Supplementary Information

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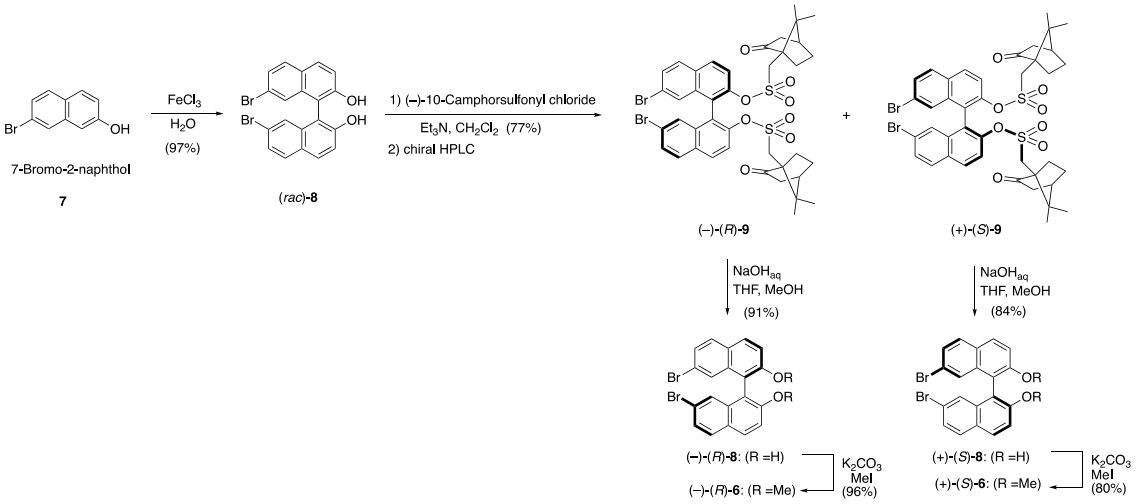
S1. General

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AVANCE-II-600 (600 MHz for ^{1}H and 150 MHz for ^{13}C) or Bruker AVANCE-III-400 (400 MHz for ^{1}H and 100 MHz for ^{13}C) instruments. Spectra are reported (in δ) referenced to internal Me_4Si. Mass spectra, including high-resolution mass spectra (HRMS) were recorded on Thermo Scientific, Exactive Plus Orbitrap Mass Spectrometer for electrospray ionization (ESI). IR spectra were recorded on JASCO FT/IR-610 spectrometer. Absorption spectra and CD spectra were recorded on JASCO V-560 spectrometer and JASCO J-720 spectrometer, respectively. Optical Rotation Measurements were recorded on JASCO P-1030 spectrometer. Recycling Preparative HPLC was carried out using HPLCLC-9204 instrument by Japan Analytical Industry (JAI) equipped with a CHIRALPAK®IA (φ = 30 mm, l = 200 mm) and JASCO OR-2090 Plus. Photoluminescence (PL) and circularly polarized luminescence (CPL) spectra were obtained at rt using a JASCO CPL-300 spectrofluoropolarimeter. The absolute value of ΦF was obtained with a Hamamatsu Photonics C9920-02 system (Hamamatsu, Japan) in air at rt. Melting points were determined with Yanaco melting point apparatus. Elemental analyses were performed on Perkin Elmer PE 2400-II CHNA/O analyzer. Starting 7-Bromo-2-naphthol and (–)-10-Camphor sulfonyl chloride were purchased from Tokyo Chemical Industry Co., Ltd (TCI). $Ni(cod)_2$ was purchased from Strem Chemicals, Inc. and stored under Ar at –20 °C. Column chromatography was carried out using Kanto Chemical silica gel 60N, 60-210mm meshes. All solvents were dried by conventional procedures and distilled before use.

S2. Preparation and Optical Resolution of 7,7'-dibromo-1,1'-bi-2-naphthol (6)

Preparation of (–)-(*R*)-**6** and (+)-(*S*)-**6** were described in Scheme S1. Synthesis and optical resolution of **6** were first reported by Lustenberger and Diederich in 2000.[1] They carried out optical resolution by using diastereomeric camphorsulfonates (**9**) by column chromatography on silica gel with the elution of CH_2Cl_2 containing 3% of AcOEt. However, this optical resolution method is not practical to give high diastereomeric excess (d.e.) isomers in multigram quantity, because two diastereomeric isomers did not exhibit sufficiently different retardation factor (R_f) values ((–)-(*R*)-**9**: 0.27, (+)-(*S*)-**9**: 0.24). Alternately, we succeeded in chiral separation of (+)/(–)-**9** by a chiral HPLC method in large quantity (Fig. S1). The retention times of each isomer on a chiral stationary phase (Chiralpak IA) were sufficiently different, and thus they were conveniently separable as optically active isomers with high d.e. (>99%).



Scheme S1. *Preparation of (R) and (S)-**6***

Synthesis of 8

Oxidative coupling from commercially available 7-Bromo-2-nathphol (**7**) to give **8** was carried out according to a similar procedure as reported previously.[2] A mixture of 7-Bromo-2-nathphol (1.0 g, 4.5 mmol) and $FeCl_3$ (1.2 g, 7.6 mmol) in H_2O (40 mL) was stirred under air for 3h at 100°C. The products were extracted by AcOEt, and the resulting organic phase was washed with saturated brine and dried over Na_2SO_4. Purification by column chromatography on silica gel with the elution of Hexane-EtOH (v/v = 6:1) gave brown solid of (*rac*)-**8** (1.0 g, 97%). Data for (*rac*)-**8**: Brown solid; Mp. = 111-116 °C;

MS (ESI-orbitrap, negative mode) *m/z* = 441, 443, 445 $[M-H]^-$; ^1H NMR (400MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.8 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.46 (dd, *J* = 8.4 and 2.0 Hz), 7.36 (d, *J* = 8.8 Hz, 2H), 7.22 (d, *J* = 2.0 Hz, 2H), 5.07 (s, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 109.7, 118.4, 122.6, 126.1, 127.9, 128.1, 130.3, 131.8, 134.8, 153.8.

Synthesis of (–)-(*R*)-9 and (+)-(*R*)-9

To a solution of racemic **8** (1.3 g, 3.1 mmol) in CH_2Cl_2 (60 mL) was added dropwise NEt_3 (1.2 mL, 8.4 mmol) and (–)-10-Camphor sulfonyl chloride (2.0 g, 8.2 mmol) at 0 °C under Ar atmosphere. The mixture was stirred for 3h at 0°C, then the reaction was quenched by the addition of H_2O. The products were extracted by CH_2Cl_2, and the combined organic phase was washed with saturated brine and dried over Na_2SO_4. After the removal of the solvent, the residue was roughly purified by column chromatography on silica gel with the elution with CH_2Cl_2-acetone (v/v=10:1). Further purification and chiral separation was carried out with a recycling HPLC method on a chiral stationary phase (chiralpak IA) with the elution of $CHCl_3$-hexane (v/v=1:2) to give (–)-(*R*)-**9** (1.2 g, 89%) and (+)-(*S*)-**9** (1.1 g, 83%) with high diastereomeric excess (>99%). The absolute configuration was determined by optical rotation measurements and compared with previous literature.[1]

Data for (–)-(*R*)-**9**: White solid; $[\alpha]_D^{25} = -90^\circ$ (c = 0.249); Mp. = 119.5-120.2 °C; MS (ESI-orbitrap) *m/z* = 893, 895, 897 ($M+Na^+$); ^1H NMR (400MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.8 Hz, 2H), 7.79–7.86 (m, 4H), 7.62 (dd, *J* = 8.8 and 2.0 Hz), 7.41 (d, *J* = 2.0 Hz, 2H), 2.99 (d, J_{AB} = 15.0 Hz, 2H), 2.57 (d, J_{AB} = 15.0 Hz, 2H), 2.12–2.28 (m, 2H), 1.78–2.07 (m, 8H), 1.24–1.35 (m, 4H), 0.83 (s, 6H), 0.63 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$) δ 213.3, 146.7, 134.5, 131.1, 130.4, 130.3, 130.0, 128.3, 122.6, 122.0, 121.7, 57.9, 49.3, 47.8, 42.9, 42.4, 26.9, 25.0, 19.6, 19.5.

Data for (+)-(*S*)-**9**: White solid; $[\alpha]_D^{25} = 88^\circ$ (c = 0.255); Mp. = 115.0-115.6 °C; MS (ESI-orbitrap) 893, 895, 897 ($M+Na^+$); ^1H NMR (400MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.8 Hz, 2H), 7.83–7.86 (m, 4H), 7.60 (dd, *J* = 8.8 and 2.0 Hz), 7.36 (d, *J* = 2.0 Hz, 2H), 3.29 (d, J_{AB} = 15.0 Hz, 2H), 2.39 (d, J_{AB} = 15.0 Hz, 2H), 2.17–2.27 (m, 2H), 1.87–1.96 (m, 8H), 1.21–1.41 (m, 4H), 0.70 (s, 6H), 0.55 (s, 6H); ^{13}C NMR (100MHz, $CDCl_3$) δ 213.3, 146.7, 134.5, 131.1, 130.4, 130.3, 130.1, 128.3, 122.6, 121.9, 121.7, 57.8, 49.3, 47.7, 42.8, 42.4,

26.9, 24.8, 19.5, 19.4.

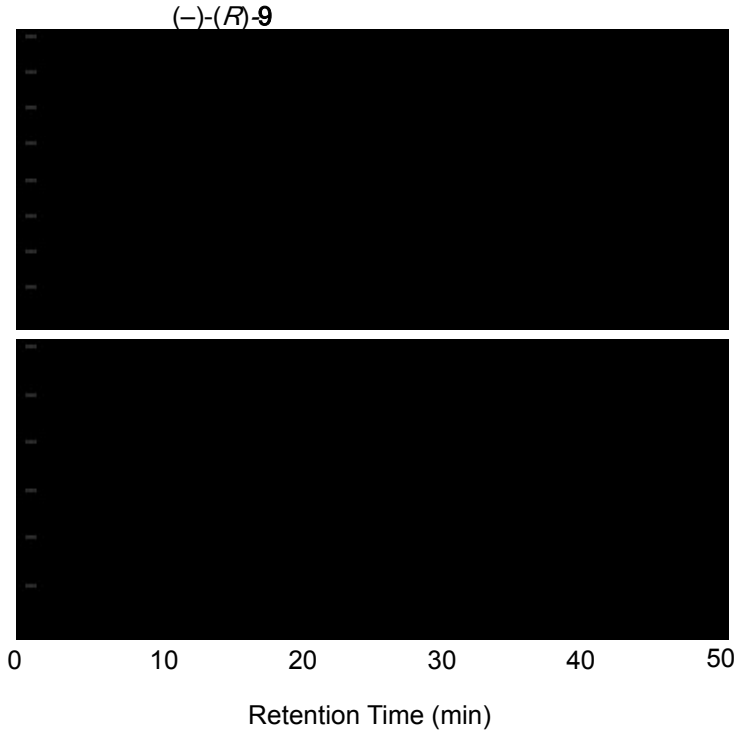


Fig. S1 *Chiral HPLC Chart of* (–)-(*S*)-**9** and (+)-(*S*)-**9**

Synthesis of (–)-(*R*)-8

To a solution of (–)-(*R*)-**9** (786 mg, 0.9 mmol) in THF (25 mL) and MeOH (25 mL) was added 1M $NaOH_{aq}$ (12.5 mL) under Ar atmosphere. The mixture was warming up to 60 °C and stirred for 14h with refluxing. Then, the mixture was further stirred for 12h at rt. The reaction was quenched by the addition of HCl. The resulting mixture was neutralized by the addition of $NaHCO_3$aq, and the products were extracted by CH_2Cl_2. The combined organic phase was washed with saturated brine and dried over Na_2SO_4. Purification by column chromatography on silica gel with $CHCl_3$ gave (–)-(*R*)-**8** (515 mg, 91 %). Data for (–)-(*R*)-**8**: White solid; $[\alpha]_D^{25} = -210^\circ$ (*c* = 0.0906); Mp. = 111-116 °C.

Synthesis of (+)-(*S*)-8

Compound (+)-(*S*)-**8** was prepared by a similar procedure to that used in the production of (–)-(*R*)-**8**, but starting with (+)-(*R*)-**9** (1.0 g, 1.2 mmol) to give (+)-(*S*)-**8** (442 mg, 84%). Data for (+)-(*S*)-**8**: White solid; $[\alpha]_D^{25} = +210^\circ$ (*c* = 0.0724); Mp. = 111-116 °C.

Synthesis of (–)-(*R*)-6

To a solution of (–)-(*R*)-**8** (322 mg, 0.73 mmol) in acetone (17 mL) K_2CO_3 (714 mg, 5.2 mmol) and CH_3I (0.40 mL, 6.4 mmol) were added under Ar atmosphere. The mixture was stirred for 14h at 60°C. Then, the mixture was filtered through Celite pad. The resulting solution was evaporated, and the residue was purified on silica gel column chromatography with $CHCl_3$ to give (–)-(*R*)-**6** (328 mg, 96%). Data for (–)-(*S*)-**9**: White solid; $[\alpha]_D^{25} = -80°$ (c = 0.0767); Mp. = 270–273 °C; MS (ESI-orbitrap) *m/z* = 441, 443, 445 $[M+H]^+$; ^{1}H NMR (400MHz, $CDCl_3$) δ 7.94 (d, *J* = 9.2 Hz, 2H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.44 (dd, *J* = 9.2 and 2.0 Hz, 2H), 7.39 (dd, *J* = 8.8 Hz and 2.0 Hz, 2H), 7.21 (d, *J* = 2.0 Hz, 2H), 3.76 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$) δ 155.8, 135.3, 129.93, 129.88, 127.8, 127.2, 127.1, 121.3, 118.1, 114.4, 56.8.

Synthesis of (+)-(*S*)-6

Compound (+)-(*S*)-**6** was prepared by a similar procedure to that used in the production of (–)-(*R*)-**6**, but starting with (+)-(*R*)-**8** (361 mg, 0.81 mmol) to give (+)-(*S*)-**6** (306 mg, 80%). The absolute configuration was also confirmed by X-ray analysis (Fig. S2). Data for (+)-(*S*)-**6**: White solid; $[\alpha]_D^{25} = -80^\circ$ (c = 0.0837); Mp. = 270-273 °C; ^{1}H NMR

(400MHz, $CDCl_3$) δ 7.94 (d, *J* = 9.2 Hz, 2H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.44 (dd, *J* = 9.2 and 2.0 Hz, 2H), 7.39 (dd, *J* = 8.8 and 2.0 Hz, 2H), 7.21 (d, *J* = 2.0 Hz, 2H), 3.76 (s, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 155.8, 135.3, 129.93, 129.88, 127.8, 127.2, 127.1, 121.3, 118.1, 114.4, 56.8.

S3. X-ray Analysis of (+)-(*S*)-6

Compound **6** was known compound. However, fortunately, we were able to obtain single crystals of (+)-**6** suitable for X-ray analysis, and confirm the absolute configuration by the irradiation of Cu-*K*α. Crystal data of (+)-(*S*)-**6**: Tetragonal space group $P4_3$, T = 120 K, $a = b$ = 8.4188(3) Å, c = 25.963(1) Å, V = 1840.17(15) Å^3, Z = 4, dcalc = 1.704 gcm^{-3}, $F_{(000)}$ = 936.0, reflections collected/unique = 4507/2604 (Rint = 0.0242), The structure was solved by direct methods (SHELXT) and refined by full-matrix least-squares methods (SHELXL) on F_2 with 237 parameters. Flack parameter 0.01(6). R_1=0.0589 (I>2σ(I)), wR_2=0.1718, GOF 1.192. CCDC 1862118 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

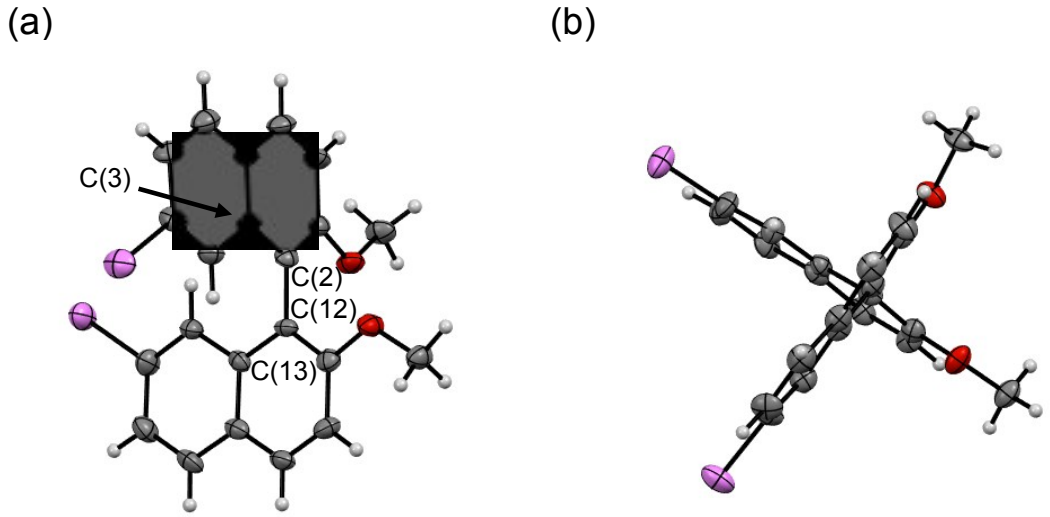
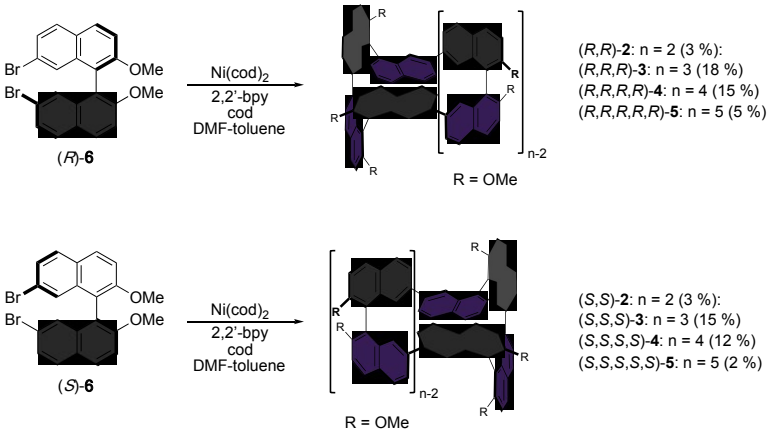


Fig. S2 *ORTEP Drawing of (+)-(S)-**6** (a) Top View and (b) Side View. Dihedral angle: C(3)–C(2)–C(12)–C(13) 85.88°. Bond length: C(2)–C(12) 1.49(1) Å.*

S4. Preparation of Cyclic Oligomers 2–5

The syntheses of cyclic chiral oligomers were carried out separately from each chiral binaphthyl precursor in a similar procedure. We chose $Ni(cod)_2$-catalyzed Yamamoto coupling reaction in a concentration of 0.08 M to obtain desired cyclic product. Interestingly, we did not obtain any acyclic (linear) product as the isolable major product. When we carried out in less concentrated (< 0.01 M), we obtained only acyclic products of 2-mer and 3-mer together with starting materials. Here described the procedure for (*R*)-isomer as the representative.



Scheme S2. *Synthesis of **2**–**5***

Synthesis of (*R*)-2, (*R*,*R*)-**2**, (*R*,*R*,*R*)-**3**, (*R*,*R*,*R*,*R*)-**4**, and (*R*,*R*,*R*,*R*,*R*)-**5**

In a sealed Schlenk tube, a mixture of 2,2'-bipyridyl (224 mg, 1.43 mmol), cod (0.2 mL, 1.63 mmol), and $Ni(cod)_2$ (384 mg, 1.4 mmol) in DMF-toluene (1.1 and 1.1 mL) was stirred for 30 min at 90 °C under Ar atmosphere. Then, (*R*)-**6** (285 mg, 0.60 mmol) in toluene (5.4 mL) was transferred to the mixture, and the solution was stirred for 4 days. The resultant mixture was filtered through a Celite pad. The products were extracted by CH_2Cl_2. The combined solution was washed with saturated brine and dried over Na_2SO_4. After the removal of the solvent, hexane was added into the residue. The resultant solid was collected through filtration, and they were subject to further purification by the column chromatography on silica gel with CH_2Cl_2 to give cyclic 2-mer **2** (5 mg, 3%), cyclic 3-mer **3** (35 mg, 18 %), cyclic 4-mer **4** (29 mg, 15 %), and cyclic 5-mer **5** (9 mg, 5%).

We also conducted the crude product into gel permeation chromatography (GPC) to investigate the product obtained from the coupling products (Fig. S3). We found the peaks corresponding to the cyclic products together with inseparable peaks.

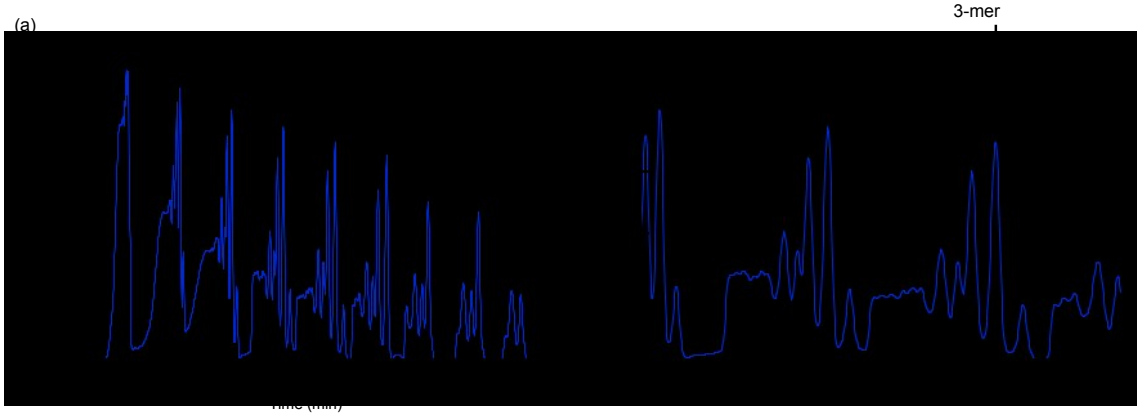


Fig. S3 *GPC charts of the crude products. (a) 0-650 min. (b) 200-400 min.*

Data for (*R,R*)-**2**:

White powder; M.p. = 193.0 °C (decomp.); MS (ESI-orbitrap) *m/z* = 625 ([M+H]$^+$: $C_{44}H_{33}O_4$); $[\alpha]_D^{28} = -106^\circ$ (CH_2Cl_2, *c* = 0.042); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 9.0 Hz, 4H), 7.70 (d, *J* = 8.0 Hz, 4H), 7.40 (d, *J* = 9.0 Hz, 4H), 7.19 (dd, *J* = 8.0 and 1.2 Hz, 4H), 6.98 (d, 1.2 Hz, 12H), 3.83 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 141.7, 132.4, 129.5, 128.4, 127.4, 127.3, 123.5, 118.6, 114.1, 57.0; IR (KBr) 3047, 3017, 3000, 2929, 2851, 1727, 1616, 1597, 1499, 1460, 1439, 1358, 1312, 1254, 1170, 1150, 1095, 1071, 1044, 958, 916, 893, 830, 753 cm^{-1}; HRMS (ESI-orbitrap) *m/z* calcd. for $C_{44}H_{33}O_4$ [M+H]$^+$: 625.23734, Found 625.23737.

Data for (*R,R,R*)-**3**: White powder; Mp. = 262.3 °C ; MS (ESI-orbitrap) *m/z* = 954 ([M+H_2O]+:$C_{66}H_{50}O_7$); $[\alpha]_D^{28} = -37^\circ$ (CH_2Cl_2, *c* = 0.0258); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (d, *J* = 9.0 Hz, 6H), 7.63 (d, *J* = 8.4 Hz, 6H), 7.41 (d, *J* = 9.0 Hz, 6H), 7.07 (dd, *J*

= 8.4 and 1.2 Hz), 6.87 (d, *J* = 1.2 Hz, 6H), 3.80 (s, 18H); ^{13}C NMR (150 Hz, $CDCl_3$) δ 155.4, 140.3, 134.4, 129.3, 128.6, 128.4, 124.6, 123.7, 120.3, 114.5, 57.4; IR (KBr) 3050, 2927, 2835, 1719, 1620, 1596, 1500, 1458, 1436, 1358, 1308, 1249, 1170, 1153, 1097, 1069, 1048, 1033, 969, 910, 829 719 cm^{-1}; Anal. Calcd. for $C_{66}H_{48}O_6$• $2CHCl_3$•$2H_2O$: C, 67.40, H, 4.49, found C, 67.08, H, 4.23; HRMS (ESI-orbitrap) *m/z* calcd. for $C_{66}H_{49}O_6$ $[M+H]^+$: 937.35237, Found 937.35236.

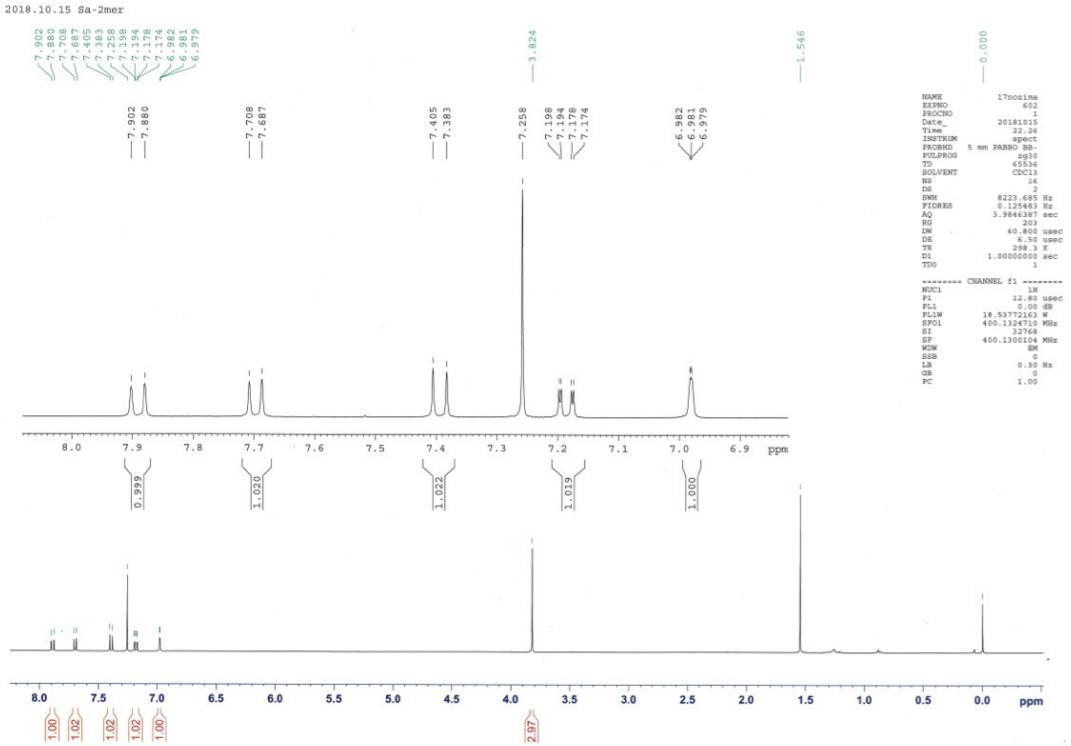
Data for (*R,R,R,R*)-**4**: White powder; Mp. = 285.3 °C ; MS (ESI-orbitrap) *m/z* = 1266 ($[M+H_2O]^+$:$C_{88}H_{66}O_9$); $[\alpha]_D^{28}$ = +397° (CH_2Cl_2, *c* = 0.0286); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.85 (d, 8.0 Hz, 8H), 7.62 (d, *J* = 8.4 Hz, 8H), 7.41 (d, *J* = 9.0 Hz, 8H), 7.29 (d, *J* = 1.6 Hz, 8H), 7.15 (dd, *J* = 1.6 and 8.4 Hz, 8H), 3.78 (s, 24H); ^{13}C NMR (100 Hz, $CDCl_3$) δ 155.2, 138.2, 134.1, 129.3, 128.5, 128.3, 123.2, 123.1, 119.9, 113.9, 56.9; IR (KBr) 3046, 3011, 2998, 2955, 2925, 2835, 1724, 1619, 1595, 1500, 1459, 1437, 1357, 1304, 1248, 1170, 1151, 1097, 1068, 1048, 1035, 957, 909, 829, 750, 718 cm^{-1}; Anal. Calcd. for $C_{66}H_{48}O_6$•$3H_2O$: C, 81.09, H, 5.41, found C 81.27, H 5.49; HRMS (ESI-orbitrap) *m/z* calcd. for $C_{88}H_{65}O_8$ $[M+H]^+$: 1249.46740, Found 1249.46741.

