Electronic Supplementary Information

Enantioselective Assembly and Recognition of Heterochiral Porous Organic Cages Deduced from Binary Chiral Components

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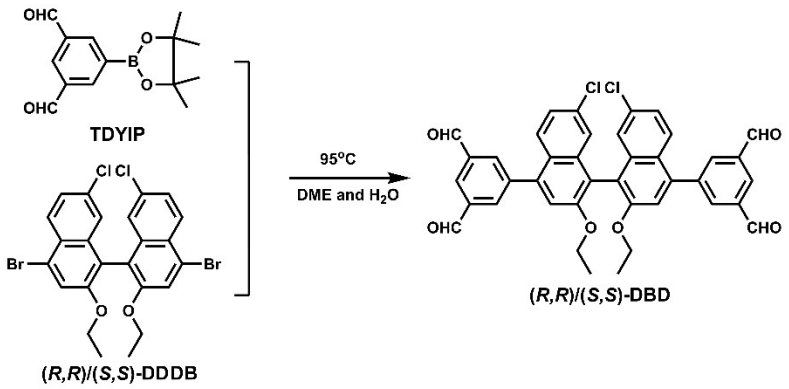
Experimental Procedures

General Remark. 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)isophthalaldehyde (TDYIP) and (*S,S*)/(*R,R*)-4,4'-dibromo-7,7'-dichloro-2,2'-diethoxy-1,1'-binaphthalene (DDDB) was prepared according to the published procedure.[1,2] Unless otherwise noted, all other reagents and solvents were of analytical grade and used as supplied without further purification.



Scheme S1. Schematic synthesis of 5,5'-(7,7'-dichloro-2,2'-diethoxy-[1,1'-binaphthalene]-4,4'-diyl)diisophthalaldehyde (DBD).

Synthesis of 5,5'-(7,7'-dichloro-2,2'-diethoxy-[1,1'-binaphthalene]-4,4'-diyl)diisophthalaldehyde (DBD). A mixture of (*S,S*)/(*R,R*)-DDDB (569.0 mg, 1.0 mmol), TDYIP (570.0 mg, 2.1 mmol), potassium carbonate (1000 mg, 7.2 mmol), tetrakis(triphenylphosphine)palladium (150.0 mg, 0.13 mmol), 1,2-dimethoxyethane (20.0 mL), and deionized water (2.0 mL) in a 25.0 mL flask was stirred at 95 ℃ for 12.0 hours. After cooling, the solvent was evaporated under reduced pressure and the residue was chromatographed on a silica gel column using

dichloromethane/tetrahydrofuran (100:1, v:v) as eluent in the yield of 30.5% and 34.5% for (*S,S*)-DBD and(*R,R*)-DBD, respectively. For (*S,S*)-DBD, ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.27 (s, 4H), 8.54 (s, 2H), 8.40 (s, 4H), 7.65 (s, 2H), 7.41 (s, 2H), 7.21 (d, J = 9.0 Hz, 4H), 4.17 – 4.08 (m, 4H), 1.15 (t, J = 6.8 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 190.83 (s), 153.87 (s), 142.37 (s), 138.14 (s), 137.44 (s), 135.84 (s), 132.79 (s), 130.37 (d, J = 24.7 Hz), 128.00 – 127.34 (m), 124.05 (s), 120.39 (s), 117.64 (s), 77.08 (dd, J = 42.2, 21.7 Hz), 76.71 (s), 76.71 (s), 65.31 (s), 15.00 (s). For (*R*,*R*)-DBD, ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.27 (s, 4H), 8.54 (s, 2H), 8.39 (s, 4H), 7.65 (s, 2H), 7.41 (s, 2H), 7.26 – 7.16 (m, 4H), 4.19 – 4.08 (m, 4H), 1.15 (t, J = 6.8 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 190.85 (s), 153.86 (s), 142.38 (s), 138.13 (s), 137.43 (s), 135.85 (s), 132.79 (s), 130.49 (s), 130.27 (s), 127.63 (d, J = 10.8 Hz), 124.05 (s), 120.37 (s), 117.62 (s), 77.34 (s), 77.03 (s), 76.71 (s), 65.30 (s), 15.00 (s).

Synthesis of HPOC-1. To a stirred dichloromethane (200.0 mL) solution of DBD (67.6 mg, 0.10 mmol) and trifluoroacetic acid (1.0 μL), cyclohexanediamine (25.1 mg, 0.22 mmol) in dichloromethane (50.0 mL) was directly added. The mixture was stirred for 36.0 hours at room temperature. Then the reaction mixture was filtered to remove very small amount insoluble matter, evaporated under reduced pressure, and recrystallized in a dichloromethane/methanol system, giving the target cages as white powder in the yield of 85.4% for (*S,R*)-HPOC-1 and 88.1% for (*R,S*)-HPOC-1. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.35 (d, J = 16.8 Hz, 12H), 8.15 (d, J = 15.5 Hz, 12H), 7.83 (d, J = 1.6 Hz, 6H), 7.40 (s, 6H), 7.13 – 7.08 (m, 6H), 7.03 (d, J = 9.1 Hz, 6H), 6.79 (s, 6H), 3.57 – 3.45 (m, 12H), 3.26 (s, 6H), 2.98 (s, 6H), 1.90 (d, J = 11.9 Hz, 24H), 1.74 (s, 12H), 0.27 (t, J = 6.5 Hz, 18H); ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 159.33, 159.20, 152.59, 140.80, 139.37, 138.26, 136.64, 133.74, 132.92, 129.75, 128.47, 127.30,

127.23, 127.16, 126.64, 124.05, 118.84, 116.87, 74.17, 62.44, 33.35, 32.73, 24.54, 24.45, 13.52. MS (MALDI-TOF) *m/z*: $[M]^+$ calcd for $C_{156}H_{144}Cl_6N_{12}O_6$, 2495.6; found: 2495.0 for (*S*,*R*)-HPOC-1 and 2495.6 for (*R,S*)-HPOC-1; Elemental analysis of (*S*,*R*)-HPOC-1 (calcd., found for $C_{156}H_{144}Cl_6N_{12}O_6{\cdot}0.5CH_2Cl_2{\cdot}3CH_3OH$): C (72.81, 72.81), H (5.90, 6.24), N (6.39, 6.30); Elemental analysis of (*R,S*)-HPOC-1 (calcd., found for $C_{156}H_{144}Cl_6N_{12}O_6{\cdot}0.75CH_2Cl_2$): C (73.56, 73.56), H (5.73, 5.99), N (6.57, 6.79).

Fluorescent Responses of (*S*,*S*)-DBD toward (*R*,*R*)/(*S*,*S*)-CA and (*R*,*R*)/(*S*,*S*)-DPA. In order to monitor the fluorescent responses of DBD toward CA and DPA, time-dependent fluorescent spectroscopic measurements were carried out in CH_2Cl_2. In a typical experiment, (*S,S*)-DBD (25.0 mg, 37.0 μmol) with trifluoroacetate (2.5 μL) were dissolved in CH_2Cl_2 (50.0 mL) in a reaction vial with stirring. The (*R*,*R*)/(*S*,*S*)-CA (8.9 mg, 78.0 μmol) or (*R*,*R*)/(*S*,*S*)-DPA (17.0 mg, 78.0 μmol) was added after recording the initial fluorescence spectrum. Then, the fluorescent spectra were recorded for different time by periodically taking out 3.0 mL CH_2Cl_2 solution from the mother solution and then transferring back. (λ_{ex} = 357 nm, Slit: 2.5/2.5 nm, PMT Voltage: 700V).

^{1}H NMR Responses of (*S*,*S*)-DBD toward (*R*,*R*)/(*S*,*S*)-CA and (*R*,*R*)/(*S*,*S*)-DPA. In order to monitor the ^{1}H NMR responses of DBD toward CA and DPA, time-dependent ^{1}H MNR spectroscopic measurements were carried out in $CDCl_3$. In a typical experiment, *(S,S)*-DBD (12.5 mg, 18.5 μmol) with trifluoroacetate (1.0 μL) were dissolved in $CDCl_3$ (2.0 mL) in a reaction vial with stirring. The (*R*,*R*)/(*S*,*S*)-CA (4.5 mg, 39 μmol) or (*R*,*R*)/(*S*,*S*)-DPA (8.5 mg, 39.0 μmol) was added after recording the initial ^{1}H NMR spectrum. Then, the ^{1}H NMR spectra were recorded for different time

by periodically taking out 0.4 mL $CDCl_3$ solution from the mother solution and then transferring back.

HPOC-1 Recognition Responses toward Chiral Substrates. Recognition of chiral substrates, such as (*D*/*L*)-carvone, (*R*/*S*)-1-phenylethanol, (*R*/*S*)-limonene, (*D*/*L*)-tartaric acid, and (*R*/*S*)-pinene, by the pure (*S*,*R*)/(*R*,*S*)-HPOC-1 was investigated in liquid state and monitored by CD spectra. Typically, 6.3 mg (*S*,*R*)-HPOC-1 or (*R*,*S*)-HPOC-1 were dissolved in 25.0 mL THF solvent to get a solution with a concentration of 100.0 μM, respectively. Then different equiv. (0, 20.0, 40.0, 80.0, and 120.0) of chiral substrates with the 0.1 mL above solution of (*S*,*R*)-HPOC-1 or (*R*,*S*)-HPOC-1 were added to 5 mL volumetric flask for CD spectrum detection, respectively.

Characterizations. ^{1}H NMR spectra were recorded on a Bruker DPX 400 spectrometer in $CDCl_3$ with the residual solvent resonances (δ = 7.26 ppm for $CDCl_3$) relative to $SiMe_4$ as internal reference at 298 K and 400 MHz. ^{13}C NMR spectra were recorded by means of the same equipment and referenced internally using the solvent resonance (δ = 77.16 ppm for $CDCl_3$) at 298 K and 100 MHz. Elemental analysis was performed on an Elementar Vavio El III. The electronic absorption spectra were collected using a Perkin-Elmer Lambda 750 UV-vis spectrophotometer. CD spectra were determined using a JASCO J-1500 CD spectropolarimeter. Steady-state emission spectra and fluorescence quantum yield were recorded on a F-7000 instrument and transient-state emission spectra were recorded on an Edinburgh FLS 980 instrument. A 375 nm laser (EPL) was used as exciting source to measure the excited singlet state lifetimes. CPL spectra were measured on JASCO CPL-200 spectrophotometer.

Single crystal crystallography. Crystallographical data of two organic cages were collected on a diffractometer of SuperNova, Dual, Cu at home/near, AtlasS2 with Cu *Kα* radiation (λ = 1.54184 Å) at 150.0 K. The structures were solved by the direct method (*SHELXS-2014*) and refined by full-matrix least-squares (*SHELXL-2014*) on F^2.[3] Anisotropic thermal parameters were used for the non-hydrogen atoms and isotropic parameters for the hydrogen atoms. Hydrogen atoms were added geometrically and refined using a riding model. Crystallographic and refinement parameters for organic cages are compiled (Table S1). Because there are seriously disordered solvent molecules in the cage pores, 'SQUEEZE' command was employed.[4] CCDC 2114815 and 2114817 for (*S,R*)-HPOC-1 and (*R,S*)-HPOC-1, respectively, contain 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.

