Unlocking Intrinsically Chiral Bipyrenyl-based Aggregation-induced Emission Luminogens: Circularly Polarized Luminescence and Dynamic Chirality Amplification

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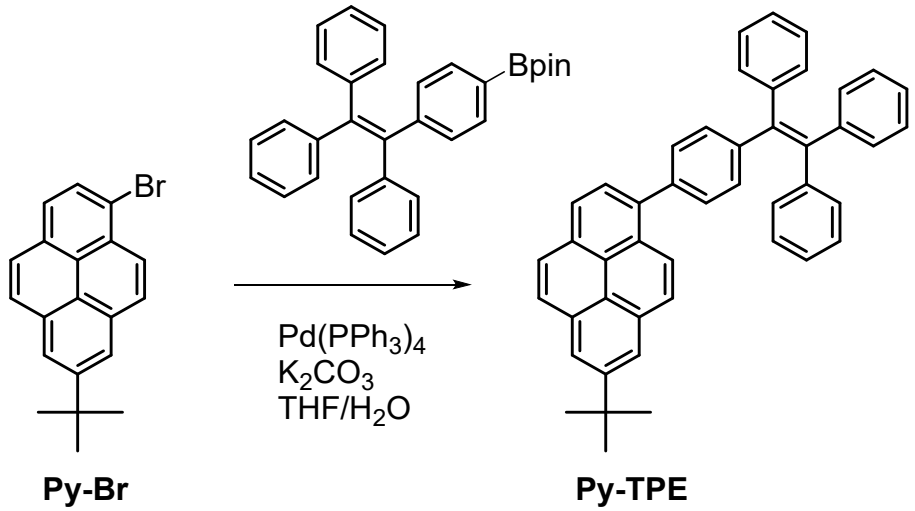
1. Experimental section

1.1 Materials

Unless otherwise stated, all reagents used were purchased from commercial sources and were used without further purification. Specpure grade solvents were used for spectroscopic measurements. The starting compound 7-*tert*-butyl-2-hydroxypyrene (**Py-OH**) was synthesized following the previously reported procedure.[1 2]

1.2 Synthetic Procedures



Scheme S1. Synthetic route for Py-TPE

2. NMR spectra

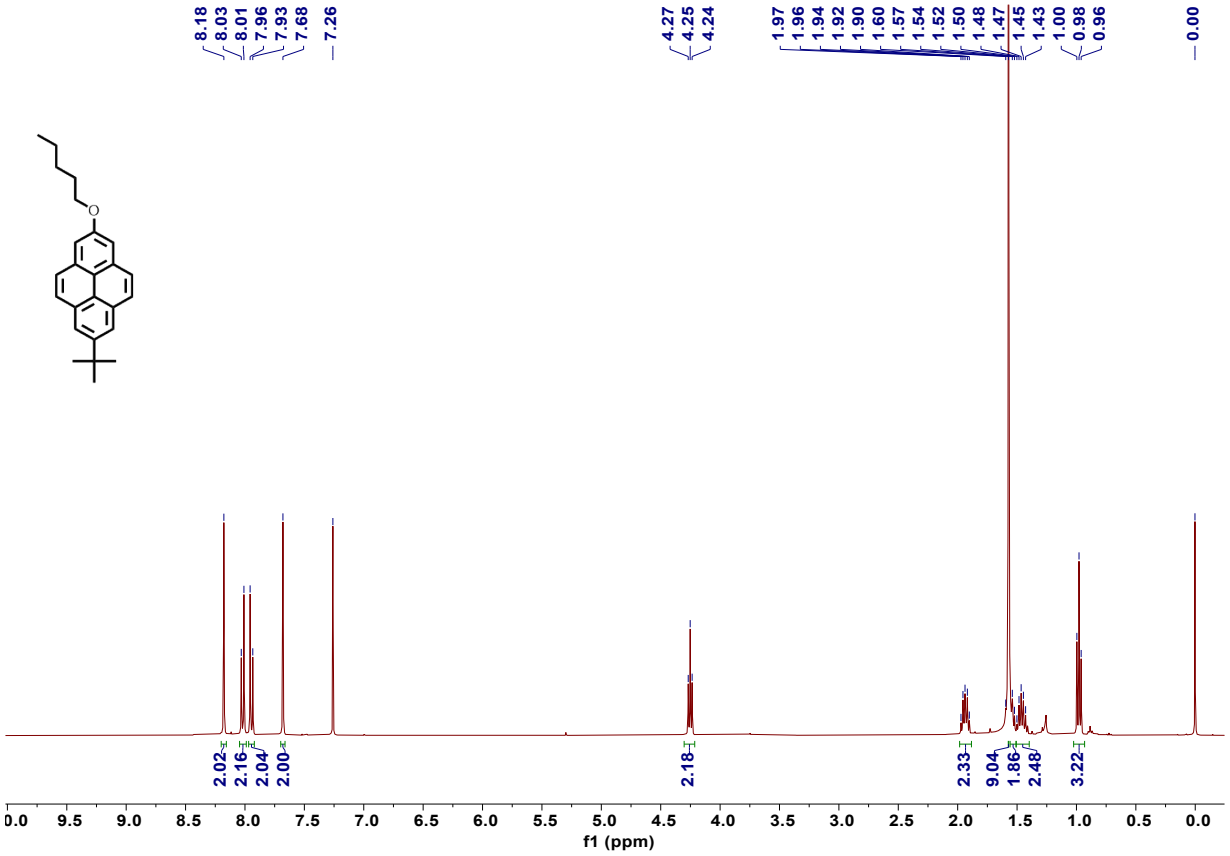


Figure S1. ^{1}H-NMR spectrum (400 MHz, 293 K, *$CDCl_3$) for **1**.

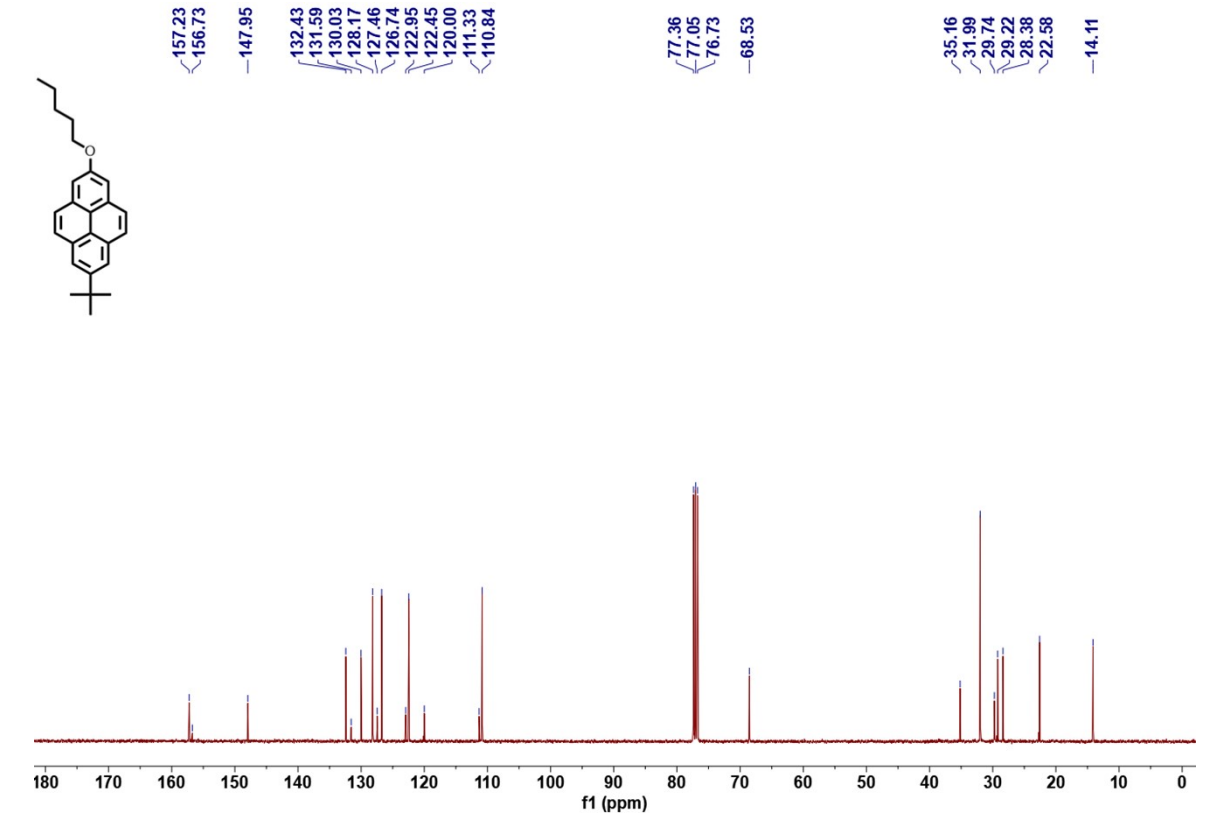


Figure S2. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for **1**.

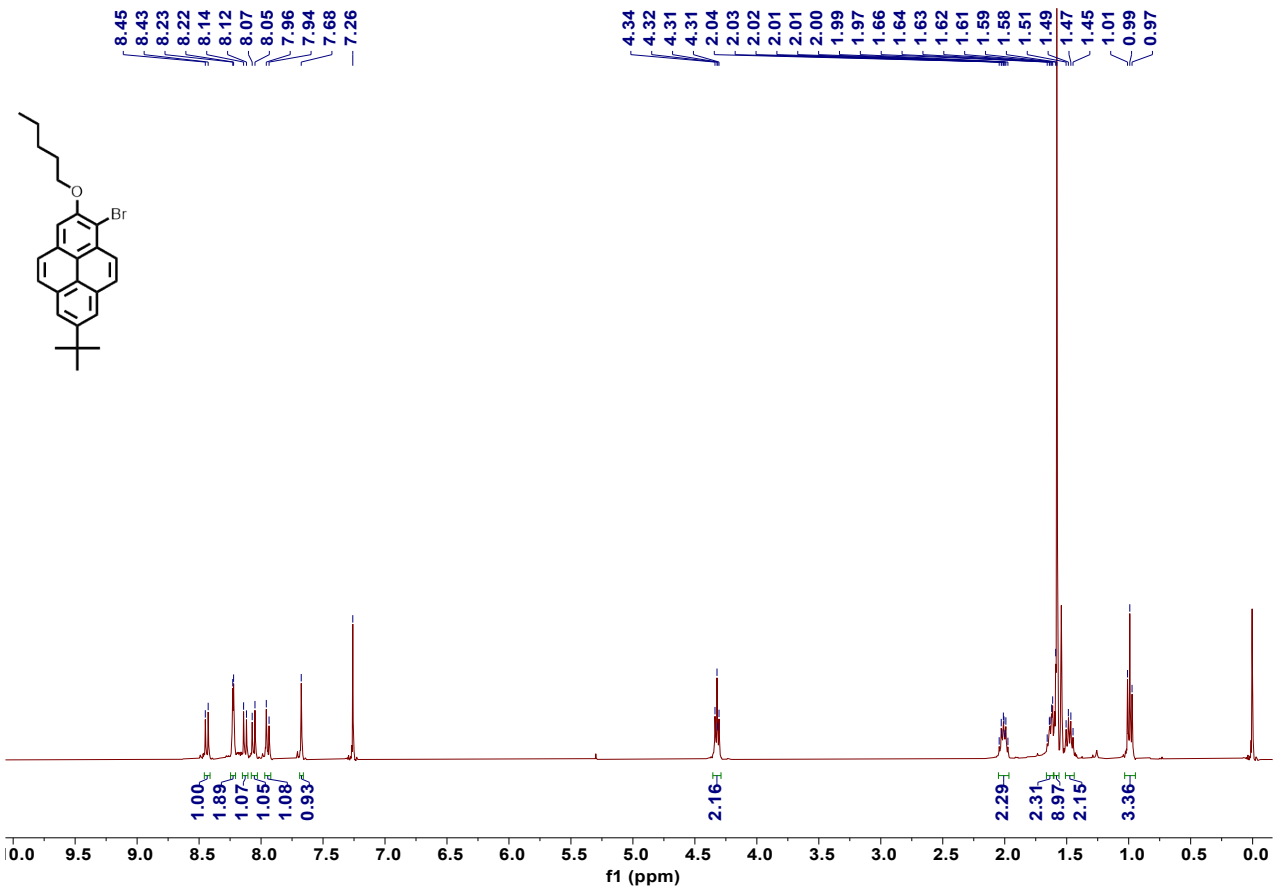


Figure S3. ^{1}H-NMR spectrum (400 MHz, 293 K, *$CDCl_3$) for **2**.

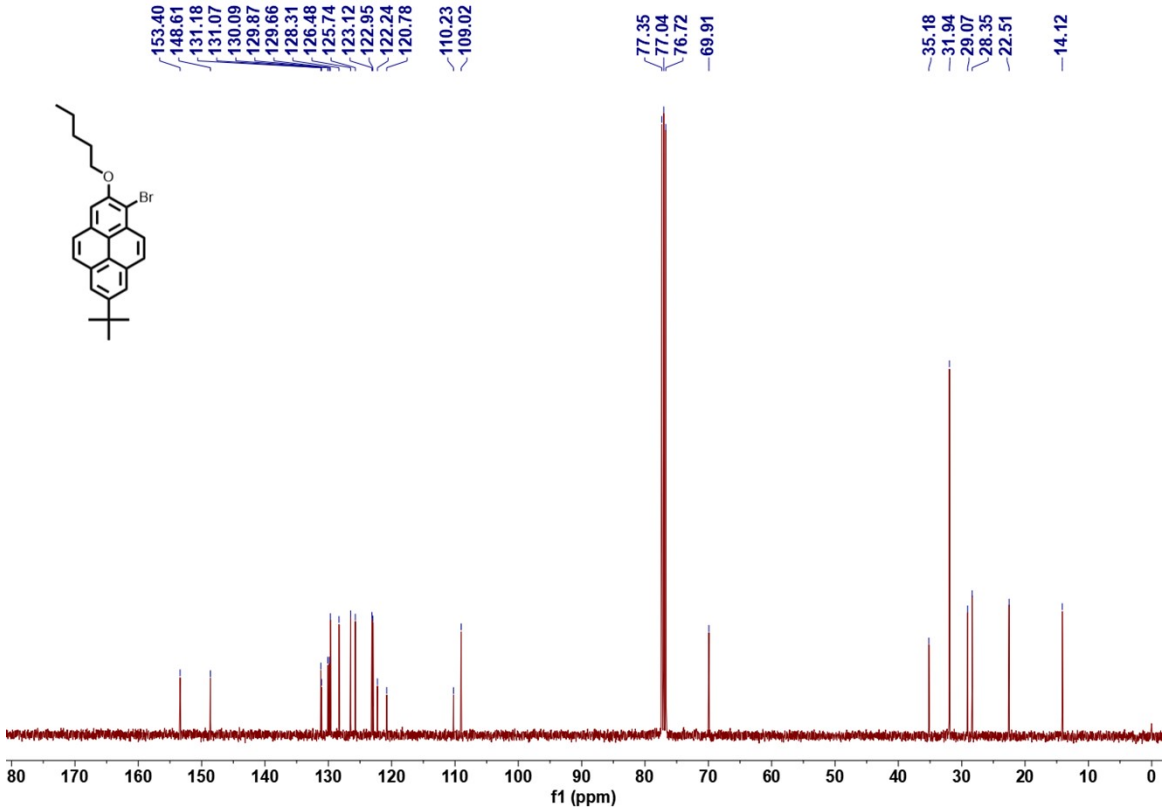


Figure S4. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for **2**.

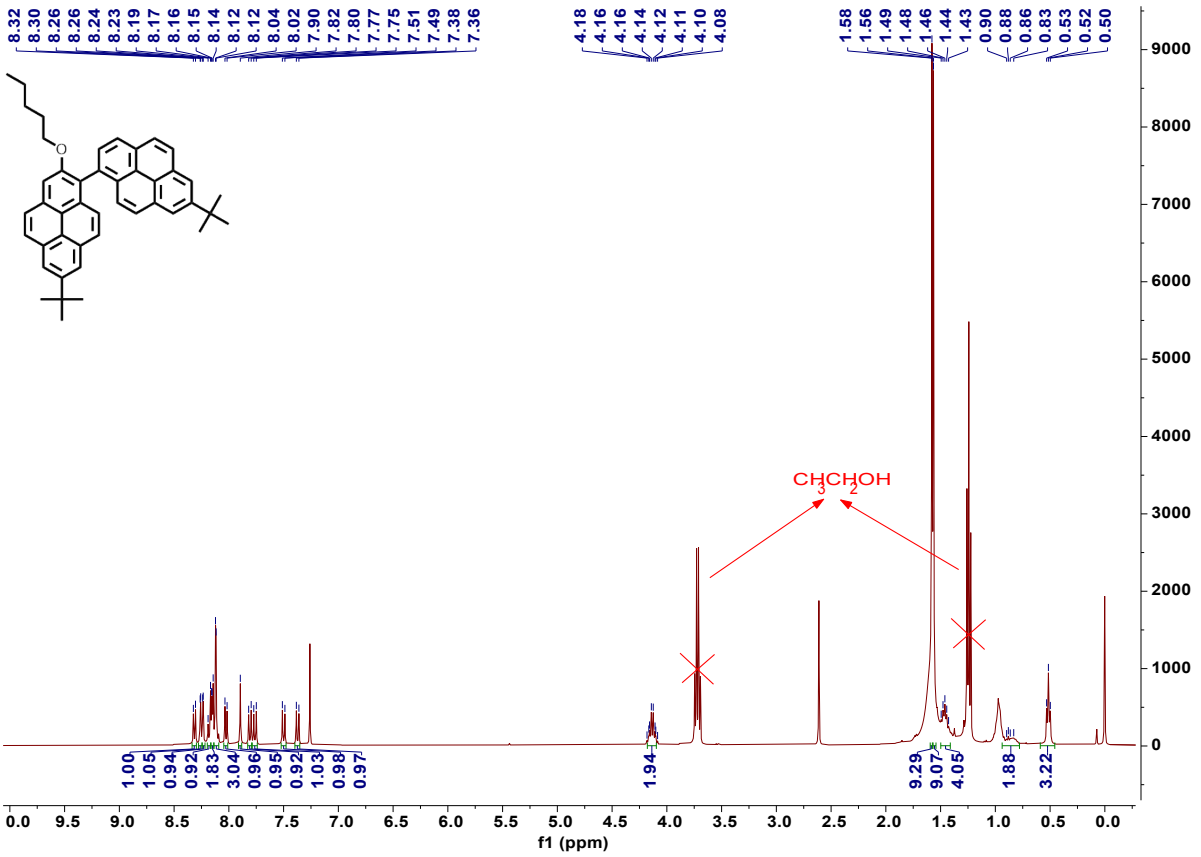


Figure S5. ^{1}H-NMR spectrum (400 MHz, 293 K, *$CDCl_3$) for **3**.

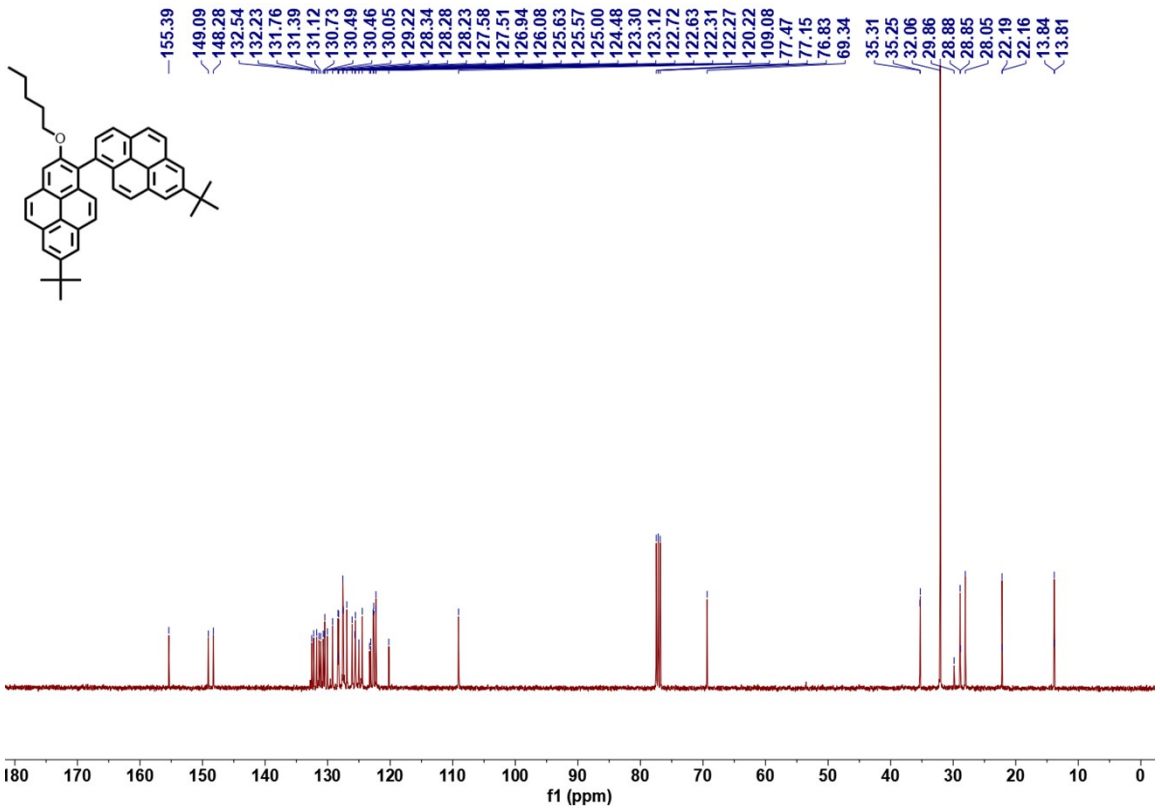


Figure S6. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for **3**.

