Supporting Information

Chiroptical Protocol for the Absolute Configurational Assignment of Alkyl-Substituted Epoxides Using Bis(zinc porphyrin) as a CD-Sensitive Bidentate Host

Shiori Takeda, Satoshi Hayashi, Masahiro Noji, and Toshikatsu Takanami*
Meiji Pharmaceutical University, 2-522-1, Noshio, Kiyose, Tokyo 204-8588, Japan
takanami@my-phram.ac.jp

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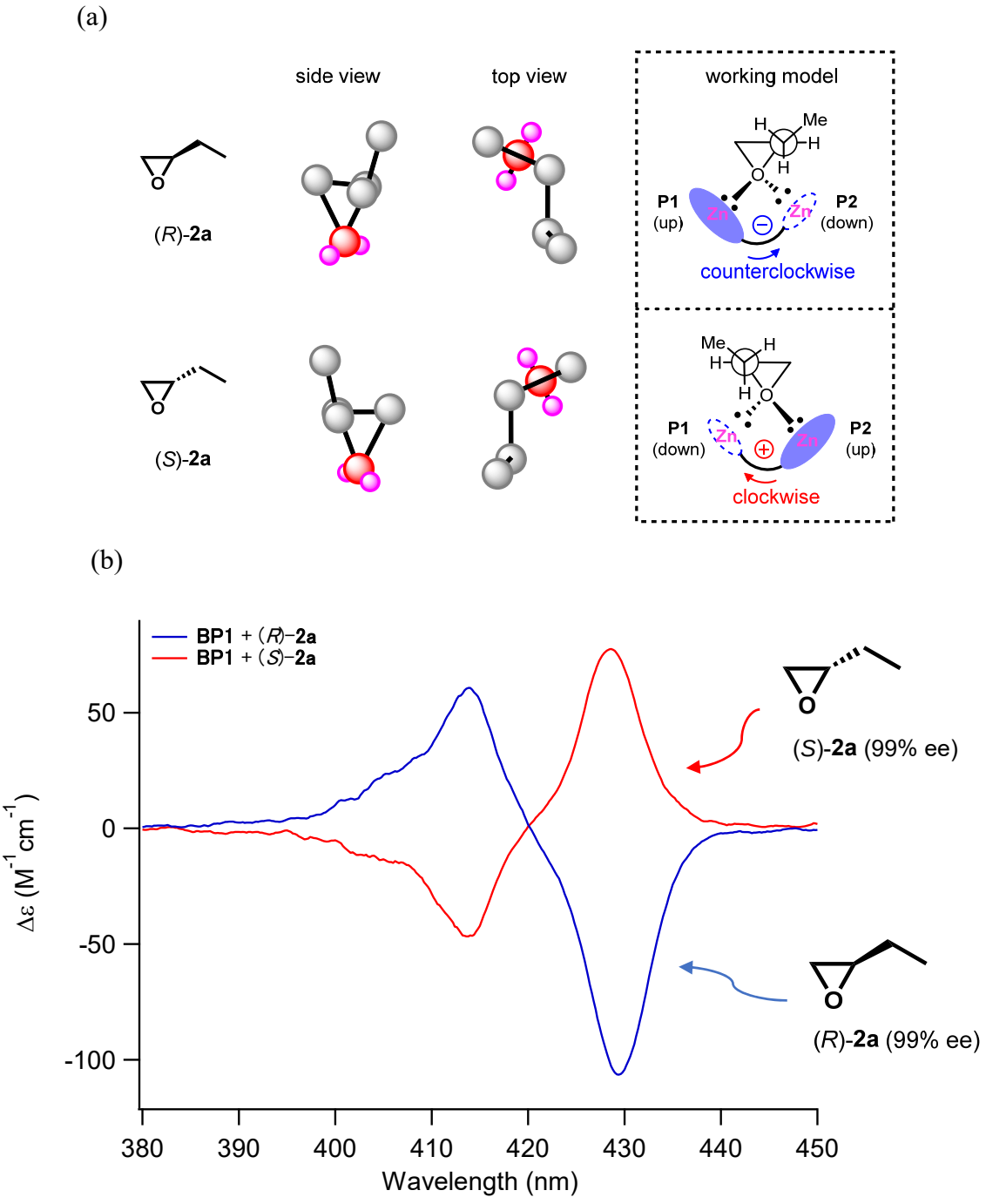


Figure S1A. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2a** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2a** (1.5×10^{-4} M) in the presence of **BP1** (1.5×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

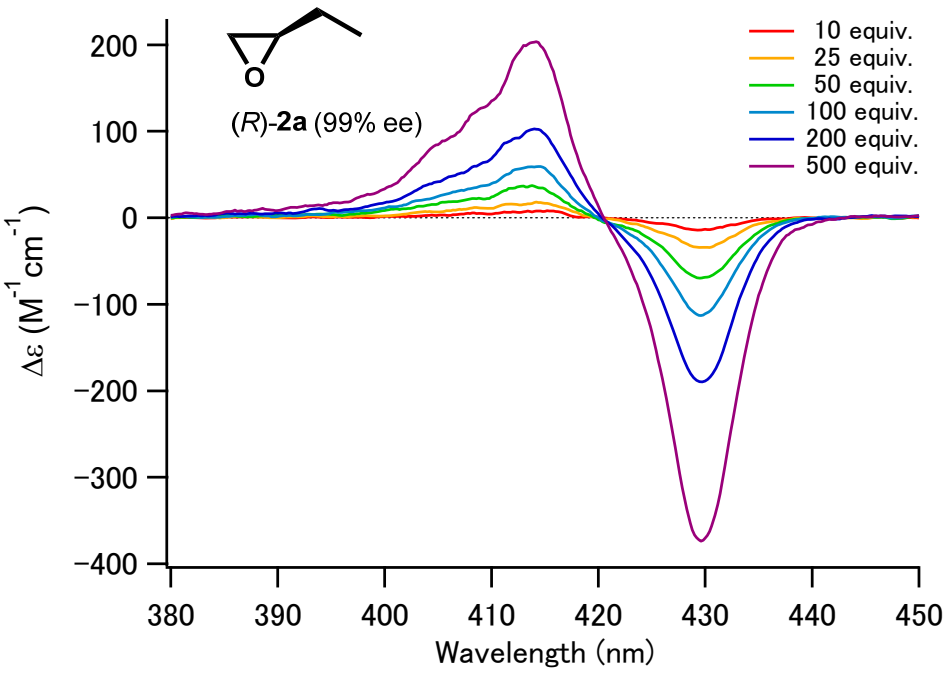


Figure S1B. ECCD titration of **BP1** (2.0×10^{-6} M) with different equivalents of epoxide (*R*)-**2a** in 1%CH_2Cl_2/*n*-hexane at 0 °C.

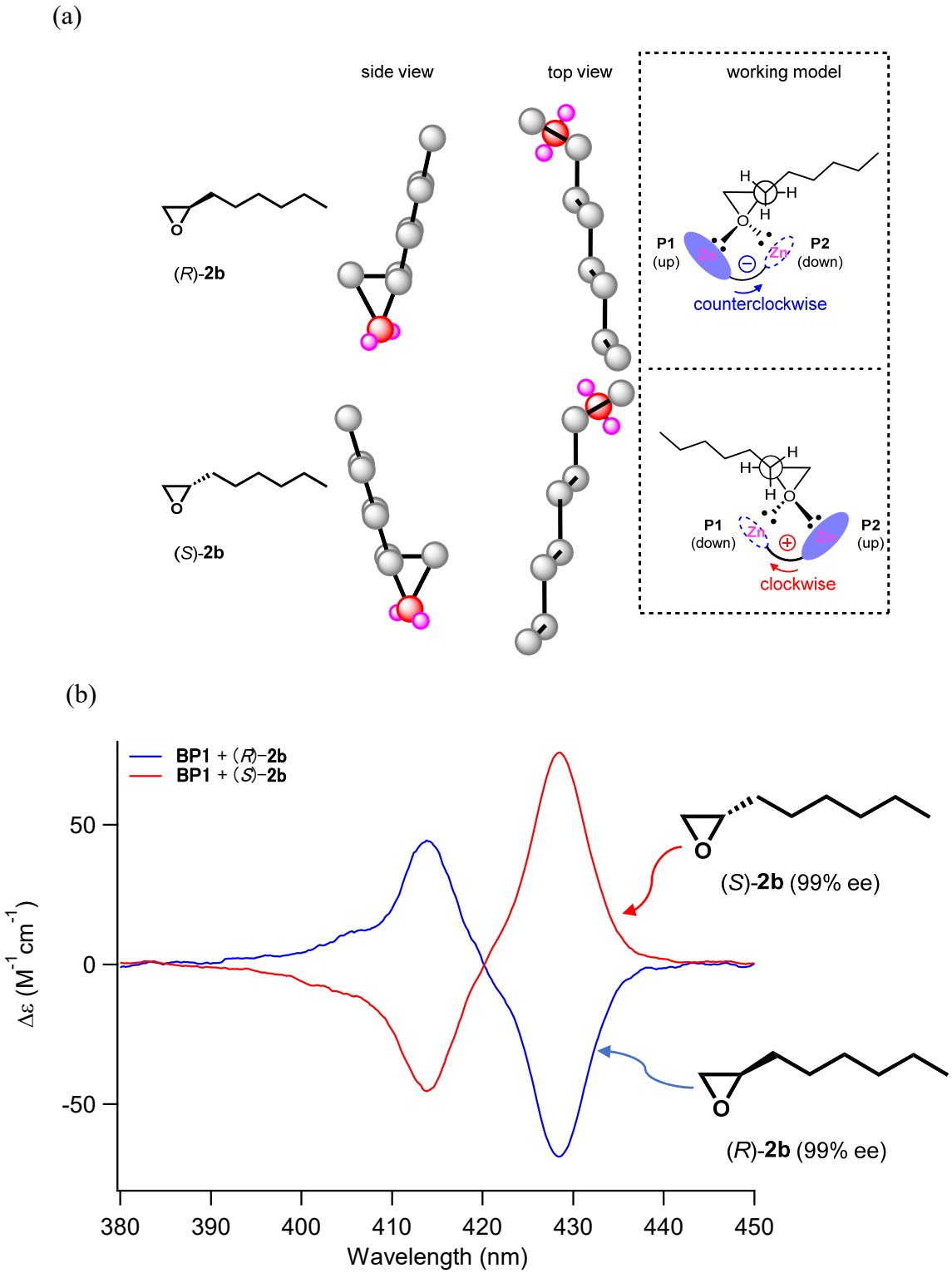


Figure S2. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2b** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2b** (2.7×10^{-4} M) in the presence of **BP1** (2.7×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

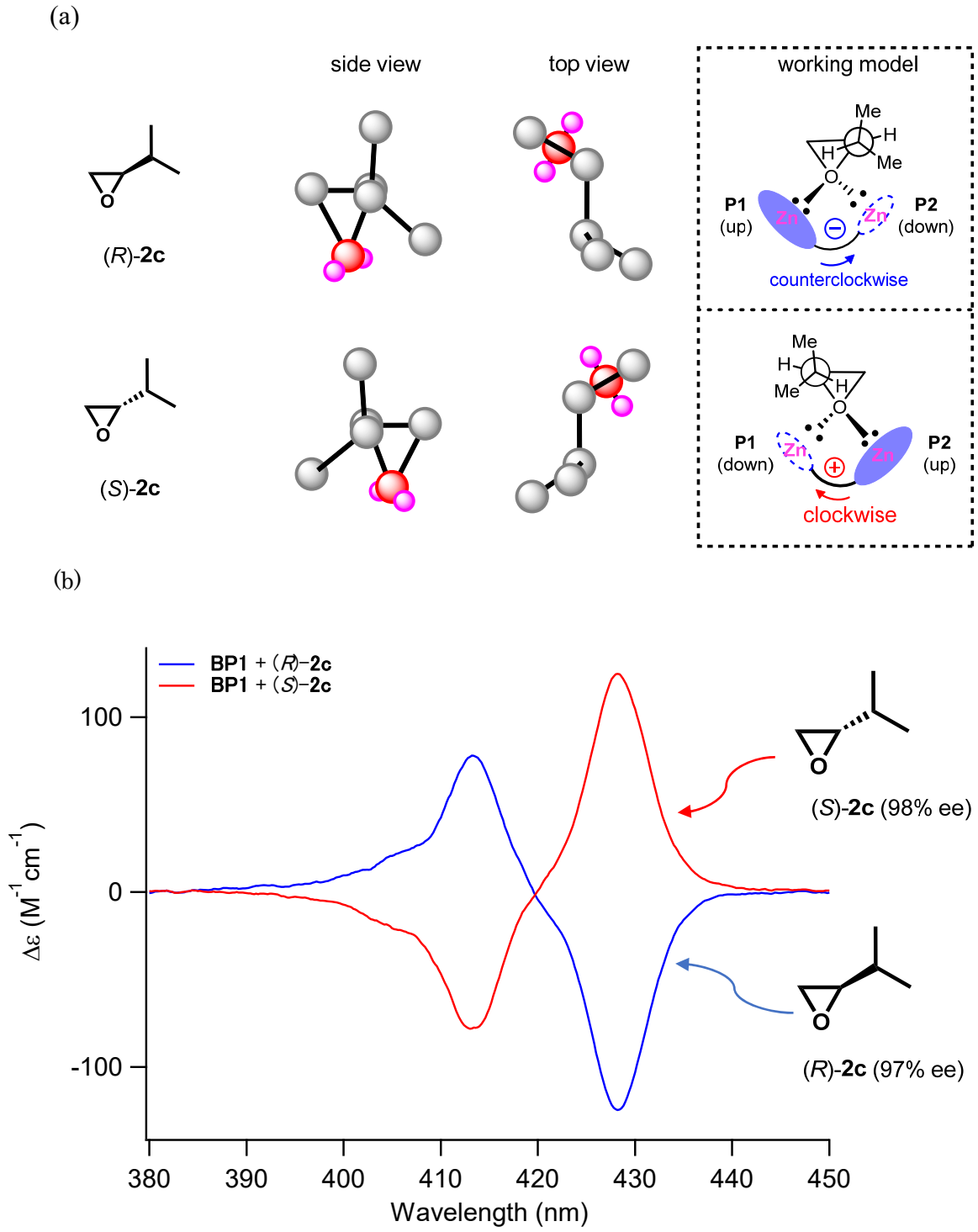


Figure S3. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2c** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2c** (2.0×10^{-4} M) in the presence of **BP1** (2.0×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

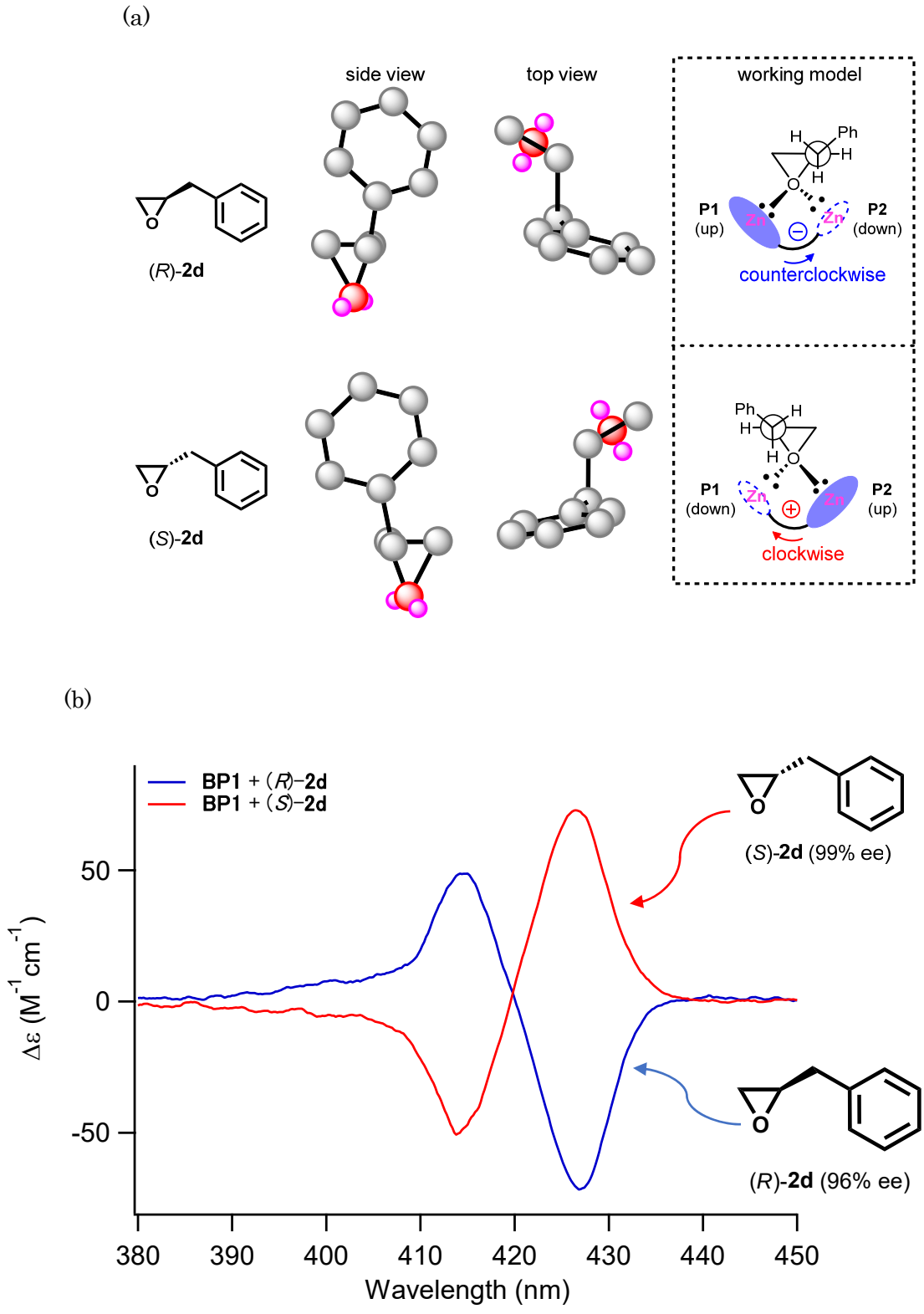


Figure S4. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2d** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2d** (2.0×10^{-4} M) in the presence of **BP1** (2.0×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

