Supplementary Information for

BIONL-like Atropoisomeric Chiral Nanographene

Sheng-Tao Li,[1] Ranran Li,[1] Yi-Kang Zhang,[1] Shutao Wang,[2] Bin Ma,[1] Bin Zhang,[1] and Peng An,[1]*

[1]School of Chemical Science and Technology, Yunnan University, Kunming 650500, P. R. China

[2]College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, P. R. China

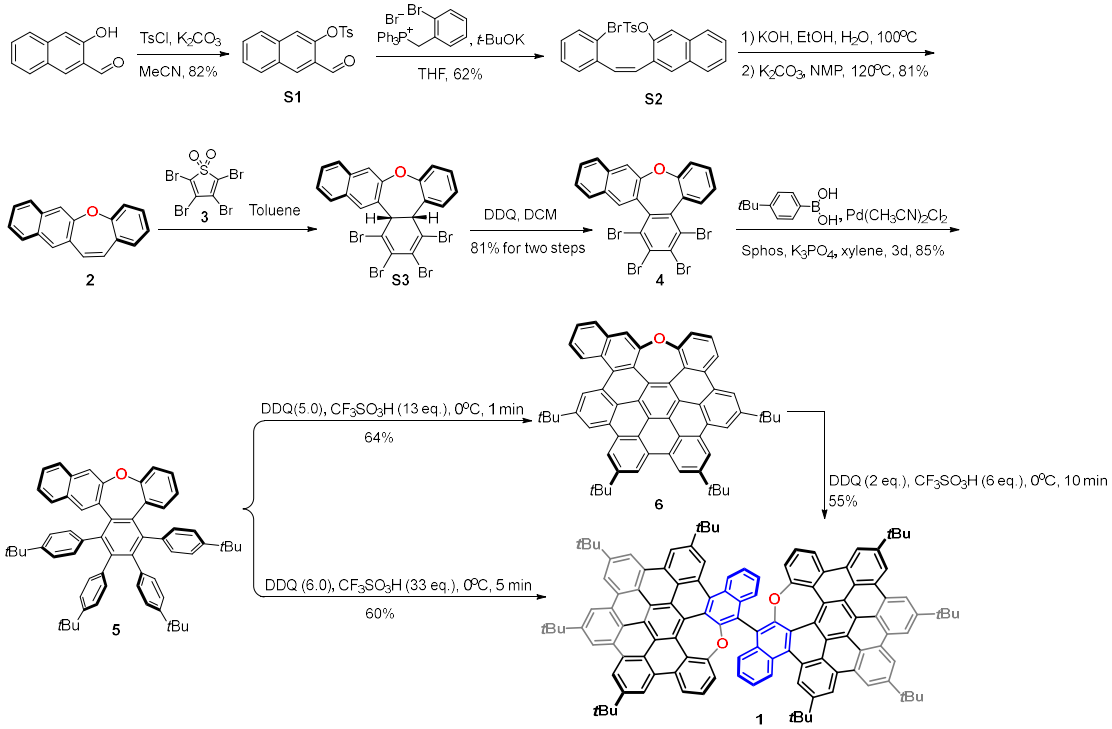
Table of Contents

General Information

Solvents and chemicals were purchased from commercial sources and used directly without further purification. Molecular sieves were activated in an oven and solvents for reaction was stored with molecular sieves. Petroleum ether (PE) used had a boiling range of 60−90 °C. Reactions were monitored by TLC on silica gel GF 254 plates. Column chromatography was generally performed through silica gel (200−300 mesh). All reactions were run open to air unless specifically described. NMR spectra were recorded with Bruker-400, 500 or 600 MHz spectrometers. Unless specified otherwise, the NMR spectra were recorded at 22 °C; they were calibrated using the residual solvent signal(^{1}H) or solvent signal (^{13}C). Chemical shifts were reported in parts per million (ppm). Chemical shifts were reported in ppm using TMS or deuterated solvents as internal standards (for ^{1}H NMR: $CDCl_3$, 7.26, C_6D_6, 7.15; for ^{13}C NMR: $CDCl_3$, 77.0, C_6D_6, 128.6). Multiplicity was reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, brs = broad. Coupling constants (J) are reported in Hertz (Hz). UV-Vis absorption spectra were recorded using a 1-cm quartz cuvette on a Shimadzu-UV-2600 spectrometer. Fluorescence spectra were recorded using a 1-cm quartz cuvette or powder form on a Gangdong F-320 spectrofluorometer at 25 ºC. High-resolution mass spectrometry was performed on a Thermo LTQ-Orbitrap XL mass spectrometer equipped with collision cells for collision induced dissociation or Bruker MALDI-TOF MS RapifleX with DCTB(*trans*-2-[3-(4-*t*-butylphenyl)-2-methyl-2-propenylidene]malononitrile) as the matrix. Crystallographic data were collected on a Bruker D8 VENTURE diffractometer.

Synthesis

Scheme S1. Synthesis of nanographene **1**.



3-Formylnaphthalen-2-yl 4-methylbenzenesulfonate (**S1**): To a solution of 3-hydroxy-2-naphthaldehyde (861 mg, 5.0 mmol, 1.0 equiv) in anhydrous acetonitrile 50 mL was added potassium carbonate (1.38 g, 10.0 mmol, 2.0 equiv). The 4-methylbenzenesulfonyl chloride (1.14 g, 6.0 mmol, 1.2 equiv) was added to the above suspension and the mixture was stirred at 80 °C overnight. Upon complete convertion (checked by TLC), The mixture was filtered through a thin pad of silica gel, and the filtrate was concentrated to give a colorless solid (1.3 g, 82%) and directly used in the following step without further purification.

(Z)-3-(2-Bromostyryl)naphthalen-2-yl 4-methylbenzenesulfonate (**S2**): To a suspension of (2-bromobenzyl) triphenylphosphonium bromide (1.54 g, 3.0 mmol, 1.2 equiv) in anhydrous tetrahydrofuran 30 mL at 0 °C was added potassium *tert*-butoxide (404 mg, 3.6 mmol, 1.4 equiv) under Ar. The mixture was allowed to stir at room temperature for 30 mins followed by adding **S1** (815 mg, 2.5 mmol, 1.0 equiv) and the mixture were stirred at room temperature overnight. Upon complete convertion (checked by TLC), the mixture was quenched with water and extracted with EtOAc. The organic phase was collected, concentrated and purified by silica gel flash chromatography using ethyl acetate/petroleum ether as eluent to give the title product as a colorless solid (742 mg, 62%) and the NMR data was identical as the reported results[S1]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.0 Hz, 2H), 7.73 (dd, J = 8.0,

0.5 Hz, 1H), 7.70 (s, 1H), 7.59 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.47–7.42 (m, 3H), 7.36 (td, *J* = 8.0, 1.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.02 (td, *J* = 8.0, 1.0 Hz, 1H), 7.59 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.88 (dd, *J* = 8.0, 0.5 Hz, 1H), 6.75 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.69 (d, *J* = 12.0 Hz, 1H), 6.66 (d, *J* = 12.0 Hz, 1H), 2.40 (s, 3H).

Benzo[b]naphtho[2,3-f]oxepine (**2**): To a solution of **S2** (479 mg, 1.0 mmol, 1.0 equiv) in mixed solvents of water (15 mL) and ethanol (15 mL) was added potassium hydroxide (1.12 g, 20 mmol, 20.0 equiv) and the mixture was stirred under reflux for around 1 h. The reaction mixture was allowed to cool to room temperature. Hydrochloric acid (10%) was added to adjust the pH to 4 and dichloromethane was added to extract the product. The organic phase was washed with aqueous $NaHCO_3$ solution and dried over anhydrous Na_2SO_4. After the solvent was evaporated, the residue was mixed with K_2CO_3 (690 mg, 5.0 mmol, 5.0 equiv) in NMP (10.0 mL). The mixture was heated at 120 °C for 20 h. The reaction mixture was quenched with water and then extracted with EtOAc, dried over anhydrous Na_2SO_4. The organic phase was concentrated and purified by silica gel column chromatography using ethyl acetate/ petroleum ether as eluent to give the title product as a colorless solid (198 mg, 81%) and the NMR data was identical as the reported results[S1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 12.0, 2H), 7.44–7.36 (m, 2H), 7.31–7.25 (m, 2H), 7.19 (dd, *J* = 4.0, 0.5 Hz, 1H), 7.14–7.10 (m, 1H), 6.86 (d, *J* = 10.0, 1H), 6.70 (d, *J* = 10.0, 1H).

1,2,3,4-Tetrabromodibenzo[b,d]naphtho[2,3-f]oxepine (**4**): A mixture of oxepine **2** (244 mg, 1.0 mmol, 1.0 equiv), tetrabromothiophene-S,S-dioxide 7[S2] (647 mg, 1.5 mmol, 1.5 equiv) in toluene (5 mL) in the sealed tube were heated to 110–120 °C until no oxepine **2** left (around 20 hours, checked by TLC: silica, PE: DCM = 2:1, UV/PMA). Then the solvent was removed in vacuo and the residue was dissolved in dichloromethane (15 mL) and 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (454 mg, 2.0 mmol, 2.0 equiv) was added and the mixture was stirred at room temperature for around 30 mins. The reaction mixture was concentrated. The residue was purified by silica gel flash chromatography (20-40% DCM in PE) to give the compound **4** (494 mg, 81% for two steps) as colorless solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 6.0 Hz, 2H), 7.81 (t, *J* = 8.0 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.67 (s, 1H), 7.50 (td, *J* = 8.0, 0.5 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 6.0 Hz, 2H), 7.15–7.11 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.72, 159.46, 138.42, 138.22, 134.22, 134.04, 133.28, 131.07, 130.76, 130.64, 130.45, 130.25, 129.76, 128.34, 127.52, 127.12, 126.47, 125.78, 123.96, 120.51, 116.24; HRMS (MALDI-TOF) calcd for $C_{22}H_{10}Br_4O$ 607.7445 [M^+], found 607.7447.

1,2,3,4-Tetrakis(4-(tert-butyl)phenyl)dibenzo[b,d]naphtho[2,3-f]oxepine (**5**): To a solution of oxepine **4** (153 mg, 0.25 mmol, 1.0 equiv) in xylene (4.0 mL) was quickly added 4-*tert*-butyllphenylboronic acid (890 mg, 5.0 mmol, 20.0 equiv), palladium(II) chloride diacetonitrile complex (13 mg, 0.05 mmol, 0.2 equiv), 2-dicyclohexylphosphino-2,6-dimethoxy-1,1-biphenyl (SPhos, 41 mg, 0.1 mmol, 0.4 equiv) and potassium phosphate tribasic (795 mg, 3.75 mmol, 15.0 equiv) under argon atmosphere.

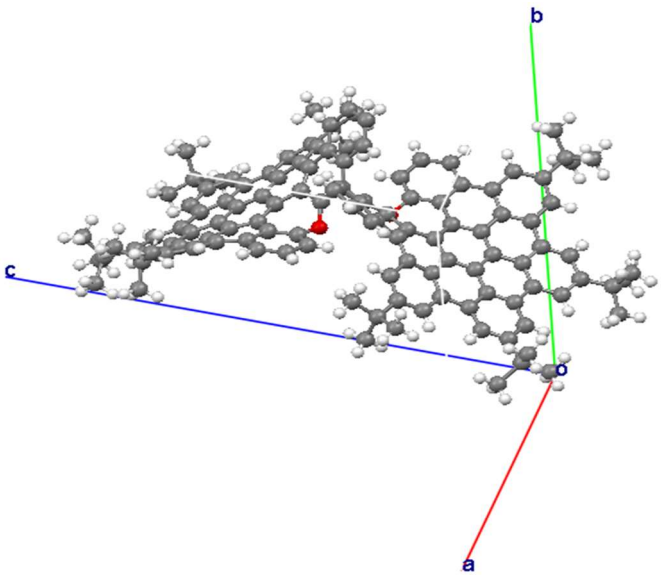
Then the mixture was carefully gas exchanged to keep stirring under argon at 150 °C for around 72 h. The mixture was extracted thrice with dichloromethane, the combined organic layers were dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (silica, 20–40 % DCM in PE, UV) to give the compound **5** (175 mg, 85%) as white solid: m. p. 56–58 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.0 Hz, 1H), 7.65 (s, 1H), 7.34–7.27 (m, 5H), 7.20–6.98 (m, 5H), 6.90–6.87 (m, 2H), 6.70–6.64 (m, 4H), 6.54 (t, J = 8.0 Hz, 2H), 6.61–6.37 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.13, 160.79, 148.22, 147.91, 147.72, 147.69, 142.99, 142.72, 141.39, 140.80, 137.92, 137.76, 137.70, 137.65, 135.06, 134.98, 134.58, 133.85, 132.86, 132.73, 132.43, 131.55, 131.50, 131.48, 130.71, 130.44, 130.29, 130.25, 130.22, 129.99, 128.27, 127.95, 126.47, 126.11, 124.48, 123.74, 123.55, 123.49, 123.38, 122.49, 119.72, 115.27, 34.19, 34.11, 34.07, 31.26, 31.18, 31.16, 31.06; HRMS (ESI) calcd for $C_{62}H_{62}NaO$ 845.4693 [M+Na$^+$], found 845.4686.

2,5,17,20-Tetra-tert-butyl-10-oxabenzo[e]benzo[5',6']tetraceno[1',12',11',10':5,6,7,8,9]tetrapheno[10,11,12,1-nopqab]pleiadene (**6**): To a solution of compound **5** (82 mg, 0.1 mmol, 1.0 equiv) in anhydrous dichloromethane (50 mL) in oven-dried flask with a magnetic stirring bar was added 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (112 mg, 0.5 mmol, 5.0 equiv). The mixture was carefully exchanged into an argon atmosphere and stirred in an ice-water bath. Then trifluoromethanesulfonic acid (0.1 mL, 1.3 mmol, 13 equiv) was added dropwise to the above reaction mixture and the mixture was stirred at 0 °C for around 1 min. Triethyl amine (1.0 mL, 7.2 mmol, 72 equiv) was added, followed by methanol (1.0 mL, 24.7 mmol, 247 equiv) to quench the reaction and the mixture was concentrated under reduced pressure. The residue was purified by flash chromatography (silica, 20–40 % DCM in PE, UV) to give the titled compound **6** (52 mg, 64%) as yellow solid: m. p. 61–63 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 9.29 (s, 1H), 9.28 (s, 1H), 9.25 (s, 1H), 9.23 (s, 1H), 9.10 (s, 1H), 9.04 (s, 1H), 8.95 (s, 1H), 8.94 (d, J = 6.0 Hz, 1H), 8.76 (dd, J = 6.0, 2.0 Hz, 1H), 8.12 (dd, J = 6.0, 2.0 Hz, 1H), 7.97 (s, 1H), 7.90–7.85 (m, 2H), 7.67–7.62 (m, 2H), 1.83 (s, 9H), 1.82 (s, 9H), 1.72 (s, 9H), 1.72 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.73, 154.22, 149.68, 149.64, 149.20, 133.96, 133.43, 130.57, 130.44, 130.41, 130.32, 130.28, 130.25, 128.78, 128.65, 128.55, 127.36, 127.06, 126.88, 126.39, 125.51, 125.02, 124.95, 124.66, 123.71, 123.53, 123.32, 123.20, 122.39, 121.29, 120.86, 120.36, 120.23, 119.26, 119.00, 118.85, 118.80, 118.63, 118.55, 118.48, 114.49, 35.75, 35.72, 35.58, 31.99, 31.97, 31.84; HRMS (MALDI-TOF) calcd for $C_{62}H_{52}O$ 813.4048 [M$^+$], found 813.4036.