Data for (*R,R,R,R,R*)-**5**: White powder; Mp. = 270.6 °C; MS (ESI-orbitrap) *m/z* = 1580 ($[M+H_2O]^+$:$C_{110}H_{82}O_{11}$); $[\alpha]_D^{28}$ = +409° (CH_2Cl_2, *c* = 0.0182); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.73 (d, *J* = 9.0 Hz, 10H), 7.53 (d, *J* = 7.8 Hz, 10H), 7.30 (d, *J* = 9.0 Hz, 10H), 7.03–7.05 (m, 20H), 3.78 (s, 30H); ^{13}C NMR (150 Hz, $CDCl_3$) δ 155.2, 139.6, 134.0, 129.2, 128.3, 128.1, 124.1, 123.5, 119.8, 114.0, 57.0; IR (KBr) 3010, 2999, 2956, 2926, 2845, 1732, 1717, 1620, 1596, 1501, 1460, 1437, 1357, 1301, 1250, 1171, 1151, 1141, 1098, 1068, 1047, 1032, 969, 909, 881, 828, 801 cm^{-1}; HRMS (ESI-orbitrap) *m/z* calcd. for $C_{110}H_{81}O_{10}$ $[M+H]^+$: 1561.58234, Found 1561.58240.

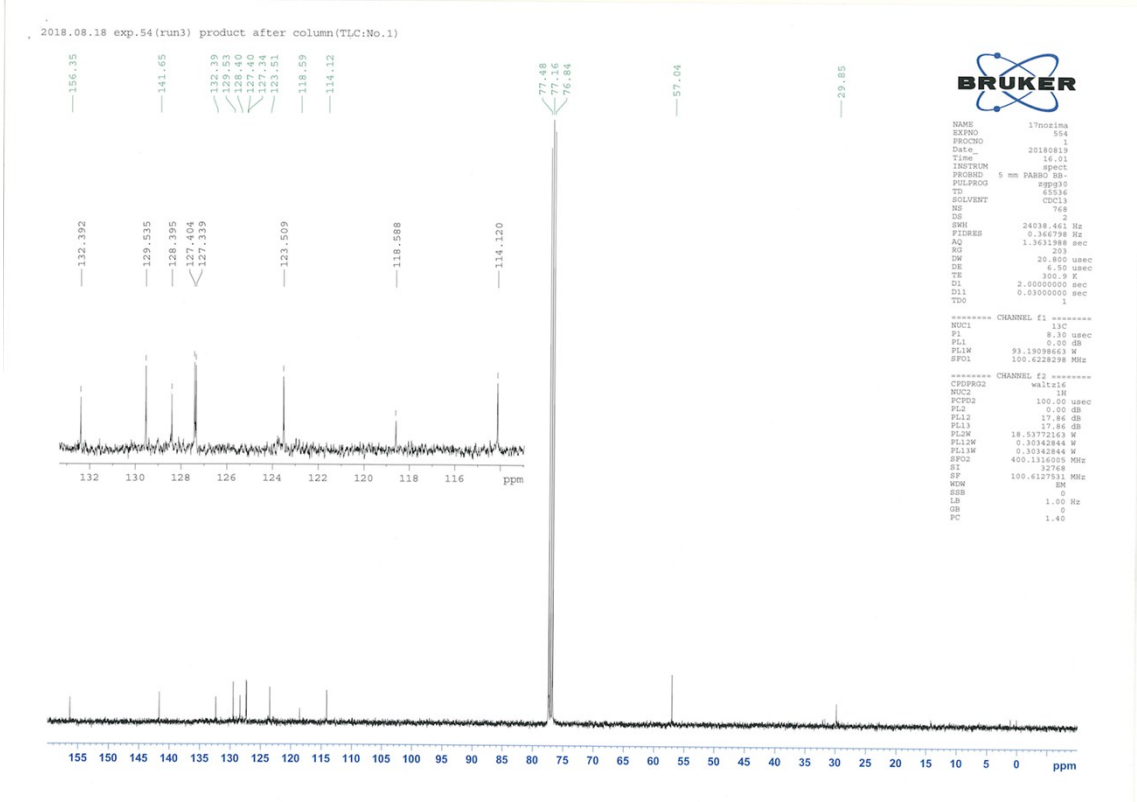
S5. Fig. S4 ^{1}H and ^{13}C NMR Charts of Cyclic Compounds

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

i) ^{1}H NMR Spectrum

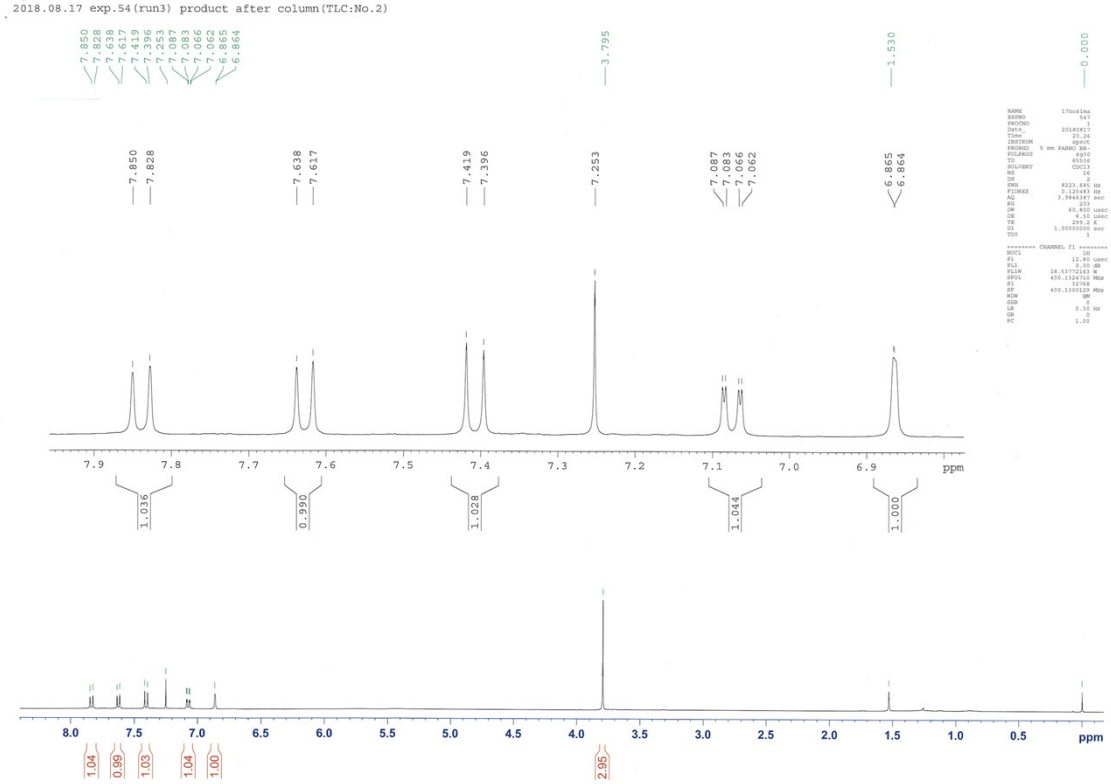


ii) ^{13}C NMR Spectrum

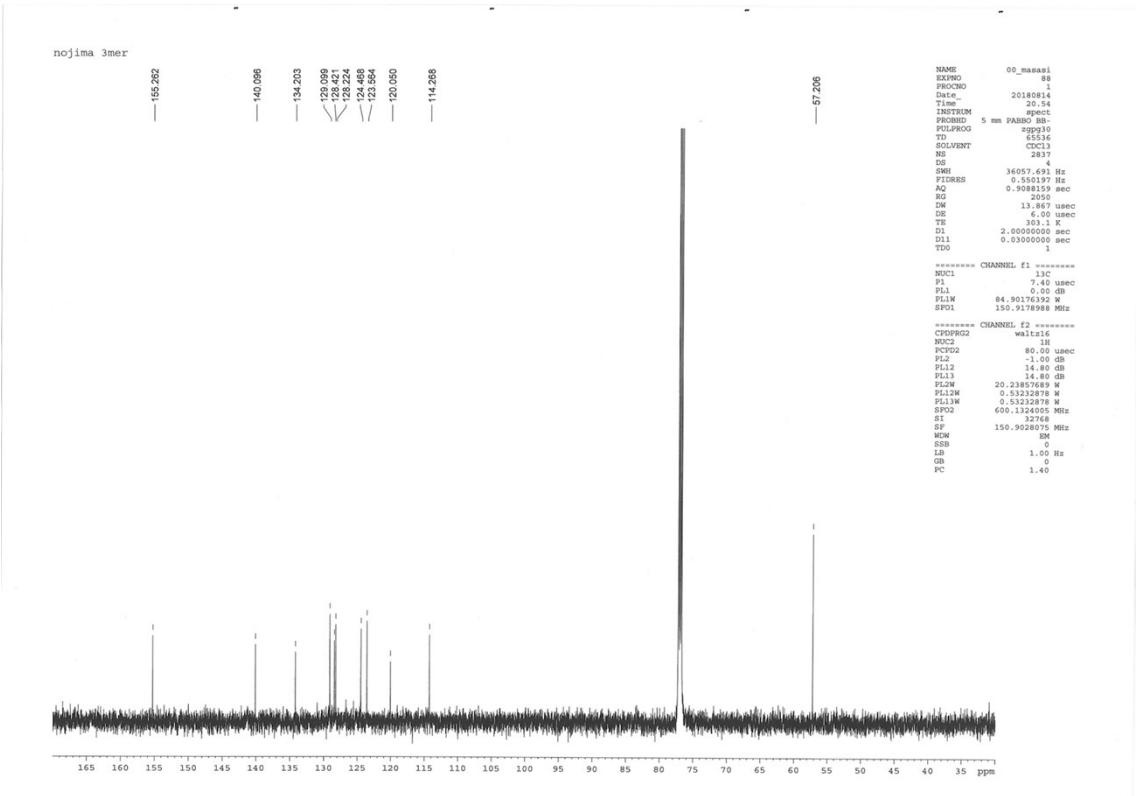


(b) (*R,R,R*)-**3**

i) ^{1}H NMR Spectrum

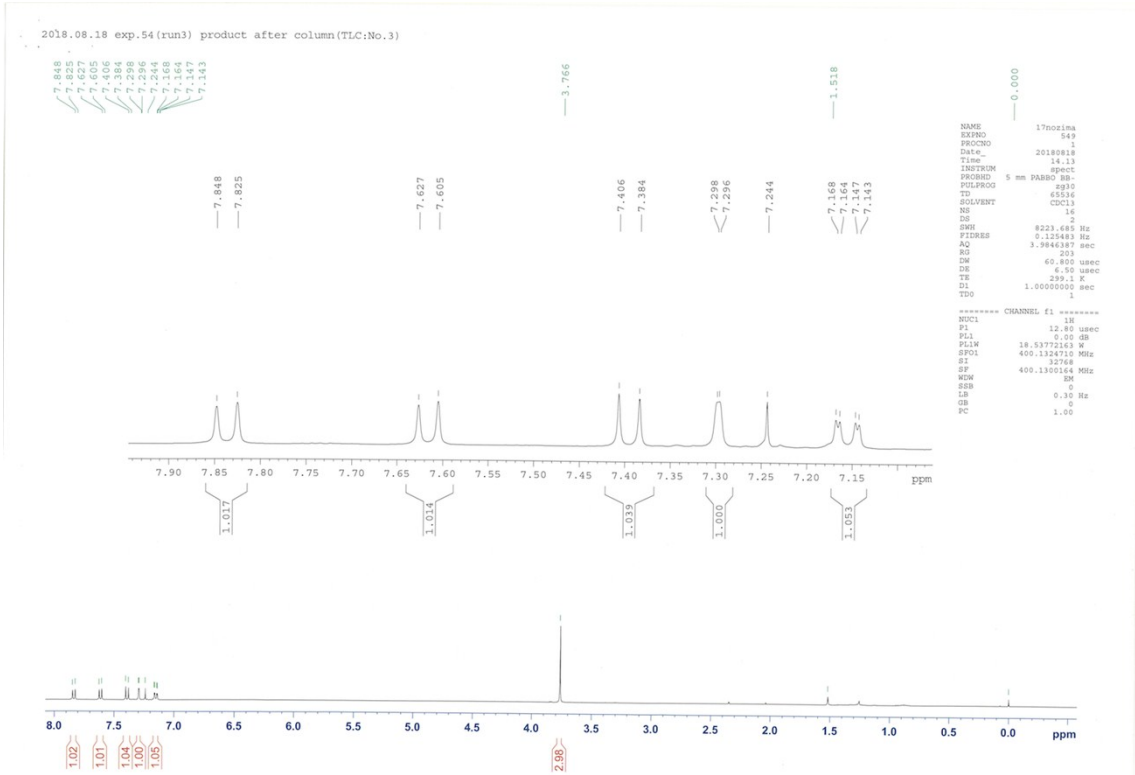


ii) ^{13}C NMR Spectrum

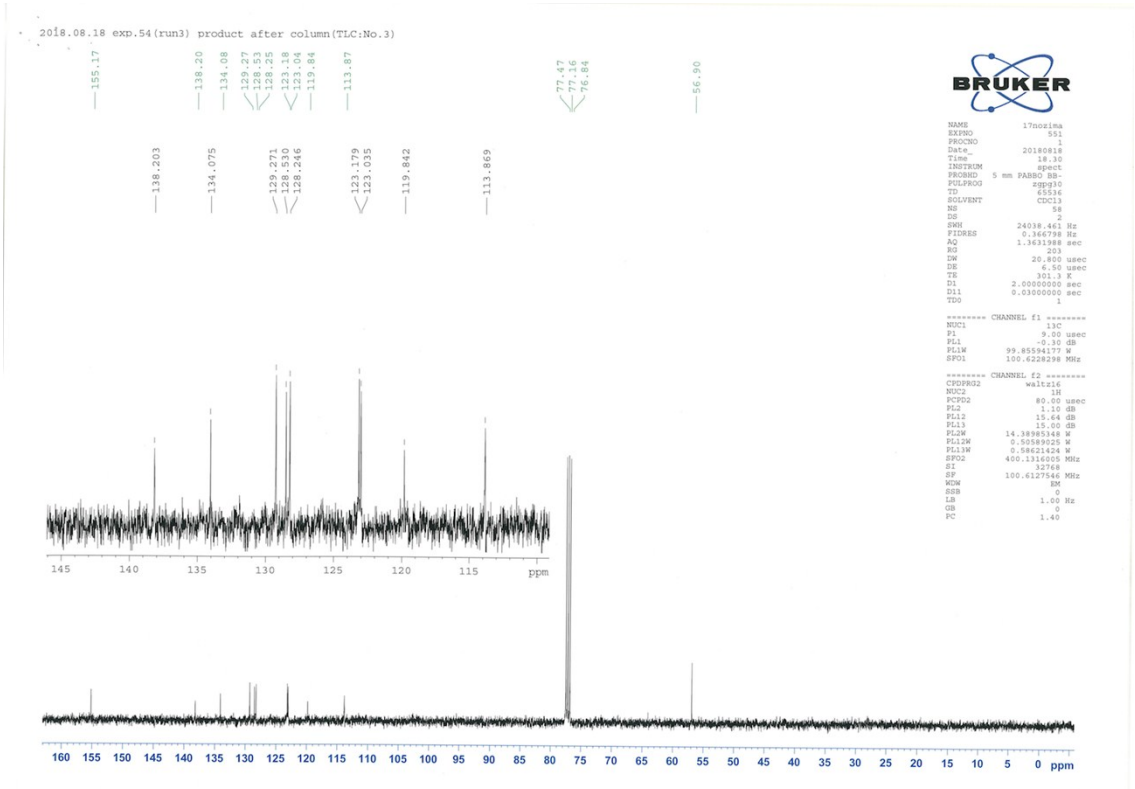


(c) (*R,R,R,R*)-**4**

i) ^{1}H NMR Spectrum

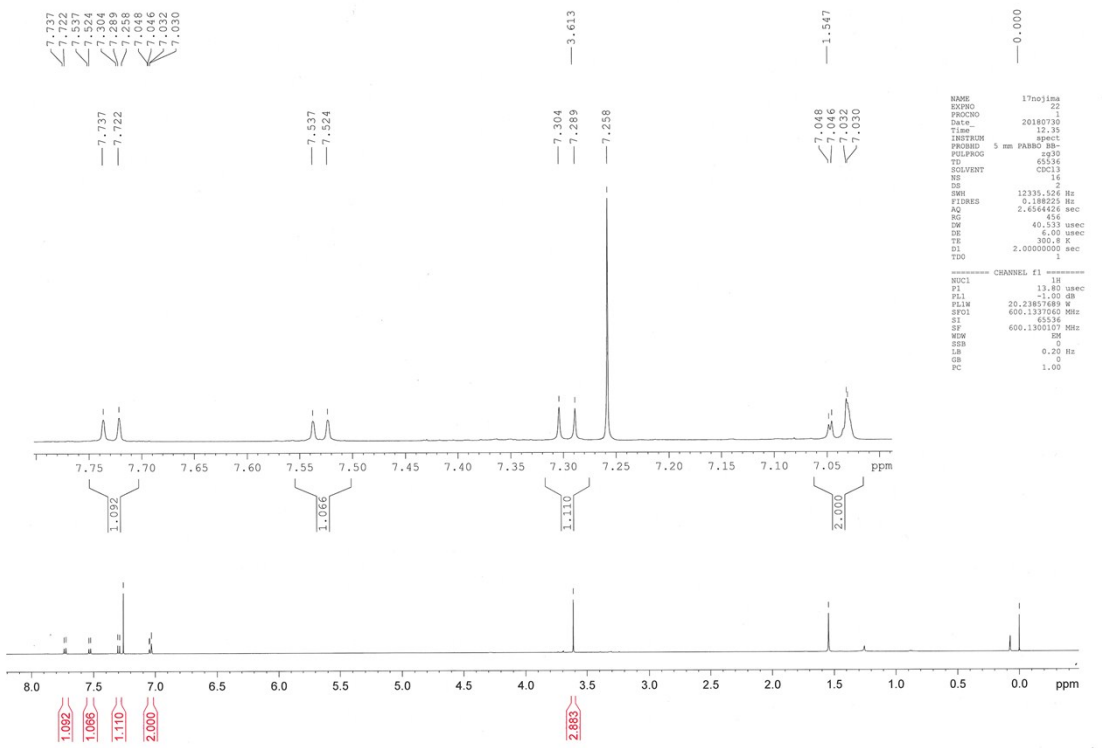


ii) ^{13}C NMR Spectrum

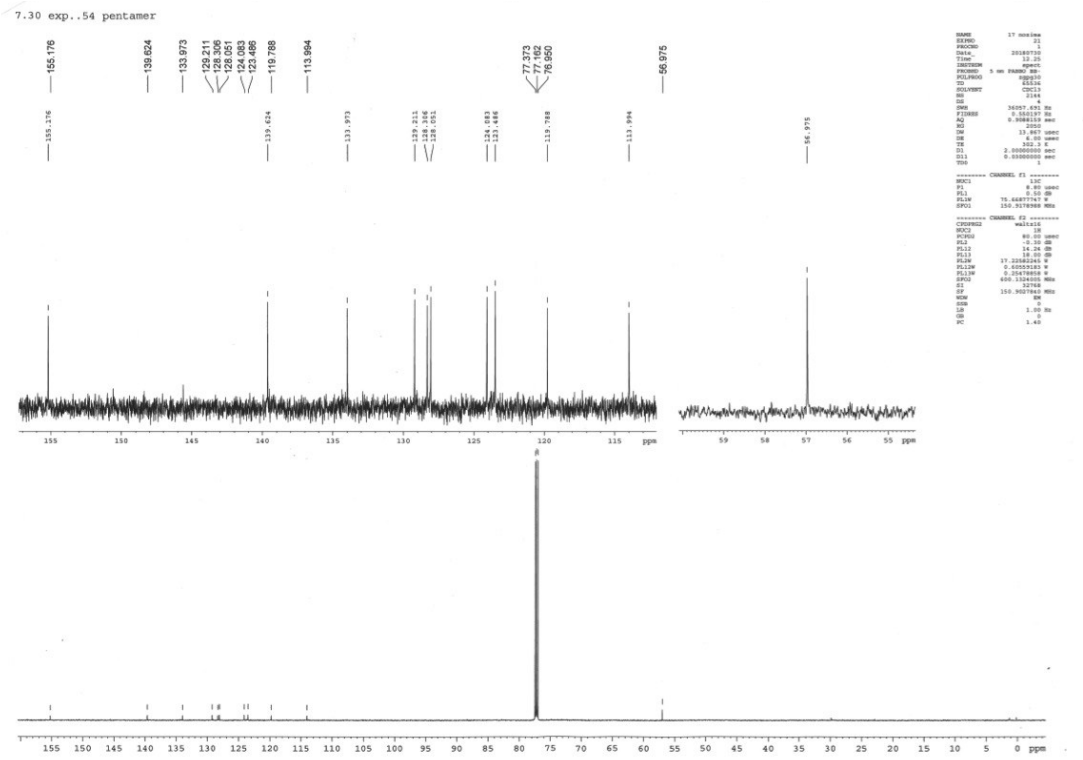


(d) (*R,R,R,R,R*)-**5**

i) ^{1}H NMR Spectrum



ii) ^{13}C NMR Spectrum



S6. UV, CD, PL, and CPL Spectra of 2–5

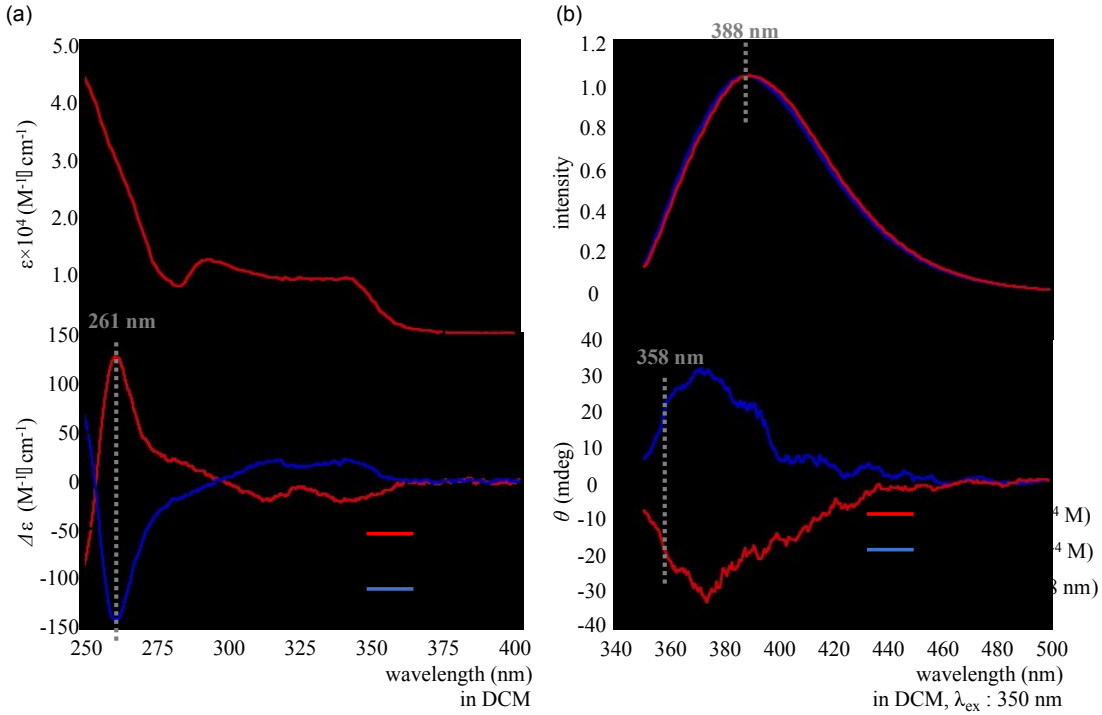


Fig. S5 *(a) UV-CD, and (b) PL-CPL spectra of* ***2*** *in* CH_2Cl_2.

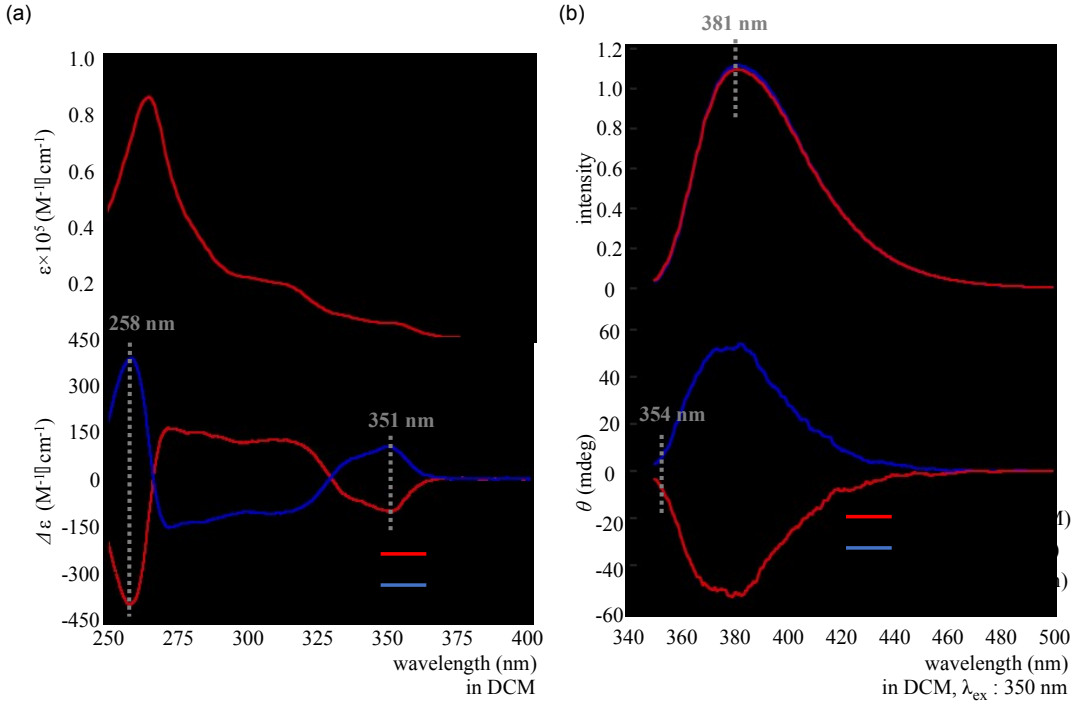


Fig. S6 *(a) UV-CD, and (b) PL-CPL spectra of* ***3*** *in* CH_2Cl_2.

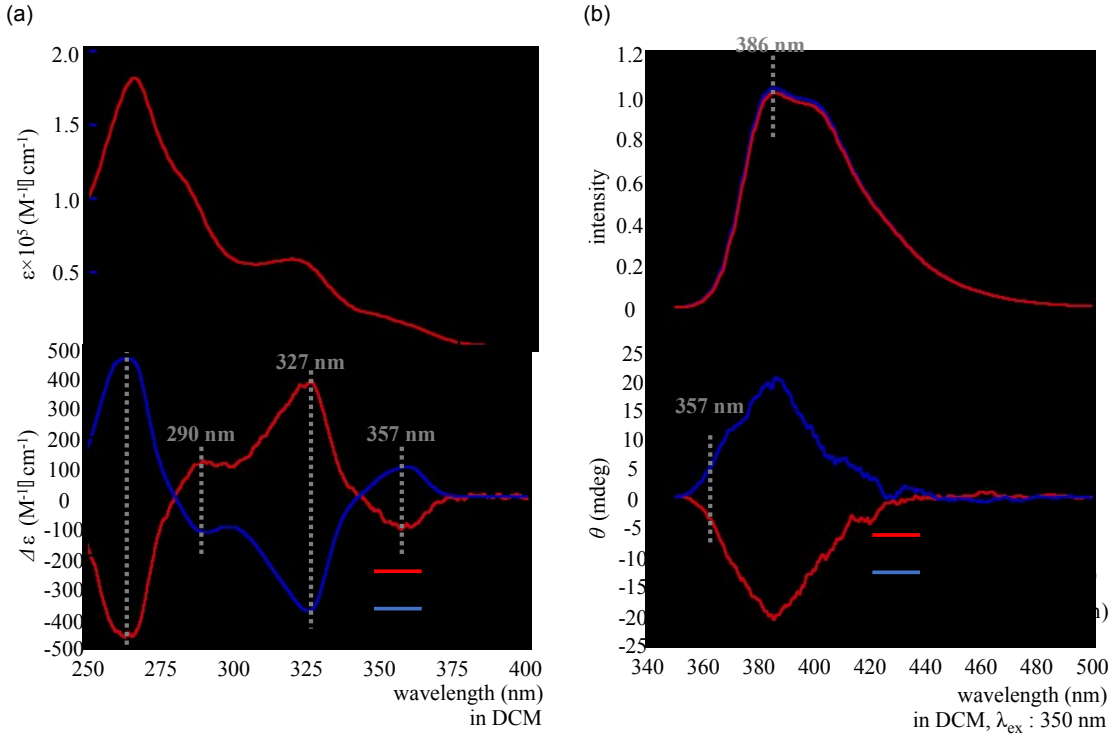


Fig. S7 *(a) UV-CD, and (b) PL-CPL spectra of* ***4*** *in* CH_2Cl_2.

