Supporting Information

A E/Z Isomers Strategy of Photosensitizers with Tunable Generation Processes of Reactive Oxygen Species

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Materials

All materials were used directly without further purification. 4-Iodobenzaldehyde, Diphenylacetylene, 1-Bromo-4-vinylbenzene, 2-(3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile, Pluronic F127 and 2-(3-cyano-4,5,5-trimethylfuran-2-ylidene)propanedinitrile were purchased from Bidepharm. Sodium hydroxide, Lithium chloride, triarylphosphines Palladium(II) acetate, 4-(Diphenylamino)phenylboronic acid, Methanol, Dimethyl sulfoxide (DMSO), Dichloromethane and Piperidine were purchased from Energy chemical.

Penicillin−streptomycin was purchased from Macgene (China). RPMI-1640 and FBS were purchased from Gibco (USA). Calcein-AM/PI Live-Dead Cell Staining Kit, Reactive Oxygen Species Assay Kit and Lyso-Tracker Green were purchased from Beijing Solarbio Science and Technology Co., Lta. The 2',7'-Dichlorofluorescein diacetate (DCFH-DA), Thiazolyl Blue (MTT), Dihydrorhodamine 123 (DHR123) and 9,10-Anthracenediyl-bis(methylene) dimalonic acid (ABDA) required for the active oxygen test were purchased from Shanghai McLean Biochemical Technology Co., Ltd.

Equipment

^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV 400 spectrometer. Mass spectra (MS) were collected using a Finnigan Biflex III mass spectrometer. The ultraviolet–visible spectra and the generation of singlet oxygen ($^{1}O_2$) were collected on the Thermo Fisher UV-2700 spectrophotometer. The PL emission spectra, reactive oxygen species (ROS) and superoxide anion (O_2^{-}•) were collected on the HORIBA FluoroMax-4 spectrofluorometer. Record cell imaging using a confocal laser PL microscope (Zeiss LSM 780). Electron spin resonance (ESR) spectra were measured on Bruker Paramagnetic Resonance Spectrometer EMXplus. *In vivo* imaging was

measured on IVIS lumina series III. Transmission Electron Microscope (TEM) was measured on Talos F200S. TD-DFT calculations were performed on Gaussian 09 program. The ground-state (S_0) geometries were optimized with B3LYP by using 6-311G(d) basis sets.

Synthetic Route of Target Compounds

Synthesis of TPB-Br-CHO: 4-Iodobenzaldehyde (1.16 g, 5 mmol), Diphenylacetylene (3.56 g, 20 mmol), 1-Bromo-4-vinylbenzene (0.75 mL, 5 mmol), Sodium hydroxide (0.84 g, 10 mmol), Lithium chloride (0.145 g, 3.5 mmol), Triarylphosphines (0.13 g, 0.5 mmol) and Palladium (II) acetate (0.055 g, 0.25) were dissolved in 25 mL N,N-Dimethylformamide, then refluxed at 100 ℃ for 6 h. After that, the solution was extracted with dichloromethane and washed with water. Later the organic layer was dried over anhydrous $MgSO_4$. The solvent was evaporated under reduced pressure and the residue was purified by silica gel column chromatography using a dichloromethane/petroleum ether mixture (1/10, V_d/V_p) as the eluent to give desired TPB-Br-CHO with 57% yield. ^{1}H NMR (400 MHz, DMSO): δ (ppm): 10.02 (s, 1H), 9.80 (s, 1H), 7.94 (d, J = 8.2 Hz, 2H), 7.56 (d, J = 8.3 Hz, 2H), 7.48-7.34 (m, 8H), 7.29-6.97 (m, 22H), 6.92-6.76 (m, 4H), 6.13 (d, J = 15.9 Hz, 2H). ^{13}C NMR (101 MHz, DMSO): δ (ppm):193.17, 192.91, 149.17, 148.38, 142.58, 142.48, 142.24, 141.44, 140.18, 139.97, 139.63, 139.46, 136.46, 136.44, 135.60, 134.46, 132.51, 132.41, 132.20, 132.17, 131.84, 131.61, 131.42, 131.37, 130.92, 129.95, 128.93, 128.77 (s), 128.69 (s), 128.58 (s), 128.51 (s), 128.26 (s), 128.18 (s), 127.85 (s), 127.67, 127.22, 128.06, 121.31. MS (APCl, *m/z*) Calcd for $C_{29}H_{21}BrO$ $[M+H]^+$: 465.08, found: 465.08. The yield of E-TPB-Br-CHO was 32%, and the yield of Z-TPB-Br-CHO was 25%.