2,2',5,5',17,17',20,20'-Octa-tert-butyl-11,11'-bi(10,10'-dioxabenzo[e]benzo[5',6']tetraceno[1',12',11',10':5,6,7,8,9]tetrapheno[10,11,12,1-nopqab]pleiadene) (**1**): From monomer **6**: to a solution of compound **6** (90 mg, 0.11 mmol, 1.0 equiv) in anhydrous dichloromethane (10 mL) in oven-dried flask with a magnetic stirring bar was added 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (50 mg, 0.22 mmol, 2.0 equiv). The mixture was carefully exchanged into an argon atmosphere and stirred in an ice-water bath. Then

trifluoromethanesulfonic acid (0.05 mL, 0.65 mmol, 6.0 equiv) was added dropwise to the above reaction mixture and the mixture was stirred at 0 °C for around 5 min. Triethyl amine (0.5 mL, 3.6 mmol, 32 equiv) was added to quench the reaction and the mixture was concentrated under reduced pressure. The residue was purified by flash chromatography (silica, 20–40 % DCM in PE, UV) then recrystallization to give the titled compound **1** (49 mg, 55%) as yellow solid. From compound **5**: to a solution of compound **5** (82 mg, 0.1 mmol, 1.0 equiv) in anhydrous dichloromethane (20 mL) in an oven-dried flask with a magnetic stirring bar was added 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (137 mg, 0.6 mmol, 6.0 equiv). The mixture was carefully exchanged to an argon atmosphere and stirred in an ice-water bath. Then trifluoromethanesulfonic acid (0.25 mL, 3.25 mmol, 32.5 equiv) was added dropwise to the above reaction mixture and the mixture was stirred at 0 °C for around 2–3 min. Triethyl amine (0.5 mL, 3.6 mmol, 36 equiv) was added to quench the reaction and the mixture was concentrated under reduced pressure. The residue was purified by flash chromatography (silica, 20–40 % DCM in PE, UV) then recrystallization to give the titled compound **1** (54 mg, 60%) as yellow solid: m. p. 130–132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.60 (s, 2H), 9.38 (s, 2H), 9.37 (s, 4H), 9.34 (s, 2H), 9.21 (d, J = 8.0 Hz, 2H), 9.14 (s, 2H), 9.09 (s, 2H), 9.89 (s, 2H), 8.44 (br, 2H), 8.07 (d, J = 8.0 Hz, 2H), 7.76 (t, J = 8.0 Hz, 2H), 7.55 (t, J = 8.0 Hz, 2H), 6.80 (br, 2H), 6.08 (d, J = 8.0 Hz, 2H), 1.91 (s, 18H), 1.88 (s, 18H), 1.86 (s, 18H), 1.78 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.45, 149.71, 149.62, 149.48, 149.25, 132.78, 130.68, 130.63, 130.50, 130.41, 130.37, 130.05, 129.01, 128.92, 128.60, 127.48, 127.02, 126.51, 125.43, 125.04, 123.72, 123.63, 123.57, 123.30, 123.24, 122.82, 122.63, 121.74, 121.36, 121.02, 120.45, 119.87, 119.49, 119.30, 119.03, 118.91, 118.81, 118.67, 118.41, 35.89, 35.81, 35.73, 35.56, 32.04, 31.99, 31.95, 31.88; HRMS (MALDI-TOF) calcd for $C_{124}H_{102}O_2$ 1622.7874 [M^+], found 1622.7792.

(a)



(b)

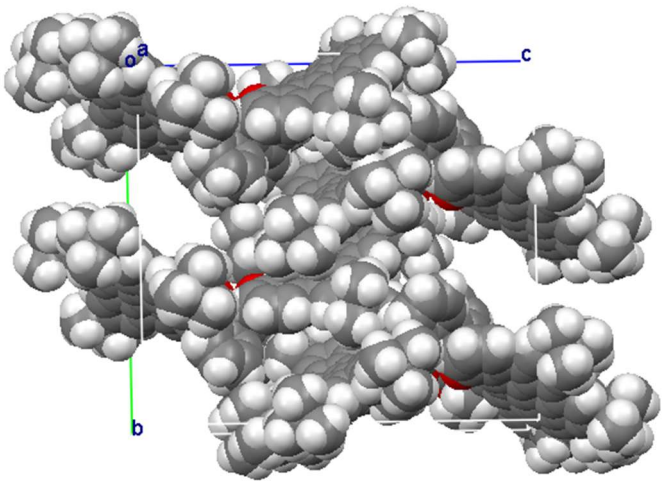


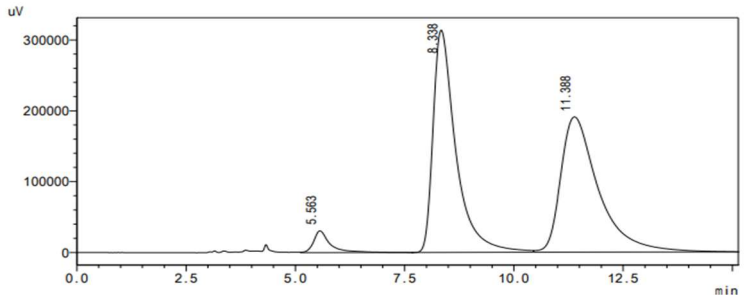
Figure S1. Single crystals suitable for X-ray diffraction analysis were obtained from solutions of **1** with 50% thermal ellipsoid probability. a) Crystal structure of compound **1** showing cell axes; b) Crystal packing as a space-filling model, along a, b, and c axes, respectively.

Table S1. Details of the Crystal Structure Analyses of Compound **1**.

	Single crystal of **1**
CCDC No.	2193890
empirical formula	$C_{124}H_{102}O_2$
formula wt	1624.05
crystal description	yellow block
crystal system	Monoclinic
space group	C12/c1
T (K)	150
a (Å)	16.1038(17)
b (Å)	24.540(3)
c (Å)	26.560(2)
α (°)	90
β (°)	90.069(4)
γ (°)	90
V (Å^3)	10455.2(18)
Z	4
ρ_{calcd} (mg/m^3)	1.032
μ (mm^{-1})	0.059
θ range (°)	2.08–24.998
F (000)	3448
collected reflcns no.	35100
unique reflcns no.	8885
R [$I > 2\sigma(I)$]	0.1053
R (ref)	0.1946
wR2 [$I > 2\sigma(I)$]	0.3087
wR2 (ref)	0.3512

(a)

Retention Time	Height	Area%	Resolution	Tailing Factor
8.338	313692	48.177	3.800	1.833
11.388	190932	48.383	2.613	1.766



(b)

Retention Time	Height	Area%	Resolution	Tailing Factor
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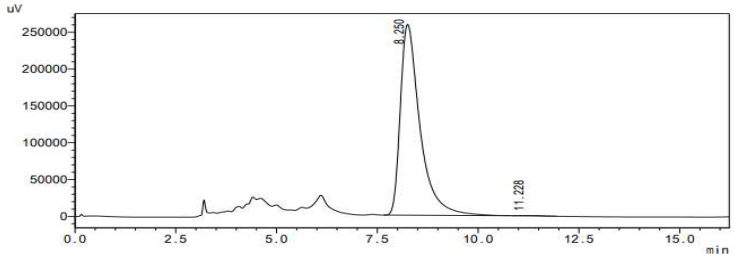
11.228	371	0.156	3.497	1.460



(c)

Retention Time	Height	Area%	Resolution	Tailing Factor
8.231	3063	0.438	--	1.463
11.121	375295	99.562	2.584	1.798

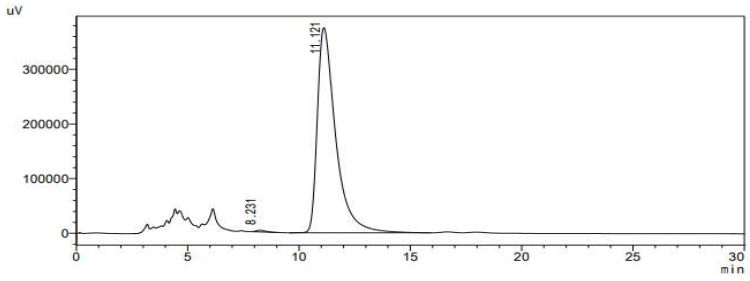
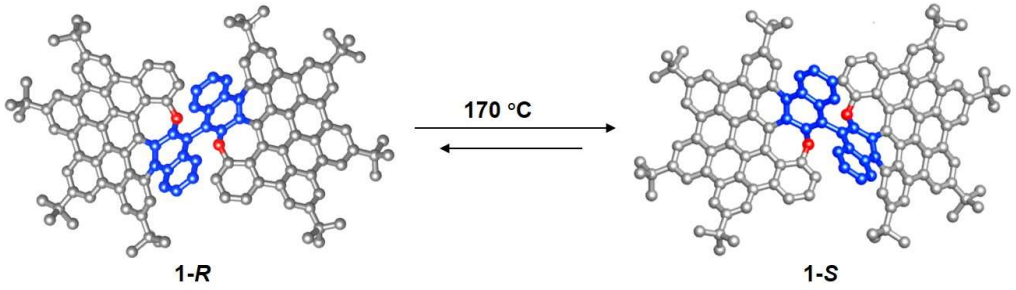


Figure S2. Racemic mixtures of **1** were separated by preparative chiral HPLC, condition: Unichiral CMD-5H column, 20mm I.D. × 250mm L, 30% n-Hexane/70% Ethanol/ 0.1%DEA(V/V/V), 25 mL/min, 254 nm. (a) Analytical HPLC trace of racemic sample; (b)

Analytical HPLC trace of enantiopure compound **1-*R***, $[\alpha]_D^{25}$ = -272.43 (c = 1.0 mg/mL) (c) Chromatogram of enantiopure compound **1-*S***, $[\alpha]_D^{25}$ = 284.04 (c = 1.0 mg/mL).

(a)



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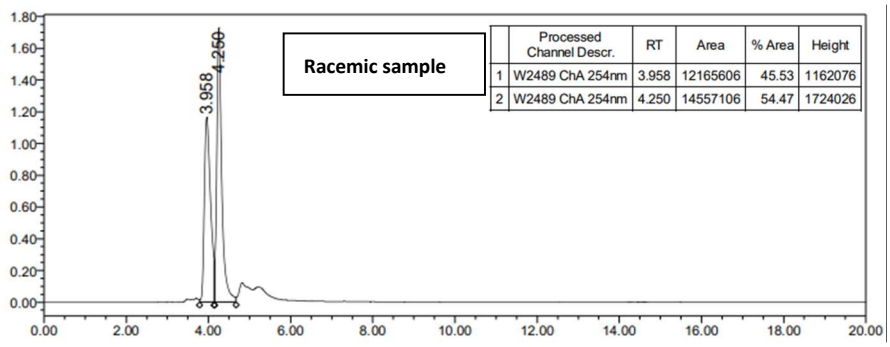

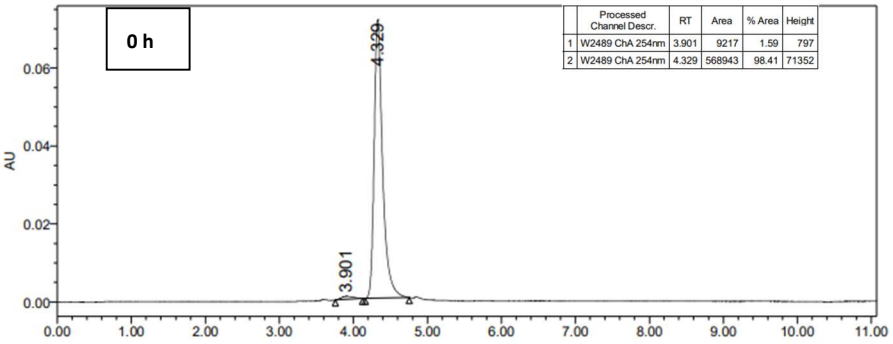

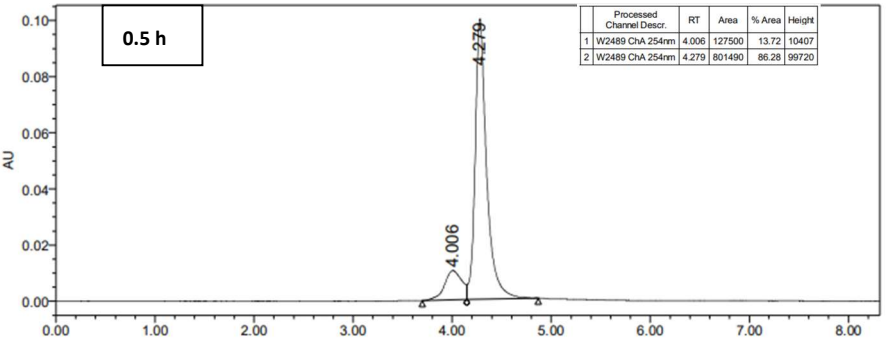

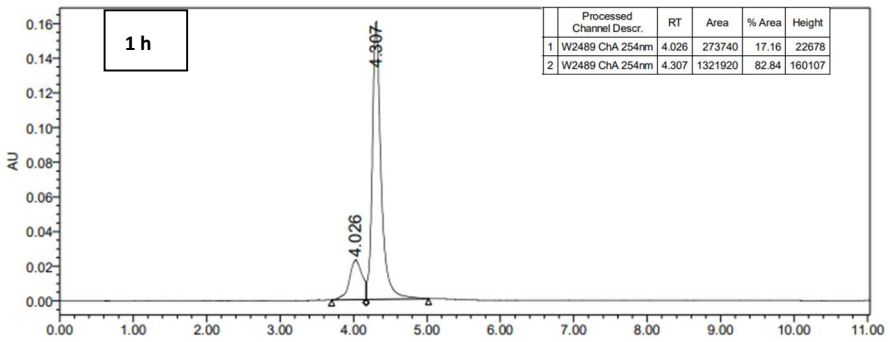

	Processed Channel Descr.	RT	Area	% Area	Height
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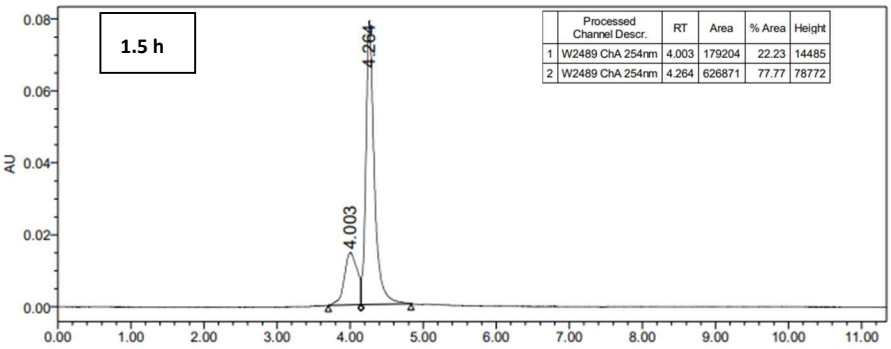

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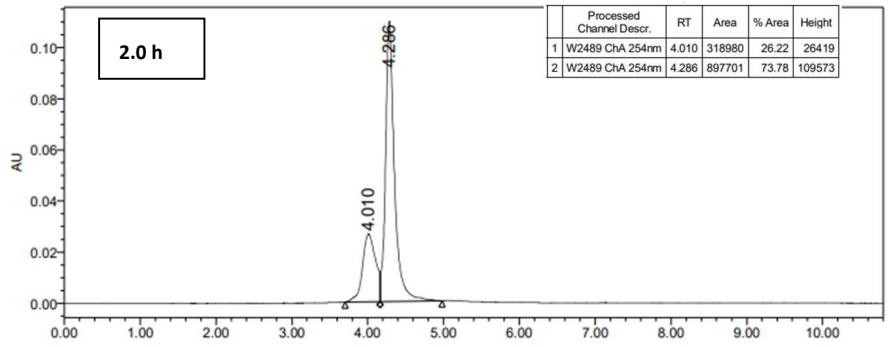

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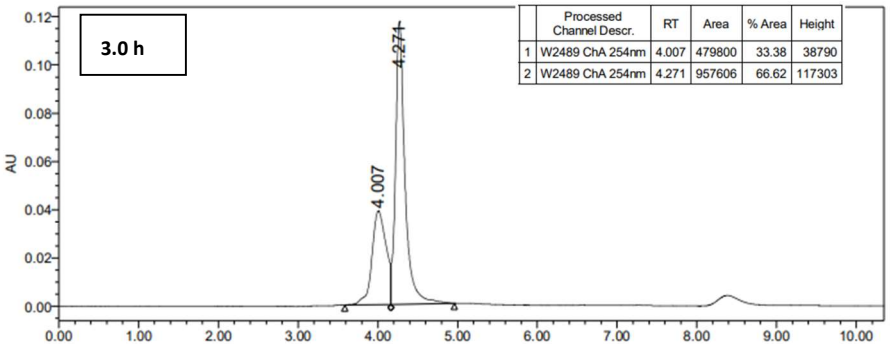

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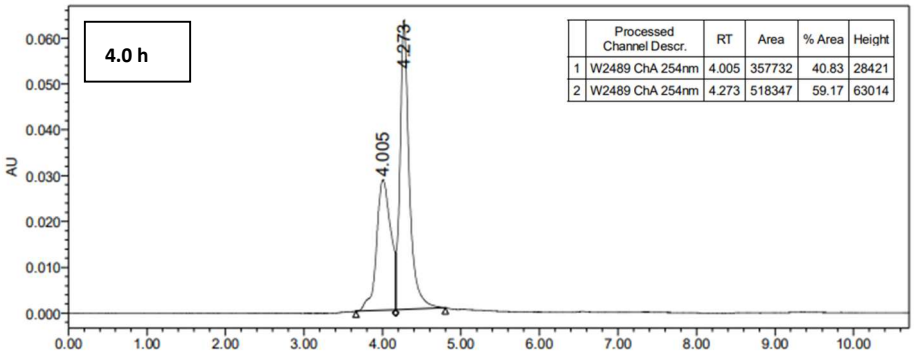
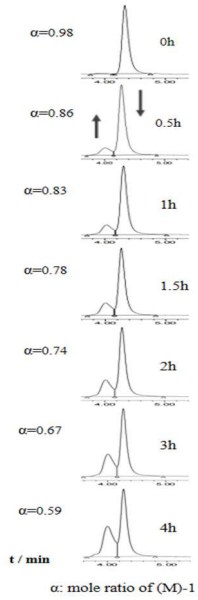