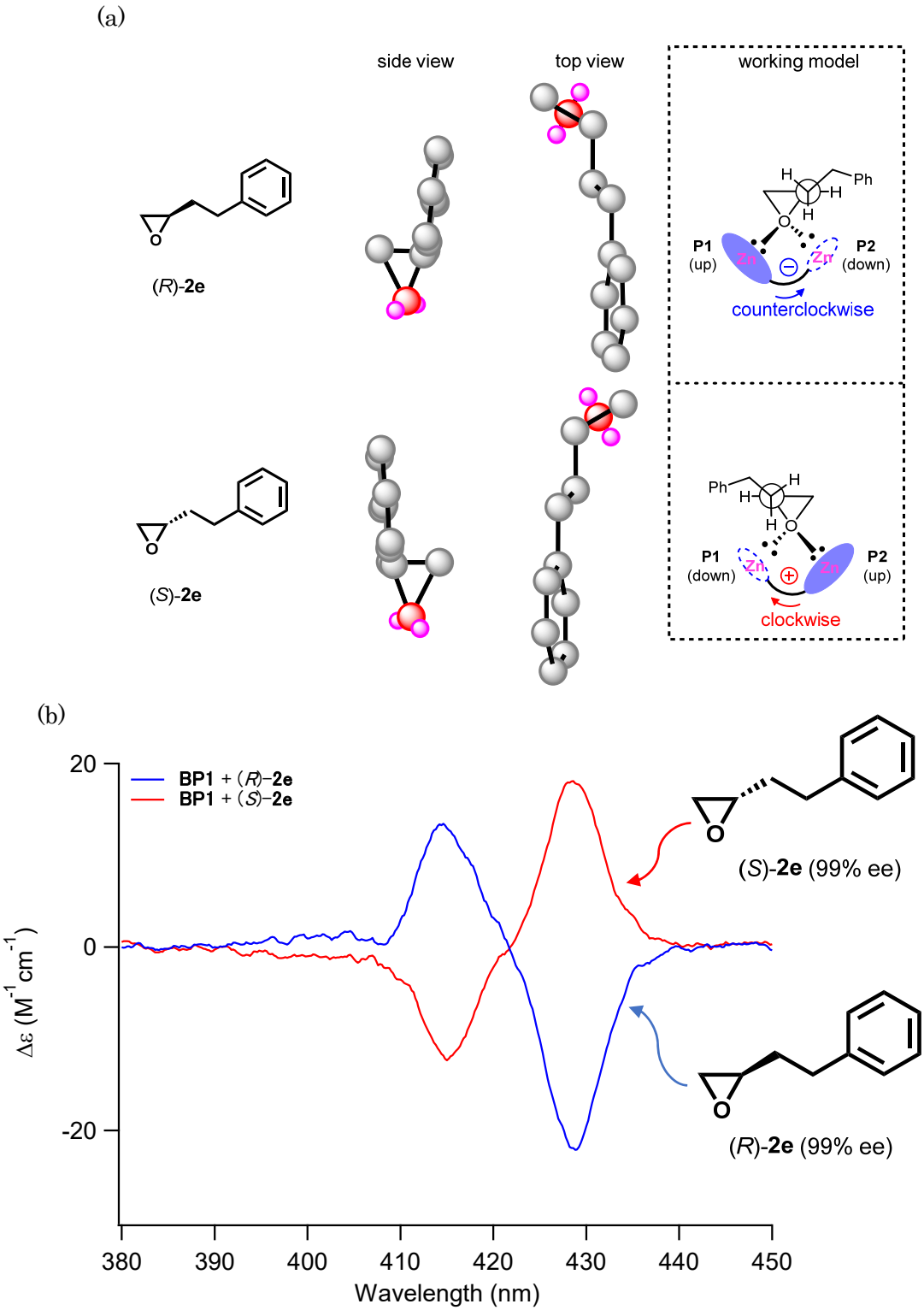


Figure S5. (a) The MM2 optimized structures of (*R*)-and (*S*)-**2e** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2e** (1.9×10^{-4} M) in the presence of **BP1** (1.9×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

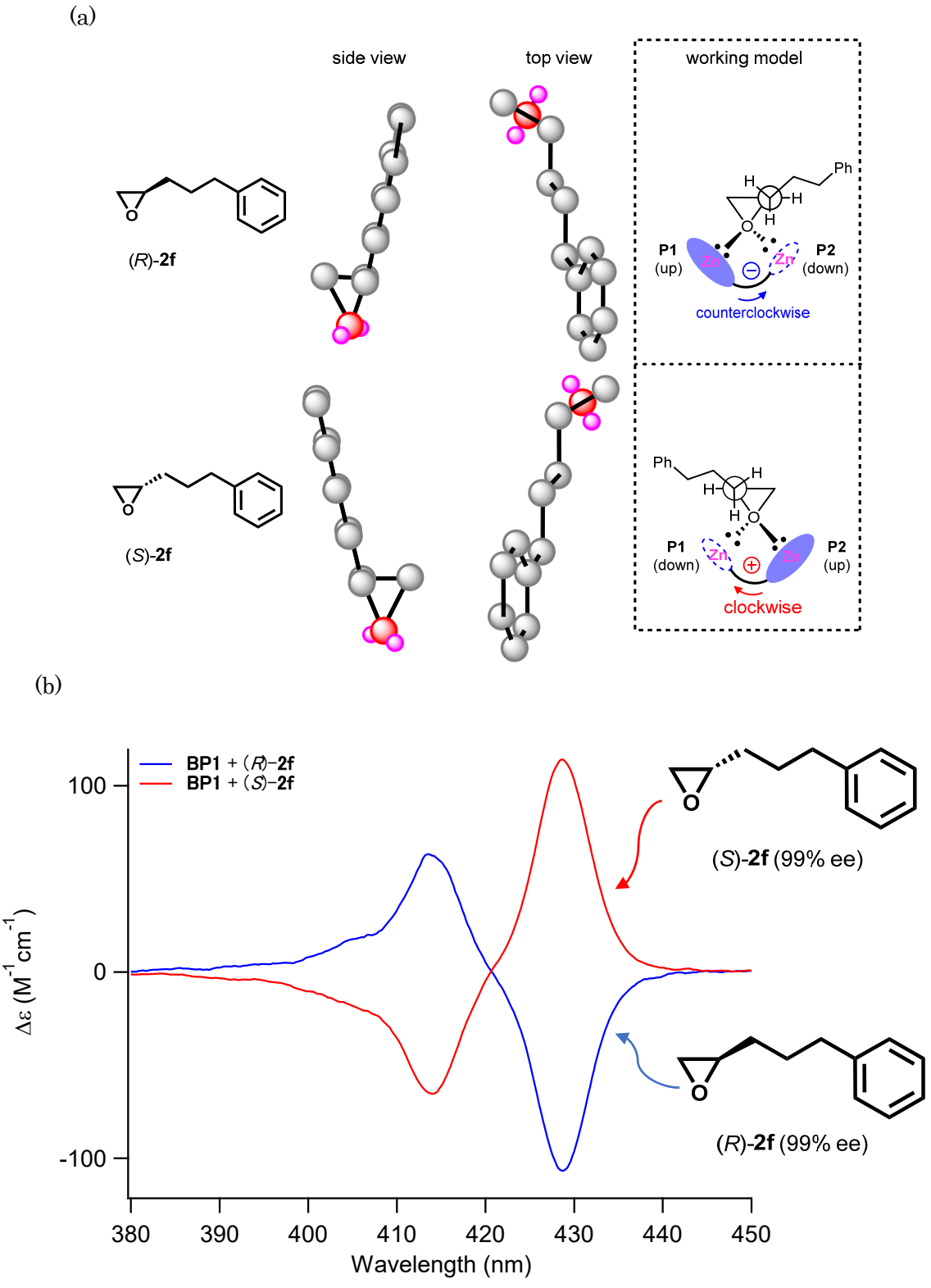
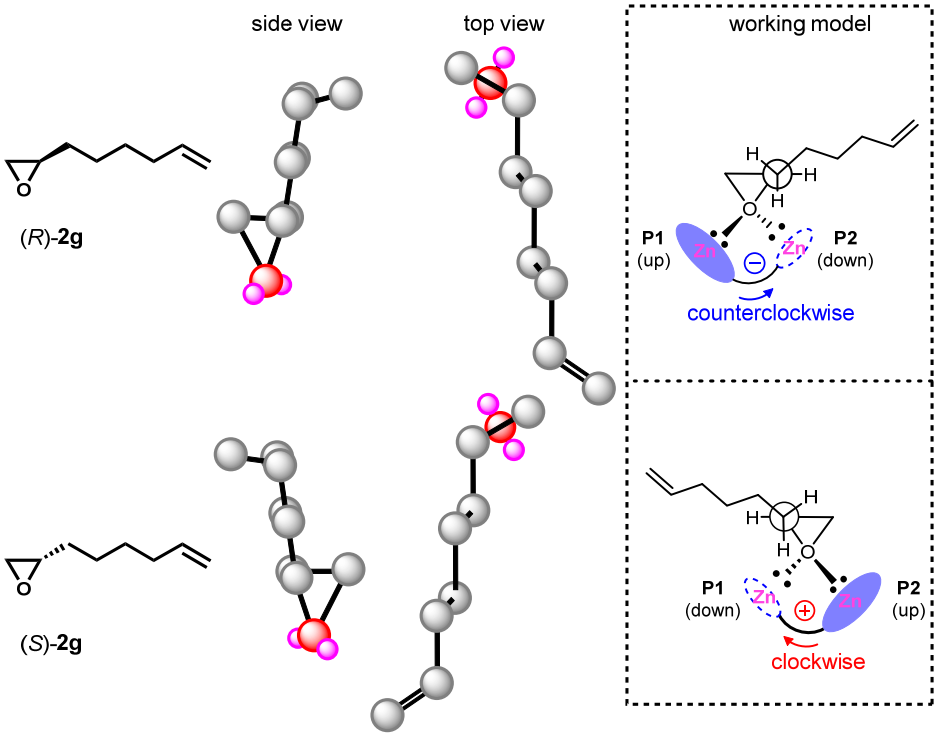


Figure S6. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2f** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2f** (2.7×10^{-4} M) in the presence of **BP1** (2.7×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

(a)



(b)

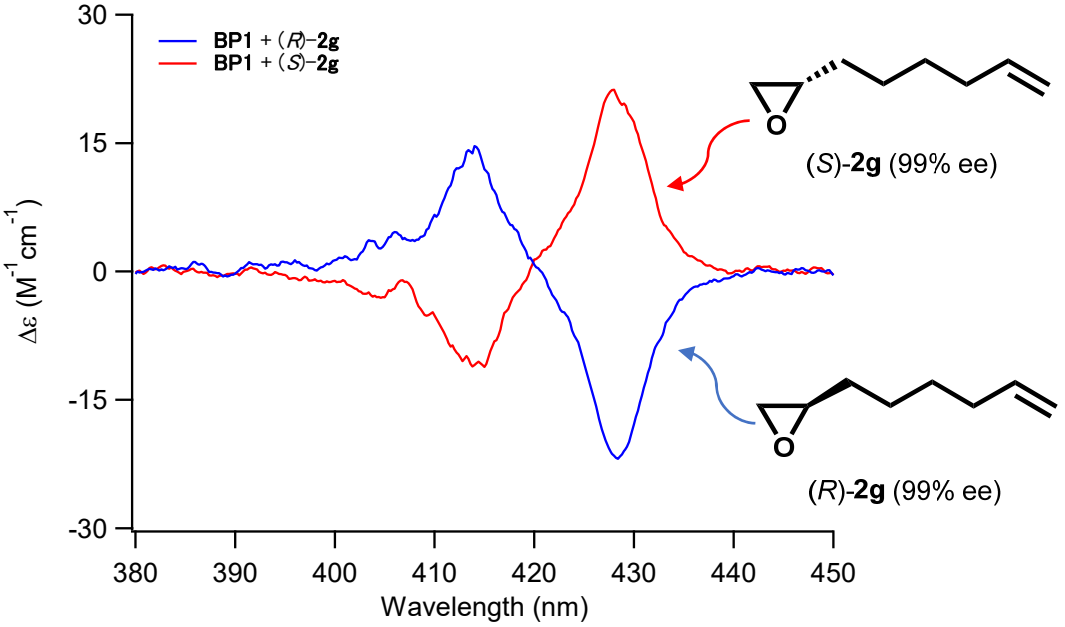


Figure S7. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2g** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2g** (2.1×10^{-4} M) in the presence of **BP1** (2.1×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

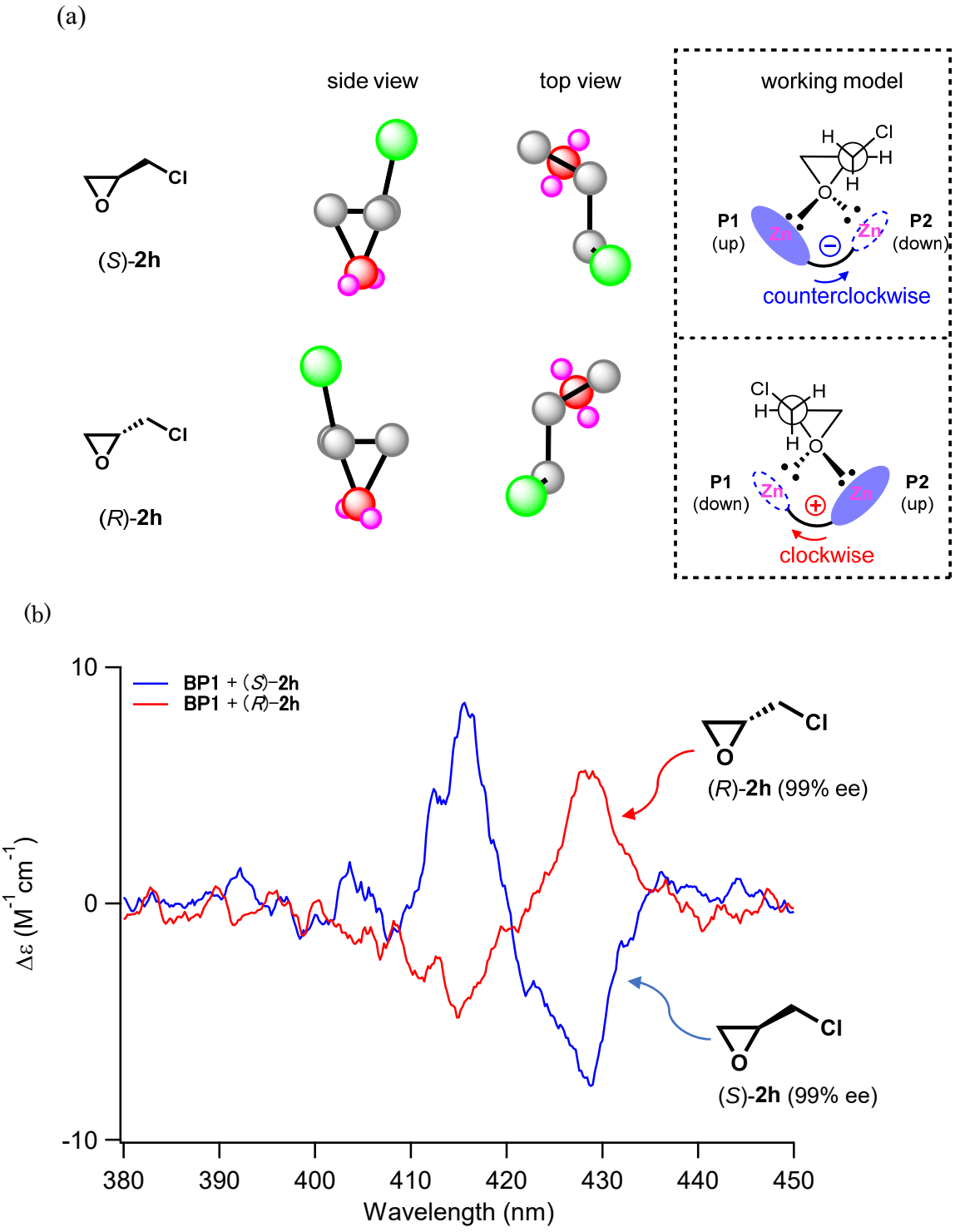
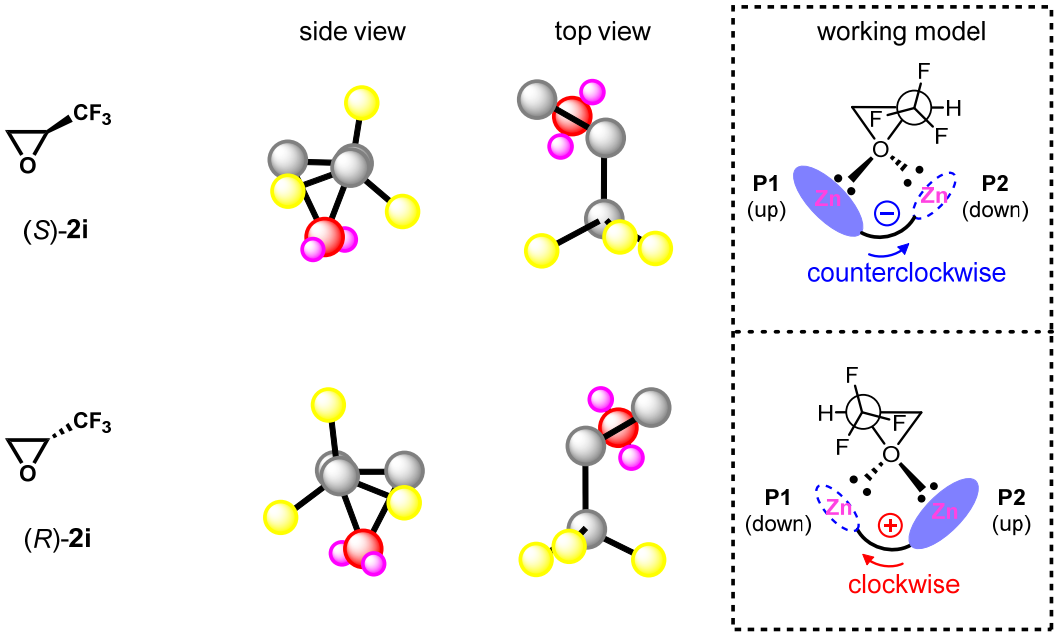


Figure S8. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2h** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2h** (1.8×10^{-4} M) in the presence of **BP1** (1.8×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

(a)



(b)