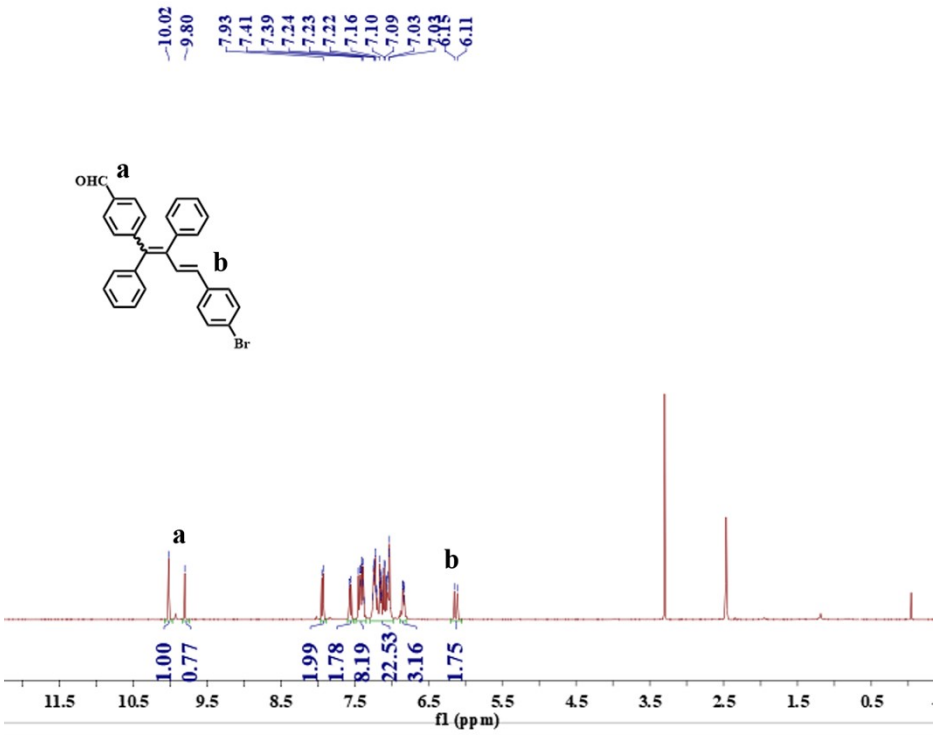

Figure S1. ^{1}H NMR spectrum of TPB-Br-CHO in DMSO-d6.