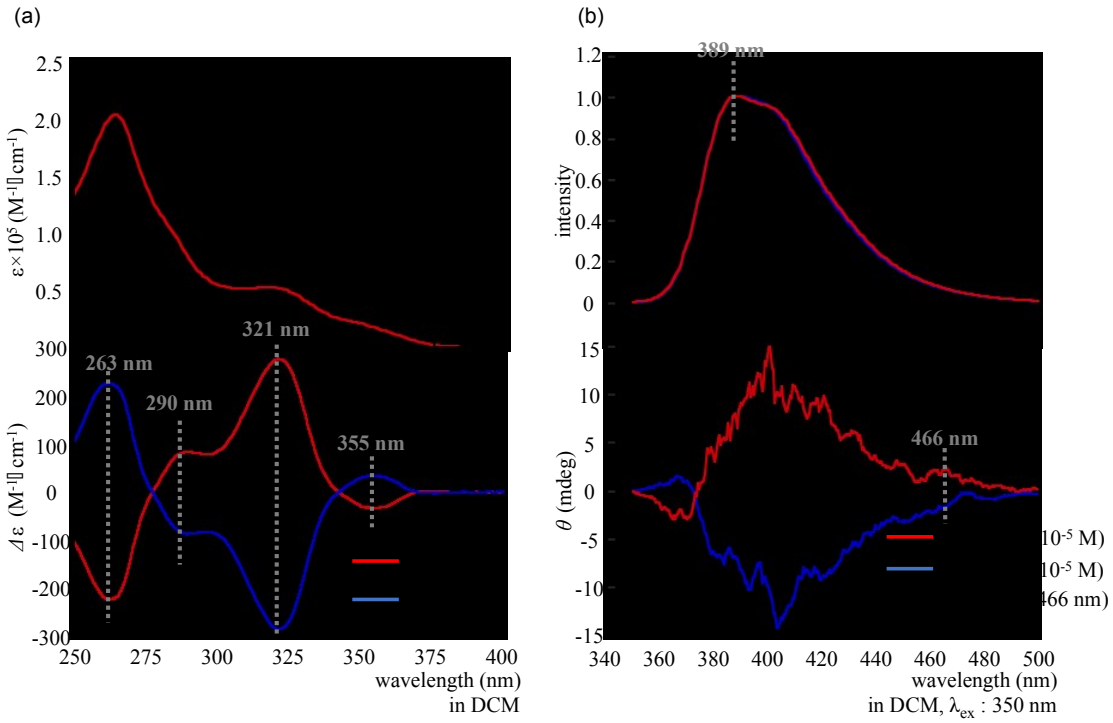


Fig. S8 *(a) UV-CD, and (b) PL-CPL spectra of* ***5*** *in* CH_2Cl_2.

S7. Summary of DFT-calculations

The geometry optimization of (*R,R*)-**2**, (*R*,*R*,*R*)-**3**, (*R*,*R*,*R*,*R*)-**4**, and (*R*,*R*,*R*,*R*,*R*)-**5** were performed by DFT calculations (Gaussian 16, Revision B.01)[2] with, B3LYP/6-31G(d,p) basis set. We found stable conformers having D_2, D_3, D_4, and D_5 symmetry for **2**, **3**, **4**, and **5** respectively. The results are summarized in Table S1 and Fig. S9.

Table S1. *Summary of DFT Calculations*

	(*R,R*)-**2**	(*R*,*R*,*R*)-**3**	(*R*,*R*,*R*,*R*)-**4**	(*R*,*R*,*R*,*R*,*R*)-**5**
Point Group	D_2	D_3	D_4	D_5
# of imaginary	0	0	0	0
Energy (HF)	–1996.8992531	–2995.3771797	–3993.8351661	–4992.2853075
Zero-point Energy (HF)	–1996.260078	–2994.417882	–3992.555651	-4990.685572
Energy/unit (HF)	–998.130039	–998.139294	–998.138912	–998.137114
Relative Energy/unit (kJ)	+24.3	0.00	+1.00	+5.72
Angle (°) θ_1	65.9	84.4	105.3	112.5
Angle (°) θ_2	76.4	39.9	32.3	26.3
E_{LUMO} (eV)	0.22	0.11	-0.02	-0.09
E_{HOMO} (eV)	-6.21	-6.32	-6.18	-6.13
E_{LUMO}-E_{HOMO} (eV)	6.43	6.43	6.16	6.04

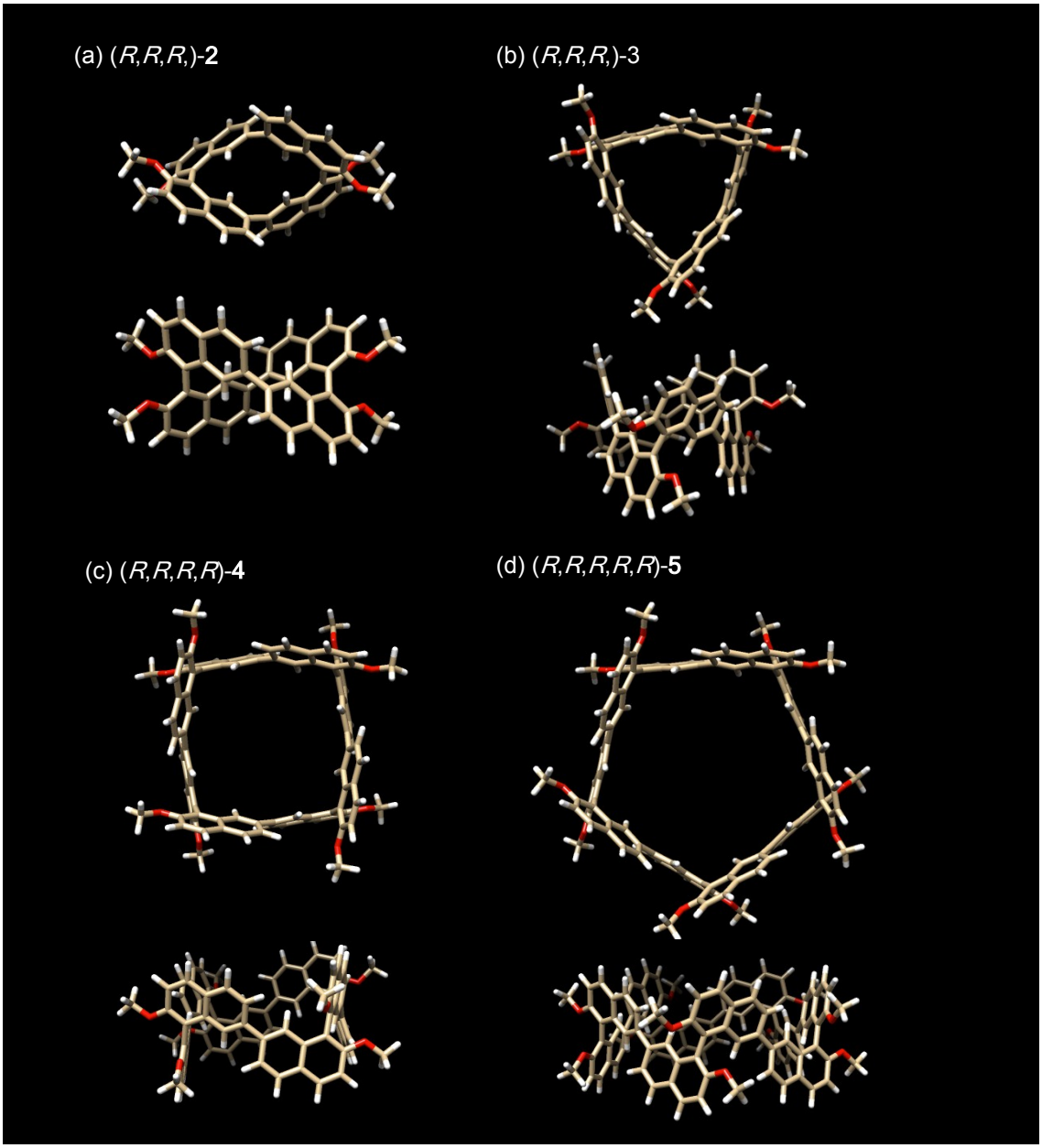


Fig. S9 *Optimized molecular structures of* ***2–5*** *in the (R)-configuration*

S8. Molecular Coordinate of Optimized Structures of 2–5

Table S2. *Atomic coordinate of optimized structure of (R,R)-**2** (D_2)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.809459	1.570105	0.186927
2	6	0	-3.794615	0.635325	0.396117
3	6	0	-2.776890	0.933170	1.359684
4	6	0	-2.805807	2.178266	2.072946
5	6	0	-3.881829	3.068073	1.848006
6	6	0	-4.861731	2.777381	0.928189
7	1	0	-1.632576	-0.882551	1.073764
8	6	0	-1.675396	0.064081	1.598178
9	6	0	-1.737417	2.503071	2.952009
10	1	0	-3.916733	4.004511	2.398641
11	1	0	-5.665400	3.484287	0.762613
12	6	0	-0.653462	1.670295	3.095145
13	6	0	-0.610652	0.431545	2.399396
14	1	0	-1.777756	3.447773	3.488765
15	1	0	0.178828	1.950709	3.733561
16	6	0	-3.794615	-0.635325	-0.396117
17	6	0	-4.809459	-1.570105	-0.186927
18	6	0	-2.776890	-0.933170	-1.359684
19	6	0	-4.861731	-2.777381	-0.928189
20	6	0	-2.805807	-2.178266	-2.072946
21	6	0	-1.675396	-0.064081	-1.598178
22	6	0	-3.881829	-3.068073	-1.848006
23	1	0	-5.665400	-3.484287	-0.762613
24	6	0	-1.737417	-2.503071	-2.952009
25	6	0	-0.610652	-0.431545	-2.399396
26	1	0	-1.632576	0.882551	-1.073764
27	1	0	-3.916733	-4.004511	-2.398641
28	6	0	-0.653462	-1.670295	-3.095145
29	1	0	-1.777756	-3.447773	-3.488765
30	1	0	0.178828	-1.950709	-3.733561
31	6	0	0.610652	-0.431545	2.399396
32	6	0	1.675396	-0.064081	1.598178
33	6	0	0.653462	-1.670295	3.095145
34	6	0	2.776890	-0.933170	1.359684
35	1	0	1.632576	0.882551	1.073764
36	6	0	1.737417	-2.503071	2.952009
37	1	0	-0.178828	-1.950709	3.733561
38	6	0	3.794615	-0.635325	0.396117

39	6	0	2.805807	-2.178266	2.072946
40	1	0	1.777756	-3.447773	3.488765
41	6	0	4.809459	-1.570105	0.186927
42	6	0	3.794615	0.635325	-0.396117
43	6	0	3.881829	-3.068073	1.848006
44	6	0	4.861731	-2.777381	0.928189
45	6	0	4.809459	1.570105	-0.186927
46	6	0	2.776890	0.933170	-1.359684
47	1	0	3.916733	-4.004511	2.398641
48	1	0	5.665400	-3.484287	0.762613
49	6	0	4.861731	2.777381	-0.928189
50	6	0	2.805807	2.178266	-2.072946
51	6	0	1.675396	0.064081	-1.598178
52	6	0	3.881829	3.068073	-1.848006
53	1	0	5.665400	3.484287	-0.762613
54	6	0	1.737417	2.503071	-2.952009
55	6	0	0.610652	0.431545	-2.399396
56	1	0	1.632576	-0.882551	-1.073764
57	1	0	3.916733	4.004511	-2.398641
58	6	0	0.653462	1.670295	-3.095145
59	1	0	1.777756	3.447773	-3.488765
60	1	0	-0.178828	1.950709	-3.733561
61	8	0	-5.729785	-1.263631	0.775174
62	8	0	-5.729785	1.263631	-0.775174
63	8	0	5.729785	-1.263631	-0.775174
64	8	0	5.729785	1.263631	0.775174
65	6	0	6.795173	-2.163289	-1.023411
66	1	0	7.389134	-1.708651	-1.817993
67	1	0	6.435430	-3.142842	-1.364221
68	1	0	7.429053	-2.302951	-0.138134
69	6	0	6.795173	2.163289	1.023411
70	1	0	7.389134	1.708651	1.817993
71	1	0	6.435430	3.142842	1.364221
72	1	0	7.429053	2.302951	0.138134
73	6	0	-6.795173	-2.163289	1.023411
74	1	0	-7.389134	-1.708651	1.817993
75	1	0	-6.435430	-3.142842	1.364221
76	1	0	-7.429053	-2.302951	0.138134
77	6	0	-6.795173	2.163289	-1.023411
78	1	0	-7.389134	1.708651	-1.817993
79	1	0	-6.435430	3.142842	-1.364221
80	1	0	-7.429053	2.302951	-0.138134

Compound: **2** (D_2)
Method: B3LYP/6-31G(d,p)
Key word: opt freq scf=(direct,tight)

Symmetry: D_2
# of imaginary frequencies: 0
Energy: –1996.8992531 Hartree

Table S3. *Atomic coordinate of optimized structure of (R,R,R)-**3** (D_3)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.322723	4.052835	1.837351
2	6	0	1.343250	4.060245	2.754490
3	6	0	2.654811	3.643871	2.400521
4	6	0	2.906057	3.207507	1.057925
5	6	0	1.827371	3.228367	0.131384
6	6	0	0.554902	3.635537	0.493482
7	1	0	3.535294	3.977229	4.346172
8	1	0	-0.668347	4.392420	2.120920
9	1	0	1.161296	4.395092	3.772797
10	6	0	3.721475	3.643038	3.328790
11	6	0	4.212438	2.760541	0.691293
12	1	0	2.010515	2.883784	-0.880034
13	6	0	5.228228	2.778780	1.642725
14	6	0	4.981519	3.224596	2.966055
15	1	0	5.779885	3.233941	3.698065
16	6	0	4.496918	2.267808	-0.691293
17	6	0	4.230811	0.912966	-1.057925
18	6	0	5.020608	3.138388	-1.642725
19	6	0	3.709533	-0.031634	-0.131384
20	6	0	4.483090	0.477198	-2.400521
21	6	0	5.283341	2.701824	-2.966055
22	6	0	3.425918	-1.337209	-0.493482
23	1	0	3.502687	0.299265	0.880034
24	6	0	4.187900	-0.866834	-2.754490
25	6	0	5.015702	1.401373	-3.328790
26	1	0	5.690617	3.388557	-3.698065
27	6	0	3.671219	-1.746931	-1.837351
28	1	0	4.386909	-1.191834	-3.772797
29	1	0	5.212028	1.073040	-4.346172
30	1	0	3.469774	-2.775016	-2.120920
31	8	0	5.252603	4.419998	-1.225702
32	8	0	6.454132	2.338889	1.225702
33	6	0	2.871016	-2.298328	0.493482
34	6	0	3.348496	-2.305904	1.837351
35	6	0	1.882162	-3.196733	0.131384
36	6	0	2.844651	-3.193411	2.754490

37	1	0	4.138121	-1.617404	2.120920
38	6	0	1.324754	-4.120473	1.057925
39	1	0	1.492172	-3.183049	-0.880034
40	6	0	1.828279	-4.121069	2.400521
41	1	0	3.225613	-3.203258	3.772797
42	6	0	0.284480	-5.028349	0.691293
43	6	0	1.294226	-5.044412	3.328790
44	6	0	-0.207620	-5.917168	1.642725
45	6	0	-0.284480	-5.028349	-0.691293
46	1	0	1.676734	-5.050268	4.346172
47	6	0	0.301822	-5.926419	2.966055
48	8	0	-1.201529	-6.758887	1.225702
49	6	0	-1.324754	-4.120473	-1.057925
50	6	0	0.207620	-5.917168	-1.642725
51	1	0	-0.089268	-6.622498	3.698065
52	6	0	-1.882162	-3.196733	-0.131384
53	6	0	-1.828279	-4.121069	-2.400521
54	6	0	-0.301822	-5.926419	-2.966055
55	8	0	1.201529	-6.758887	-1.225702
56	6	0	-2.871016	-2.298328	-0.493482
57	1	0	-1.492172	-3.183049	0.880034
58	6	0	-2.844651	-3.193411	-2.754490
59	6	0	-1.294226	-5.044412	-3.328790
60	1	0	0.089268	-6.622498	-3.698065
61	6	0	-3.348496	-2.305904	-1.837351
62	1	0	-3.225613	-3.203258	-3.772797
63	1	0	-1.676734	-5.050268	-4.346172
64	1	0	-4.138121	-1.617404	-2.120920
65	6	0	-0.554902	3.635537	-0.493482
66	6	0	-0.322723	4.052835	-1.837351
67	6	0	-1.827371	3.228367	-0.131384
68	6	0	-1.343250	4.060245	-2.754490
69	1	0	0.668347	4.392420	-2.120920
70	6	0	-2.906057	3.207507	-1.057925
71	1	0	-2.010515	2.883784	0.880034
72	6	0	-2.654811	3.643871	-2.400521
73	1	0	-1.161296	4.395092	-3.772797
74	6	0	-4.212438	2.760541	-0.691293
75	6	0	-3.721475	3.643038	-3.328790
76	6	0	-5.228228	2.778780	-1.642725
77	6	0	-4.496918	2.267808	0.691293
78	1	0	-3.535294	3.977229	-4.346172
79	6	0	-4.981519	3.224596	-2.966055
80	8	0	-6.454132	2.338889	-1.225702
81	6	0	-4.230811	0.912966	1.057925
82	6	0	-5.020608	3.138388	1.642725

83	1	0	-5.779885	3.233941	-3.698065
84	6	0	-3.709533	-0.031634	0.131384
85	6	0	-4.483090	0.477198	2.400521
86	6	0	-5.283341	2.701824	2.966055
87	8	0	-5.252603	4.419998	1.225702
88	6	0	-3.425918	-1.337209	0.493482
89	1	0	-3.502687	0.299265	-0.880034
90	6	0	-4.187900	-0.866834	2.754490
91	6	0	-5.015702	1.401373	3.328790
92	1	0	-5.690617	3.388557	3.698065
93	6	0	-3.671219	-1.746931	1.837351
94	1	0	-4.386909	-1.191834	3.772797
95	1	0	-5.212028	1.073040	4.346172
96	1	0	-3.469774	-2.775016	2.120920
97	6	0	-1.747641	-7.686173	2.147193
98	1	0	-0.991911	-8.392372	2.515073
99	1	0	-2.511757	-8.237627	1.596973
100	1	0	-2.216817	-7.185709	3.004367
101	6	0	1.747641	-7.686173	-2.147193
102	1	0	0.991911	-8.392372	-2.515073
103	1	0	2.511757	-8.237627	-1.596973
104	1	0	2.216817	-7.185709	-3.004367
105	6	0	-5.782600	5.356588	2.147193
106	1	0	-6.772052	5.055206	2.515073
107	1	0	-5.878116	6.294059	1.596973
108	1	0	-5.114598	5.512674	3.004367
109	6	0	-7.530241	2.329585	-2.147193
110	1	0	-7.763963	3.337166	-2.515073
111	1	0	-8.389873	1.943569	-1.596973
112	1	0	-7.331415	1.673034	-3.004367
113	6	0	5.782600	5.356588	-2.147193
114	1	0	6.772052	5.055206	-2.515073
115	1	0	5.878116	6.294059	-1.596973
116	1	0	5.114598	5.512674	-3.004367
117	6	0	7.530241	2.329585	2.147193
118	1	0	7.763963	3.337166	2.515073
119	1	0	8.389873	1.943569	1.596973
120	1	0	7.331415	1.673034	3.004367

Compound: **3** (D_3)
Method: B3LYP/6-31G(d,p)
Key word: opt freq scf=(direct,tight)
Symmetry: D_3
# of imaginary frequencies: 0
Energy: –2995.3771797 Hartrees

Table S4. *Atomic coordinate of optimized structure of (R,R,R,R)-**4** (D_4)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.546841	5.202090	0.502377
2	6	0	1.847169	4.883348	0.147965
3	6	0	2.918754	4.917392	1.081344
4	6	0	2.622382	5.270703	2.438543
5	6	0	1.281280	5.580422	2.791077
6	6	0	0.276450	5.555570	1.858284
7	1	0	2.065918	4.577166	-0.868250
8	6	0	4.265030	4.618282	0.704648
9	6	0	3.674991	5.310827	3.381204
10	1	0	1.065573	5.857477	3.820116
11	1	0	-0.733316	5.833015	2.142012
12	6	0	4.969761	5.023914	3.014102
13	6	0	5.267302	4.682700	1.670562
14	1	0	3.451237	5.576695	4.411058
15	1	0	5.758779	5.066915	3.754910
16	6	0	4.618282	4.265030	-0.704648
17	6	0	4.917392	2.918754	-1.081344
18	6	0	4.682700	5.267302	-1.670562
19	6	0	5.270703	2.622382	-2.438543
20	6	0	4.883348	1.847169	-0.147965
21	6	0	5.023914	4.969761	-3.014102
22	6	0	5.580422	1.281280	-2.791077
23	6	0	5.310827	3.674991	-3.381204
24	6	0	5.202090	0.546841	-0.502377
25	1	0	4.577166	2.065918	0.868250
26	1	0	5.066915	5.758779	-3.754910
27	6	0	5.555570	0.276450	-1.858284
28	1	0	5.857477	1.065573	-3.820116
29	1	0	5.576695	3.451237	-4.411058
30	1	0	5.833015	-0.733316	-2.142012
31	8	0	6.536758	4.402973	1.244111
32	8	0	4.402973	6.536758	-1.244111
33	6	0	7.603681	4.454851	2.175207
34	1	0	7.723865	5.457734	2.605132
35	1	0	8.502208	4.198666	1.611795
36	1	0	7.474738	3.729975	2.989566
37	6	0	4.454851	7.603681	-2.175207
38	1	0	5.457734	7.723865	-2.605132
39	1	0	4.198666	8.502208	-1.611795
40	1	0	3.729975	7.474738	-2.989566
41	6	0	5.202090	-0.546841	0.502377

42	6	0	4.883348	-1.847169	0.147965
43	6	0	5.555570	-0.276450	1.858284
44	6	0	4.917392	-2.918754	1.081344
45	1	0	4.577166	-2.065918	-0.868250
46	6	0	5.580422	-1.281280	2.791077
47	1	0	5.833015	0.733316	2.142012
48	6	0	5.270703	-2.622382	2.438543
49	6	0	4.618282	-4.265030	0.704648
50	1	0	5.857477	-1.065573	3.820116
51	6	0	5.310827	-3.674991	3.381204
52	6	0	4.682700	-5.267302	1.670562
53	6	0	4.265030	-4.618282	-0.704648
54	6	0	5.023914	-4.969761	3.014102
55	1	0	5.576695	-3.451237	4.411058
56	8	0	4.402973	-6.536758	1.244111
57	6	0	2.918754	-4.917392	-1.081344
58	6	0	5.267302	-4.682700	-1.670562
59	1	0	5.066915	-5.758779	3.754910
60	6	0	4.454851	-7.603681	2.175207
61	6	0	2.622382	-5.270703	-2.438543
62	6	0	1.847169	-4.883348	-0.147965
63	6	0	4.969761	-5.023914	-3.014102
64	8	0	6.536758	-4.402973	-1.244111
65	1	0	5.457734	-7.723865	2.605132
66	1	0	4.198666	-8.502208	1.611795
67	1	0	3.729975	-7.474738	2.989566
68	6	0	1.281280	-5.580422	-2.791077
69	6	0	3.674991	-5.310827	-3.381204
70	6	0	0.546841	-5.202090	-0.502377
71	1	0	2.065918	-4.577166	0.868250
72	1	0	5.758779	-5.066915	-3.754910
73	6	0	7.603681	-4.454851	-2.175207
74	6	0	0.276450	-5.555570	-1.858284
75	1	0	1.065573	-5.857477	-3.820116
76	1	0	3.451237	-5.576695	-4.411058
77	1	0	7.723865	-5.457734	-2.605132
78	1	0	8.502208	-4.198666	-1.611795
79	1	0	7.474738	-3.729975	-2.989566
80	1	0	-0.733316	-5.833015	-2.142012
81	6	0	-0.546841	-5.202090	0.502377
82	6	0	-1.847169	-4.883348	0.147965
83	6	0	-0.276450	-5.555570	1.858284
84	6	0	-2.918754	-4.917392	1.081344
85	1	0	-2.065918	-4.577166	-0.868250
86	6	0	-1.281280	-5.580422	2.791077
87	1	0	0.733316	-5.833015	2.142012

88	6	0	-4.265030	-4.618282	0.704648
89	6	0	-2.622382	-5.270703	2.438543
90	1	0	-1.065573	-5.857477	3.820116
91	6	0	-4.618282	-4.265030	-0.704648
92	6	0	-5.267302	-4.682700	1.670562
93	6	0	-3.674991	-5.310827	3.381204
94	6	0	-4.917392	-2.918754	-1.081344
95	6	0	-4.682700	-5.267302	-1.670562
96	6	0	-4.969761	-5.023914	3.014102
97	8	0	-6.536758	-4.402973	1.244111
98	1	0	-3.451237	-5.576695	4.411058
99	6	0	-4.883348	-1.847169	-0.147965
100	6	0	-5.270703	-2.622382	-2.438543
101	6	0	-5.023914	-4.969761	-3.014102
102	8	0	-4.402973	-6.536758	-1.244111
103	1	0	-5.758779	-5.066915	3.754910
104	6	0	-7.603681	-4.454851	2.175207
105	6	0	-5.202090	-0.546841	-0.502377
106	1	0	-4.577166	-2.065918	0.868250
107	6	0	-5.580422	-1.281280	-2.791077
108	6	0	-5.310827	-3.674991	-3.381204
109	1	0	-5.066915	-5.758779	-3.754910
110	6	0	-4.454851	-7.603681	-2.175207
111	1	0	-7.723865	-5.457734	2.605132
112	1	0	-8.502208	-4.198666	1.611795
113	1	0	-7.474738	-3.729975	2.989566
114	6	0	-5.202090	0.546841	0.502377
115	6	0	-5.555570	-0.276450	-1.858284
116	1	0	-5.857477	-1.065573	-3.820116
117	1	0	-5.576695	-3.451237	-4.411058
118	1	0	-5.457734	-7.723865	-2.605132
119	1	0	-4.198666	-8.502208	-1.611795
120	1	0	-3.729975	-7.474738	-2.989566
121	6	0	-4.883348	1.847169	0.147965
122	6	0	-5.555570	0.276450	1.858284
123	1	0	-5.833015	0.733316	-2.142012
124	6	0	-4.917392	2.918754	1.081344
125	1	0	-4.577166	2.065918	-0.868250
126	6	0	-5.580422	1.281280	2.791077
127	1	0	-5.833015	-0.733316	2.142012
128	6	0	-4.618282	4.265030	0.704648
129	6	0	-5.270703	2.622382	2.438543
130	1	0	-5.857477	1.065573	3.820116
131	6	0	-4.265030	4.618282	-0.704648
132	6	0	-4.682700	5.267302	1.670562
133	6	0	-5.310827	3.674991	3.381204