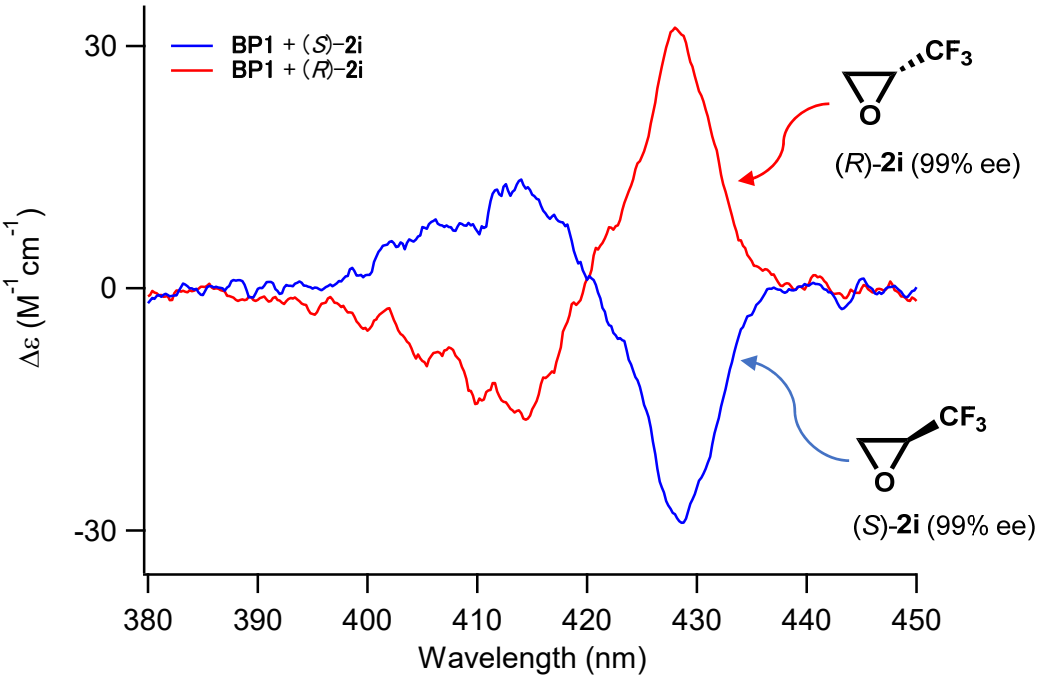


Figure S9. (a) The MM2 optimized structures of (*R*)- and (*S*)-**2i** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of **2i** (2.0×10^{-4} M) in the presence of **BP1** (2.0×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

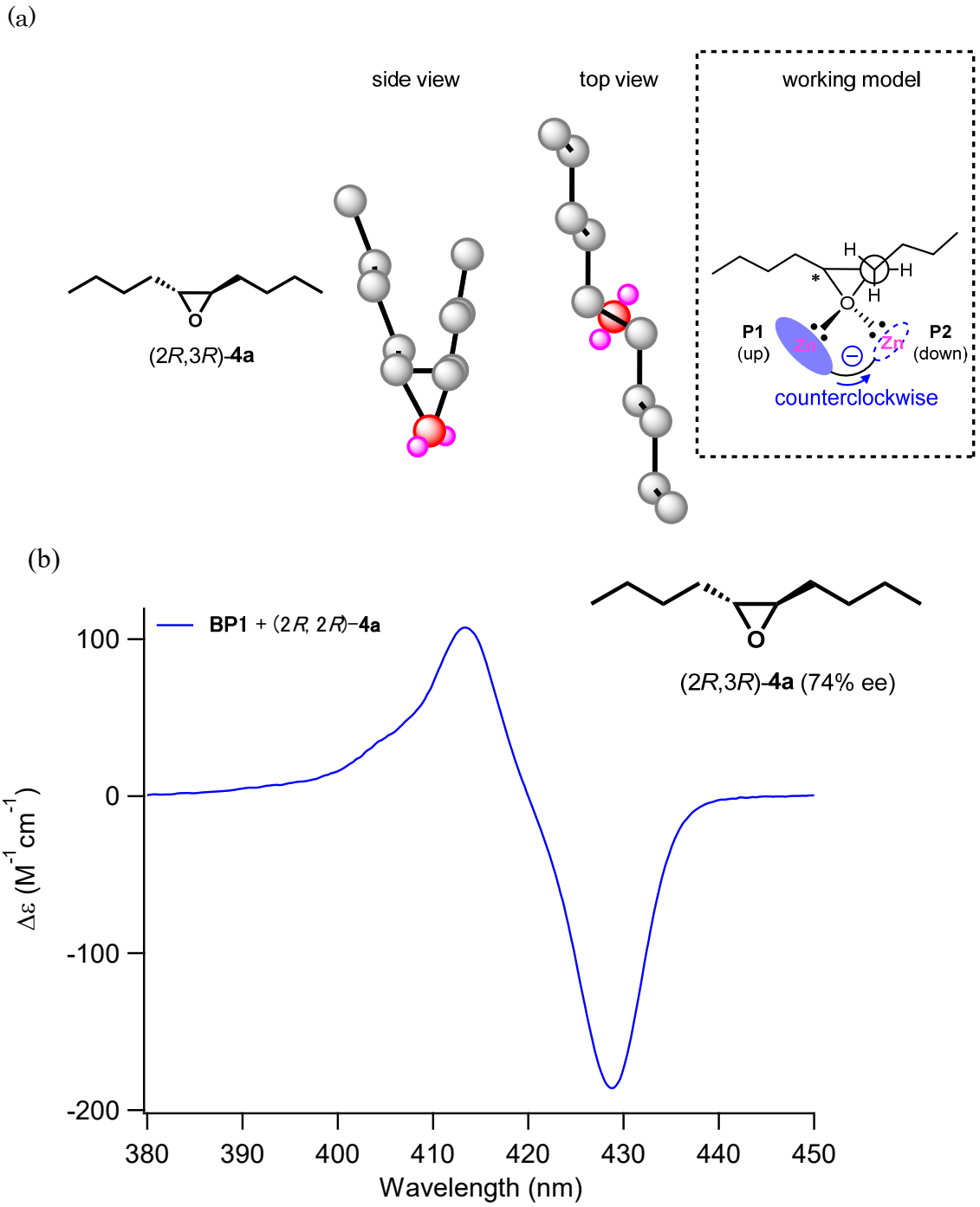


Figure S10. (a) The MM2 optimized structure of (2*R*,3*R*)-**4a** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). (b) ECCD spectra of (2*R*,3*R*)-**4a** (2.2×10^{-4} M) in the presence of **BP1** (2.2×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

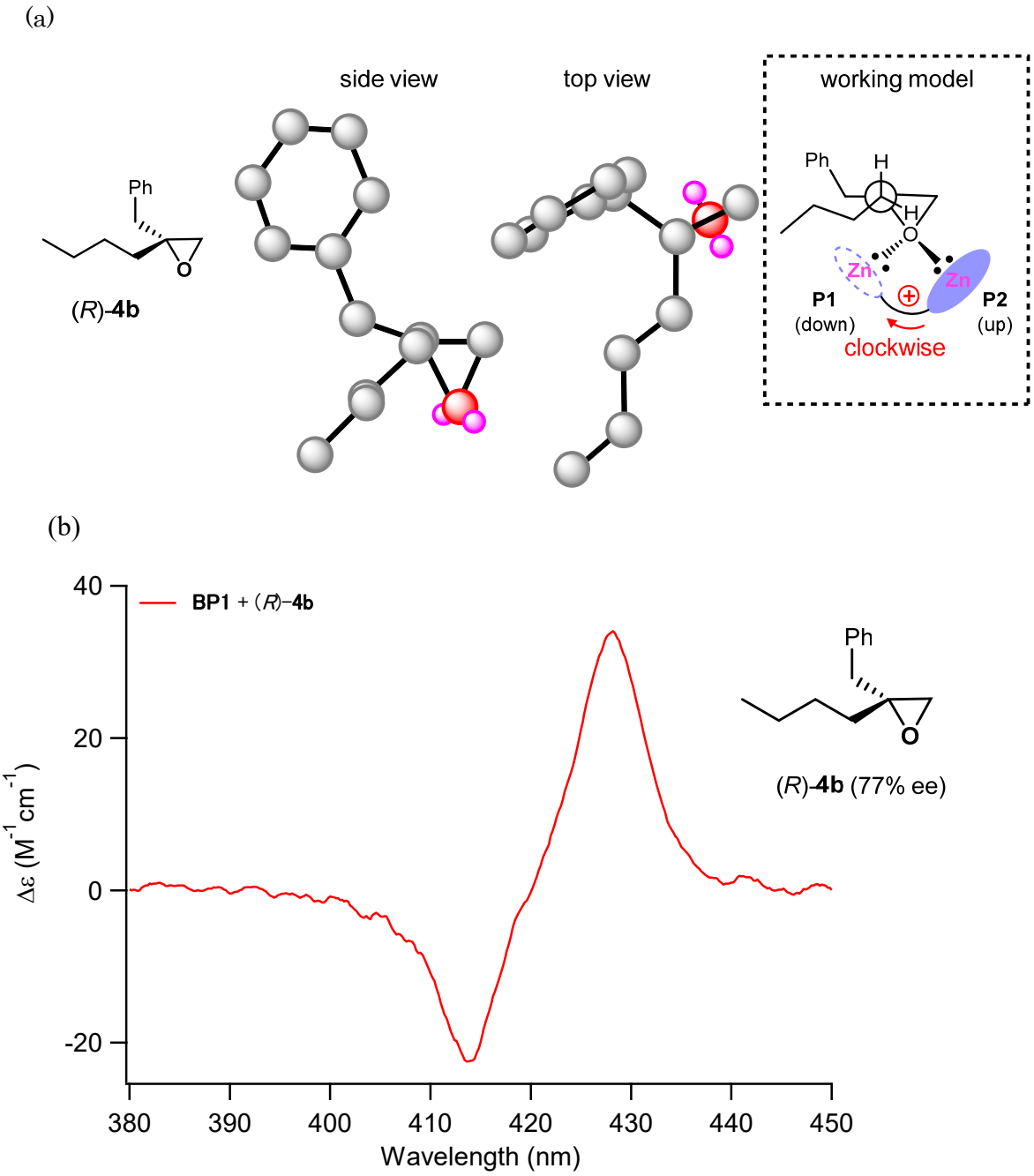


Figure S11. (a) The MM2 optimized structure of (*R*)-**4b** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). The assignment of largest group is based on the conformational energies, *A* values: Bu, 1.79 kcal/mol; Bn, 1.68 kcal/mol.[1] (b) ECCD spectra of (*R*)-**4b** (2.3×10^{-4} M) in the presence of **BP1** (2.3×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

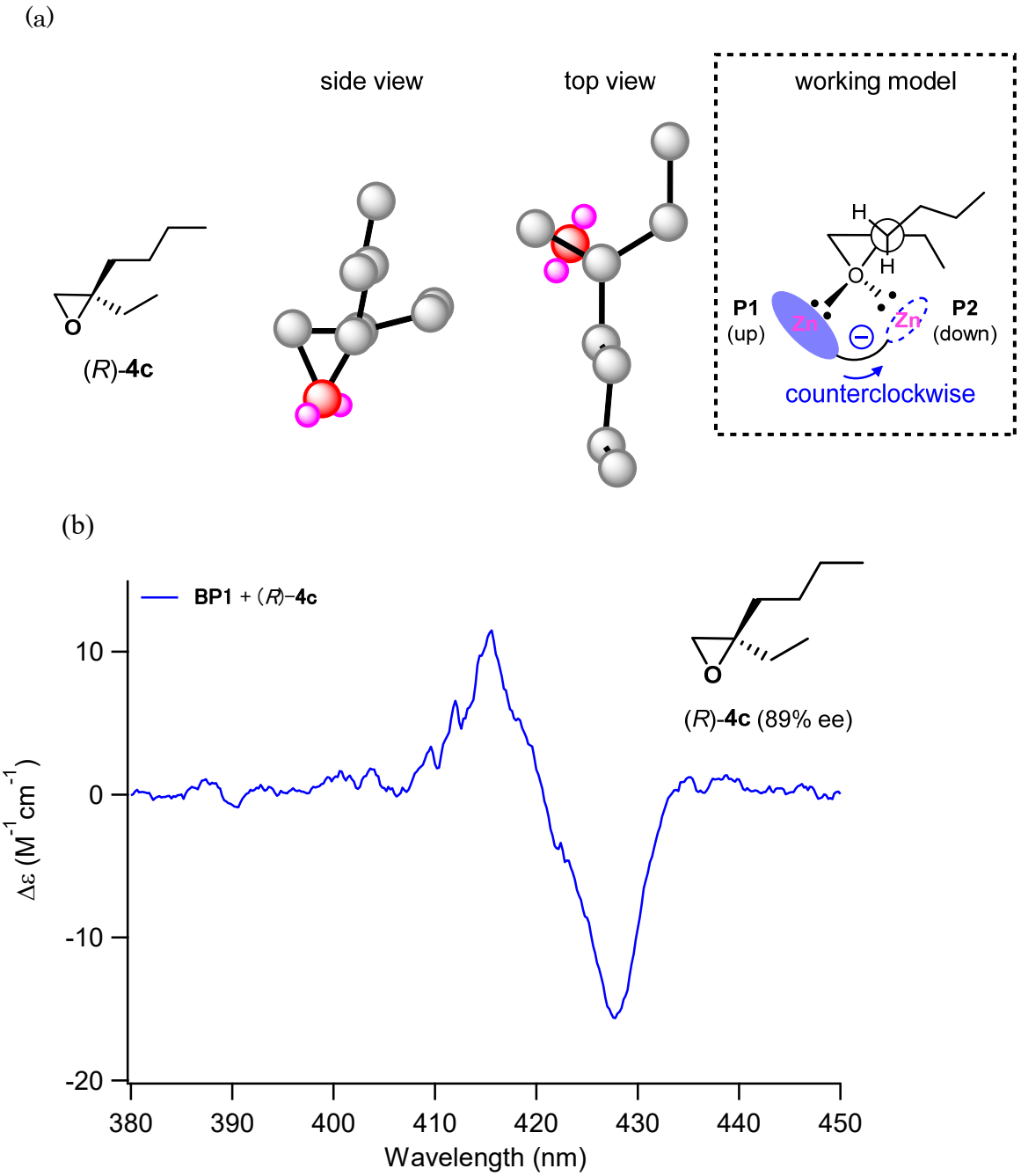


Figure S12. (a) The MM2 optimized structure of (*R*)-**4c** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). The assignment of largest group is based on the conformational energies, *A* values: Bu, 1.79 kcal/mol; Et, 1.75–1.79 kcal/mol.[1,2] (b) ECCD spectra of (*R*)-**4c** (2.2×10^{-2} M) in the presence of **BP1** (2.2×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

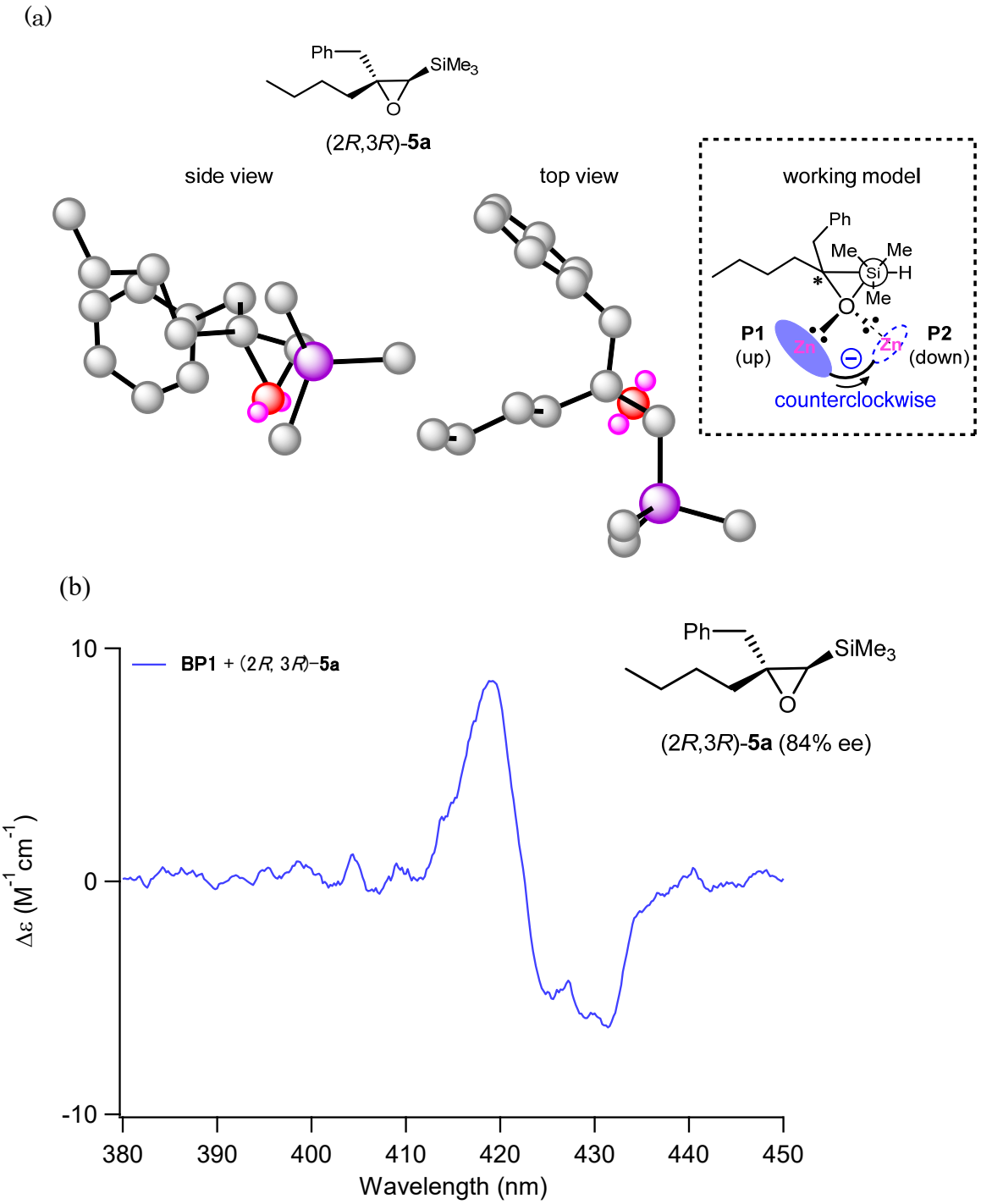


Figure S13. (a) The optimized structure of (2*R*,3*R*)-**5a** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). The assignment of largest group is based on the conformational energies, *A* values: Me_3Si, 2.5 kcal/mol; Bu, 1.79 kcal/mol; Bn, 1.68 kcal/mol.[1] (b) ECCD spectra of (2*R*,3*R*)-**5a** (1.8×10^{-3} M) in the presence of **BP1** (1.8×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