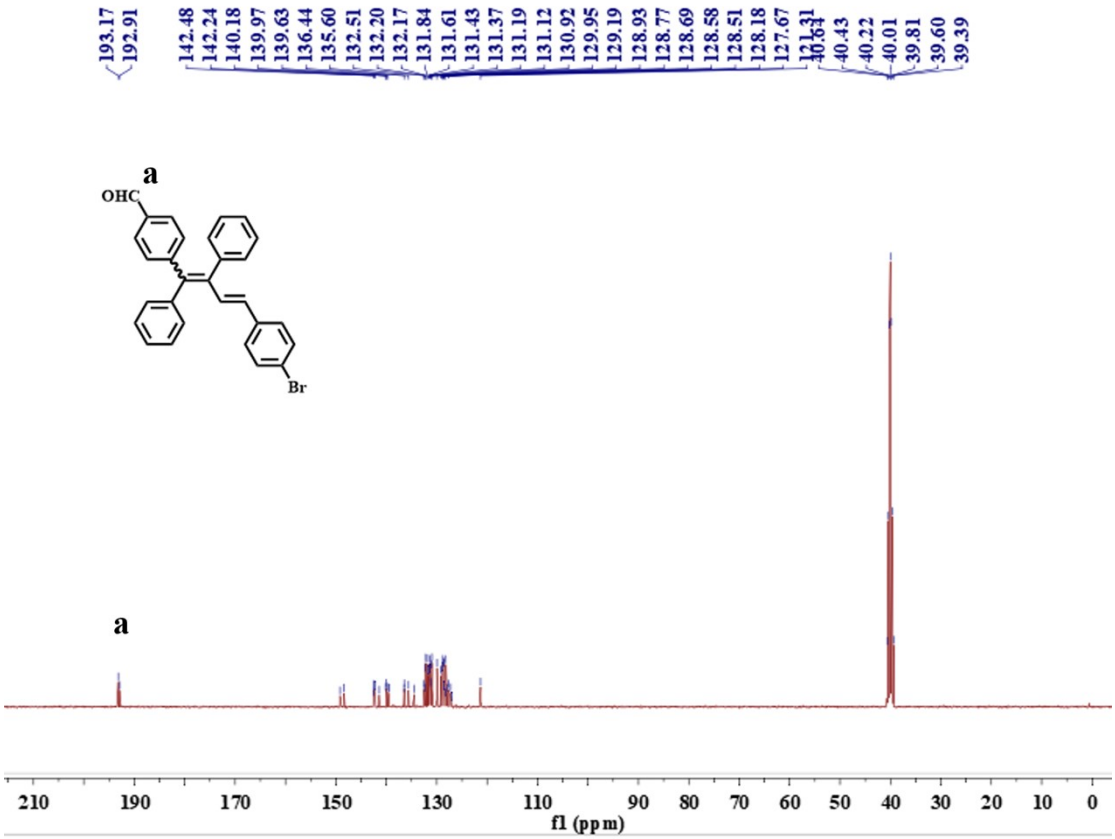

Figure S2. ^{13}C NMR spectrum of TPB-Br-CHO in DMSO-d6.

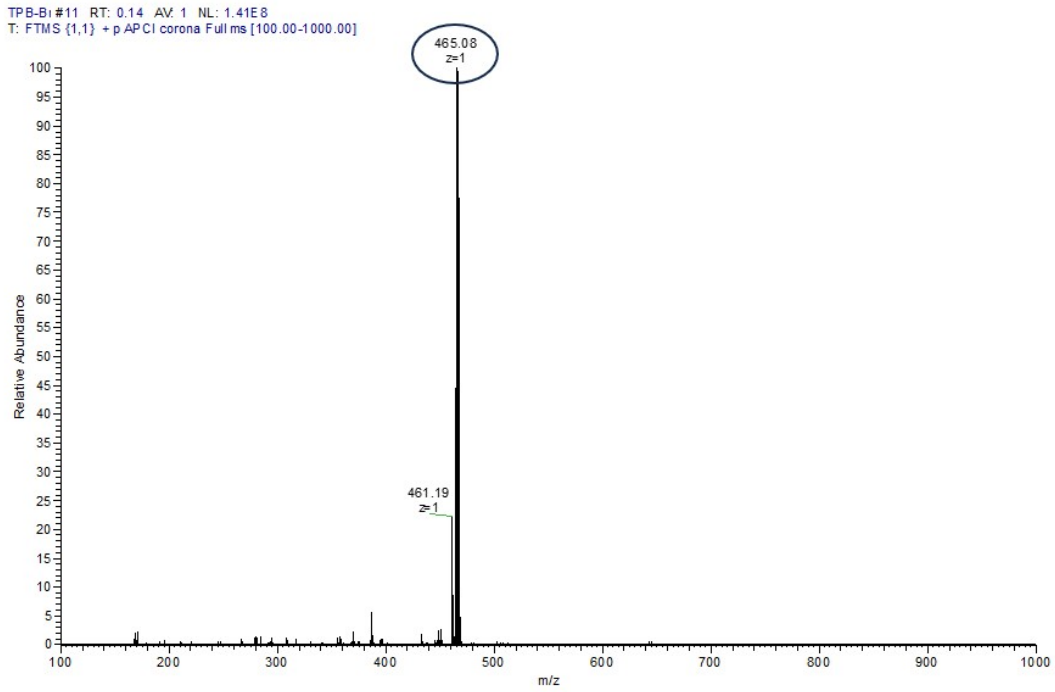

Figure S3. MS spectrum of TPB-Br-CHO.