	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	4.005	357732	40.83	28421
2	W2489 ChA 254nm	4.273	518347	59.17	63014

(c)



Best-fit values	
Slope	-9.959e-005
Y-intercept	-0.04978
X-intercept	-499.8
1/slope	-10041

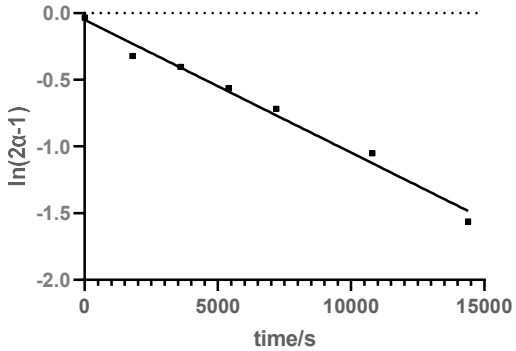
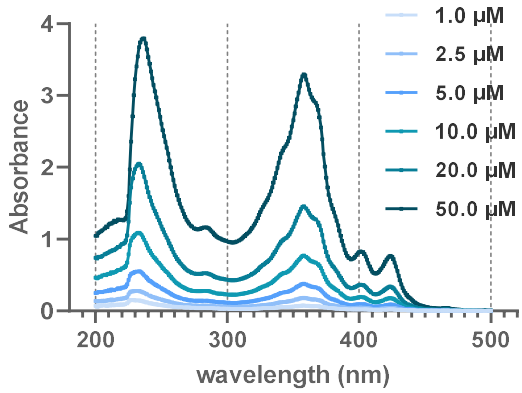
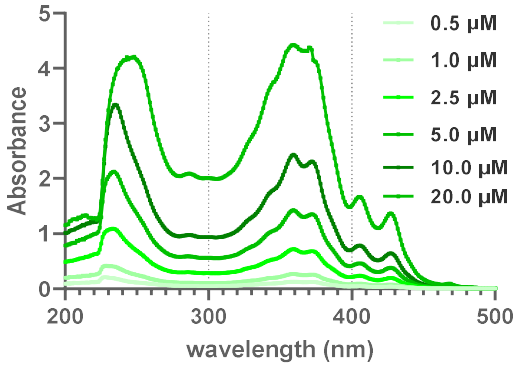


Figure S3. Thermal isomerization of **1**-*R* at 170 °C followed by chiral HPLC. (a) Scheme for thermal isomerization of **1**-*R*. (b) Chiral HPLC trace with analytic IA column after specific reaction time at 170 °C in 1,2-dichlorobenzene in 1,2-dichlorobenzene. Solvent was removed under reduced pressure before analyzing with eluent: hexane/isopropanol = 98:2, v/v; flow rate: 1.0 mL/min; detected by absorption at 254 nm. (c) Plot of HPLC-based conversion ratio of **1**-*R* (α) at time t. It switches between the (*R*)- and (*S*)-form isomers following a reversible first order reaction,[S3] with a rate constant (k), which could be obtained by fitting the experimental data using the following equation: $\ln(2\alpha - 1) = -2kt$ and k was determined as $4.98 \cdot 10^{-5}$ s^{-1}. Then the isomerization barrier ($\Delta G^{\ddagger}$) was calculated from the Eyring equation: $k = \kappa k_B T h K^{\ddagger}$ and $\Delta G^{\ddagger} = -RT\ln K^{\ddagger}$. $K^{\ddagger}$ is the thermodynamic equilibrium constant. The Gibbs activation energy can be determined as $\Delta G^{\ddagger}(T) = -RT\ln(kh/\kappa k_B T)$. R is the gas constant (R = 8.314 J K^{-1}); h is the Planck constant (h = 6.626×10^{-34} J s); k_B is the Boltzmann constant (k_B = 1.38×10^{-23} J K^{-1}); κ is the transmission coefficient (κ = 1). As a result, the isomerization energy was determined as $\Delta G^{\ddagger}$ = 146440.14 J/mol = 34.98 kcal/mol. $t_{1/2} = \ln 2/k$ = 13918.6 s = 232 min.

(a)



(b)



(c)

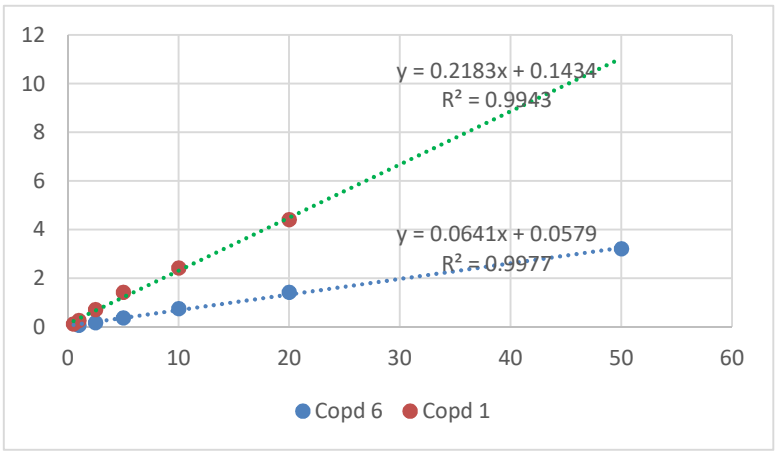
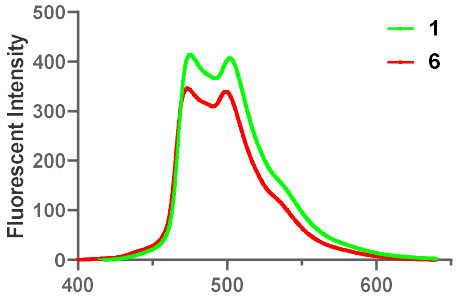
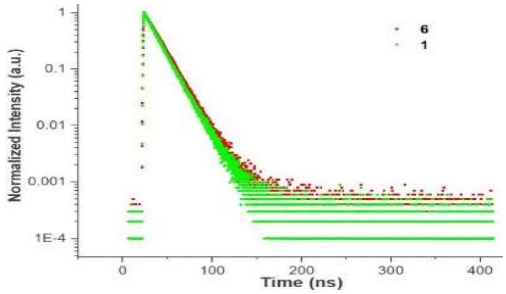


Figure S4. a) UV-vis spectra of compound **6** at different concentrations in DCM; b) UV-vis spectra of compound **1** at different concentrations in DCM; c) Absorbance vs concentration plots at the maximum wavelength at 360 nm.

(a)



(b)



(c)

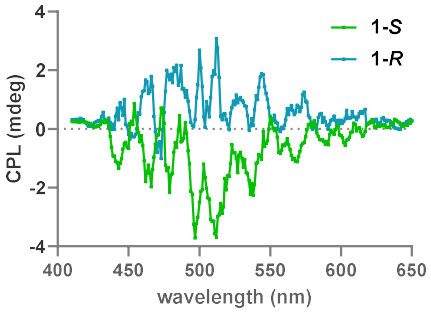


Figure S5. (a) Fluorescence spectra of monomer **6** and dimer **1**. (10 μM in DCM); (b) Fluorescence decay of compounds monomer **1** and dimer **6** in DCM. (c) CPL spectra of **1**-*S* (green line) and **1**-*R* (cyan line).

Table S2. Summary of Photophysical Properties of Compounds **1** and **6**.

Copd [a]	λ_{max} (nm)	ε_{max} (M^{-1} cm^{-1})	λ_{em} (nm)	Φ_F [b]	τ_F (ns)
6	358	6.4×10^4	474	0.03	16.22
1	358	2.2×10^5	475	0.02	15.04

[a] Measured in DCM. [b] absolute fluorescent quantum yield.

ROS Study by DCFH-DA.

2′,7′-Dichlorodihydrofluorescein diacetate (DCFH-DA) was employed for in vitro ROS evaluation according to the reported method.[S4] The ROS generation produced by compound **1** and compound **6** could be evaluated by the fluorescence emission of DCFH that is converted from DCFH-DA. First, a NaOH (400 μL, 0.01 M) solution was added to a DCFH-DA solution (10 μL, 10×10^{-3} M) to chemically hydrolyze DCFH-DA in the dark for 30 min followed by the addition of 4950 μL of a PBS buffer solution to stop the reaction. Subsequently, the solution of DCFH (600 μL) was mixed with 2400 μL of compound **1** or compound **6** in ACN to make the final concentration of 50 μM for **1** and **6** as tested samples. As the control group, the solution of DCFH (600 μL) was mixed with 2400 μL ACN. The fluorescence intensity of DCFH after incandescent light (1.5 $W \cdot cm^{-2}$) irradiation at different times (0s, 10s, 20s, 30s, 40s, 50s, 60s, 90s, 120s, 180s, 240s, 300s) was measured to estimate the ROS production ability of compound **1** and compound **6**.

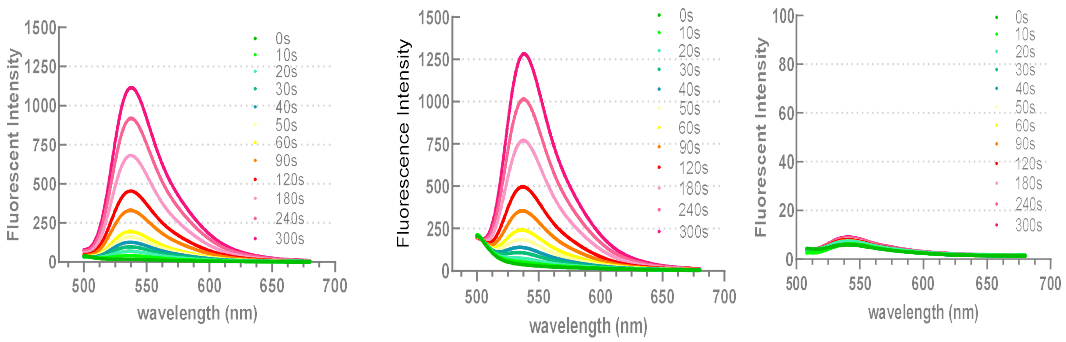
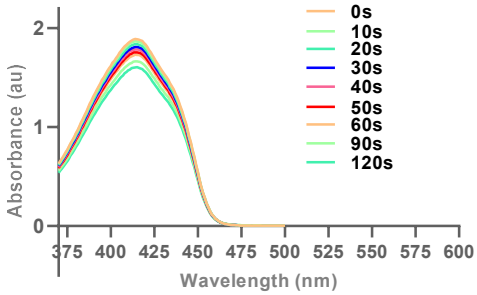


Figure S6. Fluorescence spectra of DCFH containing compounds **1** (left) or **6** (middle) as photosensitizer in PBS/ACN mixed solvents with white LED irradiation. The DCFH probe without any photosensitizer (right) was treated as control.

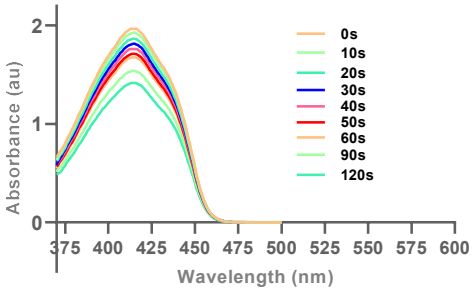
Detection of Singlet Oxygen Release by DPBF.

1,3-diphenylisobenzofuran (DPBF) was used as the singlet oxygen probe for in vitro singlet oxygen release evaluation based on the reference with modifications.[S5] First to a solution of dichloromethane was added compound **1** and compound **6** to prepare stock solution 500 μM). Then the DPBF was added into the sample solution to make the final concentration of photosensitizer at 25 μM with the DPBF probe at 100 μM. As the control group, the solution of DPBF was mixed with only dichloromethane (final concentration: 100 μM). The absorbance of DPBF after incandescent light (1.5 $W \cdot cm^{-2}$) irradiation at different times (0s, 10s, 20s, 30s, 40s, 50s, 60s, 90s, 120s) was measured to estimate the singlet oxygen releasing ability of compound **1** and compound **6**.

(a)



(b)



(c)

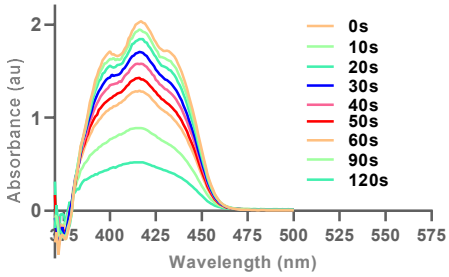
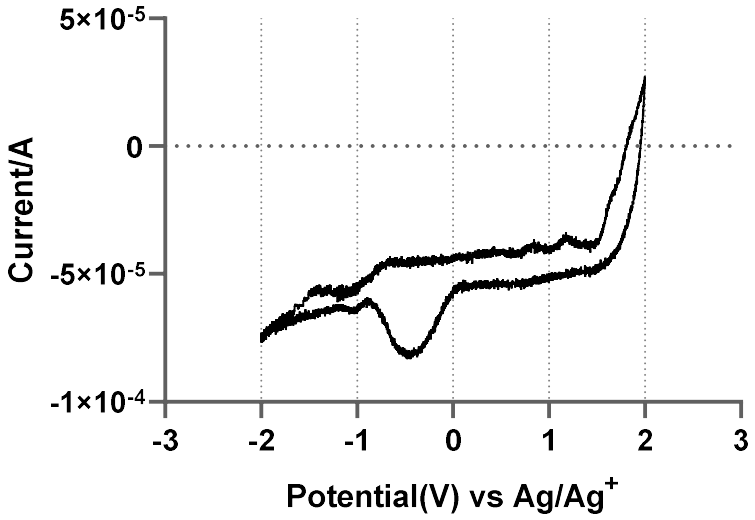


Figure S7. (a) Time-dependent absorption spectra of DPBF probe with white-light irradiation. (b) Time-dependent absorption spectra of DPBF probe in the presence of photosensitizer NG **6** with white-light irradiation. (c) Time-dependent absorption spectra of DPBF probe in the presence of photosensitizer NG **1** with white-light irradiation.

(a)



(b)

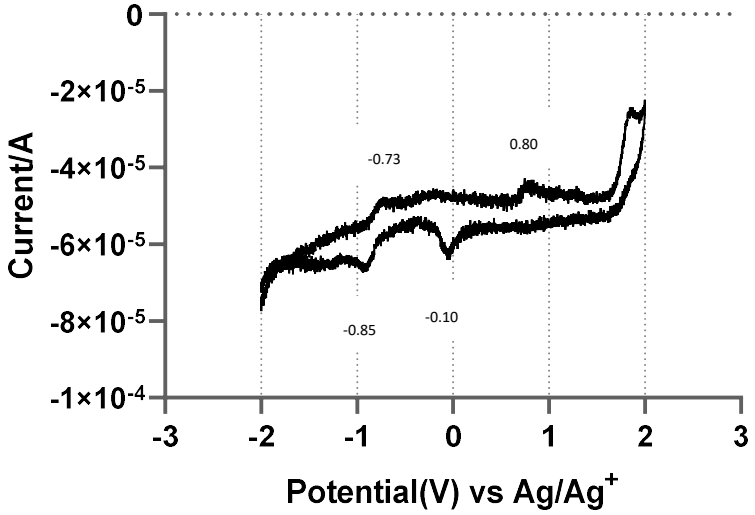


Figure S8. (a) Cyclic voltammograms of (a) monomer **6** and (b) oxa-NG **1** (supporting electrolyte: 0.1 M nBu_4NPF_6 in CH_2Cl_2).