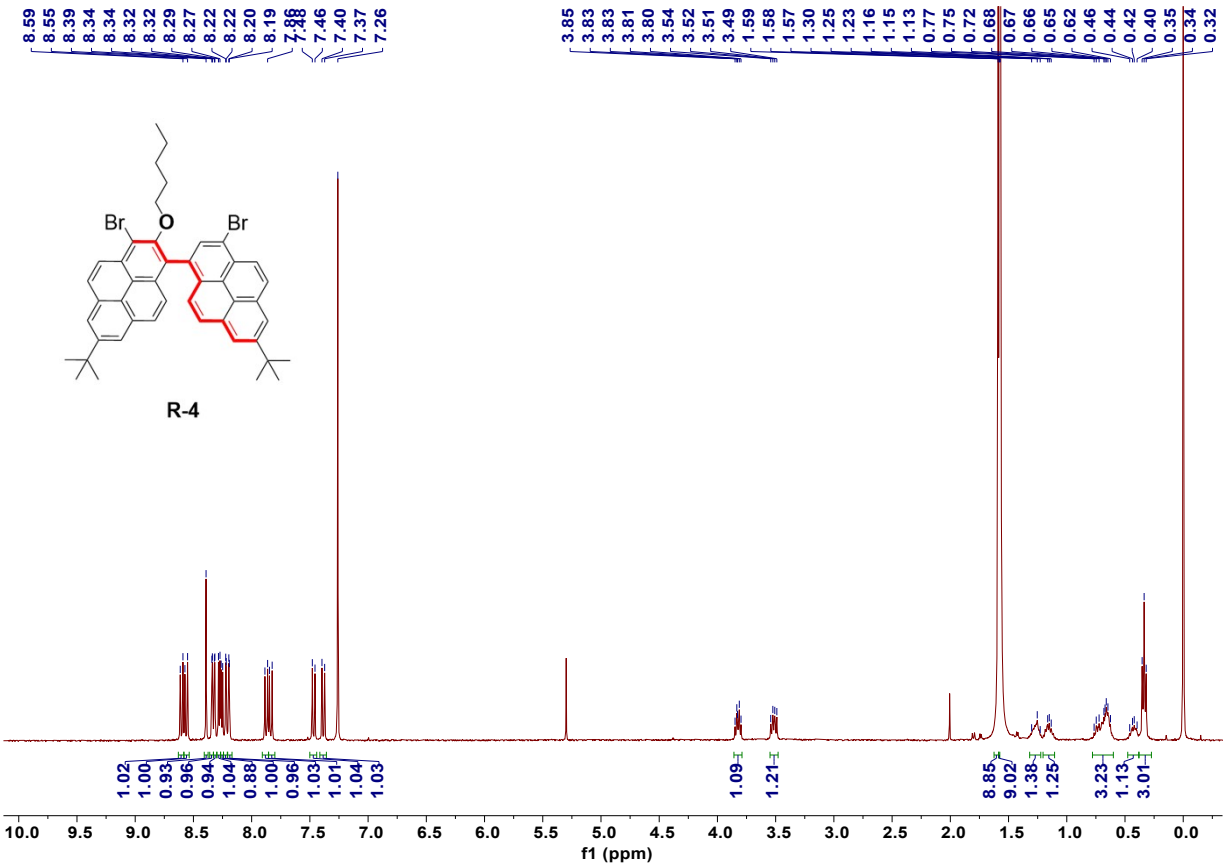


Figure S7. ^{1}H-NMR spectrum (400 MHz, 293 K, *$CDCl_3$) for ***R*-4**.

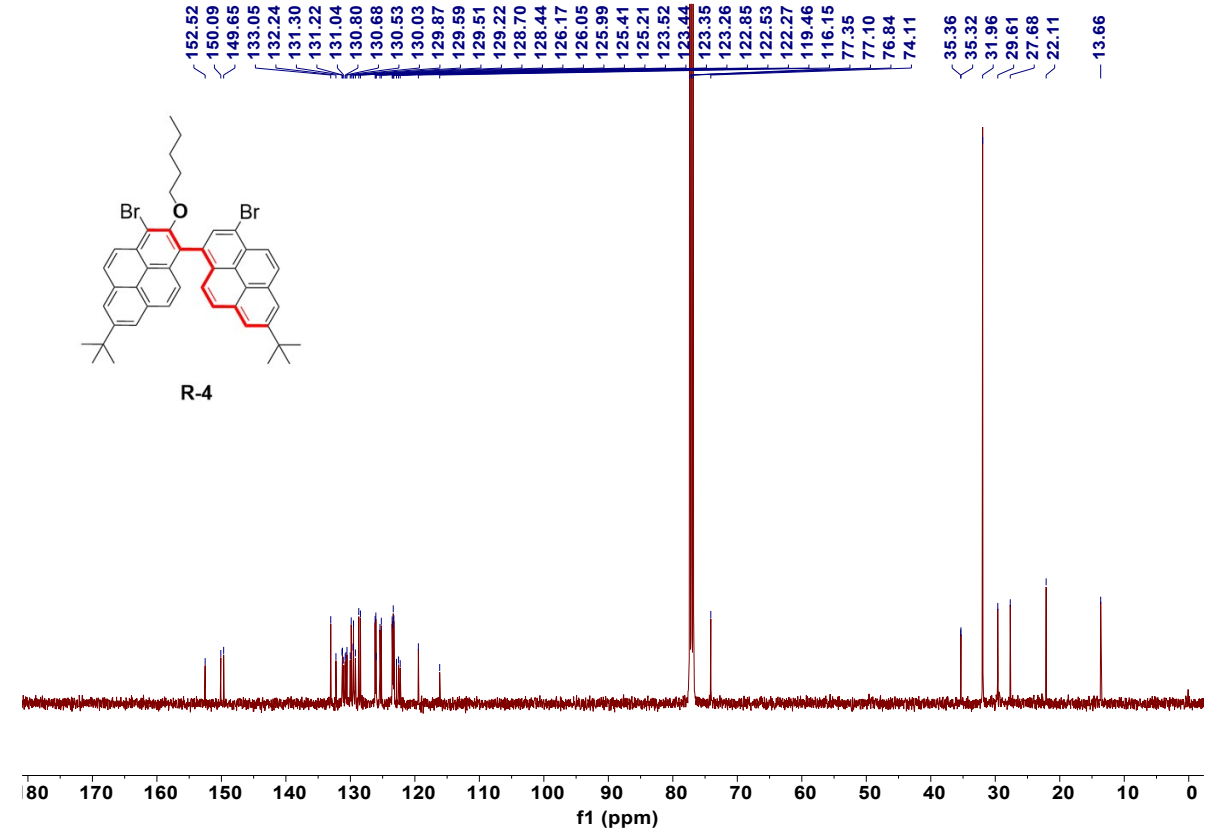


Figure S8. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for ***R*-4**.

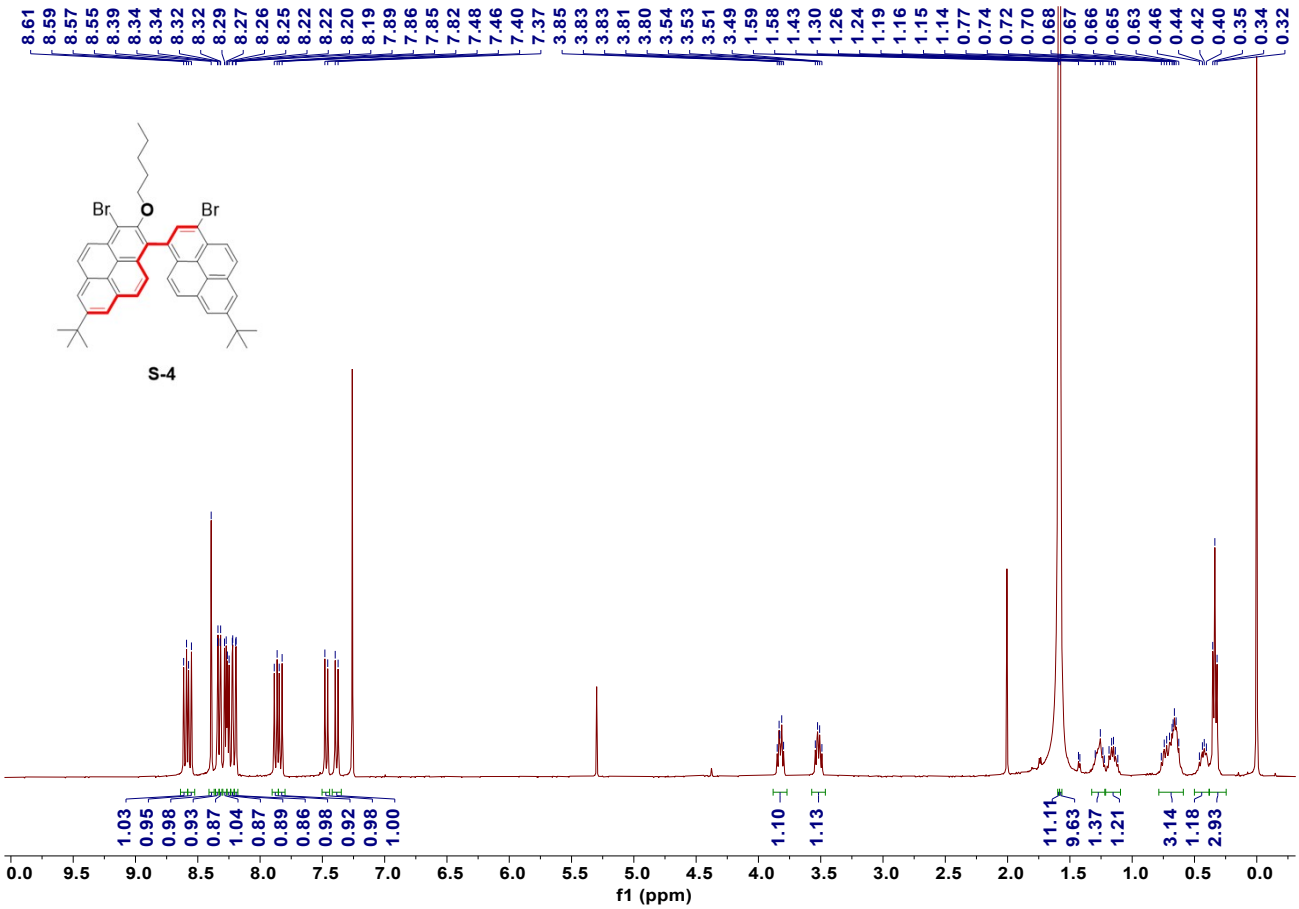


Figure S9. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for ***S*-4**.

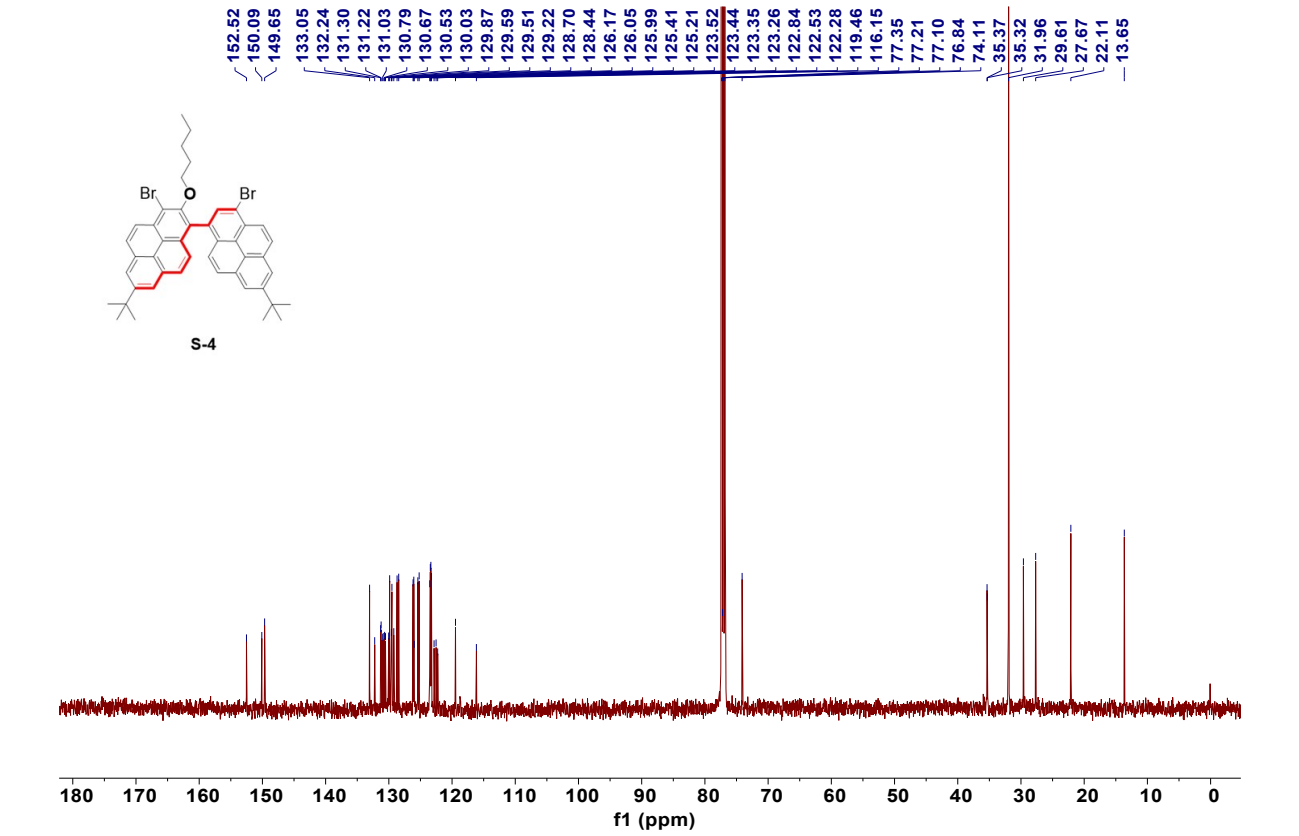


Figure S10. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for ***S*-4**.

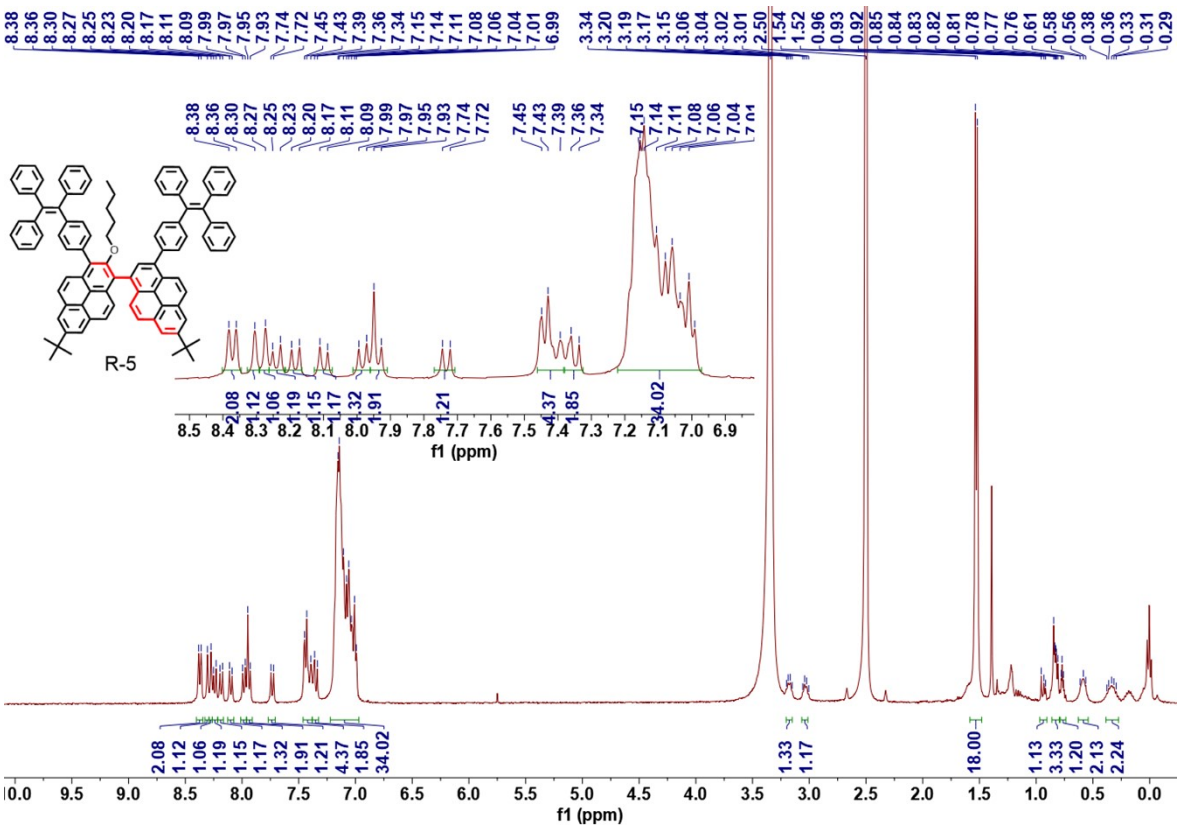


Figure S11. ^{1}H-NMR spectrum (400 MHz, 293 K, DMSO-d_6) for ***R*-5**.

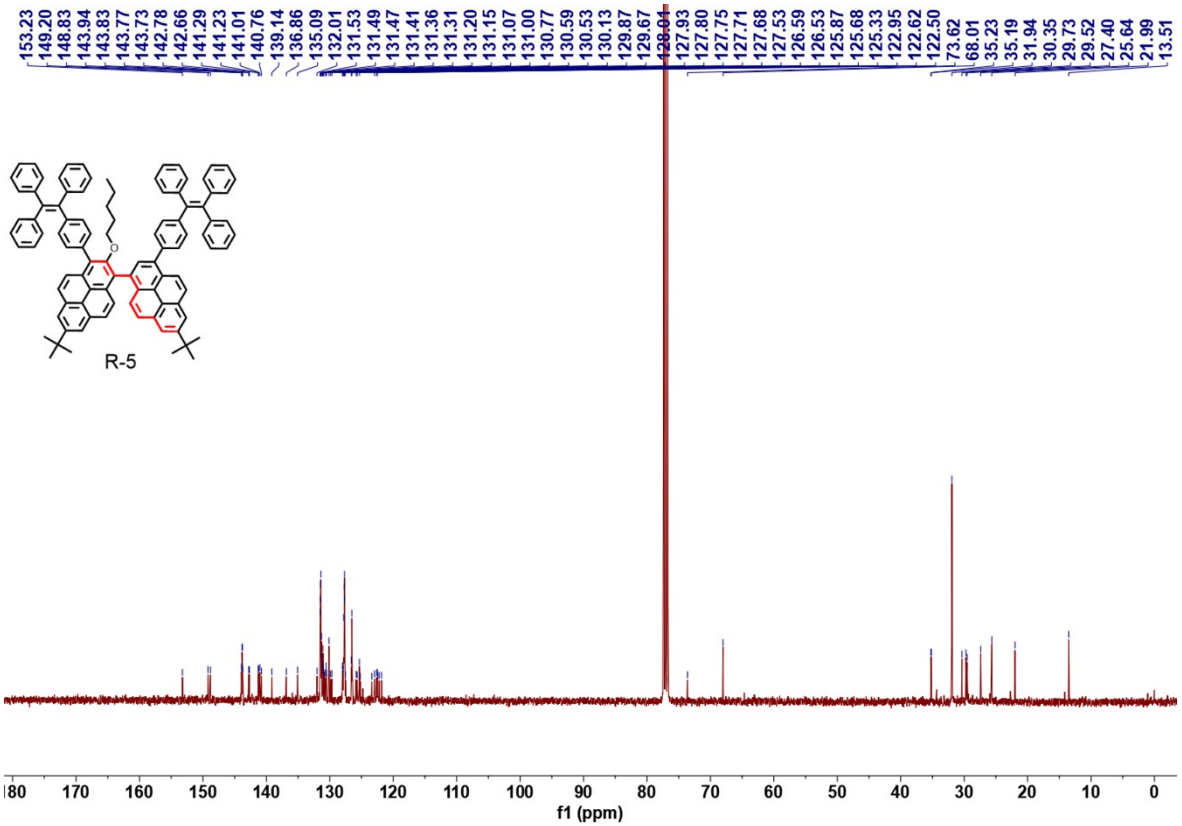


Figure S12. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for ***R*-5**.