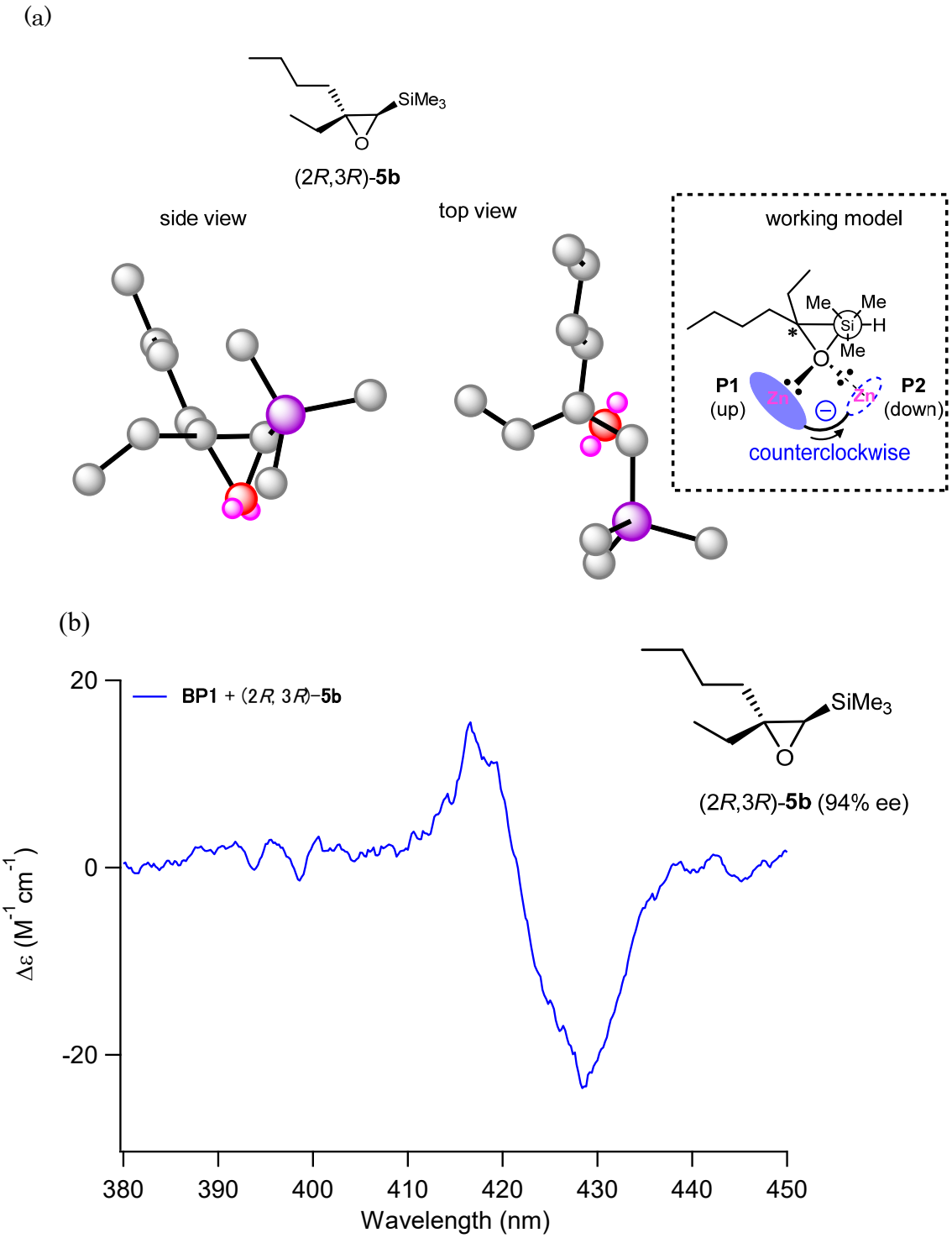
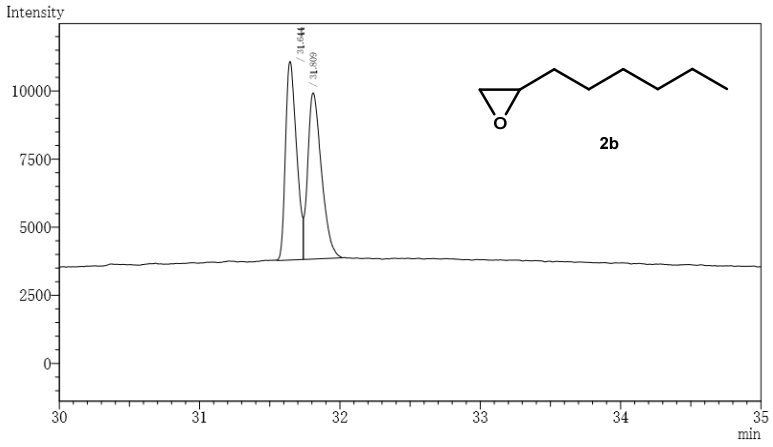


Figure S14. (a) The optimized structure of (2*R*,3*R*)-**5b** and proposed working model for assigning the absolute configuration of the chiral guest (dashed box). The assignment of largest group is based on the conformational energies, *A* values: Me_3Si, 2.5 kcal/mol; Bu, 1.79 kcal/mol; Et, 1.75-1.79 kcal/mol.[1] (b) ECCD spectra of (2*R*,3*R*)-**5b** (1.5×10^{-3} M) in the presence of **BP1** (1.5×10^{-6} M) in 1% CH_2Cl_2/*n*-hexane at 0 °C.

Determination of the optical purity of 2b

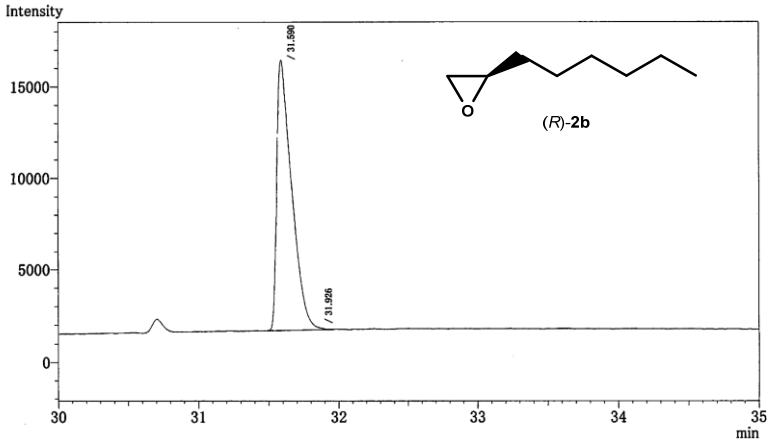
GC conditions: column, CP-Chirasil-DEX CB (0.25 mm × 25 m); carrier gas, N_2; flow rate, 15 cm/s; injection temperature, 150 °C; column temperature, 40 °C, 2°C/min, 100 °C, 8 min; detector temperature, 250 °C. Retention time: 31.6 min (*R*), 31.8 min (*S*).

Racemic **2b**



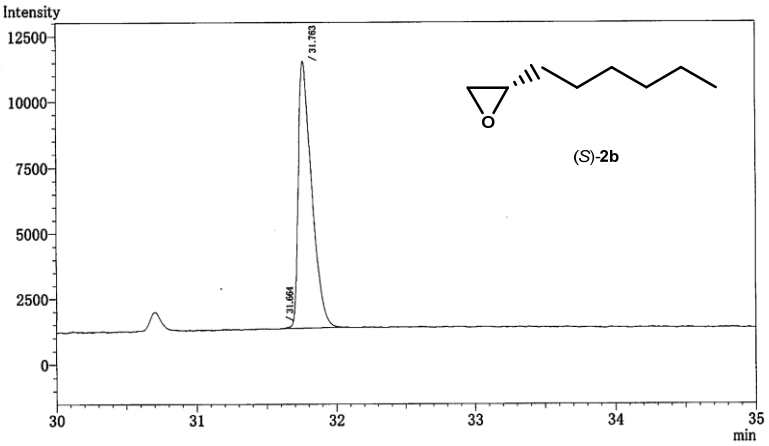
Peak No.	Rt (min)	Area	Area %
1	31.64	39951	48.936
2	31.80	41687	51.064
Total		81638	100.000

(*R*)-2-Hexyloxirane [(*R*)-2b]:[3a] colorless oil; 99 % ee; bp 60 °C / 25 mmHg; $[\alpha]_D^{27}$ +8.21° (*c* 0.99, $CHCl_3$), Lit.[4a] $[\alpha]_D^{20}$ +7.36° (*c* 1.15, $CHCl_3$).



Peak No.	Rt (min)	Area	Area %
1	31.59	108704	99.972
2	31.92	30	0.028
Total		108734	100.000

(*S*)-2-Ethyloxirane [(*S*)-2b]:[3a] colorless oil; 99 % ee; bp 60 °C / 25 mmHg; $[\alpha]_D^{29}$ -8.72° (*c* 0.96, $CHCl_3$), Lit.[4b] $[\alpha]_D^{24}$ -8.90° (*c* 1.00, $CHCl_3$).

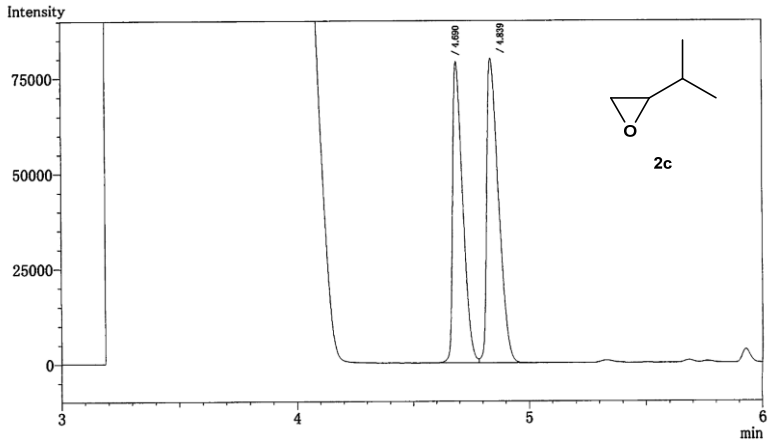


Peak No.	Rt (min)	Area	Area %
1	31.66	105	0.154
2	31.76	67959	99.946
Total		68064	100.000

Determination of the optical purity of 2c

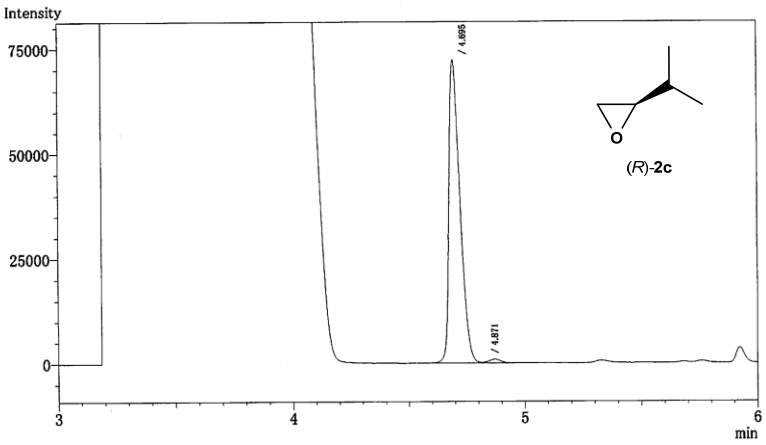
GC conditions: column, CHIRALDEX G-TA (0.25 mm × 30 m); carrier gas, N_2; flow rate, 15 cm/s; injection temperature, 150 °C; column temperature, 40 °C, 4 min, 10 °C/min, 150 °C, 10 min; detector temperature, 200 °C. Retention time: 4.7 min (*R*), 4.8 min (*S*).

Racemic **2c**



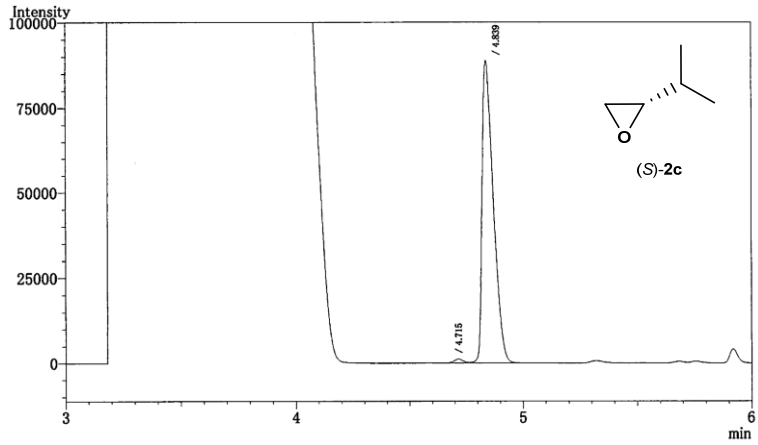
Peak No.	Rt (min)	Area	Area %
1	4.69	240075	46.020
2	4.83	281597	53.980
Total		521672	100.000

(*R*)-2-Isopropyloxirane [(*R*)-2c]:[3b] colorless oil; 97 % ee; bp 30 °C / 100 mmHg; $[\alpha]_D^{25}$ -6.25° (*c* 2.10, $CHCl_3$), Lit.[3b] $[\alpha]_D^{23}$ -6.44° (*c* 2.23, $CHCl_3$).



Peak No.	Rt (min)	Area	Area %
1	4.69	239397	98.704
2	4.87	3144	1.296
Total		242541	100.000

(*S*)-2-Isopropyloxirane [(*S*)-2c]:[3b] colorless oil; 98 % ee; bp 30 °C / 100 mmHg; $[\alpha]_D^{25}$ +5.76° (*c* 2.16, $CHCl_3$), Lit.[5] $[\alpha]_D^{25}$ +4.83° (*c* 2.43, cyclohexane)

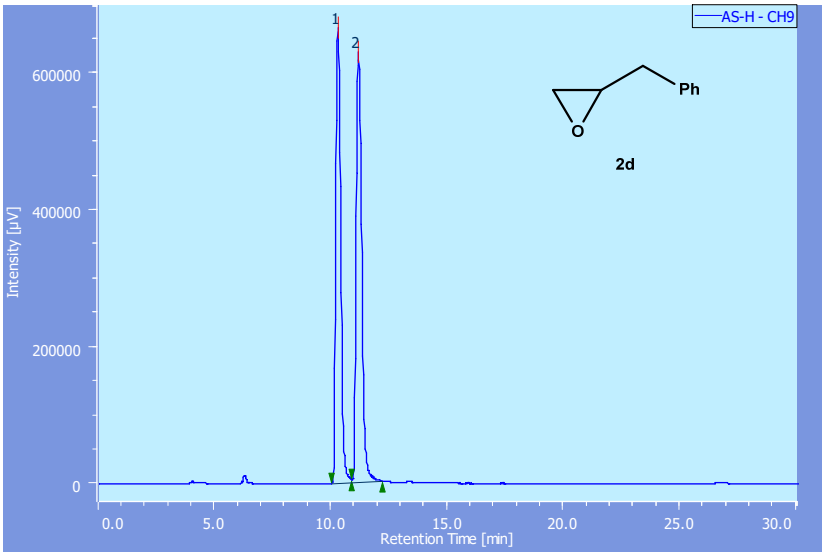


Peak No.	Rt (min)	Area	Area %
1	4.71	3293	1.069
2	4.83	304879	98.931
Total		308172	100.000

Determination of the optical purity of 2d

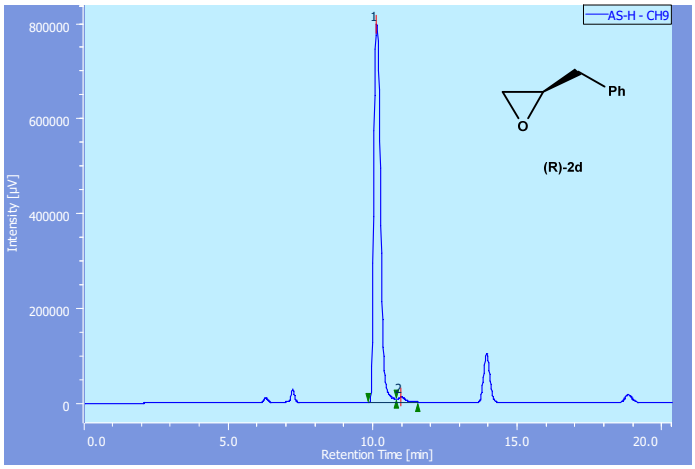
HPLC conditions: column, DAICEL CHIRALPAK AS-H; solvent, *i*-PrOH/*n*-Hexane 2/98; flow rate, 0.5 mL/min; detection at 254 nm.

Racemic **2d**



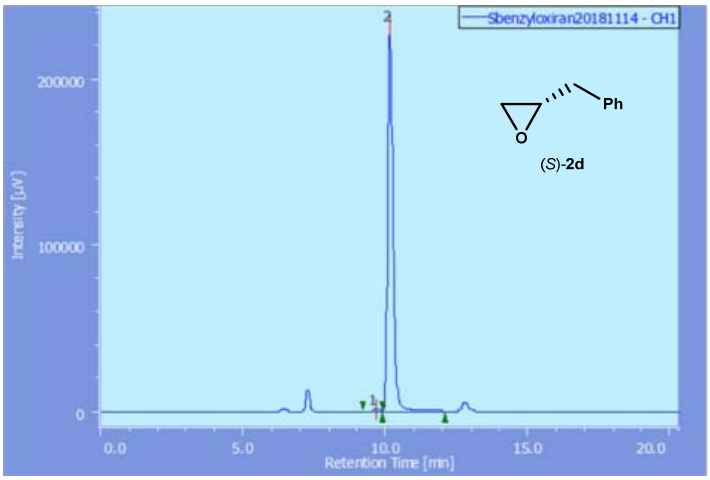
Peak No.	Rt (min)	Area	Area %
1	10.30	9926134	48.649
2	11.18	10477378	51.351
Total		20403512	100.000

(*R*)-2-Benzyloxirane [(*R*)-2d]:[3a] colorless oil; 96 % ee; bp 60 °C / 3 mmHg; $[\alpha]_D^{27}$ +16.98° (*c* 2.03, EtOH), Lit.[6] $[\alpha]_D^{25}$ +17.50° (*c* 1.94, EtOH)



Peak No.	Rt (min)	Area	Area %
1	10.25	12859807	97.927
2	11.22	272272	2.073
Total		13132079	100.000

(*S*)-2-Benzyloxirane [(*S*)-2d]:[3a] colorless oil; 99% ee; bp 60 °C / 3 mmHg; $[\alpha]_D^{25}$ -18.37° (*c* 2.01, EtOH), Lit.[6] $[\alpha]_D^{25}$ -17.30° (*c* 2.07, EtOH).