Theoretical simulations for the formation of HPOC-1 and HPOC-2. All calculations are carried out by Gaussian 09. D.01 software package[5]. Isolated cage molecules were taken from the single crystal X-ray diffraction structures and then arranged with water by hand to form HPOC-1 and HPOC-2. All structures of each compound were firstly optimized on the basis of M06L-D3/6-31G(D).[6–8] The formation energy E_f of cage is calculated according to the reported literature procedures,[9] shown by Eq. I:

$$E_f = [(E_{cage}+X_{water}) - (mE_{aldehyde} + nE_{amine})] / xn$$

where $E_{cage}+X_{water}$ is the energy of the cage with water formed, $E_{aldehyde}$ is the energy of the aldehyde, and E_{amine} is the energy of the imine. The number of aldehyde

reactants is m, n is the number of amine precursors, and xn is the number of imine bonds formed, equivalent to the number of water molecule produced in the reaction.

Theoretical simulations for the bonding of (*S,R*)-HPOC-1 and *D*/*L*-carvone. Before the preparation of (*S,R*)-HPOC-1, its formation energy was calculated by density functional theory (DFT). The structures of (*S,R*)-HPOC-1 and *D*/*L*-carvone were firstly optimized on the basis of B3LYP-D3(BJ)/6-31G(D).[6–8] The high level single point energy of each structure was calculated on the level of B3LYP-D3(BJ)/6-311G(2D,2P).[6–8] The formation energy E_f of (*S,R*)-HPOC-1 is calculated according to the reported literature procedures,[9] shown by Eq. II:

$$E_f = E_{cage+D/L\text{-carvone}} - (E_{cage} + E_{D/L\text{-carvone}})$$

where $E_{cage+D/L\text{-carvone}}$ is the total energy after adsorption, E_{cage} is the energy of the cage, and $E_{D/L\text{-carvone}}$ is the energy of the *D*/*L*-carvone. All calculations are carried out by Gaussian 09. D.01 software package.[5]

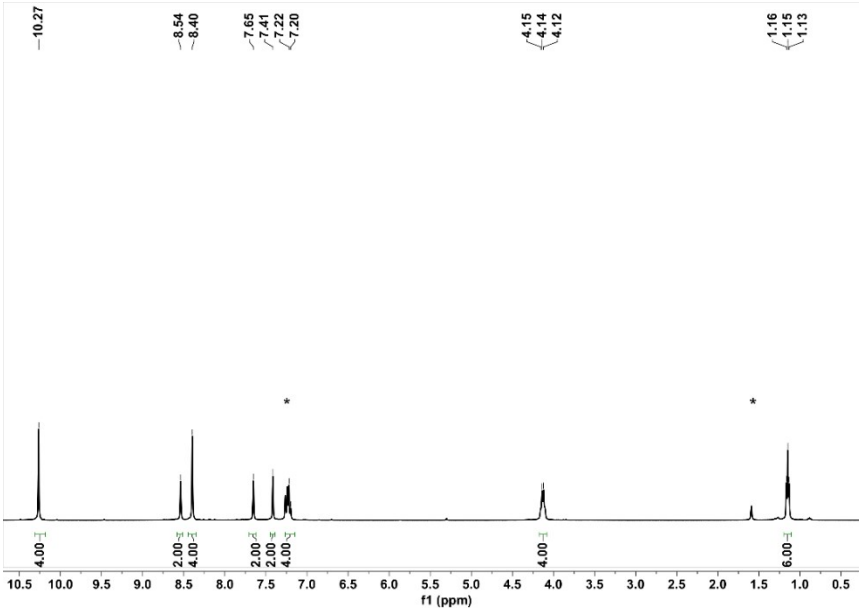


Figure S1. ^{1}H NMR spectrum of (*S*,*S*)-DBD (* denotes $CDCl_3$ solvent impurity, the protons of chloroform and (*S*,*S*)-DBD overlap).

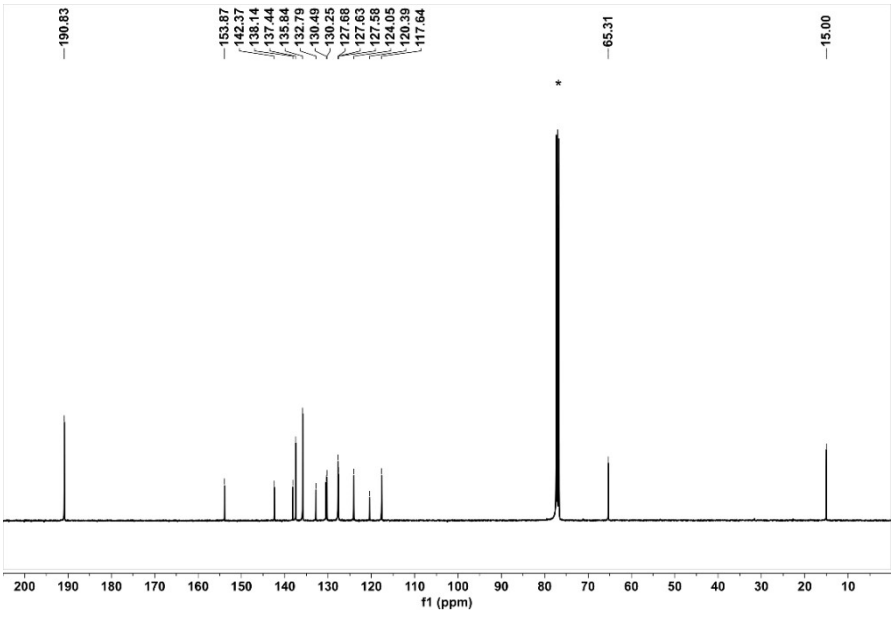


Figure S2. ^{13}C NMR spectrum of (*S*,*S*)-DBD (* denotes $CDCl_3$ solvent impurity).

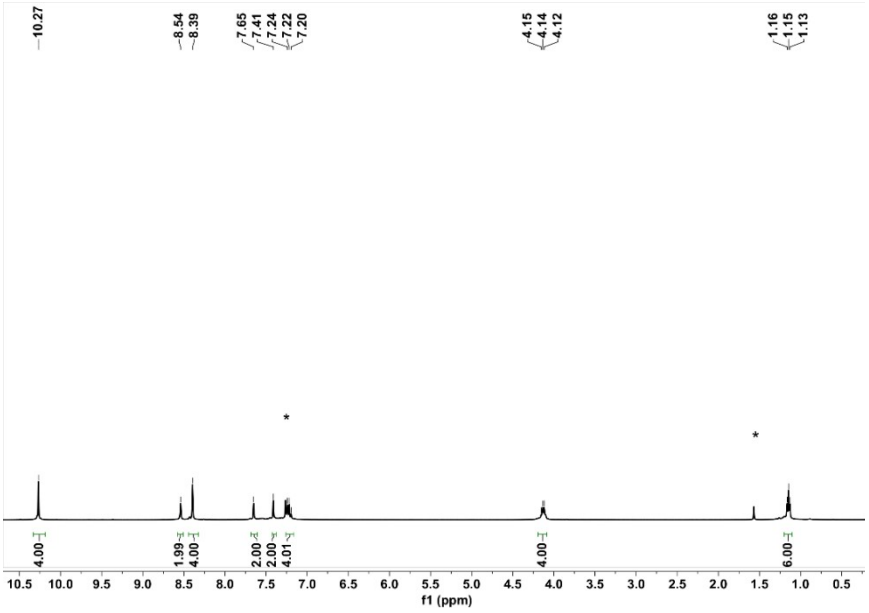


Figure S3. ^{1}H NMR spectrum of (*R,R*)-DBD (* denotes $CDCl_3$ solvent impurity, the protons of chloroform and (*R,R*)-DBD overlap).

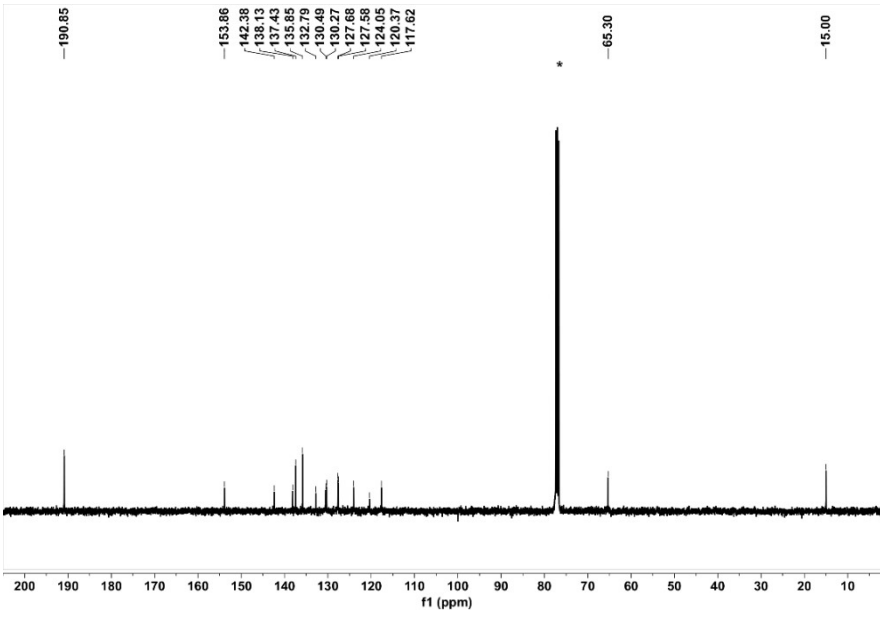


Figure S4. ^{13}C NMR spectrum of (*R,R*)-DBD (* denotes $CDCl_3$ solvent impurity).

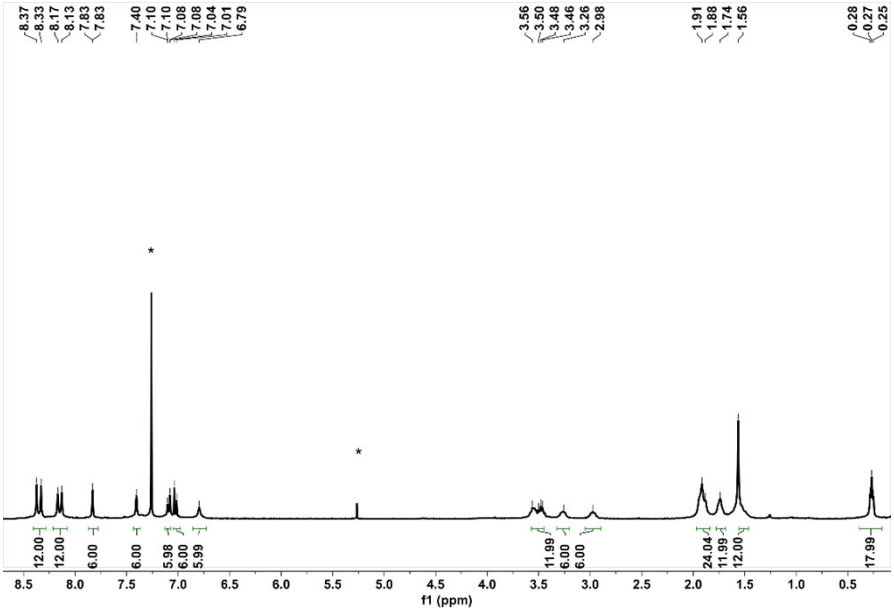


Figure S5. ^{1}H NMR spectrum of (*S,R*)-HPOC-1 (* denotes $CDCl_3$ solvent impurity).

