Electronic Supplementary Information

Chiral photoswitch based on enantiospecific interconversion between binaphthyl and helicenoid skeletons

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Contents

1 Experimental details

General

All of the synthetic reactions were carried out under a dry nitrogen atmosphere. Reagents and solvents were purchased and used as received. Flash column chromatography was carried out with Merck 230-400 mesh silica gel using chloroform and hexane as the eluent. Analytical thin-layer chromatography was performed on the Merck pre-coated 0.25-mm thick silica gel TLC plates. ^{1}H NMR Spectra were recorded in chloroform-d ($CDCl_3$) or in methanol-d_4 (CD_3OD) containing tetramethylsilane (TMS) as the internal standard on a 300 MHz NMR spectrometer (DRX300, Bruker). $^{13}C\{^{1}H, ^{19}F\}$ NMR Spectra were recorded in chloroform-d ($CDCl_3$) containing TMS as the internal standard on a 400 MHz NMR spectrometer (ECZ400, JEOL). The *J* values are expressed in Hz and quoted chemical shifts are in ppm. Splitting patterns are indicated as s, singlet; d, doublet; t, triplet; m, multiplet. Low-resolution mass spectra were measured by the electron impact ionization using a JEOL JMS-AX-600 mass spectrometer. High resolution mass spectra were measured by a Thermo-Fischer Scientific mass spectrometer, equipped with an ion-trap mass analyzer, with the atomic pressure chemical ionization method. Melting points (Mp) were measured using a Yazawa BY-2 hot stage microscope, and those were uncorrected.

Optical Measurements

Absorption spectra of **1o** in hexane (9.4×10^{-5} mol dm^{-3}) were measured on a UV-visible spectrophotometer (V-550, JASCO). Photochemical reaction was carried out in a quartz cell with 10-mm optical path length. Photoirradiation with 280-nm light was carried out using a 100 W xenon lamp (LAX-C100, Asahi spectra), separated by a LAX-UVB 240-300 mirror module and a HQBP 280-UV filter. Photoirradiation with 436-nm light was carried out using a 500 W super high-pressure mercury lamp (USH-500D, USHIO), separated by filters (a 5-cm water filter, a Y-43 glass filter, a V-44 glass filter). An ultra-high performance liquid chromatograph (JASCO, X-LC 3000) equipped with a UV/Vis detector (JASCO X-LC 3070 UV) as well as a silica gel column (ZORBAX Rx-Sil RRHT, Agilent) or a chiral column (OZ-H, Daicel) was used to determine the concentration of isomers during photoirradiation. Photocyclization quantum yield upon irradiation with 280-nm light and photocycloreversion quantum yield upon irradiation with 436-nm light were determined with the procedures described elsewhere.[1] Light intensity was measured using a power meter (Newport, 1830-C) equipped with a detector (818-UV) or a power meter (Newport, 843-R).

Theoretical calculations

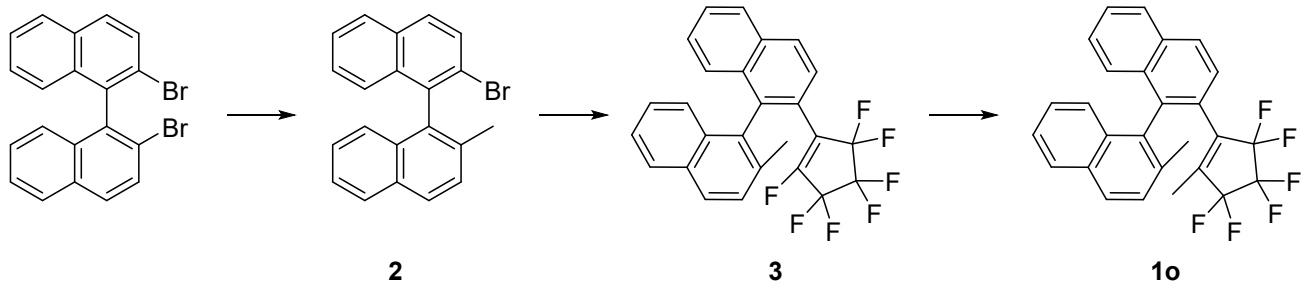
The optimization of structures and frequency calculations of (*P*)- and (*M*)-**1o**, (*P*)-(3a*S*,3b*R*)-**1c** and (*M*)-(3a*S*,3b*R*)-**1c**, the transition state determination between (*P*)-(3a*S*,3b*R*)-**1c** and (*M*)-(3a*S*,3b*R*)-**1c** and the intrinsic reaction coordinate calculation were carried out using DFT with the ωB97X-D functional[2] and 6-31G(d) basis set[3] on Spartan'20 (for optimization of structures) or Spartan'18 (for transition state determination) quantum chemistry software.[4]

CD spectra of (*P*)-**1o**, (*M*)-**1o**, (*P*)-(3a*S*,3b*R*)-**1c**, (*M*)-(3a*R*,3b*S*)-**1c**, (*P*)-(3a*R*,3b*S*)-**1c**, and (*M*)-(3a*S*,3b*R*)-**1c** were calculated for their optimized structures obtained above, using TD-DFT with the ωB97X-D functional and 6-31+G(d)[5] basis set on Gaussian 16 quantum chemistry software.[6]

All calculations were done for the molecules in vacuum.

2 Synthetic procedures

Synthesis of **1o** was carried out according to the following procedures.



2 **3** **1o**

2-1 Synthesis of 2-methyl-2'-(perfluorocyclopent-1-en-1-yl)-1,1'-binaphthalene (**3**)

To a solution of 2-bromo-2'-methyl-1,1'-binaphthalene (**2**)[7] (0.0510 g, 0.147 mmol) in dry THF (15 mL) was added dropwise an *n*-BuLi solution in hexane (2.65 mol dm^{-3}, 0.0500 mL, 0.133 mmol) at -78 °C under a N_2 atmosphere, and the resulting mixture was stirred for 30 min. To the reaction mixture was added dropwise an octafluorocyclopentene (0.038 mL, 0.28 mmol), and the reaction mixture was stirred for overnight at room temperature. The reaction was quenched by adding water, and the reaction mixture was extracted with ethyl acetate. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4, the drying agent filtered off, and the solvent evaporated. The residue was purified by column chromatography on silica gel using hexane as the eluent, to give 0.0441 g of 2-methyl-2'-(perfluorocyclopent-1-en-1-yl)-1,1'-binaphthalene (**3**) as a white solid in 65% yield.

^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ/ppm: 2.06 (3H, s), 7.00 (1H, d, *J* = 8.7 Hz), 7.18-7.23 (1H, m), 7.27-7.42 (3H, m), 7.45 (1H, d, *J* = 8.7 Hz), 7.56-7.67 (2H, m), 7.87 (2H, t, *J* = 8.1 Hz), 8.00 (1H, d, *J* = 8.3 Hz), 8.07 (1H, d, *J* = 8.7 Hz). (Fig. S1)

^{13}C {1H, ^{19}F} NMR (100 MHz, $CDCl_3$, TMS) δ/ppm: 20.15, 109.88, 115.48, 121.59, 122.73, 125.03, 125.08, 125.51, 126.05, 127.01, 127.41, 127.74, 127.85, 128.25, 128.33, 128.60 (2C), 131.84, 131.88, 132.68 (2C), 134.23, 135.26, 139.93, 152.34. There must be an overlapping of two signals in the aromatic region. (Fig. S3)

LRMS (EI, 70eV) m/z 460 (100, M^+). (Fig. S5)

HRMS (APCI-MS with ion trap) Found: m/z 460.1055. Calcd for $C_{26}H_{15}F_7$: M^+, m/z 460.1062. (Fig. S7)

Mp = 128.9-130.0 °C.

2-2 Synthesis of 2-(3,3,4,4,5,5-hexafluoro-2-methylcyclopent-1-en-1-yl)-2'-methyl-1,1'-binaphthalene (**1o**)

To a solution of **3** (0.0991 g, 0.215 mmol) in dry diethyl ether (5 mL) was added dropwise a MeLi solution in diethyl ether (1.66 mol dm^{-3}, 0.160 mL, 0.266 mmol) under a N_2 atmosphere at room temperature and the resulting mixture was stirred for overnight. The reaction was quenched by adding water, and the reaction mixture was extracted with ethyl acetate. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4, the drying agent filtered off, and the solvent evaporated. The residue was purified by column chromatography on silica gel using 1% chloroform/hexane as the eluent, to give 0.0634 g of 2-(3,3,4,4,5,5-hexafluoro-2-methylcyclopent-1-en-1-yl)-2'-methyl-1,1'-binaphthalene (**1o**) as a white solid in 65% yield.

^{1}H NMR (300 MHz, CD_3OD, TMS) δ/ppm: 1.62 (3H, br s), 2.03 (s, 3H), 6.96 (1H, d, J = 8.1 Hz), 7.19 (2H, t, J = 7.2 Hz), 7.34-7.40 (2H, m), 7.46 (1H, d, J = 7.8 Hz), 7.47 (1H, d, J = 8.1 Hz), 7.59 (1H, t, J = 7.7 Hz), 7.89 (2H, t, J = 6.0 Hz), 8.06 (1H, d, J = 8.1 Hz), 8.14 (1H, d, J = 9.0 Hz). (Fig. S2)
^{13}C {1H, ^{19}F} NMR (100 MHz, $CDCl_3$, TMS) δ/ppm: 10.03, 20.42, 110.75, 115.66, 116.28, 124.85, 125.74, 125.91, 126.88, 126.93, 127.20, 127.35, 127.93, 128.11, 128.15, 128.16, 128.24, 128.40, 128.49, 131.84, 132.35, 132.87, 133.82, 138.50, 140.77, 141.24. (Fig. S4)
LRMS (EI, 70eV) m/z 456 (100, M^+). (Fig. S6)
HRMS (APCI-MS with ion trap) Found: m/z 456.1301. Calcd for $C_{27}H_{18}F_6$: M^+, m/z 456.1313. (Fig. S8)
Mp = 138.9-140.2 °C.