134	6	0	-2.918754	4.917392	-1.081344
135	6	0	-5.267302	4.682700	-1.670562
136	6	0	-5.023914	4.969761	3.014102
137	8	0	-4.402973	6.536758	1.244111
138	1	0	-5.576695	3.451237	4.411058
139	6	0	-1.847169	4.883348	-0.147965
140	6	0	-2.622382	5.270703	-2.438543
141	6	0	-4.969761	5.023914	-3.014102
142	8	0	-6.536758	4.402973	-1.244111
143	1	0	-5.066915	5.758779	3.754910
144	6	0	-4.454851	7.603681	2.175207
145	6	0	-0.546841	5.202090	-0.502377
146	1	0	-2.065918	4.577166	0.868250
147	6	0	-1.281280	5.580422	-2.791077
148	6	0	-3.674991	5.310827	-3.381204
149	1	0	-5.758779	5.066915	-3.754910
150	6	0	-7.603681	4.454851	-2.175207
151	1	0	-5.457734	7.723865	2.605132
152	1	0	-4.198666	8.502208	1.611795
153	1	0	-3.729975	7.474738	2.989566
154	6	0	-0.276450	5.555570	-1.858284
155	1	0	-1.065573	5.857477	-3.820116
156	1	0	-3.451237	5.576695	-4.411058
157	1	0	-7.723865	5.457734	-2.605132
158	1	0	-8.502208	4.198666	-1.611795
159	1	0	-7.474738	3.729975	-2.989566
160	1	0	0.733316	5.833015	-2.142012

Compound: **4** (D_4)
Method: B3LYP/6-31G(d,p)
Key word: opt freq scf=(direct,tight)
Symmetry: D_4
# of imaginary frequencies: 0
Energy: –3993.8351661 Hartrees

***Table S5**. Atomic coordinate of optimized structure of (R,R,R,R)-**5** (D_5)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.541382	6.608690	0.509100
2	6	0	1.860883	6.368694	0.161500
3	6	0	2.927883	6.477197	1.094401
4	6	0	2.603481	6.783796	2.456201
5	6	0	1.242281	6.985492	2.809600
6	6	0	0.245581	6.918889	1.871000
7	1	0	2.105284	6.089094	-0.855700
8	6	0	4.297383	6.320400	0.708701
9	6	0	3.647581	6.904398	3.400801
10	1	0	1.004580	7.226091	3.843000
11	1	0	-0.778019	7.134087	2.157500
12	6	0	4.963281	6.756802	3.026801
13	6	0	5.290282	6.479503	1.675701
14	1	0	3.400780	7.128698	4.435201
15	1	0	5.746381	6.866304	3.767001
16	6	0	4.683093	6.040165	-0.708701
17	6	0	5.255414	4.786146	-1.094401
18	6	0	4.527586	7.033634	-1.675701
19	6	0	5.647253	4.572366	-2.456201
20	6	0	5.481943	3.737840	-0.161500
21	6	0	4.892362	6.808328	-3.026801
22	6	0	6.259712	3.340115	-2.809600
23	6	0	5.439309	5.602632	-3.400801
24	6	0	6.117942	2.557083	-0.509100
25	1	0	5.140504	3.883878	0.855700
26	1	0	4.754514	7.586938	-3.767001
27	6	0	6.504366	2.371616	-1.871000
28	1	0	6.561989	3.188397	-3.843000
29	1	0	5.728896	5.437223	-4.435201
30	1	0	7.025341	1.464614	-2.157500
31	8	0	6.582783	6.360006	1.243602
32	8	0	4.014534	8.225949	-1.243602
33	6	0	6.452534	1.527312	0.509100
34	6	0	6.632032	0.198230	0.161500
35	6	0	6.656144	1.904493	1.871000
36	6	0	7.064945	-0.783018	1.094401
37	1	0	6.441641	-0.120611	-0.855700
38	6	0	7.027484	0.977156	2.809600
39	1	0	6.544498	2.944494	2.157500
40	6	0	7.256293	-0.379750	2.456201
41	6	0	7.339022	-2.133943	0.708701

42	1	0	7.182854	1.277573	3.843000
43	6	0	7.693638	-1.335479	3.400801
44	6	0	7.797161	-3.029081	1.675701
45	6	0	7.191694	-2.587373	-0.708701
46	6	0	7.959839	-2.632394	3.026801
47	1	0	7.830693	-1.031445	4.435201
48	8	0	8.082917	-4.295249	1.243602
49	6	0	6.175907	-3.519196	-1.094401
50	6	0	8.088485	-2.132478	-1.675701
51	1	0	8.305973	-3.343328	3.767001
52	6	0	6.093676	-3.957918	-2.456201
53	6	0	5.248910	-4.058582	-0.161500
54	6	0	7.986928	-2.549024	-3.026801
55	8	0	9.063901	-1.276090	-1.243602
56	6	0	5.110996	-4.921187	-2.809600
57	6	0	7.009259	-3.441781	-3.400801
58	6	0	4.322478	-5.028326	-0.509100
59	1	0	5.282290	-3.688726	0.855700
60	1	0	8.684832	-2.177319	-3.767001
61	6	0	4.265501	-5.453150	-1.871000
62	1	0	5.060112	-5.255553	-3.843000
63	1	0	6.941432	-3.768309	-4.435201
64	1	0	3.563880	-6.228906	-2.157500
65	6	0	3.446503	-5.664759	0.509100
66	6	0	2.237938	-6.246181	0.161500
67	6	0	3.868142	-5.741848	1.871000
68	6	0	1.438494	-6.961128	1.094401
69	1	0	1.875869	-6.163636	-0.855700
70	6	0	3.100943	-6.381576	2.809600
71	1	0	4.822742	-5.314289	2.157500
72	6	0	1.881154	-7.018494	2.456201
73	1	0	3.434668	-6.436508	3.843000
74	6	0	-0.471372	-8.351578	1.675701
75	6	0	1.107349	-7.729770	3.400801
76	6	0	-7.064945	-0.783018	-1.094401
77	6	0	-7.797161	-3.029081	-1.675701
78	6	0	-0.043830	-8.383711	3.026801
79	8	0	-1.587265	-9.014616	1.243602
80	1	0	1.438855	-7.766166	4.435201
81	6	0	-6.632032	0.198230	-0.161500
82	6	0	-7.256293	-0.379750	-2.456201
83	6	0	-7.959839	-2.632394	-3.026801
84	8	0	-8.082917	-4.295249	-1.243602
85	1	0	-0.613008	-8.932595	3.767001
86	6	0	-6.452534	1.527312	-0.509100
87	1	0	-6.441641	-0.120611	0.855700

88	6	0	-7.027484	0.977156	-2.809600
89	6	0	-7.693638	-1.335479	-3.400801
90	1	0	-8.305973	-3.343328	-3.767001
91	6	0	-6.117942	2.557083	0.509100
92	6	0	-6.656144	1.904493	-1.871000
93	1	0	-7.182854	1.277573	-3.843000
94	1	0	-7.830693	-1.031445	-4.435201
95	6	0	-5.481943	3.737840	0.161500
96	6	0	-6.504366	2.371616	1.871000
97	1	0	-6.544498	2.944494	-2.157500
98	6	0	-5.255414	4.786146	1.094401
99	1	0	-5.140504	3.883878	-0.855700
100	6	0	-6.259712	3.340115	2.809600
101	1	0	-7.025341	1.464614	2.157500
102	6	0	-4.683093	6.040165	0.708701
103	6	0	-5.647253	4.572366	2.456201
104	1	0	-6.561989	3.188397	3.843000
105	6	0	-4.297383	6.320400	-0.708701
106	6	0	-4.527586	7.033634	1.675701
107	6	0	-5.439309	5.602632	3.400801
108	6	0	-2.927883	6.477197	-1.094401
109	6	0	-5.290282	6.479503	-1.675701
110	6	0	-4.892362	6.808328	3.026801
111	8	0	-4.014534	8.225949	1.243602
112	1	0	-5.728896	5.437223	4.435201
113	6	0	-1.860883	6.368694	-0.161500
114	6	0	-2.603481	6.783796	-2.456201
115	6	0	-4.963281	6.756802	-3.026801
116	8	0	-6.582783	6.360006	-1.243602
117	1	0	-4.754514	7.586938	3.767001
118	6	0	-0.541382	6.608690	-0.509100
119	1	0	-2.105284	6.089094	0.855700
120	6	0	-1.242281	6.985492	-2.809600
121	6	0	-3.647581	6.904398	-3.400801
122	1	0	-5.746381	6.866304	-3.767001
123	6	0	-0.245581	6.918889	-1.871000
124	1	0	-1.004580	7.226091	-3.843000
125	1	0	-3.400780	7.128698	-4.435201
126	1	0	0.778019	7.134087	-2.157500
127	6	0	-7.339022	-2.133943	-0.708701
128	6	0	0.238382	-7.639250	0.708701
129	6	0	-7.191694	-2.587373	0.708701
130	6	0	-6.175907	-3.519196	1.094401
131	6	0	-8.088485	-2.132478	1.675701
132	6	0	-5.248910	-4.058582	0.161500
133	6	0	-6.093676	-3.957918	2.456201

134	6	0	-7.986928	-2.549024	3.026801
135	6	0	-4.322478	-5.028326	0.509100
136	1	0	-5.282290	-3.688726	-0.855700
137	6	0	-5.110996	-4.921187	2.809600
138	6	0	-7.009259	-3.441781	3.400801
139	1	0	-8.684832	-2.177319	3.767001
140	6	0	-4.265501	-5.453150	1.871000
141	1	0	-5.060112	-5.255553	3.843000
142	1	0	-6.941432	-3.768309	4.435201
143	1	0	-3.563880	-6.228906	2.157500
144	6	0	-0.238382	-7.639250	-0.708701
145	6	0	-1.438494	-6.961128	-1.094401
146	6	0	0.471372	-8.351578	-1.675701
147	6	0	-2.237938	-6.246181	-0.161500
148	6	0	-1.881154	-7.018494	-2.456201
149	6	0	0.043830	-8.383711	-3.026801
150	6	0	-3.446503	-5.664759	-0.509100
151	1	0	-1.875869	-6.163636	0.855699
152	6	0	-3.100943	-6.381576	-2.809600
153	6	0	-1.107349	-7.729770	-3.400801
154	1	0	0.613008	-8.932595	-3.767001
155	6	0	-3.868142	-5.741848	-1.871000
156	1	0	-3.434668	-6.436508	-3.843000
157	1	0	-1.438855	-7.766166	-4.435201
158	1	0	-4.822742	-5.314289	-2.157500
159	8	0	1.587265	-9.014616	-1.243602
160	8	0	-9.063901	-1.276090	1.243602
161	6	0	2.342826	-9.774705	-2.170799
162	1	0	1.748929	-10.582407	-2.618000
163	1	0	3.163527	-10.209703	-1.598599
164	1	0	2.759425	-9.151004	-2.972399
165	6	0	10.020270	-0.792390	-2.170799
166	1	0	10.604915	-1.606813	-2.618000
167	1	0	10.687588	-0.146278	-1.598599
168	1	0	9.555831	-0.203447	-2.972399
169	6	0	3.850041	9.284981	-2.170799
170	1	0	4.805270	9.589341	-2.618000
171	1	0	3.441765	10.119298	-1.598599
172	1	0	3.146403	9.025267	-2.972399
173	6	0	-7.640814	6.530824	-2.170799
174	1	0	-7.635096	7.533352	-2.618000
175	1	0	-8.560460	6.400348	-1.598599
176	1	0	-7.611247	5.781368	-2.972399
177	6	0	-8.572324	-5.248710	-2.170799
178	1	0	-9.524018	-4.933473	-2.618000
179	1	0	-8.732421	-6.163665	-1.598599

180	1	0	-7.850413	-5.452185	-2.972399
181	6	0	-2.342826	-9.774705	2.170799
182	1	0	-1.748929	-10.582407	2.618000
183	1	0	-3.163527	-10.209703	1.598599
184	1	0	-2.759425	-9.151004	2.972399
185	6	0	8.572324	-5.248710	2.170799
186	1	0	9.524018	-4.933473	2.618000
187	1	0	8.732421	-6.163665	1.598599
188	1	0	7.850413	-5.452185	2.972399
189	6	0	7.640814	6.530824	2.170799
190	1	0	7.635096	7.533352	2.618000
191	1	0	8.560460	6.400348	1.598599
192	1	0	7.611247	5.781368	2.972399
193	6	0	-3.850041	9.284981	2.170799
194	1	0	-4.805270	9.589341	2.618000
195	1	0	-3.441765	10.119298	1.598599
196	1	0	-3.146403	9.025267	2.972399
197	6	0	-10.020270	-0.792390	2.170799
198	1	0	-10.604915	-1.606813	2.618000
199	1	0	-10.687588	-0.146278	1.598599
200	1	0	-9.555831	-0.203447	2.972399

Compound: **5** (D_5)
Method: B3LYP/6-31G(d,p)
Key word: opt freq scf=(direct,tight)
Symmetry: D_5
# of imaginary frequencies: 0
Energy: –4992.2853075 Hartrees

S9. TD-DFT Calculations

The optimized D_n structures of **2**–**5** in the (*R*) configuration were applied for the excitation energy and the simulation of the CD calculation using time-dependent density functional theory (TD-DFT) with CAM-B3LYP /6-31G(d,p) basis set. Selected excitation energies and their transition nature are listed as follow.

1. TD-DFT Calculation for (*R*,*R*)-**2**

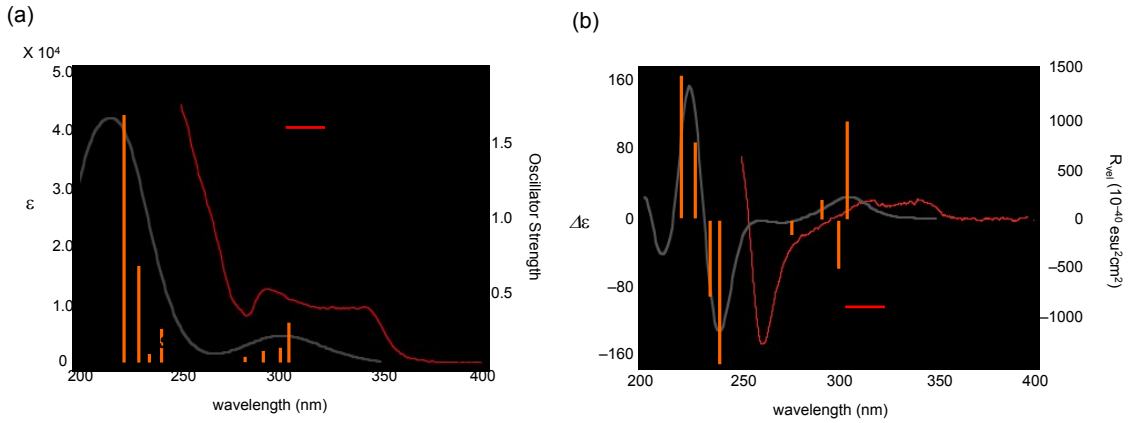


Fig. S10 *Simulated (a) UV (isovalue : 0.30) and (b) CD (isovalue : 0.15) spectra of (R,R)-**2** from TD-DFT calculation.*

Table S6. *Selected electronic transition for (R,R)-**2***

State	Excitation energies / nm (oscillator strengths, R_{vel} in CD)	Nature
S_1	303 (0.2924, +672.9)	164 -> 165 0.51714
S_2	300 (0.0810, –361.8)	163 ->165 0.45354 164 ->167 0.43087
S_3	291 (0.0609, +114.9)	162 ->165 0.30161 163 ->168 0.27105 164 ->166 0.38914
S_7	274 (0.013, –89.78)	157 ->165 -0.23395 159 ->167 -0.24960 161 ->166 -0.23311 164 ->167 0.25102
S_{13}	239 (0.3045, –1483.1)	162 ->169 -0.23689 163 ->167 0.39801 164 ->170 0.31361
S_{17}	235 (0.0483, –696.1)	163 ->167 -0.34270 164 ->165 0.35263

		164 ->170	0.24142
S_{18}	226 (0.6541, +619.2)	160 ->165 161 ->167 163 ->168	-0.30759 0.35799 -0.31523
S_{22}	223 (1.6297, +1478.3)	159 ->166 161 ->167 164 ->169	-0.24549 0.30120 0.40592

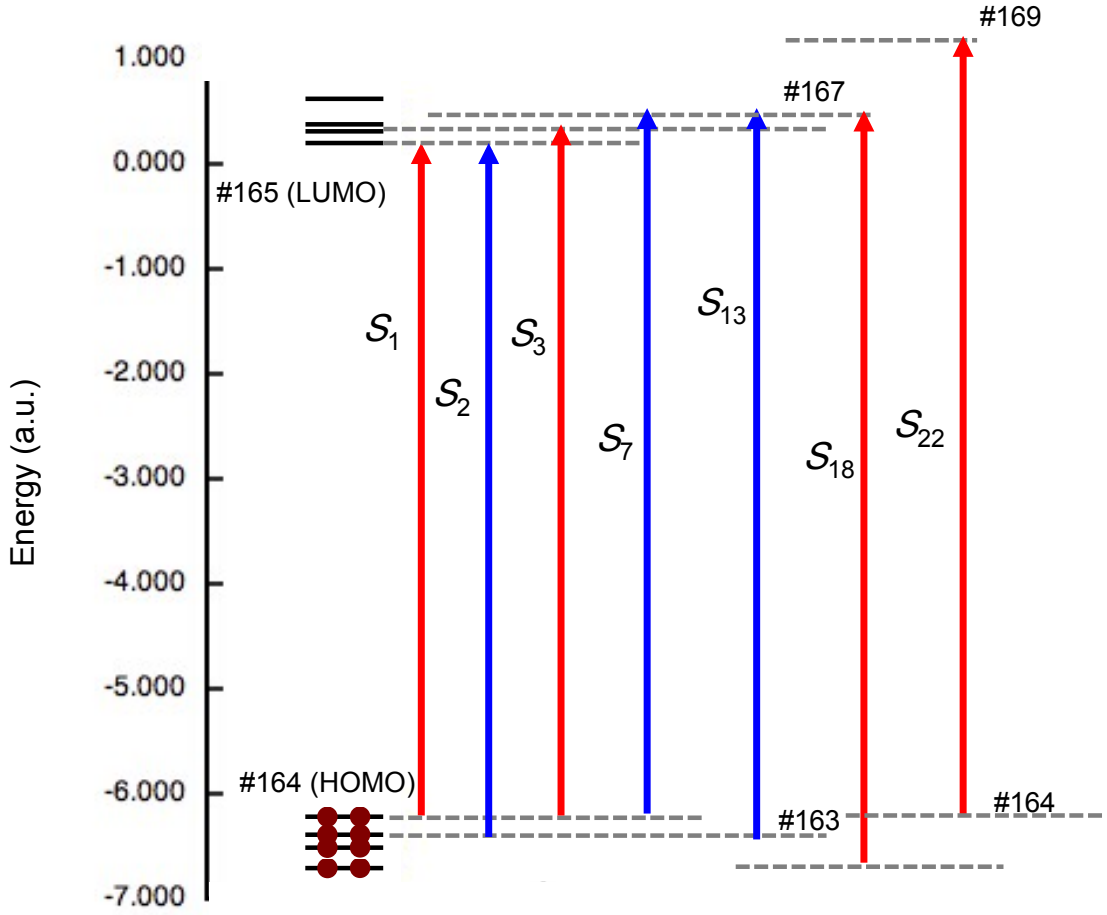
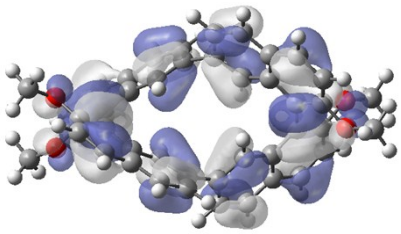
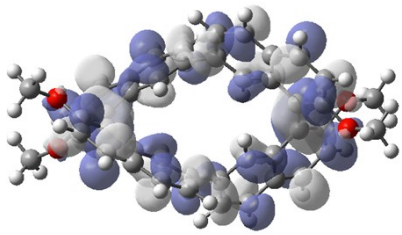


Fig. S11 *Excitation and energy diagram of (R,R)-**2***

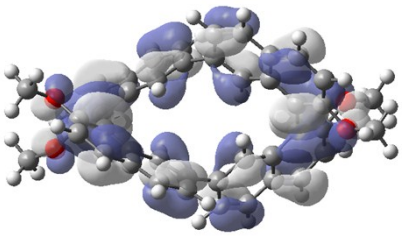
#164 (HOMO)



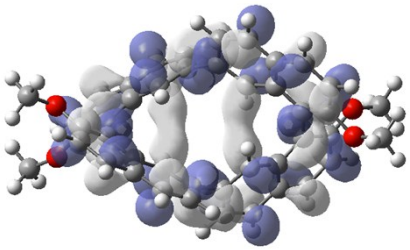
#167



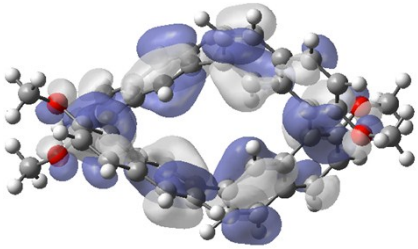
#163



#166



#162



#165 (LUMO)

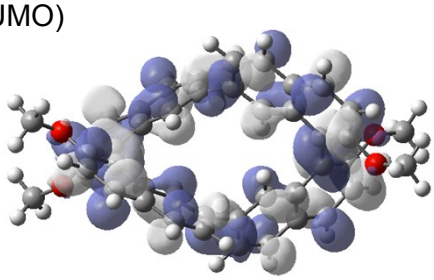


Fig. S12 *MO of (R,R)-**2***

2. TD-DFT Calculation for (*R*,*R*,*R*)-**3**

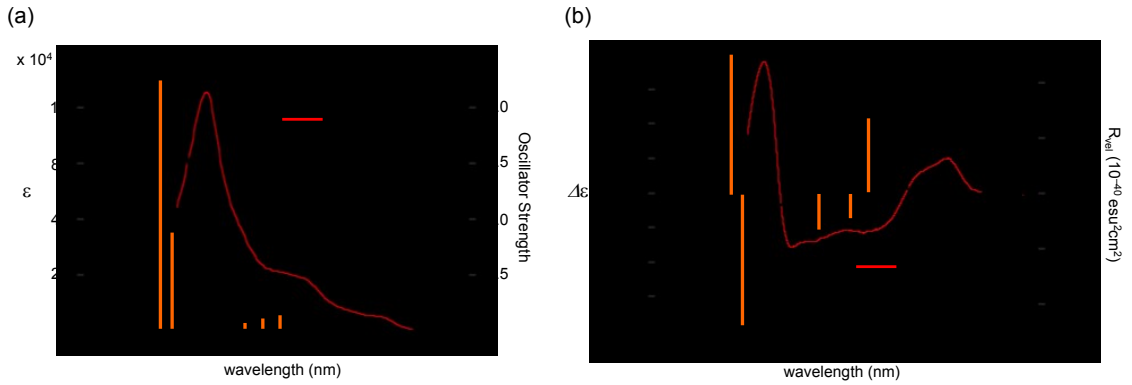


Fig. S13 *Simulated (a) UV (isovalue : 0.30) and (b) CD (isovalue : 0.15) spectra of (R,R,R)-**3** from TD-DFT calculation.*

Table S7. *Selected electronic transition for (R,R,R)-**3***

State	Excitation energies / nm (oscillator strengths, R_{vel} in CD)	Nature	
S_1	309 (0.1191, +1311)	244 -> 247	0.36550
		245 -> 249	0.36374
		246 -> 248	0.36374
S_2	301 (0.0984, –367)	241 -> 247	0.27995
		243 -> 248	0.27179
		244 -> 249	–0.20880
S_7	286 (0.0804, –736)	238 -> 247	0.32982
		239 -> 248	–0.32428
		240 -> 249	0.32428
S_{19}	247 (0.8087, –5340)	241 -> 252	–0.27404
		242 -> 251	0.27404
		243 -> 250	0.25630
		244 -> 253	0.26291
		245 -> 254	0.23618
		246 -> 255	0.23618
S_{20}	242 (2.1777, +3008)	242 -> 250	0.23963
		243 -> 251	0.28083
		244 -> 254	0.21700
		245 -> 253	0.25162