Spectra

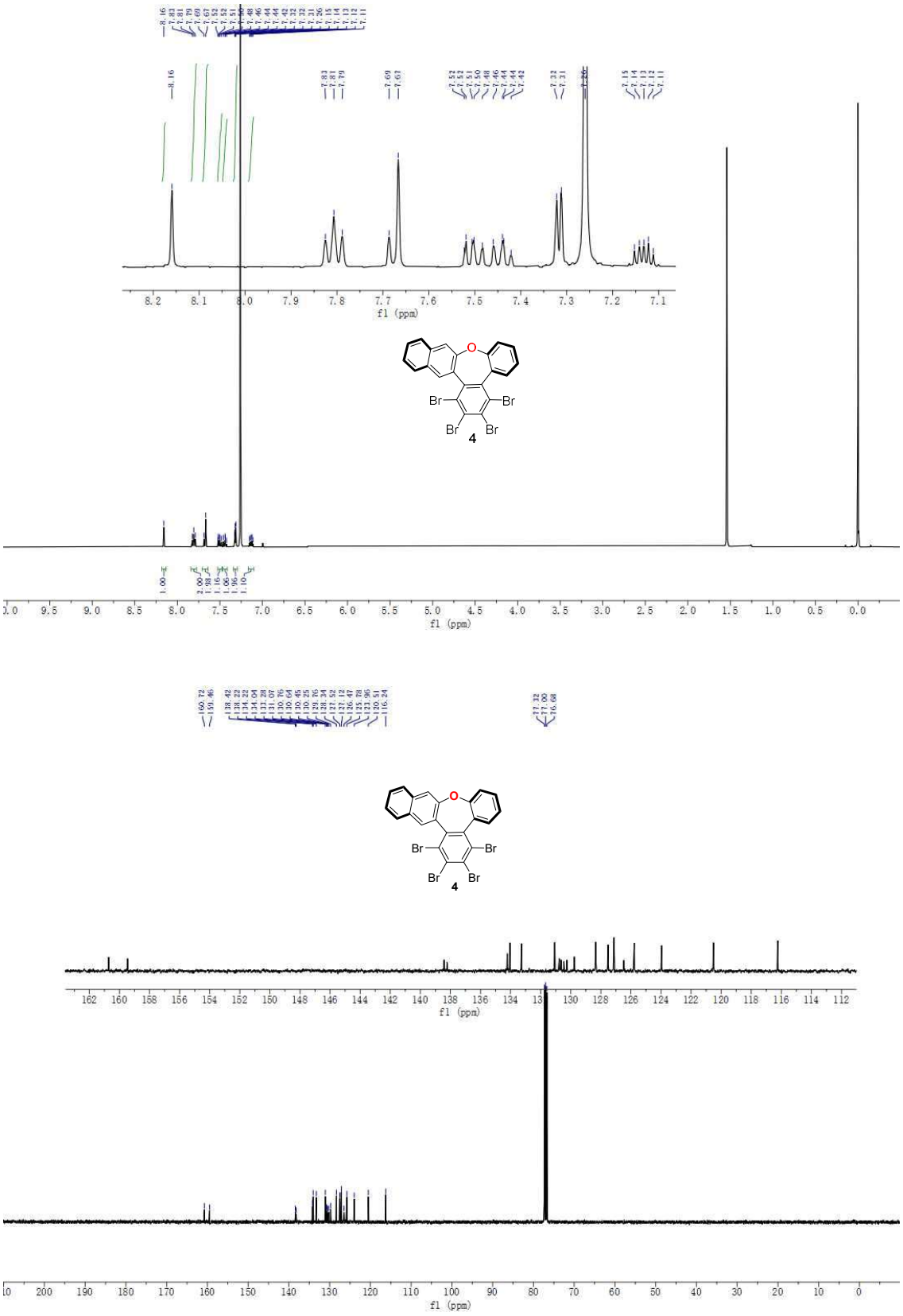


Figure S9. ^{1}H NMR (up) and ^{13}C NMR (down) of **4** in $CDCl_3$.

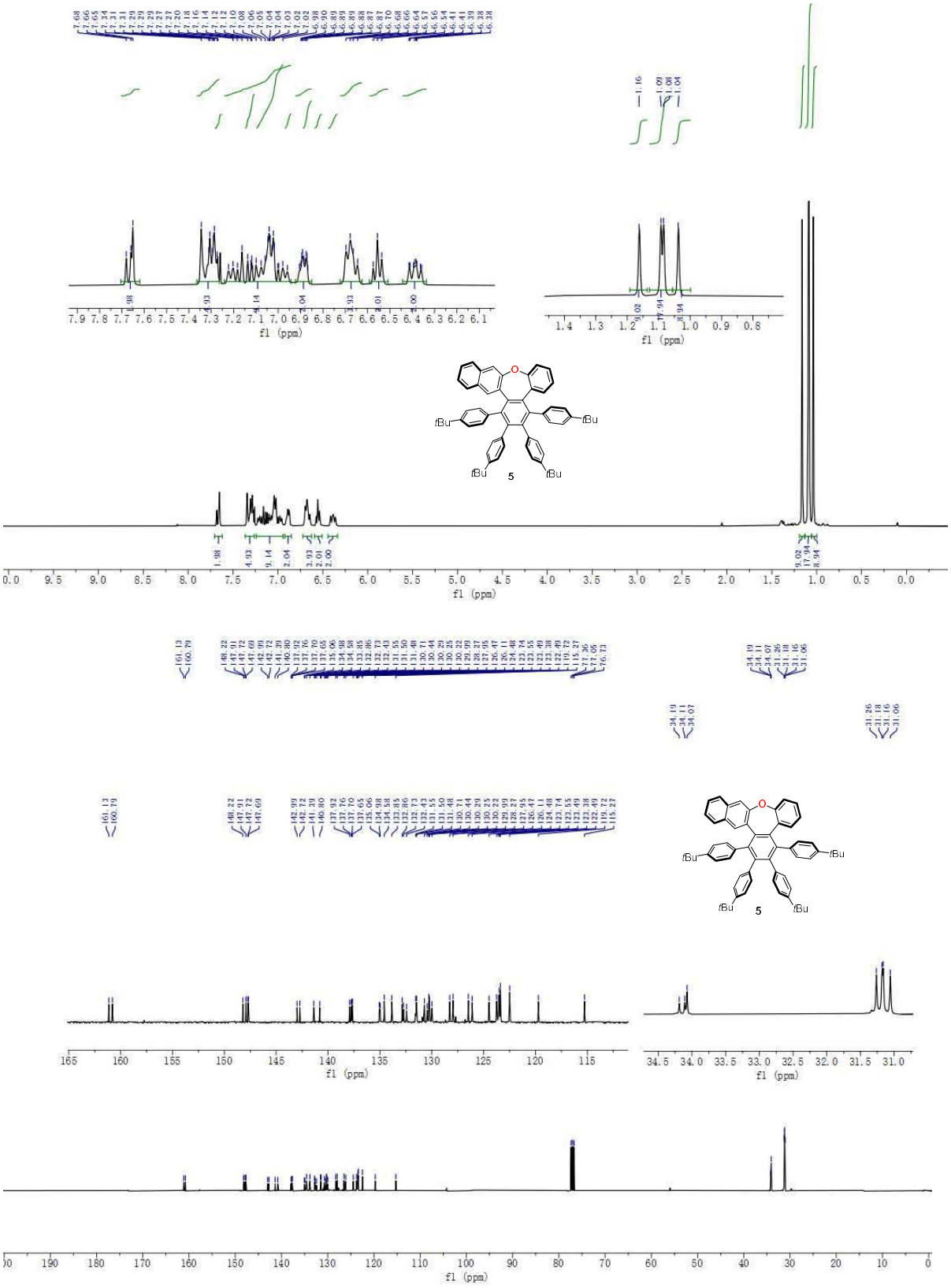


Figure S10. ^{1}H NMR (up) and ^{13}C NMR (down) of **5** in $CDCl_3$.

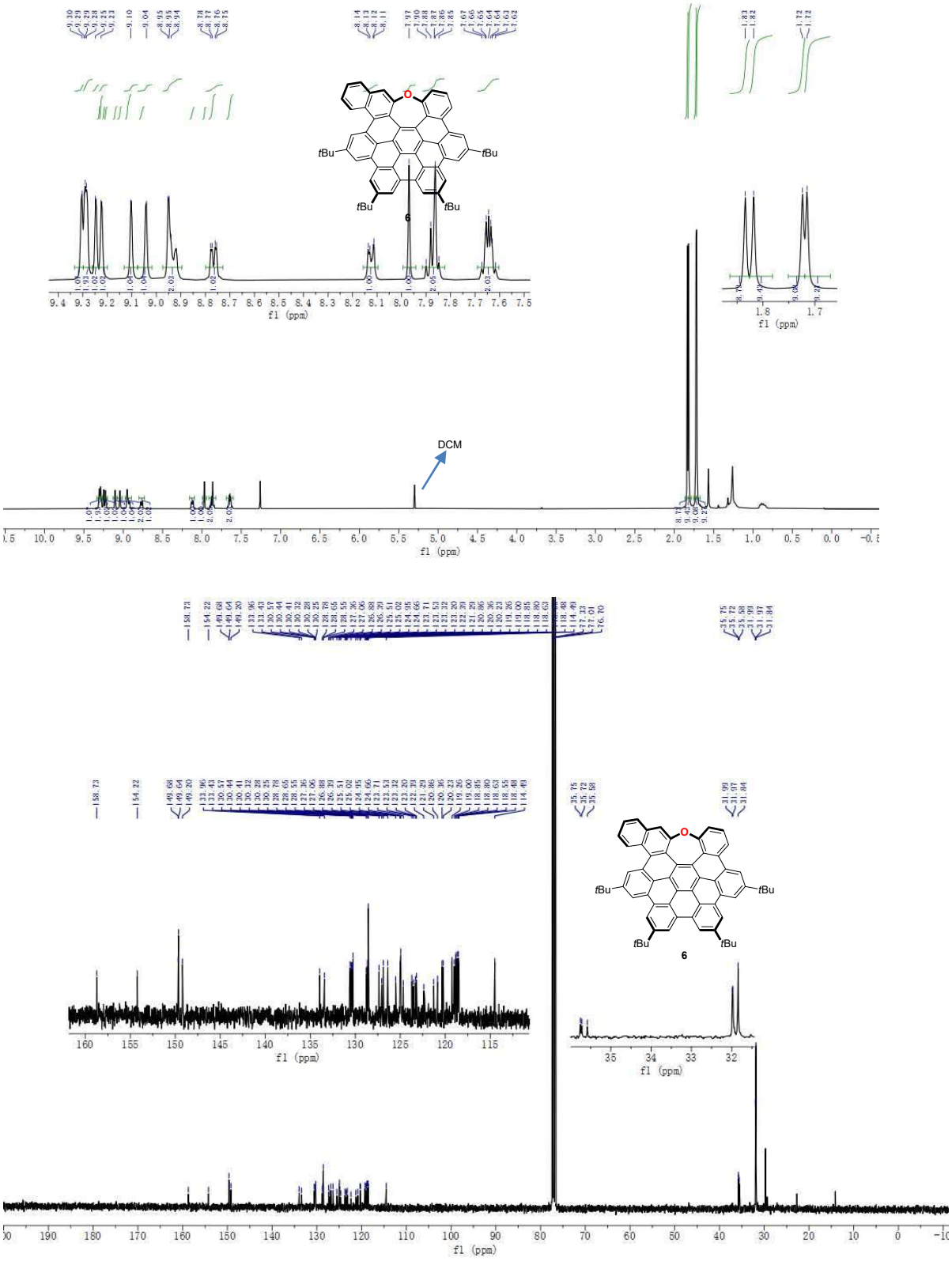


Figure S11. ^{1}H NMR (up) and ^{13}C NMR (down) of **6** in $CDCl_3$.

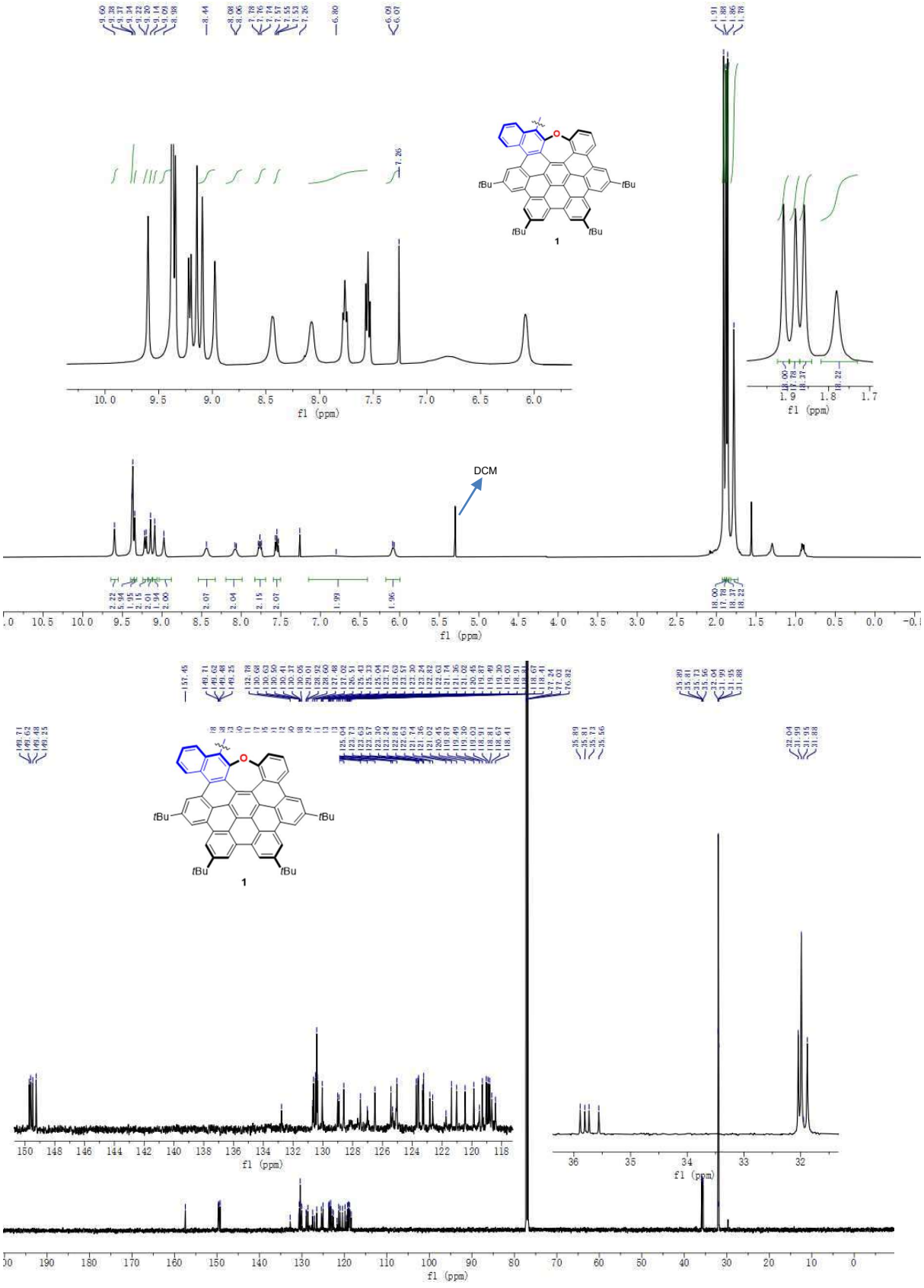


Figure S12. ^{1}H NMR (up) and ^{13}C NMR (down) of **1** in $CDCl_3$.

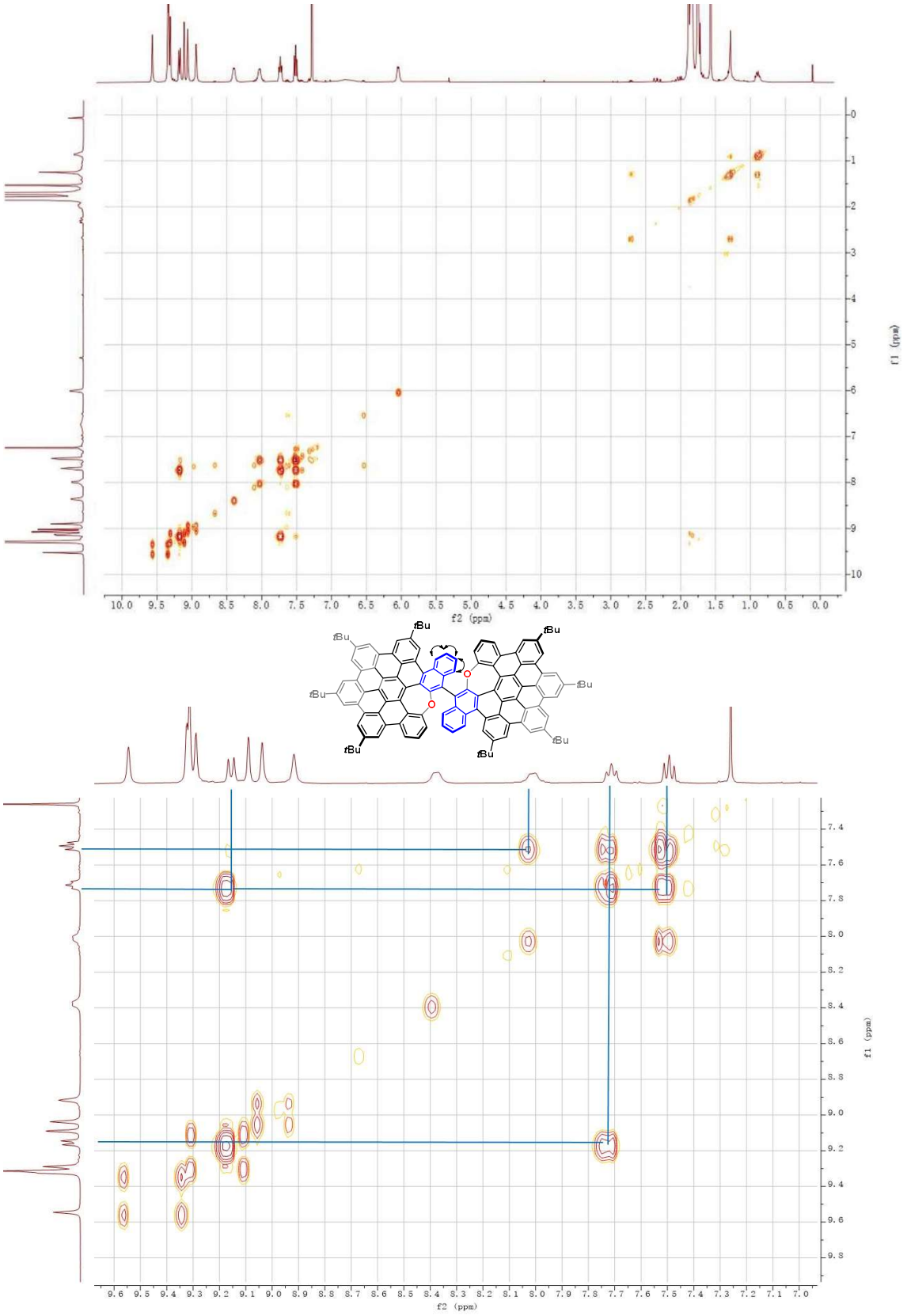


Figure S13. 2D H-H COSY spectrum (600 MHz, $CDCl_3$) of NG **1** and the spin systems of protons in naphthalene ring marked in blue.