3 Experimental data

3-1 ^{1}H NMR spectra

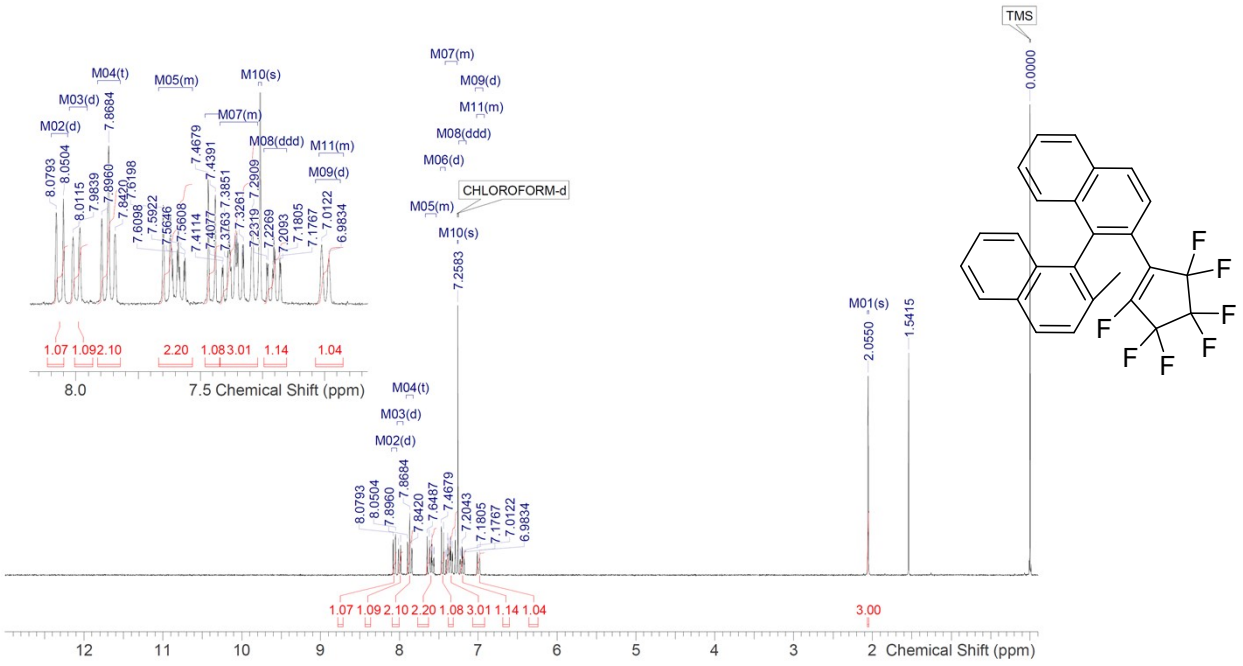


Fig. S1 ^{1}H NMR spectrum of **3** (300 MHz, $CDCl_3$, TMS).

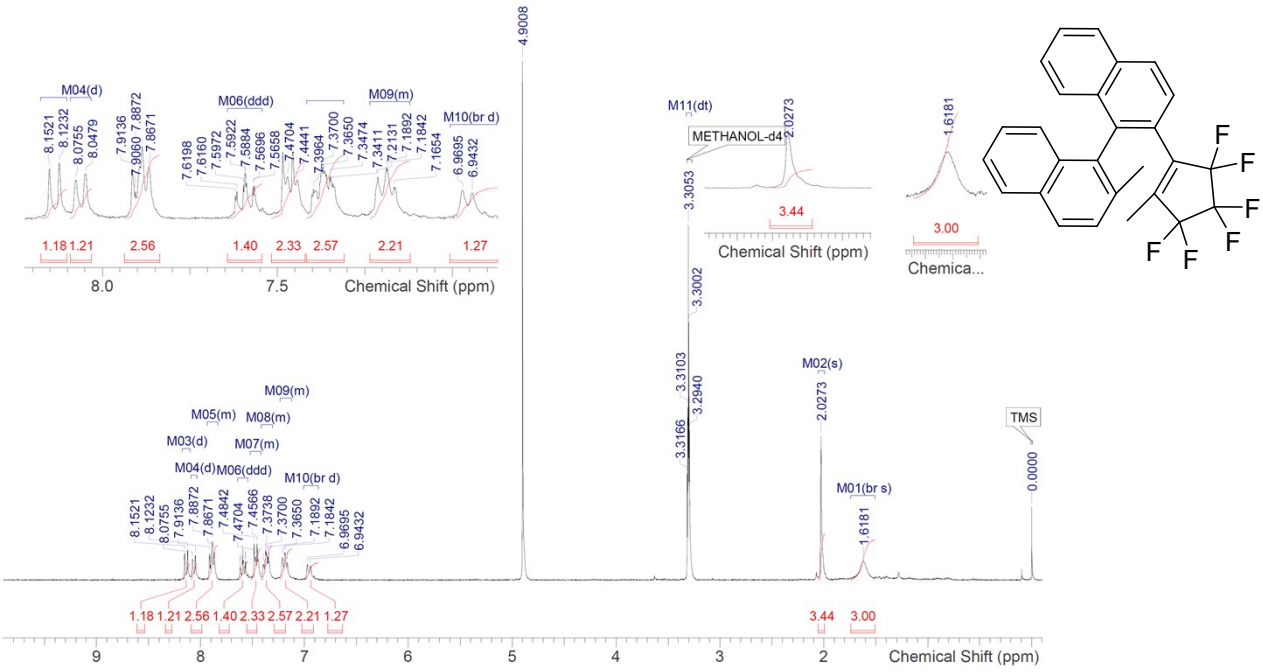


Fig. S2 ^{1}H NMR spectrum of **1o** (300 MHz, CD_3OD, TMS).

3-2 ^{13}C NMR spectra

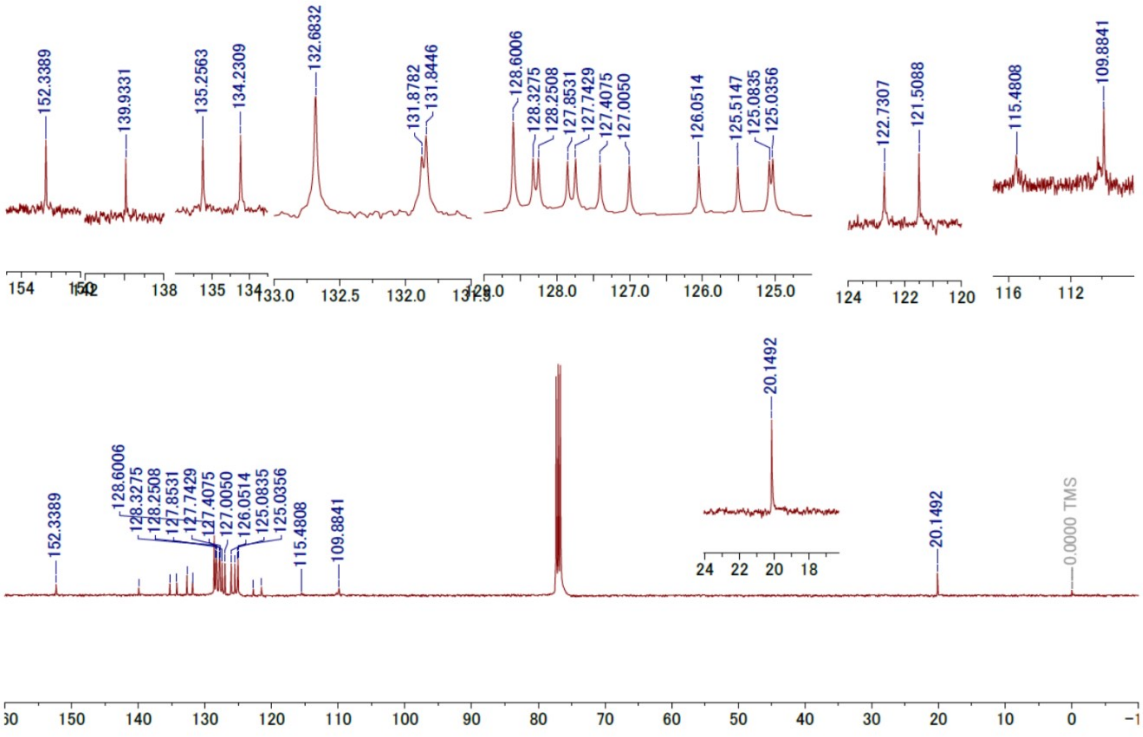


Fig. S3 ^{13}C {^{1}H,^{19}F} NMR spectrum of **3** (100 MHz, $CDCl_3$, TMS).

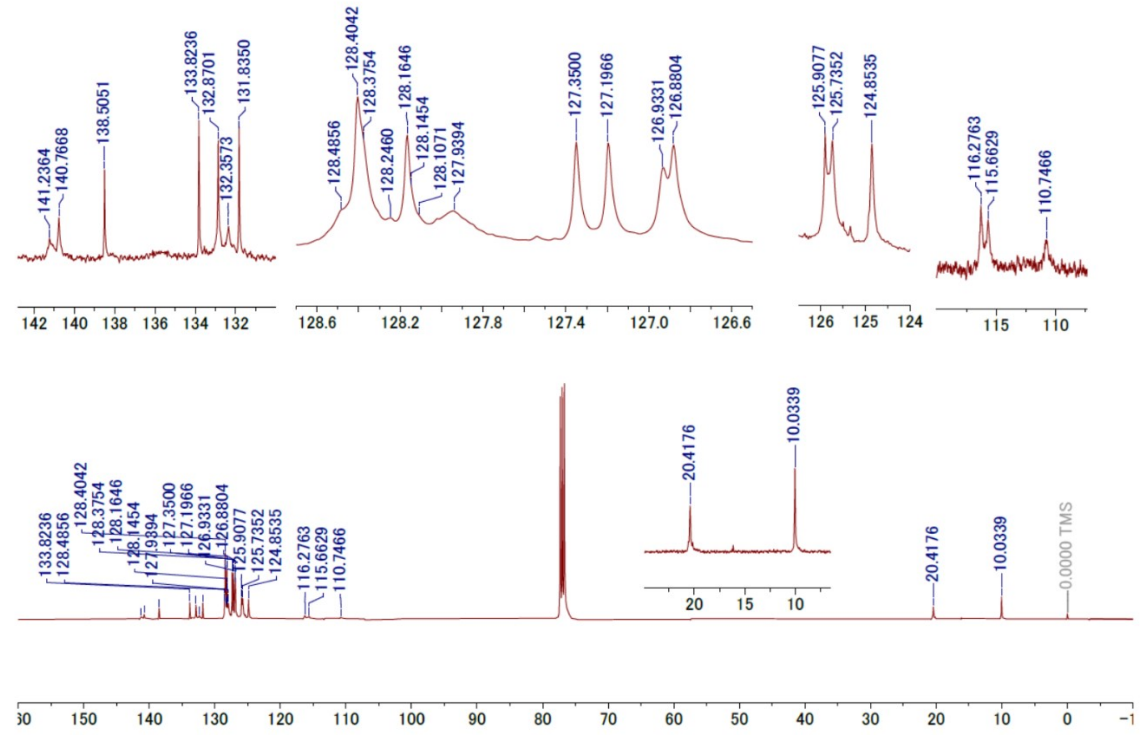


Fig. S4 ^{13}C {^{1}H,^{19}F} NMR spectrum of **1o** (100 MHz, $CDCl_3$, TMS).