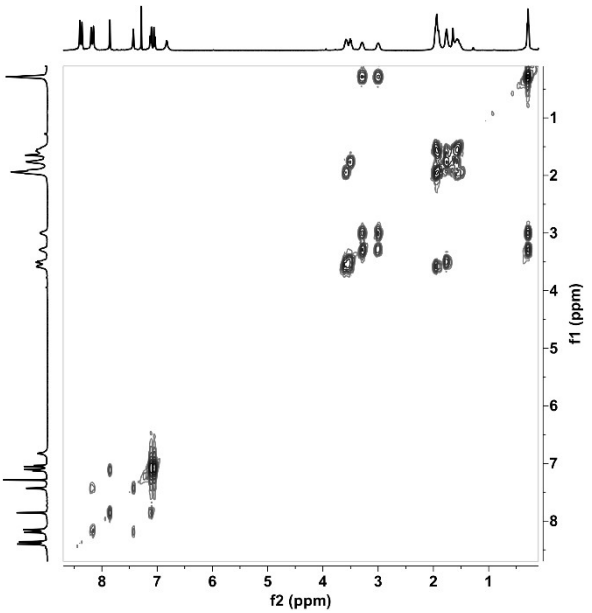


Figure S6. ^{1}H-^{1}H COSY spectrum of (*S,R*)-HPOC-1 (* denotes $CDCl_3$ solvent impurity).

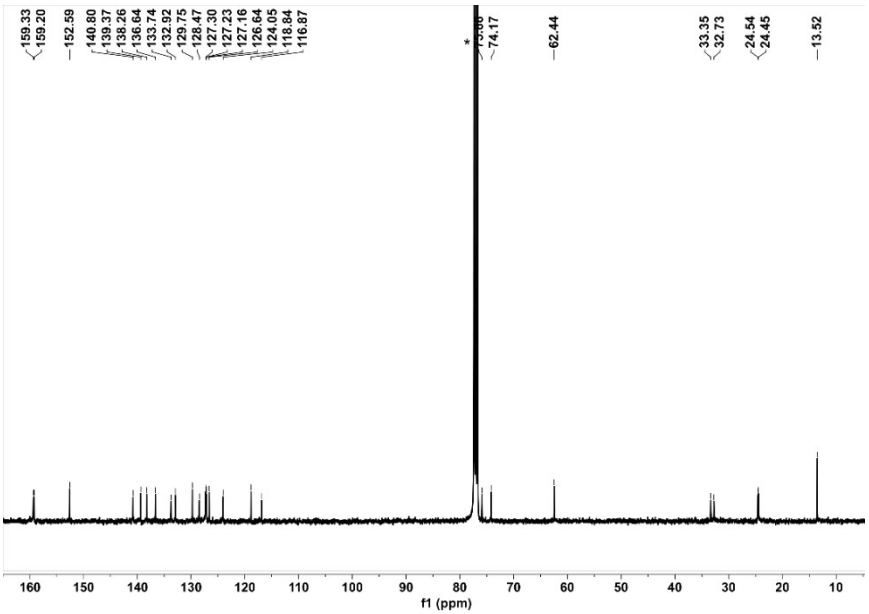


Figure S7. ^{13}C NMR spectrum of (*S,R*)-HPOC-1 (* denotes $CDCl_3$ solvent impurity).

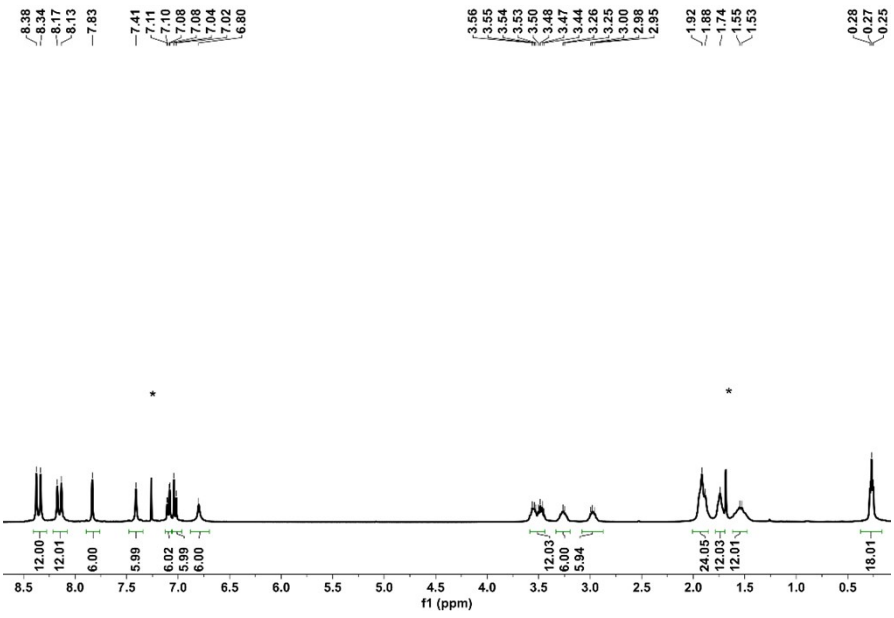


Figure S8. ^{1}H NMR spectrum of (*R,S*)-HPOC-1 (* denotes $CDCl_3$ solvent impurity).

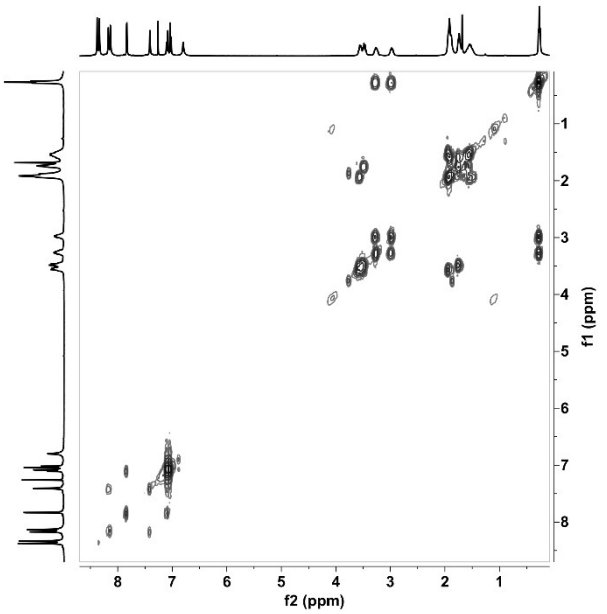


Figure S9. ^{1}H-^{1}H COSY spectrum of (*R,S*)-HPOC-1 (* denotes $CDCl_3$ solvent impurity).

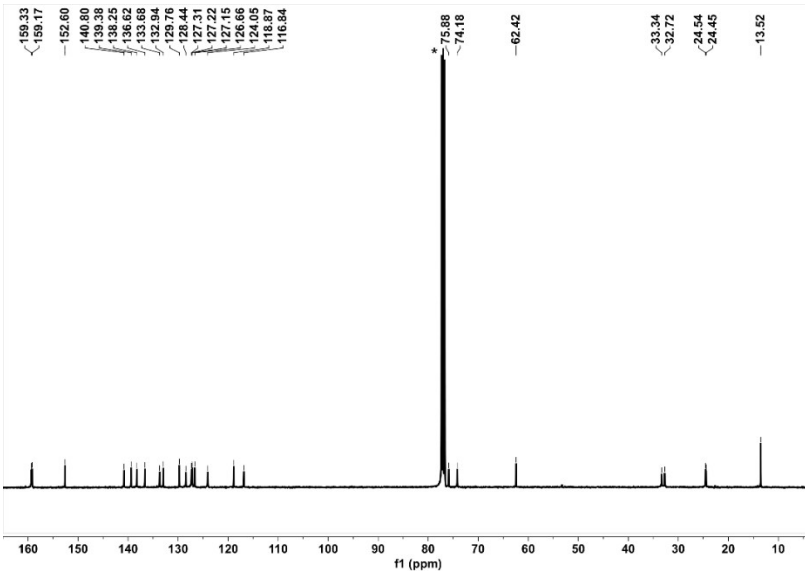


Figure S10. ^{13}C NMR spectrum of (*R,S*)-HPOC-1 (* denotes $CDCl_3$ solvent impurity).

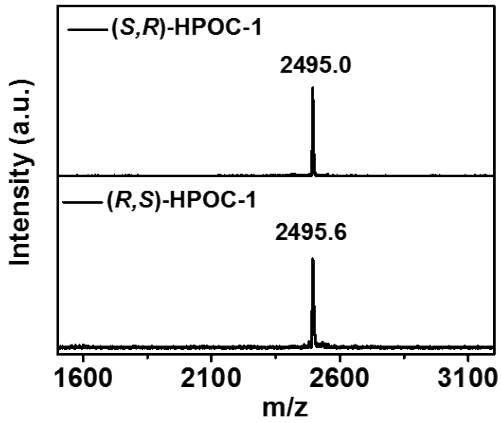


Figure S11. MALDI-TOF mass spectra of (*S,R*)/(*R,S*)-HPOC-1.

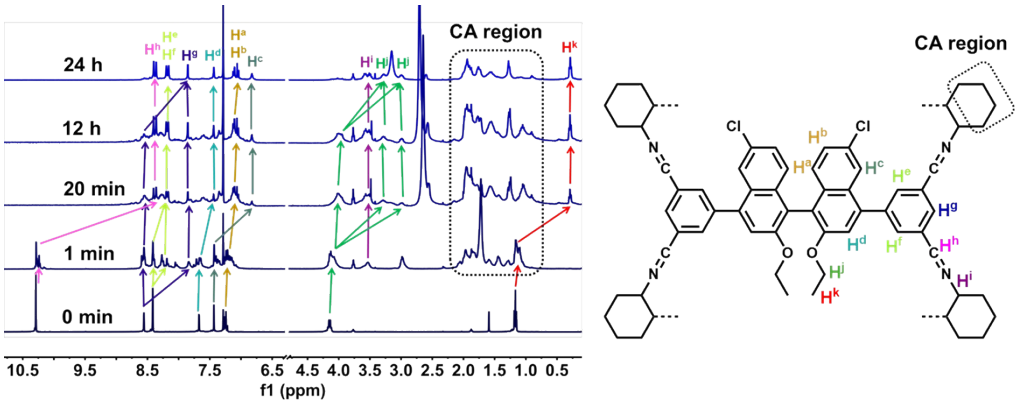


Figure S12. ^{1}H NMR spectra of the reaction mixture of (*S,S*)-DBD (9.2 mM in $CDCl_3$, 1.0 equiv.) with (*R,R*)-CA (2.0 equiv.) at various reaction times.