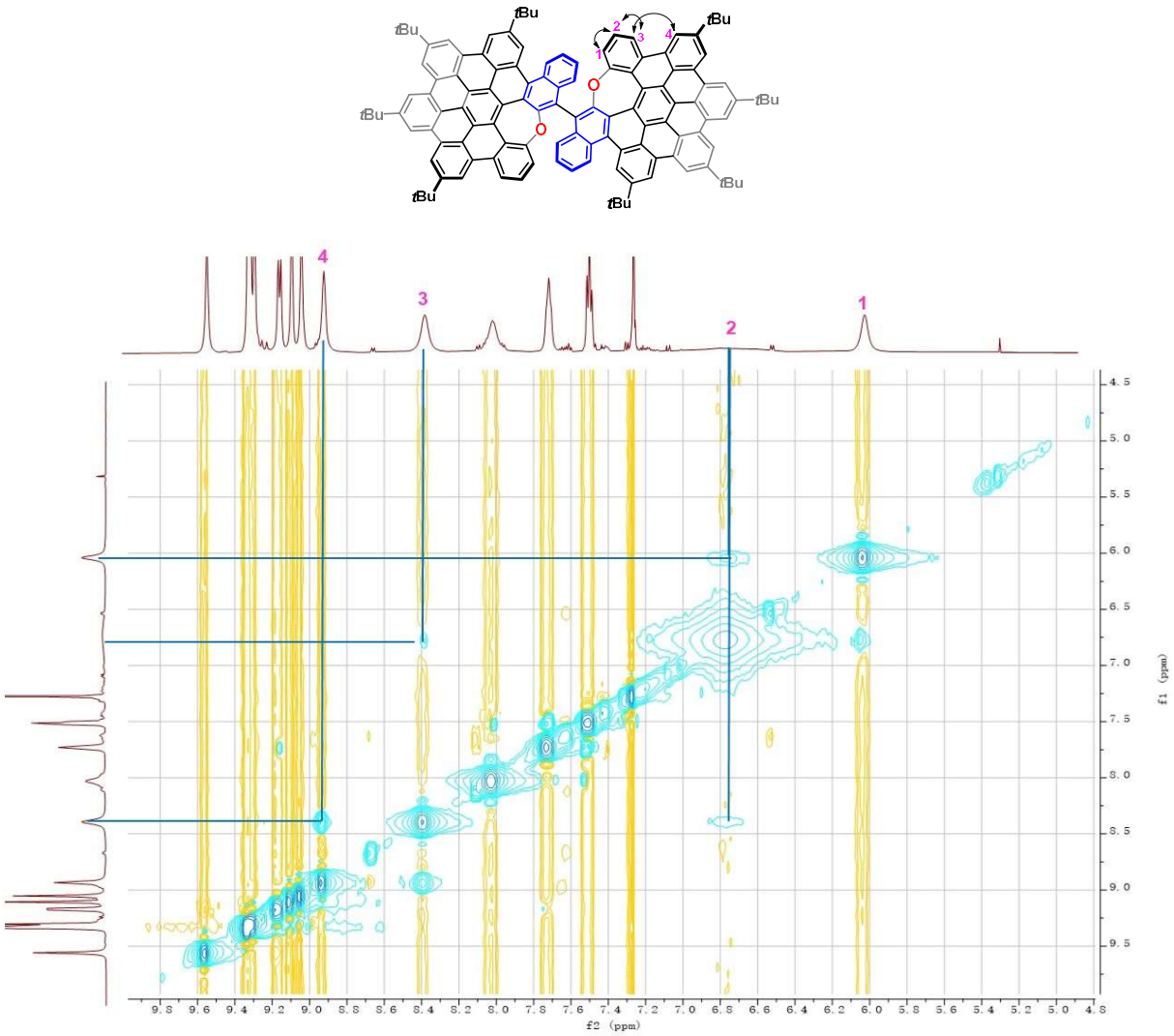


Figure S14. Partial 2D ROESY spectrum (600 MHz, $CDCl_3$) of NG **1** and depiction of representative NOEs of proton 1–4. NOEs were highlighted in blue arrow.

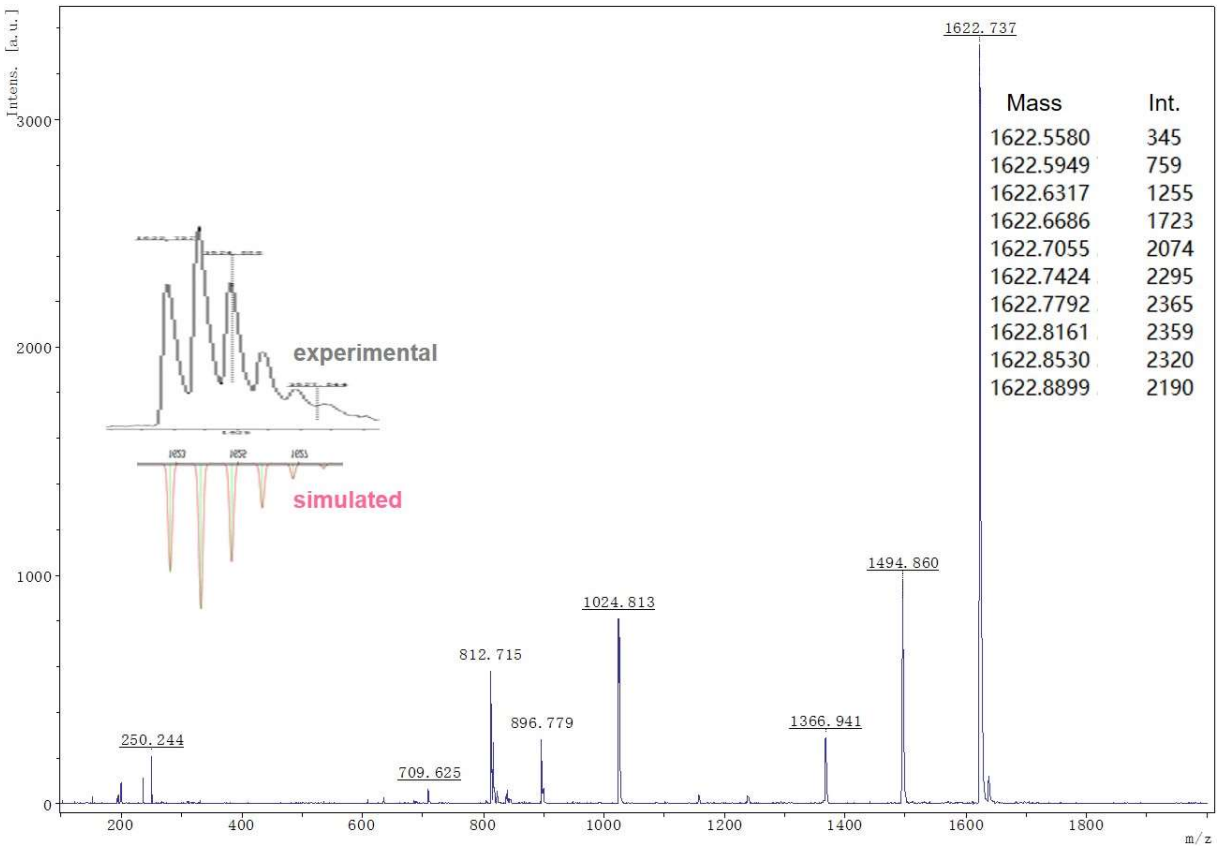


Figure S15. HR MALDI-TOF mass spectrum and isotopic distribution pattern of NG **1**.

Computational Details

Geometry calculations of the compounds **1** were carried out by DFT methods using the Gaussian 09 software.[S6] Ground state geometry were fully optimized by using density functional theory (DFT) [S7] and the M06-2X method with the 6-31G** basis set for all atoms. Frequency calculations have been performed to verify the optimized structures as local minima or transition states and to obtain Gibbs free energy at 298 K. The atomic coordinates of the calculated structures are shown in Tables S3-S5. Colour coding: C, gray; H, white; N, blue. Electronic transitions of the M and P enantiomers of **1** were calculated by means of TD-DFT methods using the Gaussian 09 software, CAM-B3LYP/6-31G** theory level was used and the first 100 excited states were considered in the gas phase.

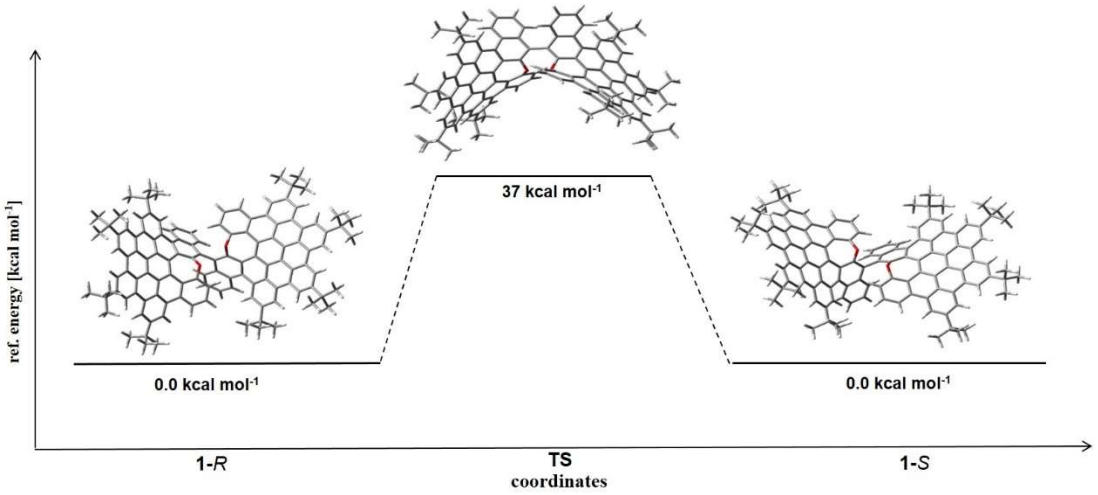


Figure S16. Computed racemization process of the NG-**1** at the B3LYP/6-31G level.

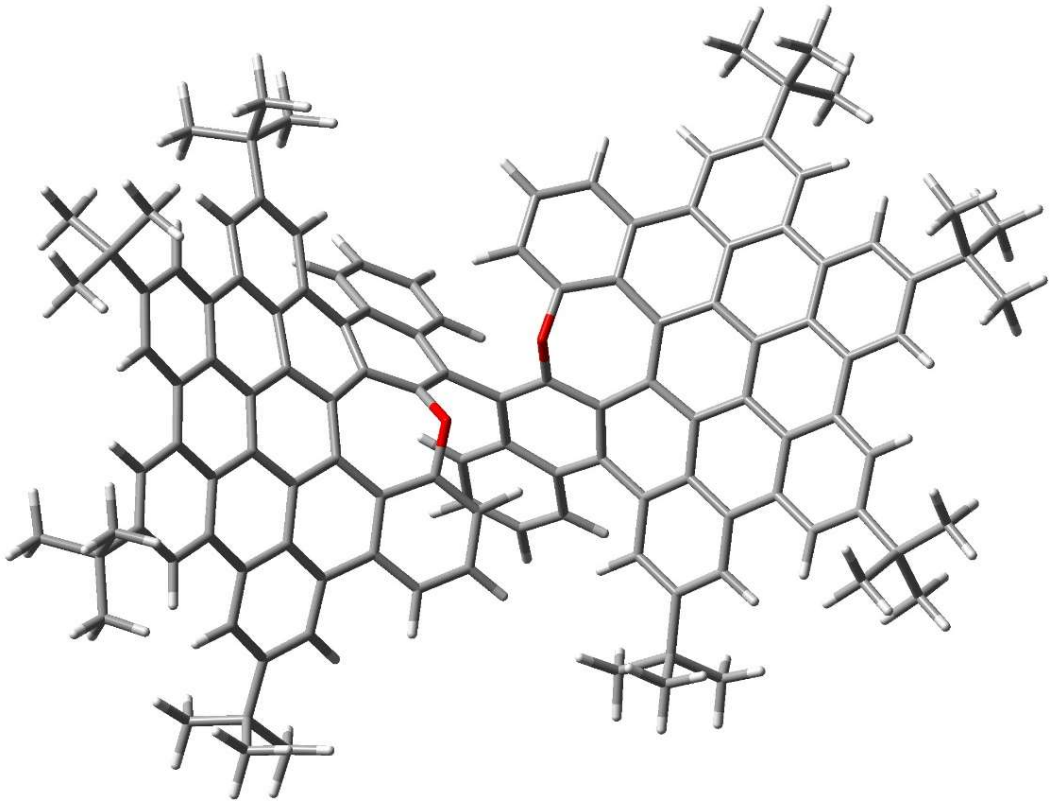


Figure S17. DFT optimized structure of **1**-*R*.

Table S3. Optimized energy and Atomic coordinates for the DFT calculated structure of **1**-*R*:

Zero-point correction=	1.914276 (Hartree/Particle)
Thermal correction to Energy=	2.017186
Thermal correction to Enthalpy=	2.018131
Thermal correction to Gibbs Free Energy=	1.774463
Sum of electronic and zero-point Energies=	-4933.697982
Sum of electronic and thermal Energies=	-4933.595071
Sum of electronic and thermal Enthalpies=	-4933.594127
Sum of electronic and thermal Free Energies=	-4933.837795

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.185976	-0.358222	0.498022
2	6	0	1.536507	0.562434	1.455249
3	6	0	2.134536	2.766047	3.028054
4	6	0	1.645154	-1.619987	0.788107
5	6	0	6.045864	0.909282	-0.605659
6	6	0	6.244500	-0.476312	-0.665748
7	6	0	4.924000	1.417194	0.093855
8	6	0	0.953557	2.014040	3.278295
9	6	0	8.046832	1.302349	-2.018304
10	6	0	3.880085	0.558352	0.514629

11	6	0	5.274148	-1.356010	-0.112152
12	6	0	7.753659	-2.367488	-1.198752
13	6	0	3.930139	3.342654	1.300195
14	6	0	0.626201	0.925780	2.406960
15	6	0	2.806044	1.181149	1.291327
16	6	0	4.031961	-0.864844	0.364890
17	6	0	0.685359	-2.578389	1.051372
18	1	0	-0.358512	-2.281478	1.037300
19	6	0	7.441562	-0.995784	-1.289366
20	6	0	6.788303	3.208937	-1.166221
21	6	0	8.840536	2.191511	-2.754057
22	1	0	9.638530	1.799157	-3.368423
23	6	0	4.868779	2.834905	0.373402
24	6	0	3.027785	-1.882905	0.737975
25	6	0	6.978022	1.808972	-1.247371
26	6	0	9.712181	-2.051134	-2.613426
27	6	0	2.976501	2.423333	1.902647
28	6	0	5.771153	3.733219	-0.249034
29	6	0	3.826259	4.731343	1.481872
30	1	0	3.012333	5.112850	2.080184
31	6	0	8.315328	-0.137479	-2.001152
32	6	0	3.401457	-3.234049	0.944619
33	6	0	4.787040	-3.639053	0.732915
34	6	0	9.429136	-0.686310	-2.639244
35	1	0	10.108839	-0.035189	-3.175939
36	6	0	5.639600	-2.751806	0.049680
37	6	0	6.904088	-3.227981	-0.375516
38	6	0	4.700867	5.620668	0.874883
39	6	0	7.325009	-4.496960	0.016564
40	1	0	8.323685	-4.823712	-0.251350
41	6	0	8.861805	-2.874367	-1.881751
42	1	0	9.047607	-3.939749	-1.855563
43	6	0	8.620926	3.563170	-2.741104
44	6	0	5.689573	5.092794	0.042044
45	1	0	6.412752	5.772628	-0.393819
46	6	0	7.592430	4.049337	-1.931340
47	1	0	7.406989	5.117237	-1.918419
48	6	0	9.455076	4.545147	-3.568419
49	6	0	5.255644	-4.899441	1.122952
50	1	0	4.613318	-5.531437	1.721223
51	6	0	4.623496	7.133115	1.096826
52	6	0	2.495514	3.759043	3.977295
53	1	0	3.457048	4.250148	3.887476
54	6	0	10.935241	-2.581726	-3.367072
55	6	0	2.426305	-4.206249	1.229130
56	1	0	2.723096	-5.241292	1.340106
57	6	0	0.110499	2.372679	4.359071
58	1	0	-0.812424	1.819181	4.502974