3-3 LRMS

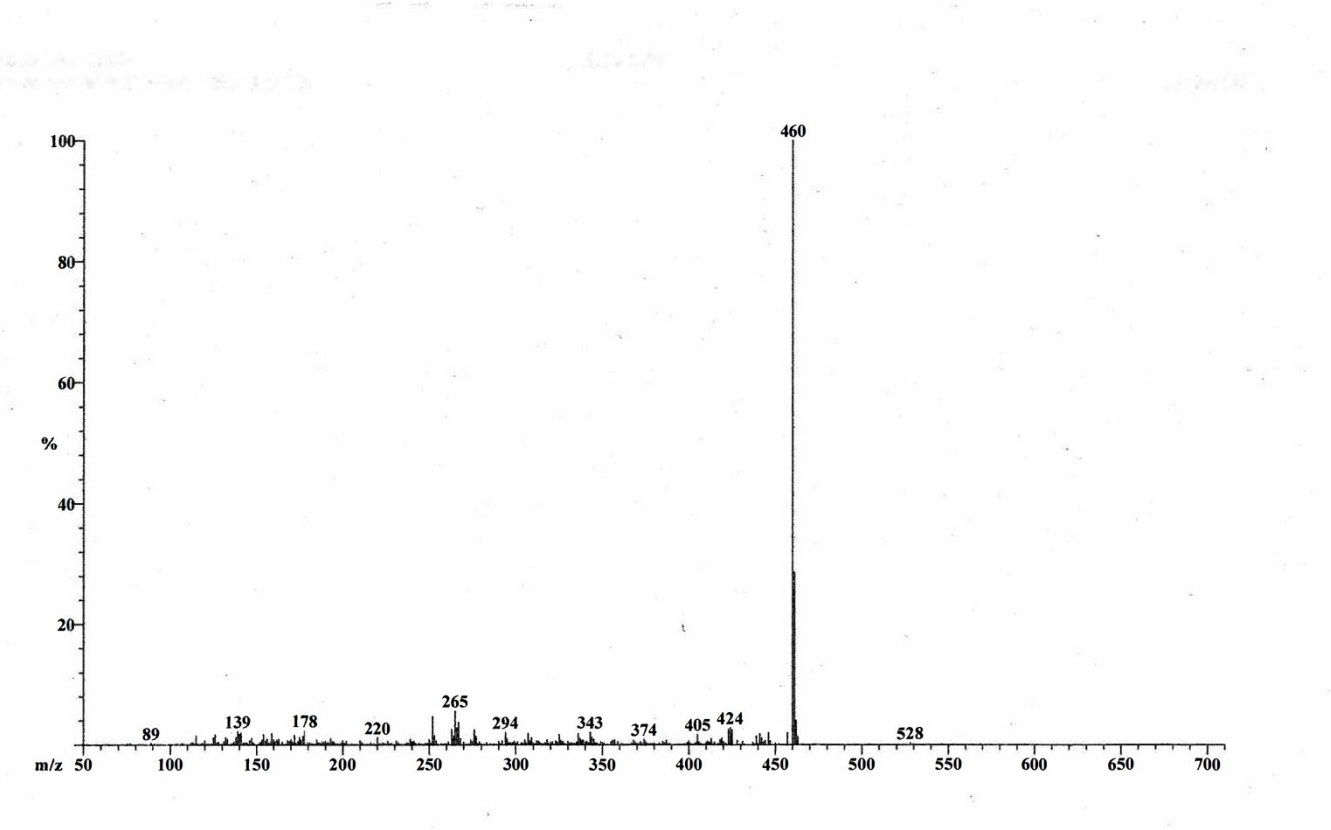


Fig. S5 EI-Mass spectrum of **3**.

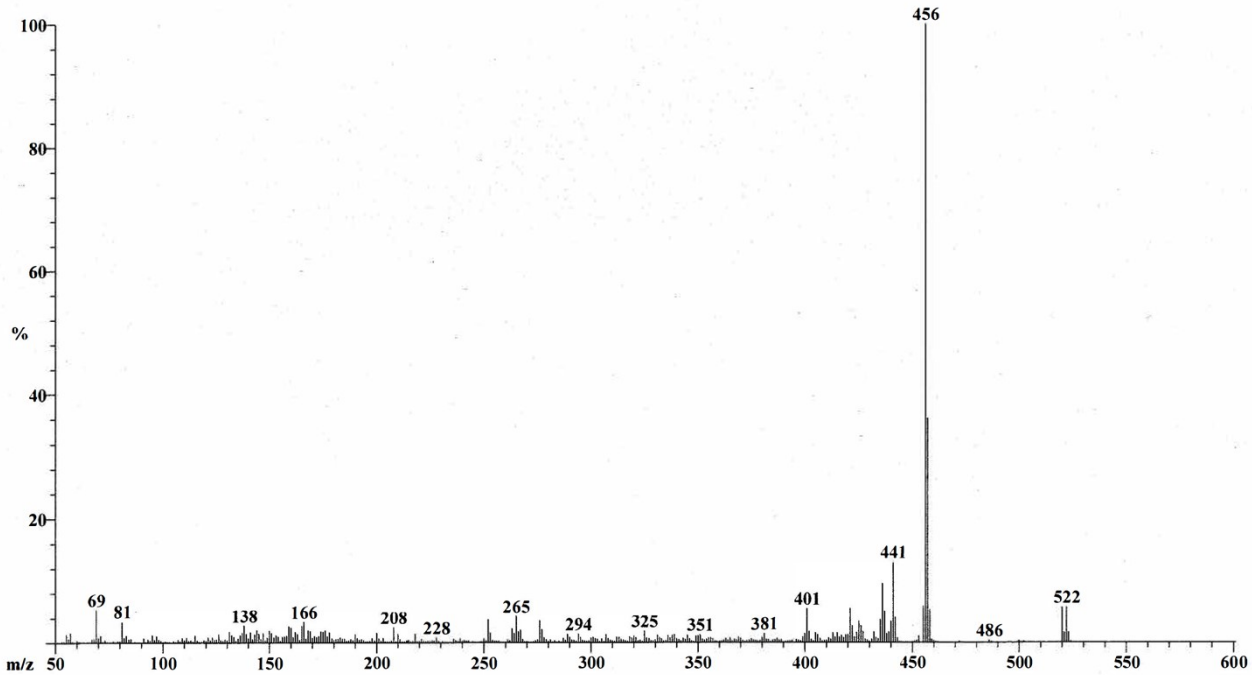


Fig. S6 EI-Mass spectrum of **1o**.

3-4 HRMS

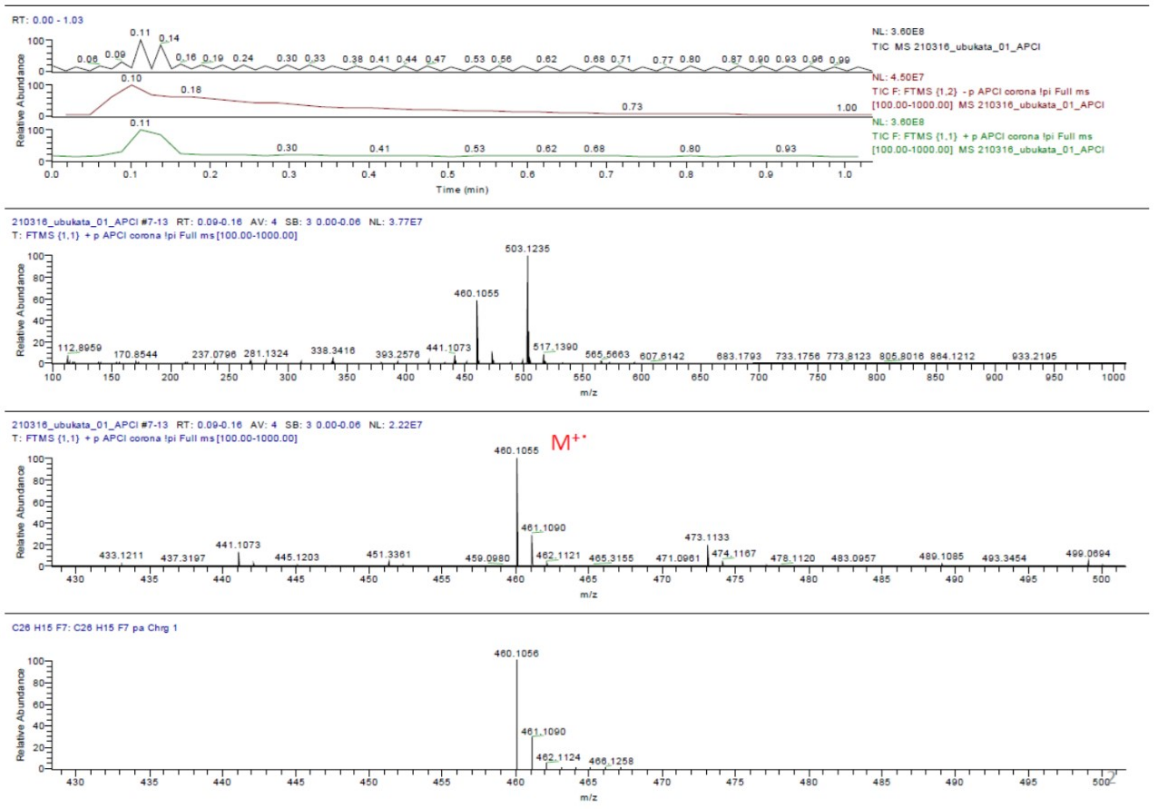


Fig. S7 APCI-Mass spectrum of **3**.

