Supporting Information

Multi-colour circularly polarized luminescence properties of chiral Schiff-base boron difluoride complexes

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1. Instrumentation and Materials

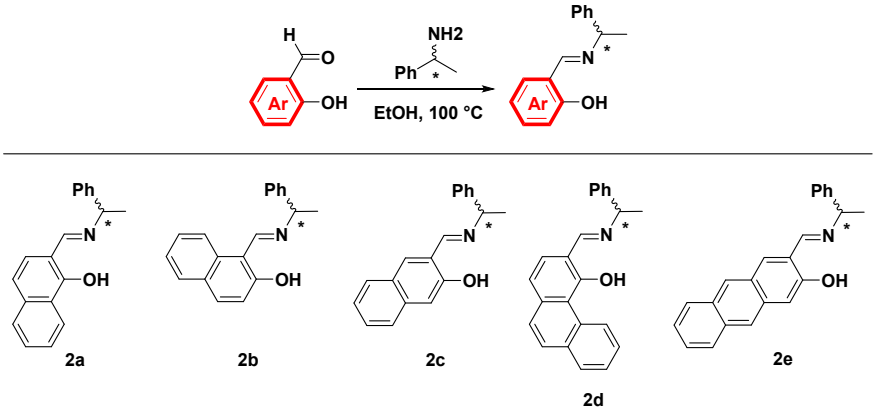
Melting points were measured by a ATM-01 melting temperature measurement device (AS ONE Corporation). IR spectra were acquired with a JASCO FT/IR4100ST spectrometer. High-resolution mass spectra were recorded on Bruker micrOTOF II spectrometer. ^{1}H and ^{13}C NMR spectra were recorded on Bruker Avance 400 and Bruker Avance III 500 spectrometers, TMS as internal standard. Elemental analyses were performed on a J-SCIENCE SCIENCE SCIENCEMICROCORDERJM10. UV–vis absorption spectra were obtained on a SHIMADZU UV-1900i spectrophotometer. CD spectra were recorded on a Jasco J-720 spectropolarimeter. Emission spectra were obtained on a FP-6500 spectrometer. CPL spectra were obtained at room temperature using a JASCO CPL-300 spectrofluoropolarimeter. Optical rotation was measured on a Jasco DIP-370 digital polarimeter.

(*R*)- and (*S*)-1-phenylethylamine (TCI), 1-hydroxy-2-naphthaldehyde (TCI), 2-hydroxy-1-naphthaldehyde (TCI), boron trifluoride- ethyl ether complex (TCI), and triethylamine (Fujifilm Wako) were obtained from commercial sources and were used without further purification. 2-Hydroxy-3-naphthaldehyde,[S1] 4-hydroxy-3-phenanthrenecarboxaldehyde[S2] and 3-hydroxy-2-anthracenecarboxaldehyde[S3] were prepared by according publish procedure.

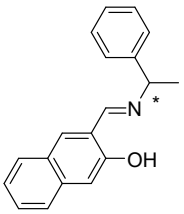
2. Synthetic Procedures and Characterization

General procedure for ligands

The ligands were prepared by condensation of corresponding aldehyde with (*R*)/(*S*)-1-phenylethylamine in boiling ethanol. The spectral data of **2a** and **2b** were corresponded with published papers.[S4] The physical properties and spectroscopic data of the ligands (*R*)/(*S*)-**2c**–**e** are as follows.

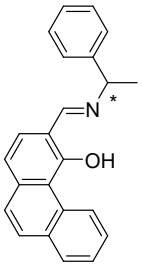


2-[[[(1*R* or 1*S*)-1-Phenylethyl)]imino]methyl]-3-naphthalenol ((*R*)- and (*S*)-2c): Yellow solid (61%); m.p. 148–150 °C; IR (KBr): ν = 1631 cm^{-1} (N=C); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 13.03 (br s, 1H), 8.57 (br s, 1H), 7.77 (s, J = 8.4 Hz, 1H), 7.75 (d, J = 8.2 Hz, 1H), 7.68 (d, J = 8.2 Hz), 7.45 (ddd, J = 8.2, 6.9, 1.3 Hz, 1H), 7.41–7.35 (m, 4H), 7.30–7.26 (m, 3H), 4.44 (q, J = 6.6 Hz, 1H), 1.67 ppm (t, J = 6.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 163.4, 156.9, 143.6, 135.9, 133.1, 128.7, 128.3, 128.1, 127.4, 127.3, 126.5, 126.3, 123.4, 121.2, 110.9, 68.9, 24.9 ppm; HRMS (APCI+): m/z [M + H]$^+$ calcd for $C_{19}H_{18}NO$: 276.1383; found: 276.1388.



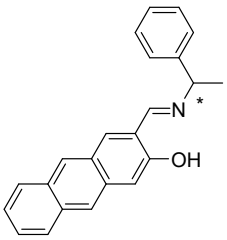
2c

3-[[[(1*R* or 1*S*)-1-Phenylethyl)]imino]methyl]-4-phenanthrenol ((*R*)- and (*S*)-2d): Yellow solid (82%); m.p. 120–121 °C; IR (KBr): ν = 1600 cm^{-1} (N=C); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 15.60 (br s, 1H, OH), 10.18 (d, J = 8.0 Hz, 1H), 8.34 (s, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 6.4 Hz, 1H), 7.69–7.59 (m, 1H), 7.52–7.48 (m, 1H), 7.38–7.26 (m, 1H), 7.28–7.20 (m, 1H), 7.04 (d, J = 8.4 Hz, 1H), 4.70 (q, J = 6.6 Hz, 1H), 1.72 ppm (t, J = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 169.1, 163.0, 142.9, 137.2, 132.3, 131.7, 129.0, 128.9, 128.20, 128.19, 127.6, 127.2, 126.9, 126.4 (2C), 125.7, 121.3, 117.5, 113.9, 65.1, 24.4 ppm; HRMS (ESI+): m/z [M$^+$] calcd for $C_{23}H_{20}NO$: 326.1539; found: 326.1538.



2d

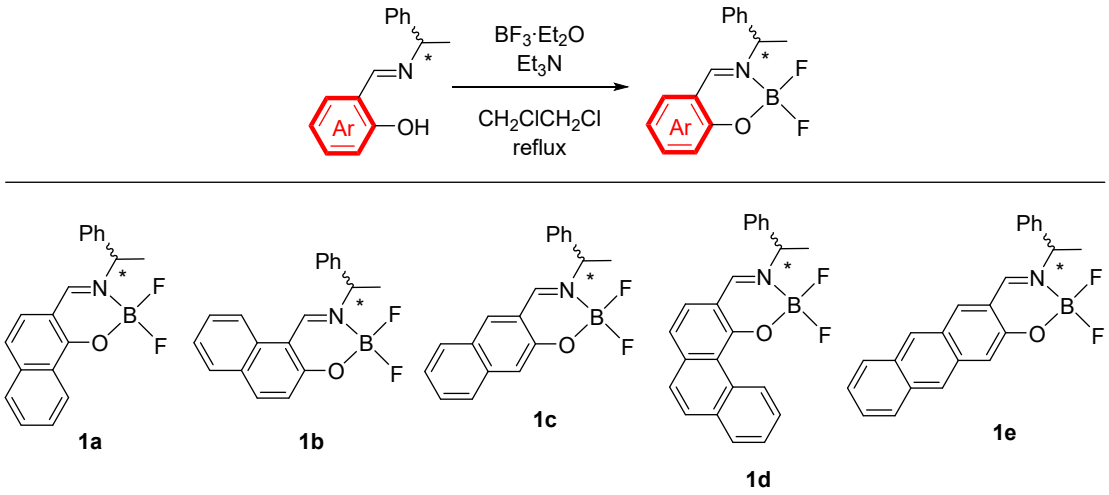
2-[[[(1*R* or 1*S*)-1-Phenylethyl)]imino]methyl]-3-anthracenol ((*R*)- and (*S*)-2e): Orange solid (90%); m.p. 263–271 °C; IR (KBr): ν = 1639 cm^{-1} (N=C); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 12.86 (br s, 1H, OH), 8.63 (s 1H), 8.38 (s, 1H), 8.22 (s, 1H), 8.01 (s, 1H), 7.92 (t, J = 8.2 Hz, 2H), 7.46–7.36 (m, 7H), 7.31–7.28 (m, 1H), 4.65 (q, J = 6.6 Hz, 1H), 1.70 ppm (t, J = 6.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 163.4, 163.0, 155.5, 143.6, 134.7, 133.4, 133.3, 130.2, 128.8, 128.4, 127.70, 127.65, 127.4, 126.8, 126.5, 126.3, 124.5, 123.6, 108.9, 69.0, 24.8 ppm; HRMS (APCI+): m/z [M + H]$^+$ calcd for $C_{19}H_{20}NO$: 326.1539; found: 326.1561.



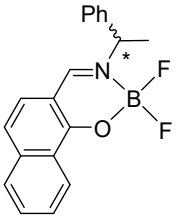
2e

General procedure for boron complexes

A solution of corresponding chiral ligands (1 equiv.) in 1,2-dichloroethane was added triethylamine (4 equiv.) and boron trifluoride-ethyl ether complex (4 equiv.) The mixture was refluxed under nitrogen atmosphere for overnight. After that, the mixture was poured into water, and was extracted with dichloromethane, followed by drying over anhydrous $MgSO_4$. After the removal of the solvent, the crude product was purified by column chromatography (SiO_2) using dichloromethane as the eluent. After recrystallization from CH_2Cl_2/EtOH, (*R*)/(*S*)-**1a**–**e** were obtained in moderate yields (44–83%).

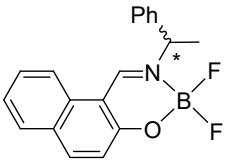


(*R*)/(*S*)-1a: Yellow crystals (83%); m.p. 122–123 °C; IR (KBr): ν = 1628 cm^{-1} (N=C); ^1H NMR ($CDCl_3$, 500 MHz) δ = 8.58 (dd, J = 7.9, 0.9 Hz, 1H), 8.07 (br, 1H), 7.73 (d, J = 7.9 Hz, 1H), 7.65 (ddd, J = 8.2, 7.0, 1.6 Hz, 1H), 7.55 (ddd, J = 8.4, 7.0, 1.3 Hz, 1H), 7.52-7.47 (m, 2H), 7.47-7.42 (m, 2H), 7.41-7.34 (m, 1H), 7.26 (d, J = 8.8 Hz, 1H), 7.13 (d, J = 8.8 Hz, 1H), 5.48 (q, J = 6.9 Hz,1H), 1.90 ppm (d, J = 6.9 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ = 162.5, 159.1, 139.0, 138.3, 130.9, 129.2, 128.7, 128.0, 127.5, 126.4, 125.3, 125.1, 124.9, 119.8, 58.5, 20.7 ppm; HRMS (APCI+): m/z $[M]^+$ calcd for $C_{19}H_{16}NOB$: 323.1291; found: 323.1320; Anal. calcd for $C_{19}H_{16}NOB$: C, 70.62; H, 4.99; N, 4.33. Found: C, 70.72; H, 4.97; N, 4.34. (*S*)-**1a**: $[\alpha]_D^{25}$ = +38 (c 0.001, $CHCl_3$).



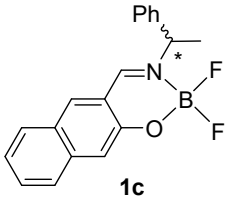
1a

(*R*)/(*S*)-1b: Yellow crystals (81%); m.p. 196–198 °C; IR (KBr): ν = 1620 cm^{-1} (N=C). ^1H NMR ($CDCl_3$, 500 MHz) δ = 8.76 (br, 1H), 8.01 (d, J = 9.1 Hz, 1H), 7.77 (dd, J = 7.9, 0.9 Hz, 1H), 7.65 (d, J = 8.2, 1H), 7.54–7.50 (m, 3H), 7.48–7.45 (m, 2H), 7.42–7.38 (m, 2H), 7.24 (d, J = 9.1 Hz, 1H), 5.51 (q, J = 6.9 Hz, 1H), 1.93 ppm (d, J = 6.9 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ = 161.1, 158.1, 139.8, 139.0, 131.2, 129.5, 129.3, 129.0, 128.9, 128.0, 127.9, 124.7, 120.50, 120.46, 118.7, 59.1, 20.9 ppm; HRMS (APCI+): m/z $[M]^+$ calcd for $C_{19}H_{16}NOB$: 323.1291, found: 373.1286; Anal. calcd for $C_{19}H_{16}NOB$: C, 70.62; H, 4.99; N, 4.33. Found: C, 70.71; H, 5.00; N, 4.36. (*S*)-**1b**: $[\alpha]_D^{25}$ = –200 (c 0.001, $CHCl_3$).



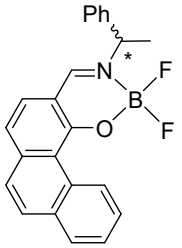
1b

(*R*)/(*S*)-1c: Yellow crystals (58%); m.p. 229–230 °C; IR (KBr): ν = 1647 cm^{-1} (N=C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 8.20 (br, 1H), 7.87 (s, 1H), 7.75–7.69 (m, 2H), 7.55–7.44 (m, 5H), 7.43–7.38 (m, 2H), 7.31 (ddd, J = 8.3, 7.0, 1.1 Hz, 1H), 5.56 (q, J = 6.9 Hz, 1H), 1.92 ppm (d, J = 6.9 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ = 163.8, 152.7, 139.4, 138.3, 130.1, 129.3, 128.2, 127.0, 124.4, 113.8, 59.5, 20.5 ppm; HRMS (APCI+): m/z $[M]^+$ calcd for $C_{19}H_{16}NOB$: 323.1291; found: 323.1274; Anal. calcd for $C_{19}H_{16}NOB$: C, 70.62; H, 4.99; N, 4.33. Found: C, 70.66; H, 4.96; N, 4.41. (*S*)-**1c**: $[\alpha]_D^{25}$ = +2 (c 0.001, $CHCl_3$).



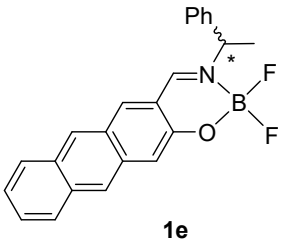
1c

(*R*)/(*S*)-1d: Yellow crystals (69%); m.p. 184–185 °C; IR (KBr): ν = 1639 cm^{-1} (N=C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 10. 05 (d, J = 8.5 Hz, 1H), 8.12 (br, 1H), 7.90 (ddd, J = 9.1, 9.1, 0.6 Hz, 1H), 7.78 (ddd, J = 8.5, 7.0, 1.2 Hz, 1H), 7.65 (ddd, J = 8.0, 7.3 Hz, 1H), 7.52 (d, J = 7.6 Hz, 2H), 7.49–7.42 (m, 2H), 7.42–7.33 (m, 2H), 7.30 (d, J = 8.5 Hz, 1H), 5.63-5.46 (q, J = 7.3 Hz, 1H), 1.94 ppm (d, J = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ = 162.7, 140.2, 138.9, 132.8, 132.5, 130.9, 129.2, 128.8, 128.7, 128.4, 128.0, 127.5, 126.8, 126.4, 120.8, 58.7, 20.7 ppm; HRMS (APCI+): m/z $[M]^+$ calcd for $C_{23}H_{18}NOB$: 373.1448; found: 373.1477; Anal. calcd for $C_{23}H_{18}NOB$: C, 74.02; H, 4.86; N, 3.75. Found: C, 74.14; H, 4.80; N, 3.79. (*S*)-**1d**: $[\alpha]_D^{25}$ = –274 (c 0.001, $CHCl_3$).