59	6	0	1.084007	-3.890155	1.285338
60	1	0	0.342460	-4.659680	1.474506
61	6	0	6.531584	-5.340919	0.796342
62	6	0	1.684727	4.058228	5.046010
63	1	0	2.000069	4.805830	5.766705
64	6	0	7.088987	-6.689881	1.256785
65	6	0	0.460034	3.384089	5.219845
66	1	0	-0.189484	3.641503	6.050013
67	6	0	10.575362	3.844600	-4.343544
68	1	0	10.178338	3.116542	-5.057807
69	1	0	11.147526	4.586829	-4.907868
70	1	0	11.268190	3.329462	-3.670185
71	6	0	8.539218	5.258554	-4.576950
72	1	0	7.730996	5.798322	-4.075134
73	1	0	9.114914	5.981901	-5.164302
74	1	0	8.086294	4.538160	-5.264650
75	6	0	10.806485	-2.231228	-4.859006
76	1	0	10.746983	-1.150485	-5.015398
77	1	0	11.676553	-2.603235	-5.410326
78	1	0	9.906776	-2.683176	-5.286969
79	6	0	7.484190	-7.528601	0.029864
80	1	0	8.247237	-7.028048	-0.572823
81	1	0	7.890167	-8.494085	0.349773
82	1	0	6.615902	-7.713842	-0.609560
83	6	0	6.069414	-7.486327	2.076665
84	1	0	5.169240	-7.708112	1.494489
85	1	0	6.511779	-8.438588	2.384027
86	1	0	5.773459	-6.948162	2.982580
87	6	0	10.096026	5.585904	-2.634533
88	1	0	10.740142	5.099848	-1.895632
89	1	0	10.704411	6.287823	-3.214423
90	1	0	9.341356	6.164973	-2.095033
91	6	0	5.924874	7.606158	1.766416
92	1	0	6.799895	7.379342	1.150640
93	1	0	5.896028	8.689284	1.925837
94	1	0	6.060319	7.118296	2.736480
95	6	0	3.446780	7.524704	1.996870
96	1	0	3.525060	7.066368	2.988287
97	1	0	3.435655	8.610428	2.130941
98	1	0	2.488337	7.231726	1.556592
99	6	0	8.330920	-6.447804	2.131411
100	1	0	8.075480	-5.844368	3.007500
101	1	0	8.741341	-7.402405	2.477467
102	1	0	9.116179	-5.924146	1.578940
103	6	0	4.455313	7.845364	-0.255342
104	1	0	3.537537	7.518895	-0.753396
105	1	0	4.401517	8.928926	-0.106605
106	1	0	5.294033	7.640122	-0.926440

107	6	0	11.077365	-4.101702	-3.240679
108	1	0	10.207707	-4.622999	-3.653221
109	1	0	11.960219	-4.432564	-3.795624
110	1	0	11.204050	-4.408583	-2.197533
111	6	0	12.205417	-1.928652	-2.796442
112	1	0	12.318061	-2.163339	-1.733731
113	1	0	13.089737	-2.296860	-3.327349
114	1	0	12.181052	-0.840217	-2.900114
115	8	0	-1.477661	1.232353	0.601399
116	6	0	-1.643444	0.326260	1.619711
117	6	0	-1.882194	-1.772098	3.421272
118	6	0	-2.170306	2.396520	0.842183
119	6	0	-5.951707	-1.001978	-0.451225
120	6	0	-6.391683	0.310166	-0.663917
121	6	0	-4.799941	-1.227132	0.343197
122	6	0	-0.791780	-0.867433	3.523767
123	6	0	-7.742692	-1.882133	-1.920809
124	6	0	-3.951607	-0.155889	0.705954
125	6	0	-5.632002	1.400951	-0.161023
126	6	0	-8.175804	1.837237	-1.455074
127	6	0	-3.545388	-2.809714	1.780319
128	6	0	-0.636362	0.149095	2.523507
129	6	0	-2.807804	-0.493283	1.555211
130	6	0	-4.351400	1.191686	0.404654
131	6	0	-1.420545	3.520162	1.129035
132	1	0	-0.342432	3.418137	1.189374
133	6	0	-7.618747	0.539512	-1.391872
134	6	0	-6.223766	-3.438756	-0.81405
135	6	0	-8.294295	-2.963531	-2.620928
136	1	0	-9.094221	-2.780744	-3.324568
137	6	0	-4.508177	-2.575656	0.771380
138	6	0	-3.572901	2.400772	0.726750
139	6	0	-6.659383	-2.112012	-1.044421
140	6	0	-9.951335	1.026270	-2.919640
141	6	0	-2.777356	-1.680920	2.288316
142	6	0	-5.196012	-3.678141	0.205408
143	6	0	-3.221557	-4.133841	2.123530
144	1	0	-2.397944	-4.306052	2.800126
145	6	0	-8.271580	-0.523782	-2.054945
146	6	0	-4.200977	3.666059	0.830337
147	6	0	-5.617157	3.794873	0.497066
148	6	0	-9.429265	-0.255115	-2.798576
149	1	0	-9.939073	-1.071783	-3.290143
150	6	0	-6.249686	2.714432	-0.148178
151	6	0	-7.547658	2.910486	-0.680637
152	6	0	-3.891120	-5.220496	1.579520
153	6	0	-8.212181	4.109853	-0.437880
154	1	0	-9.232676	4.223923	-0.787015

155	6	0	-9.306060	2.059588	-2.235000
156	1	0	-9.691208	3.068810	-2.330718
157	6	0	-7.824527	-4.261338	-2.465061
158	6	0	-4.894016	-4.965199	0.641479
159	1	0	-5.449089	-5.804109	0.237608
160	6	0	-6.797317	-4.476541	-1.542527
161	1	0	-6.421649	-5.485431	-1.415190
162	6	0	-8.382661	-5.446717	-3.257207
163	6	0	-6.327709	4.978811	0.731123
164	1	0	-5.851756	5.771121	1.292360
165	6	0	-3.560440	-6.666728	1.957960
166	6	0	-2.088223	-2.686914	4.486113
167	1	0	-2.986223	-3.293847	4.493442
168	6	0	-11.194063	1.340955	-3.756617
169	6	0	-3.437785	4.807795	1.132787
170	1	0	-3.918997	5.775943	1.185055
171	6	0	0.131387	-1.009085	4.587907
172	1	0	0.990270	-0.347440	4.627934
173	6	0	-2.068631	4.741136	1.294664
174	1	0	-1.498434	5.637781	1.512955
175	6	0	-7.634194	5.150720	0.292277
176	6	0	-1.206796	-2.770861	5.538148
177	1	0	-1.401101	-3.464138	6.350030
178	6	0	-8.449017	6.414132	0.579129
179	6	0	-0.064165	-1.948802	5.570733
180	1	0	0.645706	-2.036169	6.386658
181	6	0	-9.513124	-5.030530	-4.203591
182	1	0	-9.170238	-4.300574	-4.943611
183	1	0	-9.877523	-5.908292	-4.745468
184	1	0	-10.358650	-4.600763	-3.656867
185	6	0	-7.253417	-6.067320	-4.097290
186	1	0	-6.431351	-6.422373	-3.469228
187	1	0	-7.633441	-6.921153	-4.668252
188	1	0	-6.846736	-5.334903	-4.800906
189	6	0	-11.784904	0.088947	-4.412899
190	1	0	-12.100055	-0.647052	-3.666240
191	1	0	-12.665537	0.366122	-4.999749
192	1	0	-11.068990	-0.386963	-5.090534
193	6	0	-8.893733	7.050929	-0.747823
194	1	0	-9.517322	6.370442	-1.334525
195	1	0	-9.478300	7.956191	-0.552527
196	1	0	-8.026918	7.324330	-1.356758
197	6	0	-7.644910	7.453906	1.365837
198	1	0	-6.755905	7.775522	0.813903
199	1	0	-8.265019	8.337401	1.544380
200	1	0	-7.328542	7.066857	2.339513
201	6	0	-8.933277	-6.501074	-2.282419
202	1	0	-9.735859	-6.080370	-1.669274

203	1	0	-9.334494	-7.354243	-2.839474
204	1	0	-8.155992	-6.875587	-1.610269
205	6	0	-4.823435	-7.352728	2.505351
206	1	0	-5.629553	-7.371789	1.766741
207	1	0	-4.597806	-8.388379	2.780139
208	1	0	-5.192551	-6.832371	3.394184
209	6	0	-2.470380	-6.748887	3.031632
210	1	0	-2.766068	-6.226108	3.947296
211	1	0	-2.287431	-7.797063	3.286396
212	1	0	-1.524183	-6.322528	2.683977
213	6	0	-9.690089	6.034714	1.405224
214	1	0	-9.397083	5.571004	2.351924
215	1	0	-10.283477	6.927953	1.627185
216	1	0	-10.330404	5.329170	0.868142
217	6	0	-3.071391	-7.416624	0.707606
218	1	0	-2.172176	-6.944599	0.299859
219	1	0	-2.833457	-8.456138	0.957036
220	1	0	-3.832465	-7.423497	-0.078204
221	6	0	-10.816088	2.335836	-4.866853
222	1	0	-10.052774	1.910106	-5.524974
223	1	0	-11.696505	2.578839	-5.471172
224	1	0	-10.423034	3.269749	-4.455509
225	6	0	-12.271602	1.966353	-2.854796
226	1	0	-11.923730	2.896902	-2.397376
227	1	0	-13.167824	2.195480	-3.440798
228	1	0	-12.551005	1.279117	-2.050565

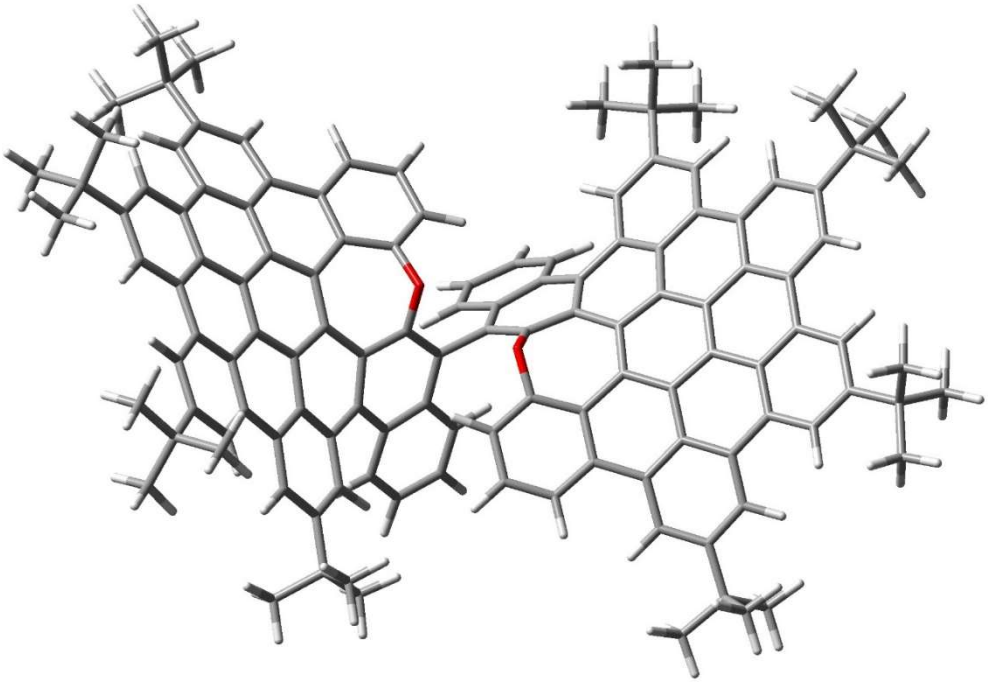


Figure S18. DFT optimized structure of **1**-*S*.

Table S4. Optimized energy and Atomic coordinates for the DFT calculated structure of **1**-*S*:

Zero-point correction=	1.914276 (Hartree/Particle)
Thermal correction to Energy=	2.017187
Thermal correction to Enthalpy=	2.018131
Thermal correction to Gibbs Free Energy=	1.774457
Sum of electronic and zero-point Energies=	-4933.697982
Sum of electronic and thermal Energies=	-4933.595071
Sum of electronic and thermal Enthalpies=	-4933.594126
Sum of electronic and thermal Free Energies=	-4933.837800

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.185589	0.358216	0.498291
2	6	0	1.536379	-0.562230	1.455621
3	6	0	2.134781	-2.765642	3.028597
4	6	0	1.644753	1.620058	0.788064
5	6	0	6.045437	-0.909185	-0.605932
6	6	0	6.244038	0.476411	-0.666124
7	6	0	4.923652	-1.417070	0.093731
8	6	0	0.953870	-2.013591	3.279024
9	6	0	8.046421	-1.302322	-2.018530
10	6	0	3.879769	-0.558217	0.514549
11	6	0	5.273693	1.356134	-0.112552
12	6	0	7.753153	2.367580	-1.199275
13	6	0	3.929987	-3.342423	1.300375
14	6	0	0.626292	-0.925479	2.407577
15	6	0	2.805890	-1.180937	1.291520
16	6	0	4.031559	0.864970	0.364636
17	6	0	0.684933	2.578441	1.051316
18	1	0	-0.358934	2.281416	1.037433
19	6	0	7.441077	0.995864	-1.289802
20	6	0	6.787920	-3.208879	-1.166308
21	6	0	8.840254	-2.191531	-2.754082
22	1	0	9.638311	-1.799227	-3.368399
23	6	0	4.868492	-2.834759	0.373397
24	6	0	3.027367	1.883026	0.737710
25	6	0	6.977599	-1.808913	-1.247585
26	6	0	9.711709	2.051157	-2.613884
27	6	0	2.976480	-2.423046	1.902950
28	6	0	5.770795	-3.733119	-0.249070
29	6	0	3.826091	-4.731094	1.482170
30	1	0	3.012270	-5.112532	2.080667
31	6	0	8.314855	0.137525	-2.001533
32	6	0	3.400996	3.234212	0.944165
33	6	0	4.786557	3.639240	0.732353
34	6	0	9.428654	0.686338	-2.639664
35	1	0	10.108341	0.035227	-3.176376
36	6	0	5.639116	2.751950	0.049167

37	6	0	6.903600	3.228109	-0.376060
38	6	0	4.700576	-5.620477	0.875079
39	6	0	7.324549	4.497087	0.015989
40	1	0	8.323267	4.823767	-0.251860
41	6	0	8.861283	2.874436	-1.882307
42	1	0	9.047042	3.939826	-1.856219
43	6	0	8.620716	-3.563200	-2.740977
44	6	0	5.689196	-5.092671	0.042089
45	1	0	6.412272	-5.772588	-0.393775
46	6	0	7.592131	-4.049311	-1.931285
47	1	0	7.406759	-5.117205	-1.918322
48	6	0	9.455107	-4.545278	-3.567922
49	6	0	5.255162	4.899658	1.122299
50	1	0	4.612867	5.531699	1.720553
51	6	0	4.623200	-7.132911	1.097119
52	6	0	2.496017	-3.758523	3.977868
53	1	0	3.457499	-4.249679	3.887799
54	6	0	10.934802	2.581750	-3.367465
55	6	0	2.425824	4.206401	1.228657
56	1	0	2.722569	5.241474	1.339484
57	6	0	0.111108	-2.372087	4.360081
58	1	0	-0.811789	-1.818593	4.504197
59	6	0	1.083538	3.890265	1.285055
60	1	0	0.342019	4.659803	1.474209
61	6	0	6.531117	5.341101	0.795698
62	6	0	1.685529	-4.057542	5.046852
63	1	0	2.001045	-4.805052	5.767565
64	6	0	7.088564	6.690006	1.256240
65	6	0	0.460888	-3.383363	5.220912
66	1	0	-0.188402	-3.640646	6.051297
67	6	0	10.575193	-3.844750	-4.343338
68	1	0	10.177962	-3.116855	-5.057666
69	1	0	11.147337	-4.587029	-4.907623
70	1	0	11.268077	-3.329414	-3.670186
71	6	0	8.539429	-5.259333	-4.576150
72	1	0	7.731275	-5.799009	-4.074122
73	1	0	9.115276	-5.982857	-5.163135
74	1	0	8.086420	-4.539334	-5.264209
75	6	0	10.806034	2.231497	-4.859459
76	1	0	10.746465	1.150770	-5.015998
77	1	0	11.676131	2.603533	-5.410706
78	1	0	9.906349	2.683569	-5.287380
79	6	0	7.484352	7.528607	0.029444
80	1	0	8.247586	7.027950	-0.572918
81	1	0	7.890322	8.494053	0.349468
82	1	0	6.616340	7.713923	-0.610324
83	6	0	6.068810	7.486679	2.075683
84	1	0	5.168854	7.708490	1.493182