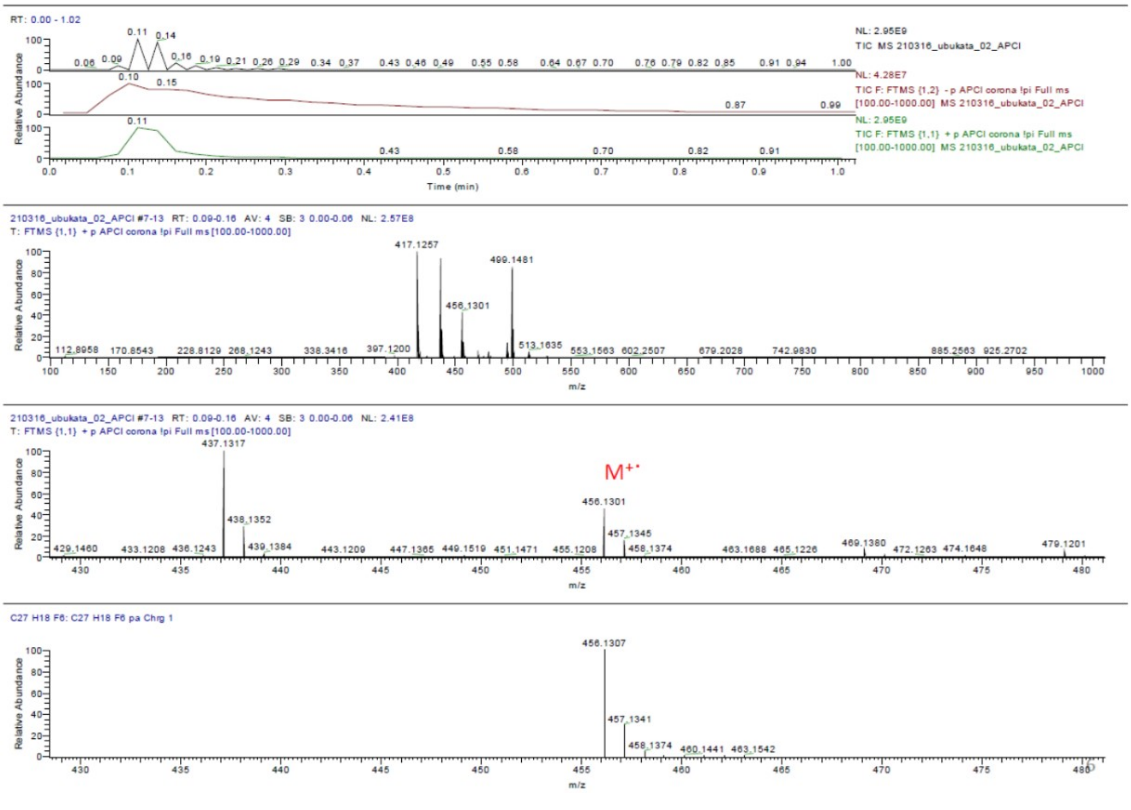


Fig. S8 APCI-Mass spectrum of **1o**.

3-5 HPLC diagrams of **1**

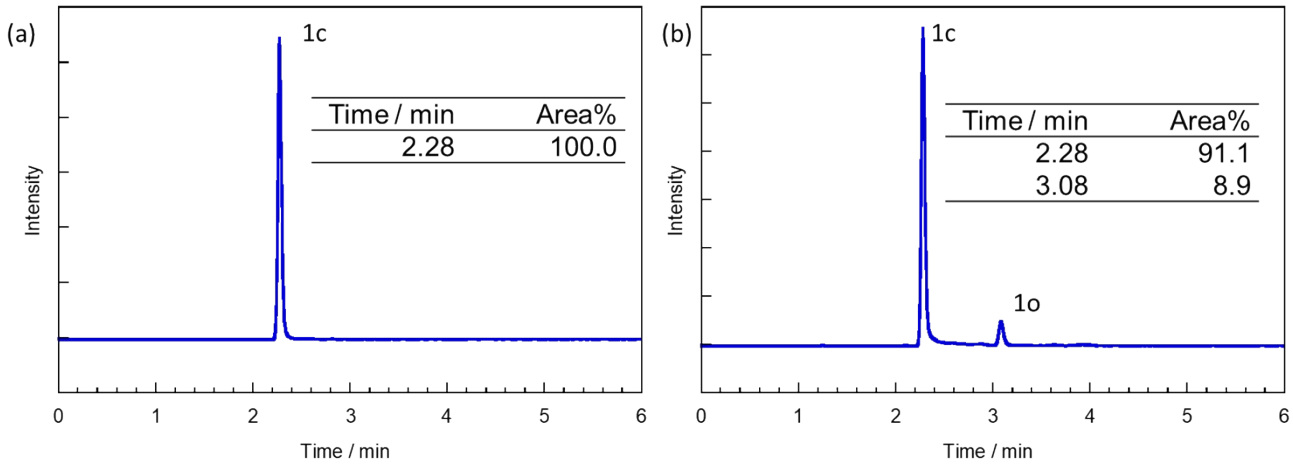
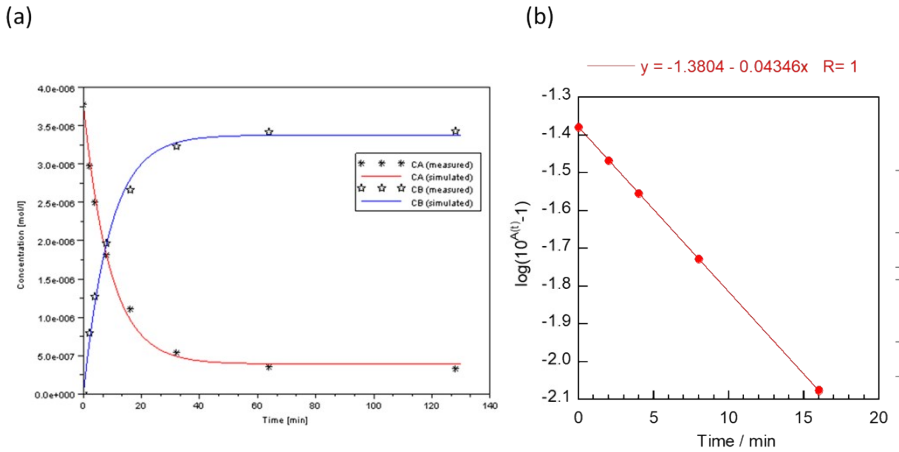


Fig. S9 HPLC diagrams of racemic **1** obtained after 280-nm (0.70 mW cm^{-2}) irradiation for 64 min in hexane (a) detected at 461 nm and (b) detected at 299 nm. Column: Agilent ZORBAX Rx-Sil RRHT 2.1 mm id x 100 mm length, Eluent: 0.2% AcOEt / Hex, Current: 0.25 mL min^{-1}.

3-6 Calculation of the quantum yields



280 nm (0.203 mW cm^{-2})			
ε_o	ε_c	Φ_{oc}	Φ_{co}
12.4×10^3	6.6×10^3	0.126	0.027

436 nm (10.5 mW cm^{-2})			
ε_o	ε_c	Φ_{oc}	Φ_{co}
-	5.3×10^3	-	0.0035

Fig. S10 (a) Concentration changes of **1o**, **1c** and results of fitting simulation upon irradiation with 280-nm light. (b) Change in absorbance of **1c** at 436 nm upon irradiation with 436-nm light. (c) Molar absorption coefficients and quantum yields at excitation wavelengths.

3-7 Calculation of the thermal cycloreversion parameters

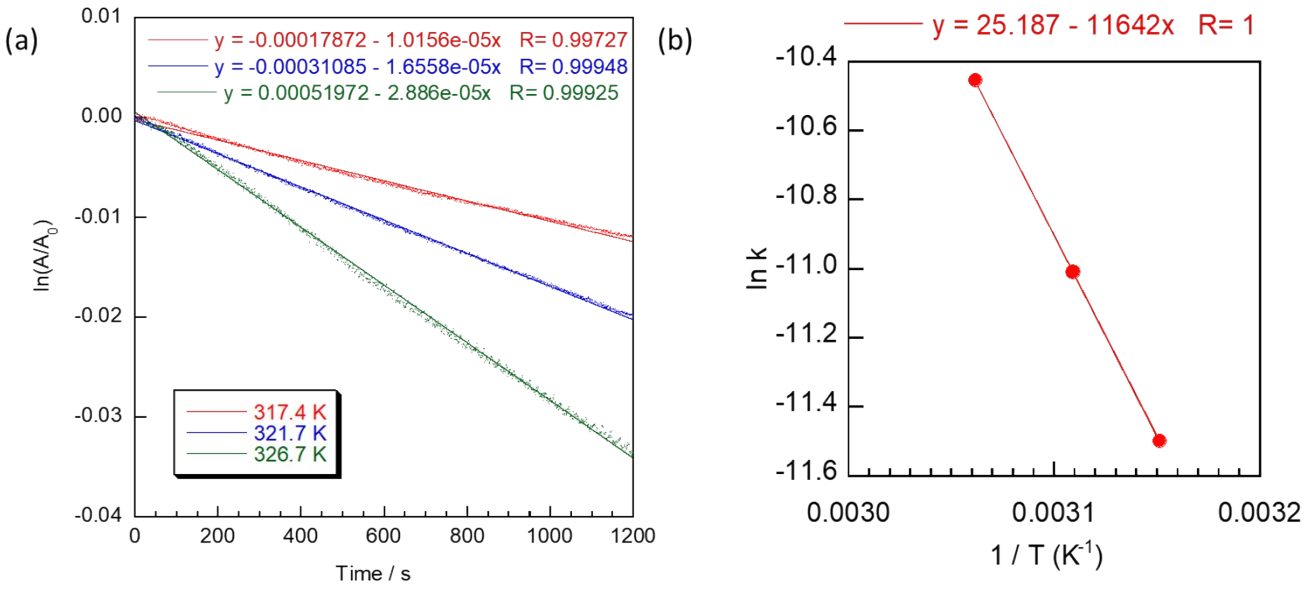


Fig. S11 (a) Decay of peak absorbance observed at 461 nm upon thermal cycloreversion of **1c** at various temperatures in hexane. (b) Arrhenius plot.