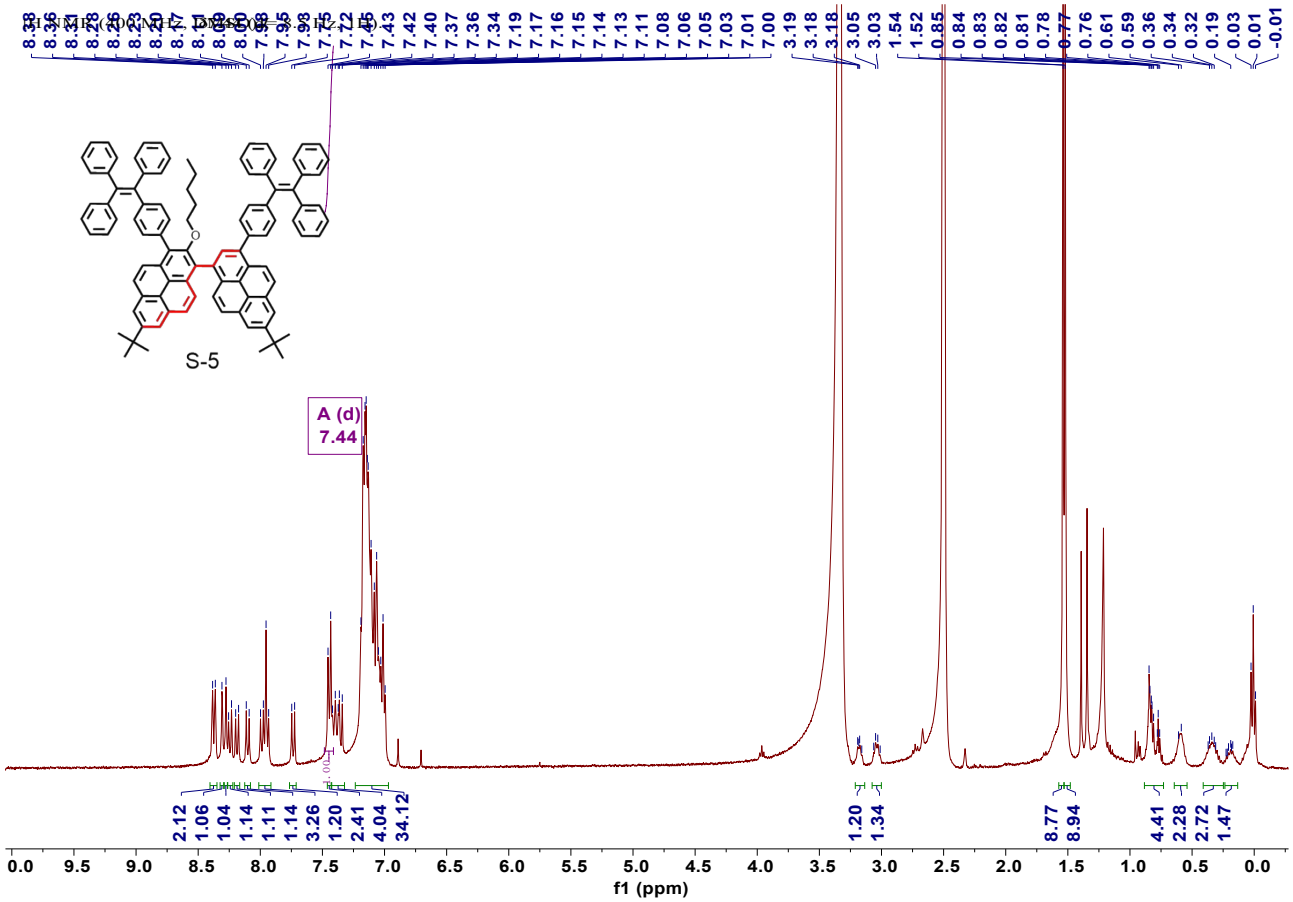


Figure S13. ^{1}H-NMR spectrum (400 MHz, 293 K, DMSO-d_6) for ***S*-5**.

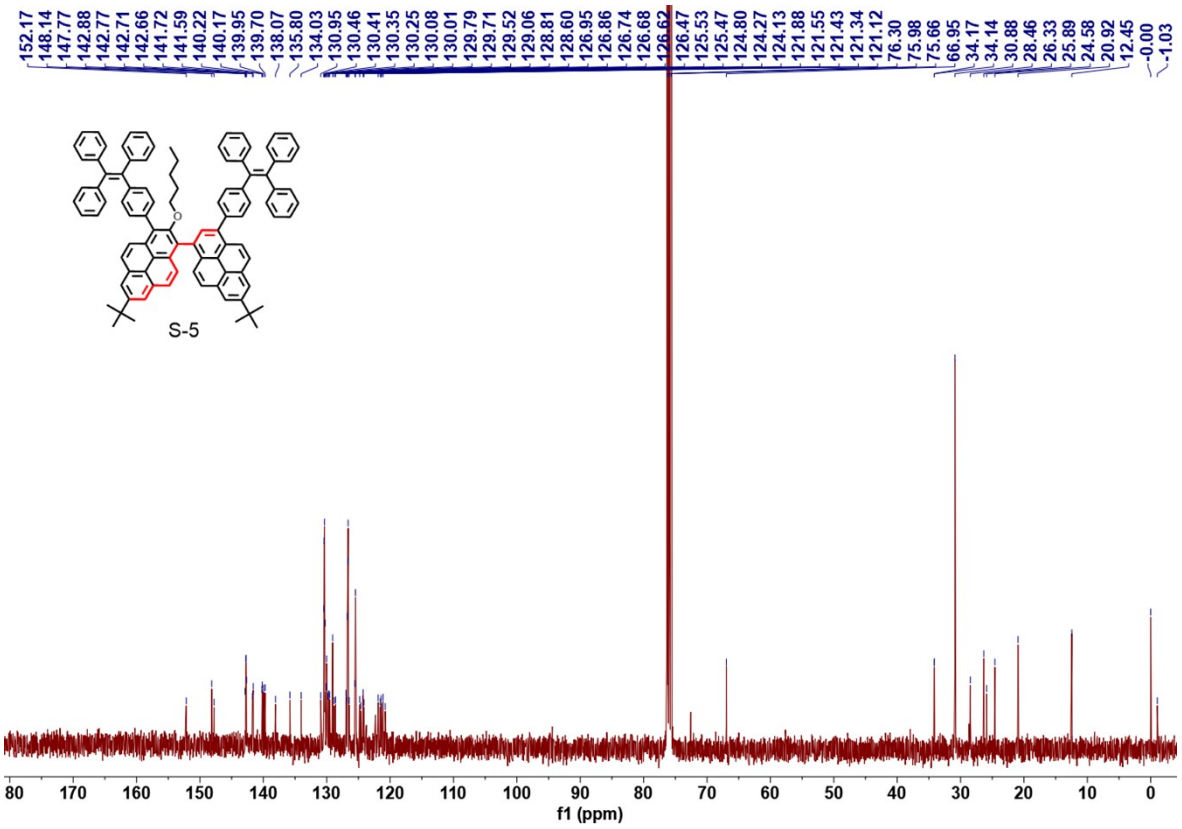


Figure S14. ^{13}C-NMR spectrum (100 MHz, 293 K, *$CDCl_3$) for ***S*-5**.

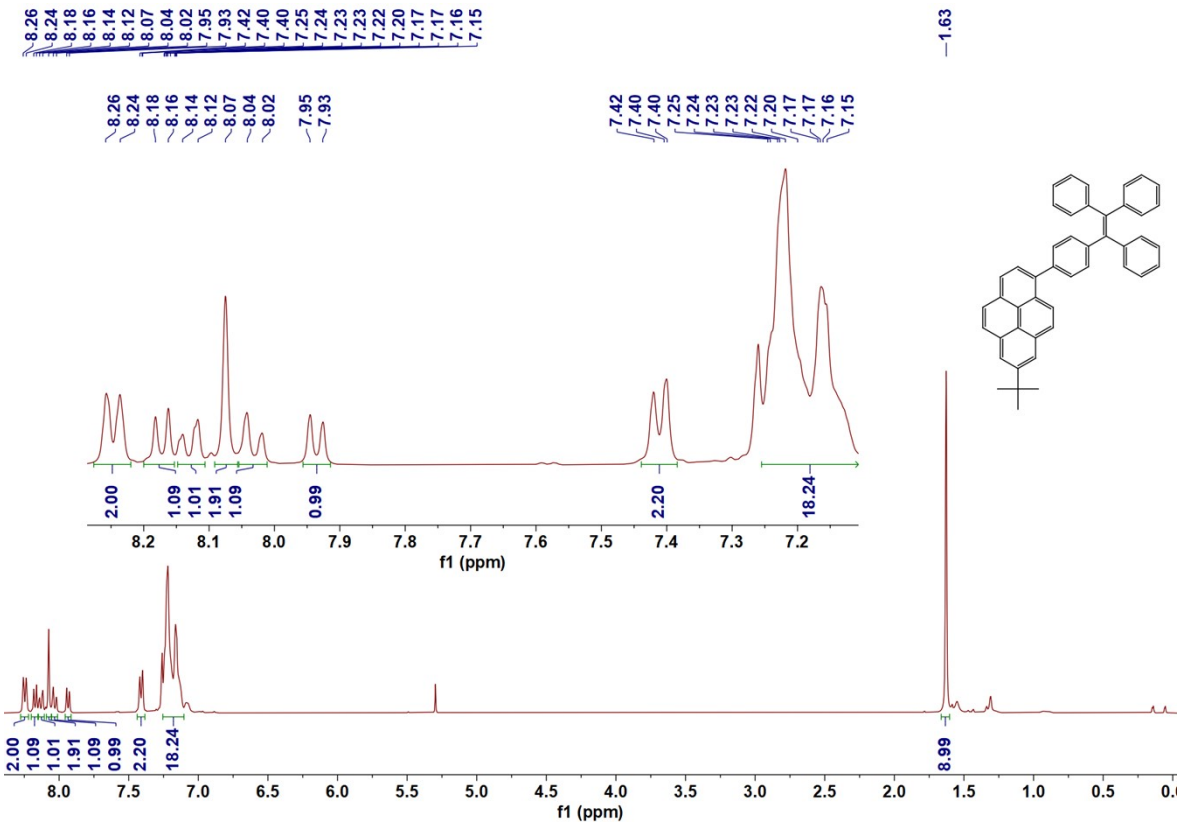


Figure S15 ^{1}H-NMR spectrum (400 MHz, 293 K, * $CDCl_3$) for **Py-TPE**

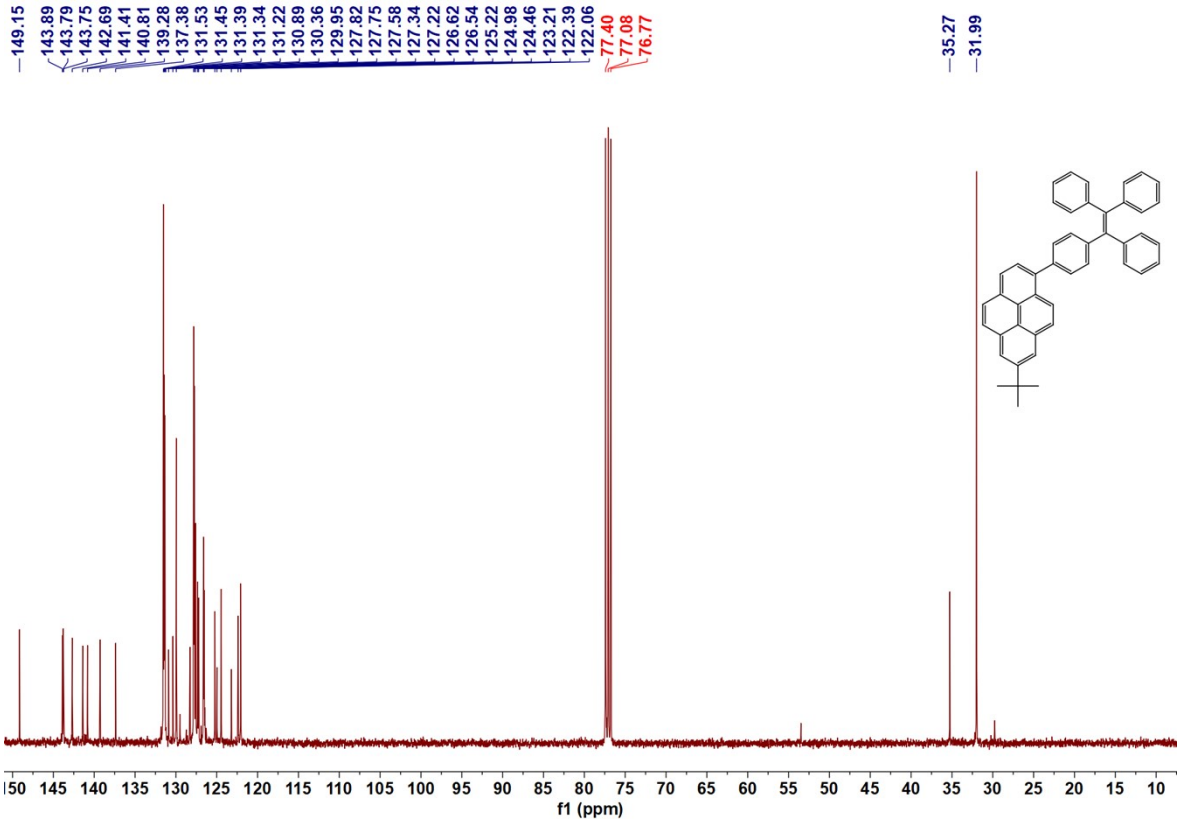


Figure S16 ^{13}C-NMR spectrum (100 MHz, 293 K, * $CDCl_3$) for **Py-TPE**

3. High-Resolution Mass Spectrometry (HRMS)

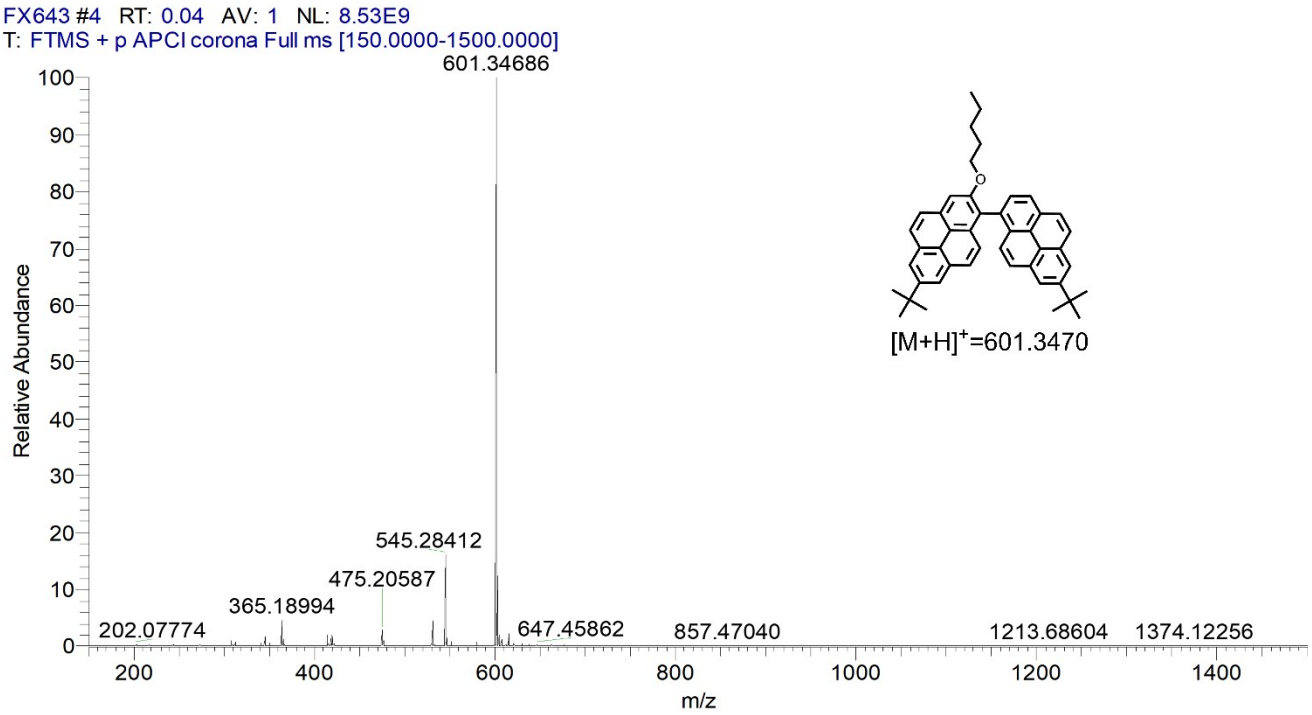


Figure S17. HRMS spectra of *racemic* **3**.

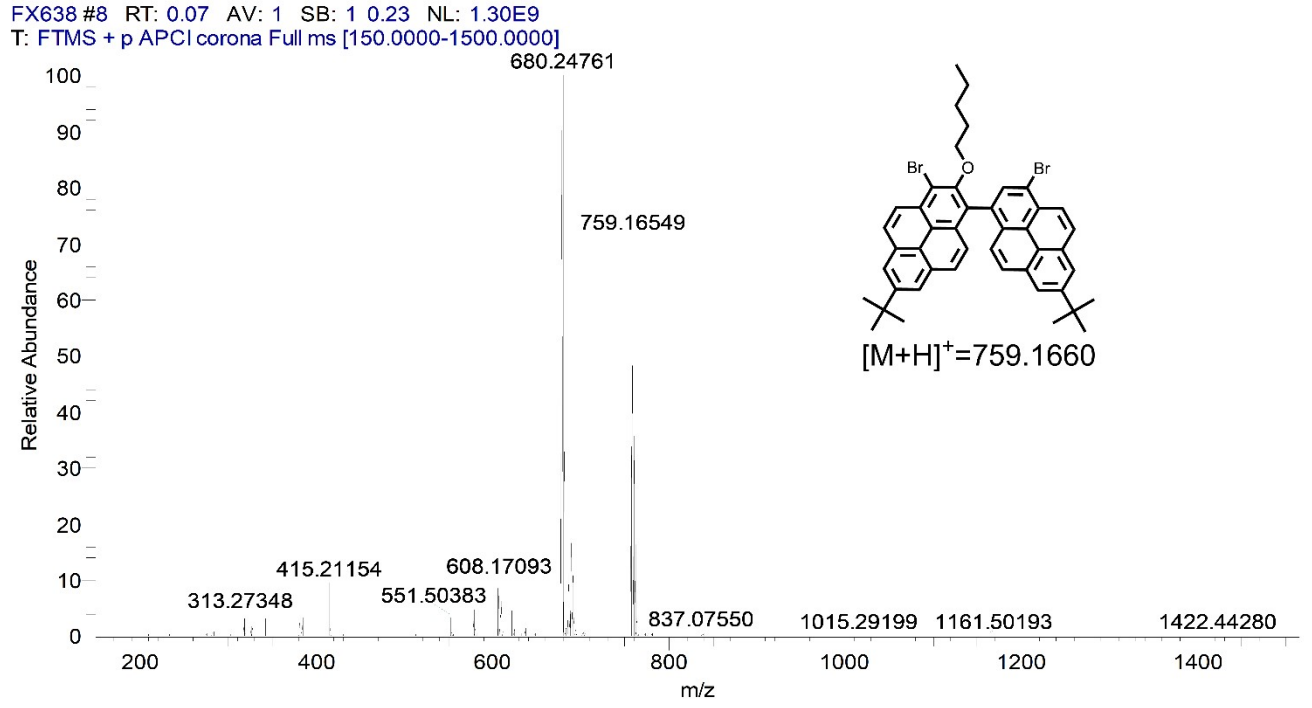


Figure S18. HRMS spectra of *racemic* **4**.