Synthesis of TPB-TPA-CHO： TPB-Br-CHO (0.465 g, 1 mmol), 4-(Diphenylamino) phenylboronic acid (1.5 g, 10 mmol), Potassium phosphate (0.212 g, 1 mmol) and Tetrakis (triphenylphosphine) palladium (0.288 g, 0.25 mmol) were dissolved in 30 mL N,N-Dimethylformamide, then refluxed at 100 ℃ for 8 h. After that, the solution was extracted with dichloromethane and washed with water. Later the organic layer was dried over anhydrous $MgSO_4$. The solvent was evaporated under reduced pressure and the residue was purified by silica gel column chromatography using a dichloromethane/petroleum ether mixture (1/5, V_d/V_p) as the eluent to give desired TPB-TPA-CHO with 83% yield. ^{1}H NMR (400 MHz, DMSO): δ (ppm): 10.00 (s, 1H), 9.79 (s, 1H), 7.92 (d, J = 8.0 Hz, 2H), 7.57-7.33 (m, 14H), 7.33-7.09 (m, 24H), 7.09-6.72 (m, 26H), 6.18 (d, J = 15.9 Hz, 2H). ^{13}C NMR (101 MHz, DMSO): δ (ppm):193.1, 192.9, 149.3, 148.6, 147.6, 147.4, 147.3, 142.3, 141.9, 141.8, 141.6, 140.5, 140.3, 139.8, 139.6, 139.3, 135.8, 135.6, 134.4, 133.6, 133.4, 133.3, 131.9, 131.7, 131.5, 131.4, 131.2, 131.0, 130.4, 130.2, 130.1, 129.9, 129.2, 128.9, 128.7, 128.6, 128.4, 128.2, 127.8, 127.6, 127.4, 127.3, 127.1, 126.8, 124.7, 124.5, 123.9, 123.8, 123.6. MS (APCl, *m/z*) Calcd for $C_{47}H_{35}NO$ $[M+H]^+$: 630.28, found: 630.28. The yield of E-TPB-TPA-CHO was 48%, and the yield of Z-TPB-TPA-CHO was 35%.

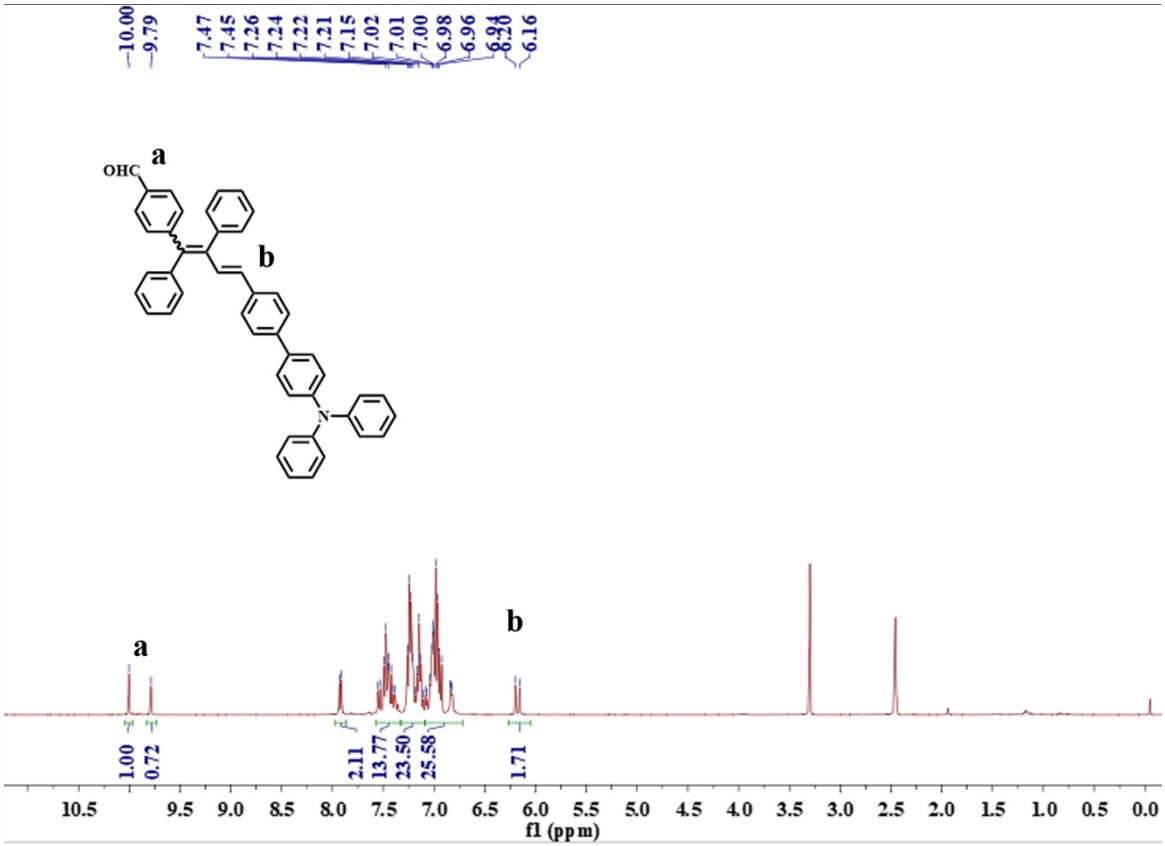

Figure S4. ^{1}H NMR spectrum of TPB-TPA-CHO in DMSO-d6.