3-8 Chiral HPLC diagrams of **1**

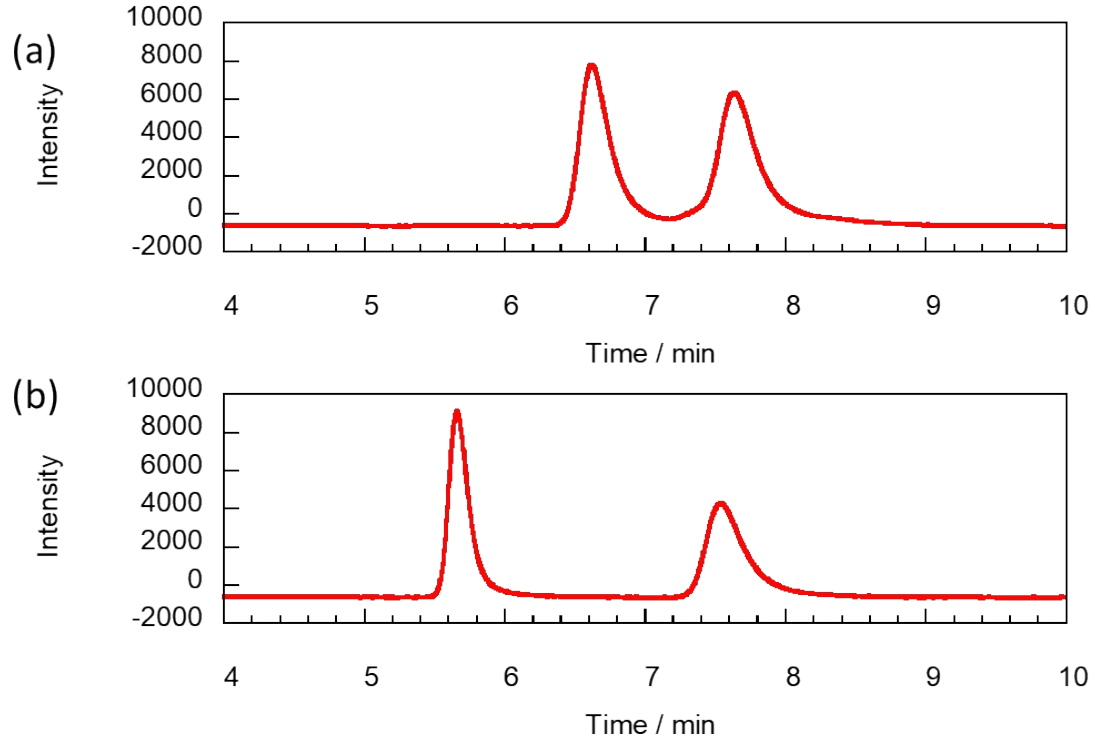


Fig. S12 Chiral HPLC diagrams of racemic **1** in hexane. (a) **1o** detected at 299 nm, (b) **1c** obtained after 280-nm light (0.25 mW cm^{-2}) irradiation for 128 min detected at 461 nm. Column: Daicel CHIRALCEL OZ-H 4.6 mm id x 250 mm length, Eluent: Hex, Current: 1.0 mL min^{-1}.

3-9 Estimation of thermal racemization

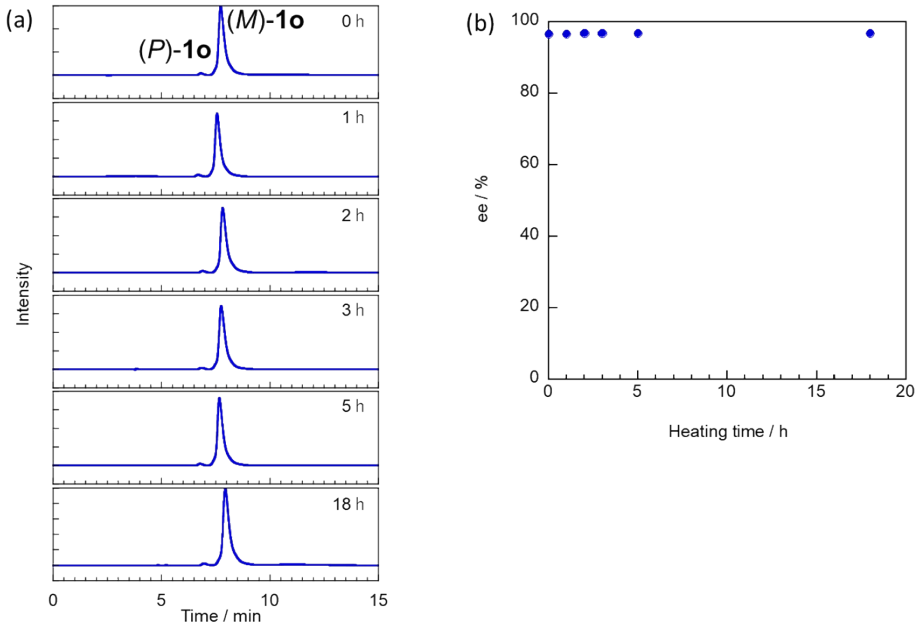


Fig. S13 (a) Chiral HPLC diagrams of optically resolved *(M)*-**1o** in hexane during heating at 60 °C. (b) Change in enantiomer excess of *(M)*-**1o**. Column: Daicel CHIRALCEL OZ-H 4.6 mm id x 250 mm length, Eluent: Hex, Current: 1.0 mL min^{-1}, Detection wavelength 285 nm.

3-10 Chiral photoswitch reactions of the other enantiomer

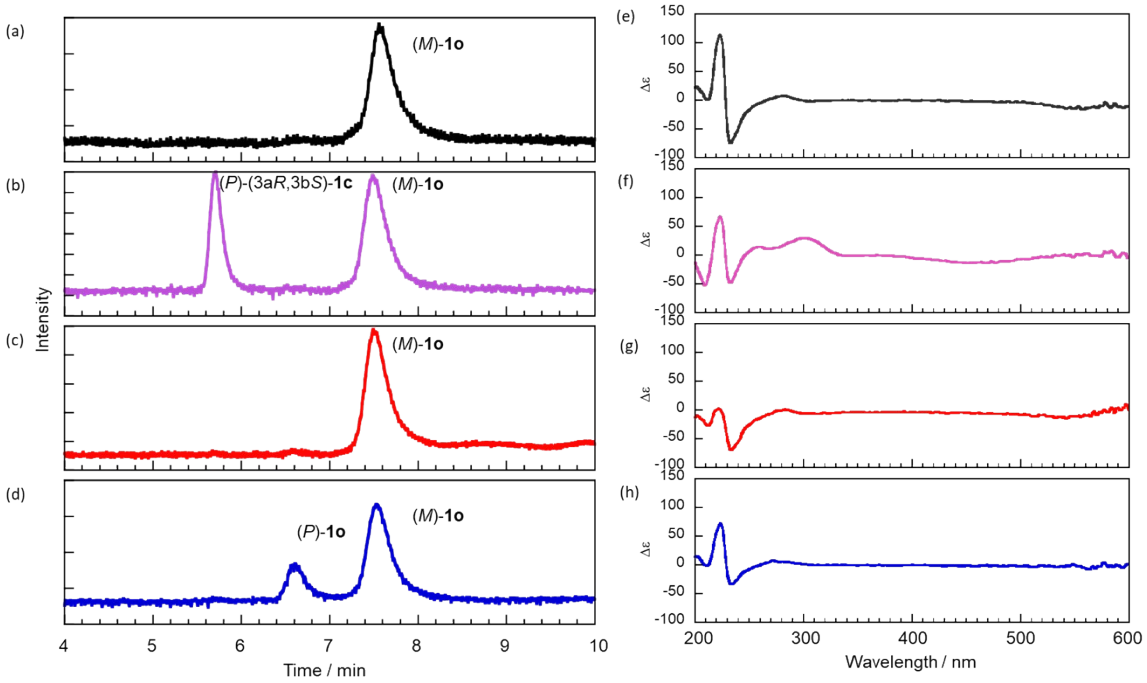


Fig. S20 Change in chiral HPLC diagrams (a-d) and CD spectra (e-h) of resolved (*M*)-**1o** (hexane: 1.0 mL min^{-1}, detected at 299 nm). (a,e) Initial state; (b,f) 280-nm light (0.21 mW cm^{-2}) irradiation for 6 min; (c,g) heating at 60 °C for 21 h after (b,f) state; (d,h) 436-nm light (5.30 mW cm^{-2}) irradiation for 64 min after (b,f) state.

4 Calculated data

4-1 Calculated most stable conformation

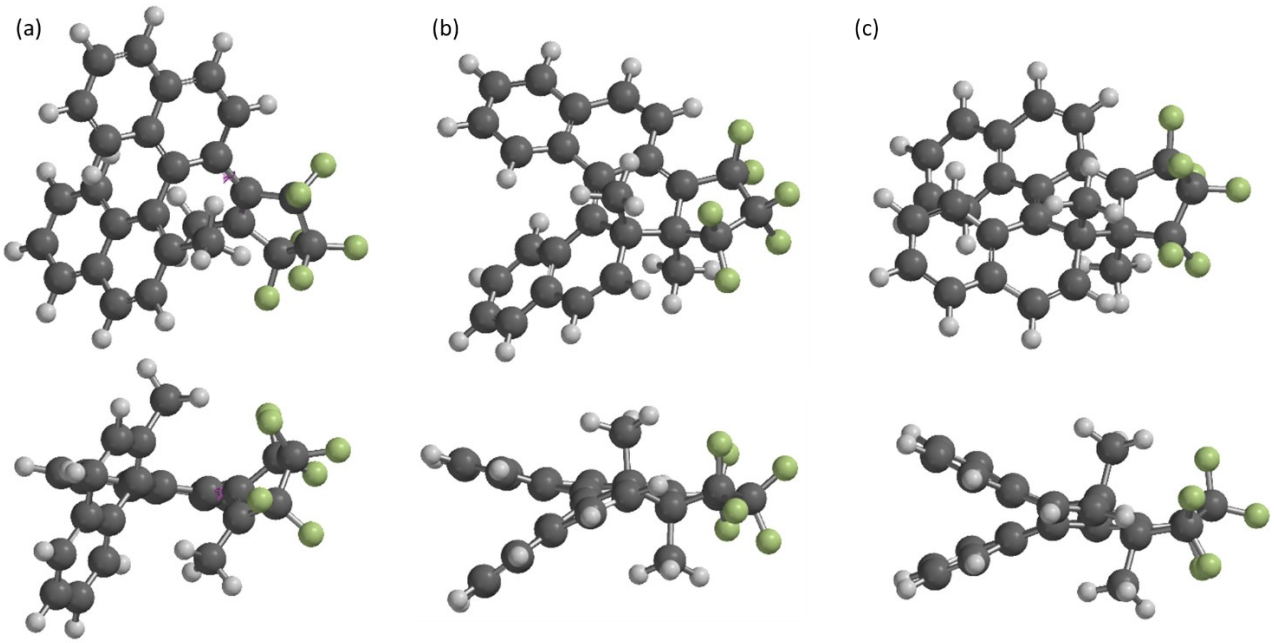


Fig. S14 The most stable conformation of (a) (*P*)-**1o**, (b) (*P*)-(3a*S*,3b*R*)-**1c**, and (c) (*M*)-(3a*S*,3b*R*)-**1c**.