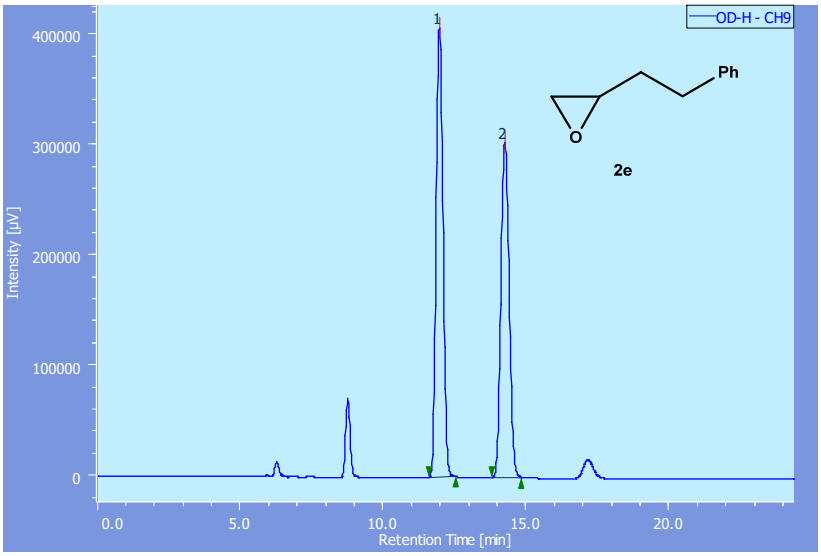


Peak No.	Rt (min)	Area	Area %
1	9.67	12620	0.418
2	10.14	3004963	99.582
Total		3017583	100.000

Determination of the optical purity of 2e

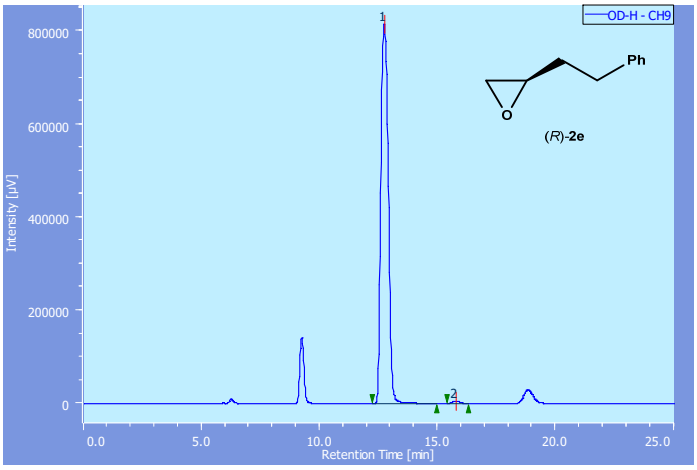
HPLC conditions: column, DAICEL CHIRALCEL OD-H; solvent, *i*-PrOH/*n*-Hexane 2/98; flow rate, 0.5 mL/min; detection at 254 nm

Racemic **2e**



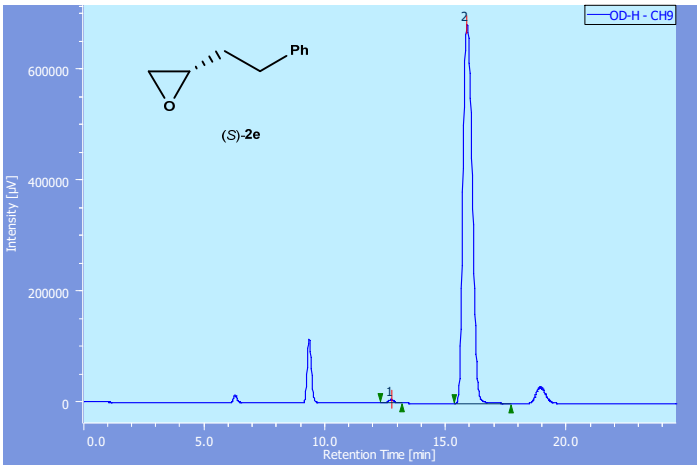
Peak No.	Rt (min)	Area	Area %
1	11.94	6840638	53.078
2	14.24	6047233	46.922
Total		12887871	100.000

(*R*)-2-Phenethyloxirane [(*R*)-2e]:[3a] colorless oil; 99 % ee; bp 65 °C / 2 mmHg; $[\alpha]_D^{27}$ +19.52° (*c* 1.04, $CHCl_3$), $[\alpha]_D^{28}$ +19.30° (*c* 1.25, acetone), Lit.[7a] $[\alpha]_D^{28}$ +15.8° (*c* 1.24, acetone).



Peak No.	Rt (min)	Area	Area %
1	12.74	17875637	99.409
2	15.78	106209	0.591
Total		17981846	100.000

(*S*)-2-Phenethyloxirane [(*S*)-2e]:[3a] colorless oil; 99 % ee; bp 65 °C / 2 mmHg; $[\alpha]_D^{27}$ -19.40° (*c* 1.21, $CHCl_3$), $[\alpha]_D^{28}$ -19.44° (C 1.04, acetone), Lit.[7b] $[\alpha]_D^{25}$ -4.65° (*c* 1.00, $CHCl_3$).

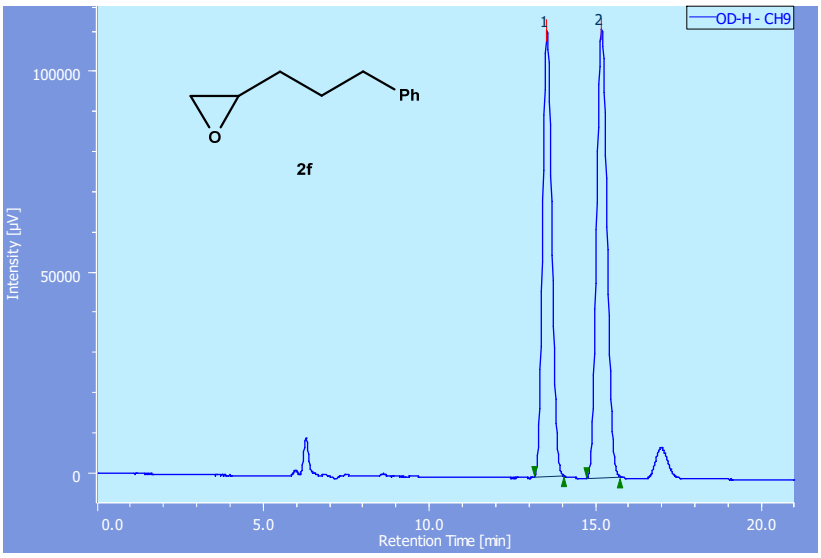


Peak No.	Rt (min)	Area	Area %
1	12.73	99431	0.551
2	15.88	17958718	99.449
Total		18058149	100.000

Determination of the optical purity of 2f

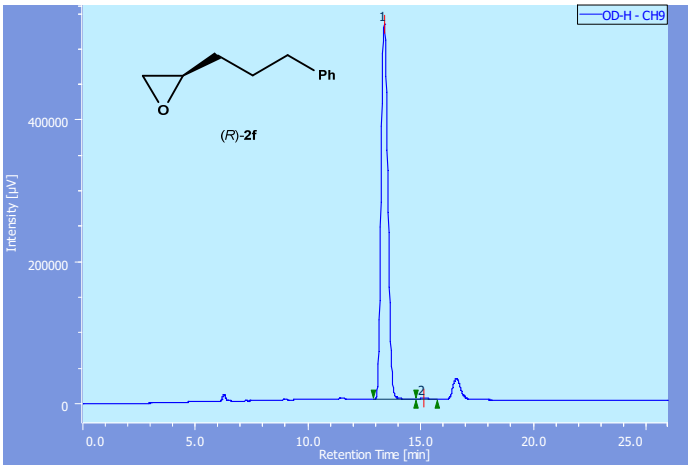
HPLC conditions: column, DAICEL CHIRALCEL OD-H; solvent, *i*-PrOH/*n*-Hexane 2/98; flow rate, 0.5 mL/min, detection at 254 nm.

Racemic **2f**



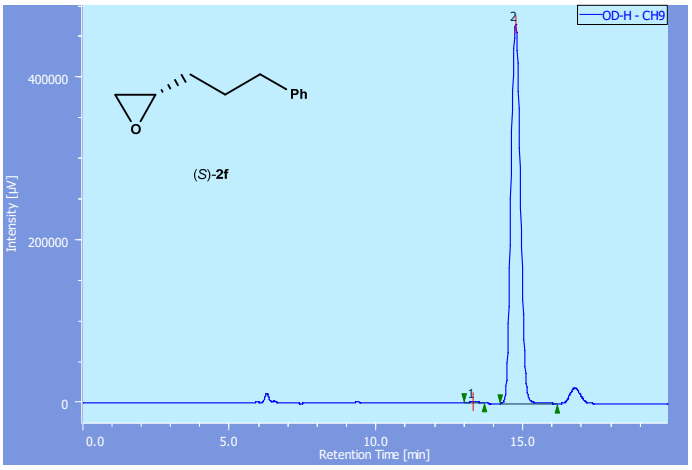
Peak No.	Rt (min)	Area	Area %
1	13.52	2113212	46.539
2	15.17	2427563	53.431
Total		4540775	100.000

(*R*)-2-(3-Phenylpropyl)oxirane [(*R*)-2f]:[3a] colorless oil; 99 % ee; bp 93 °C / 3 mmHg; $[\alpha]_D^{26}$ +7.49° (*c* 1.00, $CHCl_3$), Lit.[8a] $[\alpha]_D$ +6.66° (*c* 1.00, $CHCl_3$).



Peak No.	Rt (min)	Area	Area %
1	13.37	11136550	99.610
2	15.14	43612	0.390
Total		11180162	100.000

(*S*)-2-(3-Phenylpropyl)oxirane [(*S*)-2f]:[3a] colorless oil; 99 % ee; bp 93 °C / 3 mmHg; $[\alpha]_D^{27}$ -8.50° (*c* 1.05, $CHCl_3$), Lit.[8b] $[\alpha]_D^{23}$ -9.46° (*c* 1.04, $CHCl_3$).

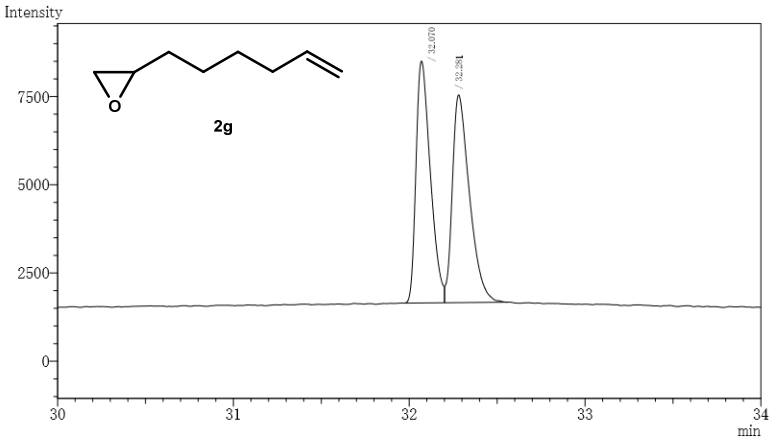


Peak No.	Rt (min)	Area	Area %
1	13.30	44869	0.429
2	14.733	10425007	99.571
Total		10469876	100.000

Determination of the optical purity of 2g

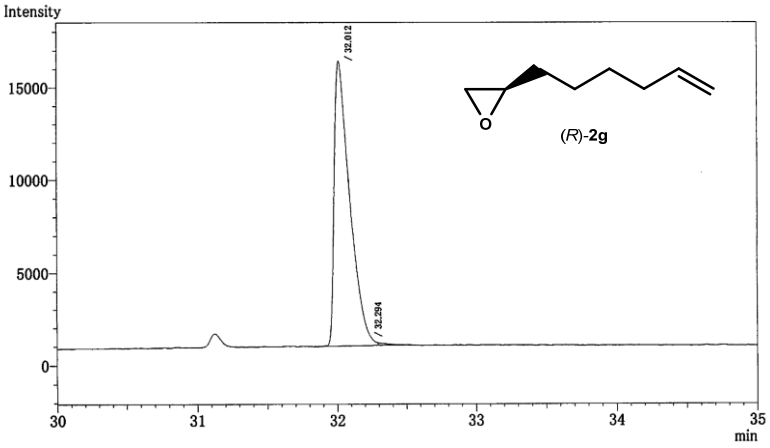
GC conditions: column, CP-Chirasil-DEX CB (0.25 mm × 25 m); carrier gas, N_2; flow rate, 15 cm/s; injection temperature, 150 °C; column temperature, 40 °C, 2 °C/min, 100 °C, 8 min; detector temperature, 250 °C. Retention time: 32.1 min (*R*), 32.3 min (*S*).

Racemic **2g**



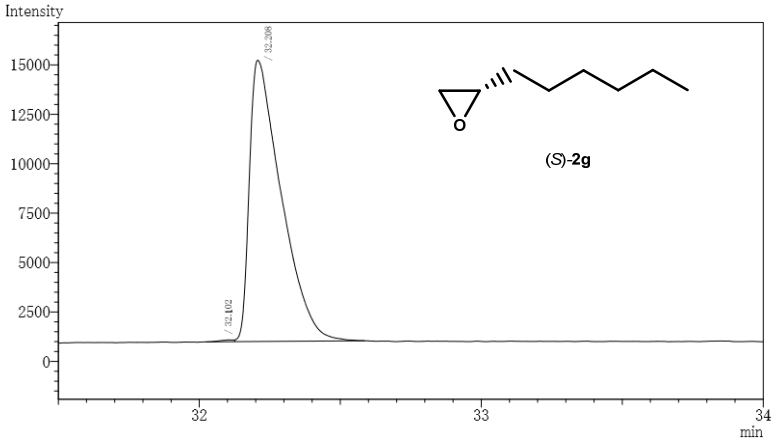
Peak No.	Rt (min)	Area	Area %
1	32.07	38921	49.304
2	32.28	40020	50.696
Total		78941	100.000

(*R*)-2-(Hex-5-en-1-yl)oxirane [(*R*)-2g]:[3a] colorless oil; 99 % ee; bp 60 °C / 5 mmHg; $[\alpha]_D^{27}$ +9.36° (*c* 0.98, $CHCl_3$), Lit.[8a] $[\alpha]_D^{20}$ +6.67° (*c* 1.00, $CHCl_3$).



Peak No.	Rt (min)	Area	Area %
1	32.01	119314	99.503
2	32.29	596	0.497
Total		119910	100.000

(*S*)-2-(Hex-5-en-1-yl)oxirane [(*S*)-2g]:[3a] colorless oil; 99 % ee; bp 60 °C / 5 mmHg; $[\alpha]_D^{27}$ -10.70° (*c* 0.98, $CHCl_3$), lit.[4b] $[\alpha]_D^{25}$ -10.40° (*c* 1.00, $CHCl_3$).

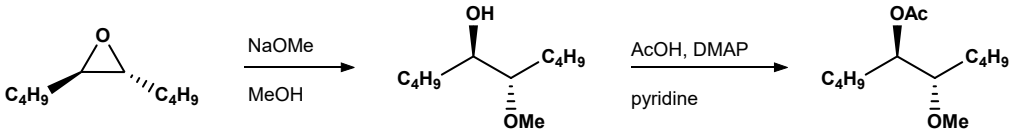


Peak No.	Rt (min)	Area	Area %
1	32.10	314	0.281
2	32.20	111706	99.719
Total		112020	100.000

Determination of the optical purity of (2R,3R)-4a

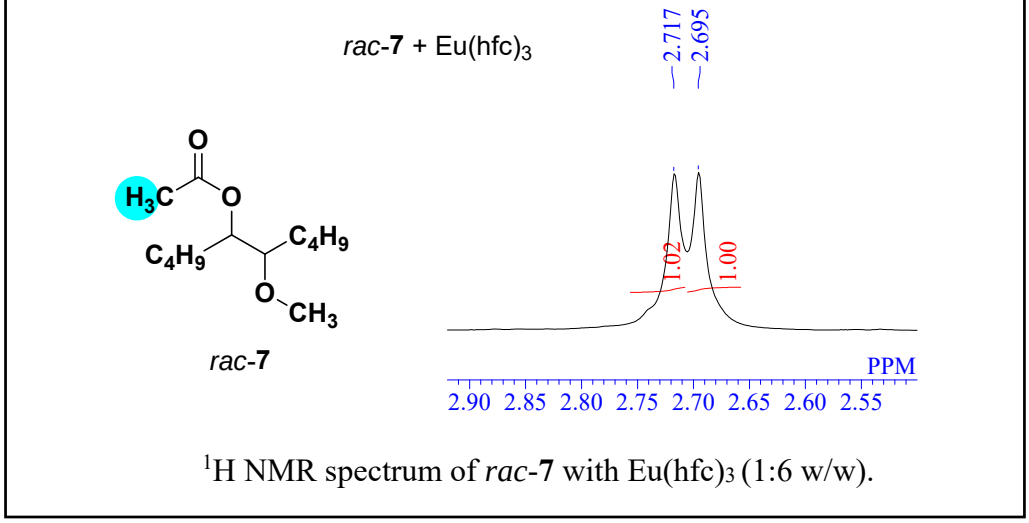
(2*R*,3*R*)-**4a** (74% ee)

The optical purity of (2*R*,3*R*)-**4a** was determined by ^{1}H NMR shift analysis of the derived acetate **7** with Eu(hfc)$_3$ in $CDCl_3$.[3c,10]



(2*R*,3*R*)-**4a** **6** **7**

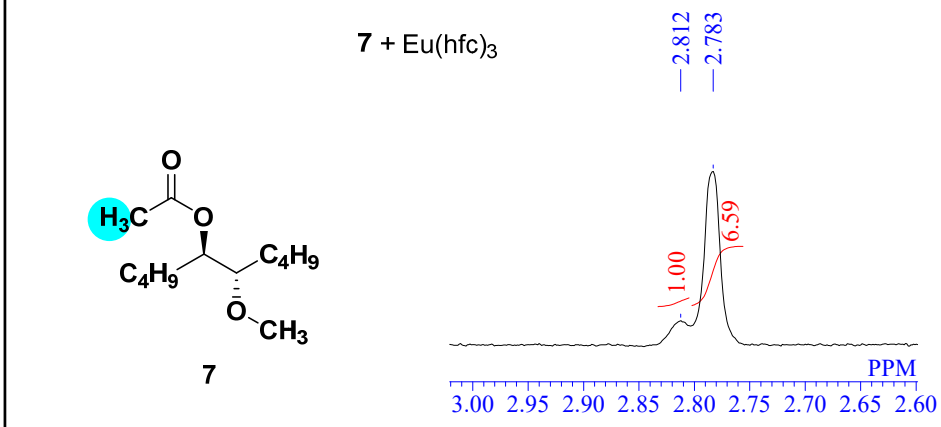
Racemic



rac-**7**

^{1}H NMR spectrum of *rac*-**7** with Eu(hfc)$_3$ (1:6 w/w).

74% ee

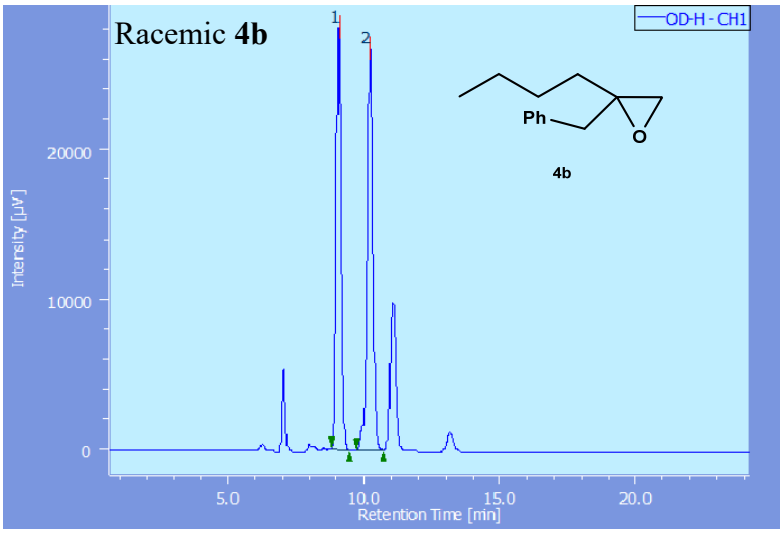


7

^{1}H NMR spectrum of **7** with Eu(hfc)$_3$ (1:6 w/w).