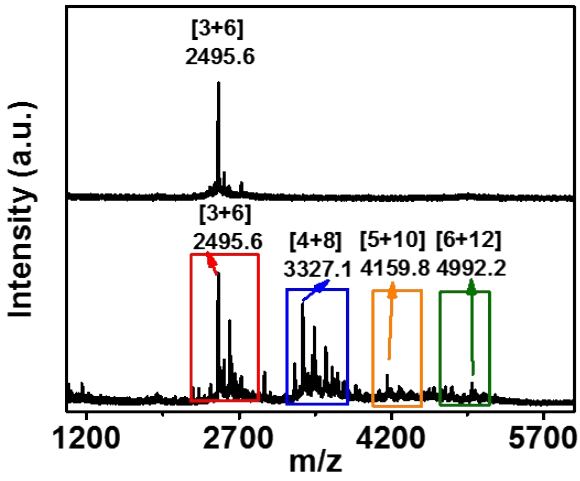


Figure S13. MALDI-TOF mass spectra of reaction mixture of (*S,S*)-DBD and (*R,R*)-CA (top) with (*S,S*)-DBD and (*S,S*)-CA (below)

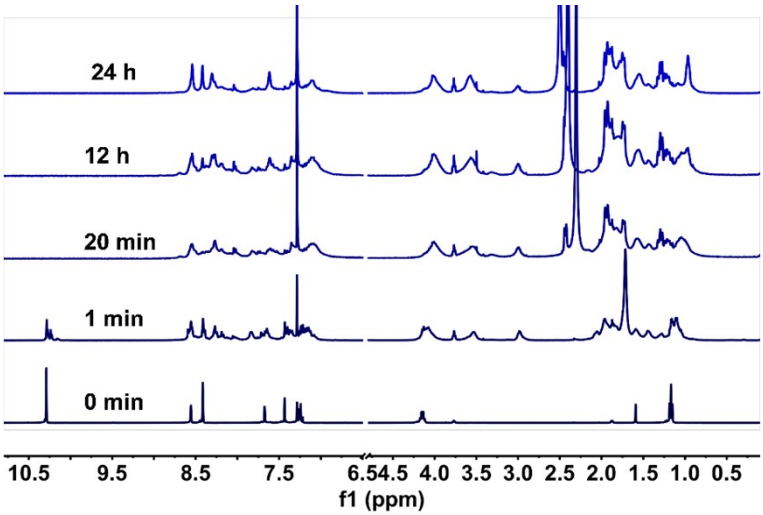


Figure S14. ^{1}H NMR spectra of the reaction mixture of (*S,S*)-DBD (9.2 mM in $CDCl_3$, 1.0 equiv.) with (*S,S*)-CA (2.0 equiv.) at various reaction times.

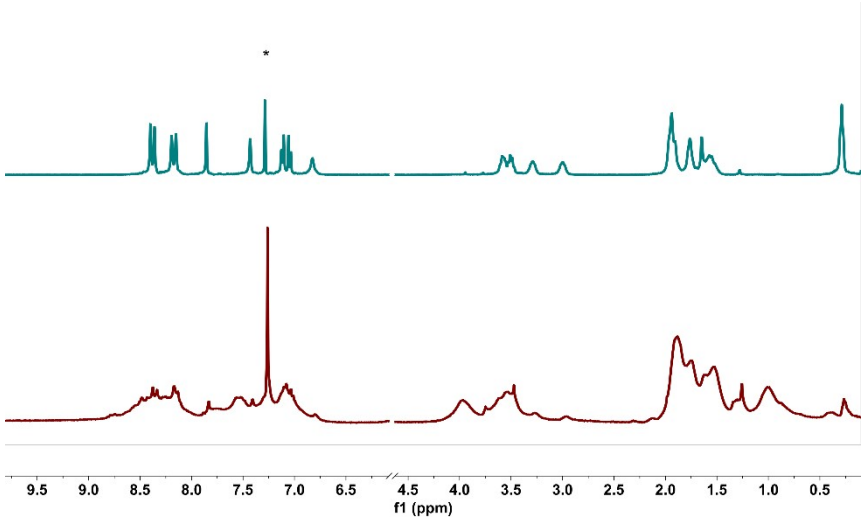


Figure S15. The ^{1}H NMR spectrum of racemic DBD and racemic CA mixed reaction (brown line) and the ^{1}H NMR spectrum of HPOC-1(cyan line).

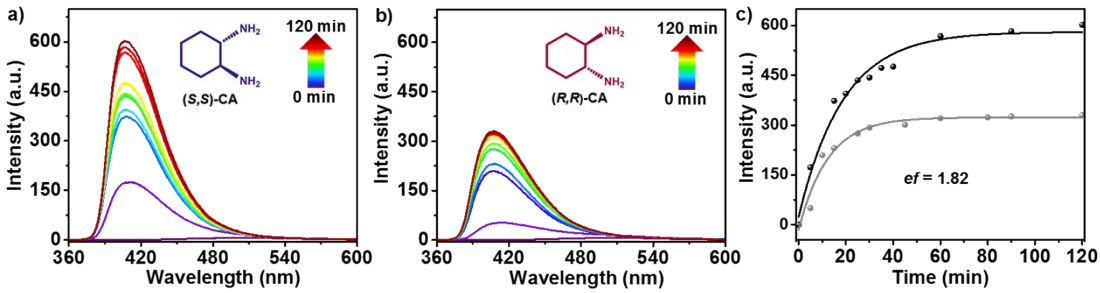


Figure S16. Fluorescent spectral changes of (*R*,*R*)-DBD upon addition of (*S*,*S*)-CA (a) or (*R*,*R*)-CA (b) (2 equiv.) in CH_2Cl_2. The spectra were collected within 120.0 min after mixing (*S*,*S*)-DBD with (*R*,*R*)-CA (a) or (*S*,*S*)-CA. (c) A plot of fluorescence intensity changes of (*R*,*R*)-DBD with (*S*,*S*)-CA (blank line) and (*R*,*R*)-CA (gray line) at 406 nm against react time from 0 to 120.0 min.

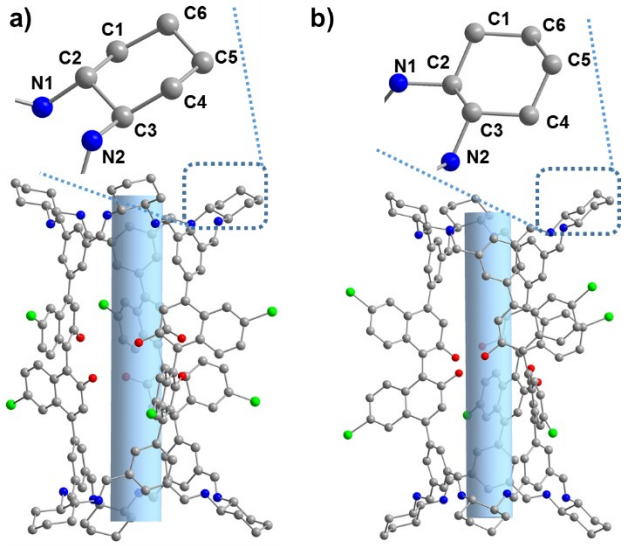


Figure 17. The two optimized structures of (*S*,*R*)-HPOC-1 (a) and (*S*,*S*)-HPOC-1 (b) (C, gray; C, gray; N, blue; O, red; Cl, green; all selected hydrogen atoms and ethoxy groups omitted for clarity).

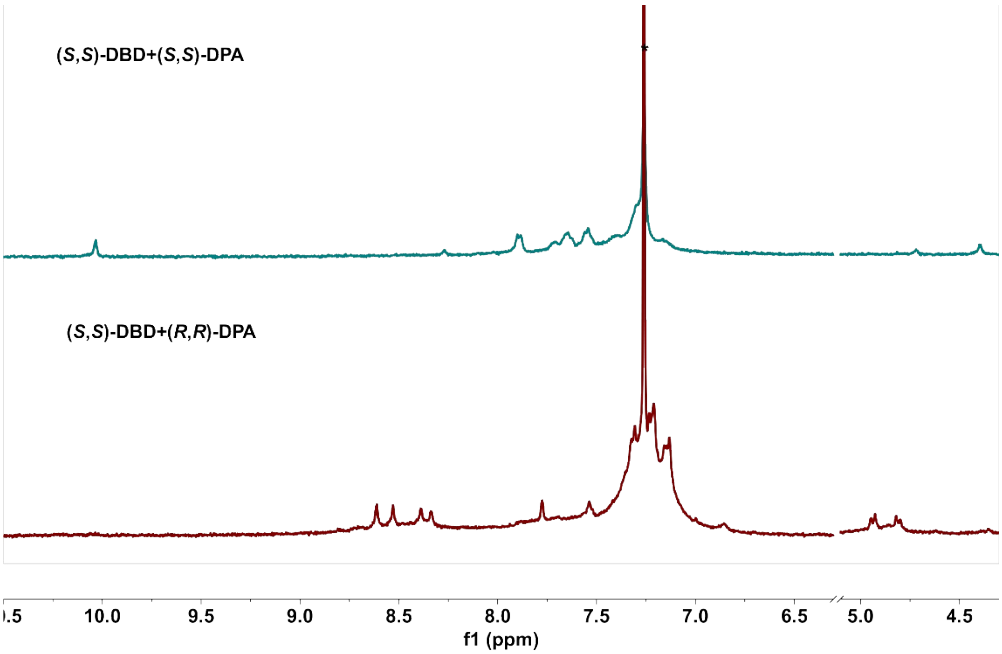


Figure S18. ^{1}H NMR spectra of the reaction mixture of (*S,S*)-DBD (9.2 mM in $CDCl_3$, 1.0 equiv.) with (*S*,*S*)-DPA and (*R*,*R*)-DPA (2.0 equiv.) after reacting for 24.0 h.