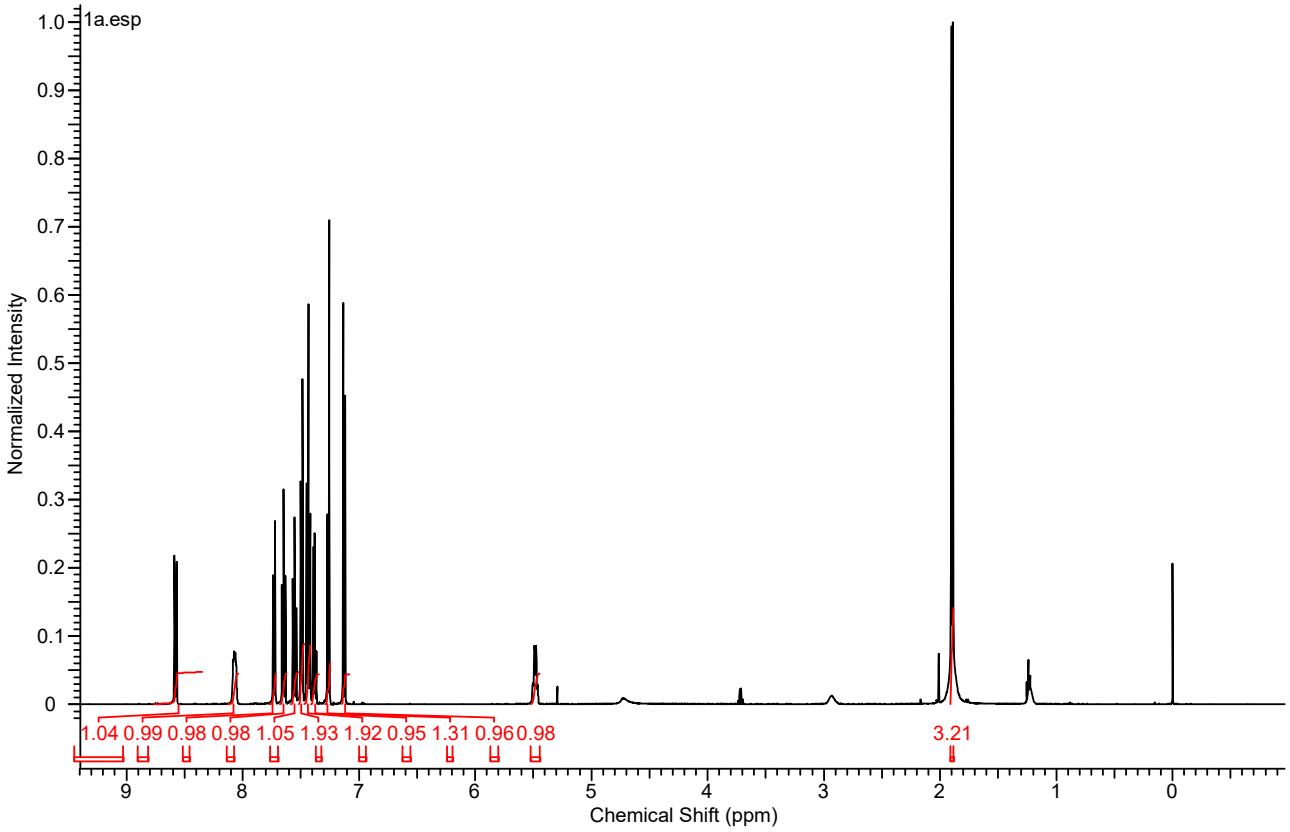
1d

(*R*)/(*S*)-1e: red solid (44%); m.p. 297–301 °C; IR (KBr): ν = 1643 cm^{-1} (N=C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 8.39 (s, 1H), 8.27 (s, 1H), 8.24 (br, 1H), 8.14 (s, 1H), 7.87 (s, 1H), 7.91 (d, J = 9.8 Hz, 1H), 7.53–7.50 (m, 3H), 7.50–7.46 (m, 3H), 7.45–7.38 (m, 2H), 5.60 (q, J = 7.3 Hz, 1H), 1.94 (d, J = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ = 159.3, 138.3, 137.2, 138.3, 134.6, 133.0, 130.6, 129.4, 129.3, 129.1, 128.7, 128.2, 127.9, 127.6, 127.5, 126.9, 126.5, 125.3, 124.6, 120.2, 59.7, 20.5 ppm; HRMS (APCI+): m/z $[M]^+$ calcd for $C_{23}H_{18}NOB$: 373.1448; found: 373.1477; (*S*)-**1e**: $[\alpha]_D^{25}$ = +70 (c 0.00044, $CHCl_3$).



1e

(a)



(b)

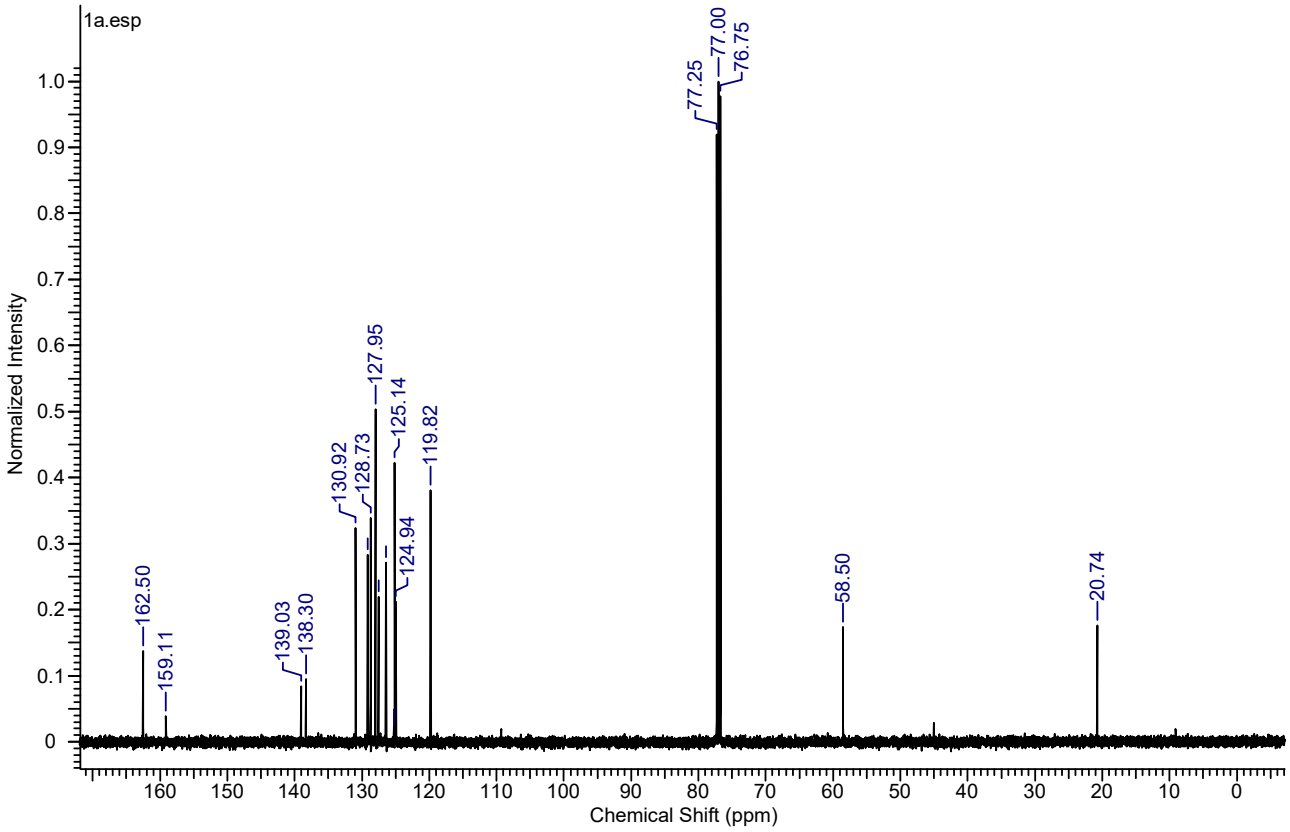
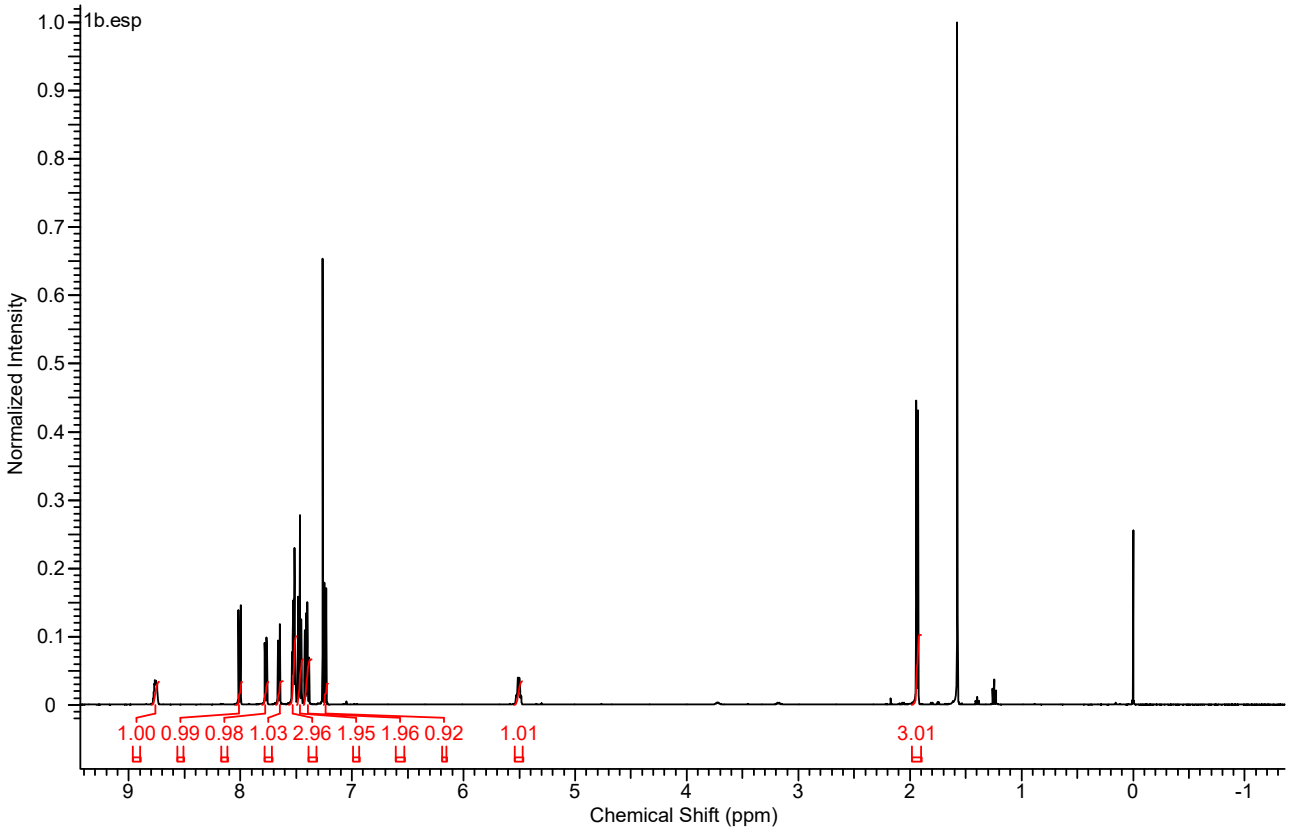


Fig. S1 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**1a** in $CDCl_3$.

(a)



(b)