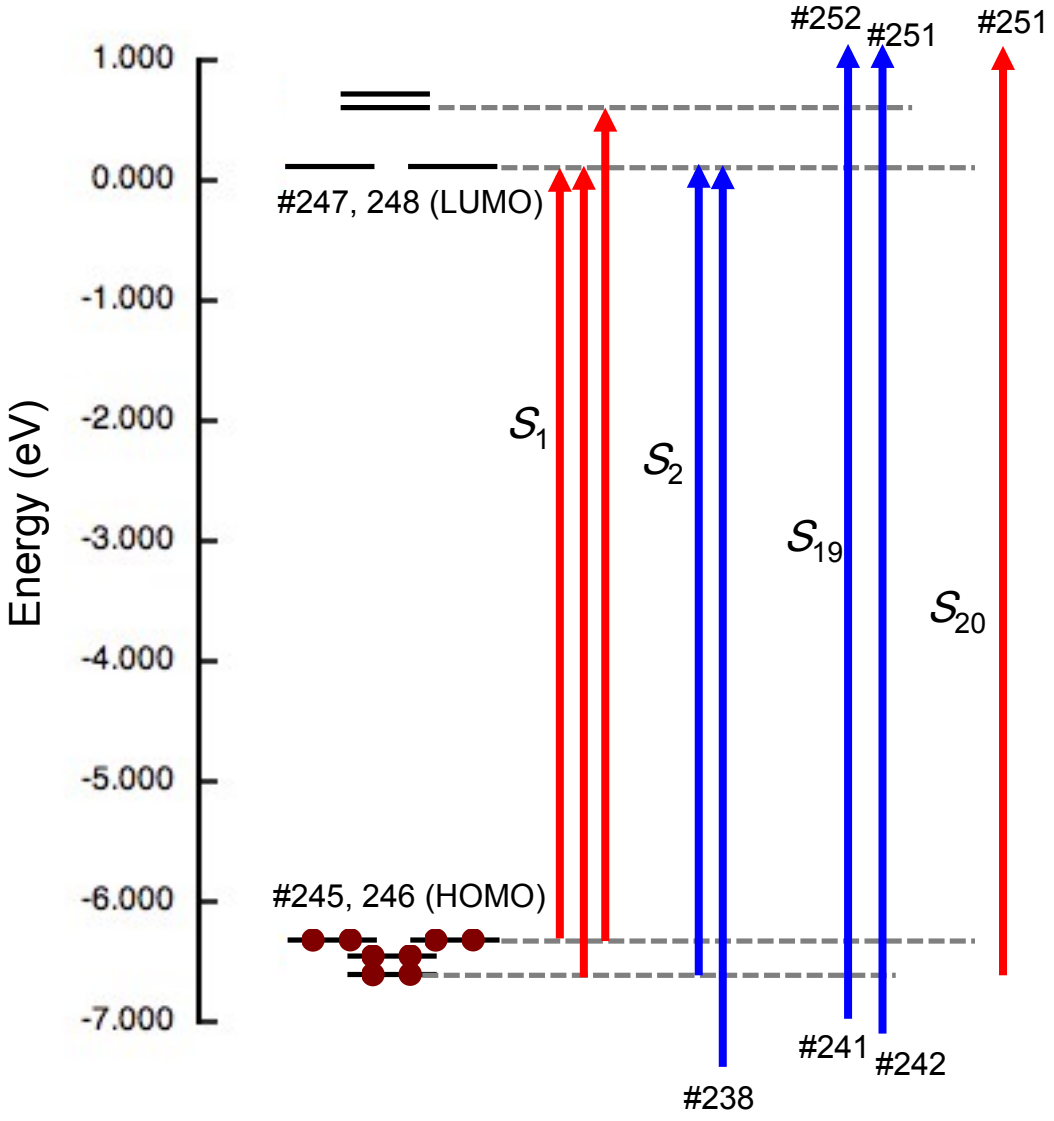


Fig. S14 *Excitation and energy diagram of (R,R,R)-**3***

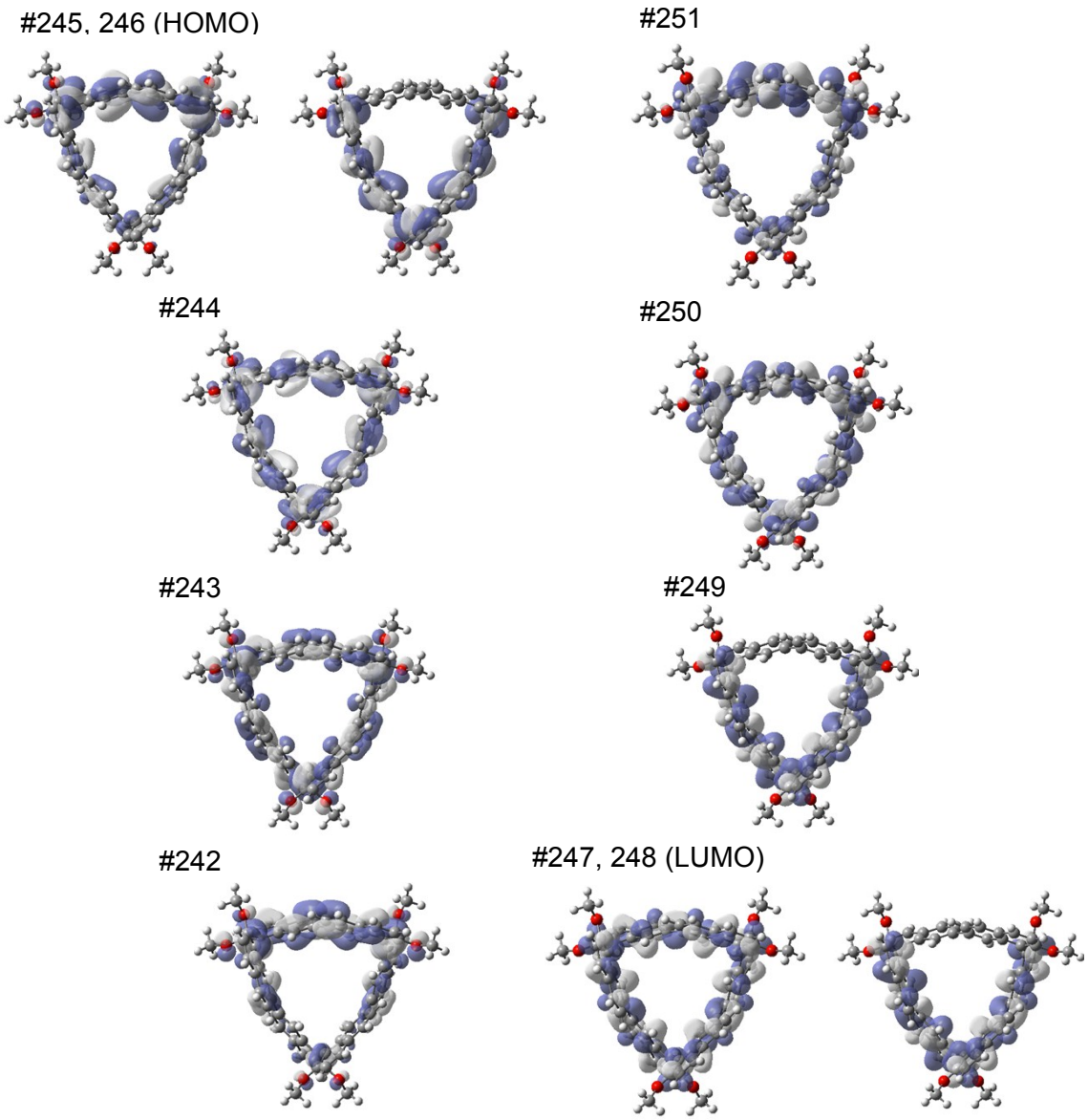


Fig. S15 *MO of (R,R,R)-**3***

3. TD-DFT Calculation for (*R*,*R*,*R*,*R*)-**4**

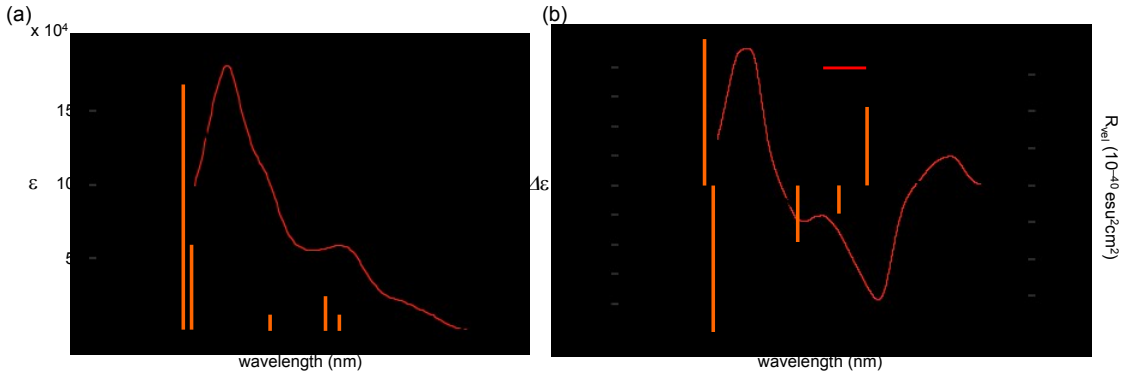


Fig. S16 *Simulated (a) UV (isovalue : 0.30) and (b) CD (isovalue : 0.15) spectra of (R,R,R,R)-**4** from TD-DFT calculation.*

Table S8. *Selected electronic transition for (R,R,R,R)-**4***

State	Excitation energies / nm (oscillator strengths, R_{vel} in CD)	Nature	
S_1	319 (0.1082, +2188)	326 -> 331	0.31718
		327 -> 330	–0.31718
		328 -> 329	0.42145
S_2	310 (0.3373, –981)	325 -> 330	0.25281
		326 -> 329	0.39239
		328 -> 331	0.32098
S_9	288 (0.1617, –1681)	317 -> 329	0.31663
		318 -> 330	–0.28394
		319 -> 331	0.28394
		320 -> 332	0.25947
S_{25}	249 (1.0587, –9096)	321 -> 336	0.20322
		325 -> 333	0.29603
		328 -> 337	0.23357
S_{27}	246 (2.5734, +5467)	321 -> 335	0.19332
		323 -> 333	0.19335
		325 -> 335	0.26352
		328 -> 339	0.22629

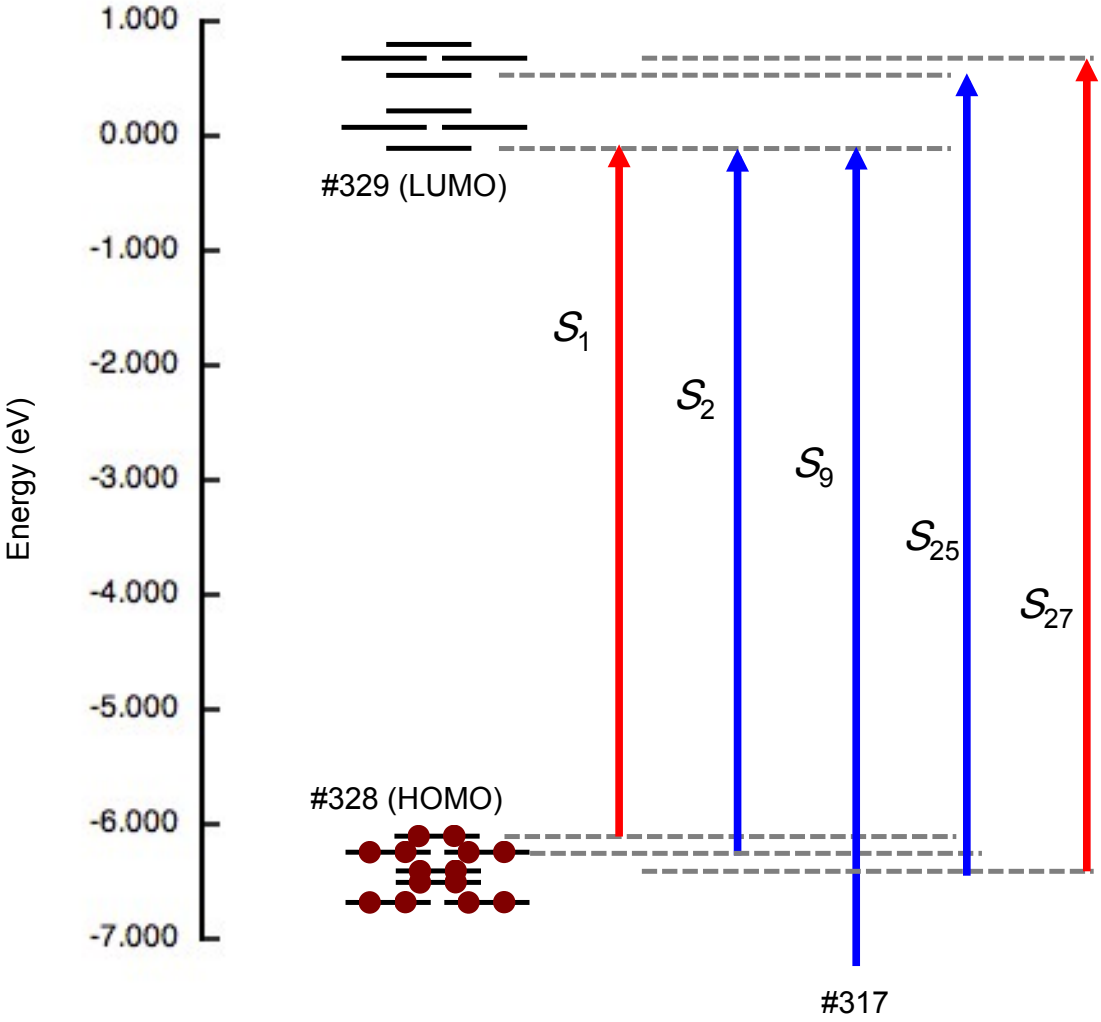


Fig. S17 *Excitation and energy diagram of (R,R,R,R)-**4***

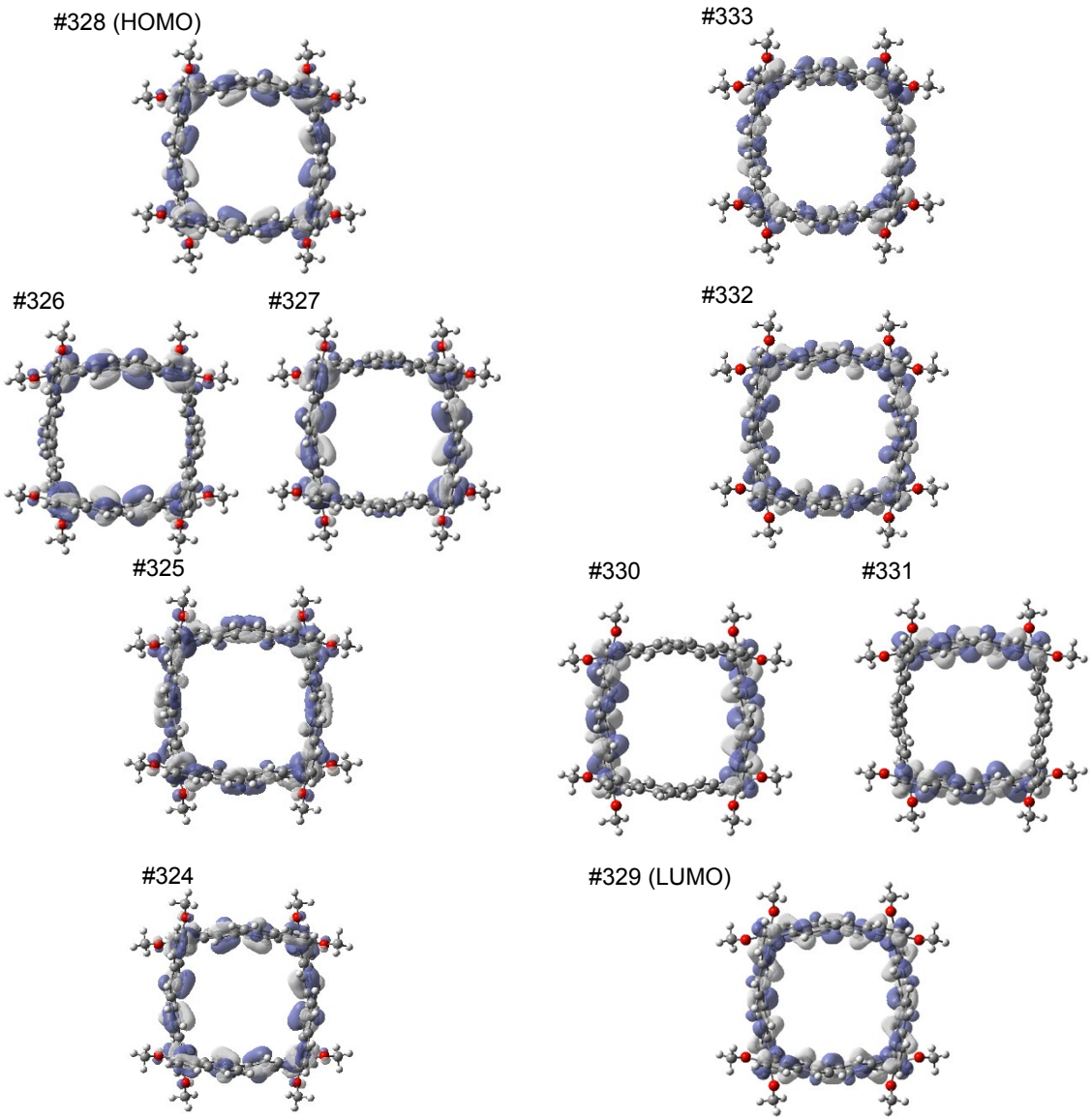


Fig. S18 *MO of (R,R,R,R)-4*

3. TD-DFT Calculation for (*R*,*R*,*R*,*R*,*R*)-**5**

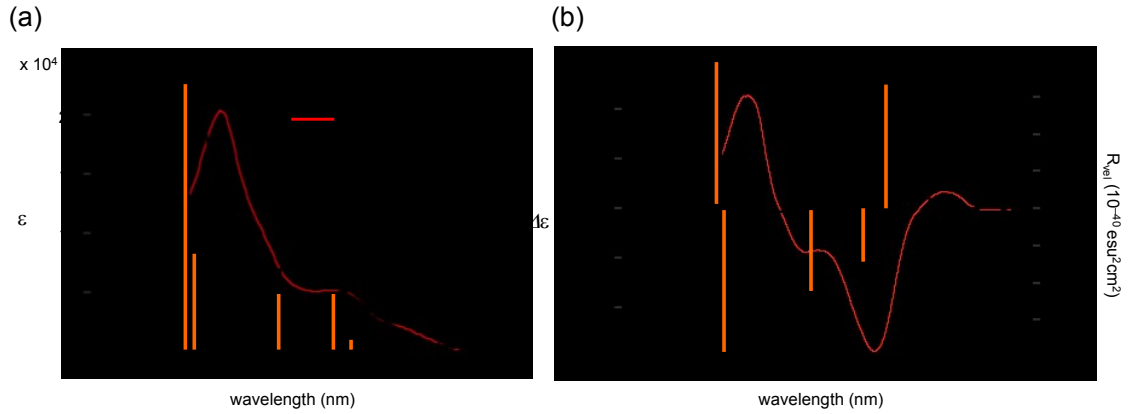


Fig. S19 *Simulated (a) UV (isovalue : 0.30) and (b) CD (isovalue : 0.15) spectra of (R,R,R,R,R)-**5** from TD-DFT calculation.*

Table S9. *Selected electronic transition for (R,R,R,R,R)-**5***

State	Excitation energies / nm (oscillator strengths, R_{vel} in CD)	Nature	
S_1	326 (0.1161, +3345)	408 -> 412	0.31987
		409 -> 413	0.31987
		410 -> 411	0.39074
S_2	318 (0.6763, –1826)	408 -> 411	0.37581
		410 -> 412	0.33351
S_{11}	290 (0.2393, –2737)	398 -> 413	0.26230
		399 -> 412	0.26230
		400 -> 411	0.29643
S_{31}	251 (1.1213, –12025)	406 -> 417	0.22449
		407 -> 416	0.22449
S_{34}	248 (2.8403, +7339)	401 -> 418	0.17075
		406 -> 417	0.17714
		407 -> 416	–0.17714
		409 -> 411	0.18532
		410 -> 422	0.19034

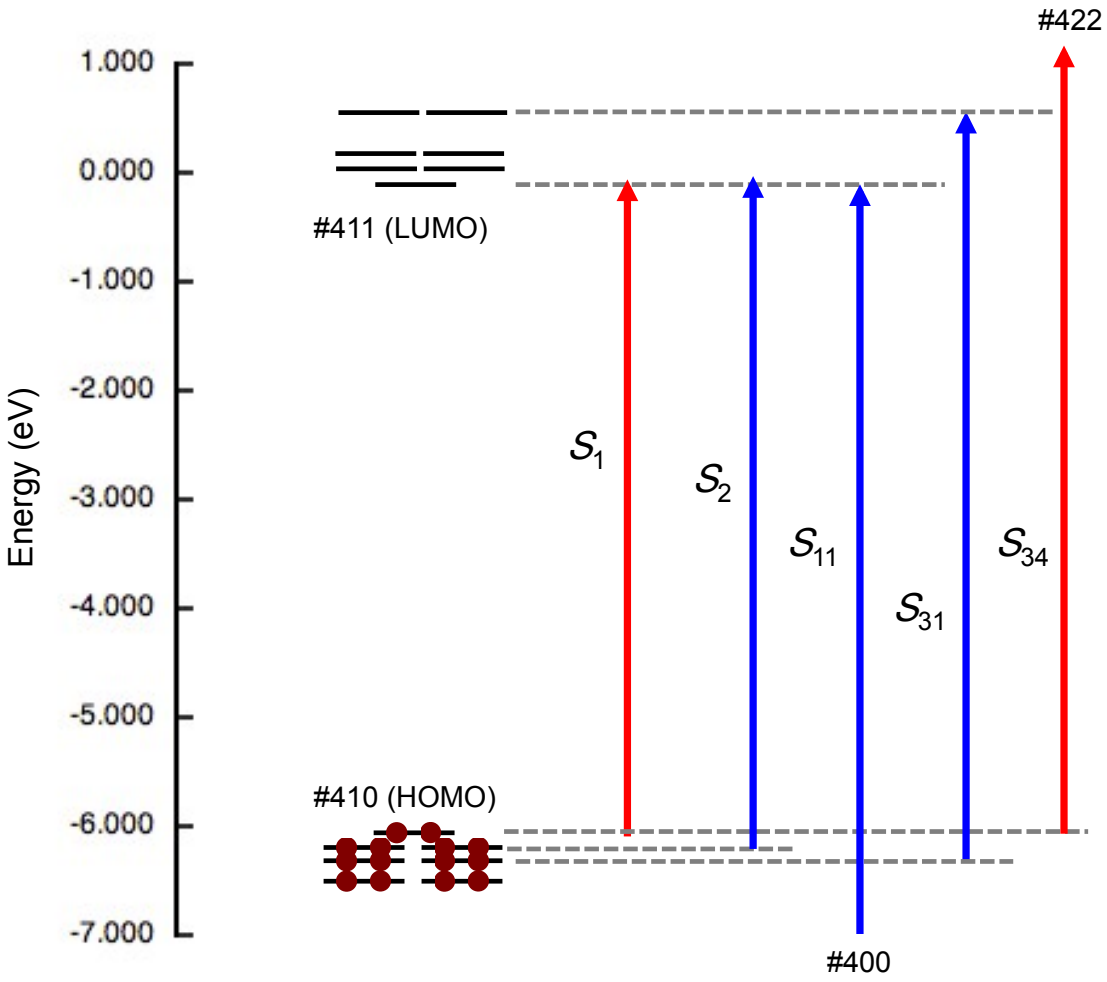


Fig. S20 *Excitation and energy diagram of (R,R,R,R,R)-**5***

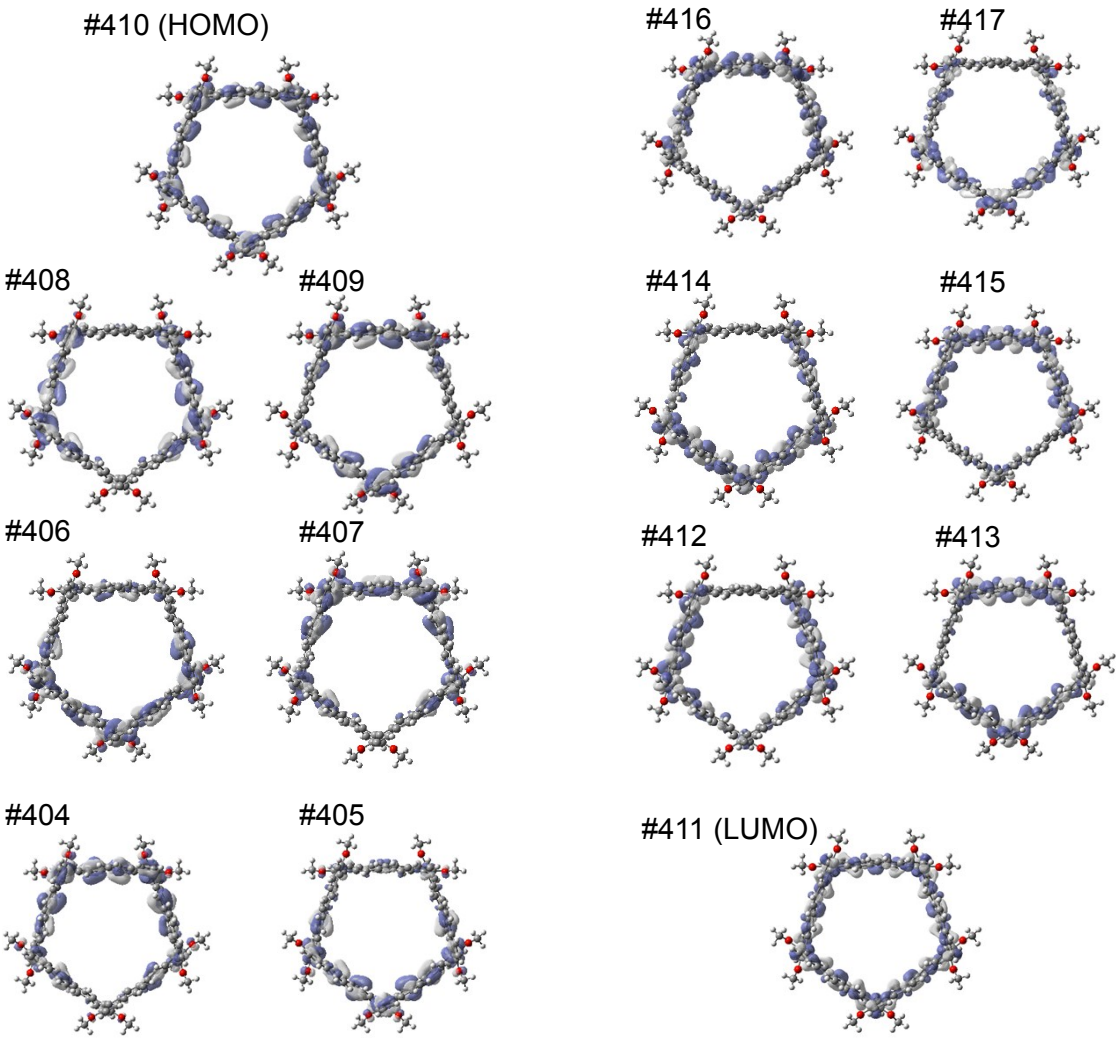


Fig. S21 *MO of (R,R,R,R,R)-**5***

S10. X-Ray Analysis of (*R,R,R*)-3 and (*R,R,R,R*)-4

Single crystal of (*R,R,R*)-**3** and (*R,R,R,R*)-**4** were grown from chloroform solution. The intensity data were collected on a Rigaku XtaLAB Synergy-R/DW with monochromated CuKα (1.54184 Å) radiation at 120 K. The structures were solved by the direct method (SHELEXT) and reined by full-matrix least-squares method by using Olex2. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were treated as the riding model.

Crystal lattice of **3** contains one $CHCl_3$ and two 1/3 $CHCl_3$ molecules. The latter $CHCl_3$ were laid on the special position passing through the midpoint of the cyclic trimer. Some $CHCl_3$ are disordered, and solved as using appropriate models.

Crystal lattice of **4** also contains $CHCl_3$ molecules and some residual electron density owing to disordered $CHCl_3$ molecules were removed with the SQUEEZE function in the PLATON software package.