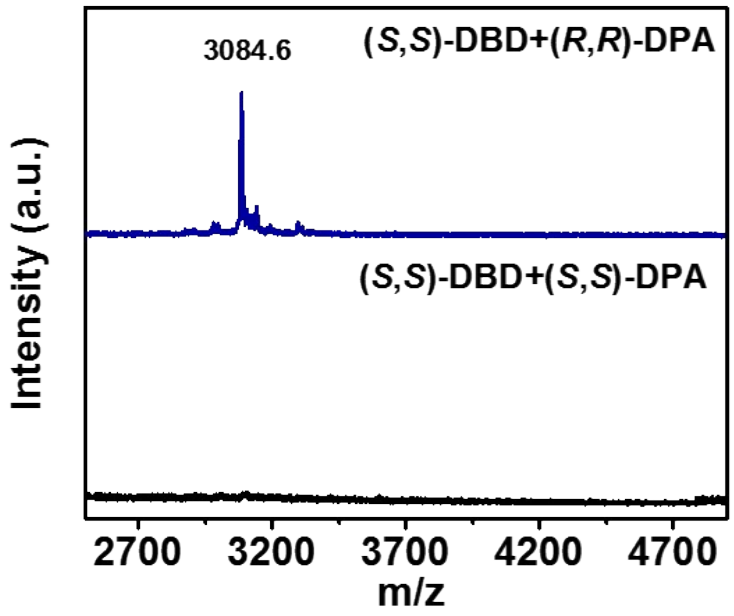


Figure S19. MALDI-TOF mass spectra of the reaction mixture of (*S,S*)-DBD with (*R,R*)-DPA (blue) or (*S,S*)-DPA (black) (2.0 equiv.) after reacting for 24.0 h.

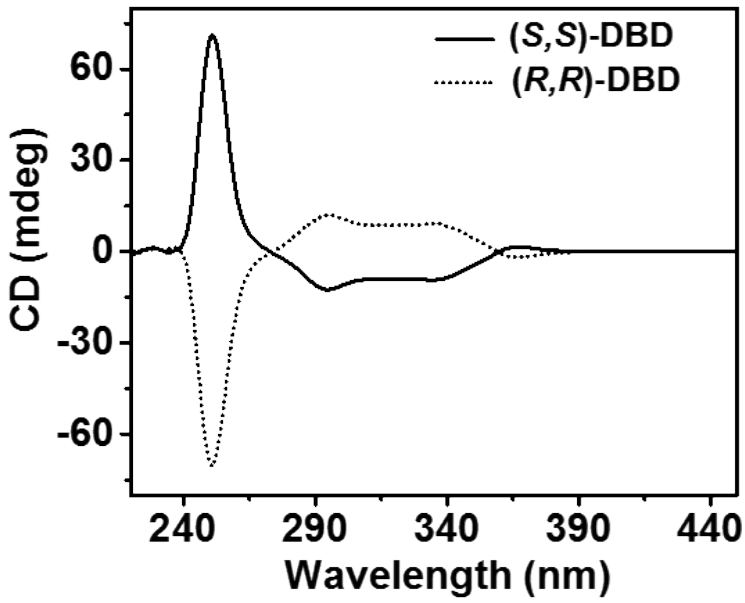


Figure S20. CD spectra of (*S,S*)-DBD and (*R,R*)-DBD with the concentration of 30.0 μM in THF.

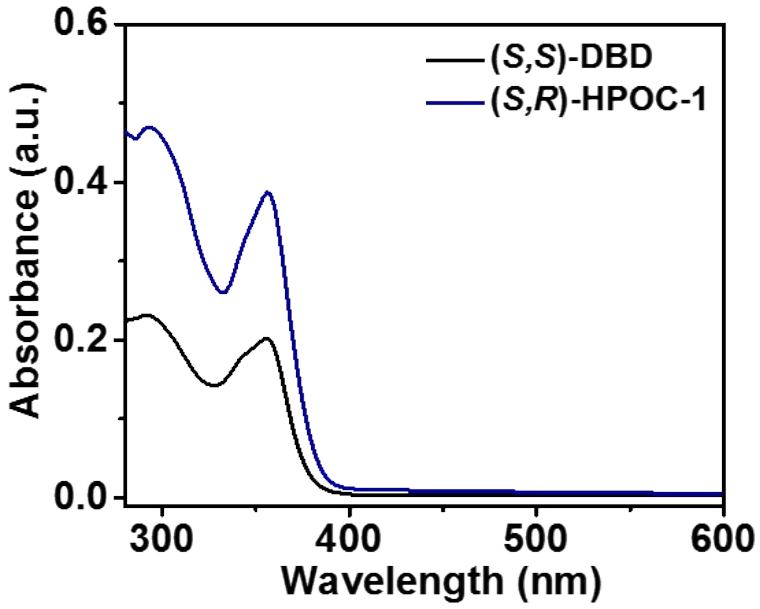


Figure S21. UV−vis spectra of (*S*,*S*)-DBD (10.0 μM) and (*S*,*R*)-HPOC-1 (10.0 μM) in THF.

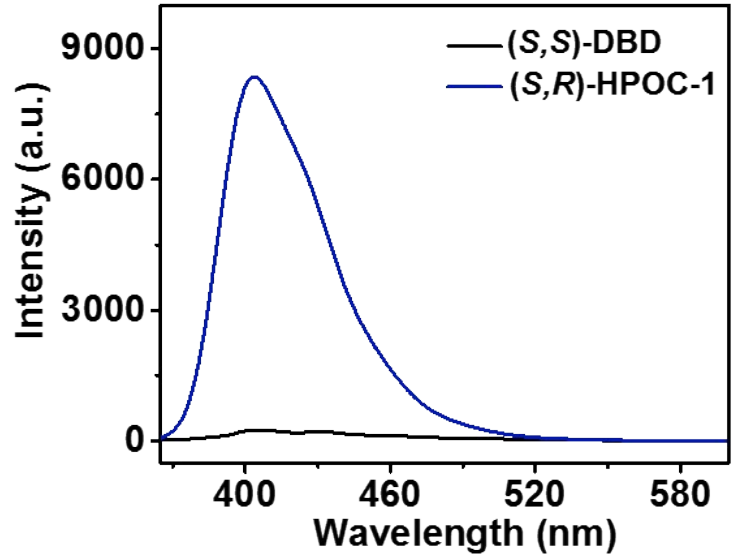


Figure S22. Fluorescence spectra of (*S*,*S*)-DBD (3.0 μM) and (*S*,*R*)-HPOC-1 (1.0 μM) in THF excited at 357 nm.

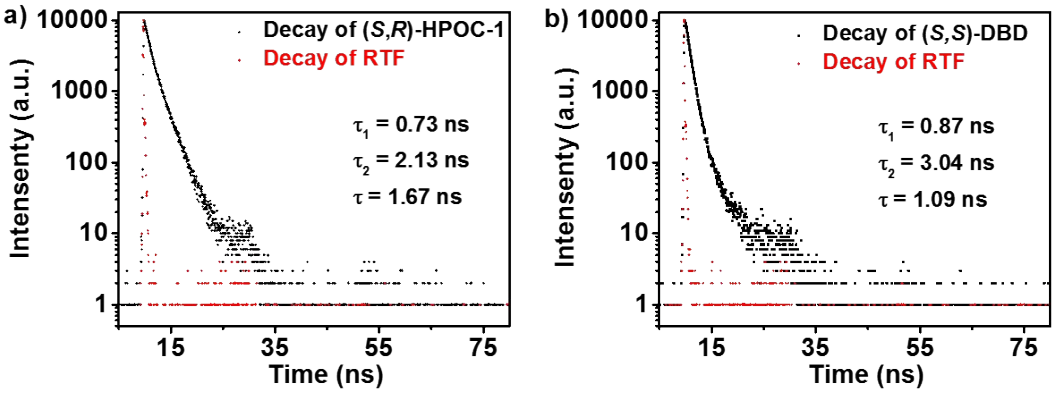


Figure S23. Fluorescence decay curves of (*S*,*R*)-HPOC-1 (10.0 μM) (a) and (*S*,*S*)-DBD (30.0 μM) (b) in THF. The time profiles of fluorescence decays were obtained with excitation at 375 nm by an EPL laser.

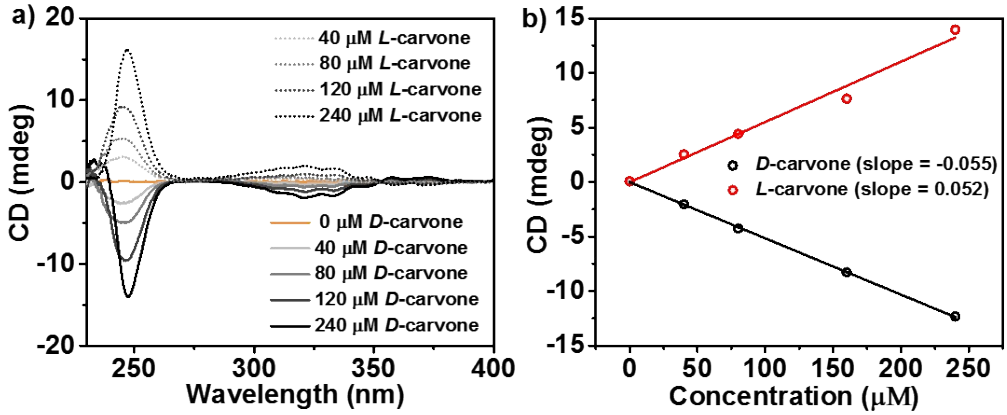


Figure S24. (a) CD spectra of *D*-carvone (solid line) and *L*-carvone (dotted line) with the concentration of 0–240.0 μM in THF. (b) The fitting curves of CD intensity at λ = 250 nm *vs.* the carvone concentration (0–240.0 μM).