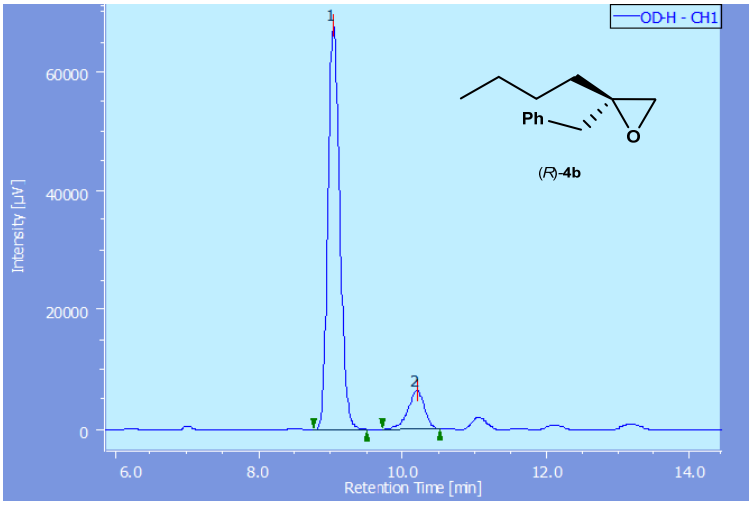
Determination of the optical purity of (R)-4b

HPLC conditions: column, DAICEL CHIRALCEL OD-H; solvent, *i*-PrOH/*n*-Hexane 2/98; flow rate, 0.5 mL/min; detection at 254 nm.



Peak No.	Rt (min)	Area	Area %
1	9.04	317698	45.255
2	10.20	384327	54.745
Total		702025	100.000

(*R*)-2-Benzyl-2-butyloxirane [(*R*)-4b]:[3d] colorless oil; 77 % ee; bp 122 °C / 8 mmHg; $[\alpha]_D^{26}$ -8.15° (C 0.92, $CHCl_3$), Lit.[3d] $[\alpha]_D^{25}$ -6.0° (C 0.29, $CHCl_3$).

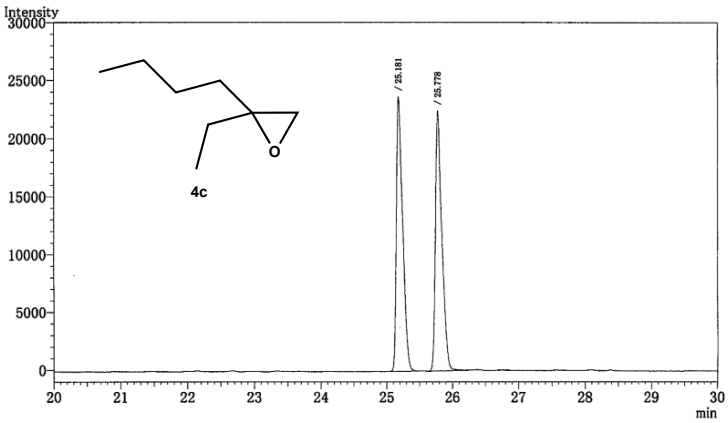


Peak No.	Rt (min)	Area	Area %
1	9.03	763692	88.330
2	10.20	100894	11.670
Total		864586	100.000

Determination of the optical purity of (R)-4c

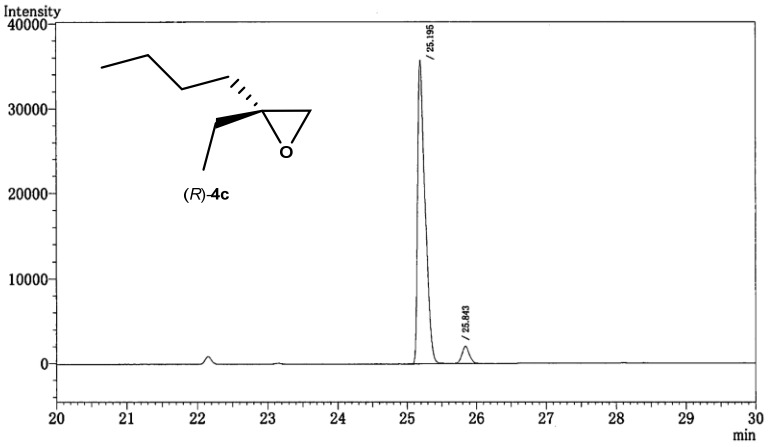
GC conditions: column, CP-Chirasil-DEX CB (0.25 mm × 25 m); carrier gas, N_2; flow rate, 15 cm/s; injection temperature, 150 °C; column temperature, 30 °C, 4 min, 2 °C/min, 100 °C, 10 min; detector temperature, 250 °C. Retention time: 25.2 min (*R*), 25.8 min (*S*).

Racemic **4c**



Peak No.	Rt (min)	Area	Area %
1	25.18	157991	50.656
2	25.77	153898	49.344
Total		311889	100.000

(R)-2-Ethyl-2-butyloxirane [**(R)-4c]**: colorless oil; 89 % ee; bp 71 °C / 38 mmHg; $[\alpha]_D^{24}$ = +0.11° (*c* 1.07, $CHCl_3$).

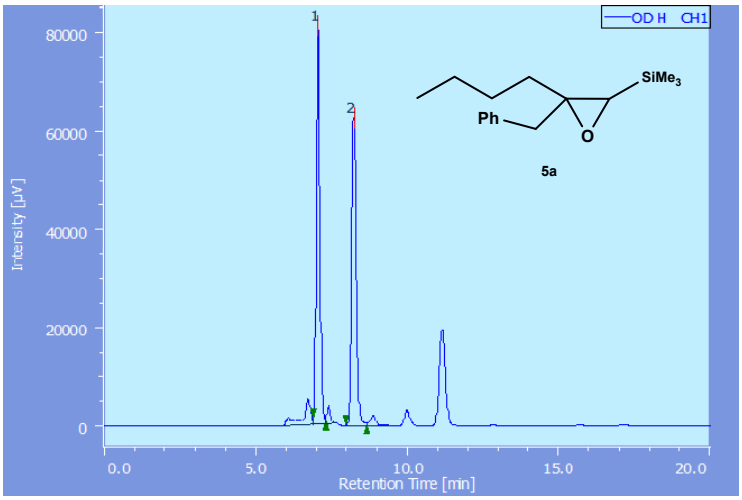


Peak No.	Rt (min)	Area	Area %
1	25.19	269461	94.696
2	25.84	15094	5.304
Total		284555	100.000

Determination of the optical purity of (2R,3R)-5a

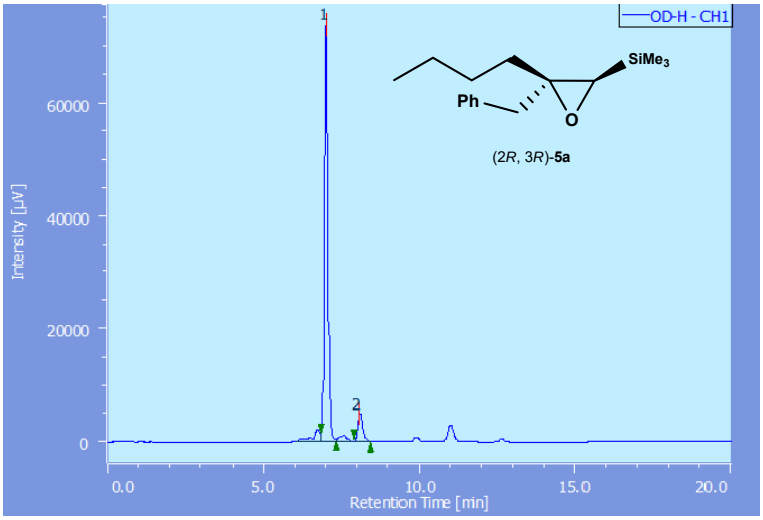
HPLC conditions: column, DAICEL CHIRALCEL OD-H; solvent, *i*-PrOH/*n*-Hexane 2/98; flow rate, 0.5 mL/min; detection at 254 nm.

Racemic **5a**



Peak No.	Rt (min)	Area	Area %
1	7.04	638624	50.385
2	8.22	628867	49.615
Total		1267491	100.000

((2*R*,3*R*)-3-Benzyl-3-butyloxiran-2-yl)trimethylsilane [(2*R*,3*R*)-5a]:[3d] colorless oil; 84 % ee; bp 121 °C / 3 mmHg; $[\alpha]_D^{25}$ +17.2° (C 1.00, $CHCl_3$).

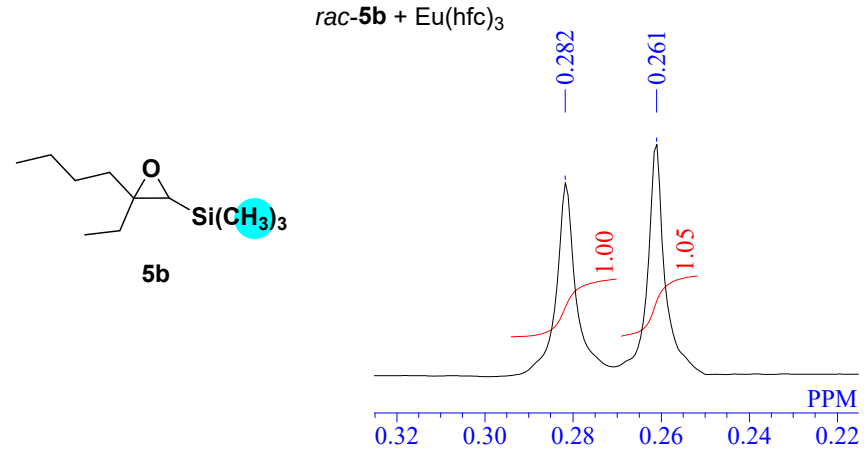


Peak No.	Rt (min)	Area	Area %
1	7.00	579803	91.865
2	8.08	51343	8.135
Total		631146	100.000

Determination of the optical purity of (2R,3R)-5b

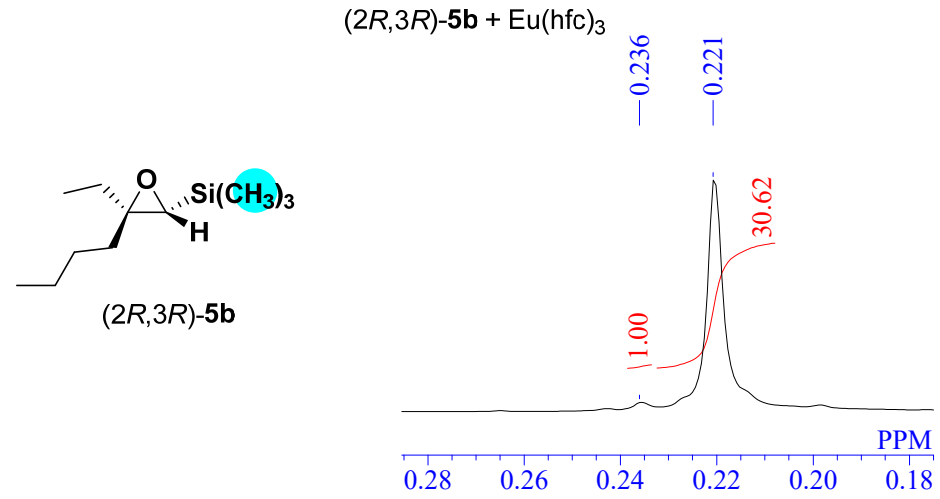
The optical purity of (2*R*, 3*R*)-**5b** was determined by ^{1}H NMR analysis with Eu(hfc)$_3$ in CDCl$_3$.[3d]

Racemic



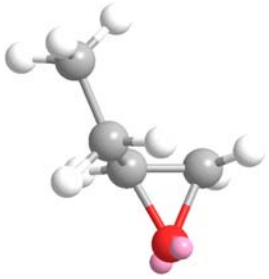
^{1}H NMR spectrum of *rac*-**5b** with Eu(hfc)$_3$ (1:5 w/w).

94% ee



^{1}H NMR spectrum of (2*R*,3*R*)-**5b** with Eu(hfc)$_3$ (1:5 w/w).

4. Cartesian Coordinates (Å) and Energies of the Optimized Structures



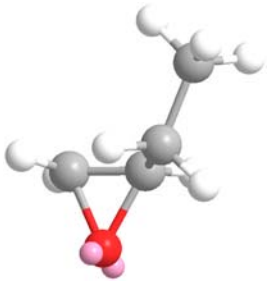
(*S*)-**2a**

MM2 Calculation

Total energy: 88.9770 kcal/mol

Cartesian coordinates for (*S*)-**2a**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-5.687	0.651	1.727
C(2)	-6.385	-0.717	1.62
C(3)	-6.946	0.339	0.897
C(4)	-6.621	0.489	-0.583
C(5)	-7.767	0.014	-1.486
H(6)	-5.695	-1.417	1.152
H(7)	-6.783	-0.974	2.601
H(8)	-7.807	0.89	1.289
H(9)	-6.414	1.567	-0.787
H(10)	-5.697	-0.074	-0.855
H(11)	-7.512	0.144	-2.563
H(12)	-7.987	-1.065	-1.314
H(13)	-8.7	0.59	-1.286
Lp(14)	-5.866	0.908	2.24
Lp(15)	-5.216	0.644	1.354



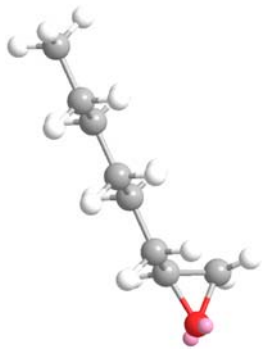
(*R*)-**2a**

MM2 Calculation

Total energy: 88.9770 kcal/mol

Cartesian coordinates for (*R*)-**2a**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-4.313	0.494	1.084
C(2)	-4.722	-0.927	0.652
C(3)	-5.241	0.137	-0.092
C(4)	-6.645	0.644	0.208
C(5)	-7.674	0.165	-0.825
H(6)	-3.83	-1.447	0.305
H(7)	-5.292	-1.379	1.462
H(8)	-4.784	0.43	-1.042
H(9)	-6.62	1.76	0.211
H(10)	-6.984	0.326	1.222
H(11)	-8.691	0.557	-0.593
H(12)	-7.733	-0.948	-0.84
H(13)	-7.404	0.507	-1.85
Lp(14)	-4.659	0.649	1.55
Lp(15)	-3.767	0.603	0.858



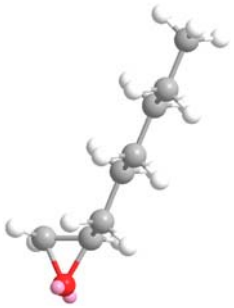
(*S*)-**2b**

MM2 Calculation

Total energy: 99.5185 kcal/mol

Cartesian coordinates for (*S*)-**2b**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-3.621	0.751	4.014	H(24)	-8.111	-1.51	-3.535
C(2)	-4.42	-0.565	3.986	H(25)	-8.689	0.197	-3.528
C(3)	-4.939	0.508	3.256	Lp(26)	-3.756	1.036	4.526
C(4)	-4.676	0.589	1.757	Lp(27)	-3.171	0.699	3.62
C(5)	-5.898	0.172	0.923				
C(6)	-5.629	0.269	-0.588				
C(7)	-6.856	-0.142	-1.417				
C(8)	-6.589	-0.046	-2.928				
C(9)	-7.816	-0.458	-3.752				
H(10)	-3.807	-1.327	3.51				
H(11)	-4.787	-0.763	4.993				
H(12)	-5.738	1.1320	3.668				
H(13)	-4.402	1.642	1.511				
H(14)	-3.808	-0.048	1.466				
H(15)	-6.177	-0.877	1.185				
H(16)	-6.765	0.823	1.188				
H(17)	-5.343	1.316	-0.845				
H(18)	-4.767	-0.388	-0.853				
H(19)	-7.143	-1.189	-1.16				
H(20)	-7.719	0.515	-1.153				
H(21)	-6.304	1.001	-3.191				
H(22)	-5.728	-0.703	-3.198				
H(23)	-7.608	-0.382	-4.844				



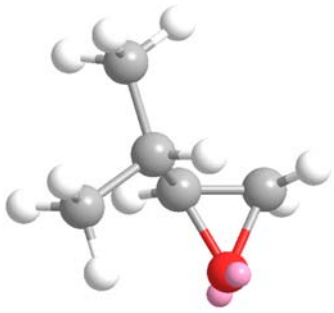
(*R*)-**2b**

MM2 Calculation

Total energy: 99.5183 kcal/mol

Cartesian coordinates for (*R*)-**2b**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	0.325	0.263	2.051	H(24)	-7.752	-1.087	-1.851
C(2)	-0.036	-1.146	1.546	H(25)	-7.393	0.419	-2.775
C(3)	-0.531	-0.063	0.814	Lp(26)	-0.049	0.396	2.502
C(4)	-1.959	0.411	1.052	Lp(27)	0.88	0.389	1.86
C(5)	-2.925	-0.051	-0.051				
C(6)	-4.36	0.443	0.192				
C(7)	-5.322	-0.014	-0.917				
C(8)	-6.757	0.479	-0.673				
C(9)	-7.713	0.025	-1.784				
H(10)	0.882	-1.64	1.23				
H(11)	-0.641	-1.637	2.306				
H(12)	-0.028	0.271	-0.099				
H(13)	-1.95	1.526	1.094				
H(14)	-2.342	0.053	2.037				
H(15)	-2.918	-1.166	-0.099				
H(16)	-2.565	0.326	-1.038				
H(17)	-4.362	1.558	0.246				
H(18)	-4.722	0.06	1.176				
H(19)	-5.319	-1.129	-0.972				
H(20)	-4.962	0.37	-1.901				
H(21)	-6.764	1.594	-0.616				
H(22)	-7.123	0.092	0.308				
H(23)	-8.749	0.389	-1.593				



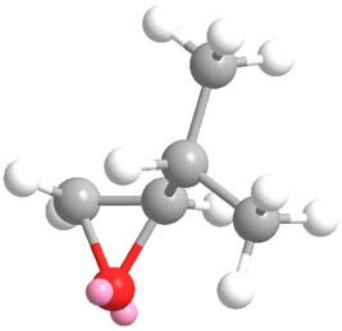
(*S*)-**2c**

MM2 Calculation

Total energy: 89.8921 kcal/mol

Cartesian coordinates for (*S*)-**2c**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-5.616	0.127	1.941
C(2)	-6.468	-1.152	1.83
C(3)	-6.897	-0.037	1.103
C(4)	-6.559	0.065	-0.383
C(5)	-7.725	-0.46	-1.241
C(6)	-6.214	1.508	-0.792
H(7)	-5.861	-1.927	1.367
H(8)	-6.9	-1.359	2.808
H(9)	-7.697	0.603	1.488
H(10)	-5.668	-0.573	-0.615
H(11)	-7.476	-0.431	-2.326
H(12)	-7.969	-1.5150	-0.98
H(13)	-8.644	0.15	-1.085
H(14)	-5.946	1.57	-1.871
H(15)	-5.346	1.894	-0.21
H(16)	-7.074	2.192	-0.614
Lp(17)	-5.768	0.405	2.451
Lp(18)	-5.147	0.066	1.571