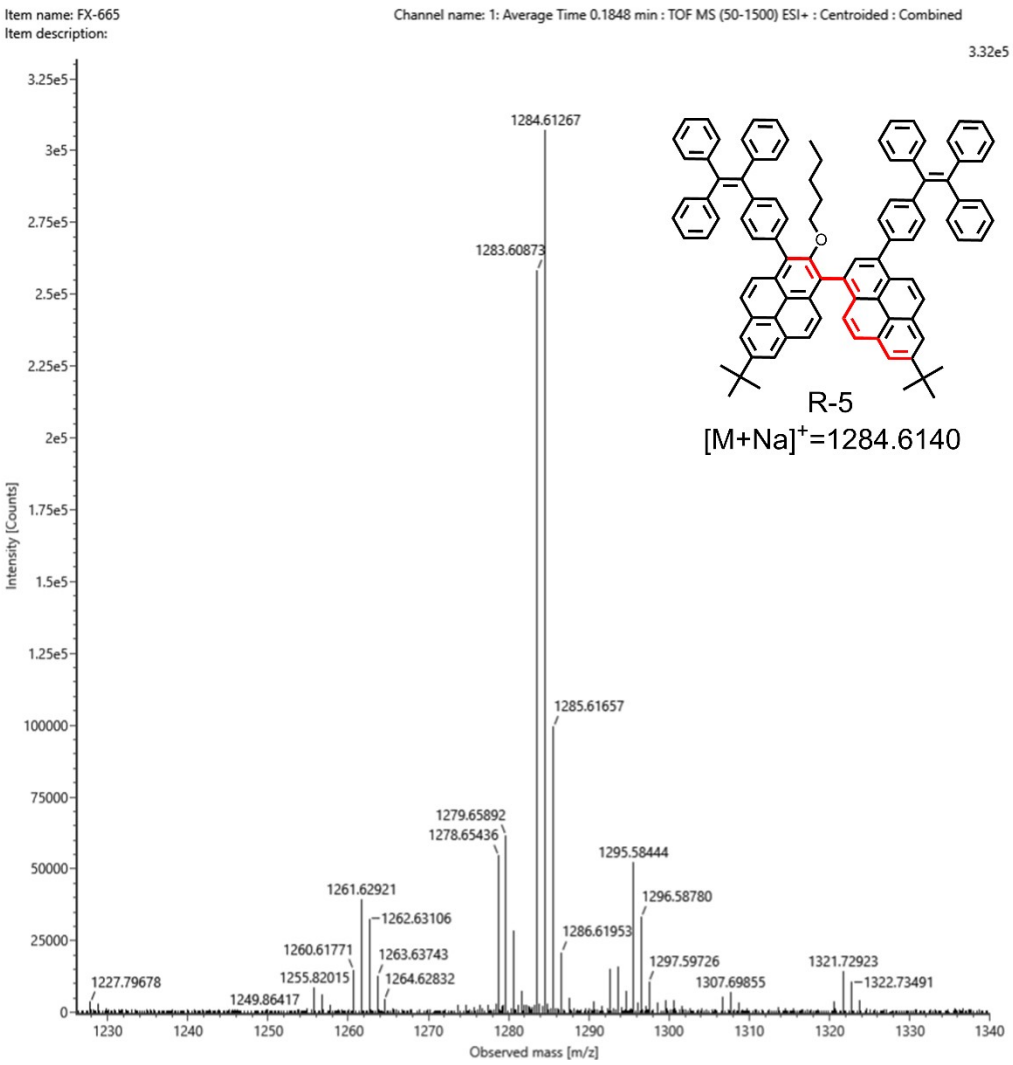


Figure S19. HRMS spectra of ***R*-5**.

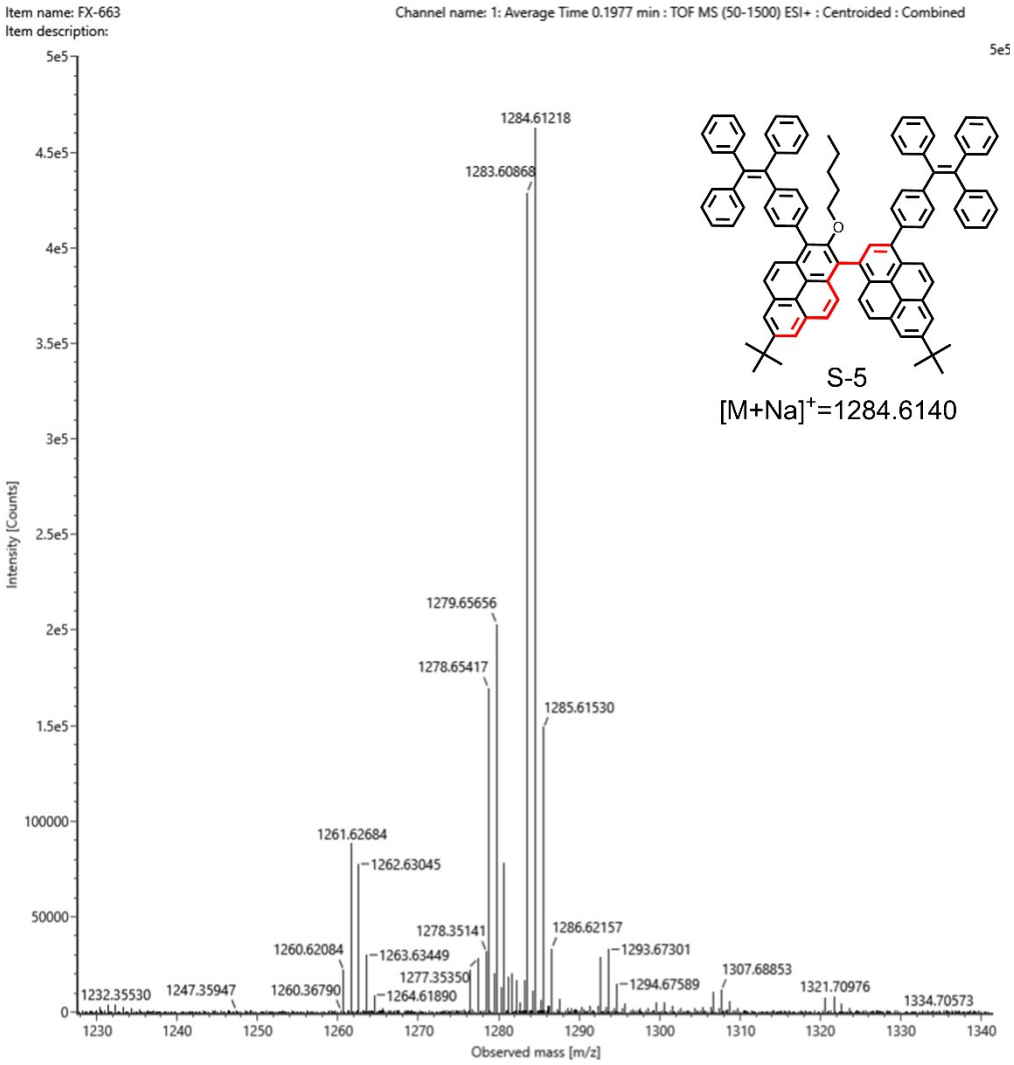
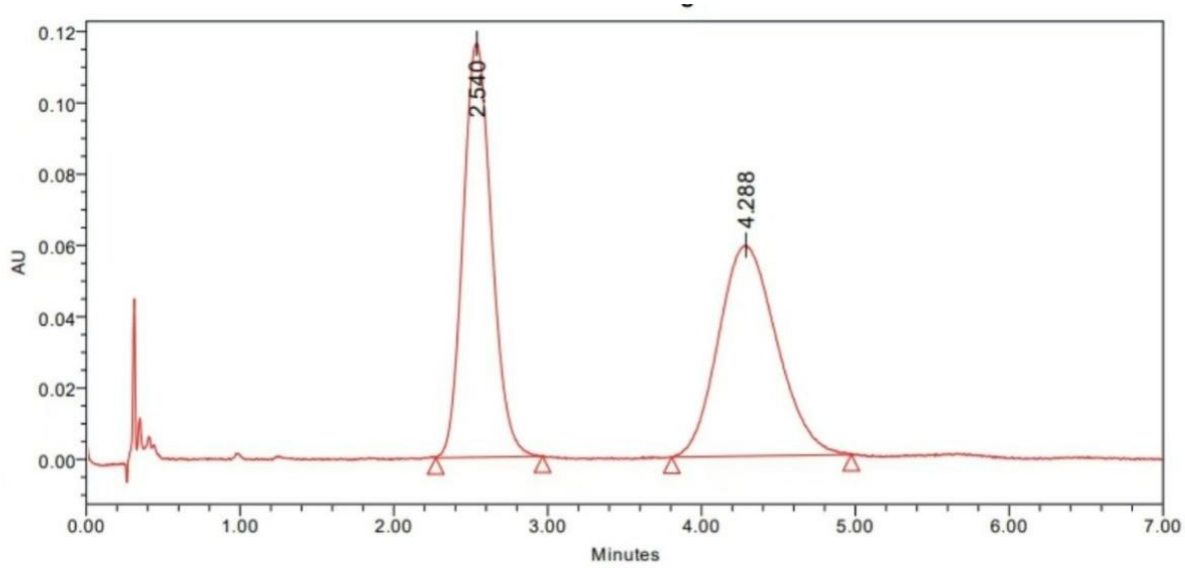


Figure S20. HRMS spectra of ***S*-5**.

4. High Performance Liquid Chromatography



Peak Results

	RT	USP Tailing	EP Plate Count	Resolution	Height	% Height	Area	% Area
1	2.540				116076	66.22	1501961	49.08
2	4.288				59200	33.78	1558116	50.92

Figure S21. Chiral HPLC chromatograms of ***R*-/*S*-5** collected at λ_{ex} = 210 nm excitation (Column: Daicel ChiralPak IH, 3mm I.D.×100mm, 3um, Mobile phase: A for CO_2 and B for MeOH, Gradient: B 35% in 7 min, Flow rate: 2.0 mL/min, Column temperature: 35°C).

5. Theoretical Calculations

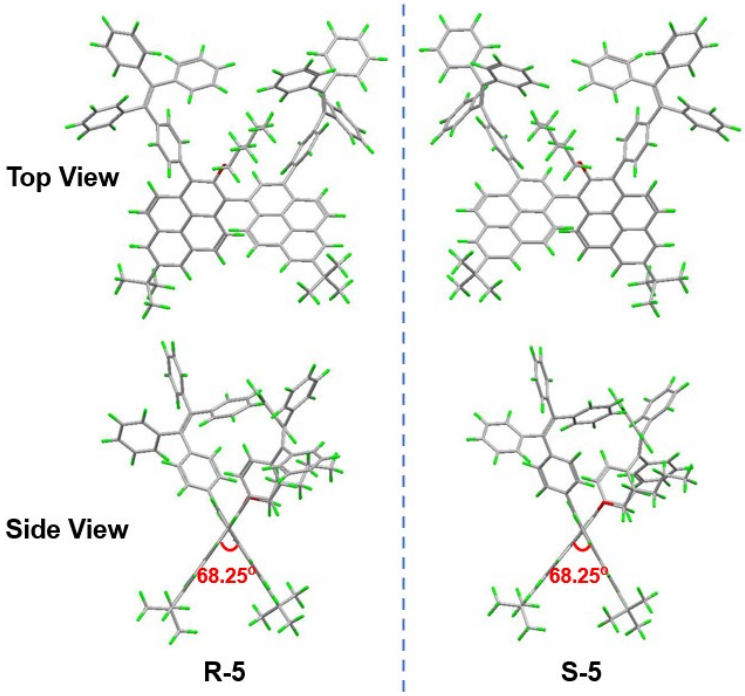


Figure S22. The optimized geometric molecular structure of ***R*-5** and ***S*-5** at ground state (CAM-B3LYP/6-311G(d,p)).

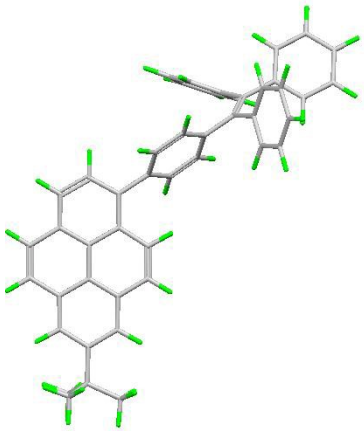


Figure S23. The optimized geometric molecular structure of **Py-TPE** at ground state (CAM-B3LYP/6-311G(d,p)).

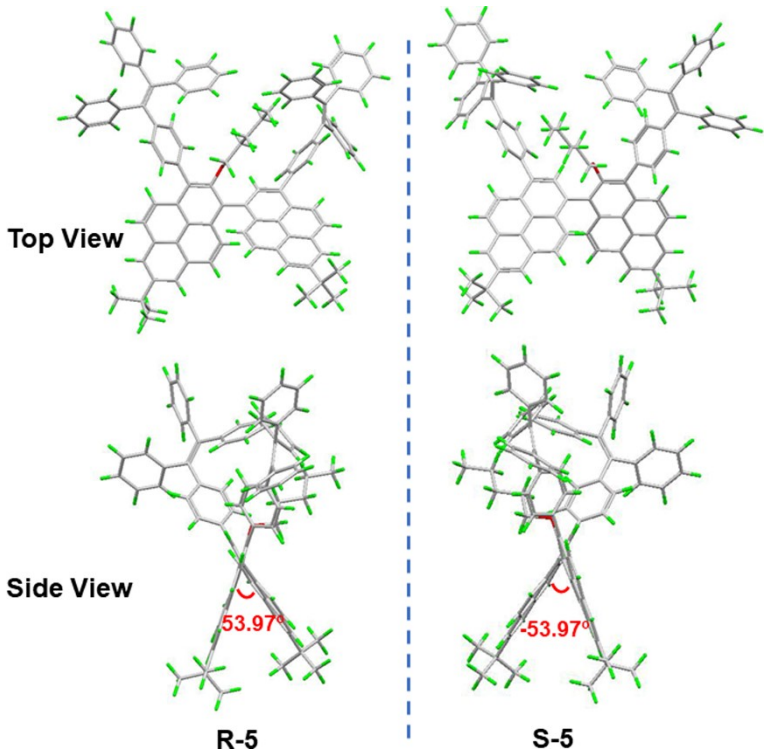


Figure S24. The optimized geometric molecular structure of ***R*-5** and ***S*-5** at excited state (CAM-B3LYP/6-311G(d,p)).

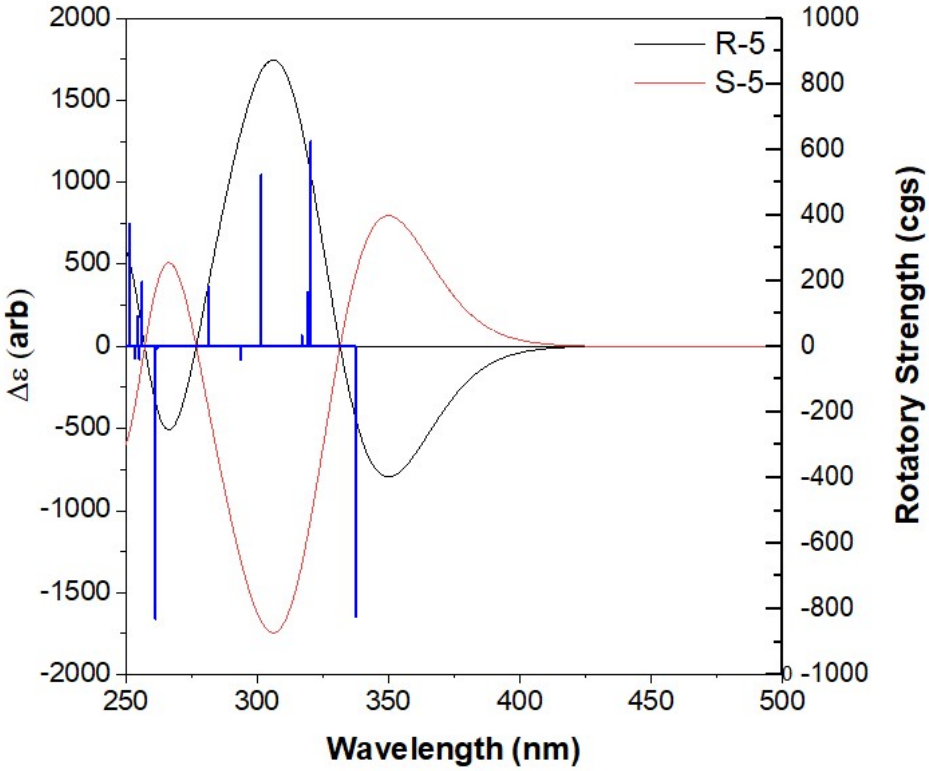
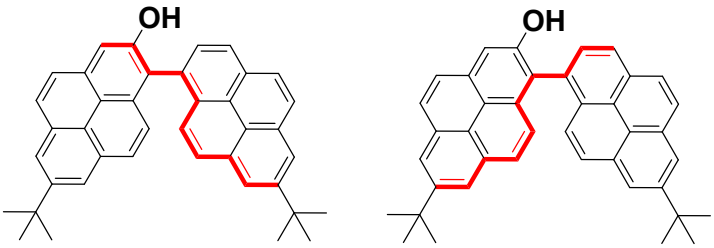


Figure S25. Simulated CD spectra of ***R*/*S*-5** based on the optimized geometric structure at ground state (CAM-B3LYP/6-311G(d,p)).



***R*-dipyrenol** **S-dipyrenol**

Scheme S1. Molecular structure of ***R/S*-dipyrenol**.

Table S1. Calculated of the parameters of the transition electric dipole moment (μ) and transition magnetic dipole moment (m), the $\theta_{\mu,m}$ and $g_{cal\ abs}$ at the ground state[a]

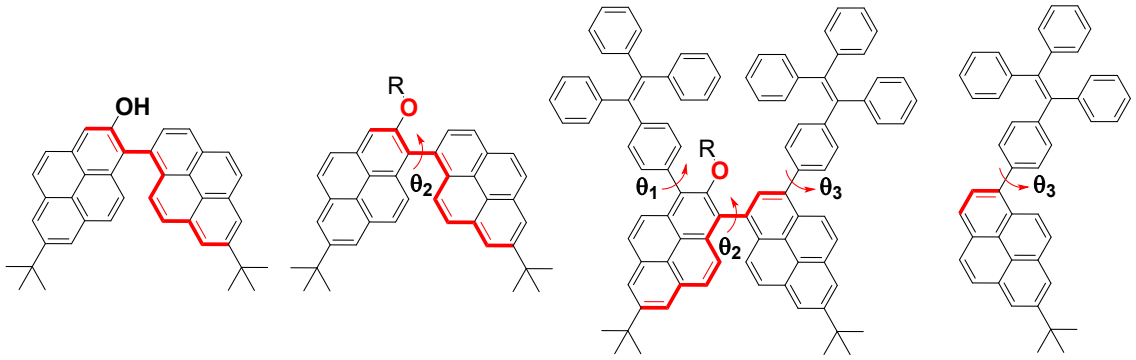
Compounds	μ	m	$\theta_{\mu,m}$	g_{cal}
***R/S*--dipyrenol**	5.92×10^{-18}	2.53×10^{-20}	100.5°	3.12×10^{-3}
***R/S*-3**	7.38×10^{-18}	4.38×10^{-20}	75.6°	5.90×10^{-3}
***R/S*-5**	7.01×10^{-18}	3.31×10^{-20}	44.1°	1.35×10^{-2}

[a] Calculated by CAM-B3LYP/6-311G(d,p)

Table S2. Calculated of the parameters of the transition electric dipole moment (μ) and transition magnetic dipole moment (m), the $\theta_{\mu,m}$ and $g_{cal\ lum}$ at the excited state[a]

Compounds	μ	m	$\theta_{\mu,m}$	g_{cal}
***R/S*--chiral dipyrenol**	7.12×10^{-18}	4.82×10^{-20}	81.9°	3.82×10^{-3}
***R/S*-3**	7.36×10^{-18}	6.81×10^{-20}	76.4°	8.70×10^{-4}
***R/S*--5**	7.97×10^{-18}	1.32×10^{-20}	55.3	3.77×10^{-3}

[a] Calculated by CAM-B3LYP/6-311G(d,p)



***R*-/*S*-dipyrenol** **R-/S-3** **R-/S-5** **Py-TPE**

Table S3. Calculated twist angle[a]

Compounds	θ_1	θ_2	θ_3
***R/S*--chiral dipyrenol**	-	97.7[b] / 46.9[c]	-
***R/S*-3**	-	69.8[b] / 46.3[c]	-
***R/S*-5**	80.7[b] / 61.6[c]	64.9[b] / 48.3[c]	53.5[b] / 53.5[c]
Py-TPE	-	-	57.1[b] /

[a] Calculated by CAM-B3LYP/6-311G(d,p)
[b] at ground state
[c] at excited state

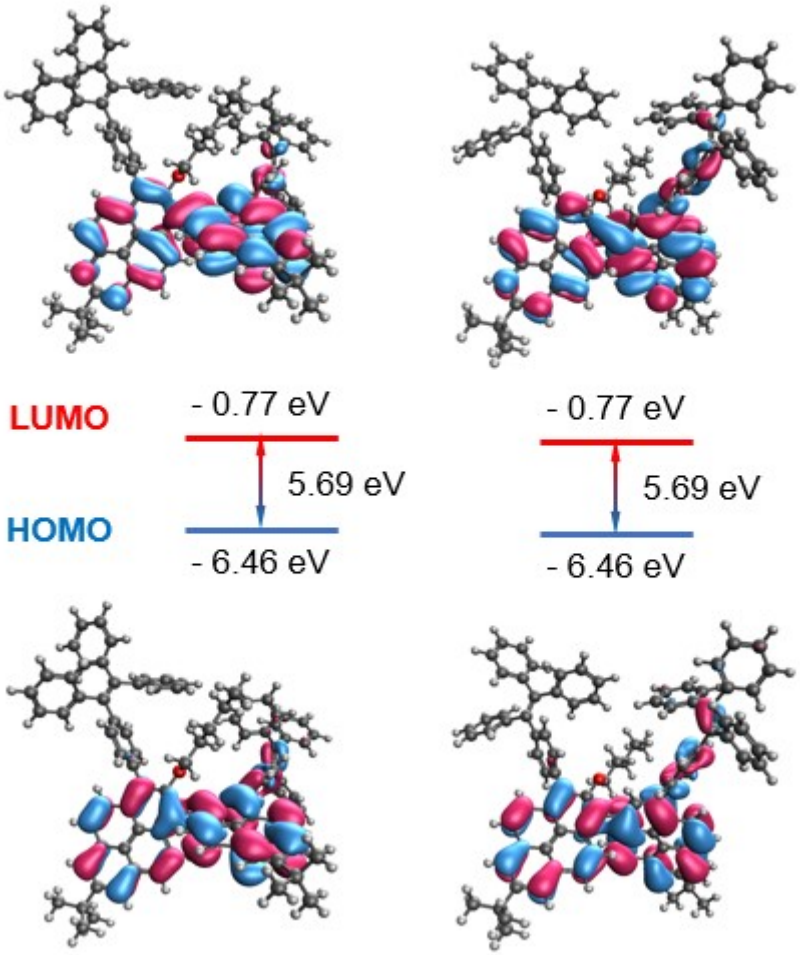


Figure S26. Molecular orbital plots of compounds ***R*/*S*-5** calculated at the ground state (CAM-B3LYP/6-311G(d,p) level).