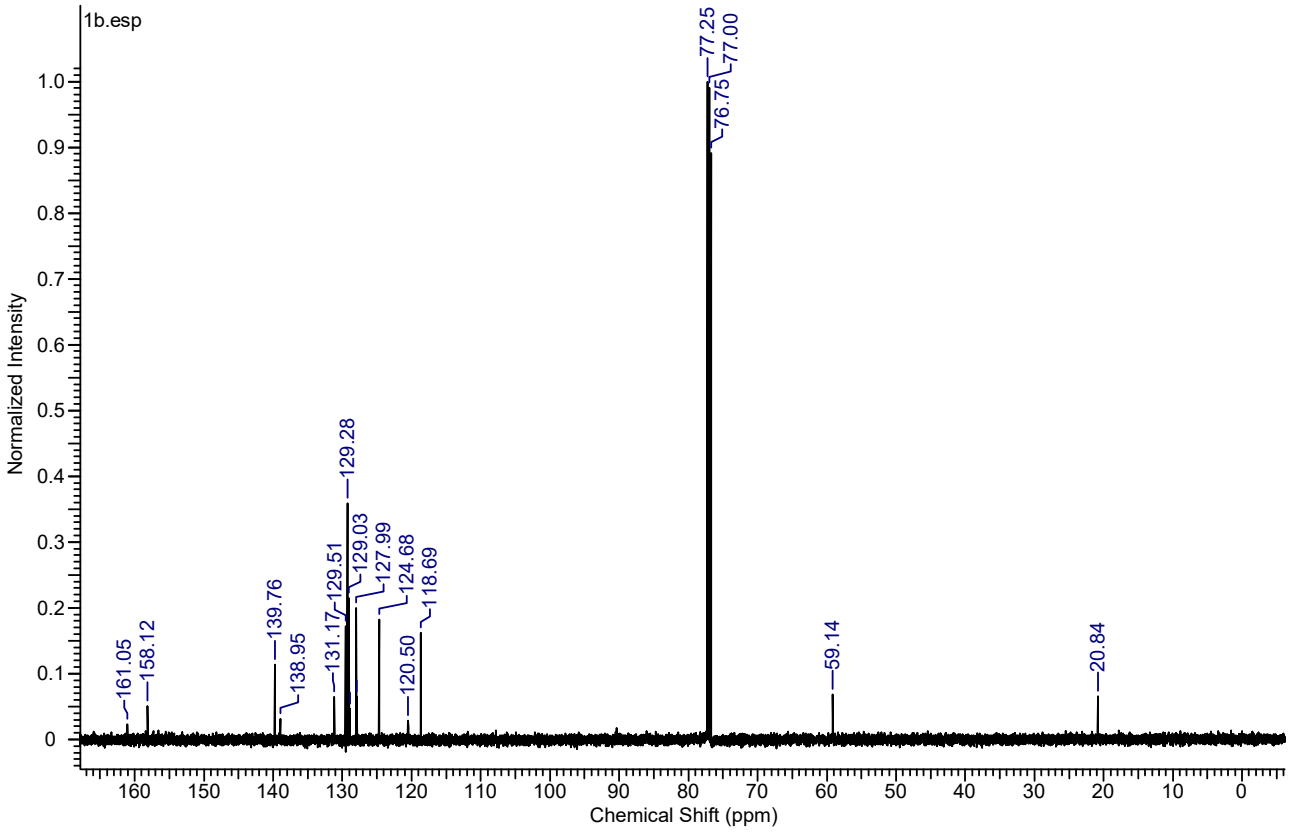
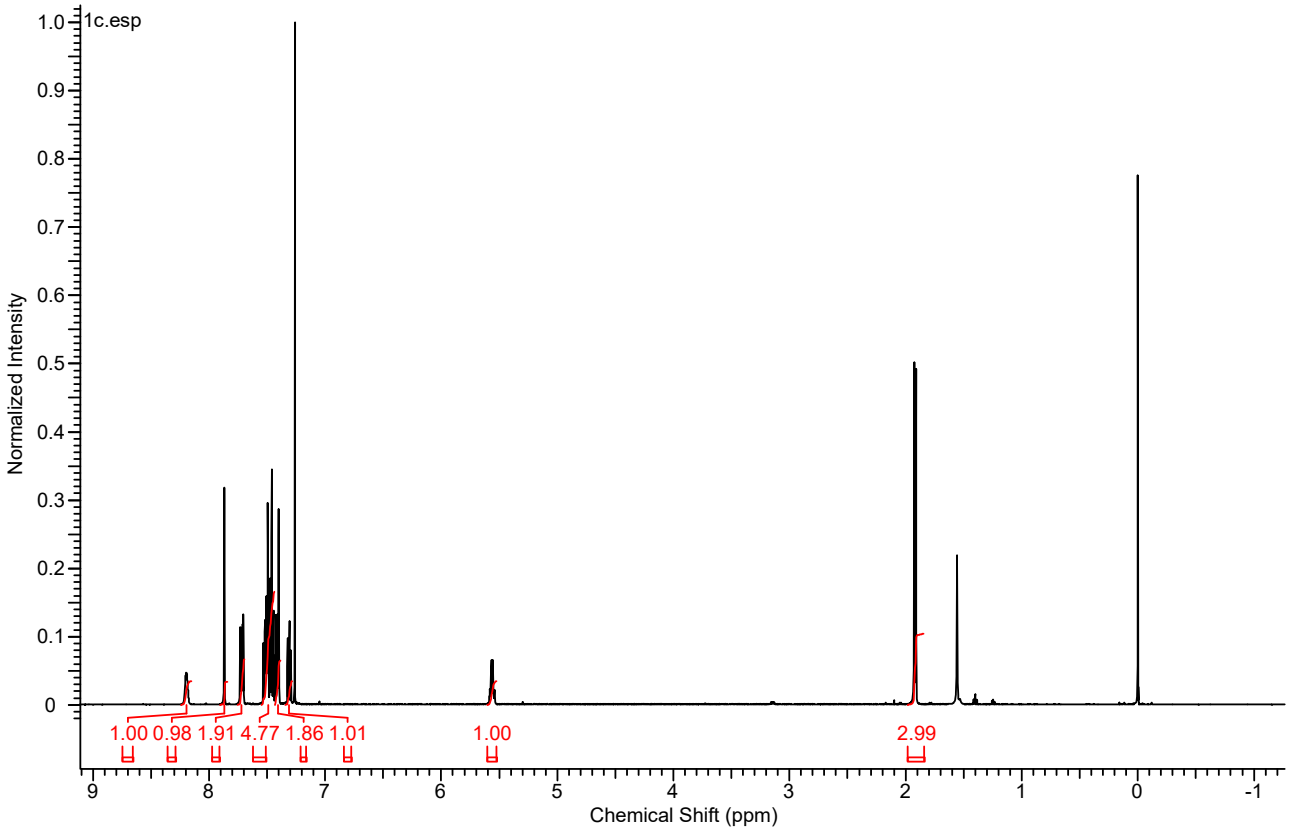


Fig. S2 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**1b** in $CDCl_3$.

(a)



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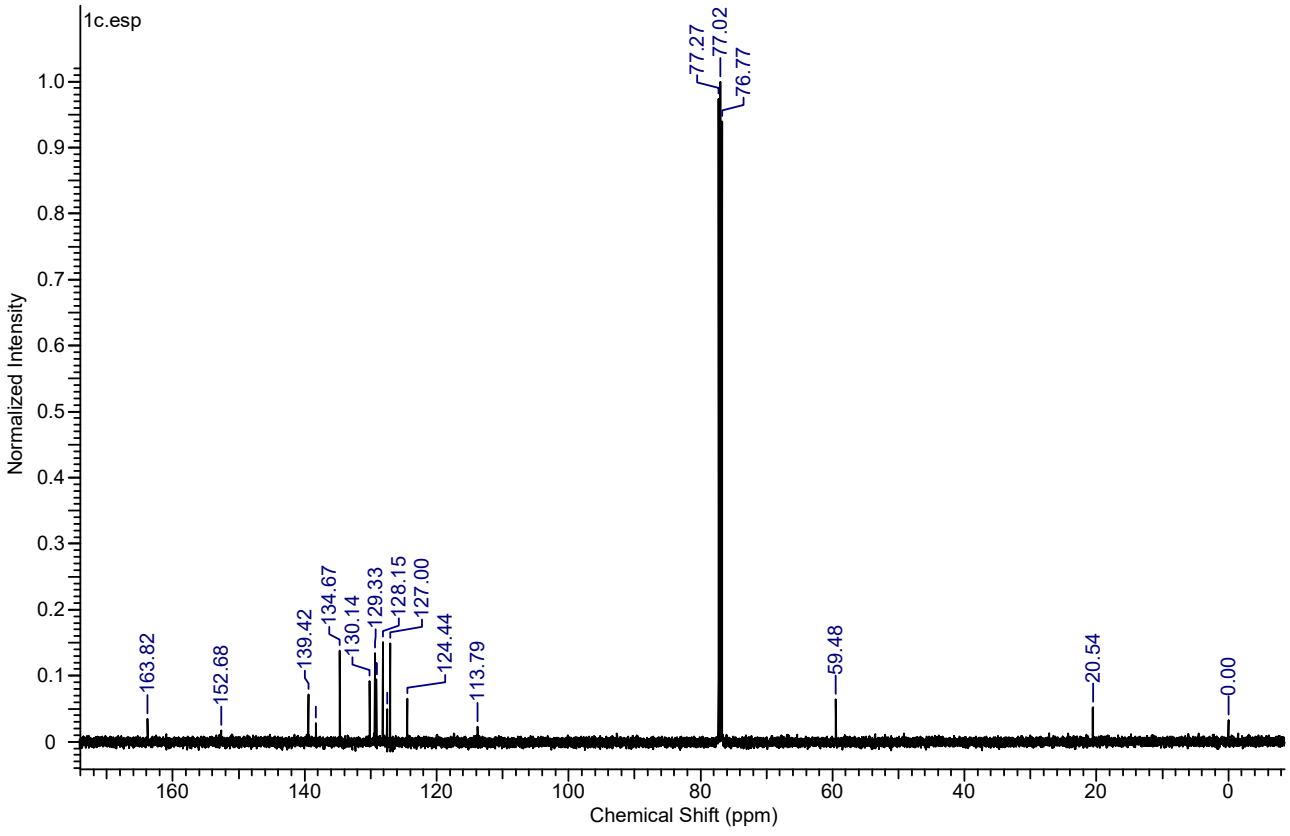
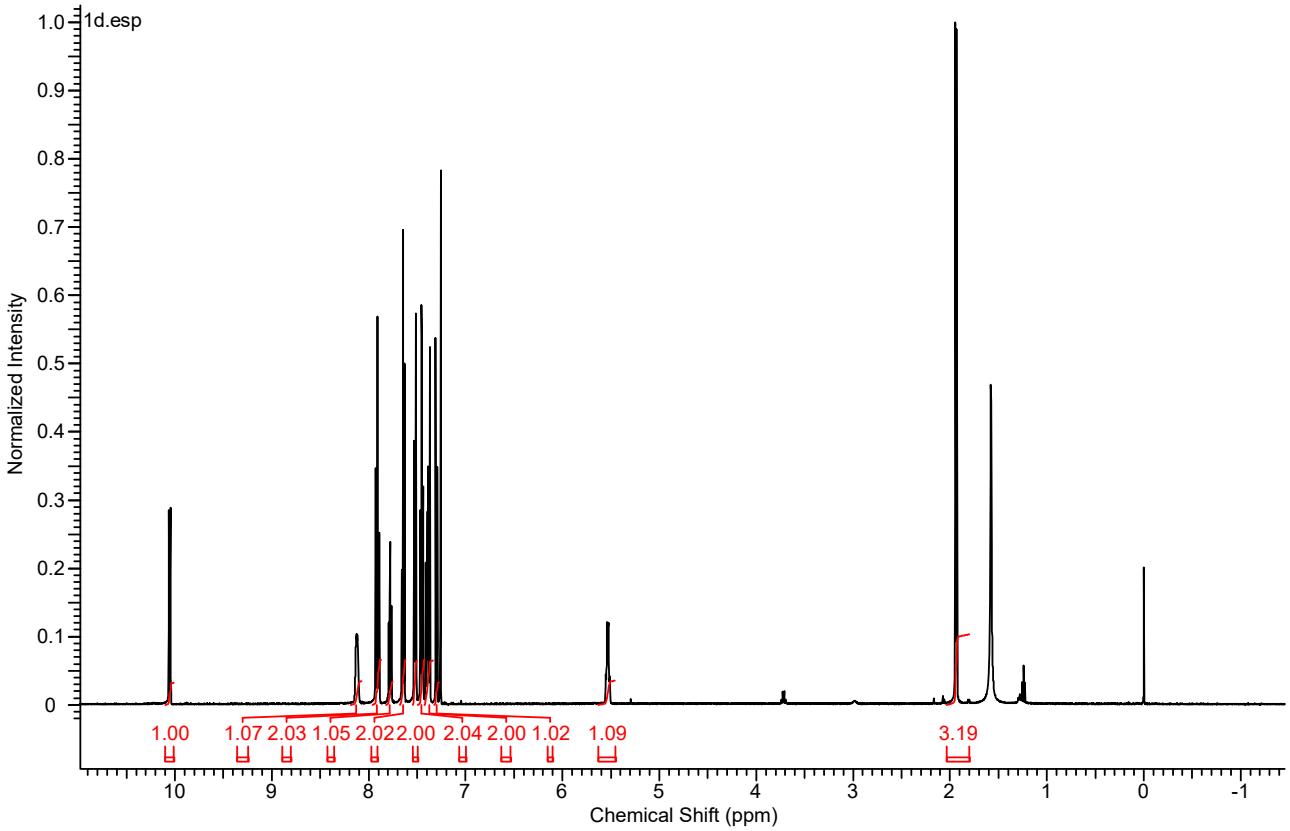


Fig. S3 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**1c** in $CDCl_3$.

(a)



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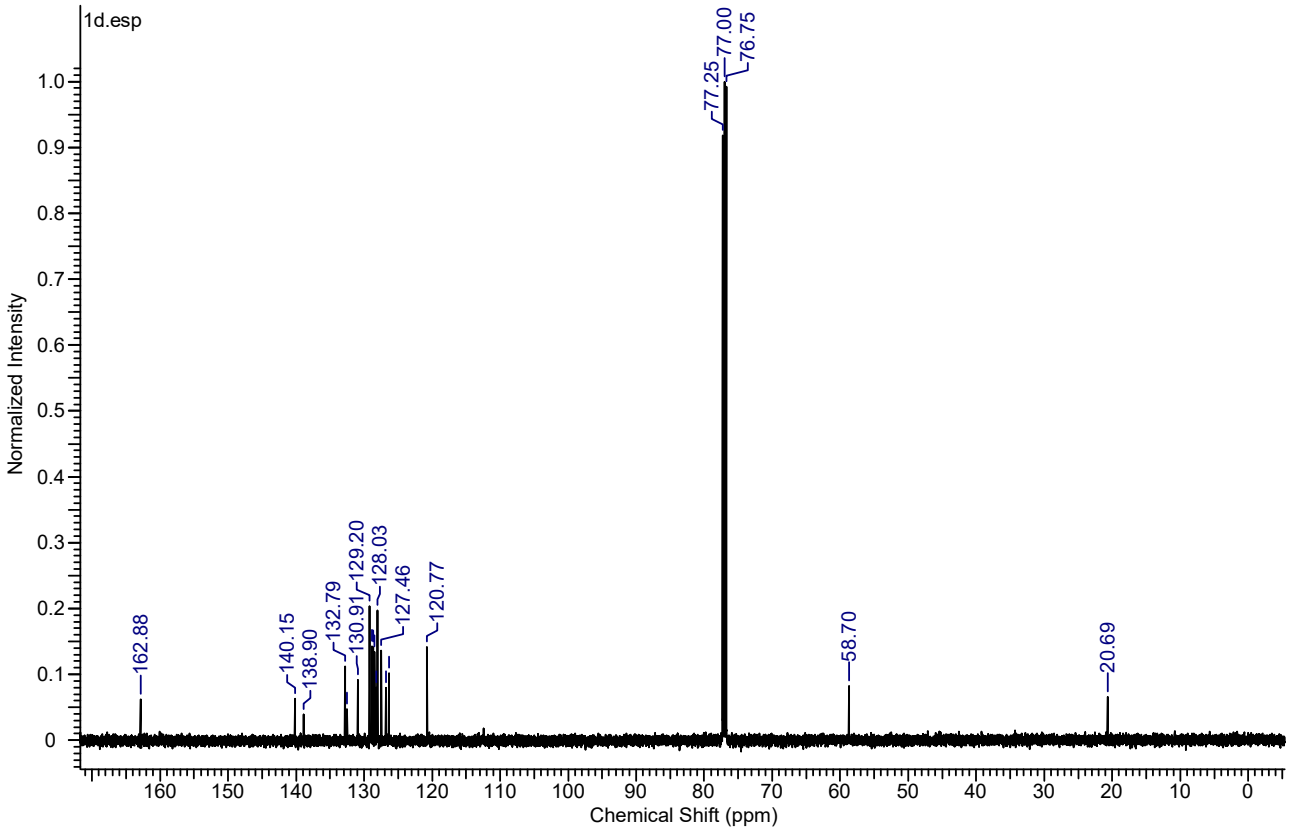
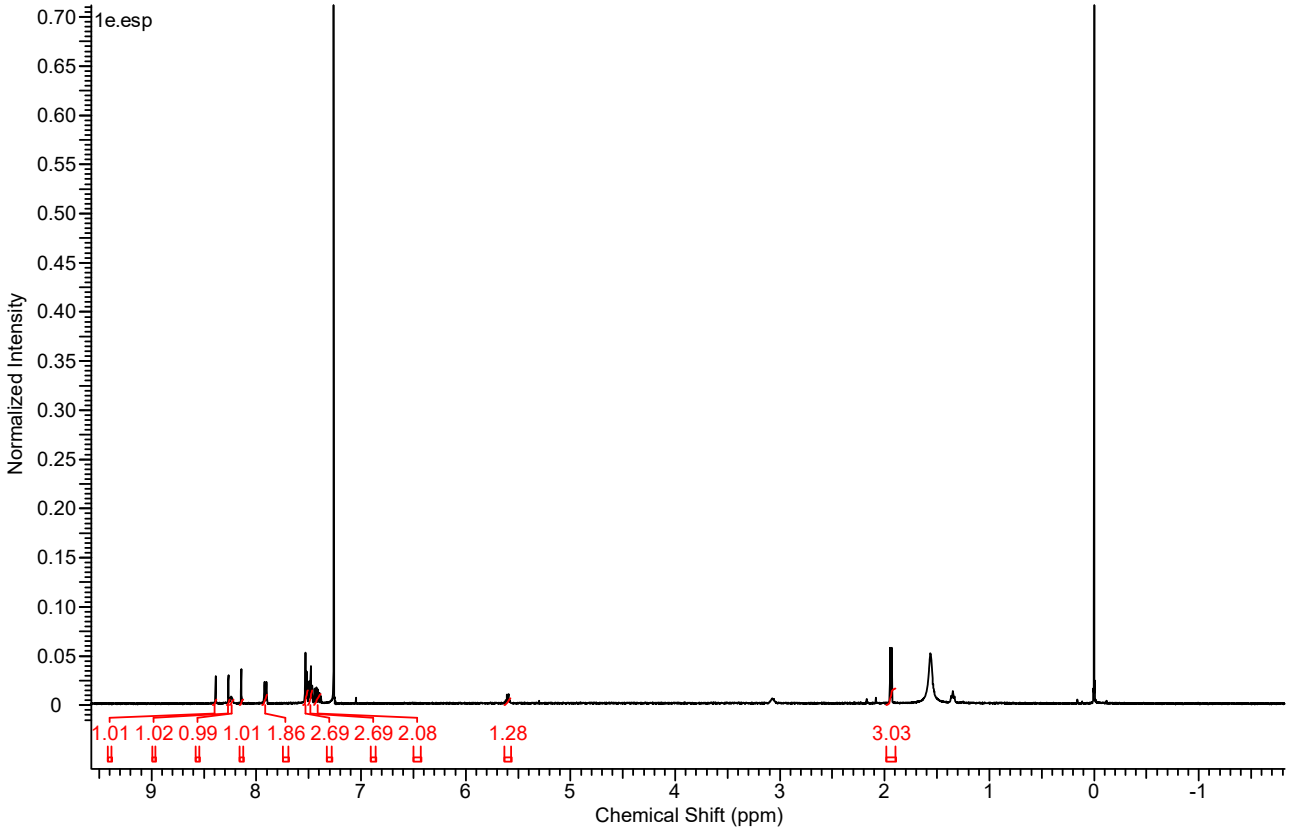