4-2 Calculated total energy

Table S1 Total energy of (*P*)-**1o**, (*P*)-(3a*S*,3b*R*)-**1c**, and (*M*)-(3a*S*,3b*R*)-**1c**

	(*P*)-**1o**	(*P*)-(3a*S*,3b*R*)-**1c**	(*M*)-(3a*S*,3b*R*)-**1c**
E [kJ/mol]	−4301352.70	−4301197.38	−4301230.34
Δ*E* to (*P*)-(3a*S*,3b*R*)-**1c** [kJ/mol]	−155.32	–	−32.96

4-3 Calculated CD spectra

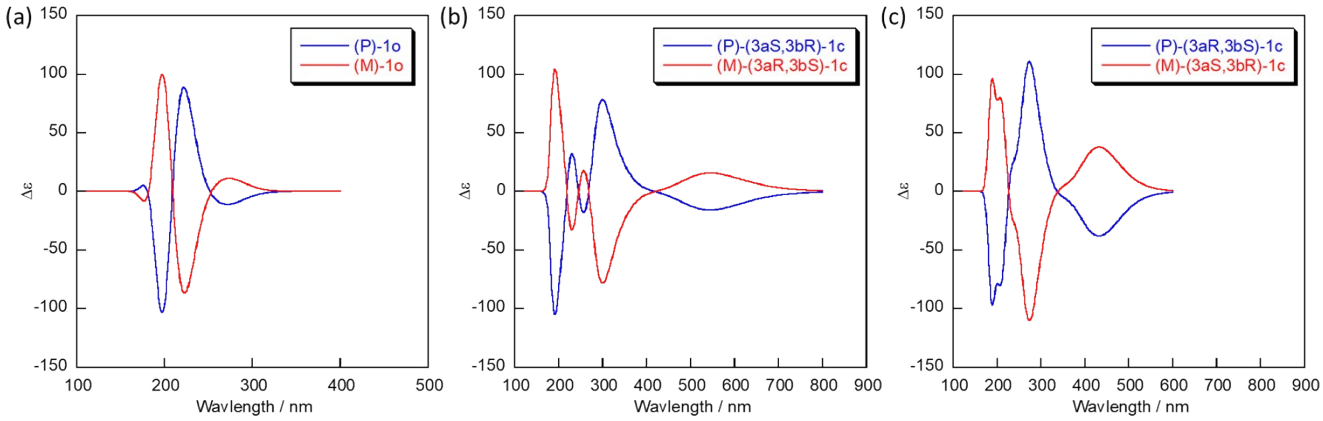


Fig. S15 Calculated CD spectra of (a) (*P*)-**1o**, (*M*)-**1o**, (b) (*P*)-(3a*S*,3b*R*)-**1c**, (*M*)-(3a*R*,3b*S*)-**1c** and (c) (*P*)-(3a*R*,3b*S*)-**1c**, (*M*)-(3a*S*,3b*R*)-

1c.

4-4 Schematic illustration of cycloreversion

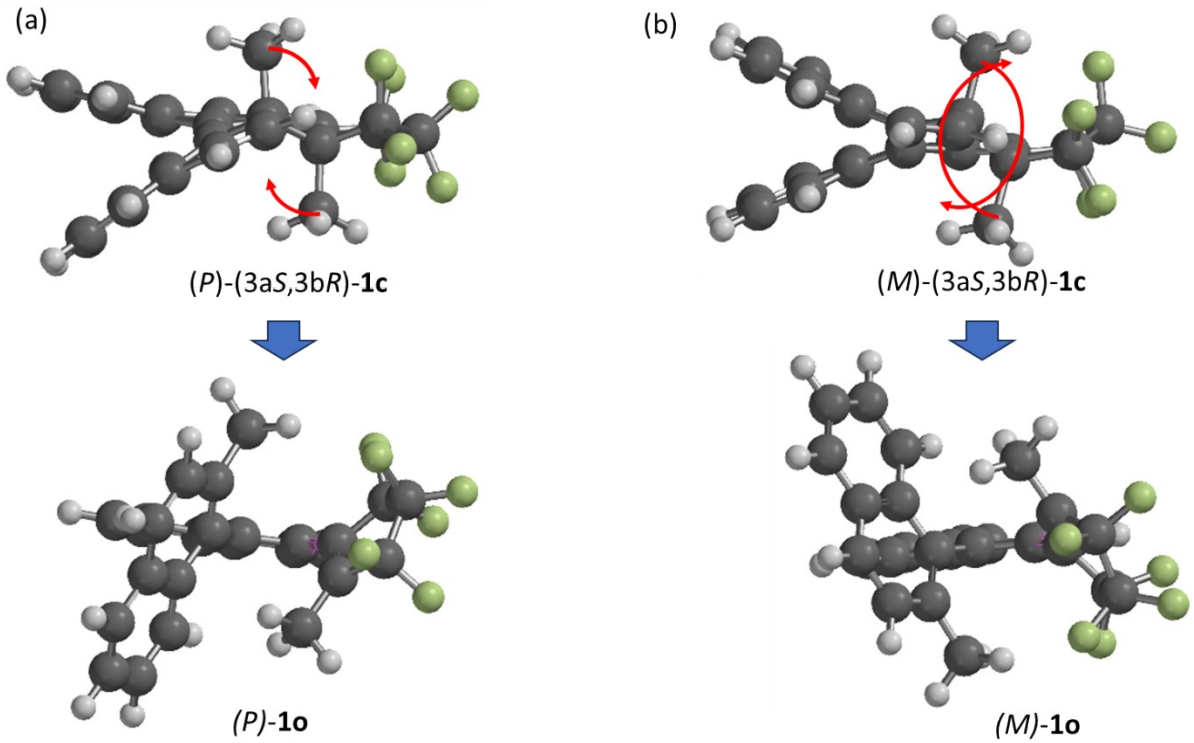


Fig. S16 Schematic illustration of cycloreversion (a) from (*P*)-(3a*S*,3b*R*)-**1c** to *(P)*-**1o** and (b) from (*M*)-(3a*S*,3b*R*)-**1c** to *(M)*-**1o.**

4-5 Energy diagram of **1**

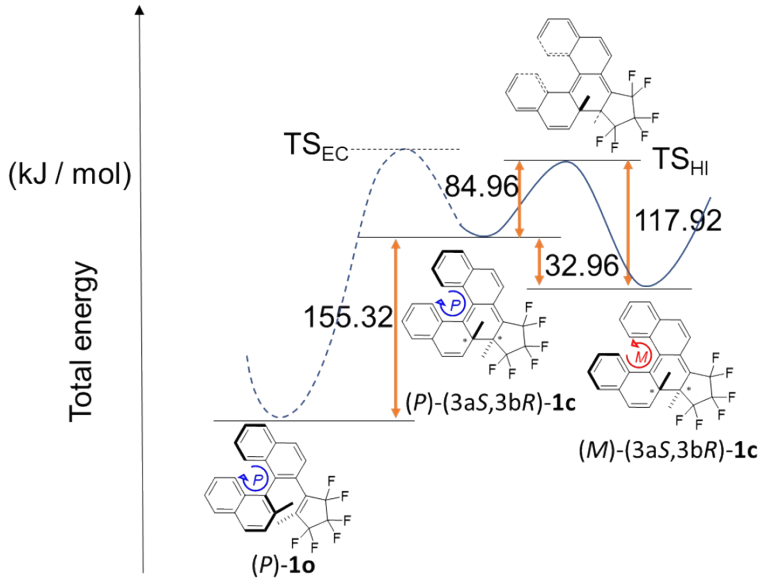


Fig. S17 Energy diagram of **1**.

4-6 Transition state

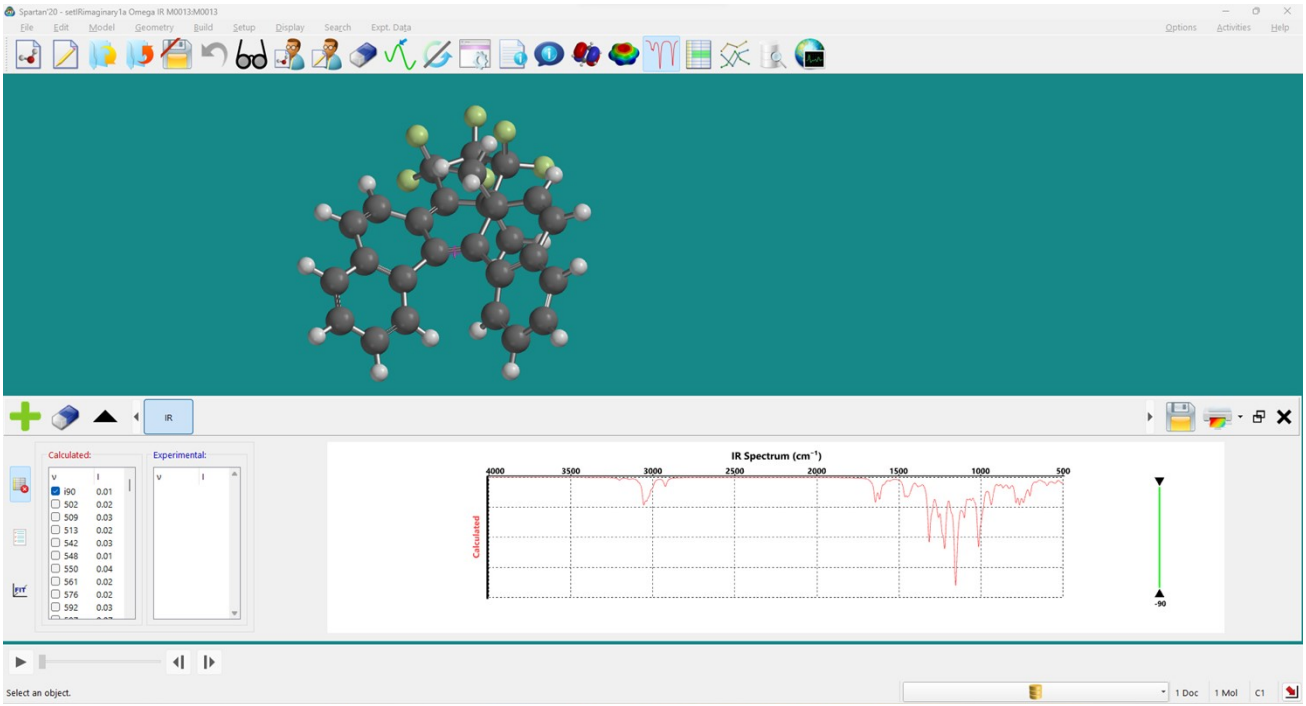


Fig. S18 Transition state structure between (*M*)-(3a*S*,3b*R*)-**1c** and (*P*)-(3a*S*,3b*R*)-**1c**.