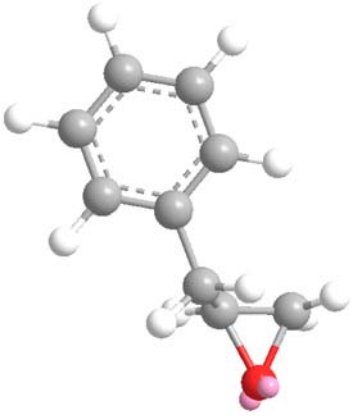
(*R*)-**2c**

MM2 Calculation

Total energy: 89.8921 kcal/mol

Cartesian coordinates for (*R*)-**2c**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-4.319	-0.076	1.078
C(2)	-4.744	-1.447	0.518
C(3)	-5.231	-0.313	-0.138
C(4)	-6.643	0.184	0.169
C(5)	-7.647	-0.368	-0.857
C(6)	-6.712	1.721	0.198
H(7)	-3.855	-1.951	0.141
H(8)	-5.335	-1.957	1.277
H(9)	-4.755	0.045	-1.056
H(10)	-6.964	-0.186	1.176
H(11)	-8.688	-0.049	-0.621
H(12)	-7.633	-1.482	-0.87
H(13)	-7.406	-0.014	-1.885
H(14)	-7.739	2.076	0.445
H(15)	-6.02	2.142	0.963
H(16)	-6.431	2.155	-0.789
Lp(17)	-4.67	0.045	1.55
Lp(18)	-3.768	0.043	0.871



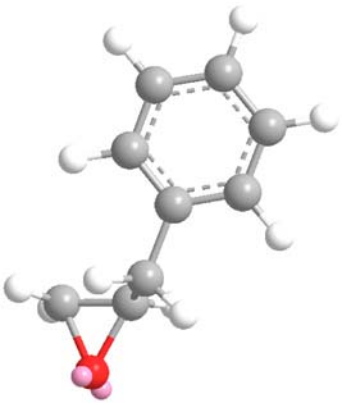
(*S*)-**2d**

MM2 Calculation

Total energy: 87.7008 kcal/mol

Cartesian coordinates for (*S*)-**2d**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-2.434	0.452	0.881
C(2)	-1.942	1.075	-0.439
C(3)	-3.317	0.859	-0.313
C(4)	-4.218	2.011	0.106
C(5)	-4.937	2.552	-1.111
C(6)	-4.323	3.42	-1.935
C(7)	-4.95	3.904	-3.019
C(8)	-6.206	3.523	-3.293
C(9)	-6.829	2.656	-2.48
C(10)	-6.196	2.176	-1.399
H(11)	-1.501	2.045	-0.214
H(12)	-1.323	0.3410	-0.953
H(13)	-3.788	-0.024	-0.758
H(14)	-3.651	2.836	0.596
H(15)	-4.945	1.642	0.867
H(16)	-3.289	3.74	-1.723
H(17)	-4.432	4.615	-3.684
H(18)	-6.724	3.918	-4.183
H(19)	-7.861	2.337	-2.703
H(20)	-6.721	1.461	-0.743
Lp(21)	-2.349	-0.142	0.847
Lp(22)	-2.471	0.89	1.289



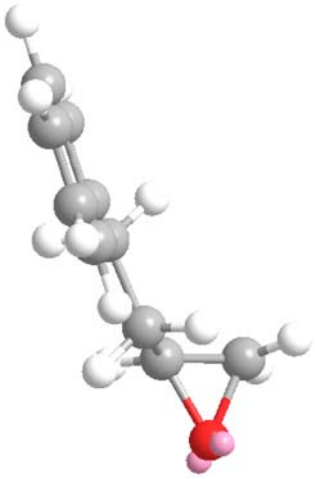
(*R*)-**2d**

MM2 Calculation

Total energy: 87.7008 kcal/mol

Cartesian coordinates for (*R*)-**2d**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-2.111	2.168	-0.213
C(2)	-2	0.668	0.113
C(3)	-3.171	1.095	-0.521
C(4)	-4.413	1.37	0.314
C(5)	-5.375	0.21	0.175
C(6)	-5.211	-0.904	0.912
C(7)	-6.057	-1.939	0.795
C(8)	-7.083	-1.874	-0.066
C(9)	-7.257	-0.77	-0.808
C(10)	-6.407	0.262	-0.686
H(11)	-1.186	0.25	-0.478
H(12)	-1.954	0.556	1.195
H(13)	-3.295	0.98	-1.602
H(14)	-4.88	2.319	-0.037
H(15)	-4.174	1.523	1.391
H(16)	-4.37	-0.973	1.621
H(17)	-5.908	-2.845	1.407
H(18)	-7.78	-2.723	-0.164
H(19)	-8.098	-0.711	-1.519
H(20)	-6.562	1.161	-1.307
Lp(21)	-2.284	2.453	0.286
Lp(22)	-1.806	2.27	-0.72



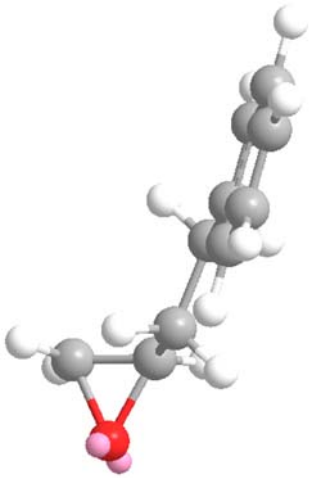
(*S*)-**2e**

MM2 Calculation

Total energy: 89.7772 kcal/mol

Cartesian coordinates for (*S*)-**2e**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-0.494	1.291	-0.763	H(21)	-7.824	-3.05	0.735
C(2)	-1.208	2.252	0.205	H(22)	-8.526	-0.706	0.676
C(3)	-1.98	1.691	-0.817	H(23)	-6.912	1.036	0.171
C(4)	-2.84	0.467	-0.522	Lp(24)	-0.202	1.624	-1.169
C(5)	-4.327	0.824	-0.366	Lp(25)	-0.459	0.755	-0.496
C(6)	-5.288	-0.309	-0.056				
C(7)	-4.922	-1.604	-0.02				
C(8)	-5.812	-2.57	0.259				
C(9)	-7.092	-2.258	0.507				
C(10)	-7.475	-0.973	0.474				
C(11)	-6.578	-0.015	0.195				
H(12)	-1.186	1.8130	1.201				
H(13)	-0.78	3.245	0.077				
H(14)	-2.191	2.255	-1.731				
H(15)	-2.707	-0.242	-1.374				
H(16)	-2.489	-0.044	0.406				
H(17)	-4.412	1.58	0.453				
H(18)	-4.675	1.314	-1.307				
H(19)	-3.883	-1.906	-0.218				
H(20)	-5.491	-3.625	0.284				



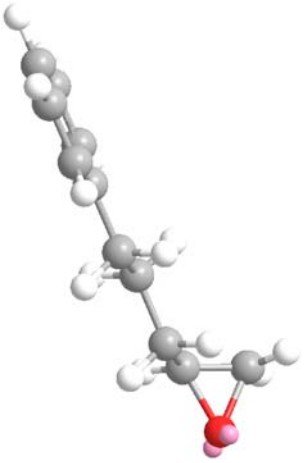
(*R*)-**2e**

MM2 Calculation

Total energy: 89.7764 kcal/mol

Cartesian coordinates for (*R*)-**2e**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-0.495	1.489	0.016	H(21)	-7.807	-3.057	0.825
C(2)	-1.229	1.879	-1.281	H(22)	-8.517	-0.975	-0.249
C(3)	-1.983	1.868	-0.103	H(23)	-6.913	0.806	-0.635
C(4)	-2.838	0.651	0.229	Lp(24)	-0.46	0.89	0.033
C(5)	-4.33	0.893	-0.053	Lp(25)	-0.199	1.974	0.211
C(6)	-5.286	-0.255	0.216				
C(7)	-4.915	-1.407	0.806				
C(8)	-5.799	-2.394	1.021				
C(9)	-7.079	-2.247	0.648				
C(10)	-7.467	-1.106	0.06				
C(11)	-6.575	-0.125	-0.151				
H(12)	-0.805	2.814	-1.645				
H(13)	-1.217	1.021	-1.951				
H(14)	-2.184	2.798	0.439				
H(15)	-2.498	-0.238	-0.353				
H(16)	-2.688	0.429	1.313				
H(17)	-4.671	1.765	0.556				
H(18)	-4.431	1.18	-1.128				
H(19)	-3.876	-1.57	1.13				
H(20)	-5.475	-3.33	1.507				



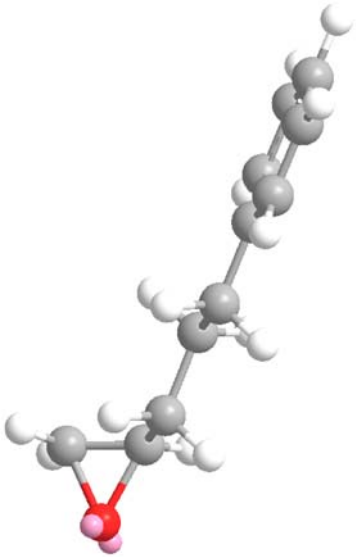
(*S*)-**2f**

MM2 Calculation

Total energy: 90.2722 kcal/mol

Cartesian coordinates for (*S*)-**2f**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	0.359	2.491	-0.298	H(21)	-4.551	1.212	-0.787
C(2)	0.262	1.217	-1.157	H(22)	-3.876	-2.051	0.428
C(3)	-0.451	1.227	0.045	H(23)	-5.528	-3.791	0.621
C(4)	-1.937	1.565	0.03	H(24)	-7.912	-3.249	0.595
C(5)	-2.826	0.317	0.168	H(25)	-8.621	-0.916	0.372
C(6)	-4.321	0.672	0.163	H(26)	-6.963	0.847	0.178
C(7)	-5.308	-0.474	0.289	Lp(27)	0.874	2.466	0.011
C(8)	-4.939	-1.763	0.413	Lp(28)	-0.022	2.895	-0.527
C(9)	-5.852	-2.741	0.521				
C(10)	-7.161	-2.447	0.507				
C(11)	-7.547	-1.169	0.385				
C(12)	-6.626	-0.1990	0.277				
H(13)	-0.217	1.476	-2.099				
H(14)	1.249	0.757	-1.197				
H(15)	-0.046	0.744	0.94				
H(16)	-2.14	2.262	0.878				
H(17)	-2.216	2.105	-0.905				
H(18)	-2.598	-0.372	-0.681				
H(19)	-2.564	-0.202	1.121				
H(20)	-4.517	1.38	1.005				



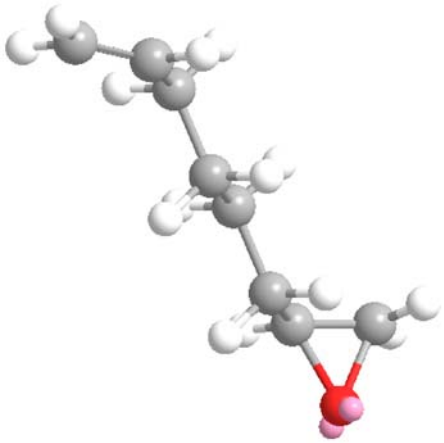
(*R*)-**2f**

MM2 Calculation

Total energy: 90.2717 kcal/mol

Cartesian coordinates for (*R*)-**2f**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	0.37	2.313	-0.971	H(19)	-2.58	-0.003	0.764
C(2)	0.29	1.591	0.386	H(20)	-4.535	1.456	0.144
C(3)	-0.448	1.044	-0.668	H(21)	-4.528	0.766	-1.518
C(4)	-1.933	1.364	-0.787	H(22)	-3.876	-1.984	0.627
C(5)	-2.824	0.206	-0.306	H(23)	-5.529	-3.602	1.292
C(6)	-4.319	0.533	-0.446	H(24)	-7.913	-3.114	1.054
C(7)	-5.307	-0.533	-0.007	H(25)	-8.62	-0.959	0.132
C(8)	-4.938	-1.723	0.503	H(26)	-6.962	0.681	-0.542
C(9)	-5.853	-2.633	0.876	Lp(27)	-0.006	2.782	-0.951
C(10)	-7.161	-2.368	0.747	Lp(28)	0.879	2.141	-1.241
C(11)	-7.547	-1.187	0.242				
C(12)	-6.625	-0.285	-0.129				
H(13)	1.277	1.193	0.62				
H(14)	-0.171	2.265	1.106				
H(15)	-0.061	0.194	-1.239				
H(16)	-2.193	2.282	-0.21				
H(17)	-2.153	1.583	-1.859				
H(18)	-2.58	-0.704	-0.905				



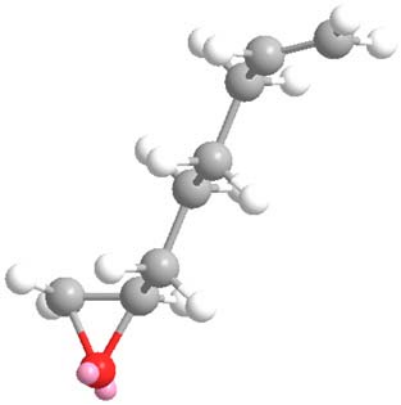
(*S*)-**2g**

MM2 Calculation

Total energy: 90.8813 kcal/mol

Cartesian coordinates for (*S*)-**2g**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-3.792	0.934	3.675	H(21)	-5.796	-0.967	-3.572
C(2)	-4.389	-0.486	3.683	H(22)	-7.242	0.301	-5.08
C(3)	-5.07	0.485	2.943	H(23)	-8.357	0.783	-3.642
C(4)	-4.845	0.574	1.439	Lp(24)	-3.96	1.205	4.184
C(5)	-5.998	-0.047	0.634	Lp(25)	-3.345	0.941	3.275
C(6)	-5.769	0.061	-0.883				
C(7)	-6.924	-0.561	-1.683				
C(8)	-6.681	-0.446	-3.167				
C(9)	-7.467	0.247	-4.003				
H(10)	-3.677	-1.159	3.209				
H(11)	-4.708	-0.716	4.699				
H(12)	-5.947	0.9910	3.359				
H(13)	-4.741	1.651	1.169				
H(14)	-3.892	0.073	1.146				
H(15)	-6.105	-1.121	0.918				
H(16)	-6.953	0.465	0.902				
H(17)	-5.663	1.136	-1.166				
H(18)	-4.814	-0.451	-1.149				
H(19)	-7.029	-1.642	-1.427				
H(20)	-7.881	-0.061	-1.405				



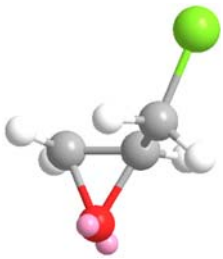
(*R*)-**2g**

MM2 Calculation

Total energy: 90.8812 kcal/mol

Cartesian coordinates for (*R*)-**2g**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	0.338	0.465	1.776	H(21)	-7.239	-0.106	0.225
C(2)	0.002	-1.011	1.492	H(22)	-8.496	1.153	-1.45
C(3)	-0.537	-0.058	0.622	H(23)	-7.042	1.061	-2.643
C(4)	-1.97	0.415	0.827	Lp(24)	-0.028	0.655	2.212
C(5)	-2.949	-0.226	-0.17	Lp(25)	0.886	0.574	1.554
C(6)	-4.391	0.268	0.033				
C(7)	-5.364	-0.377	-0.965				
C(8)	-6.772	0.119	-0.749				
C(9)	-7.47	0.812	-1.661				
H(10)	0.924	-1.526	1.227				
H(11)	-0.574	-1.397	2.331				
H(12)	-0.063	0.15	-0.342				
H(13)	-1.989	1.525	0.703				
H(14)	-2.321	0.2	1.864				
H(15)	-2.917	-1.336	-0.05				
H(16)	-2.621	0.006	-1.211				
H(17)	-4.422	1.378	-0.088				
H(18)	-4.717	0.036	1.075				
H(19)	-5.361	-1.486	-0.842				
H(20)	-5.03	-0.159	-2.005				



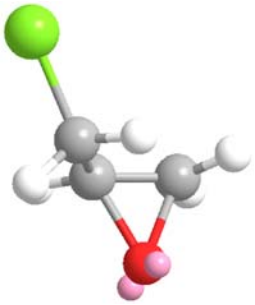
(*S*)-**2h**

MM2 Calculation

Total energy: 88.7122 kcal/mol

Cartesian coordinates for (*S*)-**2h**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-5.194	0.527	0.704
C(2)	-5.625	-0.903	0.335
C(3)	-6.185	0.14	-0.41
C(4)	-7.563	0.672	-0.038
Cl(5)	-8.78	0.025	-1.177
H(6)	-4.752	-1.433	-0.045
H(7)	-6.15	-1.33	1.188
H(8)	-5.778	0.406	-1.391
H(9)	-7.563	1.779	-0.101
H(10)	-7.865	0.387	0.991
Lp(11)	-5.533	0.722	1.16
Lp(12)	-4.675	0.6530	0.428



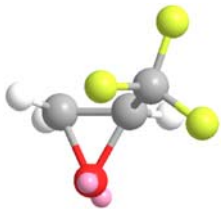
(*R*)-**2h**

MM2 Calculation

Total energy: 88.7122 kcal/mol

Cartesian coordinates for (*R*)-**2h**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-6.315	0.664	1.267
C(2)	-6.936	-0.738	1.13
C(3)	-7.513	0.287	0.374
C(4)	-7.106	0.465	-1.083
Cl(5)	-8.381	-0.201	-2.145
H(6)	-6.187	-1.401	0.7
H(7)	-7.368	-1.014	2.091
H(8)	-8.42	0.793	0.722
H(9)	-6.982	1.545	-1.304
H(10)	-6.152	-0.046	-1.323
Lp(11)	-6.548	0.935	1.75
Lp(12)	-5.846	0.706	0.895



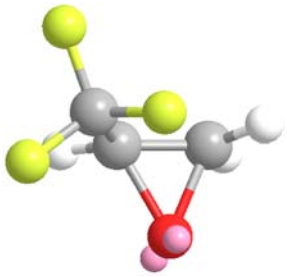
(*S*)-**2i**

MM2 Calculation

Total energy: 92.7490 kcal/mol

Cartesian coordinates for (*S*)-**2i**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-5.416	0.476	0.666
C(2)	-5.857	-0.946	0.271
C(3)	-6.424	0.115	-0.443
C(4)	-7.808	0.644	-0.062
F(5)	-8.707	0.126	-0.886
F(6)	-7.872	1.961	-0.194
F(7)	-8.197	0.344	1.168
H(8)	-4.99	-1.467	-0.132
H(9)	-6.364	-1.39	1.125
H(10)	-6.031	0.396	-1.426
Lp(11)	-5.78	0.695	1.087
Lp(12)	-4.924	0.6320	0.357