Fig. S4 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**1d** in $CDCl_3$.

(a)



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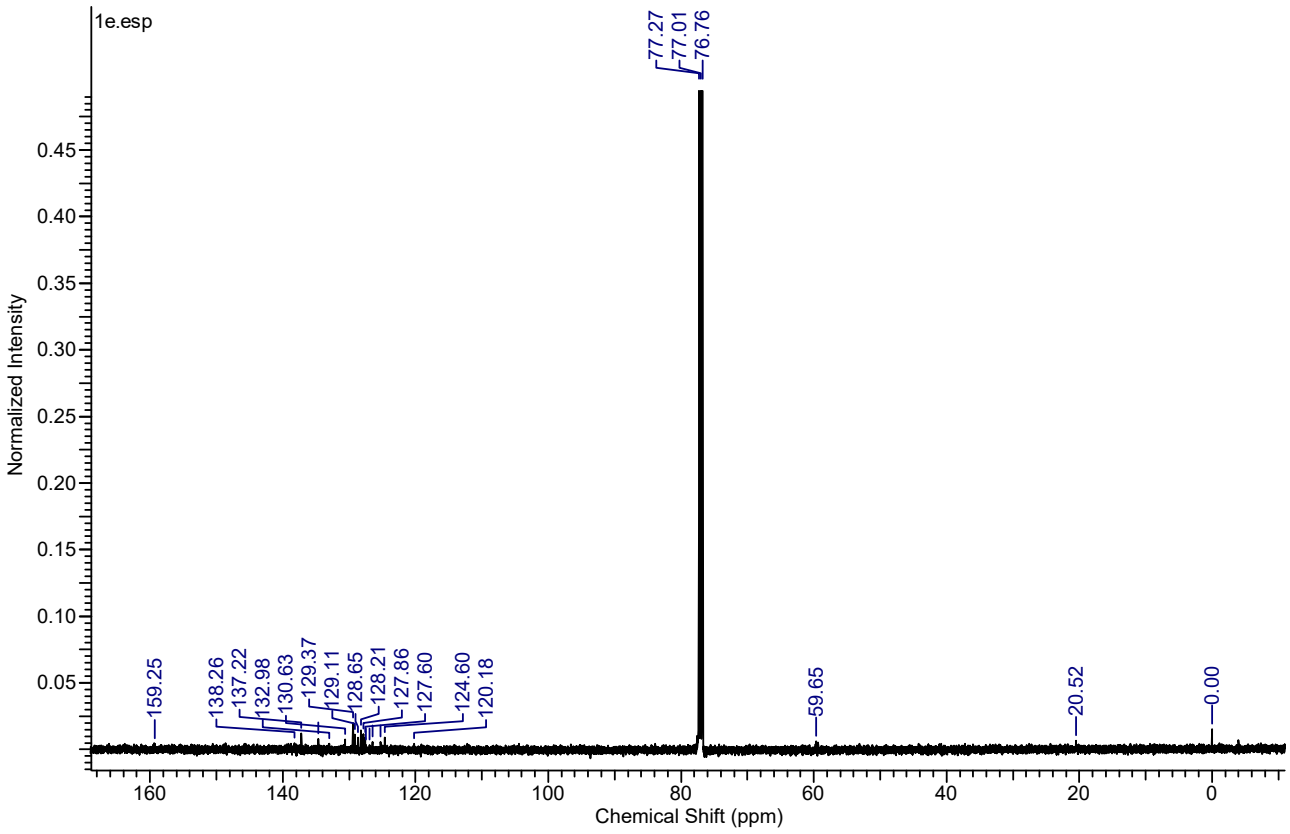
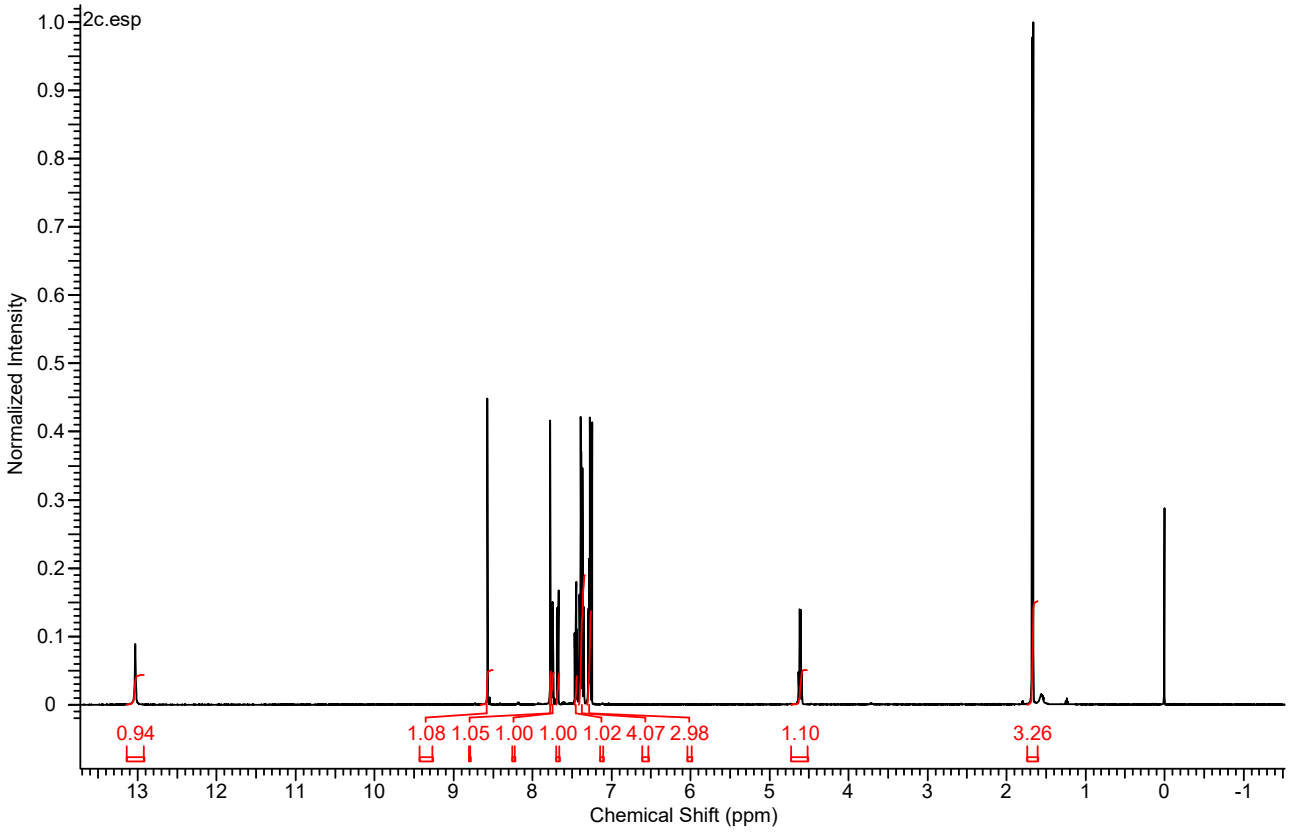


Fig. S5 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**1e** in $CDCl_3$.

(a)



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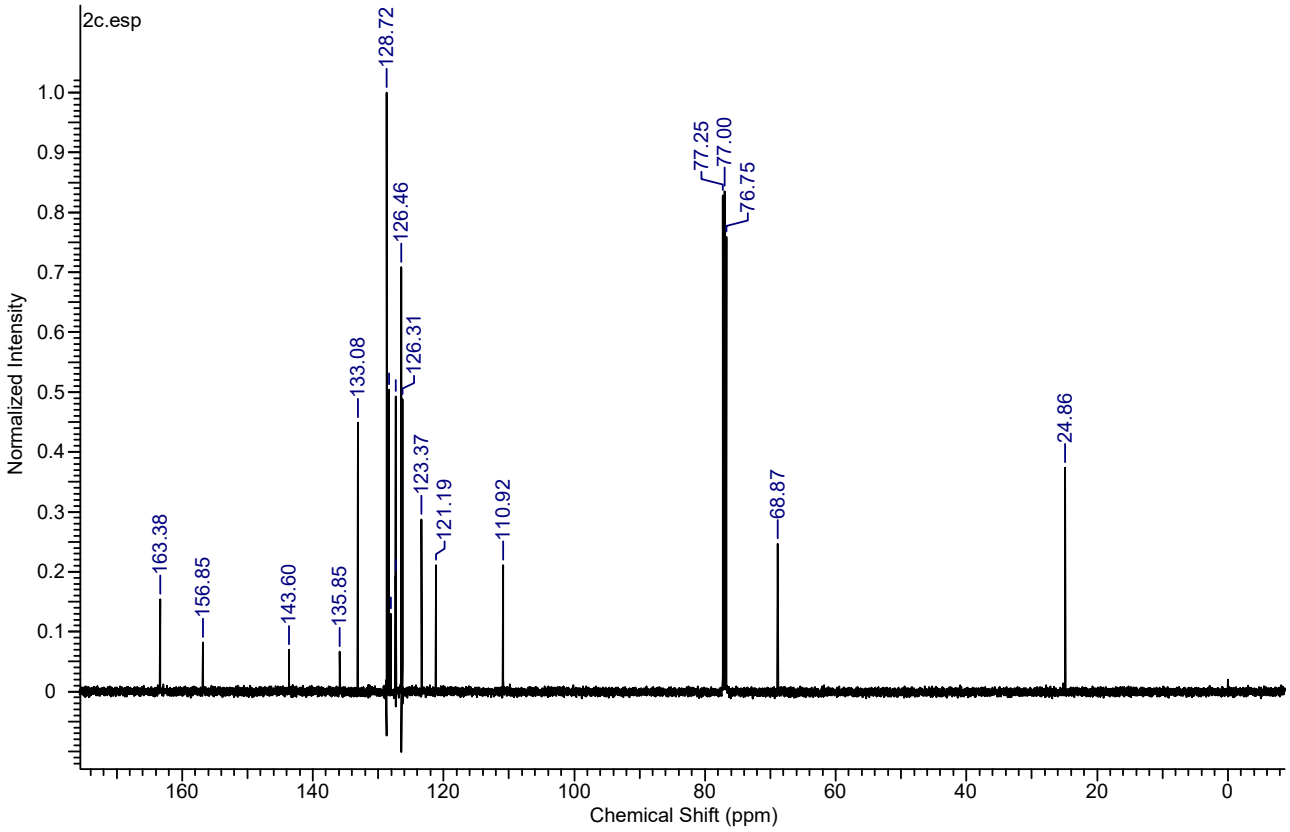
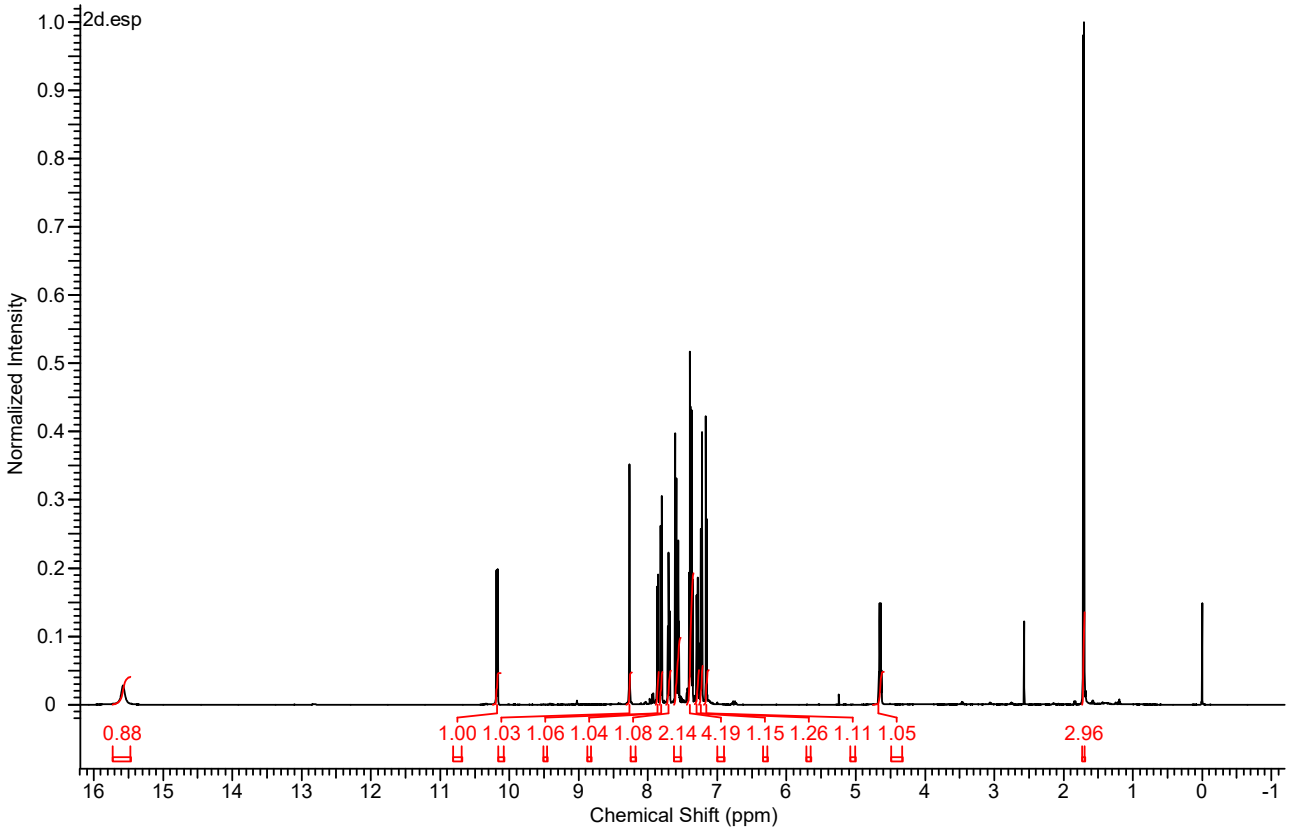


Fig. S6 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**2c** in $CDCl_3$.