85	1	0	6.511210	8.438914	2.383067
86	1	0	5.772506	6.948660	2.981571
87	6	0	10.096307	-5.585477	-2.633590
88	1	0	10.740229	-5.098922	-1.894848
89	1	0	10.704939	-6.287452	-3.213167
90	1	0	9.341763	-6.164553	-2.093908
91	6	0	5.924650	-7.605938	1.766594
92	1	0	6.799615	-7.379114	1.150742
93	1	0	5.895822	-8.689058	1.926035
94	1	0	6.060174	-7.118064	2.736642
95	6	0	3.446594	-7.524421	1.997340
96	1	0	3.525082	-7.066074	2.988734
97	1	0	3.435417	-8.610142	2.131408
98	1	0	2.488104	-7.231363	1.557224
99	6	0	8.330110	6.447770	2.131369
100	1	0	8.074233	5.844401	3.007373
101	1	0	8.740549	7.402318	2.477554
102	1	0	9.115483	5.923962	1.579207
103	6	0	4.454887	-7.845235	-0.254998
104	1	0	3.537088	-7.518753	-0.752993
105	1	0	4.401065	-8.928785	-0.106203
106	1	0	5.293569	-7.640028	-0.926149
107	6	0	11.077127	4.101694	-3.240743
108	1	0	10.207546	4.623170	-3.653213
109	1	0	11.960024	4.432574	-3.795580
110	1	0	11.203778	4.408301	-2.197516
111	6	0	12.204936	1.928441	-2.797011
112	1	0	12.317824	2.163191	-1.734335
113	1	0	13.089241	2.296433	-3.328101
114	1	0	12.180339	0.840009	-2.900600
115	8	0	-1.477331	-1.232200	0.601925
116	6	0	-1.643297	-0.326139	1.620232
117	6	0	-1.882392	1.772184	3.421734
118	6	0	-2.169901	-2.396431	0.842591
119	6	0	-5.951427	1.001800	-0.451236
120	6	0	-6.391234	-0.310377	-0.664087
121	6	0	-4.799783	1.227024	0.343350
122	6	0	-0.791930	0.867601	3.524376
123	6	0	-7.742317	1.881863	-1.921012
124	6	0	-3.951392	0.155833	0.706168
125	6	0	-5.631511	-1.401119	-0.161165
126	6	0	-8.175104	-1.837586	-1.455587
127	6	0	-3.545468	2.809690	1.780613
128	6	0	-0.636340	-0.148926	2.524170
129	6	0	-2.807718	0.493307	1.555580
130	6	0	-4.351017	-1.191763	0.404731
131	6	0	-1.420093	-3.520010	1.129574
132	1	0	-0.342004	-3.417895	1.190167

133	6	0	-7.618174	-0.539808	-1.392229
134	6	0	-6.223752	3.438574	-0.813901
135	6	0	-8.293932	2.963246	-2.621143
136	1	0	-9.093694	2.780387	-3.324966
137	6	0	-4.508171	2.575567	0.771608
138	6	0	-3.572468	-2.400804	0.726883
139	6	0	-6.659157	2.111794	-1.044445
140	6	0	-9.950588	-1.026688	-2.920231
141	6	0	-2.777414	1.680956	2.288671
142	6	0	-5.196069	3.678014	0.205623
143	6	0	-3.221757	4.133836	2.123873
144	1	0	-2.398221	4.306114	2.800547
145	6	0	-8.271039	0.523461	-2.055304
146	6	0	-4.200440	-3.666155	0.830275
147	6	0	-5.616565	-3.795059	0.496817
148	6	0	-9.428648	0.254743	-2.799043
149	1	0	-9.938502	1.071431	-3.290535
150	6	0	-6.249081	-2.714657	-0.148490
151	6	0	-7.546984	-2.910803	-0.681094
152	6	0	-3.891357	5.220438	1.579831
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154	1	0	-9.231956	-4.224252	-0.787546
155	6	0	-9.305237	-2.060001	-2.235664
156	1	0	-9.690219	-3.069264	-2.331531
157	6	0	-7.824414	4.261113	-2.465036
158	6	0	-4.894191	4.965096	0.641726
159	1	0	-5.449270	5.803984	0.237812
160	6	0	-6.797407	4.476374	-1.542283
161	1	0	-6.421963	5.485310	-1.414659
162	6	0	-8.382632	5.446502	-3.257104
163	6	0	-6.327085	-4.979017	0.730860
164	1	0	-5.851156	-5.771258	1.292207
165	6	0	-3.560839	6.666698	1.958269
166	6	0	-2.088644	2.686980	4.486556
167	1	0	-2.986702	3.293821	4.493758
168	6	0	-11.193207	-1.341429	-3.757340
169	6	0	-3.437199	-4.807854	1.132738
170	1	0	-3.918334	-5.776052	1.184761
171	6	0	0.131084	1.009334	4.588633
172	1	0	0.990013	0.347751	4.628789
173	6	0	-2.068083	-4.741070	1.294931
174	1	0	-1.497833	-5.637683	1.513203
175	6	0	-7.633538	-5.150986	0.291933
176	6	0	-1.207356	2.771006	5.538706
177	1	0	-1.401828	3.464258	6.350568
178	6	0	-8.448397	-6.414350	0.578912
179	6	0	-0.064660	1.949041	5.571428
180	1	0	0.645105	2.036468	6.387436

181	6	0	-9.512555	5.030162	-4.204062
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183	1	0	-9.876933	5.907918	-4.745971
184	1	0	-10.358219	4.600080	-3.657783
185	6	0	-7.253259	6.067711	-4.096556
186	1	0	-6.431491	6.422726	-3.468080
187	1	0	-7.633302	6.921669	-4.667326
188	1	0	-6.846165	5.335660	-4.800316
189	6	0	-11.784356	-0.089305	-4.413141
190	1	0	-12.099461	0.646410	-3.666179
191	1	0	-12.665061	-0.366413	-4.999925
192	1	0	-11.068607	0.386926	-5.090729
193	6	0	-8.892801	-7.051457	-0.747980
194	1	0	-9.516294	-6.371106	-1.334950
195	1	0	-9.477389	-7.956687	-0.552598
196	1	0	-8.025852	-7.324966	-1.356662
197	6	0	-7.644435	-7.453918	1.366037
198	1	0	-6.755347	-7.775693	0.814336
199	1	0	-8.264605	-8.337349	1.544705
200	1	0	-7.328238	-7.066578	2.339650
201	6	0	-8.934000	6.500417	-2.282269
202	1	0	-9.736622	6.079237	-1.669499
203	1	0	-9.335387	7.353538	-2.839281
204	1	0	-8.157094	6.875120	-1.609785
205	6	0	-4.823807	7.352383	2.506126
206	1	0	-5.630163	7.371294	1.767760
207	1	0	-4.598338	8.388082	2.780884
208	1	0	-5.192516	6.831904	3.395065
209	6	0	-2.470425	6.749000	3.031562
210	1	0	-2.765777	6.226232	3.947340
211	1	0	-2.287481	7.797202	3.286223
212	1	0	-1.524321	6.322674	2.683600
213	6	0	-9.689641	-6.034799	1.404697
214	1	0	-9.396840	-5.570985	2.351407
215	1	0	-10.283094	-6.928008	1.626618
216	1	0	-10.329812	-5.329305	0.867392
217	6	0	-3.072431	7.416782	0.707762
218	1	0	-2.173401	6.944846	0.299502
219	1	0	-2.834429	8.456274	0.957213
220	1	0	-3.833881	7.423750	-0.077690
221	6	0	-10.814953	-2.335825	-4.867908
222	1	0	-10.051574	-1.909762	-5.525726
223	1	0	-11.695244	-2.578710	-5.472441
224	1	0	-10.421862	-3.269833	-4.456813
225	6	0	-12.270622	-1.967421	-2.855784
226	1	0	-11.922477	-2.897969	-2.398574
227	1	0	-13.166716	-2.196711	-3.441927
228	1	0	-12.550339	-1.280485	-2.051404

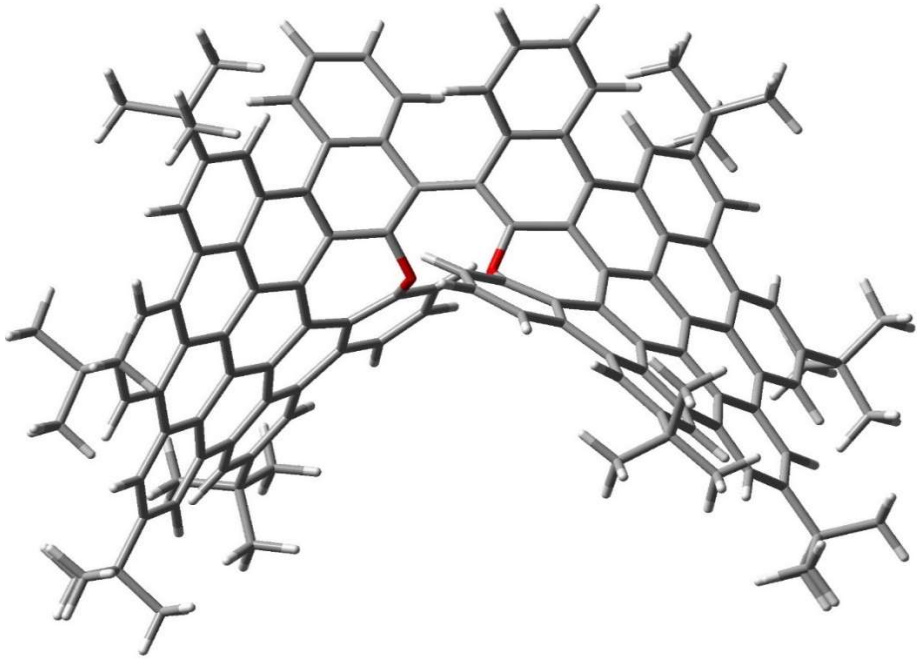

Figure S19. DFT optimized structure of *TS*.

Table S5. Optimized energy and Atomic coordinates for the DFT calculated structure of *TS*:

Zero-point correction=	1.911480 (Hartree/Particle)
Thermal correction to Energy=	2.012884
Thermal correction to Enthalpy=	2.013828
Thermal correction to Gibbs Free Energy=	1.776243
Sum of electronic and zero-point Energies=	-4933.643609
Sum of electronic and thermal Energies=	-4933.542204
Sum of electronic and thermal Enthalpies=	-4933.541260
Sum of electronic and thermal Free Energies=	-4933.778845

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.853897	1.131910	0.758094
2	6	0	1.465266	2.326589	0.510316
3	6	0	2.908444	4.672968	0.322221
4	6	0	0.932618	0.761798	2.080924
5	6	0	5.710712	-0.233660	0.218323
6	6	0	5.369186	-1.182528	1.189209
7	6	0	4.918142	0.934051	0.072981
8	6	0	1.501714	4.686050	0.504791
9	6	0	7.568571	-1.671162	-0.582235
10	6	0	3.659943	1.039838	0.717034
11	6	0	4.219696	-0.977617	1.996241
12	6	0	5.937848	-3.241124	2.436781
13	6	0	4.816927	3.289706	-0.677190

14	6	0	0.734947	3.471123	0.211413
15	6	0	2.900384	2.271284	0.465512
16	6	0	3.303155	0.052324	1.693738
17	6	0	-0.186925	0.938959	2.867874
18	1	0	-1.046505	1.447590	2.443677
19	6	0	6.187134	-2.358790	1.364958
20	6	0	7.267239	0.549613	-1.546414
21	6	0	8.598428	-1.897877	-1.504905
22	1	0	9.127166	-2.840240	-1.480889
23	6	0	5.439472	2.021351	-0.720405
24	6	0	2.095666	0.117924	2.524925
25	6	0	6.863859	-0.447272	-0.626596
26	6	0	7.626139	-4.781737	1.591031
27	6	0	3.562845	3.415305	0.029723
28	6	0	6.612277	1.861045	-1.498507
29	6	0	5.334579	4.345891	-1.447010
30	1	0	4.783116	5.274956	-1.480407
31	6	0	7.227077	-2.654517	0.450069
32	6	0	2.029079	-0.521259	3.783412
33	6	0	3.080434	-1.470995	4.151857
34	6	0	7.916802	-3.860727	0.584999
35	1	0	8.706977	-4.103999	-0.115335
36	6	0	4.063249	-1.792185	3.186801
37	6	0	4.956622	-2.853580	3.453069
38	6	0	6.497888	4.206063	-2.188987
39	6	0	4.915588	-3.496426	4.694300
40	1	0	5.647237	-4.265301	4.903439
41	6	0	6.641387	-4.445725	2.515732
42	1	0	6.393508	-5.144053	3.304064
43	6	0	8.958957	-0.955158	-2.459253
44	6	0	7.129250	2.958133	-2.181945
45	1	0	8.061004	2.848290	-2.725452
46	6	0	8.284262	0.267736	-2.453653
47	1	0	8.551781	1.010340	-3.197126
48	6	0	10.058706	-1.201179	-3.496189
49	6	0	3.086796	-2.131171	5.380227
50	1	0	2.361017	-1.853290	6.135541
51	6	0	7.108668	5.354683	-2.995409
52	6	0	3.661080	5.824512	0.654807
53	1	0	4.741128	5.788441	0.567371
54	6	0	8.399851	-6.102621	1.647480
55	6	0	0.893303	-0.334938	4.590423
56	1	0	0.832954	-0.816077	5.558328
57	6	0	0.928164	5.816704	1.130354
58	1	0	-0.120567	5.799174	1.395384
59	6	0	-0.188626	0.407614	4.156476
60	1	0	-1.057825	0.526701	4.794572
61	6	0	4.003305	-3.138326	5.681268

62	6	0	3.060357	6.939189	1.194904
63	1	0	3.661513	7.797664	1.475595
64	6	0	3.964221	-3.806206	7.058603
65	6	0	1.683059	6.921274	1.458447
66	1	0	1.211275	7.761595	1.957217
67	6	0	10.697869	-2.585536	-3.347735
68	1	0	9.962200	-3.384884	-3.481752
69	1	0	11.472278	-2.713451	-4.109739
70	1	0	11.170682	-2.708174	-2.368073
71	6	0	9.455599	-1.096119	-4.907203
72	1	0	9.017949	-0.109955	-5.086382
73	1	0	10.231074	-1.262279	-5.662325
74	1	0	8.669778	-1.844039	-5.048694
75	6	0	7.940298	-6.994844	2.804791
76	1	0	6.881636	-7.257984	2.714636
77	1	0	8.517465	-7.924173	2.799595
78	1	0	8.096854	-6.511158	3.774263
79	6	0	5.034903	-4.892118	7.206691
80	1	0	6.043298	-4.480903	7.096645
81	1	0	4.963372	-5.341089	8.201769
82	1	0	4.902745	-5.690512	6.469540
83	6	0	2.586012	-4.456566	7.268301
84	1	0	2.394139	-5.212999	6.501492
85	1	0	2.542665	-4.940528	8.249806
86	1	0	1.780139	-3.718703	7.222455
87	6	0	11.160763	-0.140695	-3.330965
88	1	0	11.602694	-0.194428	-2.331509
89	1	0	11.953475	-0.302514	-4.068932
90	1	0	10.771497	0.871378	-3.473907
91	6	0	8.504601	5.672330	-2.432762
92	1	0	9.170793	4.806742	-2.491438
93	1	0	8.963418	6.489390	-2.999624
94	1	0	8.438670	5.975375	-1.383442
95	6	0	6.258172	6.626743	-2.923319
96	1	0	6.152071	6.985072	-1.894220
97	1	0	6.738137	7.419644	-3.504649
98	1	0	5.257801	6.466459	-3.337550
99	6	0	4.198854	-2.744057	8.145807
100	1	0	3.437553	-1.959705	8.113015
101	1	0	4.163876	-3.206322	9.138053
102	1	0	5.176846	-2.270351	8.019305
103	6	0	7.235093	4.940935	-4.470952
104	1	0	6.254035	4.701845	-4.892130
105	1	0	7.671647	5.758120	-5.054858
106	1	0	7.877326	4.063719	-4.591157
107	6	0	9.898058	-5.807869	1.831697
108	1	0	10.073576	-5.261011	2.762923
109	1	0	10.464044	-6.744620	1.869409