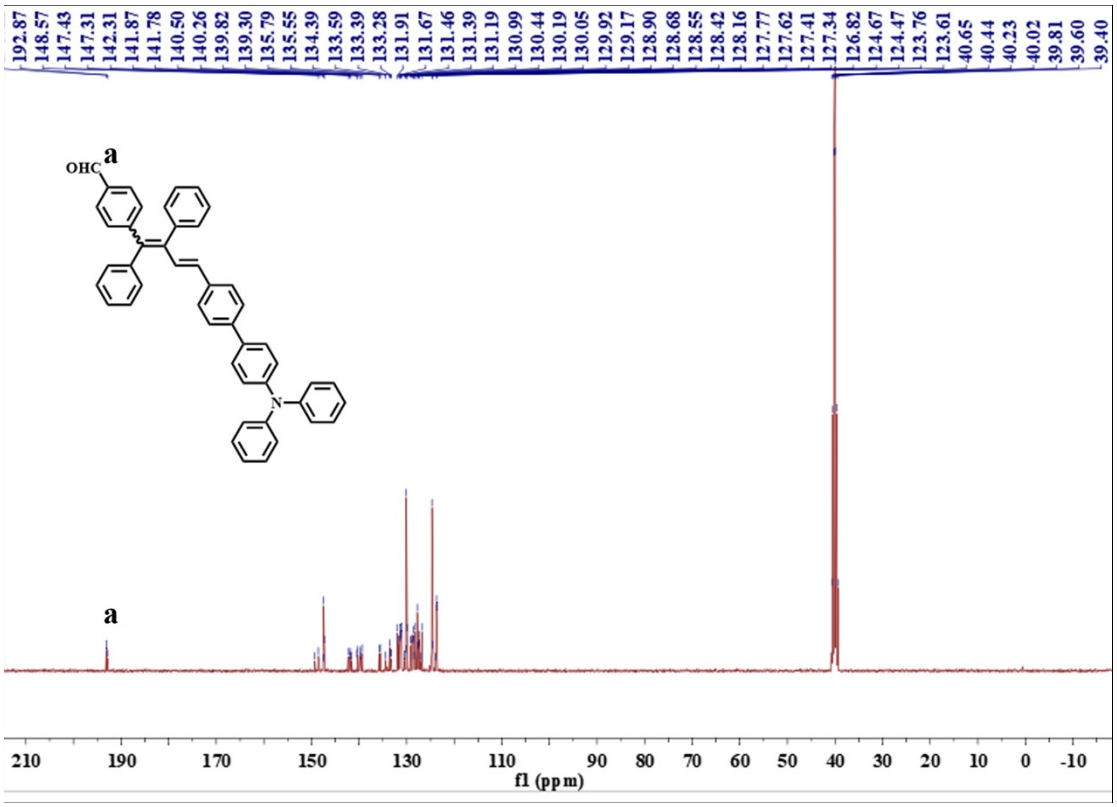

Figure S5. ^{13}C NMR spectrum of TPB-TPA-CHO in DMSO-d6.