(a)



(b)

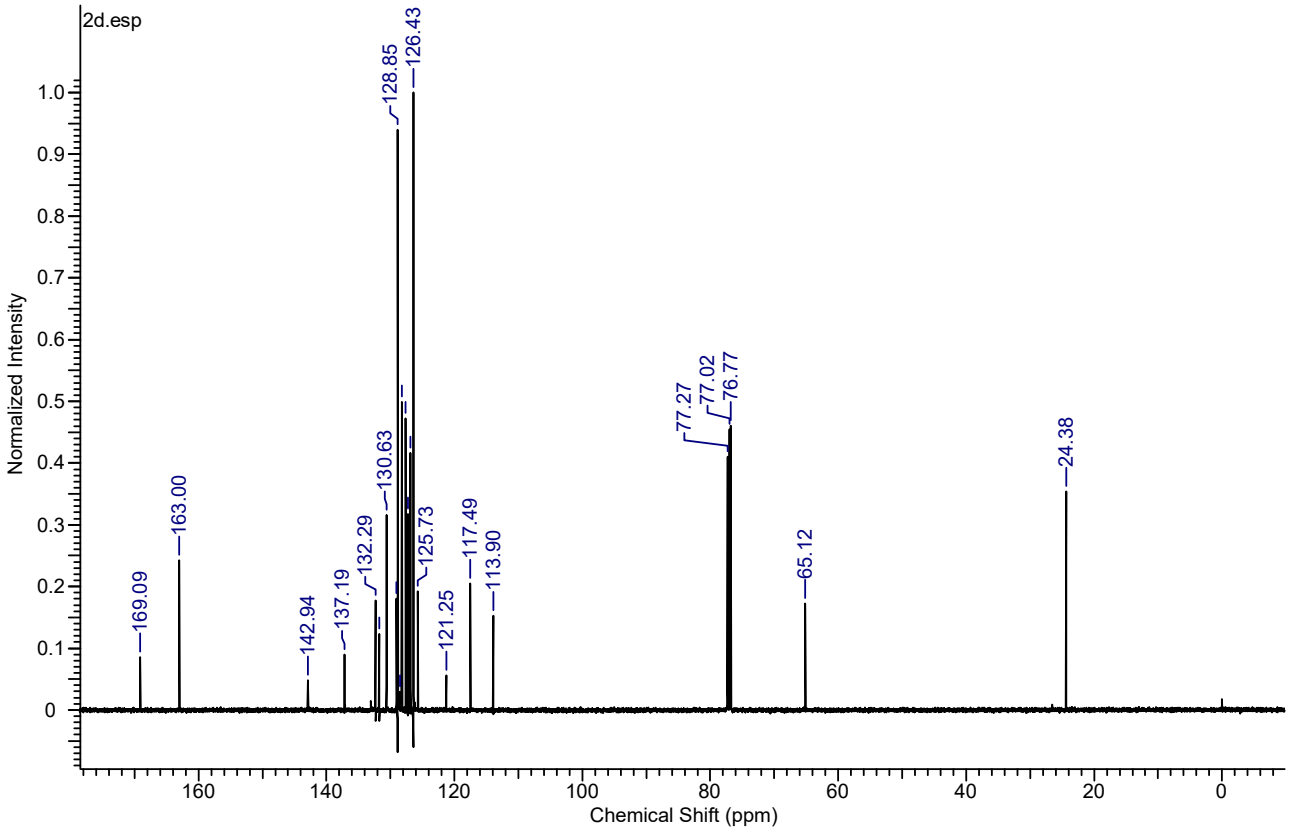
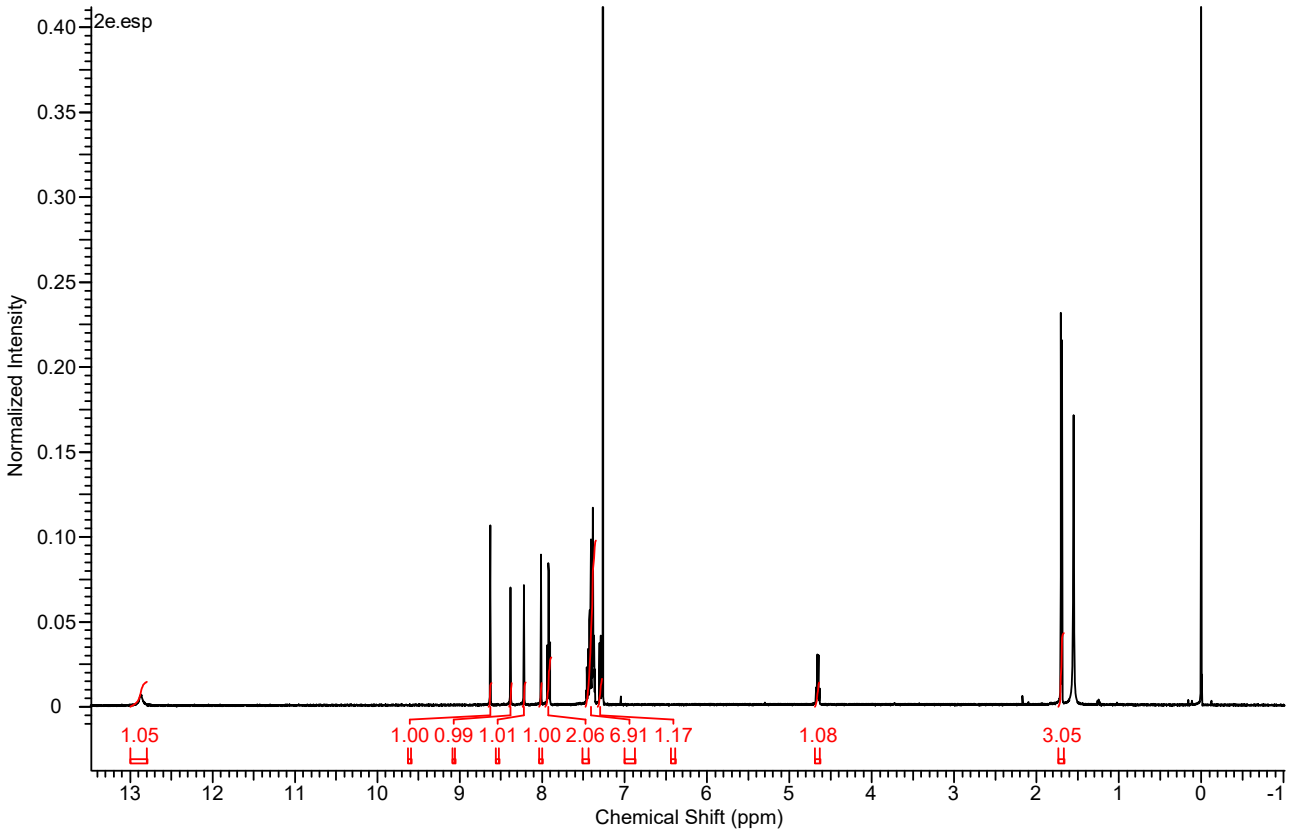


Fig. S7 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**2d** in $CDCl_3$.

(a)



(b)

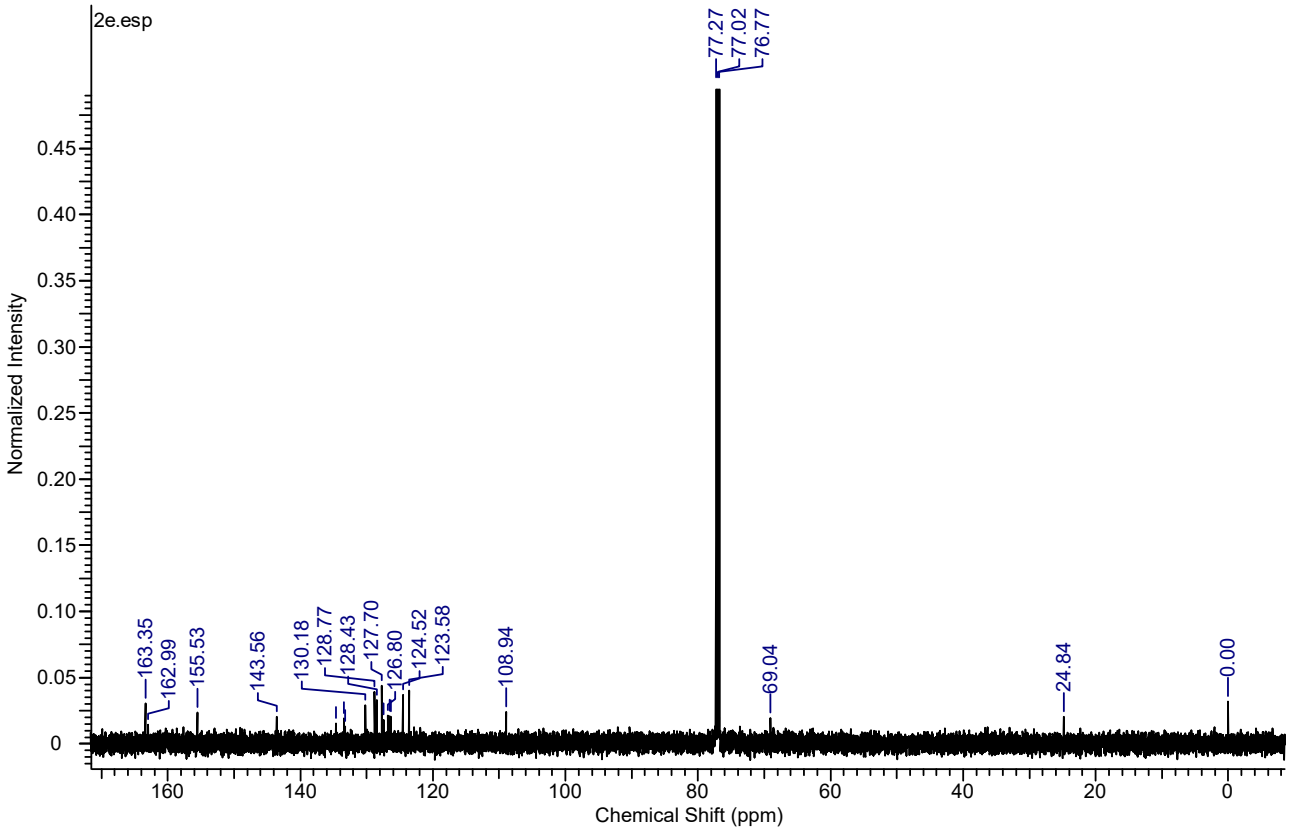


Fig. S8 (a) ^{1}H and (b) ^{13}C NMR spectra of (*S*)-**2e** in $CDCl_3$.

3. Single X-ray Structure Analysis

Crystals suitable for XRD studies were analyzed using Rigaku RAXIS-RAPID imaging plate diffractometer using Mo-K_α radiation (graphite monochromated, λ = 0.71073 Å, fine focus tube, ω-scan) and Rigaku XtaLAB mini2 benchtop X-ray crystallography system equipped with a Mo rotating-anode X-ray generator with monochromated Mo-K_α radiation (λ = 0.71073 Å). The molecular structures and packings in crystals (*S*)-**1a**–**d** were solved by direct methods and refined using the full-matrix least-squares method. In subsequent refinements, the function $\Sigma\omega(F_o^2 - F_c^2)^2$ was minimized, where F_o and F_c are the observed and calculated structure factor amplitudes, respectively. The positions of non-hydrogen atoms were found from difference Fourier electron density maps and refined anisotropically. All calculations were performed using the Crystal Structure crystallographic or CrysAlisPro program software package, and illustrations were drawn by using ORTEP.

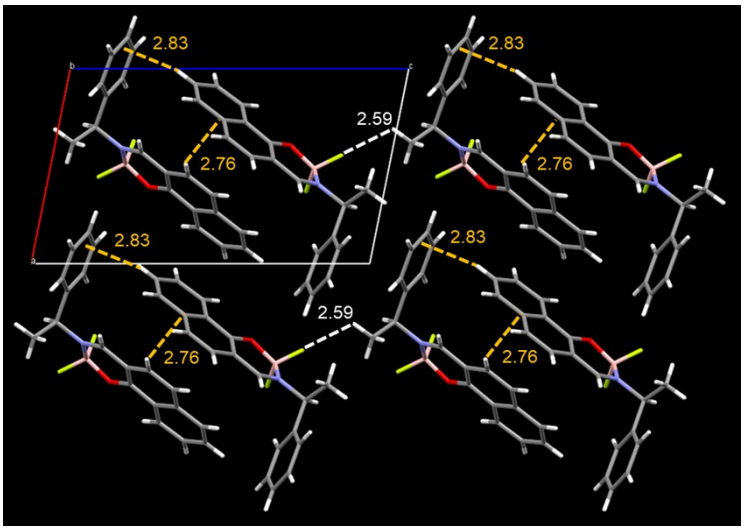


Fig. S9 Packing structure of (*S*)-**1a**. The *b*-axis projections showing CH-π (orange broken lines) and H··F (white broken lines) interactions.