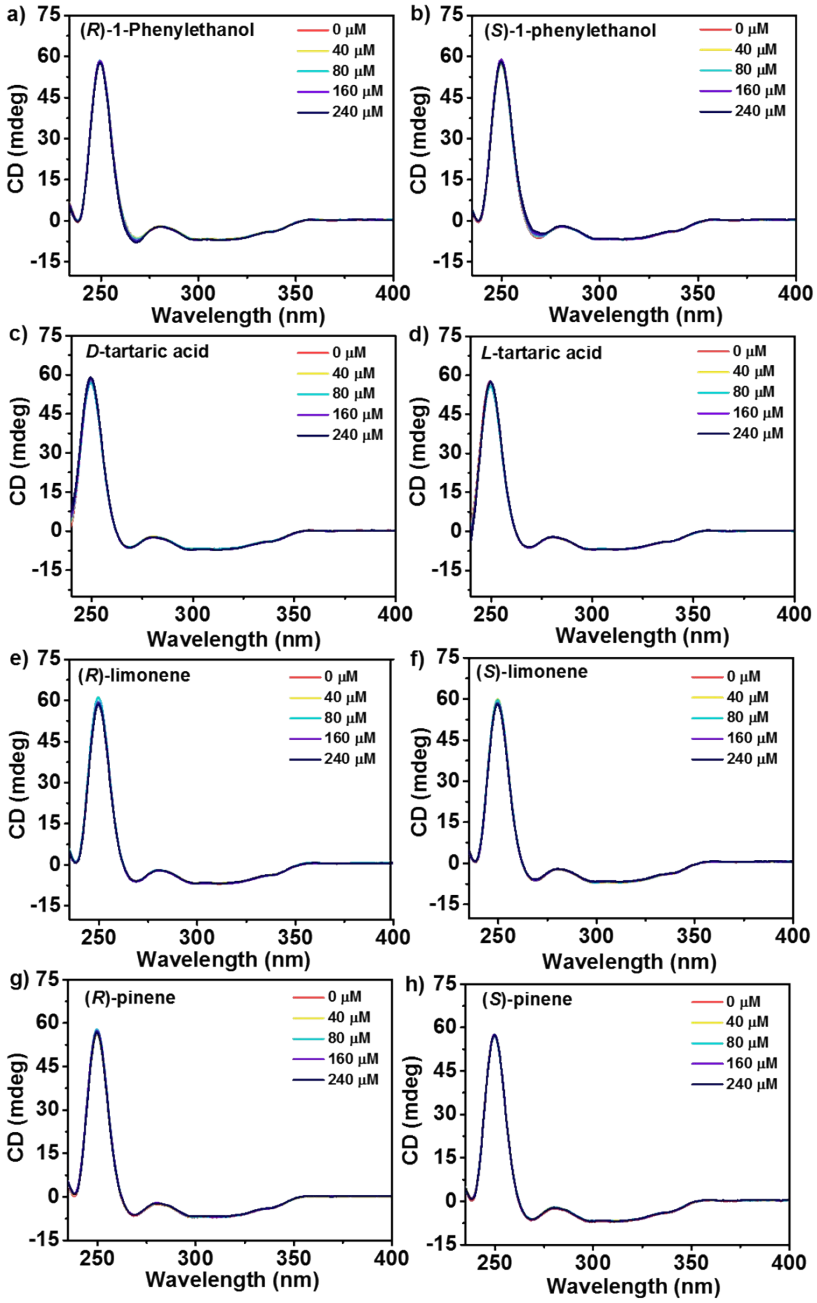


Figure S25. The CD spectra of (*S,R*)-HPOC-1 (2.0 μM) upon different concentrations of chiral substrates.

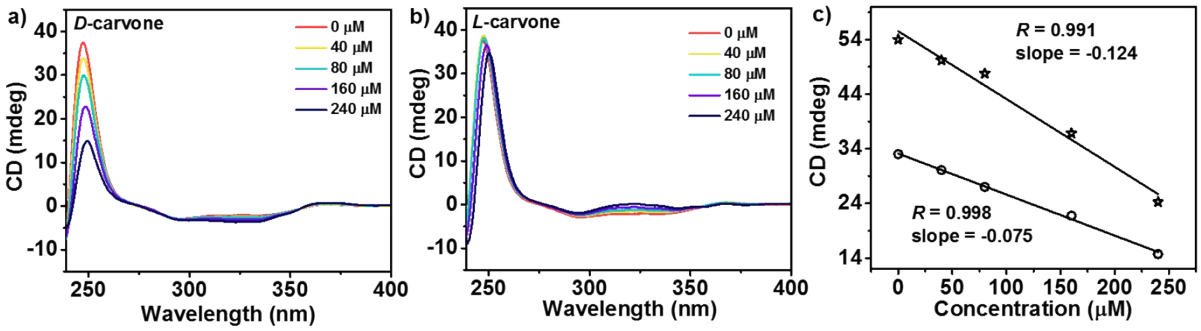


Figure S26. CD spectra of (*S,S*)-DBD (6.0 μM) upon different concentrations of *D*-carvone (a) and *L*-carvone (b). (c) The CD intensity (stars symbols for (*S,R*)-HPOC-1 and circle symbols (*S,S*)-DBD) at λ = 250 nm *vs.* the *D*-carvone concentration (0–240.0 μM).

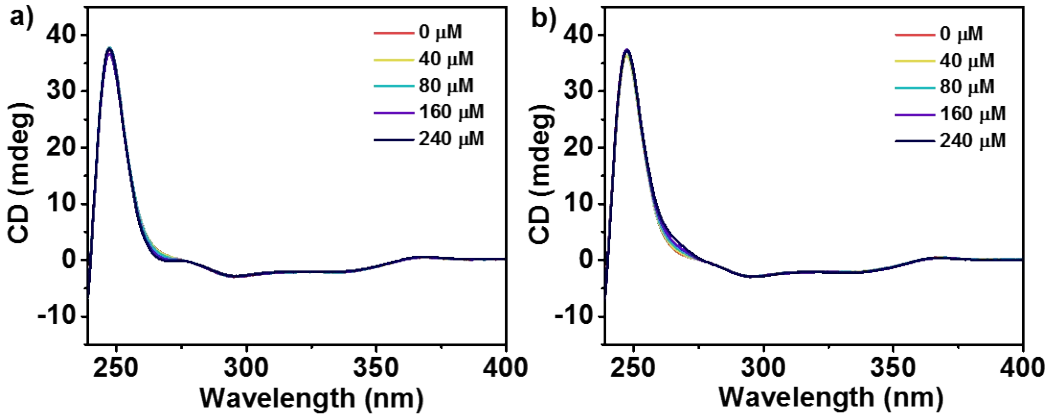


Figure S27. CD spectra of (*S,S*)-DBD (6.0 μM) upon different concentrations (0–240.0 μM) of (*R*)-1-phenylethanol (a) and (*S*)-1-phenylethanol (b).

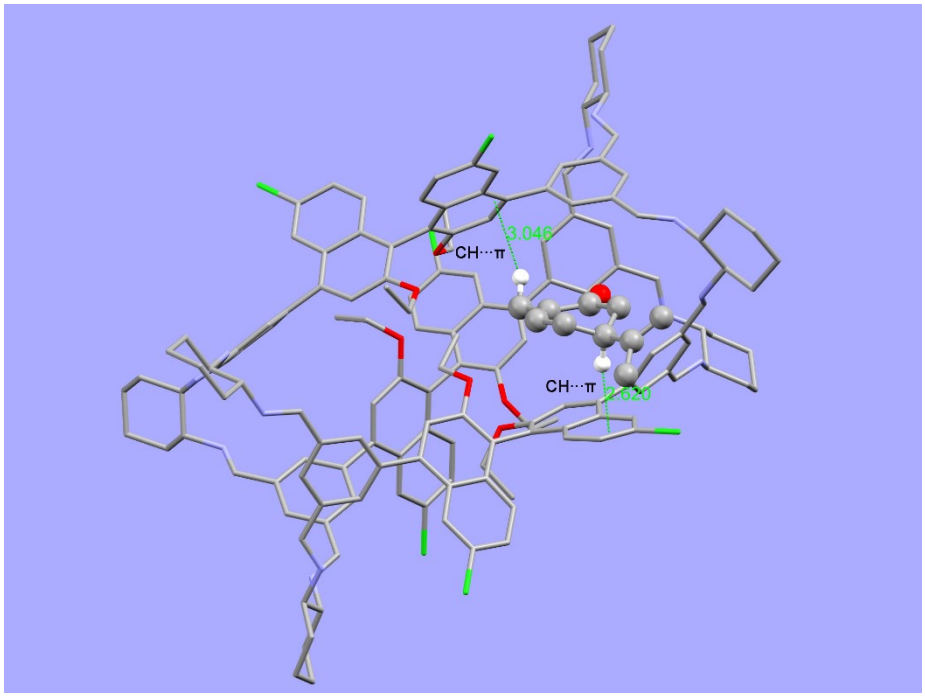


Figure S28. Binding sites of *D*-carvone in (*S,R*)-HPOC-1. C: gray; H: white; O: red; N: blue; Cl: green. The green dash lines represent double CH···π interactions.

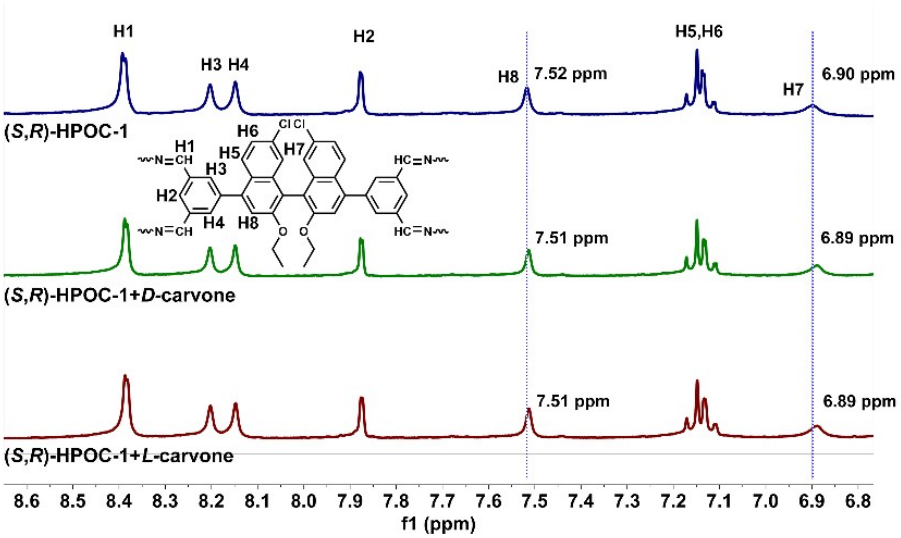


Figure S29. ^{1}H NMR spectra of (*S,R*)-HPOC-1 before and after adding *D*/*L*-carvone (12 equivalent).

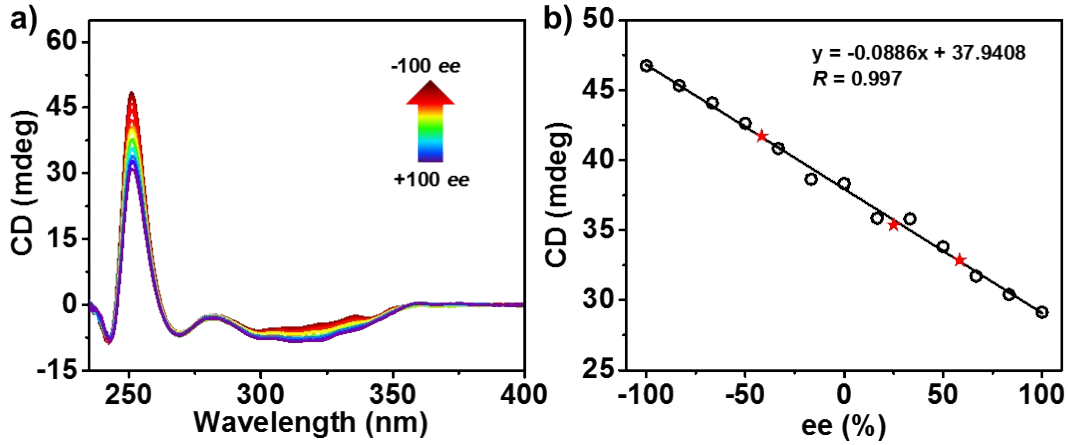


Figure S30. (a) CD spectra of (*S*,*R*)-HPOC-1 (2 μM) when titrated by *rac*-carvone (240 μM) with different *ee* values. (b) Calibration curve for the *ee* determination of carvone using the CD intensity at 250 nm (stars represent test samples 1-3).