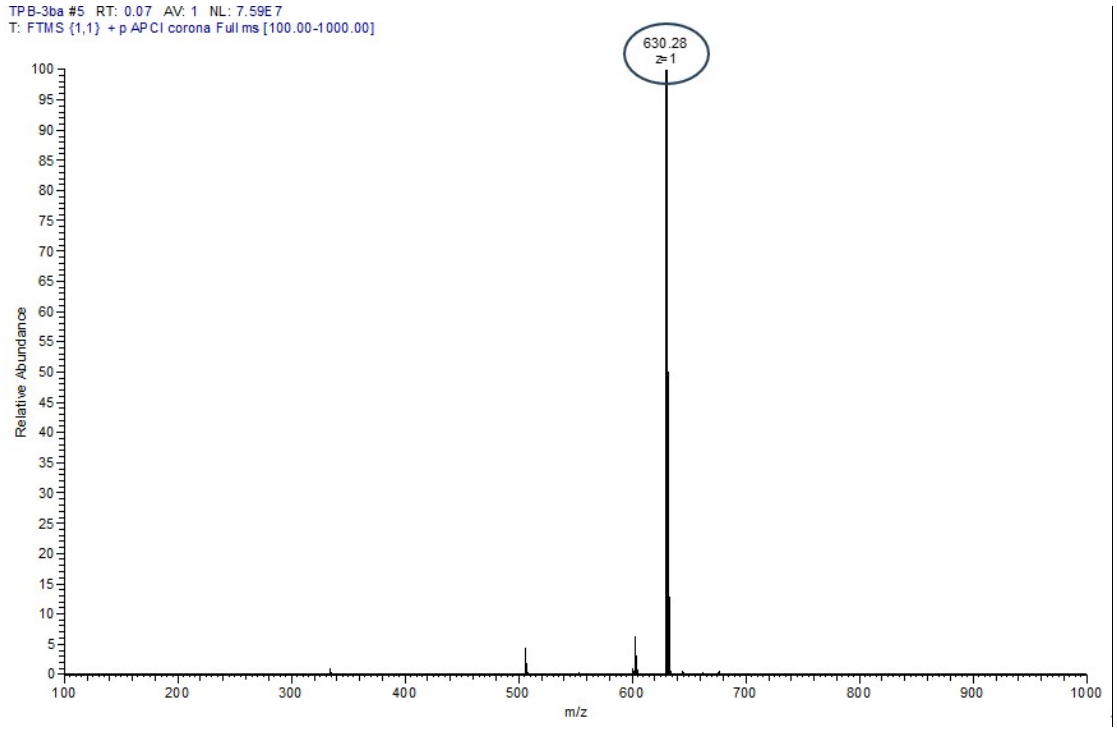

Figure S6. MS spectrum of TPB-TPA-CHO.

Synthesis of E/Z-TPB-OIY: 2-(3-Oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (0.146 g, 0.75 mmol), TPB-TPA-CHO (0.315 g, 0.5 mmol) and Piperidine (0.15 mL)

were added to a 50 mL round bottom flask and stirred at 45 ℃ for 24 h. After that, the solution was extracted with dichloromethane and washed with water. Later the organic layer was dried over anhydrous $MgSO_4$. The solvent was evaporated under reduced pressure and the residue was purified by silica gel column chromatography using a dichloromethane/petroleum ether mixture (1/2, V_d/V_p) as the eluent to give desired E-TPB-OIY with 10% yield and Z-TPB-OIY with 7% yield. E-TPB-OIY**:** ^{1}H NMR (400 MHz, DMSO): δ (ppm):8.78 (d, *J* = 5.1 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.54 (d, *J* = 8.7 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.41-7.19 (m, 14H), 7.17-7.13 (m, 3H), 7.09-7.00 (m, 12H), 6.85 (dd, *J* = 7.6, 1.7 Hz, 2H), 6.14 (d, *J* = 15.9 Hz, 1H), 5.63 (d, *J* = 4.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO): δ (ppm): 187.9, 160.6, 155.0, 147.4, 147.3, 142.8, 142.7, 142.5, 141.6, 140.1, 139.5, 139.1, 136.1, 135.2, 133.7, 132.2, 132.0, 131.5, 131.4, 130.9, 130.3, 130.1, 128.5, 128.0, 127.8, 127.4, 127.2, 126.7, 125.9, 124.6, 123.7, 123.7, 120.7, 120.5, 120.2, 110.9, 60.7, 52.4, 50.5, 40.6, 40.4, 40.2, 40.0, 39.8, 39.6, 39.4, 26.1, 24.0. MS (APCl, *m/z*) Calcd for $C_{59}H_{39}N_3O$ $[M+H]^+$: 806.32, found: 806.32.

Z-TPB-OIY**:** ^{1}H NMR (400 MHz, DMSO): δ (ppm): 8.63 (d, *J* = 5.2 Hz, 1H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.52 (dd, *J* = 13.4, 8.6 Hz, 4H), 7.38 (d, *J* = 9.4, 7.3, 4.2 Hz, 4H), 7.31-7.21 (m, 10H), 7.15 (d, *J* = 8.0 Hz, 3H), 7.01 (d, *J* = 15.0, 11.0, 6.8 Hz, 12H), 6.85 (d, *J* = 8.3 Hz, 2H), 6.12 (d, *J* = 15.9 Hz, 1H), 5.40 (d, *J* = 5.0 Hz, 1H). ^{13}C NMR (101 MHz, DMSO): δ (ppm): 187.8, 160.4, 154.9, 147.4, 147.3, 142.7, 142.3, 142.0, 140.1, 139.0, 132.1, 131.4, 131.3, 131.1, 130.9, 130.1, 128.7, 128.6, 128.1, 127.8, 127.4, 127.2, 126.8, 125.1, 124.7, 123.8, 123.6, 120.6, 60.6. MS (APCl, *m/z*) Calcd for $C_{59}H_{39}N_3O$ $[M+H]^+$: 806.32, found: 806.32.