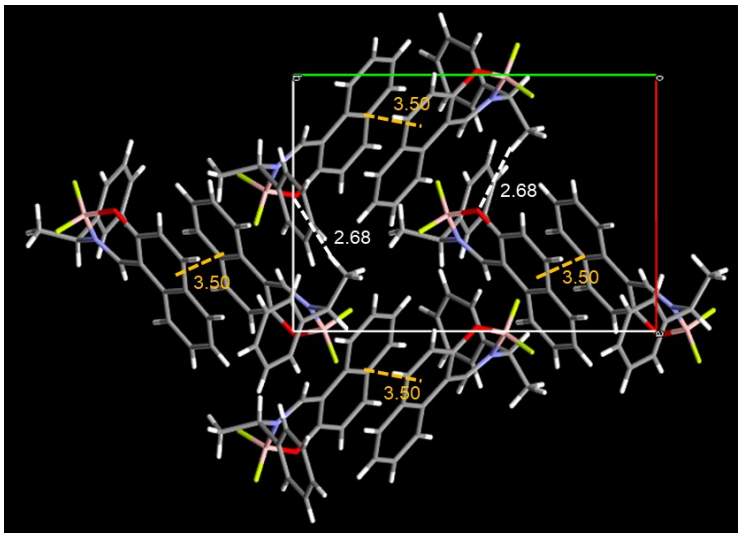


Fig. S10 Packing structure of (*S*)-**1b**. The *c*-axis projections showing π-π (orange broken lines) and H··O (white

broken lines) interactions.

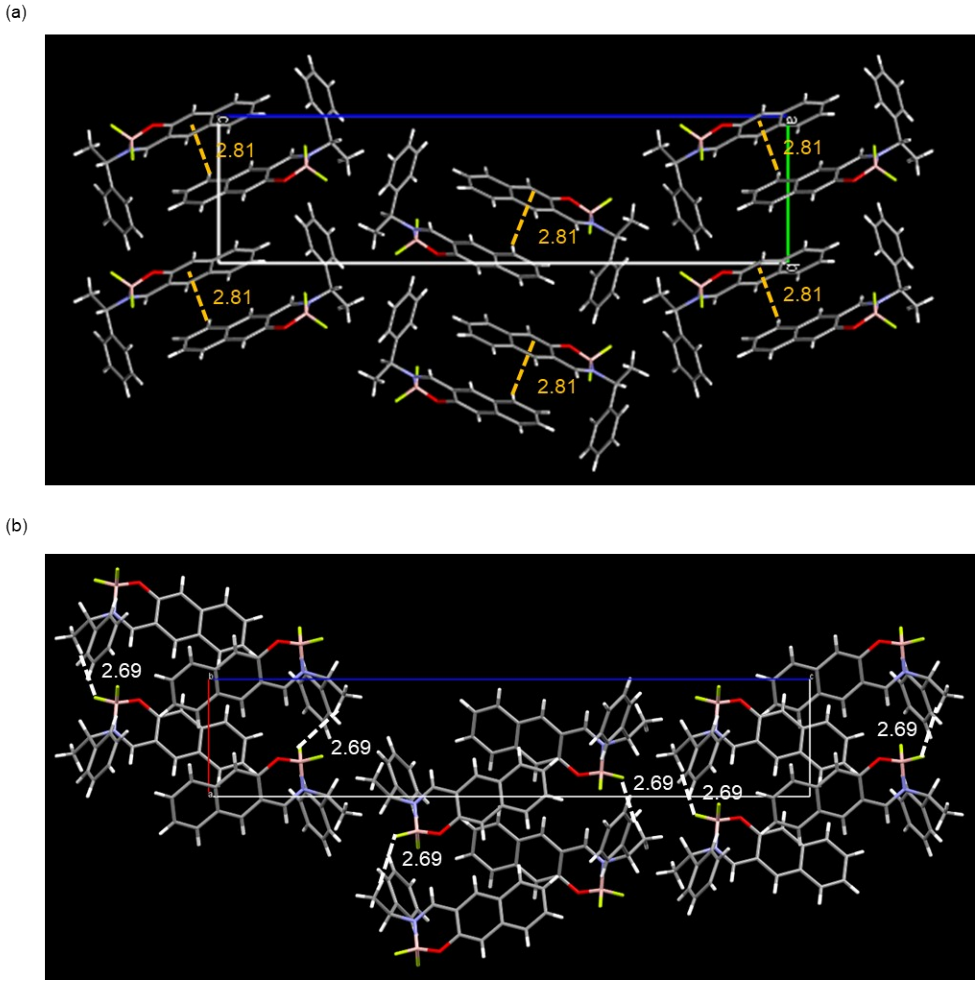


Fig. S11 Packing structure of (*S*)-**1c**. (a) The *a*-axis and (b) *b*-axis projections showing CH-π (orange broken lines) and H···F (white broken lines) interactions.

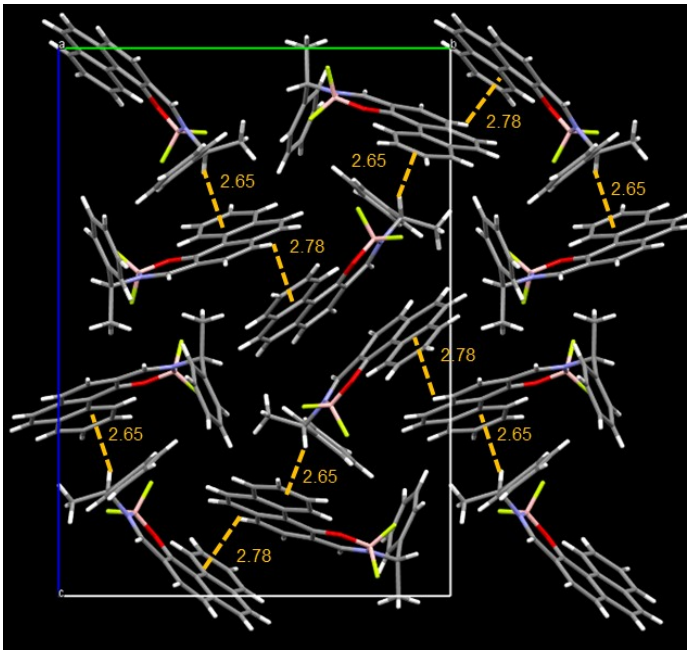


Fig. S12 Packing structure of (*S*)-**1d**. The *a*-axis projections showing CH-π (orange broken lines) interactions.

Table S1. Crystal data and structural refinement details for complexes (*S*)-**1a**–**d**.

	(*S*)-**1a**	(*S*)-**1b**	(*S*)-**1c**	(*S*)-**1d**
Formula	$C_{19}H_{16}BF_2NO$	$2(C_{19}H_{16}BF_2NO)$	$C_{19}H_{16}BF_2NO$	$C_{23}H_{18}BF_2NO$
M_F	323.14	646.27	323.14	373.19
T [K]	173.15	173.15	173.15	173.15
Crystal color, habit	colorless, plate	colorless, block	yellow, needle	colorless, plate
Crystal size [mm]	0.456×0.125×0.058	0.408×0.375×0.305	0.25×0.05×0.02	0.455×0.412×0.26
Crystal system	monoclinic	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1$ (#4)	$P2_1$ (#4)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)
a [Å]	8.7506(8)	10.3730(4)	6.1678(14)	9.7997(5)
b [Å]	6.4046(6)	13.9191(4)	8.1722(13)	16.3983(8)
c [Å]	14.9030(14)	11.5437(4)	31.570(5)	22.9360(11)
α [°]	90	90	90	90
β [°]	101.334(8)	108.664(4)	90	90
γ [°]	90	90	90	90
V [Å^3]	818.94(13)	1579.06(10)	1591.3(5)	3685.8(3)
Z	2	2	4	8
D_{calcd} [g cm^{-3}]	1.310	1.359	1.349	1.345
Abs coeff (mm^{-1})	0.095	0.099	0.098	0.095
Abs correct	multi-scan	multi-scan	multi-scan	multi-scan
Transmiss max/min	1.0000/0.58274	1.0000/0.96113	1.0000/0.24387	1.0000/0.92835
F (000)	336	672	672	1552
θ range (°)	4.748–60.886	4.144–60.998	5.148–61.086	4.334–60.712
Rflns/unique	15183/4710	27219/9216	14957/4620	38018/10595
R_{int}	0.0698	0.0347	0.1352	0.0360
Data/params	4710/1/218	9216/1/435	4620/32/218	10595/0/507
Largest diff. peak and hole (e Á$^{-3}$)	0.15/–0.19	0.16/–0.23	0.27/–0.25	0.84/–0.56
R_1 (I > 2σ(I))[a]	0.0508	0.0472	0.1104	0.0591
wR_2 (all reflections)[b]	0.1039	0.0964	0.1265	0.1493
Goodness of fit	0.957	0.981	1.004	1.049
Flack Parameter	0.2(6)	0.4(3)	0.3(10)	0.1(3)
CCDC No.	21511184	21511185	21511186	21511187

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

4. Chiroptical Properties

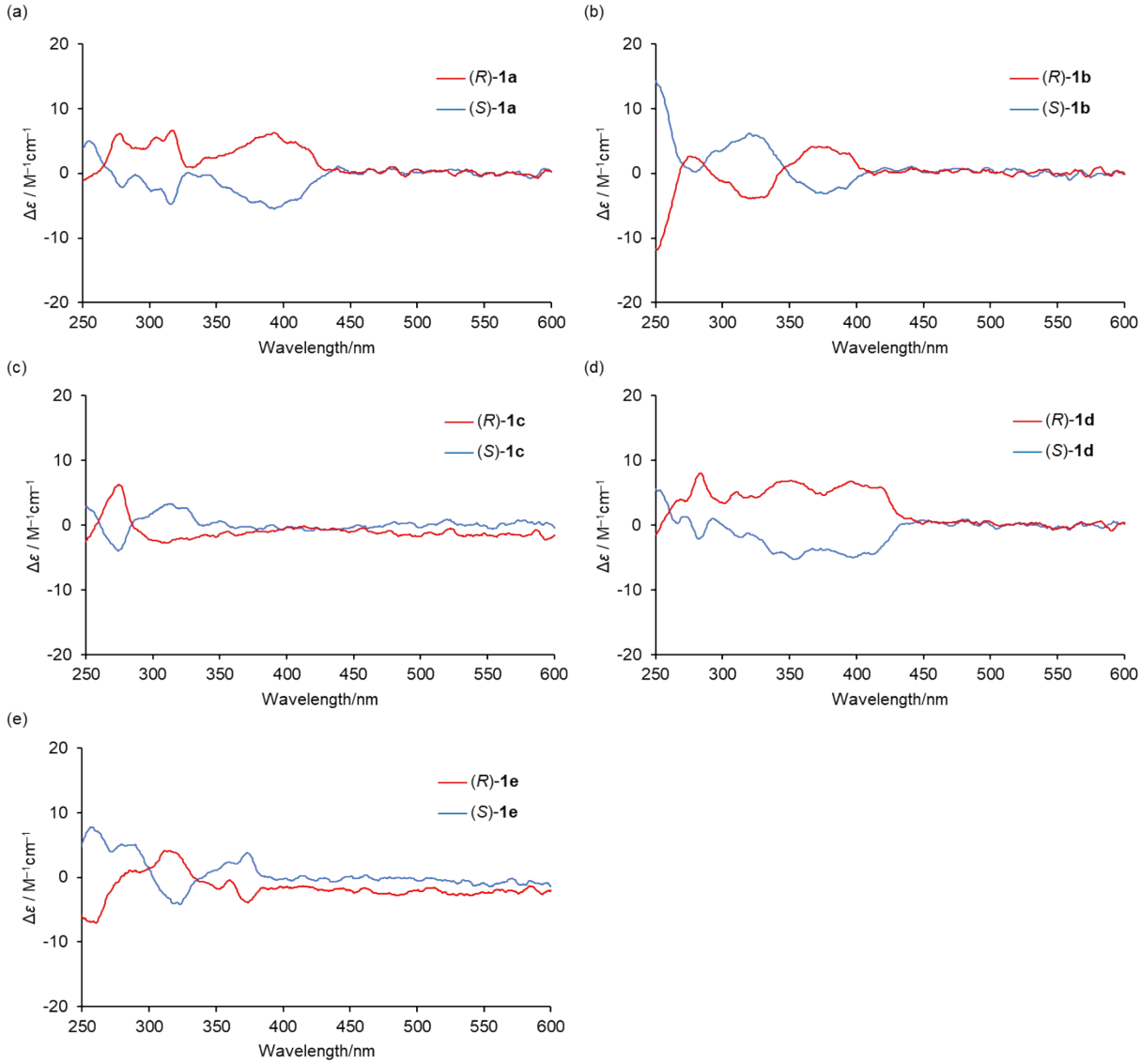


Fig. S13 CD spectra for 2.0× 10^{-4} M solutions of (a) **1a**, (b) **1b**, (c) **1c**, (d) **1d** and (e) **1e** in CH_2Cl_2 at 298 K.

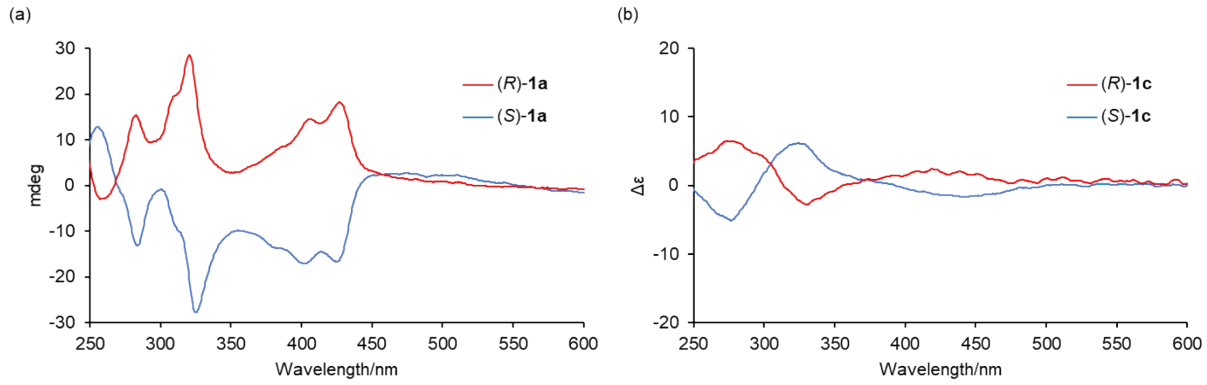


Fig. S14 CD spectra of (a) **1a** and (b) **1c** in the drop-cast film state at 298 K.