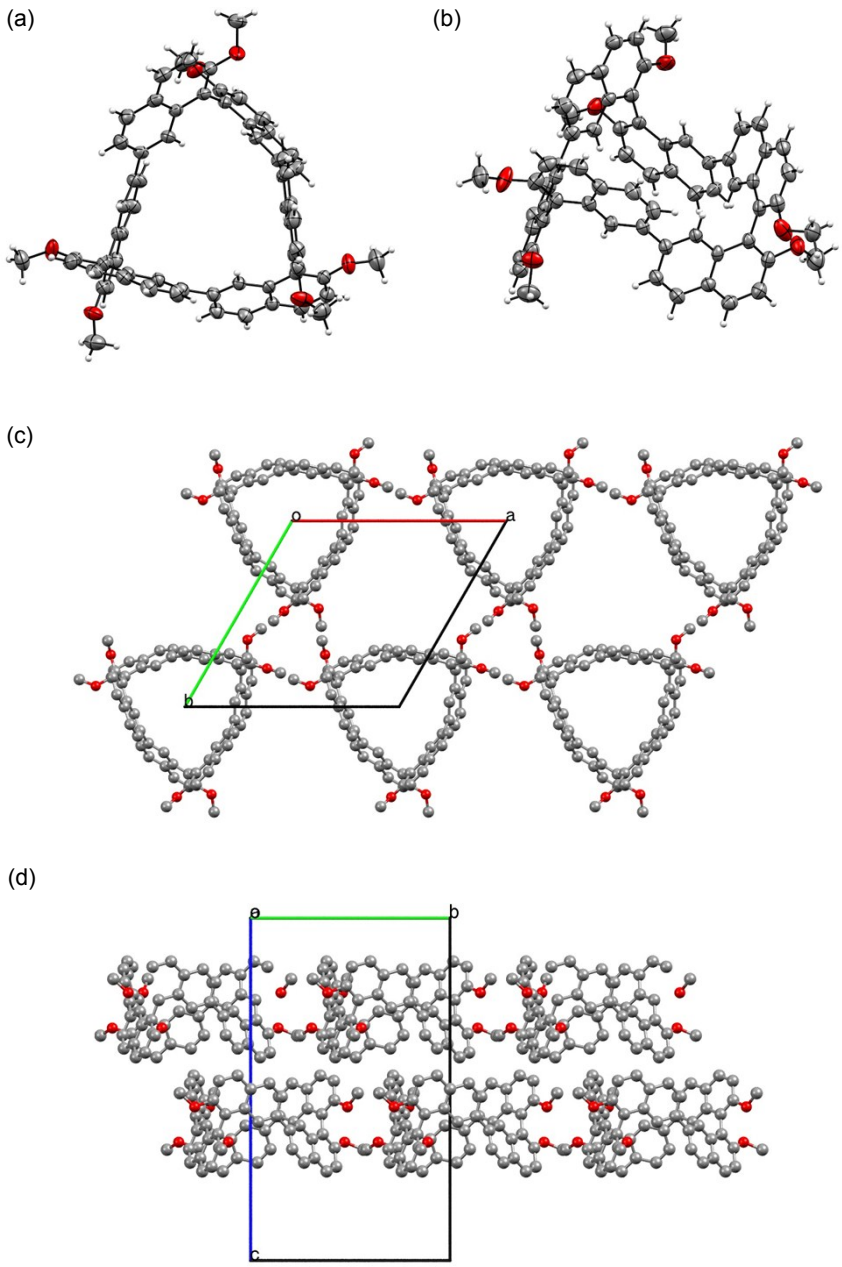


Fig. S22 *ORTEP drawing of (R,R,R)-**3***

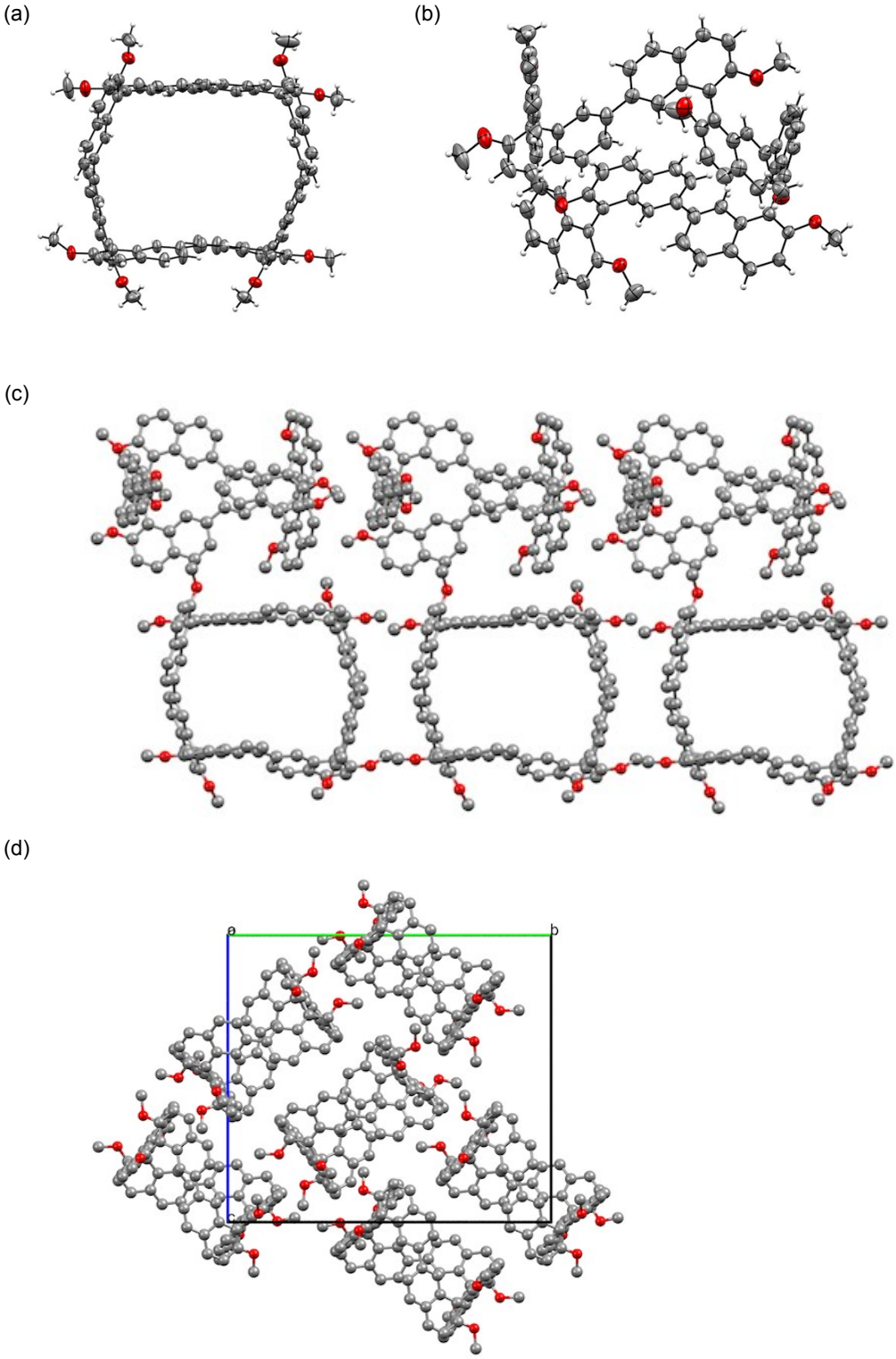


Fig. S23 *ORTEP drawing of (R,R,R,R)-**4***

Table S10 *Detailed X-ray parameters of (S)-**6**, (R,R,R)-**3**, and (R,R,R,R)-**4**.*

Identification code	(+)-(*S*)-**6**	(*R,R,R*)-**3**	(*R,R,R,R*)-**4**
Crystal description	Colorless Block	Colorless Block	Colorless Block
Empirical formula	$C_{22}H_{16}Br_2O_2$	$C_{71}H_{53}Cl_{15}O_6$	$C_{91}H_{67}Cl_9O_8$
Moiety formula	$C_{22}H_{16}Br_2O_2$	$C_{66}H_{48}O_6$•5($CHCl_3$)	$C_{88}H_{64}O_8$•3($CHCl_3$)
Formula weight	472.17	505.16	1607.49
Temperature	120 K	120 K	120 K
Wavelength	Cu*K*α 1.54184 Å	Cu*K*α 1.54184 Å	Cu*K*α 1.54184 Å
Crystal system	Tetragonal	Trigonal	Orthorhombic
Space group	$P4_3$ (#73)	R_3 (#146)	$P2_12_12_1$ (#19)
Unite cell dimensions	*a* = 8.4188(3) Å	*a* = 15.8802(4) Å	*a* = 16.0331(2) Å
	b = 8.4188(3) Å	*b* = 15.8802(4) Å	*b* = 23.3943(3) Å
	c = 25.9631(11) Å	*c* = 23.5680(6) Å	*c* = 20.8429(3) Å
	α = 90°	α = 90°	α = 90°
	β = 90°	*β* = 90°	*β* = 90°
	γ = 90°	*γ* = 120°	*γ* = 90°
Volume	1840.17(15)	5147.1(3)	7817.82(18)
Z	4	3	4
Density (calc.)	1.704 gcm^{-1}	1.485 gcm^{-1}	1.366 gcm^{-1}
Absorption coefficient	5.694	5.936	3.419
F(000)	936	2346	3320
Crystal size	0.05 x 0.05 x 0.03 cm^3	0.08 x 0.08 x 0.05 cm^3	0.01x0.01x0.01 mm^3
Index ranges	–10 <= h <= 10	–19 <= h <= 13	–19 <= h <= 20
	–7 <= k <= 9	–19 <= k <= 19	–14 <= k <= 28
	–26 <= l <= 32	–29 <= l <= 28	–25 <= l <= 26
Reflections collected	2604	5328	49303
Independent reflections	2604 [R_{int} = 0.0242]	3329 [R_{int} = 0.0220]	15856 [R_{int} = 0.0395]
Data/restraints/parameters	2604/1/237	3329/92/310	15856/0/1046
Goodness-of-fit on F^2	1.192	1.050	1.032
Final *R* indices [I > 2σ(I)]	R_1 = 0.0589, wR_2 = 0.1718	R_1 = 0.0620, wR_2 = 0.1687	R_1 = 0.0891, wR_2 = 0.2559
Final *R* indices [all data]	R_1 = 0.0611, wR_2 = 0.1756	R_1 = 0.0664, wR_2 = 0.1793	R_1 = 0.0945, wR_2 = 0.2637
CCDC deposition No.	1862118	1873110	1873111

S11. Dihedral Angle Dependence of the Theoretical CD Spectra

To gain further insight into the relationship between the dihedral angle and chiroptical properties in cyclic oligomers in (*R*)-configuration, we carried out TD-DFT calculations based on a binaphthyl conformer with various preset θ_1 and θ_2 (Fig. S23). All cyclic oligomers constitute 1,1'-binaphthyl with (*R*) configuration and 7,7'-binaphthyl with (S_A) configuration, where the notation "S_A" defines as the *S* configuration of axially chiral within 7,7'-connection. Thus, theoretical CD spectra were validated with varying dihedral angles of θ_1 in (*R*)-**1** and θ_2 in (S_A)-**1'** (Fig. S24).

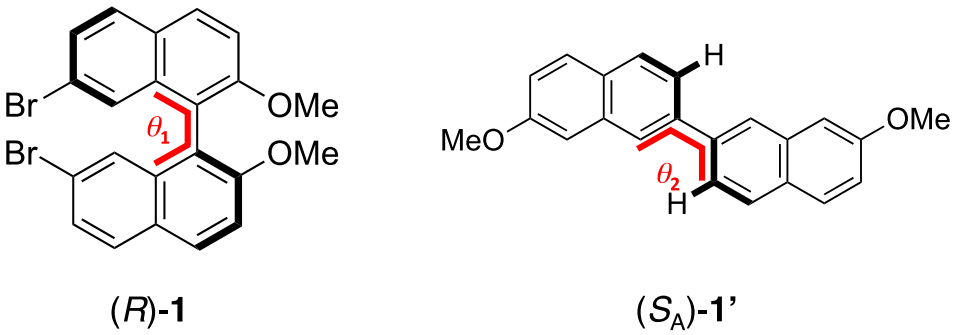


Fig. S24 *Molecular structure of (R)-**1** and (S_A)-**1'***

Theoretical CD spectra of axially chiral binaphthyl were obtained from TD-CAM-B3LYP/6-31G(d,p) calculations based on each optimized grand-state geometry with fixed dihedral angle at B3LYP/6-31G(d,p) level. The optimized structures with fixed dihedral angle were obtained by using "opt=modredundant" keyword. The theoretical CD spectra were obtained as sums of Gaussian curves with 0.15 eV exponential half-width treated with GaussView 5.0.

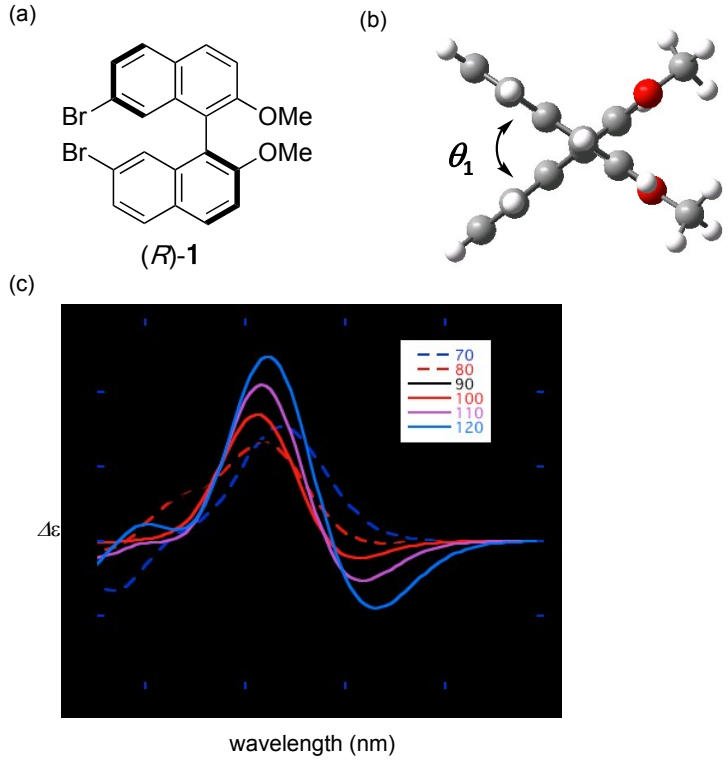


Fig. S25 *(a) Chemical structure of (R)-**1**. (b) Optimized geometry (θ_1 = 70°) (c) Dihedral angle dependence of the theoretical CD spectra of (R)-**1** at the CAM-B3LYP/6–31G(d,p) level (half-width, 0.15 eV).*

Table S11 *Optimized Geometries of (R)-**1** at the B3LYP/6–31G(d,p) level*

(*R*)-**1** (θ_1 = 70°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.064561	-2.624095	-1.731661
2	6	0	-1.187258	-1.679108	-1.252239
3	6	0	-1.614762	-0.671665	-0.338635
4	6	0	-2.997414	-0.663350	0.048637
5	6	0	-3.875332	-1.657058	-0.463530
6	6	0	-3.423816	-2.621120	-1.332831
7	1	0	-1.711802	-3.380293	-2.427272
8	1	0	-0.151488	-1.690195	-1.571248
9	6	0	-0.727742	0.326845	0.171072
10	6	0	-3.451368	0.345404	0.930772
11	1	0	-4.917466	-1.636154	-0.154238
12	1	0	-4.103463	-3.375165	-1.718537
13	6	0	-2.594632	1.305657	1.415967
14	6	0	-1.227703	1.294359	1.041162
15	1	0	-4.497415	0.355593	1.225726
16	1	0	-2.969808	2.064819	2.091311
17	6	0	0.727742	0.326841	-0.171077
18	6	0	1.614758	-0.671670	0.338632
19	6	0	1.227707	1.294352	-1.041169
20	6	0	1.187250	-1.679110	1.252238
21	6	0	2.997410	-0.663360	-0.048638
22	6	0	2.594636	1.305645	-1.415973
23	6	0	2.064550	-2.624098	1.731663
24	1	0	0.151480	-1.690193	1.571245
25	6	0	3.875325	-1.657071	0.463532
26	6	0	3.451369	0.345391	-0.930775
27	1	0	2.969815	2.064803	-2.091320
28	6	0	3.423806	-2.621129	1.332835
29	1	0	1.711788	-3.380294	2.427275
30	1	0	4.917460	-1.636171	0.154241
31	1	0	4.497416	0.355573	-1.225728
32	1	0	4.103450	-3.375175	1.718543
33	8	0	-0.327469	2.206880	1.513907
34	8	0	0.327476	2.206873	-1.513920
35	6	0	-0.775492	3.226601	2.389613
36	1	0	0.105682	3.826309	2.623131
37	1	0	-1.184609	2.816799	3.322226
38	1	0	-1.531024	3.868644	1.918588
39	6	0	0.775512	3.226616	-2.389592
40	1	0	-0.105657	3.826336	-2.623100
41	1	0	1.184633	2.816841	-3.322215
42	1	0	1.531043	3.868641	-1.918543

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6531501 Haartrees

(*R*)-**1** (θ_1 = 80°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.215804	-2.492236	1.794376
2	6	0	1.291342	-1.602771	1.297695
3	6	0	1.653221	-0.638462	0.312772
4	6	0	3.015401	-0.618767	-0.139757
5	6	0	3.943736	-1.553271	0.394172
6	6	0	3.557573	-2.473021	1.339946
7	1	0	1.914780	-3.217797	2.544785
8	1	0	0.267652	-1.625443	1.654319
9	6	0	0.714750	0.296806	-0.219802
10	6	0	3.395673	0.339709	-1.108931
11	1	0	4.970725	-1.524570	0.038342
12	1	0	4.275214	-3.182457	1.741181
13	6	0	2.487823	1.240301	-1.615858
14	6	0	1.141764	1.219960	-1.170971
15	1	0	4.425829	0.358677	-1.454999

16	1	0	2.807738	1.962496	-2.357065
17	6	0	-0.714816	0.297090	0.219382
18	6	0	-1.653628	-0.637913	-0.313048
19	6	0	-1.141449	1.220497	1.170490
20	6	0	-3.015755	-0.617791	0.139620
21	6	0	-1.292119	-1.602444	-1.297893
22	6	0	-2.487490	1.241300	1.615446
23	6	0	-3.944412	-1.552094	-0.394107
24	6	0	-3.395649	0.340901	1.108714
25	6	0	-2.216880	-2.491707	-1.794372
26	1	0	-0.268476	-1.625434	-1.654633
27	1	0	-2.807202	1.963758	2.356470
28	6	0	-3.558600	-2.472063	-1.339809
29	1	0	-4.971358	-1.523060	-0.038180
30	1	0	-4.425781	0.360241	1.454839
31	1	0	-1.916141	-3.217431	-2.544738
32	1	0	-4.276481	-3.181342	-1.740894
33	8	0	0.193724	2.083465	-1.643486
34	8	0	-0.193111	2.083990	1.642513
35	6	0	0.565009	3.049558	-2.611480
36	1	0	-0.342307	3.614614	-2.830785
37	1	0	0.927860	2.584449	-3.537268
38	1	0	1.331769	3.736948	-2.231335
39	6	0	-0.562828	3.047746	2.613442
40	1	0	0.345198	3.611240	2.833815
41	1	0	-0.925697	2.580418	3.538093
42	1	0	-1.329041	3.737073	2.235674

Keyword: opt=modredundant scf=(direct,tight)
Energy = -999.653743 Haartrees

(*R*)-**1** ($\theta_1 = 90°$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.410954	-2.322936	1.832042
2	6	0	1.428153	-1.499750	1.333151
3	6	0	1.698538	-0.594463	0.266809
4	6	0	3.028623	-0.566570	-0.271680
5	6	0	4.019618	-1.430701	0.268001
6	6	0	3.722689	-2.292040	1.297436
7	1	0	2.179973	-3.005400	2.645122
8	1	0	0.426772	-1.531682	1.748279
9	6	0	0.697183	0.269097	-0.270611
10	6	0	3.313672	0.327337	-1.331278
11	1	0	5.021922	-1.396386	-0.151947
12	1	0	4.487530	-2.948275	1.702029
13	6	0	2.344451	1.157755	-1.844464
14	6	0	1.030513	1.131089	-1.311671
15	1	0	4.319211	0.352354	-1.743135
16	1	0	2.592106	1.832080	-2.655202
17	6	0	-0.697274	0.269159	0.270469
18	6	0	-1.698805	-0.594061	-0.267166
19	6	0	-1.030385	1.130922	1.311796
20	6	0	-3.028850	-0.566129	0.271414
21	6	0	-1.428618	-1.499089	-1.333781
22	6	0	-2.344317	1.157655	1.844634
23	6	0	-4.020011	-1.429958	-0.268450
24	6	0	-3.313695	0.327520	1.331273
25	6	0	-2.411571	-2.321989	-1.832839
26	1	0	-0.427274	-1.531041	-1.748993
27	1	0	-2.591884	1.831843	2.655499
28	6	0	-3.723271	-2.291051	-1.298143
29	1	0	-5.022285	-1.395609	0.151566
30	1	0	-4.319218	0.352598	1.743170
31	1	0	-2.180746	-3.004249	-2.646134
32	1	0	-4.488234	-2.947057	-1.702877
33	8	0	0.025658	1.932058	-1.777789
34	8	0	-0.025354	1.931744	1.777871
35	6	0	0.297605	2.826409	-2.843070
36	1	0	-0.640699	3.346910	-3.041000
37	1	0	0.611214	2.297735	-3.752561
38	1	0	1.065642	3.563020	-2.573822
39	6	0	-0.296137	2.824073	2.845152
40	1	0	0.642670	3.343386	3.043811
41	1	0	-0.609868	2.293756	3.753635
42	1	0	-1.063634	3.561931	2.577758

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6538531 Haartrees

(*R*)-**1** (θ_1 = 100°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.635940	-1.818543	-2.139017
2	6	0	1.587511	-1.336700	-1.390037
3	6	0	1.746490	-0.198608	-0.548384
4	6	0	3.033767	0.434331	-0.509421
5	6	0	4.095590	-0.090681	-1.294942
6	6	0	3.906652	-1.193666	-2.093296
7	1	0	2.488920	-2.687204	-2.774683
8	1	0	0.617323	-1.819077	-1.436004
9	6	0	0.674035	0.323917	0.236129
10	6	0	3.207054	1.571936	0.314616
11	1	0	5.064406	0.400947	-1.252078
12	1	0	4.724672	-1.586172	-2.690047
13	6	0	2.170291	2.071400	1.067988
14	6	0	0.899138	1.443596	1.032884
15	1	0	4.179943	2.055429	0.347323
16	1	0	2.332532	2.942375	1.691208
17	6	0	-0.674145	-0.323573	0.236448
18	6	0	-1.746716	0.198373	-0.548288
19	6	0	-0.899074	-1.442728	1.033996
20	6	0	-3.033951	-0.434616	-0.508771
21	6	0	-1.587888	1.335895	-1.390741
22	6	0	-2.170216	-2.070553	1.069671
23	6	0	-4.095887	0.089792	-1.294545
24	6	0	-3.207084	-1.571662	0.316059
25	6	0	-2.636418	1.817157	-2.139951
26	1	0	-0.617741	1.818313	-1.437121
27	1	0	-2.332397	-2.941058	1.693546
28	6	0	-3.907090	1.192236	-2.093677
29	1	0	-5.064670	-0.401861	-1.251245
30	1	0	-4.179952	-2.055169	0.349213
31	1	0	-2.489515	2.685397	-2.776219
32	1	0	-4.725192	1.584286	-2.690616
33	8	0	-0.165730	1.887038	1.766609
34	8	0	0.165926	-1.885446	1.768015
35	6	0	-0.009048	3.035681	2.582059
36	1	0	-0.979302	3.199895	3.053289
37	1	0	0.257047	3.923214	1.993476
38	1	0	0.747048	2.883702	3.363206
39	6	0	0.010302	-3.034815	2.582658
40	1	0	0.980975	-3.199056	3.053012
41	1	0	-0.255958	-3.921965	1.993583
42	1	0	-0.745216	-2.883738	3.364547

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6537637 Haartrees

(*R*)-**1** (θ_1 = 110°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.858843	-1.755210	-1.973869
2	6	0	1.745986	-1.304018	-1.302976
3	6	0	1.791394	-0.120123	-0.512346
4	6	0	3.033124	0.595904	-0.449075
5	6	0	4.164786	0.100508	-1.152204
6	6	0	4.085918	-1.051258	-1.898085
7	1	0	2.796558	-2.660064	-2.571930
8	1	0	0.809708	-1.845955	-1.376202
9	6	0	0.647482	0.373966	0.187598
10	6	0	3.094229	1.785806	0.314623
11	1	0	5.097593	0.655531	-1.089389
12	1	0	4.956248	-1.420578	-2.432373

13	6	0	1.992087	2.256558	0.988891
14	6	0	0.766657	1.545055	0.934172
15	1	0	4.032297	2.332475	0.364560
16	1	0	2.068653	3.167576	1.569751
17	6	0	-0.647580	-0.373690	0.187813
18	6	0	-1.791572	0.120059	-0.512242
19	6	0	-0.766615	-1.544502	0.934854
20	6	0	-3.033245	-0.596036	-0.448625
21	6	0	-1.746291	1.303634	-1.303361
22	6	0	-1.992009	-2.256045	0.989946
23	6	0	-4.164985	-0.101009	-1.151892
24	6	0	-3.094223	-1.785634	0.315549
25	6	0	-2.859214	1.754465	-1.974383
26	1	0	-0.810067	1.845628	-1.376839
27	1	0	-2.068513	-3.166797	1.571226
28	6	0	-4.086236	1.050454	-1.898250
29	1	0	-5.097748	-0.656075	-1.088803
30	1	0	-4.032259	-2.332334	0.365773
31	1	0	-2.797031	2.659087	-2.572805
32	1	0	-4.956620	1.419493	-2.432644
33	8	0	-0.351992	1.952047	1.606275
34	8	0	0.352079	-1.951050	1.607167
35	6	0	-0.306086	3.151351	2.360223
36	1	0	-1.303552	3.272769	2.785228
37	1	0	-0.076660	4.021999	1.732367
38	1	0	0.426196	3.094672	3.175975
39	6	0	0.307041	-3.151198	2.359833
40	1	0	1.304845	-3.272841	2.783978
41	1	0	0.077321	-4.021208	1.731211
42	1	0	-0.424626	-3.095581	3.176216

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6533045 Haartrees

(*R*)-**1** (θ_1 = 120°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.053014	-1.669830	-1.840062
2	6	0	1.884252	-1.251382	-1.247883
3	6	0	1.829796	-0.047167	-0.488926
4	6	0	3.031092	0.729874	-0.385369
5	6	0	4.223760	0.266995	-1.005260
6	6	0	4.241682	-0.909386	-1.715356
7	1	0	3.064576	-2.591515	-2.415168
8	1	0	0.978363	-1.835520	-1.363723
9	6	0	0.621231	0.416336	0.121634
10	6	0	2.993933	1.948541	0.332619
11	1	0	5.124288	0.868554	-0.908900
12	1	0	5.157531	-1.253420	-2.186739
13	6	0	1.834926	2.387700	0.927186
14	6	0	0.650041	1.613917	0.838564
15	1	0	3.900938	2.542137	0.411839
16	1	0	1.836490	3.320047	1.478341
17	6	0	-0.621308	-0.416061	0.121825
18	6	0	-1.829930	0.047151	-0.488853
19	6	0	-0.650004	-1.613415	0.839133
20	6	0	-3.031157	-0.729962	-0.385005
21	6	0	-1.884498	1.251078	-1.248257
22	6	0	-1.834830	-2.387242	0.928092
23	6	0	-4.223877	-0.267410	-1.005042
24	6	0	-2.993887	-1.948375	0.333411
25	6	0	-3.053303	1.669204	-1.840575
26	1	0	-0.978671	1.835267	-1.364310
27	1	0	-1.836306	-3.319358	1.479645
28	6	0	-4.241906	0.908708	-1.715571
29	1	0	-5.124352	-0.869010	-0.908449
30	1	0	-3.900853	-2.542000	0.412885
31	1	0	-3.064955	2.590681	-2.416012
32	1	0	-5.157790	1.252492	-2.187068
33	8	0	-0.511343	1.982557	1.457465
34	8	0	0.511374	-1.981732	1.458227
35	6	0	-0.559660	3.207493	2.168786
36	1	0	-1.578742	3.288405	2.549762
37	1	0	-0.351341	4.067541	1.519407
38	1	0	0.140611	3.218400	3.013953
39	6	0	0.560312	-3.207489	2.168092

40	1	0	1.579665	-3.288743	2.548266
41	1	0	0.351579	-4.066801	1.517882
42	1	0	-0.139352	-3.219423	3.013758

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6520119 Haartrees

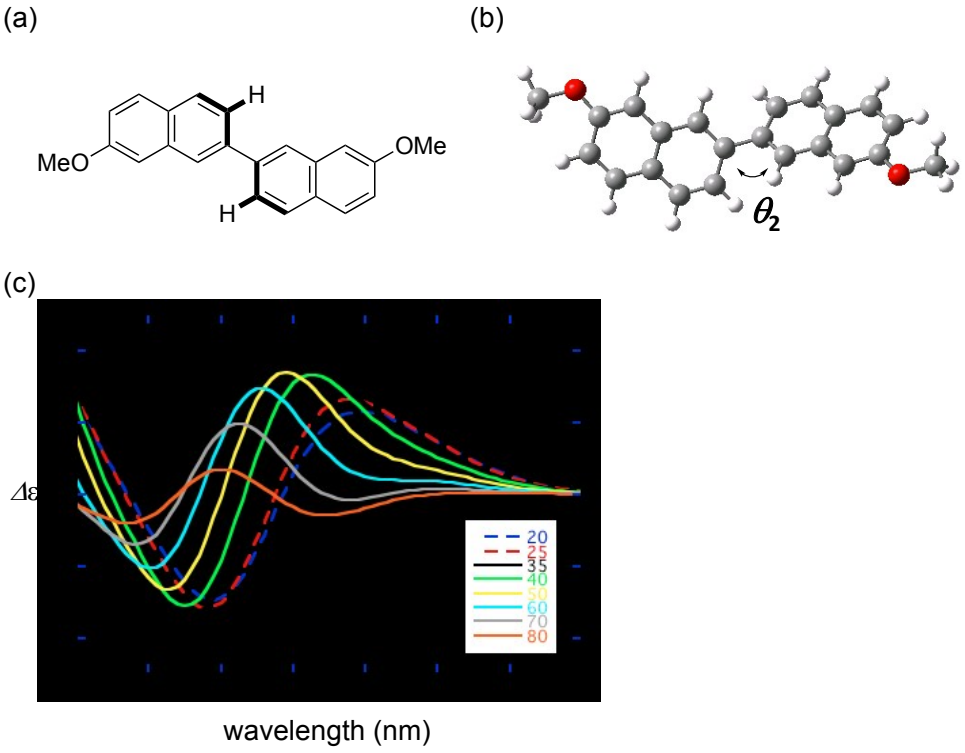


Fig. S26 *(a) Chemical structure of (S_A)-**1'**. (b) Optimized geometry (θ_2 = 35°) (c) Dihedral angle dependence of the theoretical CD spectra of (S_A)-**1'** at the CAM-B3LYP/6–31G(d,p) level (half-width, 0.15 eV).*