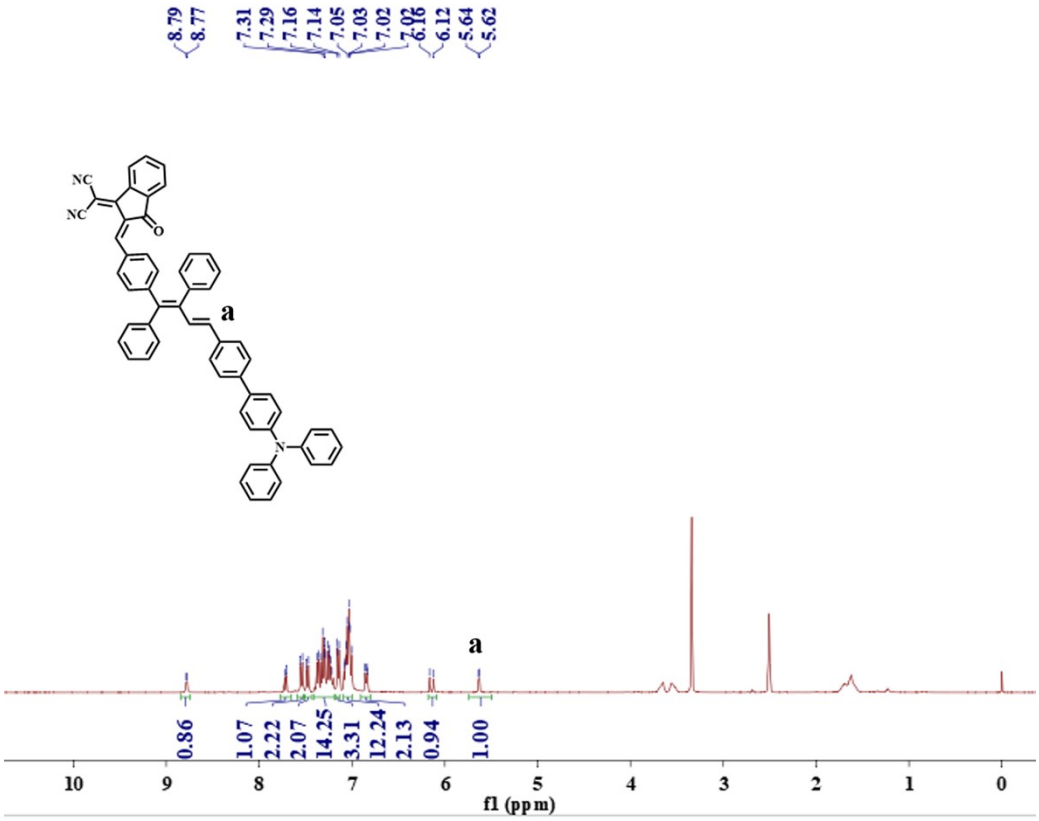

Figure S7. ^{1}H NMR spectrum of E-TPB-OIY in DMSO-d6.