5. Computational Methods

All calculations were carried out based on DFT with the B3LYP exchange-correlation functional, using the Gaussian 16W program package.[S5] The basis set used was 6-31+G(d,p) for all atoms. Molecular orbitals and their eigenvalues for **1a**–**e** were estimated using the optimized geometries determined by the DFT calculations using initial geometries obtained from XRD analysis. The singlet–singlet (*E*(Sn)) transition energies were estimated by time-dependent (TD) DFT calculation (B3LYP/6-31+G(d,p)).

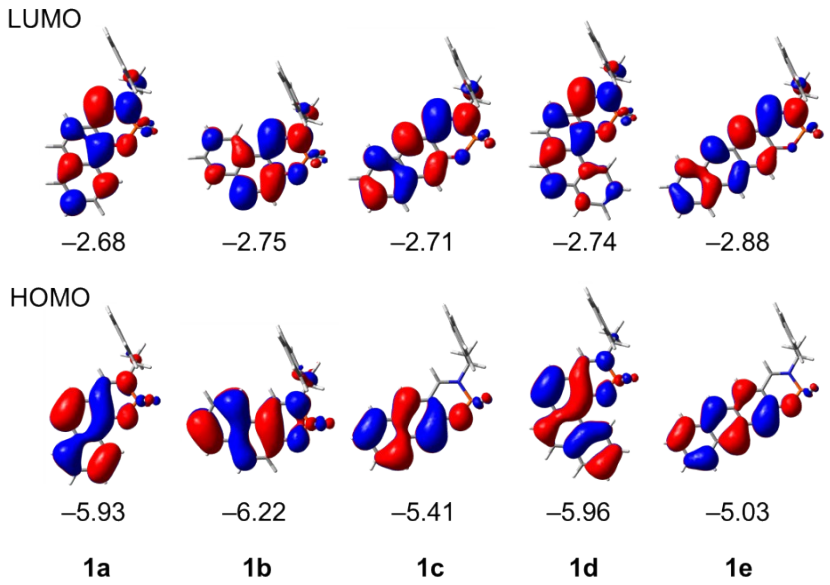


Fig. S15 Molecular orbitals (overhead views) and eigenvalues [eV] for the frontier orbitals of **1a**–**e** estimated from DFT calculations (B3LYP/6-31+G(d,p)) on the basis of the optimized geometries in the S_1 excited states.

Table S2. Selected data for excitation energy, major configuration, coefficient, and oscillator strength for **1** (for the geometries optimized in the S_0 state).[a]

Compound	State	Excitation energy (eV)	Major configuration[b]	Coefficient	Oscillator strength
(*S*)-**1a**	S_1	3.22 (385 nm)	HOMO→LUMO	0.693	0.1362
(*S*)-**1b**	S_1	3.41 (364 nm)	HOMO→LUMO	0.698	0.1775
(*S*)-**1c**	S_1	2.83 (439 nm)	HOMO→LUMO	0.700	0.0297
(*S*)-**1d**	S_1	3.15 (394 nm)	HOMO→LUMO	0.631	0.1675
(*S*)-**1e**	S_1	2.26 (549 nm)	HOMO→LUMO	0.699	0.0272

[a] Estimated by TD-DFT (B3LYP/6-31+G(d,p)) calculations based on the optimized geometries. [b] Molecular orbitals are shown in Fig. 8.

Table S3. Selected data for excitation energy, major configuration, coefficient, and oscillator strength for **1** (for the geometries optimized in the S_1 state).[a]

Compound	State	Excitation energy (eV)	Major configuration[b]	Coefficient	Oscillator strength
(*S*)-**1a**	S_1	2.82 (440 nm)	HOMO→LUMO	0.699	0.1099
(*S*)-**1b**	S_1	3.10 (401 nm)	HOMO→LUMO	0.700	0.1638
(*S*)-**1c**	S_1	2.16 (574 nm)	HOMO→LUMO	0.705	0.0236
(*S*)-**1d**	S_1	2.74 (453 nm)	HOMO→LUMO	0.684	0.0785
(*S*)-**1e**	S_1	1.67 (740 nm)	HOMO→LUMO	0.705	0.0169

[a] Estimated by TD-DFT (B3LYP/6-31+G(d,p)) calculations based on the optimized geometries. [b] Molecular orbitals are shown in Fig. S15.

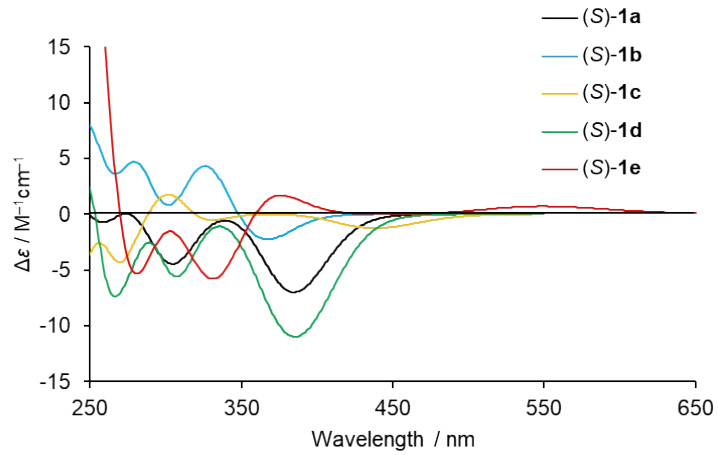


Fig. S16 Theoretical CD spectra of (*S*)-**1a**–**e** estimated by TD-DFT calculation (B3LYP/6-31+G(d,p)).

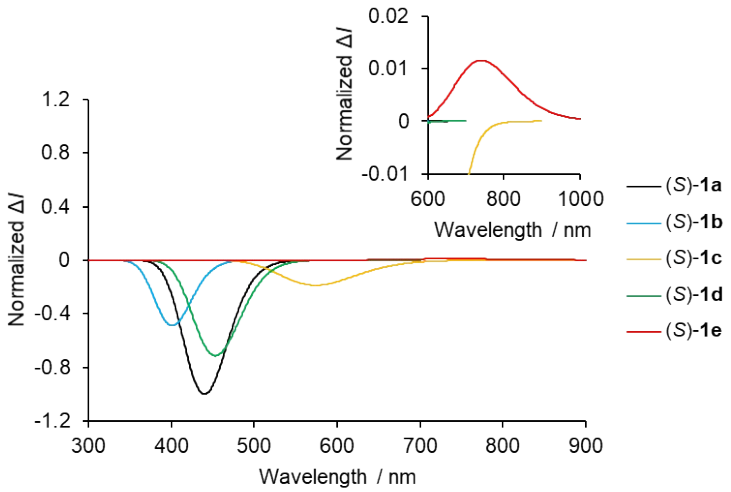


Fig. S17 Theoretical CPL spectra of (*S*)-**1a**–**e** estimated by TD-DFT calculation (B3LYP/6-31+G(d,p)). The insets show the enlarged spectra.

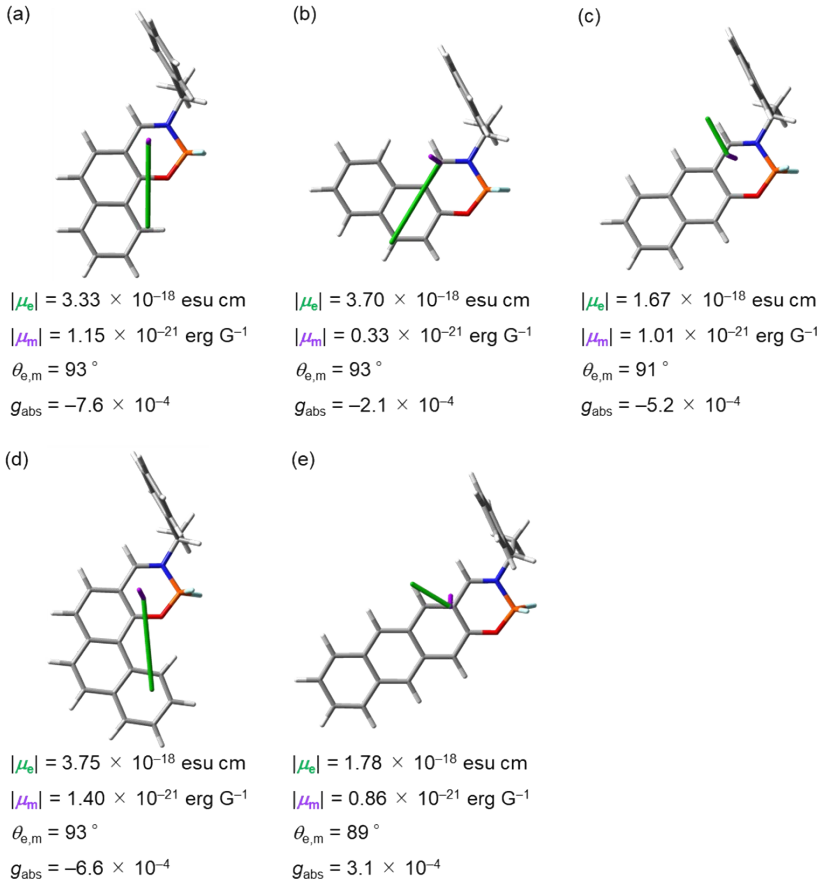


Fig. S18 Electric (μ_e, orange) and magnetic (μ_m, purple) dipole moments of the $S_0 \rightarrow S_1$ transition for (a) (*S*)-**1a**, (b) (*S*)-**1b**, (c) (*S*)-**1c**, (d) (*S*)-**1d** and (e) (*S*)-**1e** calculated at the B3LYP/6-31+G(d,p) level. Calculated values of transition dipole moments ($|\mu_e|$, $|\mu_m|$, and $\theta_{e,m}$) and g_{abs} are given under each structure.

6. Cartesian Coordinates (in Å)

Table S4. Cartesian coordinates (in angstrom) of (*S*)-**1a** in S_0 state[a].

atom	x	y	z
F	-0.525698	2.095979	1.557689
O	1.299079	1.459622	0.20891
F	-0.256406	3.056599	-0.514982
N	-1.022627	0.766223	-0.378472
C	0.814641	-0.767151	-0.477971
C	1.709178	0.235578	-0.052356
C	-0.556457	-0.4217	-0.641963
H	-1.250402	-1.182198	-1.00041
C	3.106564	-0.065506	0.085886
C	3.557235	-1.390914	-0.204933
C	1.295581	-2.08455	-0.760909
H	0.583687	-2.839787	-1.083962
C	2.620486	-2.390002	-0.628701
H	2.982136	-3.391028	-0.842996
C	4.938172	-1.675189	-0.061557
H	5.291586	-2.679391	-0.27952
C	4.031768	0.921319	0.505368
H	3.664298	1.918124	0.721912
C	5.825542	-0.697378	0.347735
H	6.880425	-0.934899	0.451578
C	5.371463	0.610265	0.633566
H	6.07787	1.369288	0.95532
B	-0.109127	1.899504	0.240031
C	-2.461468	1.102045	-0.614489
H	-2.621909	2.011126	-0.029535
C	-2.667884	1.454761	-2.092386
H	-1.991776	2.266855	-2.367817
H	-2.46438	0.60093	-2.747506
H	-3.697058	1.784879	-2.262752
C	-3.383909	0.02499	-0.049883
C	-4.181292	-0.795985	-0.856532
H	-4.172365	-0.679441	-1.935459
C	-3.438066	-0.142969	1.344545
H	-2.823623	0.490464	1.97952
C	-5.05418	-1.929429	1.099543
H	-5.700324	-2.681513	1.5428
C	-4.26332	-1.111381	1.914565
H	-4.294199	-1.224634	2.994374
C	-5.011932	-1.767942	-0.285387
H	-5.626366	-2.393212	-0.926886

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G (d,p)).

Table S5. Cartesian coordinates (in angstrom) of (*S*)-**1b** in S_0 state[a].

atom	x	y	z
F	-1.120361	-2.603597	-1.516266
F	-1.107032	-3.477998	0.612124
O	0.889832	-2.642146	-0.280121
N	-0.938303	-1.081368	0.329031
C	1.323957	-0.319214	0.082801
C	-0.051854	-0.127525	0.398837
H	-0.398258	0.850397	0.723765
C	2.293252	0.757003	0.124897
C	1.737206	-1.634275	-0.225661
C	-2.357975	-0.843287	0.736422
H	-2.90935	-1.664725	0.271916
C	3.667273	0.444822	-0.118647
C	1.958779	2.109528	0.386233
H	0.926743	2.397565	0.554671
C	-2.89573	0.459485	0.150228
C	-3.056002	0.547947	-1.24345
H	-2.789218	-0.30434	-1.863543
C	-3.545413	1.712883	-1.832572
H	-3.66521	1.761534	-2.91101
C	4.641772	1.472451	-0.080509
H	5.680224	1.211945	-0.268148
C	-3.243974	1.563935	0.93735
H	-3.145781	1.520128	2.01724
C	-3.887816	2.812671	-1.037389
H	-4.273084	3.719185	-1.495008
C	4.286335	2.779773	0.18639
H	5.039566	3.560929	0.212979
C	2.931145	3.093914	0.418714
H	2.643006	4.12156	0.620213
C	-3.73743	2.734178	0.347199
H	-4.006529	3.579378	0.974334
C	-2.485706	-0.997515	2.256708
H	-1.905452	-0.23892	2.792912
H	-3.533568	-0.911625	2.559718
H	-2.118161	-1.982526	2.551713
C	4.035293	-0.907794	-0.402895
H	5.084396	-1.127321	-0.584653
C	3.113288	-1.917082	-0.457585
H	3.390821	-2.94181	-0.67851
B	-0.576506	-2.512327	-0.233197

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

Table S6. Cartesian coordinates (in angstrom) of (*S*)-**1c** in S_0 state[a].

atom	x	y	z
F	1.113634	3.297722	0.477342
F	1.30166	2.276346	-1.570889
O	-0.762713	2.232249	-0.430029
N	1.199441	0.900003	0.369048
C	-1.811476	-1.144898	0.545885
H	-1.376153	-2.061769	0.937474
C	-3.191956	-1.091182	0.288603
C	0.414413	-0.103815	0.590779
H	0.835696	-1.024979	0.995539
C	-1.537835	1.177066	-0.209261
C	3.289557	-0.427661	0.135504
C	-0.989241	-0.046577	0.308953
C	-2.899162	1.24455	-0.46259
H	-3.307895	2.171448	-0.851074
C	2.655753	0.838612	0.697552
H	3.082029	1.688191	0.159793
C	-3.742698	0.137299	-0.226244
C	3.848717	-1.425545	0.939369
H	3.851895	-1.320582	2.019532
C	3.315972	-0.585583	-1.2601
H	2.876807	0.188358	-1.884432
C	2.844746	1.09248	2.195712
H	2.376683	2.044496	2.453214
H	3.909091	1.147781	2.440588
H	2.389152	0.304889	2.80482
C	-5.143016	0.187632	-0.48379
H	-5.568005	1.108728	-0.872196
C	4.423176	-2.562719	0.362228
H	4.856667	-3.327865	0.999673
C	-4.053858	-2.201953	0.520858
H	-3.624448	-3.12197	0.909003
C	-5.398268	-2.113709	0.260014
H	-6.049196	-2.963683	0.43908
C	3.886373	-1.718062	-1.833938
H	3.901808	-1.824991	-2.91459
C	-5.94392	-0.903747	-0.247678
H	-7.009325	-0.844682	-0.450639
C	4.442785	-2.711892	-1.022713
H	4.8909	-3.594054	-1.470362
B	0.694377	2.252855	-0.322292