Table S4. Excitation energies calculated at CAM-B3LYP/6-311G(d,p) optimized geometries.

Compound	Excitation	E/eV	λ/nm	Osc. Strength	$i \rightarrow a$	k_{ia}
***R*-5**	$S_0 \rightarrow S_1$	2.99	415	0.7204	H-1→L+1	2.3
					H→L	93.3
	$S_0 \rightarrow S_2$	3.54	350	0.8698	H-5→L	3.2
					H-4→L+1	3.7
					H-3→L	3.6
					H-1→L	68.4
					H→L+1	6.6
					H→L+5	4.5
	$S_0 \rightarrow S_3$	3.58	346	0.3502	H-5→L	5.7
					H-4→L	2.6
					H-4→L+1	3.1
					H-1→L+4	3.8
					H→L+1	68.5
					H→L+5	5.0
	$S_0 \rightarrow S_4$	3.70	335	0.0311	H-5→L	6.87
					H-5→L+1	8.85
					H-4→L	32.1
					H-2→L	7.38
					H-1→L+5	7.02
					H→L+4	22.7
***S*-5**	$S_0 \rightarrow S_1$	3.03	409	0.7318	H-1→L+1	2.6
					H→L	93.3
	$S_0 \rightarrow S_2$	3.56	348	0.8283	H-5→L	7.5
					H-1→L	62.5
					H→L+1	7.9
					H→L+5	4.4
	$S_0 \rightarrow S_3$	3.62	343	0.3487	H-5→L	11.1
					H-4→L+1	2.4
					H-1→L+4	3.3
					H→L+1	61.5
					H→L+4	3.1
					H→L+5	6.9

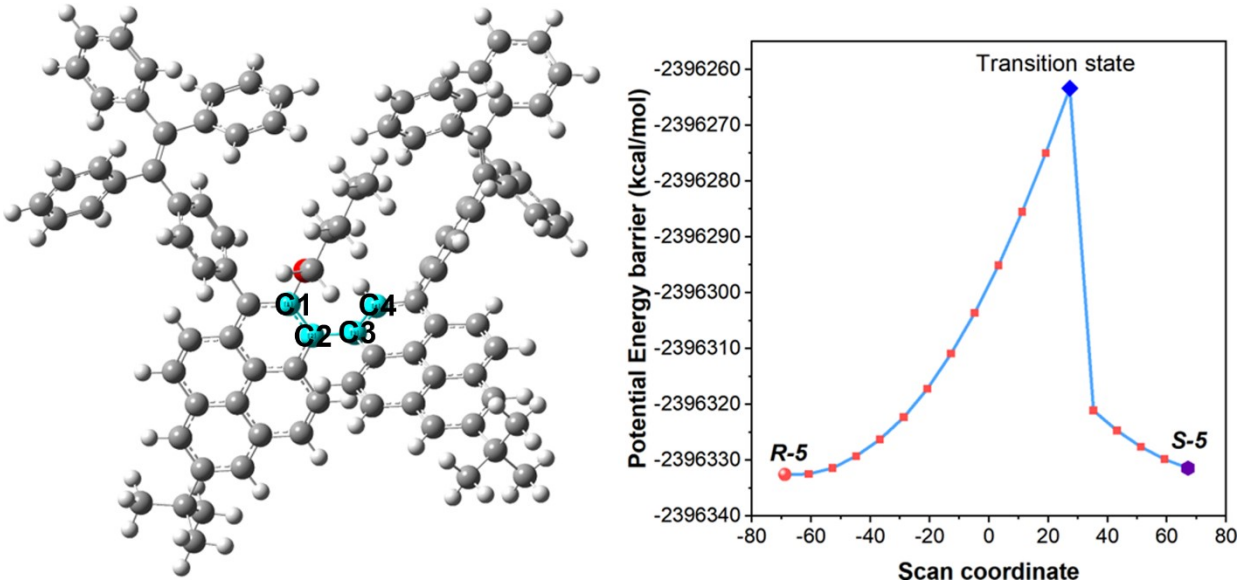


Figure S27 (Left): the molecular conformation, and (Right)the energy profile for ***R-5*** ↔ **S-5**, transition state conformational interconversion and the associated energy barrier along the C1-C4 (blue sky atom).

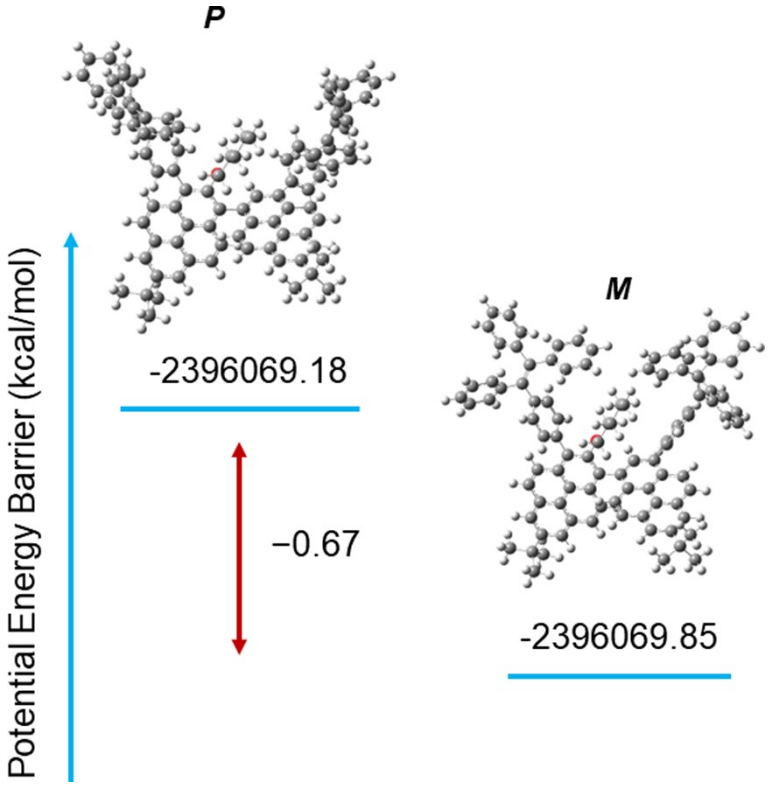


Figure S28 The energy barrier between plus (*P*) to minus (*M*) helical configurations of ***R-5*** CAM-B3LYP/6-311G(d,p).

6. Photophysical Properties

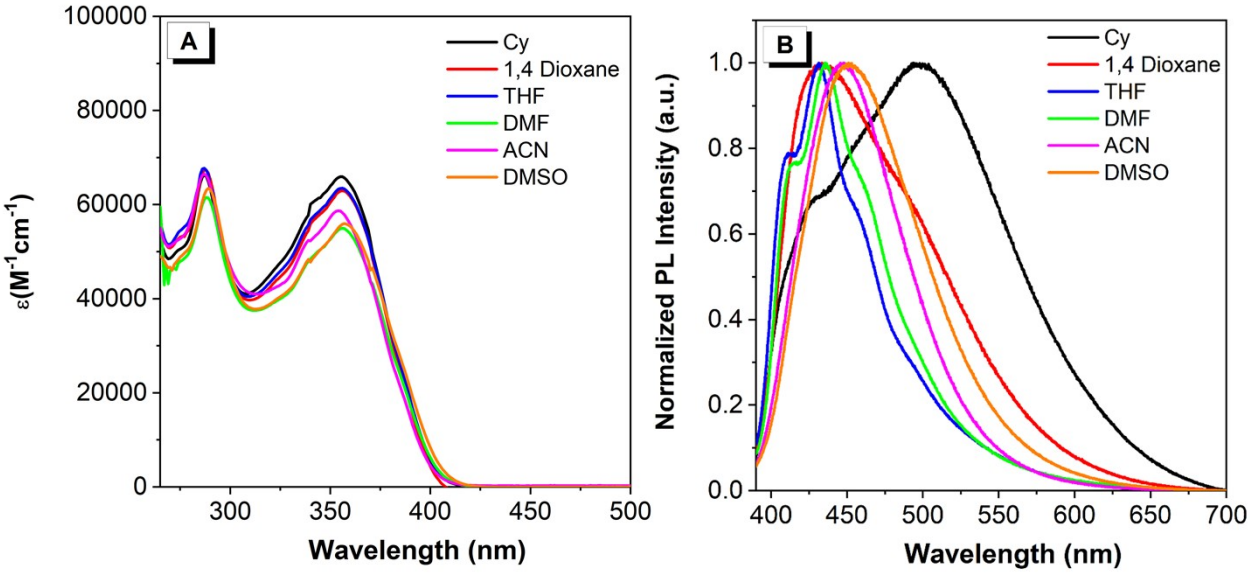


Figure S29. (A) UV-vis spectra and (B) Fluorescence spectra of the compound ***R*-5** recorded in six solvents at ~10^{-5} M and 25 °C.

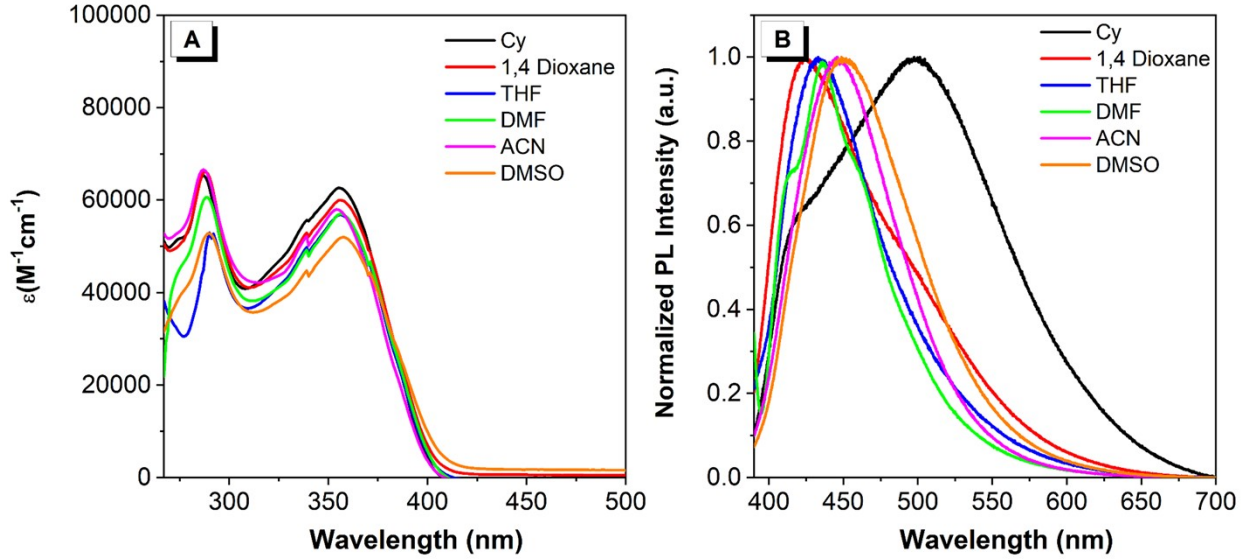


Figure S30. (A) UV-vis spectra and (B) Fluorescence spectra of the compound ***S*-5** recorded in six solvents at ~10^{-5} M and 25 °C.

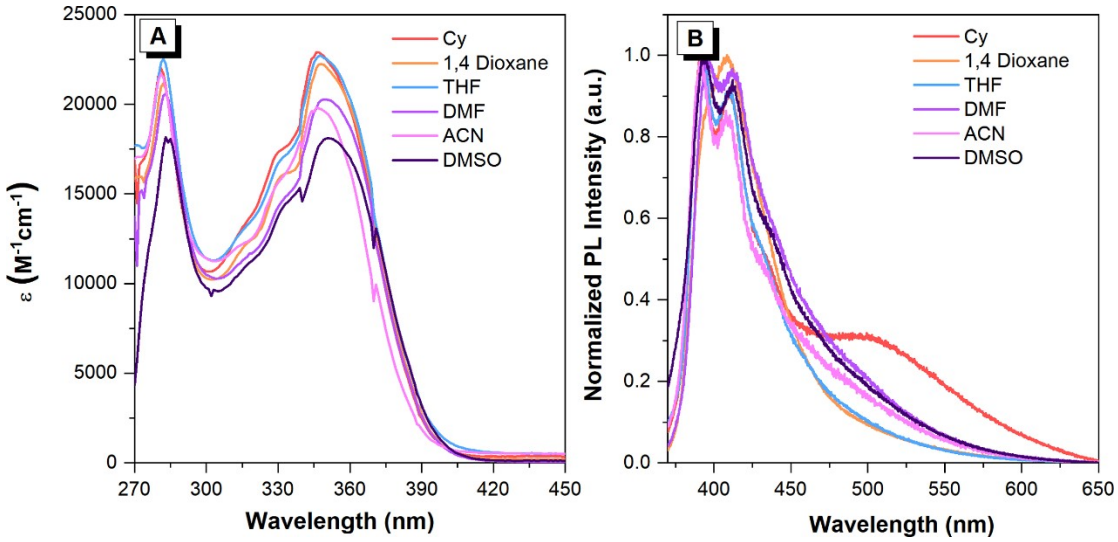


Figure S31. (A) UV-vis spectra and (B) Fluorescence spectra of the compound **Py-TPE** recorded in six solvents at ~10^{-5} M and 25 °C.

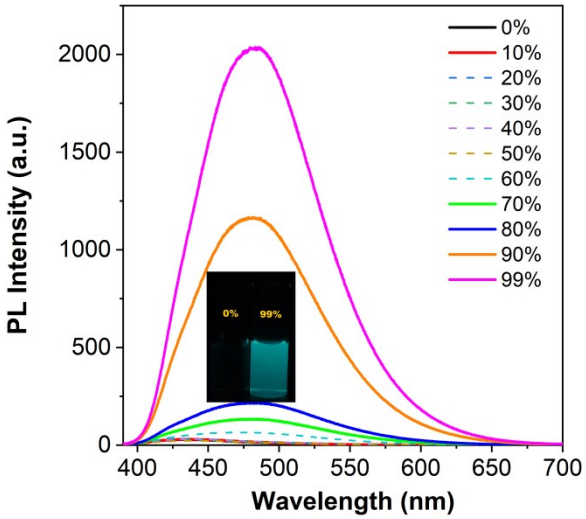


Figure S32. PL spectra of ***R*-5** in THF/water mixtures with different water fractions (f_w) (~10^{-5} m), Insert: Fluorescence images of compound ***R-5*** in f_w = 0% and 99% under 365 nm irradiation.

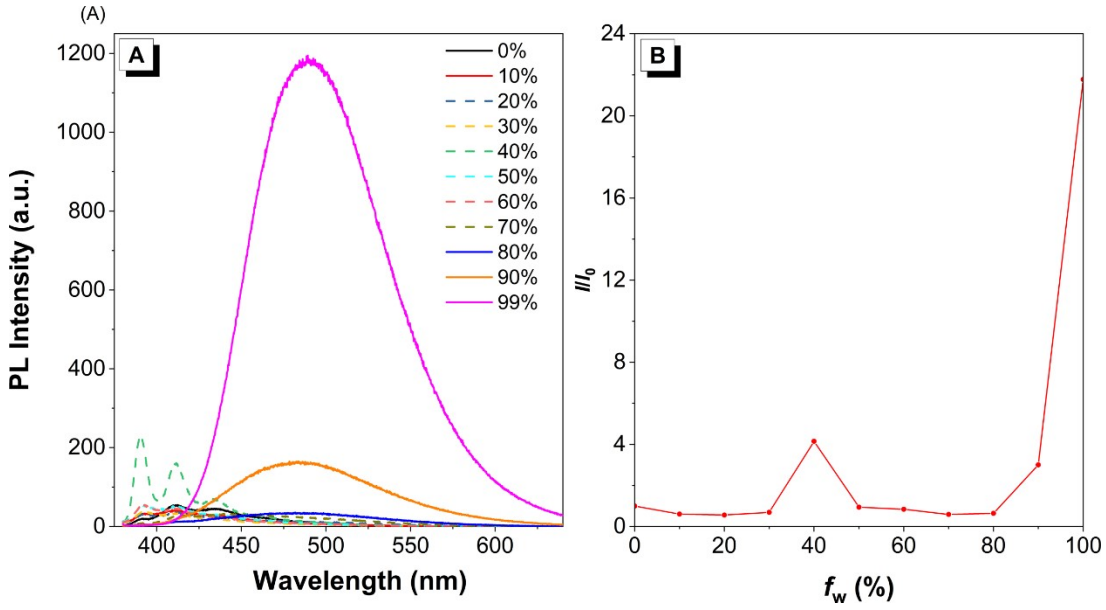


Figure S33. (A) PL spectra of **Py-TPE** in THF/water mixtures with different water fractions (f_w) (≈10^{-5} m); (B) The plot of relative PL intensity I/I_0.

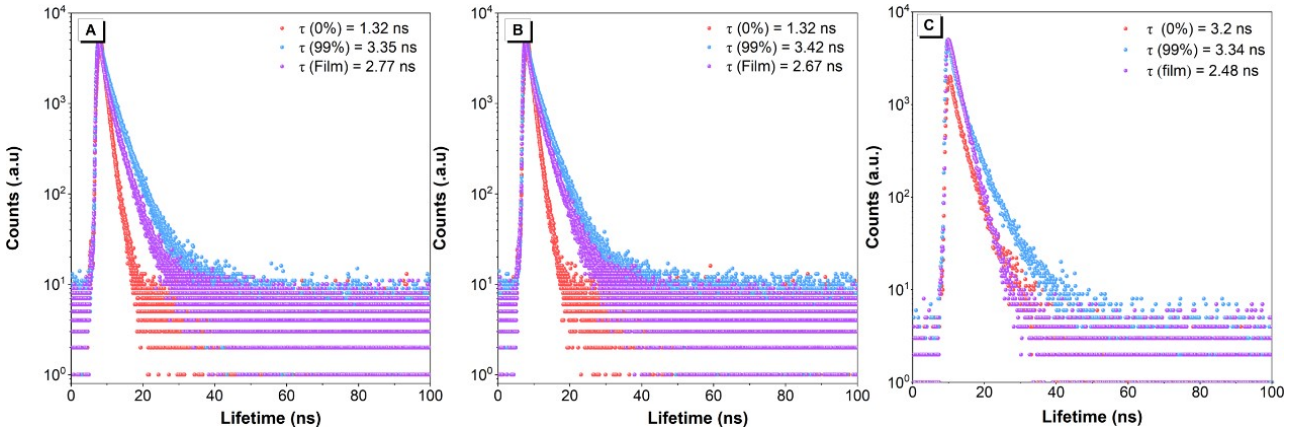


Figure S34. Time-resolved fluorescence decay profiles of (A) ***R*-5,** (B) ***S*-5** and (C) **Py-TPE** in THF solution, in f_w = 99%, and in the solid-state.

7. Circular Dichroism Spectroscopy

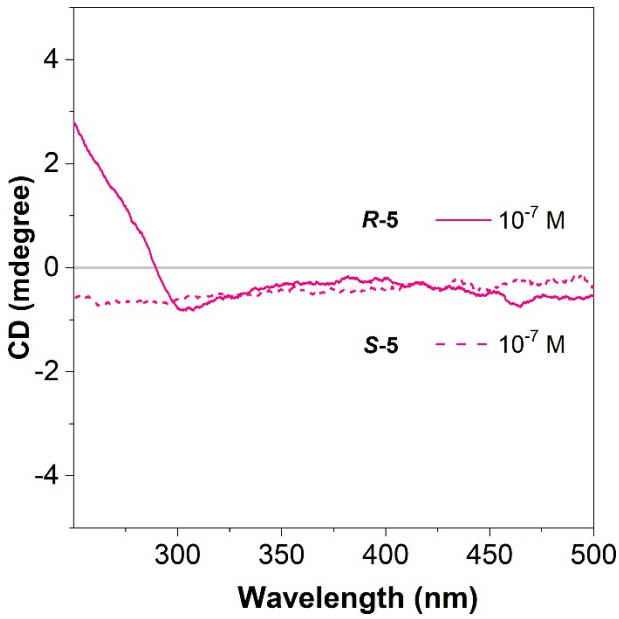


Figure S35. CD spectra of ***R*-/*S*-5** in THF solution of *ca*. 10^{-7} M.

