
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H	2.22748000	4.31706100	-3.54398500		
H	3.02310500	2.38269000	-2.20648100		
H	3.53749900	1.52138300	3.31038500		
H	2.88073000	2.86071300	5.28899000		
H	1.83395700	5.08592300	5.02521200		
H	1.40767200	6.01829500	2.76073600		
H	8.12049000	4.26979200	4.27618100		
H	8.12207500	2.30031100	5.79304800		
H	7.00721500	0.19794500	5.11516900		
H	5.88091100	0.01110300	2.91680300		
H	5.06171800	3.72108200	-1.27048400		
H	5.77960000	6.05076200	-1.57887700		
H	7.12470700	7.21256900	0.14662900		
H	7.77487900	6.02585900	2.23385800		

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