Table S12. *Optimized Geometries of (S_A)-**1'** at the B3LYP/6–31G(d,p) level*

(S_A)-**1'** (θ_2 = 20°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.511575	0.408952	-0.249164
2	6	0	4.222245	0.910425	-0.241662
3	6	0	3.115574	0.064277	0.003662
4	6	0	3.342123	-1.329828	0.242999
5	6	0	4.672607	-1.810950	0.229959
6	6	0	5.739993	-0.971330	-0.009391
7	1	0	1.633042	1.607929	-0.197674
8	1	0	4.072250	1.969289	-0.427778
9	6	0	1.781868	0.554684	0.017468
10	6	0	2.219156	-2.164171	0.489656
11	1	0	4.851311	-2.867336	0.413078
12	1	0	6.746226	-1.372518	-0.013080
13	6	0	0.944443	-1.657432	0.492935
14	6	0	0.693053	-0.272325	0.240045
15	1	0	2.385608	-3.219311	0.691885
16	1	0	0.114167	-2.315429	0.724006
17	6	0	-0.694964	0.259456	0.270605
18	6	0	-0.940805	1.649913	0.496473
19	6	0	-1.784243	-0.560424	0.023706
20	6	0	-2.214237	2.159997	0.489615
21	1	0	-0.108869	2.308553	0.719204
22	6	0	-3.116949	-0.067535	0.011195
23	1	0	-1.636176	-1.612031	-0.200311
24	6	0	-3.339770	1.327459	0.248800
25	1	0	-2.377045	3.218180	0.678447
26	6	0	-4.225386	-0.910202	-0.238044
27	6	0	-4.668805	1.812494	0.233075
28	6	0	-5.513230	-0.404942	-0.248173
29	1	0	-4.078099	-1.969534	-0.423649
30	6	0	-5.738131	0.975901	-0.008201
31	1	0	-4.844774	2.869515	0.415165
32	1	0	-6.743175	1.380027	-0.014033
33	8	0	6.509642	1.310593	-0.495336
34	8	0	-6.513393	-1.303568	-0.496682
35	6	0	-7.854432	-0.842062	-0.520399
36	1	0	-8.015304	-0.092629	-1.306063
37	1	0	-8.468464	-1.718288	-0.734081
38	1	0	-8.158715	-0.419300	0.445798
39	6	0	7.851979	0.852834	-0.517130
40	1	0	8.016182	0.104175	-1.302846
41	1	0	8.463920	1.730852	-0.729470
42	1	0	8.155932	0.430503	0.449365

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.167398 Haartrees

(S_A)-**1'** (θ_2 = 25°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.286415	5.514288	0.259672
2	6	0	0.816232	4.236519	0.259759
3	6	0	0.000580	3.111183	-0.003785
4	6	0	-1.393852	3.306396	-0.271210
5	6	0	-1.903955	4.626604	-0.266492
6	6	0	-1.093598	5.711574	-0.008248
7	1	0	1.570108	1.651201	0.219763
8	1	0	1.874092	4.109051	0.467229
9	6	0	0.517613	1.787773	-0.009320
10	6	0	-2.200457	2.167880	-0.536573
11	1	0	-2.959975	4.781962	-0.471844
12	1	0	-1.516999	6.708678	-0.013325
13	6	0	-1.668561	0.902574	-0.532651
14	6	0	-0.286415	0.685151	-0.250544
15	1	0	-3.254225	2.314089	-0.760364
16	1	0	-2.299649	0.054109	-0.775647
17	6	0	0.286415	-0.685151	-0.250544
18	6	0	1.668561	-0.902574	-0.532651

19	6	0	-0.517613	-1.787773	-0.009320
20	6	0	2.200457	-2.167880	-0.536573
21	1	0	2.299649	-0.054109	-0.775647
22	6	0	-0.000580	-3.111183	-0.003785
23	1	0	-1.570108	-1.651201	0.219763
24	6	0	1.393852	-3.306396	-0.271210
25	1	0	3.254225	-2.314089	-0.760364
26	6	0	-0.816232	-4.236519	0.259759
27	6	0	1.903955	-4.626604	-0.266492
28	6	0	-0.286415	-5.514288	0.259672
29	1	0	-1.874092	-4.109051	0.467229
30	6	0	1.093598	-5.711574	-0.008248
31	1	0	2.959975	-4.781962	-0.471844
32	1	0	1.516999	-6.708678	-0.013325
33	8	0	1.161540	6.530055	0.528942
34	8	0	-1.161540	-6.530055	0.528942
35	6	0	-0.664227	-7.858480	0.578215
36	1	0	0.098292	-7.977268	1.357641
37	1	0	-1.525599	-8.482739	0.819946
38	1	0	-0.250617	-8.172752	-0.387869
39	6	0	0.664227	7.858480	0.578215
40	1	0	-0.098292	7.977268	1.357641
41	1	0	1.525599	8.482739	0.819946
42	1	0	0.250617	8.172752	-0.387869

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6635228Haartrees

(S_A)-**1'** (θ_2 = 30°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.280926	5.491557	0.363173
2	6	0	0.800512	4.209594	0.362912
3	6	0	0.001327	3.101215	-0.003046
4	6	0	-1.365656	3.318136	-0.375021
5	6	0	-1.865700	4.642170	-0.366961
6	6	0	-1.071633	5.710431	-0.008066
7	1	0	1.537975	1.620082	0.296784
8	1	0	1.837316	4.065494	0.650373
9	6	0	0.508323	1.773942	-0.011470
10	6	0	-2.155765	2.196560	-0.742507
11	1	0	-2.900654	4.814057	-0.651226
12	1	0	-1.486614	6.711066	-0.013653
13	6	0	-1.634331	0.926907	-0.738361
14	6	0	-0.280926	0.687420	-0.353495
15	1	0	-3.187047	2.359891	-1.045267
16	1	0	-2.249378	0.092838	-1.059701
17	6	0	0.280926	-0.687420	-0.353495
18	6	0	1.634331	-0.926907	-0.738361
19	6	0	-0.508323	-1.773942	-0.011470
20	6	0	2.155765	-2.196560	-0.742507
21	1	0	2.249378	-0.092838	-1.059701
22	6	0	-0.001327	-3.101215	-0.003046
23	1	0	-1.537975	-1.620082	0.296784
24	6	0	1.365656	-3.318136	-0.375021
25	1	0	3.187047	-2.359891	-1.045267
26	6	0	-0.800512	-4.209594	0.362912
27	6	0	1.865700	-4.642170	-0.366961
28	6	0	-0.280926	-5.491557	0.363173
29	1	0	-1.837316	-4.065494	0.650373
30	6	0	1.071633	-5.710431	-0.008066
31	1	0	2.900654	-4.814057	-0.651226
32	1	0	1.486614	-6.711066	-0.013653
33	8	0	1.138199	6.489687	0.735935
34	8	0	-1.138199	-6.489687	0.735935
35	6	0	-0.647363	-7.820345	0.789685
36	1	0	0.174748	-7.920477	1.508822
37	1	0	-1.490551	-8.428234	1.120745
38	1	0	-0.315140	-8.170144	-0.195418
39	6	0	0.647363	7.820345	0.789685
40	1	0	-0.174748	7.920477	1.508822
41	1	0	1.490551	8.428234	1.120745
42	1	0	0.315140	8.170144	-0.195418

Keyword: opt=modredundant scf=(direct,tight)
Energy =–999.6639936 Haartrees

(S_A)-**1'** (θ_2 = 40°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.465447	0.402257	0.419804
2	6	0	-4.170827	0.889396	0.413327
3	6	0	-3.091191	0.076978	-0.005230
4	6	0	-3.350032	-1.270182	-0.421752
5	6	0	-4.686419	-1.736735	-0.404536
6	6	0	-5.726782	-0.929852	0.004092
7	1	0	-1.559351	1.564526	0.321330
8	1	0	-3.994961	1.911034	0.735263
9	6	0	-1.751443	0.551187	-0.020277
10	6	0	-2.256795	-2.078149	-0.834657
11	1	0	-4.890685	-2.756272	-0.721213
12	1	0	-6.737526	-1.319624	0.005737
13	6	0	-0.974241	-1.588524	-0.836404
14	6	0	-0.697828	-0.249345	-0.425492
15	1	0	-2.453033	-3.096219	-1.161750
16	1	0	-0.155271	-2.212573	-1.179639
17	6	0	0.697010	0.259677	-0.417728
18	6	0	0.977246	1.596950	-0.832306
19	6	0	1.749429	-0.545811	-0.019372
20	6	0	2.260973	2.083495	-0.830630
21	1	0	0.159757	2.222697	-1.176076
22	6	0	3.090180	-0.074458	-0.003326
23	1	0	1.555504	-1.559962	0.318659
24	6	0	3.352184	1.272681	-0.418009
25	1	0	2.459886	3.100683	-1.158855
26	6	0	4.168115	-0.890359	0.412862
27	6	0	4.689736	1.735900	-0.400716
28	6	0	5.463935	-0.406437	0.419435
29	1	0	3.989916	-1.912103	0.733171
30	6	0	5.728324	0.925780	0.006001
31	1	0	4.896360	2.755430	-0.715887
32	1	0	6.740029	1.313049	0.007747
33	8	0	-6.435948	1.268751	0.840352
34	8	0	6.432537	-1.276078	0.837878
35	6	0	7.779822	-0.833460	0.867651
36	1	0	8.139561	-0.550610	-0.130009
37	1	0	8.364808	-1.680395	1.229436
38	1	0	7.916864	0.013949	1.551627
39	6	0	-7.782135	0.822791	0.870007
40	1	0	-8.141688	0.540874	-0.127985
41	1	0	-8.369001	1.667638	1.233624
42	1	0	-7.916758	-0.026189	1.552513

Keyword: opt=modredundant scf=(direct,tight)
Energy =–999.6639579 Haartrees

(S_A)-**1'** (θ_2 = 50°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.440728	0.388950	0.502900
2	6	0	-4.143379	0.868660	0.502478
3	6	0	-3.079639	0.085524	-0.003355
4	6	0	-3.357159	-1.224694	-0.515577
5	6	0	-4.696276	-1.684293	-0.501682
6	6	0	-5.720923	-0.906014	-0.007366
7	1	0	-1.526145	1.537063	0.394437
8	1	0	-3.952865	1.861682	0.897329
9	6	0	-1.736861	0.552140	-0.013852
10	6	0	-2.280151	-2.006052	-1.013451
11	1	0	-4.915065	-2.675541	-0.890300
12	1	0	-6.733997	-1.289715	-0.011129
13	6	0	-0.994071	-1.524288	-1.009252
14	6	0	-0.702208	-0.219413	-0.510938
15	1	0	-2.491189	-2.997069	-1.407582
16	1	0	-0.183536	-2.126009	-1.408523
17	6	0	0.698973	0.274623	-0.483109
18	6	0	1.009484	1.574937	-0.982155
19	6	0	1.726734	-0.523776	-0.015078
20	6	0	2.301563	2.040399	-0.982586
21	1	0	0.206815	2.189194	-1.378449
22	6	0	3.074760	-0.072752	0.002820
23	1	0	1.505630	-1.514597	0.372692
24	6	0	3.368376	1.240646	-0.492181

25	1	0	2.525897	3.030385	-1.371946
26	6	0	4.129503	-0.877001	0.494221
27	6	0	4.713248	1.683006	-0.473825
28	6	0	5.432853	-0.413912	0.499154
29	1	0	3.927011	-1.873092	0.875134
30	6	0	5.728662	0.884814	0.007584
31	1	0	4.944078	2.676760	-0.848843
32	1	0	6.746515	1.255663	0.007656
33	8	0	-6.395190	1.225448	1.011705
34	8	0	6.377403	-1.269726	0.994183
35	6	0	7.731013	-0.847064	1.026087
36	1	0	8.117018	-0.634629	0.020785
37	1	0	8.293625	-1.677921	1.454507
38	1	0	7.867587	0.040396	1.657342
39	6	0	-7.743345	0.785380	1.039212
40	1	0	-8.128126	0.582730	0.031425
41	1	0	-8.315705	1.602788	1.480396
42	1	0	-7.867828	-0.112796	1.657678

Keyword: opt=modredundant scf=(direct,tight)
Energy =–999.6633477 Haartrees

(S_A)-**1'** (θ_2 = 60°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.375430	5.400394	-0.677298
2	6	0	-0.829335	4.104905	-0.693498
3	6	0	-0.069001	3.065932	-0.089724
4	6	0	1.166193	3.386105	0.530735
5	6	0	1.612147	4.736070	0.532963
6	6	0	0.857412	5.719480	-0.058091
7	1	0	-1.474214	1.477772	-0.575453
8	1	0	-1.786025	3.847597	-1.172317
9	6	0	-0.514867	1.715606	-0.091964
10	6	0	1.925881	2.346498	1.134403
11	1	0	2.571368	4.973837	1.016512
12	1	0	1.199448	6.764902	-0.058204
13	6	0	1.472142	1.050891	1.117999
14	6	0	0.239213	0.731881	0.498471
15	1	0	2.882625	2.603433	1.613354
16	1	0	2.058532	0.245452	1.584188
17	6	0	-0.239213	-0.731881	0.498471
18	6	0	-1.472142	-1.050891	1.117999
19	6	0	0.514867	-1.715606	-0.091964
20	6	0	-1.925881	-2.346498	1.134403
21	1	0	-2.058532	-0.245452	1.584188
22	6	0	0.069001	-3.065932	-0.089724
23	1	0	1.474214	-1.477772	-0.575453
24	6	0	-1.166193	-3.386105	0.530735
25	1	0	-2.882625	-2.603433	1.613354
26	6	0	0.829335	-4.104905	-0.693498
27	6	0	-1.612147	-4.736070	0.532963
28	6	0	0.375430	-5.400394	-0.677298
29	1	0	1.786025	-3.847597	-1.172317
30	6	0	-0.857412	-5.719480	-0.058091
31	1	0	-2.571368	-4.973837	1.016512
32	1	0	-1.199448	-6.764902	-0.058204
33	8	0	-1.137581	6.447470	-1.283646
34	8	0	1.137581	-6.447470	-1.283646
35	6	0	0.829335	-7.691556	-0.648612
36	1	0	-0.152820	-8.004351	-0.935721
37	1	0	1.541418	-8.431486	-0.949180
38	1	0	0.868522	-7.569595	0.413692
39	6	0	-0.829335	7.691556	-0.648612
40	1	0	0.152820	8.004351	-0.935721
41	1	0	-1.541418	8.431486	-0.949180
42	1	0	-0.868522	7.569595	0.413692

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6622199Haartrees

(S_A)-**1'** (θ_2 = 70°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.376251	0.321657	-0.692546
2	6	0	4.067935	0.768947	-0.729254
3	6	0	3.050993	0.098785	-0.010420
4	6	0	3.387273	-1.062128	0.761233
5	6	0	4.736560	-1.492571	0.777360
6	6	0	5.715027	-0.825492	0.072443
7	1	0	1.438940	1.407172	-0.626477
8	1	0	3.832152	1.648190	-1.320557
9	6	0	1.697091	0.534682	-0.031976
10	6	0	2.357629	-1.733901	1.472583
11	1	0	5.000229	-2.371021	1.360690
12	1	0	6.737117	-1.182920	0.106862
13	6	0	1.059353	-1.285235	1.430597
14	6	0	0.712981	-0.125046	0.678042
15	1	0	2.613561	-2.614876	2.056028
16	1	0	0.280277	-1.804063	1.980632
17	6	0	-0.708329	0.324819	0.616928
18	6	0	-1.094859	1.552433	1.229880
19	6	0	-1.674914	-0.465636	0.026292
20	6	0	-2.406233	1.963312	1.215585
21	1	0	-0.334306	2.158941	1.712093
22	6	0	-3.040585	-0.069499	-0.010805
23	1	0	-1.391703	-1.408208	-0.434740
24	6	0	-3.412957	1.174214	0.598270
25	1	0	-2.691496	2.900497	1.687095
26	6	0	-4.036494	-0.862588	-0.626714
27	6	0	-4.774816	1.561645	0.560448
28	6	0	-5.357847	-0.454363	-0.646605
29	1	0	-3.773543	-1.806400	-1.094018
30	6	0	-5.731928	0.775668	-0.044032
31	1	0	-5.065692	2.502519	1.020466
32	1	0	-6.764495	1.103232	-0.054847
33	8	0	6.282833	1.041474	-1.420408
34	8	0	-6.241642	-1.293690	-1.266499
35	6	0	-7.610192	-0.924604	-1.319097
36	1	0	-7.759558	0.015396	-1.865734
37	1	0	-8.116955	-1.730260	-1.852531
38	1	0	-8.047037	-0.829462	-0.316651
39	6	0	7.639557	0.627676	-1.420860
40	1	0	7.759039	-0.381964	-1.834467
41	1	0	8.168587	1.337713	-2.058366
42	1	0	8.076401	0.656606	-0.414328

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6609637 Haartrees

(S_A)-**1'** (θ_2 = 80°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.328127	0.683541	-0.494847
2	6	0	-4.007914	0.618562	-0.902327
3	6	0	-3.029269	-0.007625	-0.096242
4	6	0	-3.417250	-0.578470	1.160600
5	6	0	-4.777392	-0.494609	1.547138
6	6	0	-5.717987	0.118275	0.747856
7	1	0	-1.367272	0.350640	-1.438595
8	1	0	-3.732747	1.057453	-1.856247
9	6	0	-1.664063	-0.087593	-0.489375
10	6	0	-2.426380	-1.200177	1.966145
11	1	0	-5.080223	-0.925224	2.498113
12	1	0	-6.749721	0.164526	1.074991
13	6	0	-1.115946	-1.260212	1.555691
14	6	0	-0.718229	-0.703422	0.305484
15	1	0	-2.721535	-1.630642	2.919888
16	1	0	-0.366221	-1.737887	2.178970
17	6	0	0.715617	-0.763813	-0.113056
18	6	0	1.140182	-1.741010	-1.059478
19	6	0	1.649391	0.090543	0.438377
20	6	0	2.459294	-1.827913	-1.436040
21	1	0	0.403083	-2.417802	-1.480748
22	6	0	3.022442	0.030587	0.069901
23	1	0	1.335548	0.834318	1.165973
24	6	0	3.434647	-0.952015	-0.889677

25	1	0	2.774113	-2.576180	-2.159238
26	6	0	3.986810	0.906755	0.619550
27	6	0	4.803059	-1.007543	-1.251406
28	6	0	5.315590	0.826033	0.244040
29	1	0	3.693396	1.657555	1.346534
30	6	0	5.729138	-0.145505	-0.705170
31	1	0	5.124117	-1.749593	-1.977885
32	1	0	6.767769	-0.215976	-1.005043
33	8	0	-6.195023	1.308867	-1.347657
34	8	0	6.167017	1.718581	0.834183
35	6	0	7.541337	1.683020	0.484648
36	1	0	7.696932	1.883800	-0.583127
37	1	0	8.018746	2.471900	1.067912
38	1	0	8.003336	0.720526	0.739427
39	6	0	-7.561645	1.406278	-0.980150
40	1	0	-7.695849	1.977315	-0.052471
41	1	0	-8.054091	1.935303	-1.797508
42	1	0	-8.025157	0.418247	-0.863120

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.6599775 Haartrees

S12. Dihedral Angle Dependence of the Theoretical CPL Spectra

There have been extensive studies of the excited states of axially chiral. Among them, it appears that TD-DFT calculations based on the global hybrid M06-2X function together with a basis set of triple-ζ quality.[3] Therefore, we performed the TD-DFT in the excited state using M06-2X/def2-TZVP.

The theoretical CPL spectra were obtained after geometry optimization in its first singlet-excited state. Optimization and TD calculations of (*R*)-**1** and θ_2 in (S_A)-**1'** with preset (fixed) angle of θ_1 in were carried out at M06-2X/def2-TZVP level. [4] The calculations were carried out in vacuo, and obtained CPL spectra were depicted in Fig. S27 and S28.

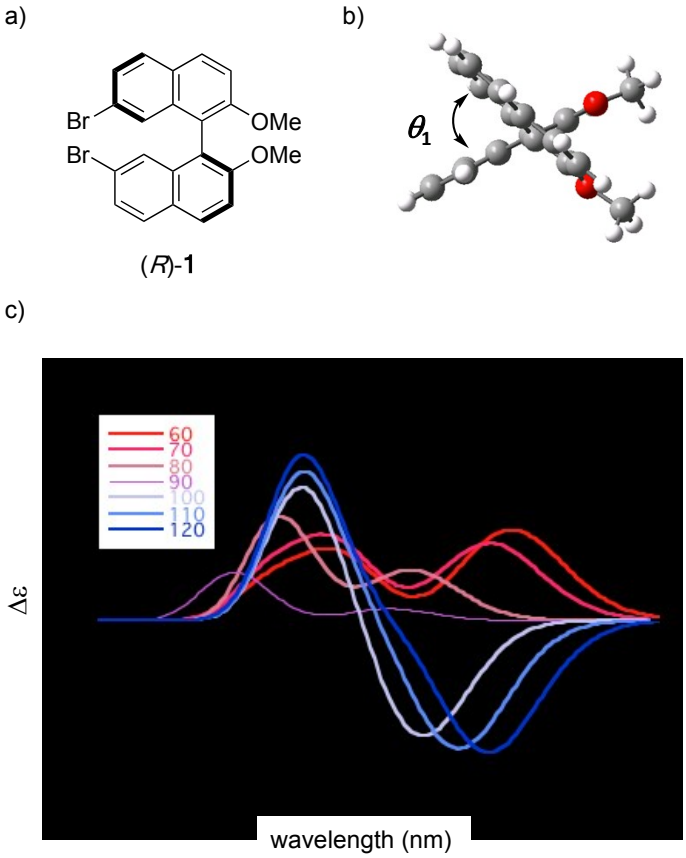


Fig. S27 *(a) Chemical structure of (R)-**1** (b) Optimized geometry (θ_1 = 70°) in the first excited state at B3LYP/6-31G(d,p) level. (c) Dihedral angle dependence of the theoretical CPL spectra of (R)-**1** at the M06-2X/def2TZVP level (width, 0.15 eV).*

Table S11. Optimized Geometries of (*R*)-**1** at the M06-2X/def2-TZVP in the first excited state

(*R*)-**1** (θ_1 = 60°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.175868	-2.880438	-1.367233
2	6	0	-1.255548	-1.920269	-0.976390
3	6	0	-1.633377	-0.805503	-0.215443
4	6	0	-3.017825	-0.638978	0.091509
5	6	0	-3.931746	-1.634050	-0.307850
6	6	0	-3.518920	-2.743610	-1.017100
7	1	0	-1.847986	-3.732369	-1.947683
8	1	0	-0.219395	-2.032339	-1.266555
9	6	0	-0.696811	0.225529	0.169435
10	6	0	-3.455641	0.536311	0.739912
11	1	0	-4.978571	-1.502086	-0.061005
12	1	0	-4.238614	-3.495319	-1.314288
13	6	0	-2.569971	1.535621	1.110445
14	6	0	-1.213305	1.378919	0.853155
15	1	0	-4.511125	0.648503	0.954686
16	1	0	-2.932630	2.397715	1.650093
17	6	0	0.696811	0.225530	-0.169433
18	6	0	1.633379	-0.805500	0.215445
19	6	0	1.213302	1.378921	-0.853155
20	6	0	1.255553	-1.920266	0.976392
21	6	0	3.017826	-0.638972	-0.091509
22	6	0	2.569968	1.535626	-1.110445
23	6	0	2.175875	-2.880434	1.367234
24	1	0	0.219400	-2.032337	1.266558
25	6	0	3.931750	-1.634044	0.307848
26	6	0	3.455640	0.536318	-0.739913
27	1	0	2.932624	2.397720	-1.650094
28	6	0	3.518927	-2.743604	1.017099
29	1	0	1.847994	-3.732365	1.947684
30	1	0	4.978574	-1.502079	0.061001
31	1	0	4.511123	0.648511	-0.954688
32	1	0	4.238622	-3.495312	1.314285
33	8	0	-0.274935	2.210211	1.340339
34	8	0	0.274930	2.210210	-1.340339
35	6	0	-0.685858	3.418912	1.937523
36	1	0	0.224729	3.959547	2.180935
37	1	0	-1.253418	3.232598	2.852581
38	1	0	-1.294619	4.007258	1.245441
39	6	0	0.685850	3.418912	-1.937525
40	1	0	-0.224738	3.959543	-2.180937
41	1	0	1.253410	3.232598	-2.852582
42	1	0	1.294610	4.007259	-1.245443

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.5663093Haartrees

(*R*)-**1** (θ_1 = 70°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.278355	-2.842344	1.373208
2	6	0	1.323160	-1.921764	0.970267
3	6	0	1.661703	-0.806380	0.191304
4	6	0	3.035481	-0.604114	-0.139410
5	6	0	3.984829	-1.556921	0.277221
6	6	0	3.613767	-2.664685	1.013874
7	1	0	1.983644	-3.695433	1.969562
8	1	0	0.290905	-2.062795	1.263811
9	6	0	0.685410	0.173168	-0.217818
10	6	0	3.422932	0.565006	-0.831700
11	1	0	5.025053	-1.396287	0.019633
12	1	0	4.360833	-3.384373	1.322494
13	6	0	2.499153	1.525204	-1.211616
14	6	0	1.153279	1.333309	-0.921106
15	1	0	4.470092	0.704580	-1.069860
16	1	0	2.824437	2.386312	-1.776256
17	6	0	-0.685407	0.172821	0.218468

18	6	0	-1.661289	-0.807101	-0.190946
19	6	0	-1.153855	1.332674	0.921665
20	6	0	-1.322178	-1.922596	-0.969505
21	6	0	-3.035252	-0.605007	0.139053
22	6	0	-2.499862	1.524335	1.211617
23	6	0	-2.277037	-2.843285	-1.372893
24	1	0	-0.289736	-2.063670	-1.262356
25	6	0	-3.984286	-1.557971	-0.278041
26	6	0	-3.423289	0.564022	0.831155
27	1	0	-2.825547	2.385316	1.776224
28	6	0	-3.612716	-2.665719	-1.014384
29	1	0	-1.981887	-3.696444	-1.968931
30	1	0	-5.024653	-1.397392	-0.020994
31	1	0	-4.470591	0.703391	1.068805
32	1	0	-4.359498	-3.385527	-1.323407
33	8	0	0.178622	2.139910	-1.377807
34	8	0	-0.179488	2.139474	1.378894
35	6	0	0.540514	3.356386	-1.991285
36	1	0	-0.390113	3.875446	-2.203641
37	1	0	1.079954	3.180088	-2.925142
38	1	0	1.159978	3.959716	-1.321972
39	6	0	-0.541963	3.356770	1.990352
40	1	0	0.388424	3.876380	2.202446
41	1	0	-1.081839	3.181833	2.924220
42	1	0	-1.161225	3.958929	1.319793

Keyword: opt=modredundant scf=(direct,tight)
Energy = –999.5664988Haartrees

(*R*)-**1** (θ_1 = 80°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.272512	-2.617070	-1.628854
2	6	0	-1.324370	-1.743250	-1.173121
3	6	0	-1.663191	-0.713787	-0.260468
4	6	0	-3.015011	-0.602197	0.157001
5	6	0	-3.973294	-1.521307	-0.333349
6	6	0	-3.614098	-2.510759	-1.204239
7	1	0	-1.992677	-3.397973	-2.324230
8	1	0	-0.297145	-1.828245	-1.504539
9	6	0	-0.690047	0.206322	0.231178
10	6	0	-3.373102	0.439830	1.039849
11	1	0	-5.001022	-1.421705	-0.004136
12	1	0	-4.353299	-3.209257	-1.573672
13	6	0	-2.445792	1.341277	1.487585
14	6	0	-1.102992	1.234484	1.072018
15	1	0	-4.404476	0.522373	1.361006
16	1	0	-2.748238	2.127206	2.164026
17	6	0	0.700295	0.194847	-0.238633
18	6	0	1.652542	-0.734830	0.257576
19	6	0	1.144864	1.289581	-1.070080
20	6	0	3.018437	-0.613511	-0.182510
21	6	0	1.311958	-1.749196	1.158572
22	6	0	2.464304	1.419594	-1.468303
23	6	0	3.949373	-1.549295	0.290956
24	6	0	3.380086	0.446278	-1.035288
25	6	0	2.268375	-2.683006	1.614050
26	1	0	0.289821	-1.815129	1.508994
27	1	0	2.780719	2.209547	-2.130172
28	6	0	3.569668	-2.577943	1.173652
29	1	0	4.981596	-1.468645	-0.027185
30	1	0	4.413708	0.517865	-1.351941
31	1	0	1.977136	-3.464691	2.301065
32	1	0	4.317612	-3.284798	1.510312
33	8	0	-0.136291	2.085082	1.490317
34	8	0	0.163342	2.104957	-1.461986
35	6	0	-0.498620	3.169470	2.313720
36	1	0	0.416379	3.726489	2.496122
37	1	0	-0.906366	2.825094	3.267698
38	1	0	-1.227859	3.817259	1.819677
39	6	0	0.490344	3.223517	-2.260123
40	1	0	-0.440373	3.758523	-2.424157
41	1	0	0.907545	2.904932	-3.217808
42	1	0	1.207214	3.866544	-1.744841