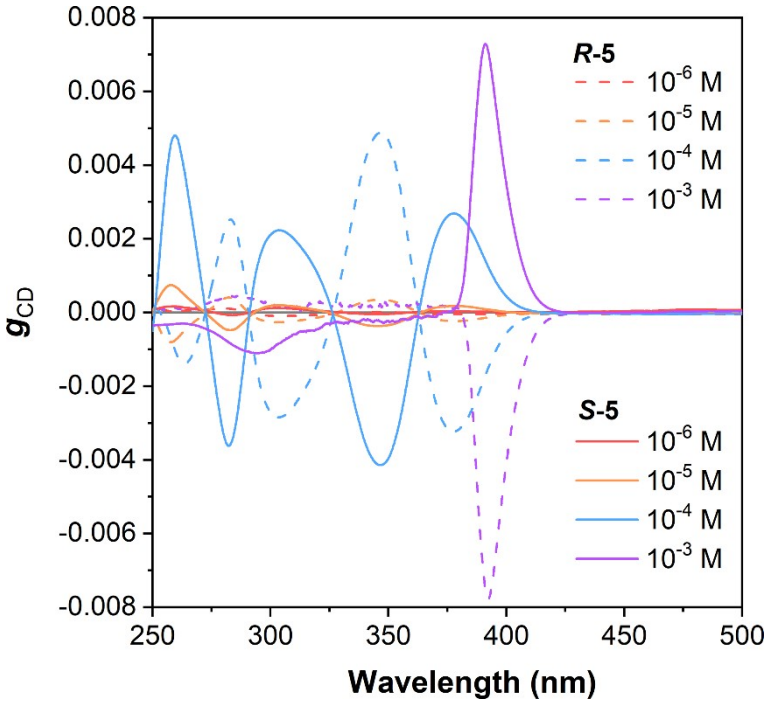


Figure S36. The g_{CD} value of concentration-dependent CD spectra of ***R*-/*S*-5** in THF solution (10^{-6}~10^{-3} M).

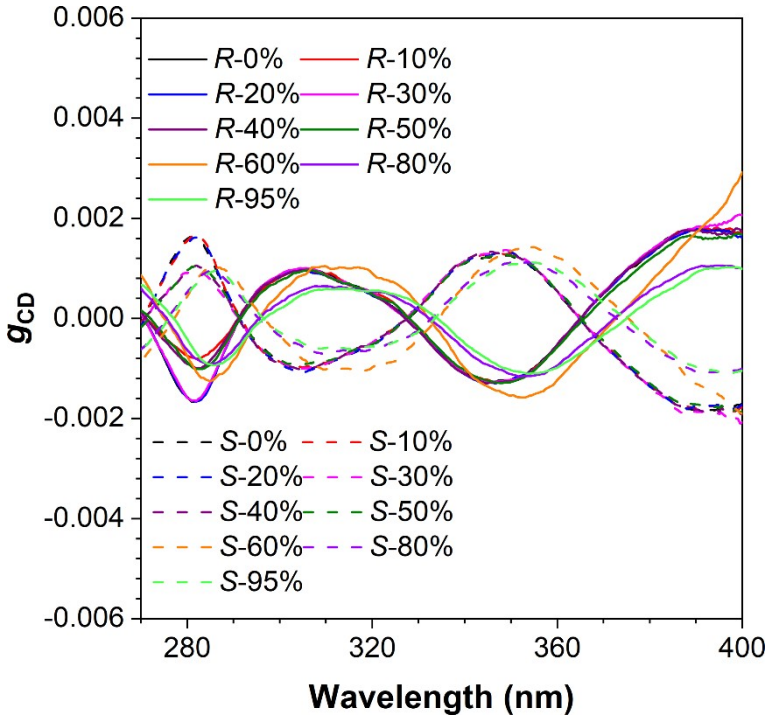


Figure S37. The g_{CD} value of compounds ***R*-/*S*-5** in THF and in THF/H_2O mixtures with various water fractions (f_w) (10 μM).

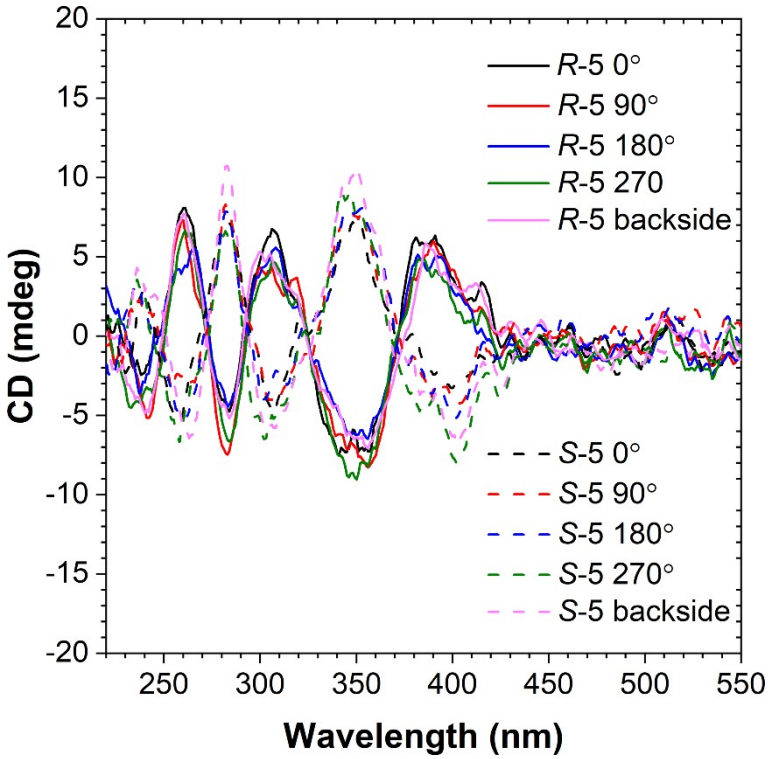


Figure S38. The g_{CD} value of compounds ***R*-/*S*-5** in KBr pellet was recorded at different rotation angles in the plane perpendicular to the light axis.

8. Circularly Polarized Luminescence Spectroscopy

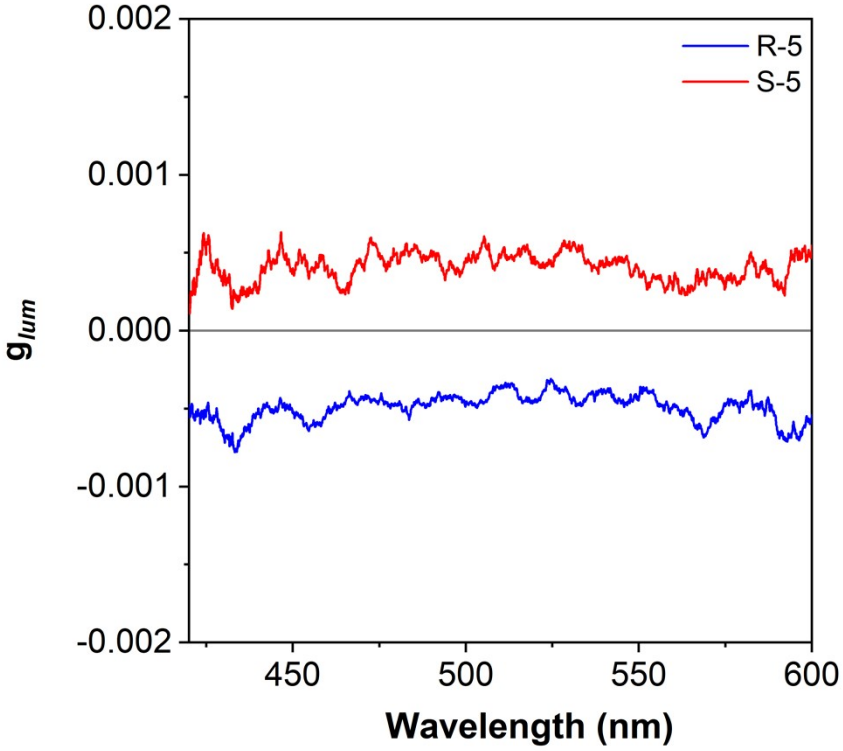
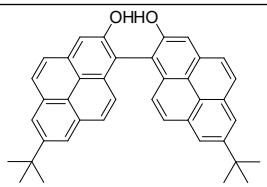
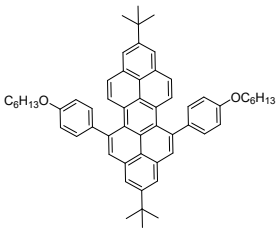
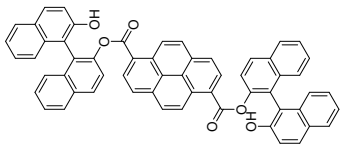
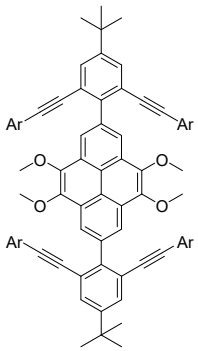
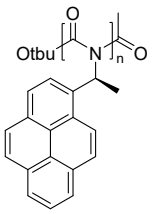
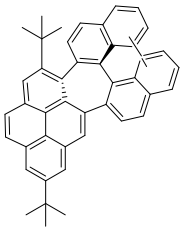
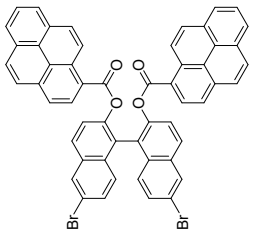
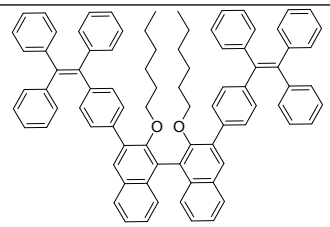
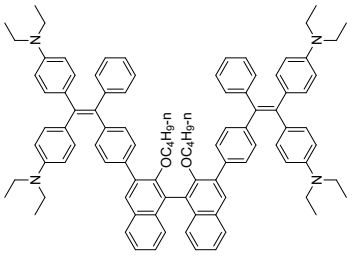
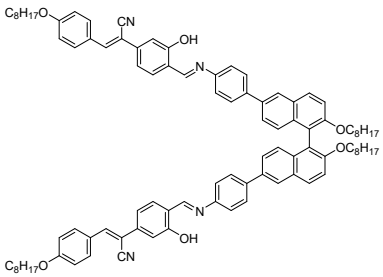
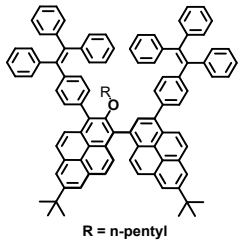


Figure S39. g_{lum} of ***R*/*S*-5** in a KBr pellet.

Table S5. Summary of chiroptical properties in pyrene-based chiral molecules

Compound	Φ_{fl}	$\lvert g_{abs}\rvert$	$\lvert g_{lum}\rvert$	Ref.
		Solution /solid state		
	0.57/nd	3.6×10^{-4}/nd	1.2×10^{-3}/nd	Ref.4
	nd	1.2×10^{-3}/nd	7.7×10^{-4}/nd	Ref.5
	nd	nd	6.9×10^{-3}/nd	Ref.6
	nd	1.0×10^{-3}/nd	nd	Ref.7
	nd	nd	nd/1.9×10^{-2}	Ref.8
	0.3/nd	2.3×10^{-3}/nd	nd	Ref.9
	nd/55.9	nd	nd/4.3×10^{-3}	Ref.10

	0.2/0.28	nd	nd	Ref.11
	nd/0.40	3×10^{-4}/7.8×10^{-4}	nd/3.6×10^{-3}	Ref.12
	0.12/nd	1.27×10^{-3}/nd	1.7×10^{-4}/nd	Ref.13
	< 0.01 / **0.66**	4.12×10^{-3}/6.48×10^{-4}	Non / 4.68×10^{-4}	**This work**

Notes: nd: no report. Non: no detect.

9. Scanning Electron Microscope Analysis

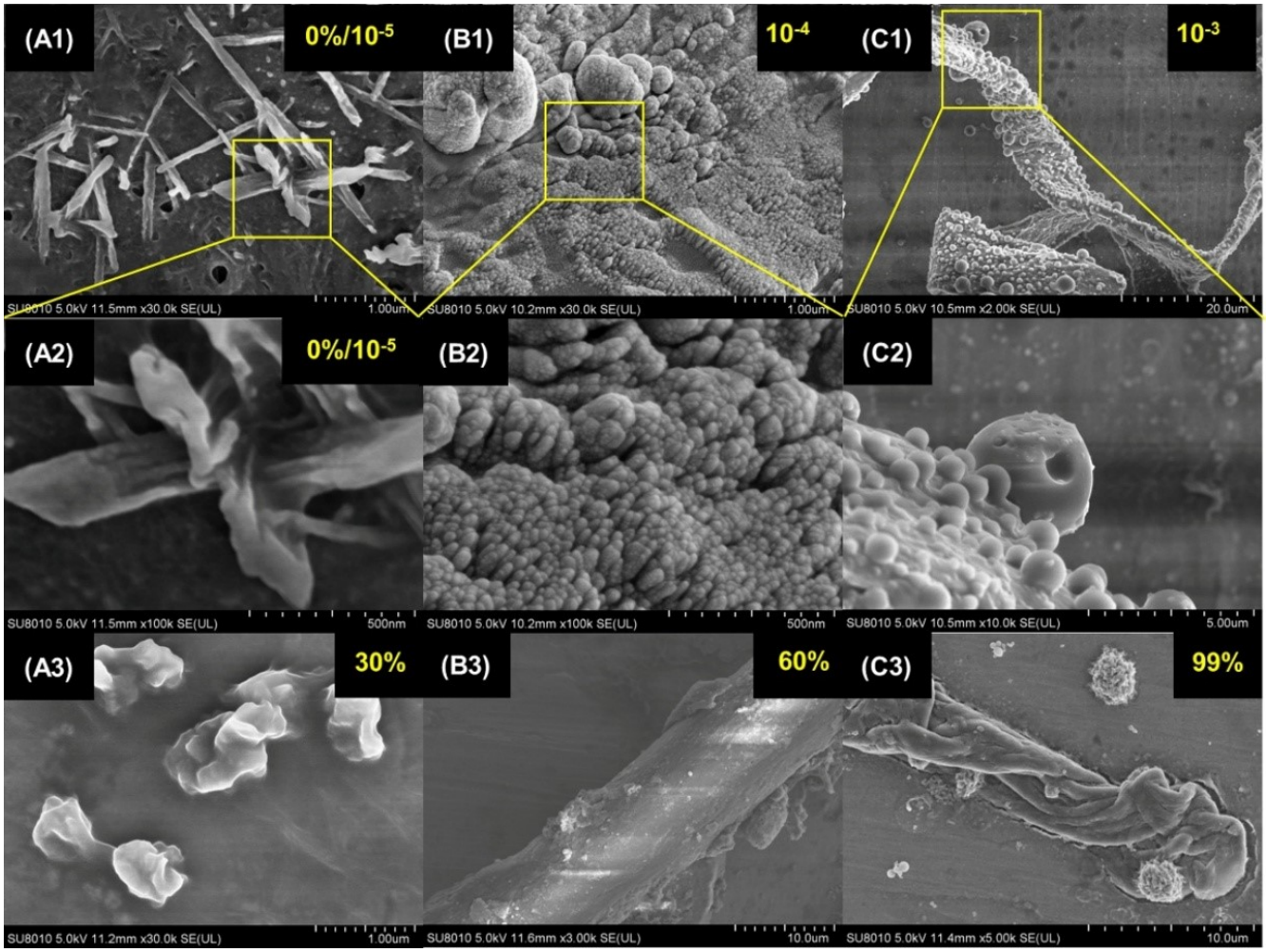


Figure S40. SEM of ***R*-5** (A1) in 10^{-5} M (in f_w = 0%), (B1) in 10^{-4} M and (C1) in 10^{-3} M, respectively, and (A2-C2) the zoom of the selected region. (A3-C3) SEM of ***R*-5** in f_w = 30%, 60% and 99% (10 μM).

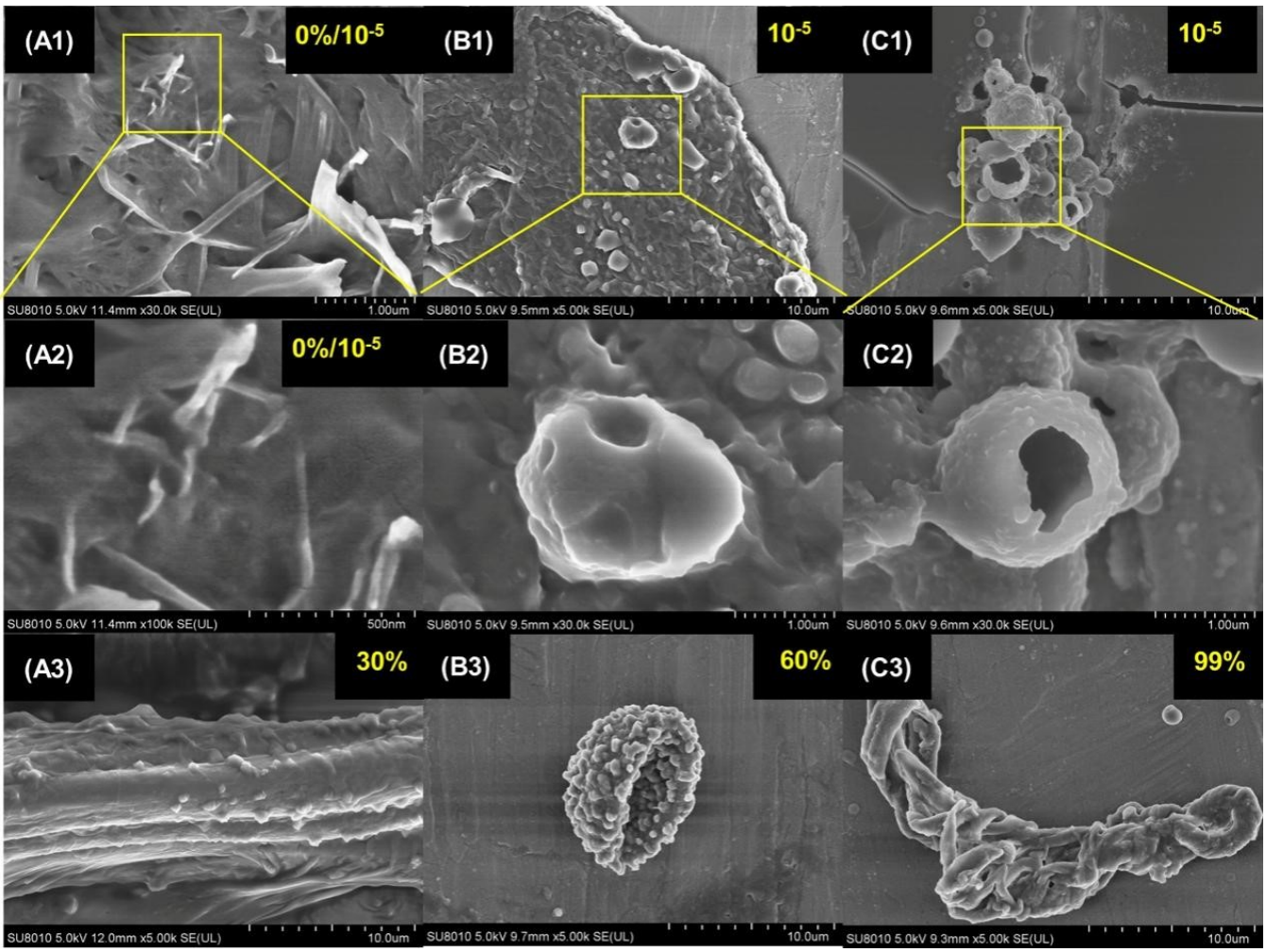


Figure S41. SEM of ***S*-5** (A1) in 10^{-5} M (in f_w = 0%), (B1) in 10^{-4} M and (C1) in 10^{-3} M, respectively, and (A2-C2) the zoom of the selected region. (A3-C3) SEM of ***S*-5** in f_w = 30%, 60% and 99% (10 μM).