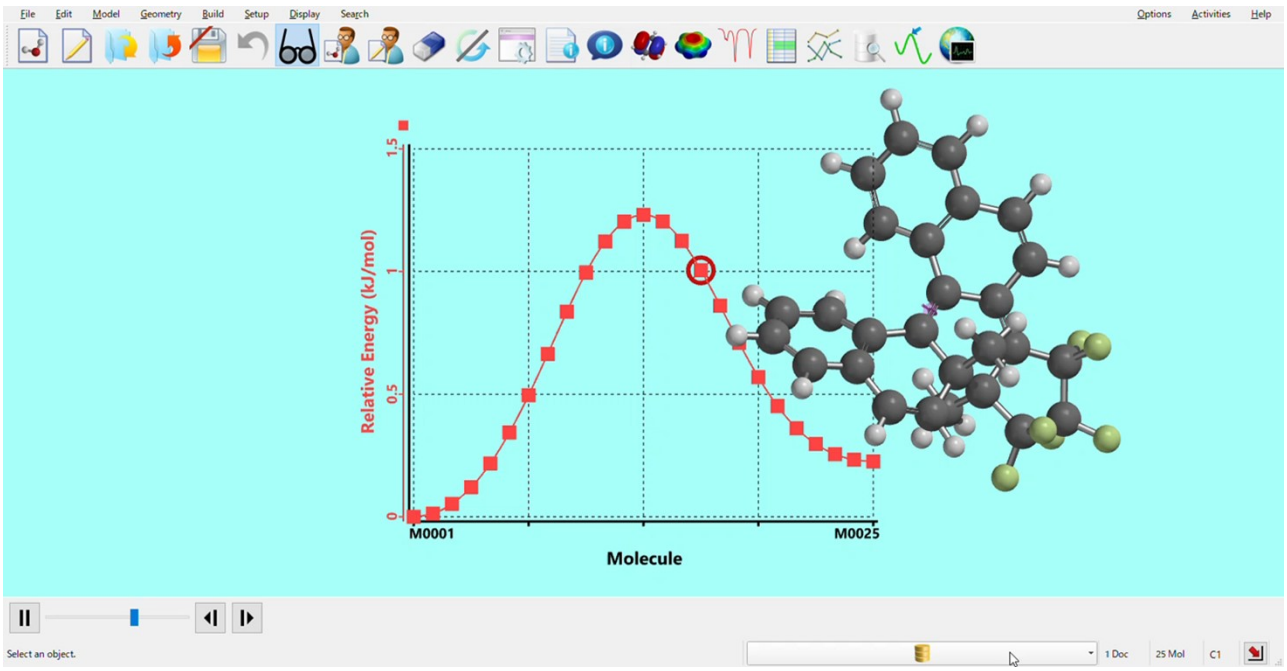
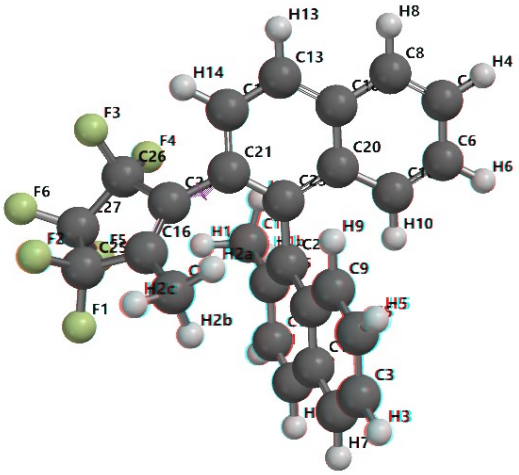


Fig. S19 Intrinsic Reaction Coordinate analysis of **1c**.

4-7 Cartesian coordinates for optimized geometries

(*P*)-**1o**

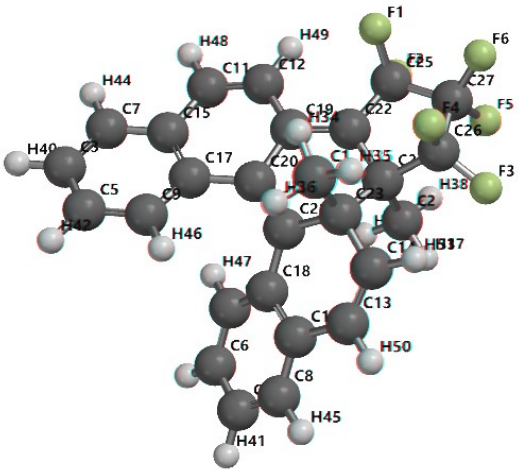


Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z
1	H	-2.2385706438	-0.7953153240	0.7979655638
2	C	-1.9996186995	-0.1125967277	1.6066935066
3	C	-1.4109225132	1.6262881333	3.7085072830
4	C	-2.7260408866	-0.1576275260	2.7687480529
5	C	-0.9327721021	0.8132256992	1.4423752343
6	C	-0.6427896292	1.6964995748	2.5173828149
7	C	-2.4304575712	0.7200685173	3.8361979539
8	H	-1.1727701359	2.3080033415	4.5210662872
9	H	-3.5356300435	-0.8741524983	2.8704750658
10	H	-3.0123854795	0.6742420572	4.7515976239
11	C	0.4169263697	2.6278707950	2.3725345714
12	C	1.1325363092	2.6859862086	1.2113062094
13	C	0.8594681365	1.8167079989	0.1214731073
14	C	-0.1405571724	0.8713787092	0.2465632488
15	H	0.6441508451	3.3007295538	3.1953152646
16	H	1.9324429068	3.4139524620	1.1030570035
17	C	-0.4395484966	-0.0843903913	-0.8651556156
18	C	-1.0706698487	-1.8654761410	-2.9644269864
19	C	0.3914502839	-1.1537725940	-1.1616213139
20	C	-1.6126649184	0.1335973026	-1.6622138612
21	C	-1.9354420052	-0.7715942148	-2.7100816351

22	C	0.0633549284	-2.0394248796	-2.2265466176
23	H	-1.3149553561	-2.5575592580	-3.7656052540
24	H	0.7322671360	-2.8648695832	-2.4430440400
25	C	-3.1024018445	-0.5536346656	-3.4867567367
26	C	-3.9136927198	0.5236141182	-3.2462605592
27	C	-3.5877241177	1.4360028431	-2.2175024238
28	C	-2.4694461426	1.2478431785	-1.4476238252
29	H	-3.3371330416	-1.2569145201	-4.2814532788
30	H	-4.8037631752	0.6831123746	-3.8471729974
31	H	-4.2280107250	2.2940269272	-2.0372305496
32	H	-2.2275674881	1.9563366452	-0.6634477648
33	C	1.6785535377	-1.3854373007	-0.4673580291
34	C	2.9449092347	-1.5076637853	-1.2815051676
35	C	4.0789131846	-1.3127131969	-0.2512811585
36	C	3.4162978721	-1.7298661417	1.0790285003
37	C	1.9404920745	-1.5732604257	0.8354102804
38	C	1.6880826280	1.9732396807	-1.1266369121
39	H	1.2273265562	1.4981245746	-1.9943809395
40	H	1.8333831198	3.0347323558	-1.3520351085
41	H	2.6791801001	1.5300667182	-0.9927090012
42	C	1.0125923785	-1.6966527549	1.9929668948
43	H	-0.0135828288	-1.8643392451	1.6654519844
44	H	1.0326364199	-0.7894657346	2.6055519011
45	H	1.3277880310	-2.5342881161	2.6239301804
46	F	3.0618374883	-2.7507859421	-1.8310557591
47	F	3.0303817720	-0.6239677116	-2.2971905558
48	F	4.4140060521	-0.0053069008	-0.1970043111
49	F	5.1758329469	-2.0247883968	-0.5398816774
50	F	3.8446635461	-0.9645861551	2.1087585086
51	F	3.7393794561	-3.0152423433	1.3738291264

(*P*)-(3a*S*,3b*R*)-**1c**



Standard Nuclear Orientation (Angstroms)

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3	C	1.1239526042	-4.9003651271	1.0369579189
4	C	-0.9940266334	-1.5372216665	-4.4506258285
5	C	1.4698257240	-4.2254976666	-0.1350984107
6	C	-1.3199409491	-2.2417833248	-3.2915474923
7	C	0.5296712934	-4.1951809523	2.0686758661
8	C	-0.3548273796	-0.3127962109	-4.3417929288
9	C	1.1663420877	-2.8826945584	-0.2833120833
10	C	-0.9453441804	-1.7489749273	-2.0533593380
11	C	-0.1993583350	-2.0694986069	3.0923719495
12	C	-0.2721588590	-0.7311332971	3.0704227216
13	C	0.4696612821	1.5877294830	-3.0003605470
14	C	0.6182372030	2.1930335186	-1.8242527572
15	C	0.2321458358	-2.8321531396	1.9336965327
16	C	0.0109257878	0.2044976747	-3.0942011362
17	C	0.4786170249	-2.1696283662	0.7124351199
18	C	-0.2083001456	-0.5578156318	-1.9242210502
19	C	-0.0950113815	0.0188001354	1.8344102690
20	C	0.1726646904	-0.7273195474	0.5783712477
21	C	0.1641276264	-0.0211543661	-0.6051085002
22	C	-0.3446885997	1.3468788153	1.7931372513