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Table S1. Mass spectroscopic and elemental analysis data for (*S,R*)/(*R,S*)-HPOC-1.[a]

Compound	m/z[b]	Analysis		
		C	H	N
(*S,R*)-HPOC-1	2495.0 (2495.6)	72.91 (72.81)[c]	6.24 (5.90)[c]	6.30 (6.39)[c]
(*R,S*)-HPOC-1	2495.6 (2495.6)	73.56 (73.56)[d]	5.99 (5.73)[d]	6.79 (6.57)[d]

[a] Calculated values given in parentheses. [b] By MALDI-TOF mass spectrometry. [c] Contain 0.5 equiv. solvated CH_2Cl_2 and 3 equiv. solvated CH_3OH. [d] Contain 0.75 equiv. solvated CH_2Cl_2.

Table S2. Bond lengths comparison of cyclohexanediamine moieties of (*S*,*R*)-HPOC-1 and (*S*,*S*)-HPOC-1.

Bond (Å)	(*R*,*R*)-CA	(*S*,*R*)-HPOC-1	(*S*,*S*)-CA	(*S*,*S*)-HPOC-1
C2-N1	1.46605	1.45013	1.45869	1.51642
C3-N2	1.45865	1.45020	1.46598	1.51087
C2-C3	1.53829	1.53827	1.53831	1.61373
C1-C2	1.52301	1.53028	1.52295	1.59198
C3-C4	1.52963	1.52865	1.52957	1.61513
C1-C5	1.52367	1.52212	1.52302	1.59480
C5-C6	1.52479	1.52419	1.52479	1.59571
C4-C6	1.52303	1.52245	1.52361	1.57132
Rate of change[a]		0.18%		4.32%

[a] The total bond length change rate of $[\sum(L_{CA} - L_{HPOC\text{-}1})/L_{CA}]/8$.

Table S3. Crystal data and structure refinements for (*S,R*)/(*R,S*)-HPOC-1.

Compound	(*S,R*)-HPOC-1	(*R,S*)-HPOC-1
formula	$C_{156}H_{144}Cl_6N_{12}O_6$	$C_{156}H_{144}Cl_6N_{12}O_6$
fw	2495.52	2495.52
crystal system	Monoclinic	Monoclinic
space group	$P2_1$	$P2_1$
a /Å	13.9655(4)	14.1106(3)
b /Å	39.9035(10)	40.2961(10)
c /Å	15.4673(3)	15.5297(3)
α /°	90	90
β /°	100.516(2)	101.091(2)
γ /°	90	90
V /Å^3	8474.7(4)	8665.3(3)
Z	2	2
θ range (deg)	2.906-74.277	2.193-73.116
Density (g/cm^3)	0.978	0.956
μ(mm^{-1})	1.309	1.280
F(000)	2628	2628
R_1 ($I>2\theta$)[a]	0.0821	0.0551
R_{w2} for all[b]	0.2295	0.1669
GOF on F^2	0.905	1.078
CCDC No.	2114815	2114817

[a] $R_1 = \Sigma|F_o-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S4. Enantioselective recognition of chiral substrates with (*S*,*R*)-HPOC-1 by CD spectra.

Entry	Chiral molecules	ΔI[a]
1	*D*-carvone	29.7
	L-carvone	6.3
2	(*R*)-1-phenylethanol	0.1
	(*S*)-1-phenylethanol	0.5
3	*D*-tartaric acid	1.2
	L-tartaric acid	0.3
4	(*R*)-limonene	0.9
	(*S*)-limonene	1.1
5	(*R*)-pinene	0.9
	(*S*)-pinene	0.4

[a] ΔI is the CD spectral intensity difference at 250 nm between I_0 (CD intensity without chiral guest molecule) and I_{240} (CD intensity with 240.0 equiv. chiral guest molecule).

Table S5. Calibration curve for the *ee* determination of carvone using the CD intensity of the complexes at 250 nm.

samples	CD intensity (mdeg)	theoreti value (ee/%)	found value (ee/%)
1	32.85	+58.33	+57.46
2	35.37	+25.00	+29.02
3	41.71	-41.67	-42.54

Table S6. Cartesian coordinates (Å) of (*R*,*R*)-Diaminocyclohexane, (*S*,*S*)-Diaminocyclohexane, (*S*,*R*)-HPOC-1, (*S*,*S*)-HPOC-1, and *D*-carvone + (*S*,*R*)-HPOC-1 at 298.15 K and 1 atm for the optimized structures.

(*R*,*R*)-Diaminocyclohexane

Cartesian coordinates (Å)			
atom	x	y	z
N	1.90263	1.32753	0.09905
N	1.77031	-1.54644	-0.06487
C	-0.61597	1.46809	0.11011
H	-0.60625	1.60552	1.20568
H	-0.58496	2.47827	-0.32492
C	0.63994	0.69034	-0.28684
H	0.65996	0.59327	-1.38749
C	-1.89118	0.73954	-0.2956
H	-1.93597	0.67434	-1.39481
H	-2.77782	1.30859	0.01426
C	-1.91882	-0.66736	0.29163
H	-1.97243	-0.59865	1.38993
H	-2.82361	-1.20189	-0.02657
C	-0.67366	-1.45147	-0.10128
H	-0.66852	-1.59956	-1.1958
H	-0.67334	-2.45473	0.34327
C	0.6117	-0.73495	0.29116
H	0.62021	-0.62903	1.39337
H	2.58725	-0.94224	0.03082
H	1.71482	-1.74464	-1.06439
H	1.85591	1.55134	1.09335
H	1.98206	2.2266	-0.37105

(*S*,*S*)-Diaminocyclohexane

Cartesian coordinates (Å)			
atom	x	y	z
N	1.90259	1.3275	-0.09876
N	1.77038	-1.54639	0.06449
C	0.61161	-0.73486	-0.29113
H	0.61978	-0.62867	-1.39334
C	0.63987	0.69042	0.28695
H	0.65946	0.59333	1.38762
C	-1.89103	0.73961	0.2955
H	-1.93568	0.67461	1.39471
H	-2.77769	1.30863	-0.01432
C	-1.91886	-0.66743	-0.29139
H	-1.97274	-0.59894	-1.38968
H	-2.82359	-1.20185	0.02715
C	-0.67361	-1.45144	0.10139
H	-0.6733	-2.45472	-0.34312
H	-0.66833	-1.59949	1.19592
C	-0.6159	1.46804	-0.11046

H	-0.60601	1.605	-1.20609
H	-0.58497	2.47841	0.32414
H	1.85587	1.55161	-1.09307
H	1.98201	2.22649	0.37165
H	2.58738	-0.94222	-0.03053
H	1.7146	-1.74592	1.06369

(*S*,*R*)-HPOC-1

Cartesian coordinates (Å)			
atom	x	y	z
Cl	2.61998	5.89752	-6.36695
Cl	-2.6354	-4.83557	6.91471
Cl	3.10554	1.9536	8.05005
Cl	2.67726	-8.20595	-2.811
Cl	-2.73324	8.58335	1.55861
Cl	-3.20324	-2.96008	-7.92146
O	1.25671	-2.33653	2.56223
O	-1.11287	0.75369	2.83208
O	-1.1011	-3.2762	-0.87796
O	1.09695	3.23159	0.34143
O	0.94269	-1.02119	-2.52727
N	7.78638	4.56397	1.49308
O	-1.10016	2.07425	-1.96264
N	7.98439	-3.85172	3.17632
N	8.44574	-1.27925	4.35045
N	7.94755	-0.71511	-4.42159
N	7.94285	4.98163	-1.2938
N	-7.74672	-4.96206	-0.10407
N	-8.29362	-0.62623	4.67993
C	1.23424	-4.97444	0.05917
C	0.77782	-4.0206	1.01319
C	8.1775	3.37048	1.74039
H	9.21875	3.05032	1.55787
N	8.49006	-3.27033	-3.20387
C	-1.56649	1.99919	2.50575
C	3.09082	-3.29679	1.30877
H	3.79945	-2.61858	1.77977
C	1.06985	2.13234	-4.33335
C	1.72608	-3.2127	1.64472
C	7.10048	1.28232	-3.35929
C	-8.07877	-4.02033	0.69209
H	-9.12761	-3.67757	0.77366
C	-2.7875	-0.64726	-4.65075
C	-0.5957	-0.88492	-5.7162
H	0.46703	-0.6463	-5.7451
C	5.87936	2.64727	2.30812
H	5.50685	3.55486	1.83739
C	-2.55616	4.57784	1.9509
C	8.15499	0.34589	-3.73983
H	9.17487	0.61791	-3.40994

C	6.45443	3.36689	-2.30136
C	5.00613	-4.15072	0.04893
C	5.12282	3.09854	-2.62703
H	4.34962	3.80717	-2.32362
C	5.754	1.02576	-3.66446
H	5.48298	0.10962	-4.18986
C	-0.66355	3.04856	2.43174
C	-3.02343	5.90069	1.75569
H	-4.08855	6.08768	1.63982
C	2.63082	-5.07658	-0.26922
C	3.5562	-4.18728	0.35777
C	0.76364	-6.83699	-1.44812
H	0.06179	-7.52846	-1.90852
C	5.9253	-4.12469	1.10032
H	5.56793	-4.21777	2.12654
C	-7.11061	-3.33576	1.55249
C	4.96917	1.79767	2.93062
C	9.06092	-3.64473	4.12455
H	9.99348	-3.34859	3.6037
C	7.25544	2.38037	2.31159
C	-4.8031	-2.97365	2.25464
C	0.58985	0.93752	-3.73918
C	5.46056	0.64257	3.55189
H	4.77009	-0.04095	4.05069
C	1.48221	0.08355	-3.10013
C	4.75647	1.92728	-3.30539
C	-1.15685	4.36135	2.17514
C	0.33595	-5.87752	-0.56515
H	-0.72145	-5.81687	-0.31439
C	2.13914	-6.94193	-1.7338
C	1.63689	2.83898	1.52354
C	2.45745	2.47991	-4.24191
N	-7.97386	2.21709	4.38291
C	8.70365	5.53637	0.93834
H	9.68262	5.08245	0.68569
C	-5.7403	-3.59551	1.43165
H	-5.40635	-4.3168	0.68657
C	-2.51754	-1.97604	-6.65275
C	-3.59692	-0.07902	-3.62437
C	8.6657	-2.51125	5.08857
H	7.73155	-2.83445	5.59
C	3.33401	1.60064	-3.54133
C	2.7148	2.18243	4.04753
C	7.29754	-3.9586	0.85727
C	2.91935	3.65407	-4.88527
H	3.97724	3.90446	-4.86641
C	2.99246	2.48259	1.65563
H	3.63162	2.45104	0.77671
C	-3.44599	3.46055	1.9902
N	-8.2848	4.3921	-1.66636