10. Femtosecond Transient Absorption Spectroscopy Analysis

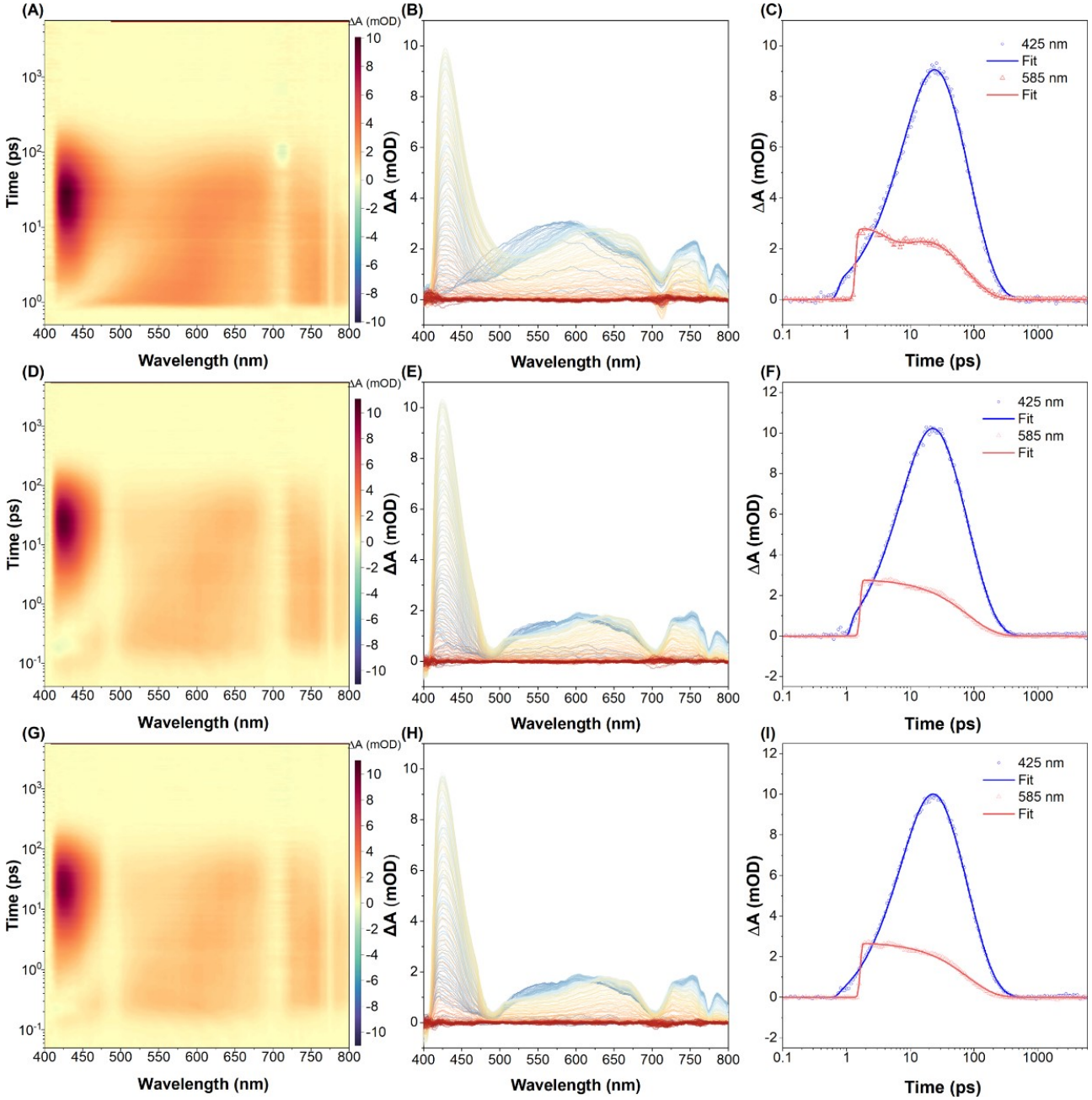


Figure S42. Femtosecond transient absorption spectroscopy analysis. (A, D and G) Pseudocolor 2D plots of TA data; (B, E, and H) TA spectra at various time delays and TA traces (C, F, and I) at 425 nm and 585 nm probe wavelengths of ***R*-5** in THF solution**.** Among them, the excitation wavelength is linear polarization for (A, B, and C), left circularly polarized (LCP) for (D, E, and F), and right circularly polarized (RCP) (G, H, respectively.

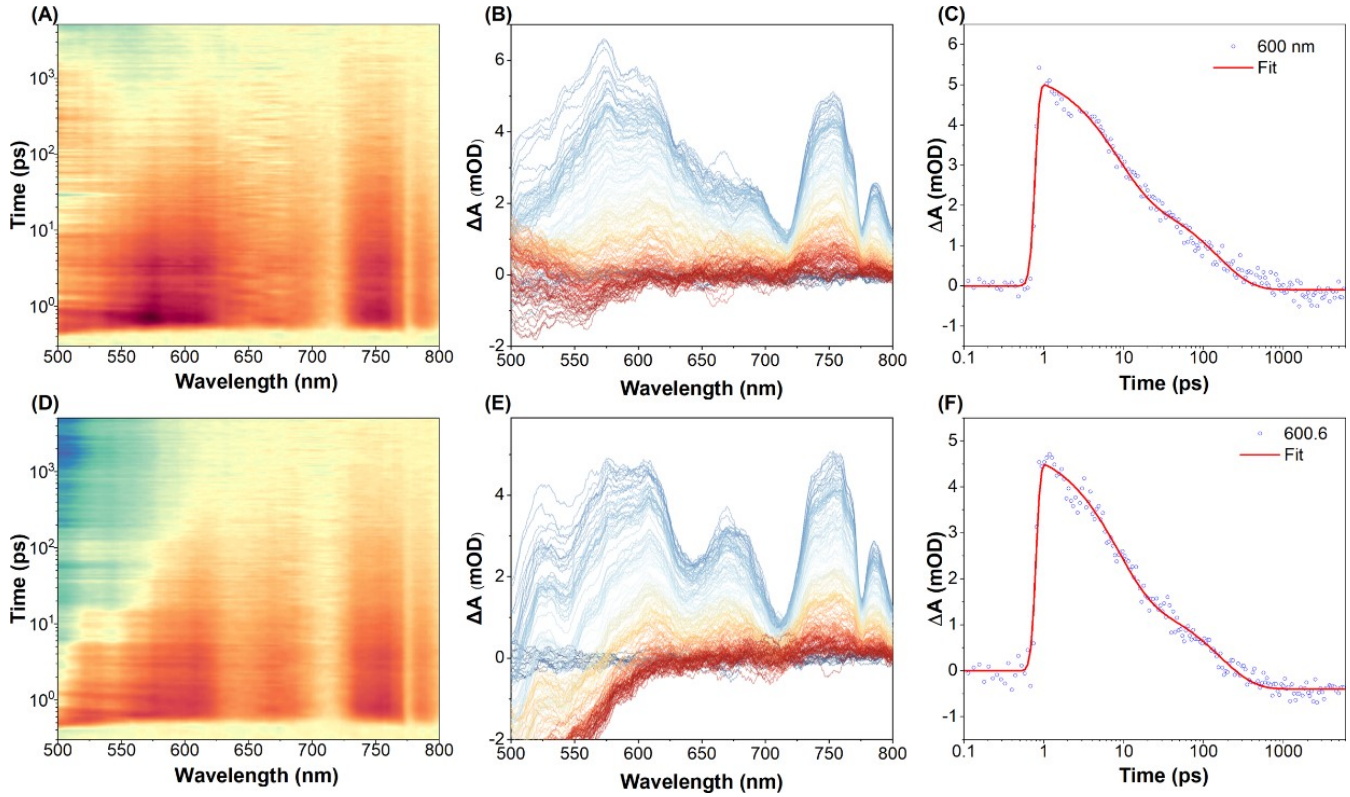


Figure S43. (A and D) Pseudocolor 2D plots of TA data; (B and E) TA spectra at various time delays and TA traces (C and F) at 600 nm probe wavelengths of ***R*-5** in solid state. Among them, the excitation wavelength is left circularly polarized (LCP) for (A, B, and C), and right circularly polarized (RCP) (D, E, and F) under 350 nm excitation.

Table S6. TA kinetics fitting results for compounds ***R*-/*S*-5** (fitted from Fig. 4A-4C and S39A-C) in THF solution.

Compound	λ_{probe} (nm)	ι (ps)	A_1	ι_2 (ps)	A_2	ι_3 (ps)	A_3	c^2
R-5[a)]	425	10±2	-0.95	82±10	1			0.9843
	585	2±0.3	0.26	11±1	-0.05	71±2	0.74	0.9581
	750	69±1	1					0.9933
S-5[a)]	425	11±1	-0.94	78±2	1			0.9988
	585	2±0.3	0.20	9±1	-0.05	68±2	0.80	0.9416
	750	66±1	1					0.9956

[a)] probed using linear polarization at 350 nm excitation

Table S7. TA kinetics fitting results for compounds ***R*-/*S*-5** (fitted from Fig. 4D-4H and S39D-I) in THF solution.

Compound	λ_{probe} (nm)	ι (ps)	A_1	ι_2 (ps)	A_2	ι_3 (ps)	A_3	c^2
***R*-5**[a)]	425	8.9±0.1	-0.94	79±1	1			0.9991
	585	80±1	1					0.9971
***R*-5**[b)]	425	9.1±0.1	-0.96	78±1	1			0.9992
	585	80±1	1					0.997
***R*-5**[c)]	485	0.6±0.1	1					0.8521
***S*-5**[a)]	425	9.4±0.1	-0.94	84±1	1			0.9989
	585	84±2	1					0.9934
	750	0.7±0.2	-0.1	72±1	1			0.9951
***S*-5**[b)]	425	9.2±0.1	-0.93	84±1	1			0.9987
	585	83±2	1					0.9914
	750	0.8±0.2	-0.1	72±1	1			0.9958
***S*-5**[c)]	440	0.11±0.03	1					0.8901
	450	0.12±0.02	1					0.8223
	465	0.13±0.04	1					0.7613
	565	0.15±0.02	1					0.8118

[a)] probed using left polarization at 350 nm excitation, [b)] probed using right polarization at 350 nm excitation. c) fitting results from the transient dynamics of differential TA spectra (H) at different wavelengths in THF solution.

Table S8. TA kinetics fitting results for compounds ***R***-/***S***-**5** (fitted from Fig. 5 and S40) in thin film.

Compound	λ_{probe} (nm)	ι (ps)	A_1	ι_2 (ps)	A_2	ι_3 (ps)	A_3	c^2
R-**5**[a)]	600	8±1	0.55	148±12	0.45			0.978
R-**5**[b)]	600	8±0.6	0.33	159±16	0.67			0.983
R-**5**[c)]	630	60±12	1					0.691
	675	50±10	1					0.7501
S-**5**[a)]	540	3±0.5	0.51	45±3	0.49			0.982
S-**5**[b)]	540	3±0.5	0.55	52±3	0.45			0.981
S-**5**[c)]	525	25±1	1					0.8978
	615	30±4	1					0.7481

[a)] probed using left polarization at 350 nm excitation. [b)] probed using right polarization at 350 nm excitation. c) fitting results from the transient dynamics of differential TA spectra (H) at different wavelengths in film state.

Table S9. Atom coordinates and absolute energies for ***R*-5** Standard orientation

AtomicType	Coordinates(Angstroms)		
	X	Y	Z
C	2.73639000	1.41598000	-0.60923500
C	3.23273000	2.44670200	-1.42225100
C	2.38661300	3.53051000	-1.76537000
C	1.05275300	3.57973900	-1.28623900
C	0.57757300	2.55558400	-0.45158100
C	1.42350300	1.48359900	-0.14769800
C	2.87792000	4.57117000	-2.60852600
C	2.04359600	5.65251500	-2.97825200
C	0.69105400	5.66203700	-2.49625200
C	0.22142200	4.68231600	-1.69888100
C	4.20390800	4.53932300	-3.09233800
C	4.66600700	5.57243900	-3.91201200
C	3.85766000	6.64199500	-4.27687100
C	2.54729800	6.65770700	-3.79774300
C	4.57565000	2.43579000	-1.93868700
C	5.03573200	3.42988800	-2.72599100
C	4.34899200	7.78304000	-5.17517000
C	5.80772900	7.59811800	-5.60517100
C	4.23948000	9.11533100	-4.41458700
C	3.48065900	7.84604400	-6.44303000
O	0.94062600	0.43266500	0.58854200
C	0.98977000	0.58900400	2.00791300
C	-0.81796100	2.55710400	0.07577500
C	-1.25870500	3.49646000	1.02368200
C	-2.61043600	3.45780400	1.45614400
C	-3.50168300	2.46638800	0.96792100
C	-3.01729600	1.49713200	0.07164800
C	-1.69843500	1.57797300	-0.36324300
C	-3.07621400	4.42662100	2.39623000
C	-4.42715500	4.43029400	2.81842100
C	-5.31460400	3.44670800	2.26626400
C	-4.87673500	2.51817100	1.39253600

C	-2.19836300	5.39915700	2.92391700
C	-2.67416300	6.33382100	3.84691100
C	-3.99838700	6.34638700	4.26802900
C	-4.85661700	5.38387700	3.73675700
C	-0.38644500	4.49065200	1.58974100
C	-0.83065400	5.38918200	2.49214100
C	-4.53628100	7.36598100	5.27866900
C	-3.45446600	8.34168300	5.75263900
C	-5.08486600	6.62480800	6.50959500
C	-5.66605600	8.18260000	4.62889100
C	3.58159800	0.24057600	-0.24974000
C	-3.84393600	0.36150600	-0.41310000
C	-4.46234200	-0.51564200	0.47836900
C	-5.15795600	-1.62246400	0.02331800
C	-5.26233900	-1.89503700	-1.34014100
C	-4.67509400	-0.99837000	-2.23276600
C	-3.96738500	0.10156200	-1.77765700
C	-5.99629600	-3.09144700	-1.84364700
C	-5.77569700	-4.33415200	-1.36451200
C	-6.63263800	-5.50186200	-1.72297400
C	-4.65645300	-4.64982000	-0.42860700
C	-6.98438700	-2.80636200	-2.92497700
C	3.46619300	-0.95789400	-0.94914300
C	4.27184300	-2.04159500	-0.64237600
C	5.21692200	-1.96834900	0.38164900
C	5.33489000	-0.76366100	1.07551400
C	4.52717400	0.32045200	0.76904200
C	6.12837100	-3.10656000	0.69641000
C	5.71072600	-4.38357500	0.82274500
C	7.56209900	-2.72068700	0.86011700
C	6.65927900	-5.53013300	0.94573300
C	4.27121500	-4.77542900	0.84959000
C	8.27634000	-3.06228800	2.00743700
C	9.60058000	-2.67947700	2.15948100
C	10.23564200	-1.95094900	1.16429600

C	9.53263300	-1.59670300	0.02071900
C	8.20530700	-1.96834800	-0.12365200
C	3.81274300	-5.80317600	0.02341500
C	2.48375800	-6.19480100	0.04603900
C	1.59142000	-5.58178700	0.91488400
C	2.03955300	-4.57372000	1.75694000
C	3.36691600	-4.17262500	1.72311600
C	6.49978700	-6.46594300	1.96884600
C	7.36519100	-7.54180700	2.08911600
C	8.39325000	-7.71583700	1.17270900
C	8.54751200	-6.80575100	0.13697000
C	7.68943900	-5.72225100	0.02577800
C	-6.97040000	-3.51606200	-4.12530200
C	-7.87749400	-3.22470200	-5.13259700
C	-8.81772600	-2.21962200	-4.95701500
C	-8.83552300	-1.49858900	-3.77097700
C	-7.91971600	-1.78215900	-2.77000600
C	-6.04959500	-6.69695600	-2.14722000
C	-6.83259700	-7.79322500	-2.47295600
C	-8.21412800	-7.72265100	-2.35758300
C	-8.80437100	-6.54789600	-1.91415400
C	-8.02087300	-5.44762500	-1.60131100
C	-4.90347200	-5.36627100	0.74376800
C	-3.87620800	-5.66009700	1.62639200
C	-2.57699600	-5.26223200	1.34123400
C	-2.31299000	-4.57447600	0.16508700
C	-3.34418700	-4.27195800	-0.71136600
H	0.04351600	6.47935300	-2.79383700
H	-0.80444000	4.70961100	-1.35802900
H	5.68795500	5.51490600	-4.26264300
H	1.88391700	7.47258400	-4.06441100
H	5.21829000	1.60452900	-1.68159500
H	6.05225500	3.40149900	-3.10270100
H	6.10954700	8.43401000	-6.23995300
H	5.94812300	6.67998600	-6.17989400

H	6.48371500	7.57413000	-4.74756900
H	4.58656700	9.93971000	-5.04315600
H	3.21113300	9.33088400	-4.12008700
H	4.84957900	9.09731600	-3.50876000
H	3.54160100	6.91028200	-7.00307100
H	3.81992600	8.65595000	-7.09426400
H	2.43059400	8.02591300	-6.20709300
H	0.41220700	1.47177900	2.30238000
H	2.03006800	0.73775500	2.31974300
H	-1.33148100	0.82573000	-1.04961300
H	-6.35750600	3.46909900	2.56252600
H	-5.57011100	1.79798100	0.98063700
H	-1.97113000	7.06090600	4.23113800
H	-5.89777200	5.36250400	4.03793600
H	0.64913400	4.50450600	1.27691800
H	-0.15294700	6.12665300	2.90766600
H	-3.88569700	9.04448300	6.46876300
H	-3.04277700	8.92434900	4.92561300
H	-2.63220100	7.82458700	6.25211100
H	-5.47234000	7.33977100	7.24023000
H	-5.89667100	5.94515700	6.24550600
H	-4.30032200	6.03698900	6.99126900
H	-5.30179900	8.72045900	3.75080800
H	-6.05969600	8.91518600	5.33845800
H	-6.49470700	7.54761100	4.31137500
H	-4.37583700	-0.34120400	1.54411900
H	-5.61257100	-2.29785200	0.73691200
H	-4.76731700	-1.17103400	-3.29855400
H	-3.50862000	0.77660000	-2.49061400
H	2.74068600	-1.03690900	-1.74963900
H	4.16986700	-2.95863800	-1.20833000
H	6.07556800	-0.67187400	1.86086800
H	4.64048600	1.24759500	1.31934400
H	7.78737000	-3.63626700	2.78457700
H	10.13793000	-2.95264400	3.05990400

H	11.27134200	-1.65510700	1.28123200
H	10.01894500	-1.02399700	-0.76022200
H	7.65693500	-1.67749800	-1.01209500
H	4.50899300	-6.29746300	-0.64377900
H	2.14446400	-6.98628700	-0.61163500
H	0.55462900	-5.89536900	0.93884500
H	1.35209700	-4.09609300	2.44497800
H	3.70999100	-3.38249400	2.37947500
H	5.68889200	-6.34453300	2.67746300
H	7.23262600	-8.25056200	2.89806700
H	9.06596900	-8.56048900	1.26162300
H	9.34002100	-6.93888400	-0.58990800
H	7.81804600	-5.01319400	-0.78222200
H	-6.24161800	-4.30421300	-4.26662700
H	-7.84829600	-3.78560300	-6.05923300
H	-9.52841300	-1.99401000	-5.74308200
H	-9.56197600	-0.70751800	-3.62687600
H	-7.92797900	-1.20558500	-1.85244600
H	-4.97066200	-6.76303600	-2.22392500
H	-6.36176500	-8.70821500	-2.81268000
H	-8.82667400	-8.58134400	-2.60524200
H	-9.88119700	-6.48640100	-1.81016900
H	-8.48780600	-4.53239600	-1.25986700
H	-5.91386600	-5.68932900	0.96534900
H	-4.09014200	-6.20416200	2.53881100
H	-1.77418500	-5.49168000	2.03218900
H	-1.30065000	-4.26823600	-0.07073500
H	-3.13321700	-3.72876700	-1.62385700
C	0.41489900	-0.66301100	2.63245300
H	1.00311300	-1.51964000	2.29030200
H	-0.60091500	-0.80458500	2.25173700
C	0.40046700	-0.60186400	4.15653000
H	-0.19333500	0.25999800	4.48244600
H	1.41755300	-0.43008400	4.52875300
C	-0.15988000	-1.86596500	4.80262600

H	0.44521400	-2.72578000	4.49462700
H	-1.16836600	-2.04983500	4.41751100
C	-0.19840900	-1.79121700	6.32499400
H	0.80239300	-1.63767300	6.73743500
H	-0.60012400	-2.70818100	6.76124300
H	-0.82461700	-0.96089300	6.66175900

Total Energy (CAM-RB3LYP) = -3818.515304 Hartree

Table S10. Atom coordinates and absolute energies for ***S*-5** Standard orientation

AtomicType	Coordinates(Angstroms)		
	X	Y	Z
C	-2.73639000	1.41598000	-0.60923500
C	-3.23273000	2.44670200	-1.42225100
C	-2.38661300	3.53051000	-1.76537000
C	-1.05275300	3.57973900	-1.28623900
C	-0.57757300	2.55558400	-0.45158100
C	-1.42350300	1.48359900	-0.14769800
C	-2.87792000	4.57117000	-2.60852600
C	-2.04359600	5.65251500	-2.97825200
C	-0.69105400	5.66203700	-2.49625200
C	-0.22142200	4.68231600	-1.69888100
C	-4.20390800	4.53932300	-3.09233800
C	-4.66600700	5.57243900	-3.91201200
C	-3.85766000	6.64199500	-4.27687100
C	-2.54729800	6.65770700	-3.79774300
C	-4.57565000	2.43579000	-1.93868700
C	-5.03573200	3.42988800	-2.72599100
C	-4.34899200	7.78304000	-5.17517000
C	-5.80772900	7.59811800	-5.60517100
C	-4.23948000	9.11533100	-4.41458700
C	-3.48065900	7.84604400	-6.44303000
O	-0.94062600	0.43266500	0.58854200
C	-0.98977000	0.58900400	2.00791300
C	0.81796100	2.55710400	0.07577500
C	1.25870500	3.49646000	1.02368200
C	2.61043600	3.45780400	1.45614400
C	3.50168300	2.46638800	0.96792100
C	3.01729600	1.49713200	0.07164800
C	1.69843500	1.57797300	-0.36324300
C	3.07621400	4.42662100	2.39623000
C	4.42715500	4.43029400	2.81842100
C	5.31460400	3.44670800	2.26626400
C	4.87673500	2.51817100	1.39253600