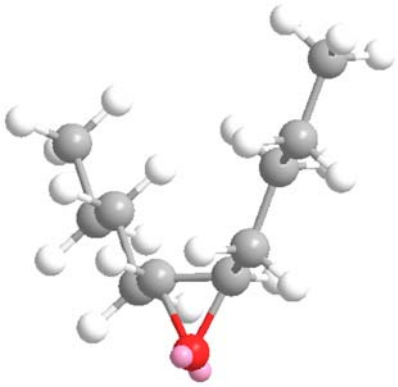
(*R*)-**2i**

MM2 Calculation

Total energy: 92.7490 kcal/mol

Cartesian coordinates for (*R*)-**2i**

Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-6.501	0.623	1.277
C(2)	-7.151	-0.765	1.134
C(3)	-7.691	0.27	0.363
C(4)	-7.273	0.434	-1.099
F(5)	-8.205	-0.102	-1.874
F(6)	-6.127	-0.148	-1.419
F(7)	-7.181	1.714	-1.432
H(8)	-6.406	-1.447	0.729
H(9)	-7.606	-1.023	2.09
H(10)	-8.595	0.793	0.691
Lp(11)	-6.759	0.927	1.726
Lp(12)	-6.061	0.687	0.876



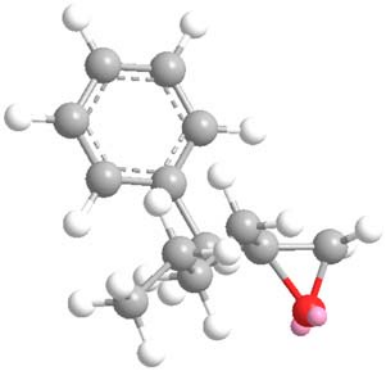
(2*R*,3*R*)-**4a**

MM2 Calculation

Total energy: 93.1546 kcal/mol

Cartesian coordinates for (2*R*,3*R*)-**4a**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-1.981	1.979	1.223	H(21)	-2.687	-2.192	1.34
C(2)	-2.606	0.574	1.128	H(22)	-0.295	-2.933	0.973
C(3)	-2.995	1.511	0.162	H(23)	-0.426	-2.489	-0.765
C(4)	-1.523	-0.438	0.78	H(24)	-0.789	-4.959	-0.441
C(5)	-4.306	2.263	0.35	H(25)	-2.291	-4.186	-1.059
C(6)	-5.431	1.703	-0.534	H(26)	-2.157	-4.633	0.682
C(7)	-2.103	-1.825	0.462	H(27)	-6.595	3.546	-0.591
C(8)	-1.007	-2.847	0.118	H(28)	-7.07	2.41	0.72
C(9)	-1.594	-4.23	-0.192	H(29)	-8.817	2.469	-1.092
C(10)	-6.751	2.468	-0.348	H(30)	-8.067	0.836	-1.005
C(11)	-7.867	1.906	-1.239	H(31)	-7.594	1.977	-2.317
H(12)	-3.225	0.37	2.007	Lp(32)	-2.283	2.285	1.643
H(13)	-2.543	1.526	-0.833	Lp(33)	-1.435	1.954	0.976
H(14)	-0.828	-0.514	1.649				
H(15)	-0.916	-0.094	-0.09				
H(16)	-4.13	3.335	0.095				
H(17)	-4.638	2.234	1.415				
H(18)	-5.588	0.626	-0.286				
H(19)	-5.121	1.756	-1.605				
H(20)	-2.811	-1.737	-0.396				



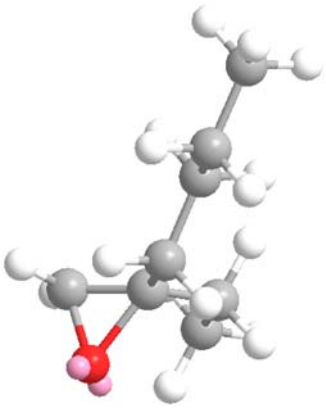
(*R*)-**4b**

MM2 Calculation

Total energy: 44.9667 kcal/mol

Cartesian coordinates for (*R*)-**4b**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
C(1)	3.914	1.066	0.432	H(21)	2.977	1.712	-2.092
O(2)	5.004	1.886	0.871	C(22)	3.542	0.659	-4.541
C(3)	4.518	0.908	1.799	H(23)	2.44	-0.509	-3.089
C(4)	2.538	1.656	0.276	H(24)	4.216	-0.893	-3.19
C(5)	3.651	0.161	-0.741	H(25)	3.342	-0.046	-5.378
C(6)	3.734	0.897	-2.072	H(26)	4.557	1.097	-4.67
H(7)	2.643	-0.299	-0.635	H(27)	2.791	1.479	-4.57
C(8)	3.459	-0.077	-3.21	H(28)	2.984	-0.851	1.219
C(9)	1.513	0.656	0.714	H(29)	1.276	-2.517	1.949
C(10)	1.914	-0.597	1.176	H(30)	-1.149	-1.941	1.852
C(11)	0.96	-1.528	1.584	H(31)	-1.867	0.301	1.025
C(12)	-0.396	-1.206	1.53	H(32)	-0.16	1.967	0.295
C(13)	-0.798	0.047	1.068	Lp(33)	5.546	1.814	0.624
C(14)	0.157	0.978	0.66	Lp(34)	5.089	2.479	0.903
H(15)	5.116	0.032	2.034				
H(16)	4.146	0.921	2.82				
H(17)	2.366	1.918	-0.792				
H(18)	2.453	2.572	0.902				
H(19)	4.385	-0.675	-0.734				
H(20)	4.753	1.328	-2.193				



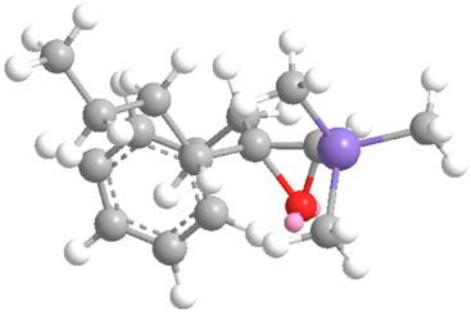
(*R*)-**4c**

MM2 Calculation

Total energy: 48.1453 kcal/mol

Cartesian coordinates for (*R*)-**4c**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
O(1)	-5.878	2.857	0.196	H(21)	-4.032	-2.04	-0.614
C(2)	-6.401	1.348	0.303	H(22)	-4.613	-1.494	-2.226
C(3)	-6.966	2.359	-0.545	H(23)	-4.752	-3.999	-2.028
C(4)	-5.396	0.363	-0.288	H(24)	-6.4	-3.296	-2.195
C(5)	-6.992	1.041	1.674	H(25)	-5.813	-3.848	-0.583
C(6)	-8.009	2.02	2.279	Lp(26)	-6.086	3.144	0.681
C(7)	-5.967	-1.034	-0.576	Lp(27)	-5.385	2.842	-0.147
C(8)	-4.937	-1.949	-1.26				
C(9)	-5.508	-3.348	-1.531				
H(10)	-7.88	2.875	-0.26				
H(11)	-6.728	2.356	-1.608				
H(12)	-4.537	0.282	0.418				
H(13)	-4.981	0.769	-1.241				
H(14)	-7.478	0.038	1.622				
H(15)	-6.134	0.953	2.383				
H(16)	-8.309	1.694	3.302				
H(17)	-7.588	3.046	2.373				
H(18)	-8.94	2.072	1.671				
H(19)	-6.867	-0.934	-1.229				
H(20)	-6.294	-1.513	0.376				



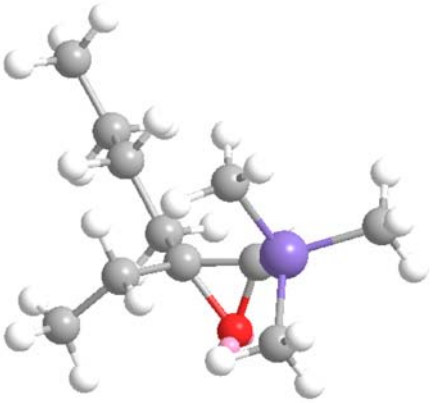
(2*R*,3*R*)-**5a**

MM2 Calculation

Total energy: 45.3313 kcal/mol

Cartesian coordinates for (2*R*,3*R*)-**5a**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
C(1)	0.165	1.372	-1.765	H(24)	0.471	1.644	-2.779
C(2)	1.01	0.579	-0.908	H(25)	-3.476	-0.339	-1.675
O(3)	0.799	2.164	-0.792	H(26)	-2.248	-0.779	-0.414
Si(4)	-1.7	1.358	-1.554	H(27)	-1.865	-1.022	-2.191
C(5)	-2.389	-0.386	-1.443	H(28)	-3.512	2.176	-3.031
C(6)	-2.403	2.151	-3.12	H(29)	-1.995	3.182	-3.205
C(7)	-2.254	2.401	-0.089	H(30)	-2.096	1.535	-3.994
C(8)	0.558	-0.117	0.372	H(31)	-1.828	3.422	-0.204
C(9)	2.381	0.201	-1.466	H(32)	-3.365	2.446	-0.102
H(10)	2.312	-0.846	-1.843	H(33)	-1.904	1.94	0.859
C(11)	-0.09	-2.279	1.558	H(34)	-0.429	0.258	0.712
H(12)	1.521	-2.064	0.125	C(35)	0.498	-1.651	0.285
H(13)	-0.111	-1.954	-0.598	H(36)	2.654	0.817	-2.353
H(14)	1.268	0.17	1.183	H(37)	-0.763	-4.145	0.613
H(15)	0.524	-1.978	2.441	C(38)	-0.135	-3.81	1.47
C(16)	3.489	0.329	-0.44	H(39)	-1.124	-1.893	1.724
C(17)	3.873	1.54	0.005	H(40)	3.385	2.449	-0.382
H(18)	-0.565	-4.252	2.398	H(41)	5.148	2.668	1.269
H(19)	0.886	-4.234	1.335	H(42)	6.268	0.677	2.146
C(20)	4.849	1.667	0.916	H(43)	5.606	-1.537	1.344
C(21)	5.465	0.577	1.397	H(44)	3.845	-1.762	-0.305
C(22)	5.1	-0.636	0.957	Lp(45)	1.274	2.425	-1.049
C(23)	4.123	-0.754	0.044	Lp(46)	0.413	2.255	-0.343



(2*R*,3*R*)-**5b**

MM2 Calculation

Total energy: 46.6033 kcal/mol

Cartesian coordinates for (2*R*,3*R*)-**5b**

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
C(1)	1.242	0.609	-0.117	H(21)	1.081	-1.856	1.187
C(2)	0.168	-0.349	-0.122	C(22)	-2.297	0.367	0.038
O(3)	1.47	-0.412	-1.055	H(23)	-1.361	-0.739	-1.597
Si(4)	2.452	0.615	1.315	H(24)	-0.361	-3.751	0.676
C(5)	3.321	2.293	1.262	H(25)	0.235	-3.071	-0.88
C(6)	3.766	-0.718	1.137	H(26)	-1.453	-2.752	-0.331
C(7)	0.093	-1.602	0.746	H(27)	0.663	1.153	2.928
C(8)	-1.096	0.067	-0.874	H(28)	2.255	0.827	3.76
C(9)	-0.399	-2.858	0.011	H(29)	1.255	-0.563	3.154
C(10)	1.555	0.49	2.964	C(30)	-4.717	1.142	0.159
H(11)	-0.9	0.972	-1.494	H(31)	-3.806	0.088	-1.511
H(12)	-2.001	1.142	0.785	H(32)	-3.255	1.789	-1.313
H(13)	1.156	1.588	-0.598	C(33)	-3.518	0.858	-0.756
H(14)	3.842	2.387	0.283	H(34)	-2.583	-0.551	0.603
H(15)	2.554	3.09	1.376	H(35)	-5.594	1.498	-0.429
H(16)	4.053	2.334	2.098	H(36)	-4.471	1.926	0.911
H(17)	4.252	-0.599	0.143	H(37)	-5.029	0.224	0.709
H(18)	3.303	-1.724	1.222	Lp(38)	1.306	-0.211	-1.597
H(19)	4.513	-0.575	1.949	Lp(39)	1.842	-0.811	-0.808
H(20)	-0.592	-1.393	1.601				

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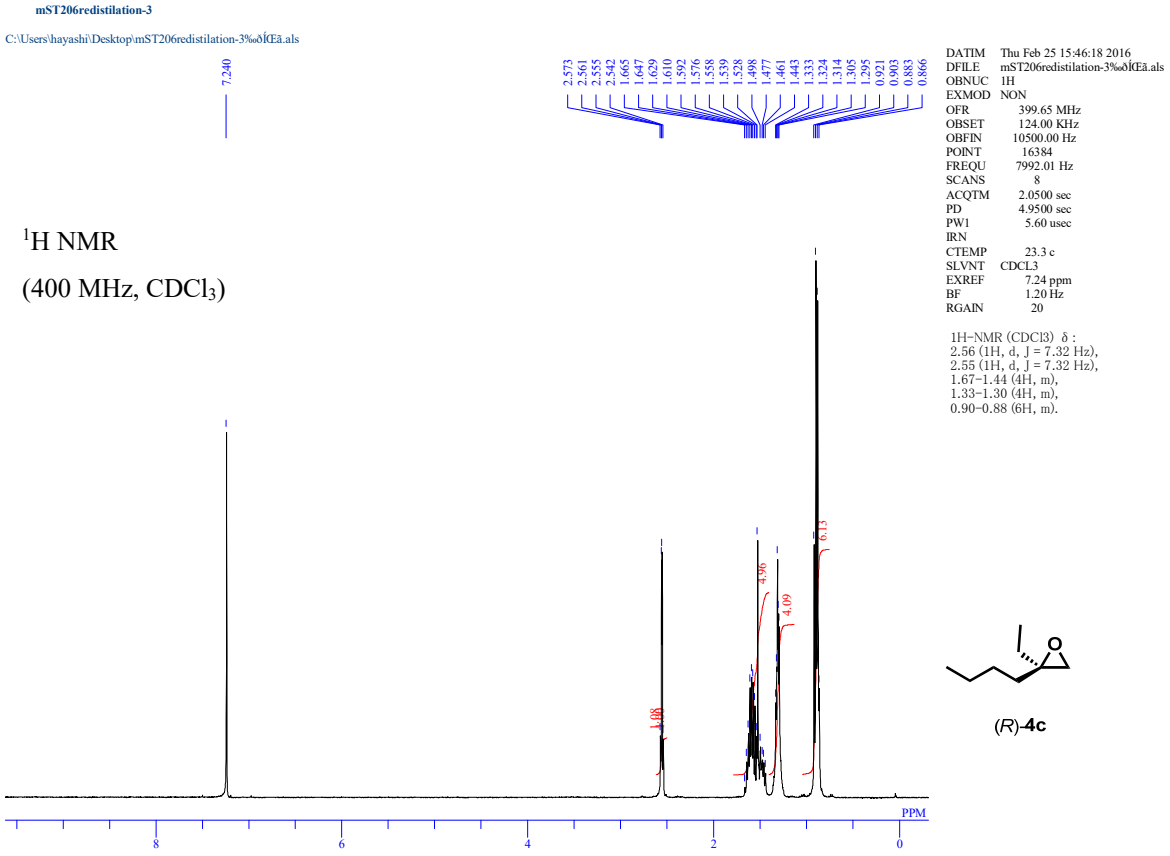
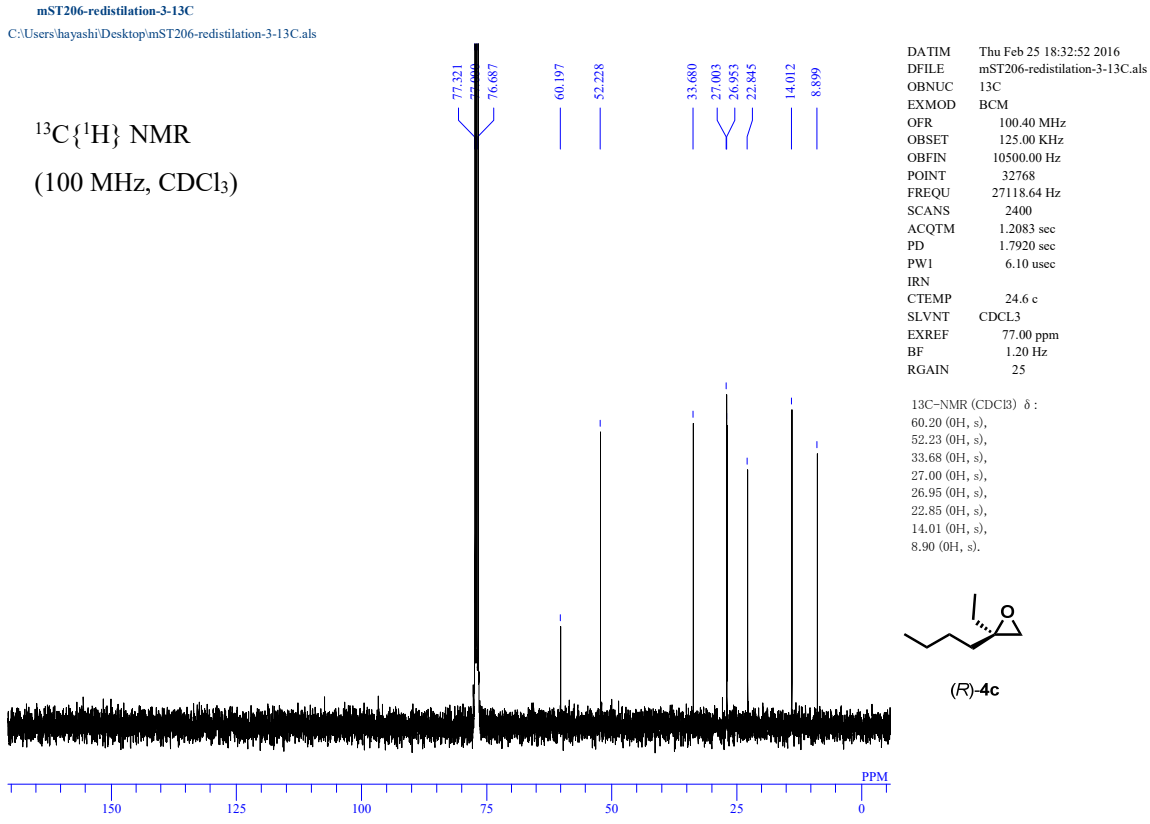


^{1}H NMR

(400 MHz, $CDCl_3$)

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



^{13}C{^{1}H} NMR

(100 MHz, $CDCl_3$)

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