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

Table S7. Cartesian coordinates (in angstrom) of (*S*)-**1d** in S_0 state[a].

atom	x	y	z
O	-0.711719	-1.054567	-0.123207
F	0.6556	-2.787444	-0.894841
F	0.900185	-2.060303	1.273107
N	1.711145	-0.648818	-0.487454
C	-0.968544	0.237926	-0.220196
C	-3.484747	-0.129507	0.119799
C	-3.439761	-1.543556	0.252672
H	-2.493814	-2.054614	0.183765
C	-2.317184	0.721531	-0.110603
C	3.101244	-1.154402	-0.70732
H	3.107744	-2.133842	-0.222186
C	1.421006	0.614187	-0.610701
H	2.228621	1.309931	-0.838581
C	0.1043	1.135873	-0.458924
C	-0.129767	2.530687	-0.577272
H	0.710405	3.196281	-0.756717
C	-2.499542	2.134347	-0.233013
C	-4.773995	0.491424	0.218704
C	-3.810041	2.697647	-0.124859
H	-3.916315	3.774424	-0.220355
C	-4.589889	-2.285724	0.469365
H	-4.509388	-3.364617	0.565398
C	4.131156	-0.282401	0.005685
C	-5.931155	-0.293044	0.440876
H	-6.891912	0.210551	0.510978
C	-1.402381	3.015795	-0.462541
H	-1.600558	4.079726	-0.546243
C	-5.848807	-1.665675	0.56602
H	-6.742551	-2.258555	0.736423
C	5.070684	0.500523	-0.676067
H	5.099154	0.501964	-1.760924
C	-4.899221	1.910265	0.092107
H	-5.889396	2.351463	0.172436
C	3.331869	-1.374572	-2.207259
H	2.567551	-2.051261	-2.595099
H	4.314677	-1.824485	-2.377089
H	3.277402	-0.436248	-2.769517
B	0.614816	-1.689414	-0.043172
C	4.138393	-0.272689	1.411176
H	3.413381	-0.8778	1.949924
C	5.995656	1.28074	0.028605
H	6.719731	1.878842	-0.517293

C	5.990795	1.286601	1.423545
H	6.709801	1.889747	1.970223

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

Table S8. Cartesian coordinates (in angstrom) of (*S*)-**1e** in S_0 state[a].

atom	x	y	z
F	-2.670913	-3.233049	0.547445
F	-2.652756	-2.242514	-1.52474
O	-0.630177	-2.509374	-0.336386
N	-2.366258	-0.855448	0.386587
C	0.913166	0.705449	0.521499
H	0.620611	1.691498	0.875762
C	2.280332	0.436904	0.279264
C	-1.437724	0.021768	0.583743
H	-1.712183	1.01039	0.954128
C	0.304132	-1.579855	-0.154152
C	-4.222188	0.776472	0.104166
C	-0.057322	-0.261372	0.316411
C	1.632295	-1.862794	-0.391311
H	1.897049	-2.854892	-0.741337
C	-3.797668	-0.561198	0.696713
H	-4.346367	-1.345321	0.170618
C	2.645908	-0.886704	-0.188019
C	-4.626318	1.865019	0.882867
H	-4.654508	1.783692	1.9647
C	-4.212264	0.908261	-1.294383
H	-3.89326	0.063146	-1.899132
C	-4.035215	-0.752387	2.197358
H	-3.72299	-1.760209	2.477364
H	-5.097093	-0.63668	2.431547
H	-3.467152	-0.032913	2.796108
C	4.002753	-1.154361	-0.42622
H	4.290473	-2.142129	-0.776948
C	-5.012859	3.065462	0.278052
H	-5.327779	3.901226	0.896125
C	3.277115	1.406549	0.480066
H	2.989153	2.39515	0.830525
C	4.624447	1.131418	0.240649
C	-4.595422	2.103539	-1.895765
H	-4.585214	2.189672	-2.978324
C	4.994918	-0.188465	-0.225974
C	-4.99778	3.187735	-1.109582
H	-5.30012	4.119354	-1.578706
B	-2.069942	-2.291847	-0.264865
C	6.379254	-0.457897	-0.467407
H	6.660933	-1.447136	-0.817701
C	5.651889	2.107404	0.440279
H	5.366371	3.095898	0.790498

C	6.964163	1.806055	0.196677
H	7.735535	2.554264	0.351524

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

Table S9. Cartesian coordinates (in angstrom) of (*S*)-**1a** in S_1 state[a].

atom	x	y	z
F	0.530165	1.964817	1.577399
O	-1.284564	1.453445	0.173615
F	0.311491	3.049884	-0.440419
N	1.049706	0.748891	-0.440521
C	-0.817638	-0.766441	-0.561254
C	-1.713003	0.238127	-0.092376
C	0.577844	-0.46728	-0.748359
H	1.258952	-1.233724	-1.101359
C	-3.1108	-0.043846	0.080847
C	-3.620082	-1.360944	-0.219763
C	-1.347292	-2.029109	-0.837854
H	-0.680116	-2.808912	-1.19709
C	-2.719497	-2.336919	-0.675148
H	-3.072392	-3.337206	-0.90679
C	-5.007546	-1.629898	-0.045063
H	-5.376258	-2.626071	-0.274676
C	-4.009816	0.933814	0.540265
H	-3.631876	1.923857	0.769652
C	-5.875548	-0.646408	0.408842
H	-6.930908	-0.860651	0.538556
C	-5.368806	0.635709	0.700559
H	-6.040988	1.410448	1.057263
B	0.162771	1.840119	0.230891
C	2.474385	1.073295	-0.671943
H	2.641458	2.006933	-0.127182
C	2.716751	1.365904	-2.161285
H	2.051544	2.17237	-2.478166
H	2.513272	0.489106	-2.785284
H	3.751293	1.681706	-2.330074
C	3.39698	0.020958	-0.051255
C	4.273474	-0.769396	-0.804081
H	4.326725	-0.652536	-1.881712
C	3.366495	-0.152391	1.343327
H	2.685244	0.453392	1.93528
C	5.061716	-1.877035	1.202545
H	5.705557	-2.606262	1.686055
C	4.189435	-1.090703	1.964556
H	4.154251	-1.206499	3.044276
C	5.100849	-1.713135	-0.182099
H	5.77664	-2.314471	-0.784067

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G (d,p)).

Table S10. Cartesian coordinates (in angstrom) of (*S*)-**1b** in S_1 state[a].

atom	x	y	z
F	-1.162399	-2.572116	-1.462523
F	-1.073053	-3.455737	0.66274
O	0.882465	-2.615815	-0.304247
N	-0.942559	-1.061758	0.396441
C	1.331816	-0.296414	0.124441
C	-0.03918	-0.082143	0.473968
H	-0.385403	0.892091	0.796026
C	2.315803	0.733183	0.142655
C	1.75552	-1.63195	-0.256192
C	-2.343913	-0.817912	0.804658
H	-2.903393	-1.665322	0.398118
C	3.694276	0.417431	-0.165188
C	1.988815	2.0978	0.459327
H	0.960028	2.362068	0.671291
C	-2.903175	0.447853	0.152356
C	-3.010568	0.481737	-1.249227
H	-2.687527	-0.382123	-1.824575
C	-3.518228	1.605839	-1.898938
H	-3.598451	1.610931	-2.982328
C	4.637528	1.451274	-0.117466
H	5.676004	1.220737	-0.339574
C	-3.316932	1.568321	0.88315
H	-3.256613	1.56769	1.966768
C	-3.928755	2.721366	-1.159364
H	-4.327795	3.59627	-1.664592
C	4.283713	2.776356	0.207368
H	5.051141	3.543708	0.230613
C	2.949993	3.098693	0.492804
H	2.667602	4.117988	0.732805
C	-3.827054	2.698551	0.231963
H	-4.148499	3.556017	0.816778
C	-2.467104	-0.883206	2.33599
H	-1.882005	-0.096378	2.824112
H	-3.513446	-0.78082	2.641352
H	-2.096487	-1.850414	2.682386
C	4.064947	-0.9196	-0.50678
H	5.102752	-1.139464	-0.733962
C	3.101783	-1.913652	-0.555259
H	3.349234	-2.935406	-0.822022
B	-0.593116	-2.465845	-0.187573

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

Table S11. Cartesian coordinates (in angstrom) of (*S*)-**1c** in S_1 state[a].

atom	x	y	z
F	0.997533	3.261329	0.531807
F	1.332141	2.29289	-1.523374
O	-0.764362	2.115855	-0.495017
N	1.227323	0.873633	0.408144
C	-1.862823	-1.142253	0.601697
H	-1.487081	-2.063765	1.041731
C	-3.273879	-1.074376	0.302183
C	0.419043	-0.168365	0.667115
H	0.843809	-1.075954	1.08061
C	-1.52853	1.095295	-0.228327
C	3.33932	-0.399949	0.146567
C	-0.982921	-0.111836	0.362479
C	-2.899781	1.192849	-0.52954
H	-3.248648	2.120493	-0.971403
C	2.655802	0.814244	0.776759
H	3.099974	1.701741	0.317086
C	-3.799488	0.124836	-0.27465
C	3.951183	-1.410477	0.893893
H	3.959214	-1.359227	1.977925
C	3.356938	-0.49307	-1.254673
H	2.875164	0.288034	-1.83657
C	2.822861	0.957696	2.295659
H	2.34513	1.886881	2.613688
H	3.881096	0.996832	2.570791
H	2.354206	0.129134	2.836283
C	-5.174329	0.203352	-0.569421
H	-5.567287	1.116407	-1.007544
C	4.567976	-2.493488	0.258568
H	5.039918	-3.268905	0.85555
C	-4.140663	-2.134214	0.556325
H	-3.751046	-3.049497	0.993582
C	-5.517197	-2.038631	0.254712
H	-6.16885	-2.880883	0.46389
C	3.971216	-1.569686	-1.887763
H	3.978792	-1.6241	-2.97275
C	-6.031176	-0.875108	-0.305385
H	-7.08777	-0.797466	-0.538876
C	4.580118	-2.576313	-1.131759
H	5.061281	-3.415708	-1.625509
B	0.741329	2.17254	-0.275578

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

Table S12. Cartesian coordinates (in angstrom) of (*S*)-**1d** in S_1 state[a].

atom	x	y	z
O	-0.69248	-1.019022	-0.222558
F	0.689707	-2.729623	-1.009231
F	0.908242	-2.025938	1.168704
N	1.742095	-0.594694	-0.588136
C	-0.974314	0.263544	-0.282436
C	-3.464059	-0.152232	0.135307
C	-3.365296	-1.577657	0.271532
H	-2.39768	-2.042547	0.178446
C	-2.339903	0.713651	-0.122034
C	3.12594	-1.062925	-0.816473
H	3.140881	-2.088893	-0.436768
C	1.438683	0.706923	-0.706871
H	2.233673	1.418363	-0.902223
C	0.094722	1.182477	-0.532216
C	-0.211569	2.53946	-0.615632
H	0.588903	3.249982	-0.806489
C	-2.591472	2.144831	-0.227135
C	-4.786875	0.432403	0.27078
C	-3.916405	2.667818	-0.084632
H	-4.051074	3.742319	-0.171897
C	-4.474848	-2.362677	0.518281
H	-4.356825	-3.437064	0.615353
C	4.132913	-0.263905	0.015486
C	-5.890625	-0.39834	0.519941
H	-6.872204	0.057003	0.616973
C	-1.528739	3.015941	-0.466599
H	-1.721054	4.081886	-0.540761
C	-5.748988	-1.777656	0.643995
H	-6.619495	-2.397379	0.837866
C	5.155038	0.506032	-0.551882
H	5.266032	0.558534	-1.630133
C	-4.97853	1.851096	0.153527
H	-5.981835	2.251401	0.260617
C	3.42379	-1.131187	-2.32257
H	2.682549	-1.773808	-2.803248
H	4.418069	-1.552397	-2.502627
H	3.374047	-0.142536	-2.791185
B	0.681174	-1.628734	-0.156132
C	4.030185	-0.314796	1.416366
H	3.236227	-0.905418	1.866143
C	6.054327	1.211577	0.257791
H	6.842298	1.801418	-0.202458

C	5.942289	1.154299	1.64688
H	6.641165	1.698679	2.275601

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

Table S13. Cartesian coordinates (in angstrom) of (*S*)-**1e** in S_1 state[a].

atom	x	y	z
F	-2.521505	-3.225929	0.625362
F	-2.686481	-2.280222	-1.459836
O	-0.596852	-2.379362	-0.403052
N	-2.38838	-0.835796	0.432089
C	0.949745	0.740422	0.587977
H	0.701335	1.720586	0.989014
C	2.328304	0.462658	0.308188
C	-1.438929	0.0817	0.659028
H	-1.732759	1.051465	1.047988
C	0.3066	-1.473656	-0.168058
C	-4.291015	0.723512	0.110961
C	-0.067349	-0.172403	0.375098
C	1.647956	-1.774277	-0.447585
H	1.868195	-2.757581	-0.849525
C	-3.795639	-0.555569	0.786125
H	-4.36155	-1.384054	0.350922
C	2.681652	-0.836572	-0.222813
C	-4.757651	1.834292	0.81983
H	-4.782276	1.818902	1.904708
C	-4.283148	0.773954	-1.292637
H	-3.913941	-0.086227	-1.844562
C	-3.987698	-0.624011	2.306696
H	-3.649071	-1.601053	2.658054
H	-5.041874	-0.502949	2.573451
H	-3.408527	0.146596	2.82574
C	4.024394	-1.121288	-0.498341
H	4.284543	-2.098471	-0.897171
C	-5.206823	2.974092	0.144491
H	-5.567374	3.827578	0.711893
C	3.331359	1.389005	0.528332
H	3.073639	2.367902	0.926511
C	4.705859	1.112543	0.251841
C	-4.730625	1.907272	-1.965376
H	-4.720839	1.928149	-3.051497
C	5.057554	-0.175242	-0.274121
C	-5.194875	3.014097	-1.247709
H	-5.545897	3.897981	-1.772519
B	-2.092937	-2.21342	-0.208523
C	6.414261	-0.455227	-0.549703
H	6.679488	-1.430672	-0.948047
C	5.722535	2.057217	0.477093
H	5.458518	3.033213	0.875192

C	7.054195	1.755533	0.196573
H	7.825006	2.498103	0.377147

[a] The geometry was optimized by DFT calculation (B3LYP/6-31+G(d,p)).

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