C	2.19836300	5.39915700	2.92391700
C	2.67416300	6.33382100	3.84691100
C	3.99838700	6.34638700	4.26802900
C	4.85661700	5.38387700	3.73675700
C	0.38644500	4.49065200	1.58974100
C	0.83065400	5.38918200	2.49214100
C	4.53628100	7.36598100	5.27866900
C	3.45446600	8.34168300	5.75263900
C	5.08486600	6.62480800	6.50959500
C	5.66605600	8.18260000	4.62889100
C	-3.58159800	0.24057600	-0.24974000
C	3.84393600	0.36150600	-0.41310000
C	4.46234200	-0.51564200	0.47836900
C	5.15795600	-1.62246400	0.02331800
C	5.26233900	-1.89503700	-1.34014100
C	4.67509400	-0.99837000	-2.23276600
C	3.96738500	0.10156200	-1.77765700
C	5.99629600	-3.09144700	-1.84364700
C	5.77569700	-4.33415200	-1.36451200
C	6.63263800	-5.50186200	-1.72297400
C	4.65645300	-4.64982000	-0.42860700
C	6.98438700	-2.80636200	-2.92497700
C	-3.46619300	-0.95789400	-0.94914300
C	-4.27184300	-2.04159500	-0.64237600
C	-5.21692200	-1.96834900	0.38164900
C	-5.33489000	-0.76366100	1.07551400
C	-4.52717400	0.32045200	0.76904200
C	-6.12837100	-3.10656000	0.69641000
C	-5.71072600	-4.38357500	0.82274500
C	-7.56209900	-2.72068700	0.86011700
C	-6.65927900	-5.53013300	0.94573300
C	-4.27121500	-4.77542900	0.84959000
C	-8.27634000	-3.06228800	2.00743700
C	-9.60058000	-2.67947700	2.15948100
C	-10.23564200	-1.95094900	1.16429600

C	-9.53263300	-1.59670300	0.02071900
C	-8.20530700	-1.96834800	-0.12365200
C	-3.81274300	-5.80317600	0.02341500
C	-2.48375800	-6.19480100	0.04603900
C	-1.59142000	-5.58178700	0.91488400
C	-2.03955300	-4.57372000	1.75694000
C	-3.36691600	-4.17262500	1.72311600
C	-6.49978700	-6.46594300	1.96884600
C	-7.36519100	-7.54180700	2.08911600
C	-8.39325000	-7.71583700	1.17270900
C	-8.54751200	-6.80575100	0.13697000
C	-7.68943900	-5.72225100	0.02577800
C	6.97040000	-3.51606200	-4.12530200
C	7.87749400	-3.22470200	-5.13259700
C	8.81772600	-2.21962200	-4.95701500
C	8.83552300	-1.49858900	-3.77097700
C	7.91971600	-1.78215900	-2.77000600
C	6.04959500	-6.69695600	-2.14722000
C	6.83259700	-7.79322500	-2.47295600
C	8.21412800	-7.72265100	-2.35758300
C	8.80437100	-6.54789600	-1.91415400
C	8.02087300	-5.44762500	-1.60131100
C	4.90347200	-5.36627100	0.74376800
C	3.87620800	-5.66009700	1.62639200
C	2.57699600	-5.26223200	1.34123400
C	2.31299000	-4.57447600	0.16508700
C	3.34418700	-4.27195800	-0.71136600
H	-0.04351600	6.47935300	-2.79383700
H	0.80444000	4.70961100	-1.35802900
H	-5.68795500	5.51490600	-4.26264300
H	-1.88391700	7.47258400	-4.06441100
H	-5.21829000	1.60452900	-1.68159500
H	-6.05225500	3.40149900	-3.10270100
H	-6.10954700	8.43401000	-6.23995300
H	-5.94812300	6.67998600	-6.17989400

H	-6.48371500	7.57413000	-4.74756900
H	-4.58656700	9.93971000	-5.04315600
H	-3.21113300	9.33088400	-4.12008700
H	-4.84957900	9.09731600	-3.50876000
H	-3.54160100	6.91028200	-7.00307100
H	-3.81992600	8.65595000	-7.09426400
H	-2.43059400	8.02591300	-6.20709300
H	-0.41220700	1.47177900	2.30238000
H	-2.03006800	0.73775500	2.31974300
H	1.33148100	0.82573000	-1.04961300
H	6.35750600	3.46909900	2.56252600
H	5.57011100	1.79798100	0.98063700
H	1.97113000	7.06090600	4.23113800
H	5.89777200	5.36250400	4.03793600
H	-0.64913400	4.50450600	1.27691800
H	0.15294700	6.12665300	2.90766600
H	3.88569700	9.04448300	6.46876300
H	3.04277700	8.92434900	4.92561300
H	2.63220100	7.82458700	6.25211100
H	5.47234000	7.33977100	7.24023000
H	5.89667100	5.94515700	6.24550600
H	4.30032200	6.03698900	6.99126900
H	5.30179900	8.72045900	3.75080800
H	6.05969600	8.91518600	5.33845800
H	6.49470700	7.54761100	4.31137500
H	4.37583700	-0.34120400	1.54411900
H	5.61257100	-2.29785200	0.73691200
H	4.76731700	-1.17103400	-3.29855400
H	3.50862000	0.77660000	-2.49061400
H	-2.74068600	-1.03690900	-1.74963900
H	-4.16986700	-2.95863800	-1.20833000
H	-6.07556800	-0.67187400	1.86086800
H	-4.64048600	1.24759500	1.31934400
H	-7.78737000	-3.63626700	2.78457700
H	-10.13793000	-2.95264400	3.05990400

H	-11.27134200	-1.65510700	1.28123200
H	-10.01894500	-1.02399700	-0.76022200
H	-7.65693500	-1.67749800	-1.01209500
H	-4.50899300	-6.29746300	-0.64377900
H	-2.14446400	-6.98628700	-0.61163500
H	-0.55462900	-5.89536900	0.93884500
H	-1.35209700	-4.09609300	2.44497800
H	-3.70999100	-3.38249400	2.37947500
H	-5.68889200	-6.34453300	2.67746300
H	-7.23262600	-8.25056200	2.89806700
H	-9.06596900	-8.56048900	1.26162300
H	-9.34002100	-6.93888400	-0.58990800
H	-7.81804600	-5.01319400	-0.78222200
H	6.24161800	-4.30421300	-4.26662700
H	7.84829600	-3.78560300	-6.05923300
H	9.52841300	-1.99401000	-5.74308200
H	9.56197600	-0.70751800	-3.62687600
H	7.92797900	-1.20558500	-1.85244600
H	4.97066200	-6.76303600	-2.22392500
H	6.36176500	-8.70821500	-2.81268000
H	8.82667400	-8.58134400	-2.60524200
H	9.88119700	-6.48640100	-1.81016900
H	8.48780600	-4.53239600	-1.25986700
H	5.91386600	-5.68932900	0.96534900
H	4.09014200	-6.20416200	2.53881100
H	1.77418500	-5.49168000	2.03218900
H	1.30065000	-4.26823600	-0.07073500
H	3.13321700	-3.72876700	-1.62385700
C	-0.41489900	-0.66301100	2.63245300
H	-1.00311300	-1.51964000	2.29030200
H	0.60091500	-0.80458500	2.25173700
C	-0.40046700	-0.60186400	4.15653000
H	0.19333500	0.25999800	4.48244600
H	-1.41755300	-0.43008400	4.52875300
C	0.15988000	-1.86596500	4.80262600

H	-0.44521400	-2.72578000	4.49462700
H	1.16836600	-2.04983500	4.41751100
C	0.19840900	-1.79121700	6.32499400
H	-0.80239300	-1.63767300	6.73743500
H	0.60012400	-2.70818100	6.76124300
H	0.82461700	-0.96089300	6.66175900

Total Energy (CAM-RB3LYP) = -3818.515304 Hartree

Table S11. Atom coordinates and absolute energies for ***R*-Bipyrene-OH** Standard orientation

AtomicType	Coordinates(Angstroms)		
	X	Y	Z
C	-1.91335700	-2.98209900	-1.72193200
C	-3.02734800	-2.17474500	-1.50398200
C	-2.95000700	-1.14735200	-0.53584600
C	-1.75098200	-0.95557100	0.19933500
C	-0.64515500	-1.78432600	-0.03258700
C	-0.74627000	-2.78904000	-0.99988900
C	-4.07753800	-0.31011600	-0.30426900
C	-4.01522400	0.72621400	0.65635800
C	-2.78647000	0.90585900	1.38005600
C	-1.71639000	0.11399100	1.16577400
C	-5.27347100	-0.50006400	-1.03073700
C	-6.36744100	0.33434300	-0.78552700
C	-6.31989100	1.35527300	0.15603300
C	-5.13015300	1.53130700	0.86470400
C	-4.25423500	-2.34900800	-2.23069000
C	-5.32094700	-1.55388600	-2.00489200
C	-7.51084600	2.27925700	0.43644800
C	-8.72684300	1.94083900	-0.43180500
C	-7.10772100	3.73525100	0.14815000
C	-7.92473700	2.14670700	1.91177700
O	0.35273500	-3.56539000	-1.19860300
C	0.62160400	-1.64066400	0.74194100
C	1.72573900	-0.94844200	0.21853900
C	2.91006400	-0.84423600	0.99142000
C	2.97925300	-1.43232600	2.27796300
C	1.86530700	-2.11036800	2.76605200
C	0.71089700	-2.20954100	2.00781400
C	4.03888300	-0.14335100	0.47655100
C	5.22632200	-0.03478500	1.24036100
C	5.26330700	-0.64583700	2.54216500
C	4.19691200	-1.30790600	3.03306500
C	3.98892200	0.45250400	-0.80192600

C	5.10719600	1.13524600	-1.28762200
C	6.27882400	1.24890700	-0.54908300
C	6.31374600	0.65467200	0.71335700
C	1.70494600	-0.32943300	-1.07916200
C	2.77620500	0.33434100	-1.56111400
C	7.51451000	1.99375500	-1.06791600
C	7.29561600	2.58185800	-2.46553400
C	8.70459600	1.02204700	-1.13899900
C	7.85482700	3.14869500	-0.11097800
H	-2.73322500	1.70490300	2.11137400
H	-0.80208500	0.27350000	1.72179700
H	-7.26874300	0.16189700	-1.35885800
H	-5.05500800	2.31842600	1.60638700
H	-4.30591000	-3.13996200	-2.97059000
H	-6.23995100	-1.69925800	-2.56192500
H	-9.54533300	2.62409900	-0.19526000
H	-9.08354800	0.92419200	-0.25223600
H	-8.50705300	2.04559900	-1.49659000
H	-7.94793800	4.40666400	0.34412000
H	-6.27230400	4.05624400	0.77244400
H	-6.81053700	3.85708000	-0.89581900
H	-8.21798300	1.12020700	2.14274000
H	-8.77395700	2.80065800	2.12703300
H	-7.11298000	2.42177500	2.58712700
H	-0.14586600	-2.74425100	2.40047800
H	6.17431000	-0.56143400	3.12422500
H	4.23750700	-1.76395300	4.01602200
H	5.03535900	1.58074900	-2.27094700
H	7.21118000	0.72315900	1.31763500
H	0.79967300	-0.40262000	-1.66800500
H	2.73691300	0.79511700	-2.54203200
H	8.20085000	3.10037500	-2.78880000
H	6.47820200	3.30618100	-2.47763900
H	7.07865600	1.80585700	-3.20290000
H	9.59417000	1.53936700	-1.50813600

H	8.94484100	0.60258000	-0.16072600
H	8.48850800	0.19140600	-1.81454800
H	7.02446000	3.85503500	-0.04324500
H	8.73471800	3.68998400	-0.46875600
H	8.07105000	2.79025600	0.89671000
H	1.90802400	-2.56558700	3.74918800
H	-1.96323400	-3.77482000	-2.46274700
H	0.16946200	-4.20811600	-1.88893000

Total Energy (CAM-RB3LYP) = -1619.520470 Hartree

Table S12. Atom coordinates and absolute energies for ***R*-3** Standard orientation

AtomicType	Coordinates(Angstroms)		
	X	Y	Z
C	2.15138800	3.27294400	-0.28831600
C	3.26129700	2.44162000	-0.40558200
C	3.16632600	1.10741800	0.05707000
C	1.95632200	0.63450600	0.62736700
C	0.84429200	1.49006300	0.71781100
C	0.97145100	2.80745700	0.26566600
C	4.29752500	0.24718800	-0.04348800
C	4.22912900	-1.08492300	0.42657500
C	2.99746900	-1.53331800	1.01455800
C	1.92444700	-0.72243600	1.11204700
C	5.50403600	0.71211800	-0.61229700
C	6.59839000	-0.15137000	-0.70385800
C	6.54314800	-1.46380500	-0.24888900
C	5.34609500	-1.90717900	0.31424600
C	4.50035800	2.89225200	-0.97657700
C	5.56486600	2.07006600	-1.07725000
C	7.73591200	-2.42263000	-0.34266000
C	8.96222300	-1.76519000	-0.98380100
C	7.34578600	-3.64158600	-1.19554700
C	8.12767700	-2.89134700	1.06883800
O	-0.07318300	3.68639400	0.40331400
C	-1.02704900	3.67480700	-0.65987100
C	-0.44177000	1.04692600	1.32989000
C	-1.30560800	0.14862200	0.67856500
C	-2.51221300	-0.24226100	1.31619600
C	-2.84504500	0.27014000	2.59334400
C	-1.97243300	1.16876100	3.20335800
C	-0.79878000	1.54919200	2.57807200
C	-3.39953100	-1.15271900	0.67154400
C	-4.60253100	-1.55187400	1.30312600
C	-4.90611000	-1.01664600	2.60298700
C	-4.07193900	-0.15138600	3.21317900

C	-3.09360800	-1.66781700	-0.60638400
C	-3.97693400	-2.55905400	-1.22055900
C	-5.15953600	-2.96103400	-0.61100300
C	-5.45007100	-2.44269700	0.65161100
C	-1.02676700	-0.38853500	-0.62787600
C	-1.87335100	-1.24671300	-1.23438200
C	-6.13933900	-3.93875400	-1.27038800
C	-5.65948600	-4.40222900	-2.64949000
C	-7.50555600	-3.25413700	-1.44435800
C	-6.30049300	-5.18069900	-0.37754800
H	2.94625900	-2.54981700	1.38881500
H	1.01255600	-1.08546200	1.56672200
H	7.50729500	0.23564200	-1.14513200
H	5.26612000	-2.92336800	0.68324800
H	4.56018700	3.91627200	-1.32755200
H	6.49299900	2.42420700	-1.51199200
H	9.78130400	-2.48623600	-1.02764400
H	9.31017000	-0.90551600	-0.40682600
H	8.75854900	-1.43495000	-2.00482300
H	8.18720100	-4.33541900	-1.27135400
H	6.50340300	-4.18512600	-0.76469600
H	7.06448200	-3.33560200	-2.20564600
H	8.41042200	-2.04295200	1.69595900
H	8.97839100	-3.57602600	1.01765000
H	7.30850100	-3.41447900	1.56476700
H	-1.44407700	2.66840900	-0.77344900
H	-0.52609200	3.94336300	-1.59862900
H	-0.13460600	2.25288100	3.06395500
H	-5.82758700	-1.32506100	3.08412600
H	-4.31272400	0.24705500	4.19245500
H	-3.71152500	-2.93430600	-2.20000000
H	-6.36414100	-2.73314100	1.15686100
H	-0.11334900	-0.08785600	-1.12422400
H	-1.64067200	-1.63605200	-2.21939800
H	-6.38873400	-5.09461100	-3.07551500

H	-4.70249600	-4.92546500	-2.59166400
H	-5.55328900	-3.56629400	-3.34441600
H	-8.21521300	-3.93995600	-1.91458600
H	-7.92790300	-2.94204400	-0.48784900
H	-7.41876400	-2.36763200	-2.07650600
H	-5.34271000	-5.68714100	-0.23905500
H	-6.99705200	-5.88798000	-0.83542100
H	-6.68778500	-4.92343200	0.60963600
C	-2.11600900	4.66980900	-0.32436300
H	-1.65706500	5.65173200	-0.17377600
H	-2.56470500	4.38074300	0.63042100
C	-3.18856400	4.74973500	-1.40587100
H	-3.63175100	3.75847400	-1.55615300
H	-2.72768900	5.02643600	-2.36166600
C	-4.29603200	5.74752200	-1.07871000
H	-3.85426100	6.73824000	-0.92735800
H	-4.75733200	5.47101200	-0.12481000
C	-5.36705400	5.82497100	-2.16105200
H	-4.93781700	6.13053400	-3.11903200
H	-6.14650800	6.54462000	-1.90218300
H	-5.84721700	4.85417400	-2.30962000
H	-2.22006300	1.57112400	4.17921400
H	2.19680300	4.30518800	-0.61495500

Total Energy (CAM-RB3LYP) = -1816.004626 Hartree

Table S13. Atom coordinates and absolute energies for **Py-TPE** Standard orientation

AtomicType	Coordinates(Angstroms)		
	X	Y	Z
C	1.56574000	1.07453300	-1.29121700
C	2.67148000	0.45451100	-0.67716500
C	3.97889900	0.93314400	-0.95713000
C	4.17204800	2.01226100	-1.85412600
C	3.05875400	2.58446900	-2.46358000
C	1.78606100	2.12062200	-2.18473700
C	5.11164600	0.32705600	-0.33862400
C	6.41809300	0.80693600	-0.60204100
C	6.57493300	1.91023000	-1.51093400
C	5.50815400	2.47900800	-2.10627100
C	2.54454000	-0.67690400	0.20374400
C	3.62120700	-1.24951600	0.78169300
C	4.94930000	-0.76262000	0.54322200
C	6.07187800	-1.34011000	1.14224500
C	7.35792000	-0.87461400	0.89757500
C	7.50489500	0.20037900	0.01977700
C	0.16422800	0.66065900	-1.01807800
C	-0.36862400	0.69536400	0.27045800
C	-1.68978200	0.35330500	0.50522000
C	-2.52706700	-0.04003800	-0.53836600
C	-1.98797100	-0.09455000	-1.82365200
C	-0.67130500	0.26317800	-2.06136700
C	-3.94375700	-0.43839900	-0.29563200
C	-4.80387700	0.31820500	0.41801600
C	-4.33439900	-1.74201500	-0.90863400
C	-6.15317400	-0.16626800	0.83211600
C	-4.48356200	1.70821800	0.85638200
C	-4.67571700	2.08853600	2.18544100
C	-4.39154600	3.37921000	2.60313200
C	-3.93226200	4.32163800	1.69330600
C	-3.76056400	3.96250600	0.36417600
C	-4.03239800	2.66746600	-0.04975500

C	-5.46359500	-1.85114800	-1.71959500
C	-5.80308100	-3.06149600	-2.30456500
C	-5.02078300	-4.18650300	-2.08690000
C	-3.88836900	-4.08898100	-1.29001300
C	-3.54294900	-2.87539000	-0.71650700
C	-7.28236400	0.62348700	0.60994600
C	-8.54006100	0.19061000	0.99959600
C	-8.68946100	-1.03121300	1.64124600
C	-7.57161200	-1.81473800	1.88935700
C	-6.31571900	-1.38671500	1.48712800
C	8.59993900	-1.49445200	1.54853500
C	8.24905300	-2.66069600	2.47798200
C	9.54225000	-2.02217800	0.45357000
C	9.32945700	-0.42437500	2.37816700
H	3.19528300	3.40941500	-3.15375800
H	0.93021700	2.59431400	-2.65076500
H	7.57647800	2.27476300	-1.71023000
H	5.63823700	3.30810300	-2.79287500
H	1.55793900	-1.07814100	0.39021800
H	3.49669200	-2.10463000	1.43692600
H	5.91020200	-2.17421200	1.81206600
H	8.49347600	0.58846500	-0.19752100
H	0.25708300	1.00984900	1.09727800
H	-2.08253900	0.39928600	1.51309500
H	-2.61008200	-0.42259200	-2.64806100
H	-0.27578200	0.21641400	-3.06935000
H	-5.04931700	1.36137200	2.89679800
H	-4.53464000	3.65180400	3.64211400
H	-3.71603300	5.33255100	2.01754600
H	-3.41338500	4.69419600	-0.35570700
H	-3.89283500	2.39173800	-1.08750400
H	-6.08048200	-0.97770400	-1.88947400
H	-6.68292700	-3.12492700	-2.93382900
H	-5.28779400	-5.13300600	-2.54155700
H	-3.26765200	-4.96060900	-1.11896300

H	-2.64927700	-2.80167700	-0.10797900
H	-7.16987200	1.58557700	0.12409300
H	-9.40624500	0.81259000	0.80681200
H	-9.67130300	-1.36725500	1.95263200
H	-7.67638200	-2.76491300	2.39958200
H	-5.44782100	-2.00462000	1.67993300
H	9.16381300	-3.06569000	2.91607700
H	7.60182200	-2.34476700	3.29911000
H	7.75291200	-3.47233700	1.94127100
H	10.43280900	-2.46858700	0.90383800
H	9.87115600	-1.22663200	-0.21694300
H	9.04718100	-2.78533000	-0.15100700
H	8.68086500	-0.03343000	3.16525300
H	10.21820000	-0.85204900	2.84971700
H	9.65116100	0.41700300	1.76231800

Total Energy (CAM-RB3LYP) = -1774.002627 Hartree

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