23	C	0.5974418115	1.4629414818	-0.5106268752
24	C	-0.3649736468	2.1238629685	0.4975663664
25	C	-0.6621092386	2.2330935732	2.9570969157
26	C	-0.0470577828	3.5537162008	0.9670059006
27	C	-0.7032819093	3.6797800272	2.3707743690
28	F	0.2920693038	2.1756771442	3.9242590211
29	F	-1.8449242005	1.9482822735	3.5656807682
30	F	-0.4979331081	4.5123295798	0.1266520213
31	F	1.2818404775	3.7661933251	1.1399719802
32	F	-1.9805209295	4.0985600340	2.2472038370
33	F	-0.0493072319	4.5542396265	3.1474520022
34	H	2.1994358357	1.0697427526	0.9594353831
35	H	2.5702927416	2.3887406559	-0.1665156809
36	H	2.6169837778	0.7121553279	-0.7273394398
37	H	-1.8612242843	2.6437475960	-1.0175497982
38	H	-2.5168418152	2.5606264350	0.6266497902
39	H	-2.1195312666	1.0707568833	-0.2376366951
40	H	1.3521730205	-5.9552333991	1.1532936067
41	H	-1.2748010055	-1.9223700636	-5.4260451631
42	H	1.9903793629	-4.7467046093	-0.9327101073
43	H	-1.8773301892	-3.1711975232	-3.3524348762
44	H	0.3127199353	-4.6867159750	3.0135908809
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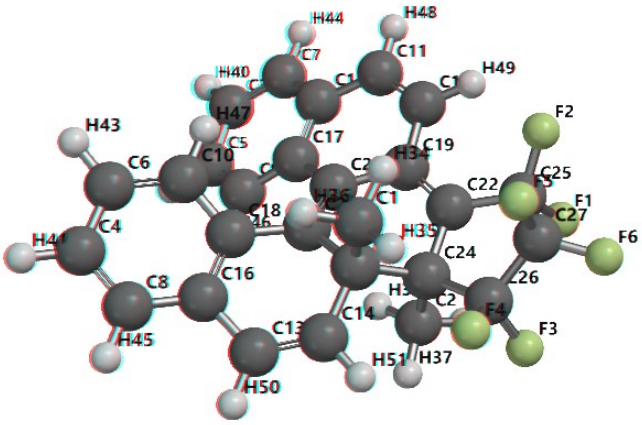
46	H	1.4666731565	-2.3750914413	-1.1922753017
47	H	-1.2286401741	-2.2983155542	-1.1641309266
48	H	-0.3862124570	-2.6106019807	4.0162427213
49	H	-0.5232905641	-0.1818063123	3.9694368936
50	H	0.5792862000	2.1447815788	-3.9272363646
51	H	0.8519569710	3.2532707480	-1.7726830034

(*M*)-(3a*S*,3b*R*)-**1c**



Standard Nuclear Orientation (Angstroms)

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3	C	-1.0423808574	0.1869822969	-4.9227818485
4	C	1.1691774865	4.6052924223	-0.7769265832
5	C	-1.4305016631	1.1362850510	-3.9772214406
6	C	1.5768205304	3.5840915754	-1.6323224778
7	C	-0.4027866935	-0.9701238030	-4.5056813259
8	C	0.4947549176	4.2911204211	0.3963690886
9	C	-1.1350076136	0.9461754596	-2.6352052147
10	C	1.2633641908	2.2639572567	-1.3363809490
11	C	0.4089770059	-2.4596477962	-2.6921576039
12	C	0.4251729729	-2.7950741876	-1.3925128303
13	C	-0.3588796604	2.6035984074	2.0186017223
14	C	-0.3046116144	1.3486400738	2.4628681826
15	C	-0.1168605955	-1.1806184505	-3.1519258553
16	C	0.1960561994	2.9644856682	0.7127991586
17	C	-0.4319240270	-0.1856552778	-2.2057645067
18	C	0.5280415866	1.9382075147	-0.1921369729
19	C	0.0162775506	-1.8409392975	-0.3667042016
20	C	-0.1017420353	-0.4224668856	-0.7824108853
21	C	0.1648468552	0.5409178033	0.1427738661
22	C	-0.1583182957	-2.1483047740	0.9312552358
23	C	0.2482602205	0.1986714328	1.6368059394

24	C	-0.6125417040	-1.0775177060	1.9068921889
25	C	0.0449378974	-3.4537980889	1.6240160726
26	C	-0.4087981276	-1.7478850833	3.3050437626
27	C	0.4063415619	-3.0425487507	3.0660648693
28	F	-1.1075658697	-4.1846098894	1.6686203232
29	F	1.0050175892	-4.2521788971	1.1027882436
30	F	-1.5936160983	-2.1234384726	3.8459198379
31	F	0.1980804771	-0.9657907407	4.2310197374
32	F	1.7270952027	-2.7607388369	3.1166542325
33	F	0.1390854463	-3.9938160872	3.9699372261
34	H	2.1792649305	-0.8084090967	1.3948205706
35	H	1.9355734023	-0.1305564553	3.0170930758
36	H	2.2827256385	0.9430997070	1.6533076879
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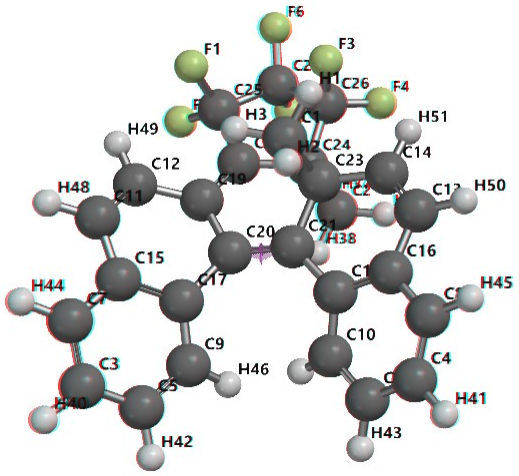
38	H	-2.6924940514	-1.7038384023	1.7446621780
39	H	-2.2740842360	-0.3165879801	0.7282079324
40	H	-1.2650407256	0.3383240677	-5.9745001051
41	H	1.4006020853	5.6400781078	-1.0104547048
42	H	-1.9720944194	2.0249602355	-4.2862964123
43	H	2.1428281170	3.8144797473	-2.5294949602
44	H	-0.1395464929	-1.7398784205	-5.2265947986
45	H	0.2166076585	5.0774034917	1.0933258907
46	H	-1.4515497436	1.6856209129	-1.9079137120
47	H	1.5888110665	1.4733502113	-2.0036073084
48	H	0.7089271016	-3.1854148647	-3.4436016625
49	H	0.7232697874	-3.7880087209	-1.0816607075
50	H	-0.7242134329	3.4018144014	2.6596094854
51	H	-0.6110497528	1.1140481764	3.4767926737

TS of (*M*)-(3a*S*,3b*R*)-**1c** between (*P*)-(3a*S*,3b*R*)-**1c**



Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z
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4	C	2.0327339327	0.2510326590	4.4737211228
5	C	4.4146853386	1.1379879937	-0.8114085768
6	C	2.3992691631	1.1326328764	3.4658946584
7	C	3.8823586870	-0.4807398874	-2.4729241115
8	C	0.9016105357	-0.5332120716	4.2869735311
9	C	3.0665189894	1.2184969027	-0.4704567512
10	C	1.7317418892	1.1042565255	2.2472189467
11	C	1.5551576278	-0.8502463435	-3.1306722907
12	C	0.2674386437	-0.4945074989	-3.0464460158
13	C	-1.1620058268	-1.0338682955	3.0547430959
14	C	-1.9144701136	-0.8992978183	1.9670101384
15	C	2.5258693273	-0.3698713239	-2.1604122440
16	C	0.2071225670	-0.5309130070	3.0761895497
17	C	2.0946175922	0.3880607956	-1.0362160976
18	C	0.7223197426	0.1801513945	1.9560206560
19	C	-0.2596854523	0.0529327803	-1.8042623337
20	C	0.6575821233	0.2264769701	-0.6314806010
21	C	0.1086861826	0.0139602850	0.6203771338
22	C	-1.5877410980	0.2227728333	-1.6440329386

23	C	-1.3099151762	-0.6405332408	0.6161381573
24	C	-2.1861373090	0.2949471431	-0.2551456383
25	C	-2.6396131239	0.0251415942	-2.6930985245
26	C	-3.6511574845	-0.1478370107	-0.4909039588
27	C	-3.9744138783	0.2667978627	-1.9470507270
28	F	-2.6584417894	-1.2516189701	-3.1819912912
29	F	-2.5177602643	0.8460736729	-3.7620831463
30	F	-3.8180917706	-1.4943506330	-0.4241693822
31	F	-4.5249220638	0.3950271530	0.3844854606
32	F	-4.2807043647	1.5832891277	-1.9893450279
33	F	-4.9984800600	-0.4230428162	-2.4649424739
34	H	-2.8764737740	2.3709335065	-0.2415826069
35	H	-1.1976950404	2.1610292118	0.2693738459
36	H	-2.5182525052	1.7176535434	1.3679524025
37	H	5.8955204073	0.1400011088	-2.0208171730
38	H	2.5637143045	0.2354665849	5.4206526439
39	H	5.1221134441	1.8009258169	-0.3224815723
40	H	3.1908594065	1.8585842056	3.6243615751
41	H	4.1728522717	-1.1035207045	-3.3153152909
42	H	0.5052398010	-1.1198451953	5.1118901045
43	H	2.7861701601	2.0122106300	0.1968054576
44	H	1.9411456346	1.8813119563	1.5389634726
45	H	1.9285653388	-1.3766699673	-4.0050670150
46	H	-0.4248652506	-0.7209446220	-3.8474951487
47	H	-1.5863917482	-1.3752660064	3.9953471882
48	H	-2.9719090870	-1.1467536608	1.9833175375
49	H	-0.8786603185	-2.1335049957	-0.9904546781
50	H	-1.9946257963	-2.7111800439	0.2535858347
51	H	-0.2760059218	-2.5446819587	0.6240585159

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