Key word: td scf=(direct, tight) opt=modredundant
Energy: HF= -999.5707631

(*R*)-**1** (θ_1 = 90°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.373319	-2.223159	-1.907771
2	6	0	-1.396607	-1.431871	-1.372742
3	6	0	-1.677336	-0.572327	-0.278352
4	6	0	-2.991708	-0.568371	0.259131
5	6	0	-3.981500	-1.400517	-0.320051
6	6	0	-3.684302	-2.207332	-1.379999
7	1	0	-2.141868	-2.874690	-2.740622
8	1	0	-0.390454	-1.455122	-1.772919
9	6	0	-0.681611	0.265069	0.289240
10	6	0	-3.270332	0.264924	1.362015
11	1	0	-4.981021	-1.384292	0.098610
12	1	0	-4.446368	-2.840250	-1.815478
13	6	0	-2.303480	1.058455	1.914339
14	6	0	-0.997333	1.057835	1.373934
15	1	0	-4.272287	0.269837	1.774398
16	1	0	-2.545713	1.688403	2.757673
17	6	0	0.695445	0.280511	-0.253301
18	6	0	1.681474	-0.596642	0.241873
19	6	0	1.014251	1.199803	-1.312710
20	6	0	3.005474	-0.517292	-0.327794
21	6	0	1.415321	-1.534359	1.250028
22	6	0	2.284023	1.274226	-1.868978
23	6	0	3.986518	-1.381918	0.176913
24	6	0	3.264222	0.407391	-1.356417
25	6	0	2.425771	-2.395759	1.738385
26	1	0	0.413378	-1.592544	1.655115
27	1	0	2.521096	1.968903	-2.657849
28	6	0	3.690858	-2.308718	1.200991
29	1	0	4.989373	-1.335565	-0.229315
30	1	0	4.265960	0.443648	-1.767828
31	1	0	2.201733	-3.110106	2.517270
32	1	0	4.479515	-2.958438	1.559709
33	8	0	0.001347	1.833762	1.864347
34	8	0	-0.013727	1.958628	-1.692628
35	6	0	-0.247002	2.602952	3.018512
36	1	0	0.689975	3.099835	3.255054
37	1	0	-0.544015	1.972193	3.860509
38	1	0	-1.019290	3.355632	2.838432
39	6	0	0.180429	2.895215	-2.734208
40	1	0	-0.777034	3.386577	-2.877695
41	1	0	0.481757	2.389400	-3.653640
42	1	0	0.938777	3.628759	-2.453403

Key word: td scf=(direct, tight) opt=modredundant
Energy: HF= -999.571898

(*R*)-**1** (θ_1 = 100°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.708097	-1.768789	-1.939459
2	6	0	1.629229	-1.295839	-1.210913
3	6	0	1.736581	-0.143455	-0.414964
4	6	0	2.965856	0.581526	-0.422929
5	6	0	4.051079	0.073643	-1.169680
6	6	0	3.926970	-1.084539	-1.906626
7	1	0	2.602762	-2.661110	-2.541790
8	1	0	0.679162	-1.812989	-1.261725
9	6	0	0.639411	0.341700	0.370378
10	6	0	3.046452	1.805053	0.269109
11	1	0	4.986374	0.620744	-1.163540
12	1	0	4.770516	-1.455090	-2.474792
13	6	0	1.950851	2.341827	0.926823
14	6	0	0.750055	1.630798	0.954174
15	1	0	3.982485	2.350045	0.256540
16	1	0	2.040960	3.290522	1.433678
17	6	0	-0.643801	-0.332271	0.372652
18	6	0	-1.742311	0.145094	-0.413701
19	6	0	-0.746257	-1.631769	0.961855
20	6	0	-2.970546	-0.589673	-0.409331

21	6	0	-1.642594	1.290370	-1.213198
22	6	0	-1.936097	-2.351725	0.940215
23	6	0	-4.058359	-0.087053	-1.150521
24	6	0	-3.041081	-1.811345	0.285786
25	6	0	-2.732934	1.763543	-1.941913
26	1	0	-0.694311	1.810001	-1.269693
27	1	0	-2.020672	-3.299963	1.448017
28	6	0	-3.941474	1.075676	-1.896763
29	1	0	-4.993322	-0.634405	-1.138835
30	1	0	-3.975172	-2.359757	0.277228
31	1	0	-2.633755	2.655643	-2.544966
32	1	0	-4.792854	1.438619	-2.458394
33	8	0	-0.349961	2.066146	1.591237
34	8	0	0.360115	-2.048473	1.592872
35	6	0	-0.339237	3.354068	2.166488
36	1	0	-1.335733	3.510066	2.569632
37	1	0	-0.122997	4.116933	1.414543
38	1	0	0.395652	3.418002	2.972739
39	6	0	0.368222	-3.332824	2.178016
40	1	0	1.368217	-3.473576	2.577668
41	1	0	0.156457	-4.101668	1.431218
42	1	0	-0.363672	-3.397513	2.986602

Key word: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5705258

(*R*)-**1** (θ_1 = 110°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.945096	-1.663546	-1.821846
2	6	0	1.796452	-1.234762	-1.169325
3	6	0	1.787656	-0.064784	-0.398755
4	6	0	2.970340	0.734363	-0.358153
5	6	0	4.126686	0.272500	-1.021559
6	6	0	4.116221	-0.910716	-1.733335
7	1	0	2.925840	-2.574499	-2.404735
8	1	0	0.882529	-1.807258	-1.266266
9	6	0	0.611698	0.381133	0.301698
10	6	0	2.937891	1.982513	0.292010
11	1	0	5.026371	0.874557	-0.975497
12	1	0	5.014178	-1.243759	-2.237826
13	6	0	1.775059	2.474672	0.871876
14	6	0	0.622431	1.695092	0.864362
15	1	0	3.838730	2.583646	0.309930
16	1	0	1.784010	3.439818	1.354851
17	6	0	-0.611666	-0.381070	0.301848
18	6	0	-1.787722	0.064726	-0.398523
19	6	0	-0.622311	-1.694937	0.864717
20	6	0	-2.970388	-0.734434	-0.357645
21	6	0	-1.796634	1.234581	-1.169279
22	6	0	-1.774925	-2.474531	0.872502
23	6	0	-4.126828	-0.272692	-1.020978
24	6	0	-2.937840	-1.982478	0.292710
25	6	0	-2.945369	1.663246	-1.821718
26	1	0	-0.882734	1.807076	-1.266431
27	1	0	-1.783803	-3.439602	1.355630
28	6	0	-4.116473	0.910412	-1.732939
29	1	0	-5.026496	-0.874756	-0.974706
30	1	0	-3.838667	-2.583623	0.310839
31	1	0	-2.926201	2.574108	-2.404752
32	1	0	-5.014498	1.243363	-2.237368
33	8	0	-0.521096	2.066596	1.459582
34	8	0	0.521306	-2.066336	1.459843
35	6	0	-0.613833	3.360376	2.014197
36	1	0	-1.631203	3.455593	2.382424
37	1	0	-0.422955	4.124239	1.256371
38	1	0	0.089266	3.483293	2.841509
39	6	0	0.614138	-3.360036	2.014623
40	1	0	1.631564	-3.455193	2.382715
41	1	0	0.423157	-4.124009	1.256933
42	1	0	-0.088837	-3.482849	2.842056

Key word: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.570475

(*R*)-**1** (θ_1 = 120°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.121439	-1.574654	-1.726998
2	6	0	1.921866	-1.177440	-1.152220
3	6	0	1.825240	-0.002121	-0.396831
4	6	0	2.973671	0.839493	-0.302984
5	6	0	4.184997	0.409601	-0.885623
6	6	0	4.260022	-0.782190	-1.577269
7	1	0	3.167609	-2.491920	-2.298484
8	1	0	1.035227	-1.780716	-1.300970
9	6	0	0.585919	0.415830	0.214092
10	6	0	2.858599	2.098069	0.317227
11	1	0	5.057953	1.044931	-0.794358
12	1	0	5.198083	-1.090923	-2.020477
13	6	0	1.649031	2.552488	0.826978
14	6	0	0.526878	1.732180	0.776038
15	1	0	3.733673	2.733973	0.372080
16	1	0	1.598818	3.521255	1.300244
17	6	0	-0.585904	-0.415799	0.214187
18	6	0	-1.825285	0.002087	-0.396665
19	6	0	-0.526802	-1.732097	0.776242
20	6	0	-2.973707	-0.839516	-0.302612
21	6	0	-1.921984	1.177319	-1.152181
22	6	0	-1.648949	-2.552401	0.827382
23	6	0	-4.185092	-0.409685	-0.885173
24	6	0	-2.858572	-2.098029	0.317715
25	6	0	-3.121616	1.574473	-1.726878
26	1	0	-1.035360	1.780576	-1.301093
27	1	0	-1.598685	-3.521123	1.300732
28	6	0	-4.260186	0.782032	-1.576940
29	1	0	-5.058040	-1.045004	-0.793750
30	1	0	-3.733639	-2.733929	0.372720
31	1	0	-3.167841	2.491676	-2.298463
32	1	0	-5.198292	1.090718	-2.020086
33	8	0	-0.644438	2.059793	1.341444
34	8	0	0.644582	-2.059662	1.341539
35	6	0	-0.804920	3.348997	1.890483
36	1	0	-1.836429	3.403855	2.226355
37	1	0	-0.621283	4.119461	1.137450
38	1	0	-0.133454	3.500588	2.739055
39	6	0	0.805132	-3.348823	1.890655
40	1	0	1.836682	-3.403654	2.226408
41	1	0	0.621406	-4.119345	1.137703
42	1	0	0.133768	-3.500352	2.739320

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5698584

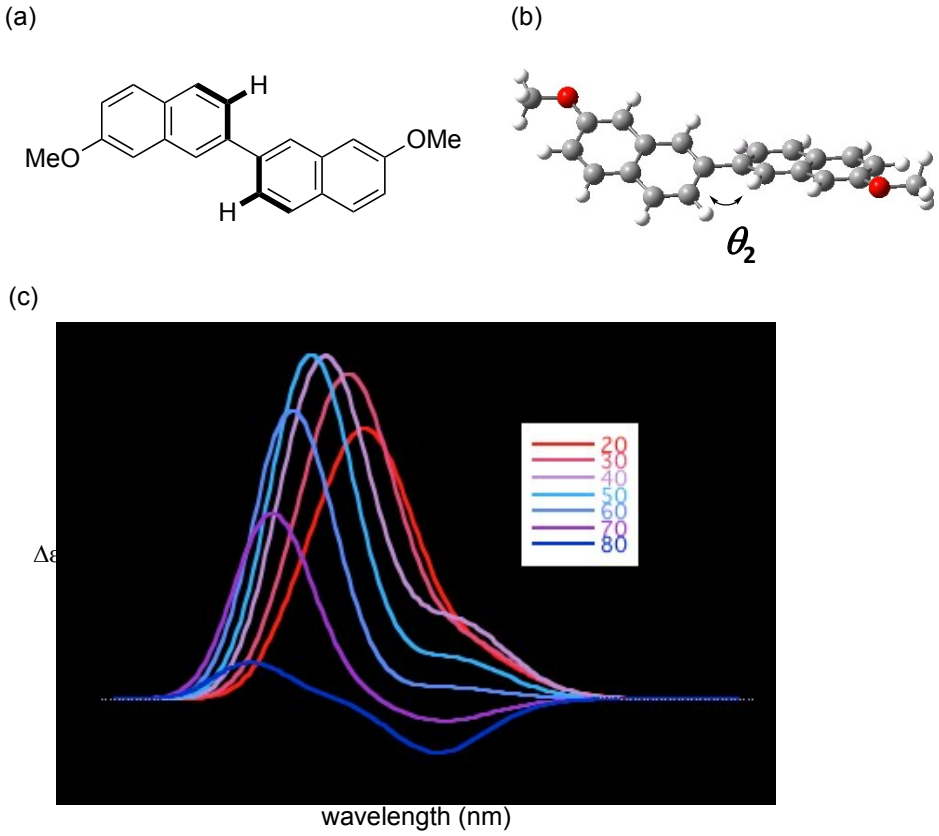


Fig. S28 *(a), (b) Molecular geometry of (S_A)-**1'**. (c) Dihedral angle dependence of the theoretical CPL spectra of (R)-**1** at the M06-2X/def2TZVP level (width, 0.15 eV).*

Table S12. Optimized Geometries of (S_A)-**1'** at the CAM-B3LYP/6–31G(d,p) in the first excited state

(S_A)-**1'** (θ_1 = 20°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.510822	-0.407011	0.217579
2	6	0	4.236841	-0.917375	0.225111
3	6	0	3.119073	-0.083056	0.001518
4	6	0	3.336718	1.305313	-0.226366
5	6	0	4.653058	1.795545	-0.229147
6	6	0	5.729453	0.970577	-0.014244
7	1	0	1.665184	-1.631925	0.228072
8	1	0	4.100760	-1.976341	0.404948
9	6	0	1.800371	-0.580060	0.009956
10	6	0	2.207072	2.137337	-0.440900
11	1	0	4.815692	2.852487	-0.405796
12	1	0	6.728580	1.379798	-0.023405
13	6	0	0.944858	1.631599	-0.423586
14	6	0	0.699701	0.239847	-0.199312
15	1	0	2.367807	3.192487	-0.630413
16	1	0	0.112829	2.292645	-0.624447
17	6	0	-0.659449	-0.271384	-0.208703
18	6	0	-0.940272	-1.629739	-0.419805
19	6	0	-1.791608	0.570748	0.004010
20	6	0	-2.236314	-2.143067	-0.432258
21	1	0	-0.124611	-2.312345	-0.618660
22	6	0	-3.101519	0.082923	-0.001685
23	1	0	-1.649158	1.622193	0.216368
24	6	0	-3.356842	-1.319293	-0.225385
25	1	0	-2.385728	-3.199929	-0.618268
26	6	0	-4.216041	0.904105	0.217946
27	6	0	-4.673157	-1.798941	-0.226604
28	6	0	-5.532238	0.381213	0.212796
29	1	0	-4.101876	1.966064	0.396014
30	6	0	-5.783499	-0.975484	-0.011787
31	1	0	-4.829347	-2.857626	-0.398802
32	1	0	-6.781844	-1.380475	-0.019233
33	8	0	6.521117	-1.290807	0.441253
34	8	0	-6.482095	1.292446	0.436875
35	6	0	-7.835381	0.874789	0.452046
36	1	0	-8.001418	0.138681	1.240624
37	1	0	-8.422109	1.766544	0.649466
38	1	0	-8.117482	0.450628	-0.513239
39	6	0	7.842755	-0.805578	0.443475
40	1	0	7.993131	-0.058932	1.228093
41	1	0	8.480176	-1.664034	0.639243
42	1	0	8.110821	-0.371094	-0.523511

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5780161

(S_A)-**1'** (θ_1 = 30°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.495971	0.402117	0.294148
2	6	0	-4.220008	0.907818	0.307279
3	6	0	-3.111361	0.087515	0.004497
4	6	0	-3.337342	-1.282248	-0.309139
5	6	0	-4.655724	-1.768057	-0.315033
6	6	0	-5.723815	-0.956585	-0.022733
7	1	0	-1.634298	1.611605	0.307220
8	1	0	-4.075649	1.952338	0.553045
9	6	0	-1.789089	0.578506	0.019698
10	6	0	-2.216511	-2.103981	-0.599536
11	1	0	-4.826404	-2.810771	-0.556657
12	1	0	-6.724310	-1.362421	-0.036691
13	6	0	-0.952063	-1.603705	-0.577487
14	6	0	-0.702572	-0.228917	-0.276515

15	1	0	-2.387114	-3.144542	-0.850938
16	1	0	-0.120341	-2.247103	-0.833728
17	6	0	0.659699	0.278553	-0.264097
18	6	0	0.950236	1.613658	-0.567758
19	6	0	1.777238	-0.561151	0.017046
20	6	0	2.252431	2.117413	-0.586785
21	1	0	0.138599	2.279551	-0.833019
22	6	0	3.091549	-0.083828	0.004963
23	1	0	1.613878	-1.596632	0.288578
24	6	0	3.360643	1.300343	-0.301783
25	1	0	2.415703	3.157058	-0.844008
26	6	0	4.195212	-0.896298	0.296377
27	6	0	4.681009	1.770193	-0.305973
28	6	0	5.516847	-0.381881	0.286506
29	1	0	4.070383	-1.944701	0.536604
30	6	0	5.782371	0.955074	-0.016023
31	1	0	4.848637	2.814762	-0.541704
32	1	0	6.783285	1.353556	-0.027628
33	8	0	-6.497848	1.271586	0.597125
34	8	0	6.453493	-1.284477	0.586128
35	6	0	7.809545	-0.875800	0.604444
36	1	0	7.964456	-0.093428	1.349548
37	1	0	8.384926	-1.757588	0.868715
38	1	0	8.114635	-0.513577	-0.378911
39	6	0	-7.820998	0.790321	0.596211
40	1	0	-7.957332	-0.005557	1.333575
41	1	0	-8.450848	1.635657	0.861179
42	1	0	-8.111318	0.420555	-0.391057

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5786087

(S_A)-**1'** ($\theta_1 = 40°$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.497695	0.369328	0.373843
2	6	0	-4.173469	0.881462	0.385027
3	6	0	-3.081403	0.093415	-0.000186
4	6	0	-3.360989	-1.265073	-0.399831
5	6	0	-4.683175	-1.731785	-0.402045
6	6	0	-5.775277	-0.938993	-0.021569
7	1	0	-1.581663	1.578338	0.351297
8	1	0	-4.039050	1.908319	0.700963
9	6	0	-1.765284	0.567188	0.007429
10	6	0	-2.263858	-2.063223	-0.767539
11	1	0	-4.860181	-2.756126	-0.708753
12	1	0	-6.777150	-1.334997	-0.035491
13	6	0	-0.957221	-1.563038	-0.748439
14	6	0	-0.664445	-0.247211	-0.386135
15	1	0	-2.437233	-3.083988	-1.086117
16	1	0	-0.148169	-2.211906	-1.061400
17	6	0	0.703483	0.252171	-0.342540
18	6	0	0.978711	1.593951	-0.745484
19	6	0	1.764645	-0.554325	0.023837
20	6	0	2.250939	2.074570	-0.769197
21	1	0	0.156970	2.222038	-1.067035
22	6	0	3.096348	-0.082619	0.011747
23	1	0	1.580512	-1.566363	0.365370
24	6	0	3.349802	1.258434	-0.389381
25	1	0	2.446359	3.089645	-1.095382
26	6	0	4.182749	-0.895980	0.397508
27	6	0	4.675951	1.723808	-0.394812
28	6	0	5.467105	-0.410575	0.383321
29	1	0	4.015172	-1.918789	0.710629
30	6	0	5.723160	0.919324	-0.019793
31	1	0	4.869395	2.744513	-0.703728
32	1	0	6.730022	1.309240	-0.035930
33	8	0	-6.421511	1.247767	0.769282
34	8	0	6.446881	-1.270935	0.771158
35	6	0	7.777159	-0.809420	0.771724
36	1	0	8.097887	-0.513155	-0.230829
37	1	0	8.386730	-1.642974	1.110980
38	1	0	7.907375	0.033826	1.455620
39	6	0	-7.777604	0.840339	0.796159
40	1	0	-8.112219	0.554628	-0.202733
41	1	0	-8.342458	1.699630	1.144092
42	1	0	-7.913057	0.002977	1.483065

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5785863

(S_A)-**1'** (θ_1 = 50°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.463509	0.368113	0.450028
2	6	0	-4.185042	0.868054	0.483173
3	6	0	-3.097125	0.104461	0.012112
4	6	0	-3.339158	-1.202234	-0.492964
5	6	0	-4.660323	-1.683789	-0.515372
6	6	0	-5.709819	-0.927168	-0.058549
7	1	0	-1.583607	1.569149	0.470871
8	1	0	-4.023871	1.863787	0.876522
9	6	0	-1.768787	0.589139	0.045641
10	6	0	-2.236900	-1.973967	-0.946632
11	1	0	-4.846415	-2.678405	-0.903661
12	1	0	-6.712137	-1.327788	-0.090254
13	6	0	-0.969702	-1.479119	-0.905986
14	6	0	-0.712087	-0.160045	-0.428827
15	1	0	-2.424124	-2.968296	-1.335535
16	1	0	-0.140999	-2.072054	-1.273480
17	6	0	0.661716	0.335353	-0.368697
18	6	0	0.996862	1.603875	-0.833050
19	6	0	1.734076	-0.506349	0.040456
20	6	0	2.321651	2.065597	-0.863955
21	1	0	0.209133	2.247760	-1.206237
22	6	0	3.065670	-0.073067	0.020427
23	1	0	1.516188	-1.501673	0.409957
24	6	0	3.388100	1.256410	-0.439225
25	1	0	2.529763	3.058894	-1.242443
26	6	0	4.129242	-0.876250	0.446666
27	6	0	4.725496	1.682265	-0.448612
28	6	0	5.470752	-0.403258	0.429521
29	1	0	3.961405	-1.884375	0.804025
30	6	0	5.790560	0.876080	-0.017653
31	1	0	4.936767	2.684409	-0.803012
32	1	0	6.803514	1.242651	-0.036261
33	8	0	-6.446790	1.179224	0.924251
34	8	0	6.361408	-1.292404	0.873022
35	6	0	7.729186	-0.926357	0.898478
36	1	0	8.082490	-0.694033	-0.107799
37	1	0	8.263436	-1.786747	1.289303
38	1	0	7.883172	-0.064586	1.550411
39	6	0	-7.771212	0.701224	0.907310
40	1	0	-8.105314	0.485795	-0.111340
41	1	0	-8.384938	1.495106	1.325007
42	1	0	-7.879291	-0.197981	1.520006

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.577469

(S_A)-**1'** (θ_1 = 60°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.447246	0.329804	0.528017
2	6	0	-4.168073	0.826665	0.585092
3	6	0	-3.090382	0.114283	0.022551
4	6	0	-3.340030	-1.137425	-0.601973
5	6	0	-4.661875	-1.617900	-0.645522
6	6	0	-5.701991	-0.911058	-0.097997
7	1	0	-1.564593	1.535189	0.584953
8	1	0	-3.999394	1.780354	1.069082
9	6	0	-1.759865	0.597694	0.076584
10	6	0	-2.247031	-1.859399	-1.149449
11	1	0	-4.855381	-2.570743	-1.124248
12	1	0	-6.704544	-1.309235	-0.149085
13	6	0	-0.979834	-1.364906	-1.088215
14	6	0	-0.717777	-0.096416	-0.494303
15	1	0	-2.441009	-2.813500	-1.625862
16	1	0	-0.153945	-1.916869	-1.520467
17	6	0	0.664198	0.389845	-0.409718
18	6	0	1.032625	1.621954	-0.931808

19	6	0	1.706462	-0.458401	0.055261
20	6	0	2.372105	2.052369	-0.960352
21	1	0	0.265199	2.264195	-1.347818
22	6	0	3.050222	-0.059363	0.035055
23	1	0	1.456069	-1.432542	0.459421
24	6	0	3.410307	1.239166	-0.481436
25	1	0	2.609906	3.022021	-1.380089
26	6	0	4.086232	-0.868539	0.511172
27	6	0	4.759811	1.630610	-0.490365
28	6	0	5.441588	-0.430163	0.491550
29	1	0	3.888199	-1.855011	0.910911
30	6	0	5.798622	0.818067	-0.007291
31	1	0	5.001687	2.609413	-0.887585
32	1	0	6.820653	1.158692	-0.027523
33	8	0	-6.421246	1.089720	1.096033
34	8	0	6.301868	-1.321921	0.986568
35	6	0	7.678397	-0.991001	1.014217
36	1	0	7.847075	-0.105977	1.630443
37	1	0	8.185032	-1.847295	1.448474
38	1	0	8.049357	-0.811311	0.003484
39	6	0	-7.745896	0.613019	1.058619
40	1	0	-7.842159	-0.340536	1.585044
41	1	0	-8.351550	1.362465	1.561408
42	1	0	-8.098999	0.494855	0.030519

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5759543

(S_A)-**1'** (θ_1 = 70°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.415149	0.265651	0.634088
2	6	0	-4.131689	0.747067	0.723259
3	6	0	-3.076556	0.121234	0.031982
4	6	0	-3.350152	-1.025749	-0.759352
5	6	0	-4.676394	-1.492887	-0.832534
6	6	0	-5.694754	-0.871076	-0.157288
7	1	0	-1.525214	1.451308	0.738523
8	1	0	-3.942361	1.620462	1.334432
9	6	0	-1.740720	0.592232	0.113433
10	6	0	-2.278955	-1.662396	-1.438546
11	1	0	-4.889883	-2.365696	-1.438373
12	1	0	-6.700752	-1.256012	-0.235460
13	6	0	-1.007442	-1.182007	-1.344970
14	6	0	-0.724052	-0.013842	-0.581968
15	1	0	-2.492256	-2.538161	-2.040510
16	1	0	-0.194648	-1.667472	-1.871346
17	6	0	0.669811	0.452372	-0.472087
18	6	0	1.076691	1.662678	-1.006029
19	6	0	1.675454	-0.414839	0.033029
20	6	0	2.431615	2.058144	-1.011144
21	1	0	0.335021	2.318738	-1.446206
22	6	0	3.031095	-0.051921	0.036252
23	1	0	1.388182	-1.376150	0.443238
24	6	0	3.435462	1.226664	-0.496571
25	1	0	2.703739	3.015488	-1.437984
26	6	0	4.032551	-0.879494	0.549836
27	6	0	4.797082	1.580553	-0.482716
28	6	0	5.401464	-0.478175	0.552740
29	1	0	3.798606	-1.851981	0.964058
30	6	0	5.802511	0.748673	0.039119
31	1	0	5.075163	2.544078	-0.893136
32	1	0	6.833751	1.061305	0.035673
33	8	0	-6.367186	0.936607	1.335158
34	8	0	6.224415	-1.383909	1.084660
35	6	0	7.608212	-1.089326	1.138039
36	1	0	7.786383	-0.197022	1.741049
37	1	0	8.081818	-1.950085	1.599924
38	1	0	8.006387	-0.938820	0.132855
39	6	0	-7.695747	0.473696	1.268594
40	1	0	-7.783004	-0.546045	1.653379
41	1	0	-8.281196	1.143445	1.893011
42	1	0	-8.079603	0.507516	0.245318

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5743201

(S_A)-**1'** (θ_1 = 80°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.363714	0.015759	-0.774681
2	6	0	-4.069445	-0.383191	-1.003440
3	6	0	-3.053141	-0.102879	-0.070787
4	6	0	-3.375345	0.605212	1.116604
5	6	0	-4.712528	0.998789	1.323150
6	6	0	-5.692269	0.716890	0.407729
7	1	0	-1.453639	-1.026435	-1.197975
8	1	0	-3.841149	-0.920438	-1.915273
9	6	0	-1.706522	-0.499888	-0.284872
10	6	0	-2.343707	0.895407	2.045575
11	1	0	-4.964559	1.537101	2.229249
12	1	0	-6.707249	1.033757	0.597356
13	6	0	-1.060871	0.496642	1.812341
14	6	0	-0.730433	-0.238312	0.640193
15	1	0	-2.594941	1.438102	2.949506
16	1	0	-0.275527	0.716985	2.524820
17	6	0	0.678368	-0.626383	0.406407
18	6	0	1.122122	-1.917975	0.609249
19	6	0	1.645373	0.369027	0.109208
20	6	0	2.489685	-2.262166	0.487202
21	1	0	0.406972	-2.686298	0.877823
22	6	0	3.010166	0.058761	-0.013045
23	1	0	1.323337	1.393278	-0.038609
24	6	0	3.457451	-1.299686	0.177016
25	1	0	2.795273	-3.288266	0.649435
26	6	0	3.975634	1.017947	-0.323783
27	6	0	4.828346	-1.597233	0.047060
28	6	0	5.355199	0.671839	-0.454102
29	1	0	3.706287	2.055006	-0.478365
30	6	0	5.798629	-0.630454	-0.271262
31	1	0	5.141340	-2.623451	0.198414
32	1	0	6.836962	-0.902816	-0.366327
33	8	0	-6.276870	-0.299848	-1.730391
34	8	0	6.139589	1.707309	-0.760061
35	6	0	7.528133	1.479133	-0.913861
36	1	0	7.711831	0.770092	-1.723315
37	1	0	7.966955	2.441910	-1.156886
38	1	0	7.957984	1.096415	0.013758
39	6	0	-7.615194	0.091340	-1.530353
40	1	0	-7.706635	1.178405	-1.456578
41	1	0	-8.165150	-0.256065	-2.400981
42	1	0	-8.035469	-0.368433	-0.631722

Keyword: td scf=(direct, tight) opt=modredundant
Energy: HF=-999.5730533

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