C	-2.94276	2.21076	2.2885
H	-3.61741	1.35651	2.34095
C	-4.89283	3.5792	1.69676
C	6.82443	0.33398	3.53664
C	-0.74108	-4.83157	4.96431
H	-0.08792	-5.26666	5.7167
C	1.31768	2.46928	3.89581
C	-2.07524	-4.52094	5.29221
C	7.44525	2.44958	-2.67588
H	8.48444	2.64698	-2.4134
C	-2.90343	-3.14364	0.72898
H	-3.58222	-2.75664	-0.02888
C	-1.13624	-1.70041	-6.67955
H	-0.52201	-2.11733	-7.4738
N	-8.01376	2.5253	-3.79671
C	8.96619	7.18913	-0.94419
H	9.95055	6.76291	-1.19633
H	8.53223	7.54606	-1.88644
C	-0.65489	-3.8474	1.35658
C	3.53381	2.13903	2.88079
C	-0.29203	-4.59578	3.69022
H	0.73266	-4.85453	3.42865
C	-2.938	-4.00385	4.35858
H	-3.97312	-3.8119	4.62732
C	-6.6308	-1.78673	3.35929
C	-1.39489	-0.31468	-4.69034
C	0.20072	3.00858	-5.03594
H	-0.8555	2.75247	-5.10847
C	-1.68972	1.19366	-2.81484
C	2.42653	2.10769	6.44763
C	-5.02343	-0.43376	-3.48302
C	-5.84148	3.11342	2.60576
H	-5.51805	2.75727	3.58458
C	7.72708	1.20822	2.90677
H	8.79664	0.98879	2.92078
C	-3.05261	0.84283	-2.75033
H	-3.69541	1.27803	-1.98651
C	-7.0652	-0.85501	4.40629
H	-6.25384	-0.36355	4.97721
C	-0.85118	0.59644	-3.74945
C	9.10125	-1.51504	-4.78484
H	9.97091	-1.26491	-4.14363
C	8.78591	-3.00918	-4.59935
H	7.91013	-3.24074	-5.23775
C	2.85004	0.41563	-3.02069
H	3.54106	-0.23851	-2.49322
C	0.51028	2.50607	5.06287
H	-0.55489	2.70231	4.95845
C	2.03684	4.46213	-5.56098
C	8.27917	-3.84356	1.93227

H	9.32408	-3.70735	1.59864
C	6.75564	4.56175	-1.51397
H	5.87956	5.07899	-1.07831
C	-1.56673	-3.42693	0.38943
C	0.78045	2.7778	2.61738
C	-8.22218	2.57817	3.18528
H	-9.23769	2.48335	2.75802
C	7.28839	-3.58918	-2.89916
H	6.50267	-3.6493	-3.6715
C	9.12981	8.32813	0.05404
H	8.14555	8.7876	0.23599
H	9.76505	9.11704	-0.36804
C	-7.20826	3.11225	2.27825
C	7.23381	-0.89277	4.22122
H	6.4053	-1.48596	4.65139
C	9.46159	-1.22714	-6.24395
H	8.57313	-1.42576	-6.86553
H	9.67964	-0.15661	-6.35307
C	-2.13907	6.95345	1.75637
N	-8.27578	-3.96422	-2.70848
C	-5.26404	-2.06452	3.22059
H	-4.54557	-1.5534	3.86492
C	-8.60214	0.30497	5.7526
H	-7.70263	0.51397	6.36565
C	-1.13228	-4.04981	2.68524
C	-8.86956	-7.06416	-0.62491
H	-7.88024	-7.51757	-0.78758
H	-9.10418	-7.19838	0.4396
C	-9.43057	2.61646	6.28756
H	-8.52452	2.81477	6.88263
H	-9.73401	3.5758	5.84758
C	3.05489	-6.09283	-1.16193
H	4.11391	-6.22095	-1.37068
C	-2.49264	-3.75307	3.03734
C	-9.05703	1.65228	5.16021
H	-9.94762	1.46639	4.5259
C	-6.68567	4.03878	0.10137
C	-8.76823	-5.56808	-0.93258
H	-9.75304	-5.08326	-0.76755
C	-3.33035	-1.47326	-5.6656
H	-4.39727	-1.68029	-5.68554
C	-0.28734	5.48023	2.14028
H	0.77805	5.3185	2.29738
C	8.08634	6.08694	-0.36676
H	7.09869	6.5114	-0.10293
C	-7.55015	-2.42422	2.5111
H	-8.61703	-2.22224	2.61338
C	6.85367	-3.83078	-1.52159
C	-2.05328	-3.17512	-1.93872
H	-2.87909	-3.88224	-1.74835

H	-2.48135	-2.157	-1.95581
C	8.87446	6.68038	1.93976
H	9.31829	6.28959	2.86521
H	7.86828	7.04319	2.20637
C	0.66434	4.15434	-5.63581
H	-0.00605	4.81318	-6.18044
C	1.04241	2.32906	6.31568
H	0.41489	2.37806	7.20153
C	-3.37252	-3.27301	2.02324
C	3.24822	2.02677	5.35051
H	4.31709	1.87987	5.4859
C	9.70401	7.82456	1.37297
H	9.75881	8.64085	2.10499
H	10.7387	7.48266	1.21447
C	7.75731	-3.817	-0.45033
H	8.82005	-3.67835	-0.64056
C	-5.99222	0.56281	-3.50576
H	-5.68557	1.59911	-3.65158
C	-7.09934	-3.49607	-2.87064
H	-6.21813	-4.16471	-2.80825
C	9.98088	-3.8491	-5.05031
H	9.75384	-4.91133	-4.89648
H	10.83244	-3.62751	-4.38846
C	-5.33256	4.05272	0.45072
H	-4.59793	4.39931	-0.27683
C	5.49109	-4.01314	-1.26227
H	4.79164	-3.99189	-2.09951
C	-6.78351	-2.08931	-3.12053
C	10.63164	-2.08009	-6.71332
H	11.53536	-1.79433	-6.15231
H	10.84664	-1.86923	-7.76968
C	-7.62327	3.57206	1.03051
H	-8.68352	3.56204	0.77353
C	2.17993	-1.67504	3.43442
H	2.70343	-0.88155	2.87313
H	2.93382	-2.39485	3.79009
C	-5.43527	-1.75825	-3.29104
H	-4.68901	-2.55498	-3.26388
C	-10.53104	2.04643	7.17099
H	-11.45843	1.95536	6.58471
H	-10.75624	2.74604	7.98417
C	2.39664	-2.84084	-3.24923
H	1.60023	-3.14006	-3.9422
H	2.87341	-3.7603	-2.89032
H	3.14119	-2.26521	-3.81117
C	1.36786	-1.10801	4.56776
H	0.63312	-0.38123	4.20132
H	2.02057	-0.60212	5.28809
H	0.83341	-1.91196	5.0872
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H	-10.90831	-7.33325	-1.27287
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H	-0.08133	7.60675	1.92433
C	-9.71521	-0.27722	6.62466
H	-9.37948	-1.23227	7.04835
C	1.99779	3.67411	-0.68022
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C	-8.33987	1.33569	-3.45897
H	-9.38475	1.07299	-3.21327
C	1.80693	-2.0781	-2.08543
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H	-6.2575	4.7782	-1.90968
C	10.39693	-4.72375	5.97092
H	10.55074	-5.65181	6.53612
H	11.35129	-4.50674	5.46733
C	-9.60861	-7.51139	-2.98665
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H	-10.39888	-7.94645	-3.6111
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H	-2.32483	-0.24465	1.45884
H	-1.11547	-1.20284	2.34773
C	-7.35453	0.25407	-3.37855
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H	9.57965	-5.73437	4.22408
H	8.36862	-5.22885	5.40044
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H	0.72601	-0.19344	1.03206
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H	-8.80859	-1.3309	-3.07976
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H	0.56217	3.93063	-2.27678
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H	0.61763	5.26265	-1.09318
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H	9.4648	-1.48315	6.80256
C	10.04711	-3.57407	6.90758
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H	9.15773	-3.84422	7.49877
C	-8.5578	4.77278	-3.03231
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H	6.27816	-3.86975	4.03753
H	5.37418	-4.69271	4.95616
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H	10.06392	-0.24311	4.01009
H	10.63704	1.02872	4.61609
O	10.74944	4.16569	-1.56923
H	9.81948	4.45643	-1.65703
H	11.2488	4.98926	-1.51671
O	5.14113	5.78927	1.28546
H	4.92736	6.24451	2.11104
H	6.01629	5.37896	1.46779
O	10.85823	-4.00335	-1.65987
H	10.12915	-3.62223	-2.191
H	11.63502	-3.49452	-1.91805
O	5.52249	-2.18107	-5.1779
H	6.3139	-1.63281	-4.98029
H	5.59363	-2.36079	-6.12459

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H	-6.48935	2.81078	5.4931
H	-6.02758	3.84702	6.52001
O	-10.65912	-2.00247	3.56312
H	-9.91295	-1.49653	3.95022
H	-10.583	-2.86298	3.99441
O	-5.48274	3.6309	-4.9104
H	-6.34078	3.26937	-4.60401
H	-5.51304	4.55939	-4.64885
O	-5.54234	-6.69073	-0.97636
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H	-4.66005	-6.30707	-0.92092
H	-10.57134	-0.51344	5.97271
H	-8.33521	4.32376	-5.71018

(*S*,*S*)-HPOC-1

Cartesian coordinates (Å)			
atom	x	y	z
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H	-1.527	3.5216	2.3595
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N	-8.9415	-4.3806	1.6795
O	-1.2271	1.6918	3.3188
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C	5.0893	-3.8395	-1.3033
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C	2.887	2.343	-2.3112
H	3.2643	1.2763	-2.4322
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C	-7.6481	-4.0774	1.8645
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H	-3.0606	-0.6422	-3.0529
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C	-1.1523	-4.1937	5.6995
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C	2.0748	-5.6392	-5.5706
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C	9.9875	-0.6301	-6.941
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C	0.8302	3.1195	1.1958
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C	11.1509	7.4766	1.2524
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H	11.1532	5.3038	3.2408
C	-2.7263	3.5945	4.2712
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C	11.0177	-3.0348	-7.1759
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H	11.2787	-3.8838	-7.9075
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C	8.8692	-4.9702	3.8193
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C	9.3969	-3.6076	4.5266
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H	11.8074	-4.6949	5.8101
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C	2.7795	-3.9436	4.0825
H	3.2796	-4.9712	3.965
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D-carvone + (*S*,*R*)-HPOC-1

Cartesian coordinates (Å)			
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H	0.61847	-0.10622	-1.29664
H	-0.37593	-1.33967	-0.46049
H	0.66167	-0.22427	0.50973
H	-1.8171	0.94674	3.70283
H	-2.11964	2.47757	2.87206
H	-0.58359	3.66369	4.47892
H	-0.2029	2.08675	5.27093
H	-1.87294	2.75771	5.3476
H	5.11796	5.04498	-3.28537
H	5.31732	5.40752	-1.51706
H	2.85786	5.7859	-4.45674
H	1.60166	6.55529	-3.42343
H	1.99817	2.02766	-1.0249
H	6.01428	7.08658	-3.36371
H	5.62199	8.8901	-3.38734
H	2.96848	9.34982	-3.47642
H	3.60786	9.52591	-1.79141
H	3.03531	6.30124	-1.42194

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