110	1	0	10.296233	-5.208295	1.008258
111	6	0	8.188058	-6.872037	0.332873
112	1	0	8.546121	-6.303102	-0.529811
113	1	0	8.733445	-7.821373	0.359500
114	1	0	7.126856	-7.087470	0.176850
115	8	0	-0.841201	1.189441	-0.896729
116	6	0	-1.432696	2.371642	-0.558440
117	6	0	-2.841647	4.722132	-0.218379
118	6	0	-0.985328	0.884229	-2.231338
119	6	0	-5.683958	-0.166192	-0.209544
120	6	0	-5.390314	-1.076253	-1.230194
121	6	0	-4.878038	0.992481	-0.051825
122	6	0	-1.439363	4.725528	-0.428677
123	6	0	-7.509075	-1.630396	0.614628
124	6	0	-3.647240	1.116037	-0.740768
125	6	0	-4.274319	-0.844125	-2.077379
126	6	0	-6.020970	-3.084731	-2.531808
127	6	0	-4.732902	3.316533	0.781525
128	6	0	-0.682808	3.489040	-0.208145
129	6	0	-2.867304	2.330006	-0.470235
130	6	0	-3.338954	0.165854	-1.771543
131	6	0	0.096115	1.095536	-3.061195
132	1	0	0.976156	1.583507	-2.655455
133	6	0	-6.220854	-2.242564	-1.413863
134	6	0	-7.161418	0.554488	1.646296
135	6	0	-8.500723	-1.888626	1.571696
136	1	0	-9.034128	-2.827922	1.535580
137	6	0	-5.361391	2.050531	0.801662
138	6	0	-2.169837	0.262287	-2.650510
139	6	0	-6.800079	-0.409107	0.674424
140	6	0	-7.665114	-4.660248	-1.656804
141	6	0	-3.503341	3.460041	0.036947
142	6	0	-6.503945	1.865754	1.618771
143	6	0	-5.216680	4.346764	1.607338
144	1	0	-4.660010	5.272176	1.653218
145	6	0	-7.213927	-2.574189	-0.466074
146	6	0	-2.164465	-0.321602	-3.937678
147	6	0	-3.235015	-1.251604	-4.297303
148	6	0	-7.910300	-3.783348	-0.607867
149	1	0	-8.658608	-4.048696	0.125599
150	6	0	-4.173895	-1.607419	-3.307195
151	6	0	-5.088352	-2.654344	-3.578433
152	6	0	-6.351155	4.184036	2.387666
153	6	0	-5.105591	-3.236272	-4.842461
154	1	0	-5.851280	-3.993357	-5.060377
155	6	0	-6.723766	-4.281476	-2.618429
156	1	0	-6.517932	-4.955724	-3.442868
157	6	0	-8.817689	-0.980557	2.573310

158	6	0	-6.988458	2.938847	2.360873
159	1	0	-7.898467	2.812427	2.936824
160	6	0	-8.140107	0.241444	2.584024
161	1	0	-8.374371	0.956978	3.364367
162	6	0	-9.875250	-1.261391	3.644607
163	6	0	-3.295803	-1.859978	-5.557875
164	1	0	-2.599942	-1.548895	-6.324491
165	6	0	-6.924412	5.304474	3.258799
166	6	0	-3.584858	5.896440	-0.483794
167	1	0	-4.663356	5.870028	-0.375003
168	6	0	-8.381038	-6.006412	-1.799653
169	6	0	-1.066629	-0.098814	-4.788113
170	1	0	-1.053023	-0.533642	-5.779398
171	6	0	-0.860585	5.875818	-1.011535
172	1	0	0.184471	5.856942	-1.292004
173	6	0	0.035585	0.623026	-4.371772
174	1	0	0.873489	0.772057	-5.044424
175	6	0	-4.231223	-2.841803	-5.858007
176	6	0	-2.978989	7.026083	-0.986349
177	1	0	-3.573372	7.903572	-1.218491
178	6	0	-4.333604	-3.500767	-7.235960
179	6	0	-1.606797	7.003207	-1.275735
180	1	0	-1.133552	7.859831	-1.744497
181	6	0	-10.519767	-2.641086	3.476886
182	1	0	-9.779185	-3.443308	3.555974
183	1	0	-11.263787	-2.794493	4.264029
184	1	0	-11.030514	-2.733272	2.513044
185	6	0	-9.217295	-1.201562	5.033444
186	1	0	-8.773437	-0.221035	5.227655
187	1	0	-9.962821	-1.393364	5.812349
188	1	0	-8.426376	-1.952518	5.120168
189	6	0	-9.141419	-6.043251	-3.135958
190	1	0	-8.466900	-5.919804	-3.988049
191	1	0	-9.653792	-7.004205	-3.251134
192	1	0	-9.889198	-5.245686	-3.179217
193	6	0	-5.734249	-3.244251	-7.817296
194	1	0	-5.916050	-2.171209	-7.929453
195	1	0	-5.826350	-3.714709	-8.801944
196	1	0	-6.518775	-3.653217	-7.174416
197	6	0	-4.108908	-5.015431	-7.092095
198	1	0	-4.853000	-5.472456	-6.433473
199	1	0	-4.181608	-5.502547	-8.070285
200	1	0	-3.118278	-5.221874	-6.675876
201	6	0	-10.982521	-0.197381	3.557120
202	1	0	-11.461400	-0.217113	2.573480
203	1	0	-11.747804	-0.384469	4.317781
204	1	0	-10.587910	0.809753	3.719499
205	6	0	-8.338655	5.649041	2.761650

206	1	0	-9.006221	4.783905	2.810712
207	1	0	-8.771862	6.444357	3.377435
208	1	0	-8.309999	5.993325	1.723468
209	6	0	-6.069495	6.574357	3.202213
210	1	0	-5.999021	6.969948	2.183833
211	1	0	-6.522572	7.347292	3.830139
212	1	0	-5.055596	6.393751	3.573019
213	6	0	-3.296135	-2.951679	-8.220320
214	1	0	-2.274332	-3.132456	-7.871637
215	1	0	-3.411814	-3.449530	-9.187594
216	1	0	-3.423794	-1.876465	-8.380943
217	6	0	-6.997316	4.836035	4.721669
218	1	0	-6.003140	4.572226	5.094520
219	1	0	-7.402249	5.633880	5.353072
220	1	0	-7.643358	3.960587	4.834044
221	6	0	-9.383910	-6.254918	-0.668994
222	1	0	-10.172106	-5.495280	-0.654066
223	1	0	-9.861751	-7.228392	-0.813164
224	1	0	-8.892473	-6.265831	0.309092
225	6	0	-7.336832	-7.135514	-1.774769
226	1	0	-6.780436	-7.127158	-0.832790
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228	1	0	-6.616144	-7.037254	-2.591451

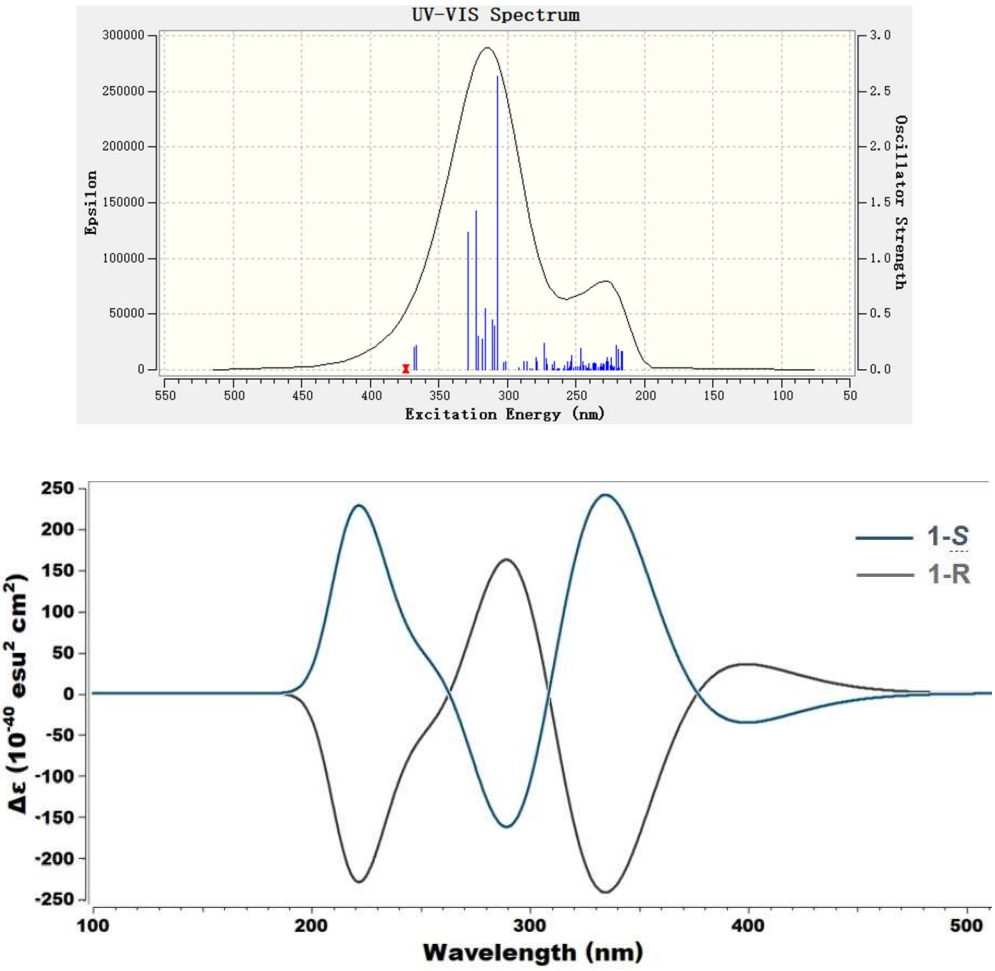

Figure S20. Calculated UV-vis spectrum of **1** (a) and ECD spectra of **1-*R* and 1-*S*** (b).

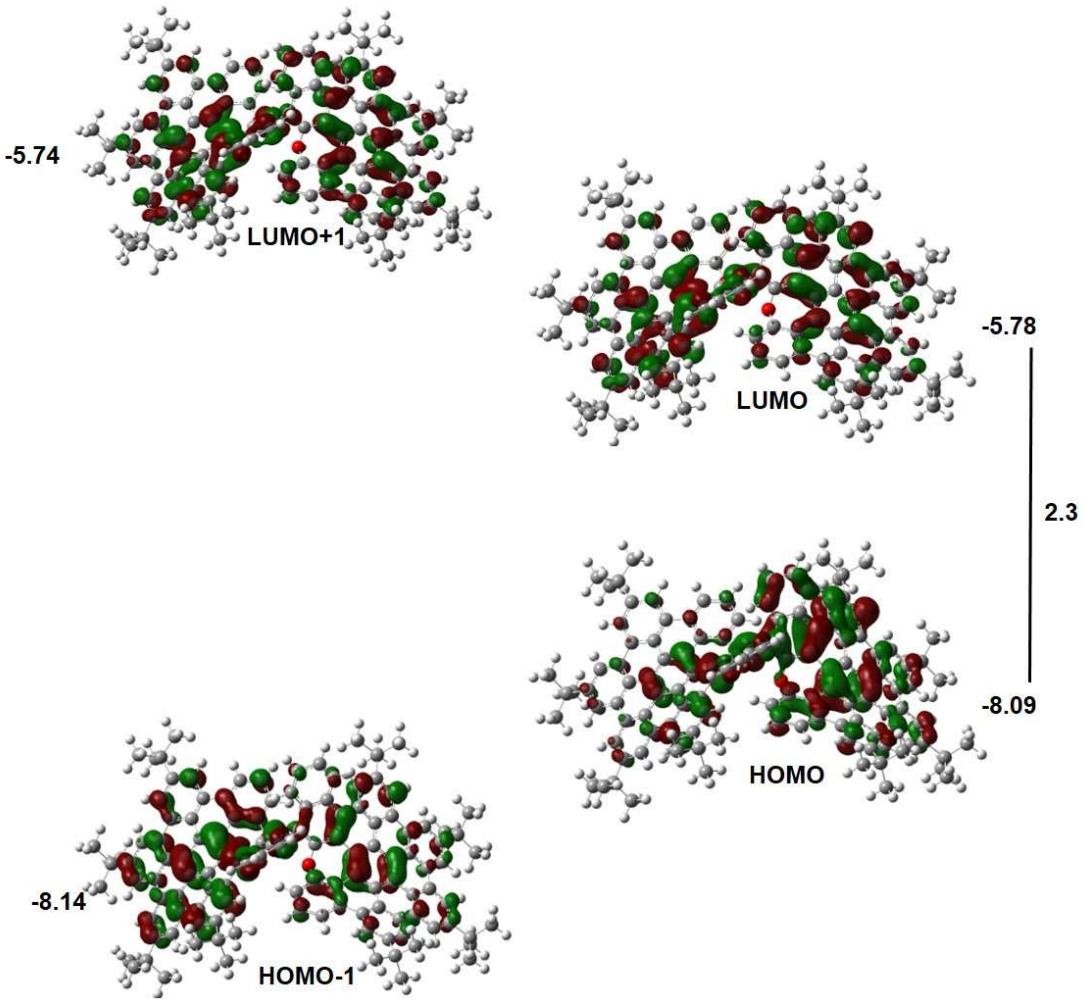

Figure S21. DFT calculated molecular orbitals (from HOMO-1 to LUMO+1) of compound **1** with energies.

Table S6. Major transitions of **1** calculated by TD-DFT.

Excited state	Energy (eV)	Wavelength (nm)	oscillator strength (f)	Description	
1	3.3158	373.92	0.0210	H-3 -> L	0.21139
				H-3 -> L+1	0.26901
				H-2 -> L	0.21161
				H-2 -> L+1	0.22486
				H-1 -> L+3	-0.19561
				H -> L+1	0.13112
				H -> L+3	0.36805
2	3.3229	373.12	0.0066	H-3 -> L	0.24717
				H-3 -> L+1	-0.18951
				H-2 -> L	-0.27862
				H-2 -> L+1	0.23720
				H-1 -> L+2	0.37430
				H -> L+2	0.21626
3	3.3744	367.43	0.1983	H-3 -> L+3	-0.17695
				H-2 -> L+3	-0.15282
				H-1 -> L	-0.21952
				H-1 -> L+1	-0.17198
				H -> L	0.33642
				H -> L+1	0.41538
				H -> L+3	-0.10436
4	3.3831	366.48	0.2162	H-3 -> L+2	-0.17049
				H-2 -> L+2	0.19399
				H-1 -> L	0.40170
				H-1 -> L+1	-0.33619
				H -> L	0.27911
				H -> L+1	-0.16957
5	3.7728	328.62	1.2362	H-7 -> L	0.11995
				H-5 -> L+1	0.15310
				H-4 -> L	-0.23398
				H-3 -> L+1	-0.11336
				H-2 -> L	-0.16259
				H-1 -> L+4	0.10767
				H-1 -> L+5	0.23541
				H ->L+4	0.37322
				H -> L+5	-0.12040
				H -> L+6	-0.10616
6	3.8454	322.42	1.4257	H-3 -> L+1	0.22046
				H-2 -> L	0.26810

				H-1 -> L+2	0.21161
				H-1 -> L+3	0.10830
				H-1 -> L+5	0.13171
				H -> L+2	0.13523
				H -> L+4	0.17922
7	3.8567	321.47	0.3038	H-3 -> L	-0.16237
				H-2 -> L+1	-0.14208
				H-2 -> L+2	0.11777
				H-1 -> L+2	0.13817
				H-1 -> L+3	-0.15794
				H-1 -> L+4	0.30682
				H -> L+2	0.12881
				H -> L+3	0.25440
				H -> L+5	0.27149
8	3.9008	317.84	0.2758	H-6 -> L	0.12140
				H-6 -> L+1	0.12436
				H-5 -> L	-0.11560
				H-5 -> L+1	-0.11540
				H-4 -> L+1	0.20087
				H-4 -> L+2	0.10928
				H-3-> L+1	-0.12362
				H-3 -> L+3	0.22837
				H-3 ->L+4	-0.11646
				H-3 -> L+5	0.11648
				H-2 -> L+3	0.20510
				H-2 -> L+4	-0.10817
				H-> L+3	0.10476
				H -> L+4	0.10886
				H ->L+8	-0.11126
9	3.9212	316.19	0.5501	H-7 -> L	0.10807
				H-5 -> L	-0.17676
				H-5 -> L+1	0.12307
				H-5 -> L+2	0.10931
				H-4 -> L	-0.13606
				H-4 -> L+1	0.14559
				H-3-> L+1	0.11797
				H-3 -> L+2	-0.19786
				H-3 ->L+4	-0.13790
				H-2 -> L+2	0.24134
				H-2 -> L+4	0.16302
				H -> L+4	-0.13001

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