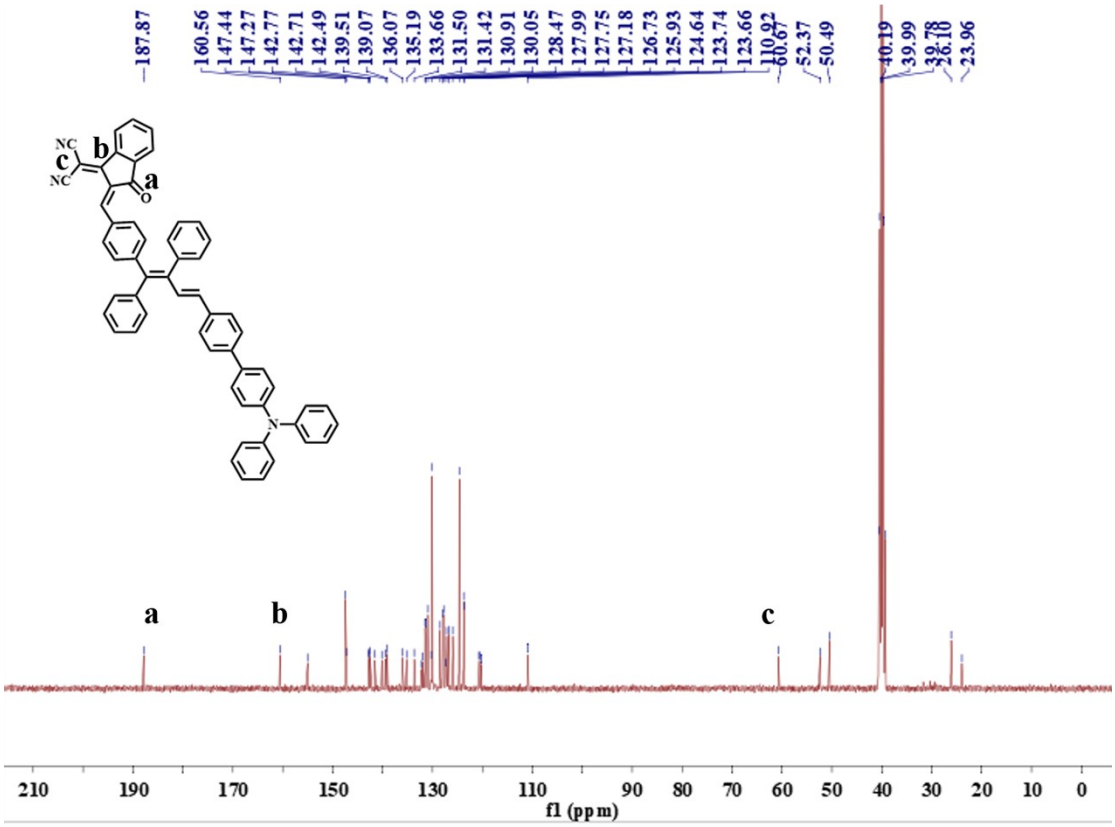

Figure S8. ^{13}C NMR spectrum of E-TPB-OIY in DMSO-d6.

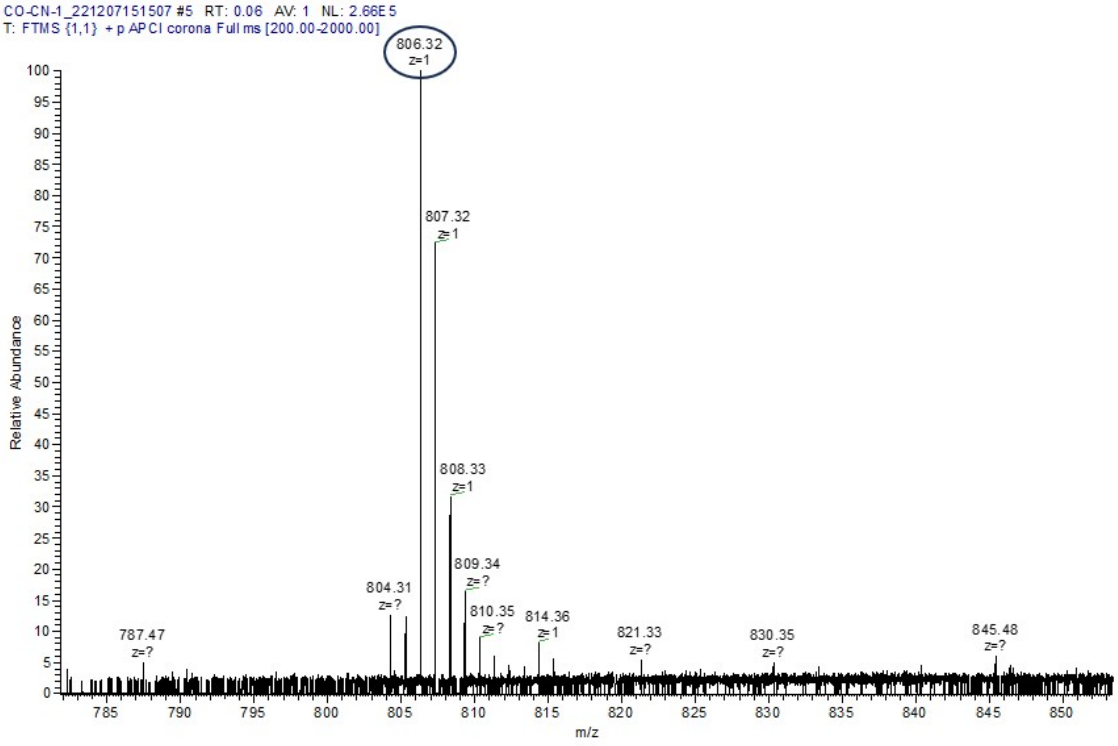

Figure S9. MS spectrum of E-TPB-OIY.

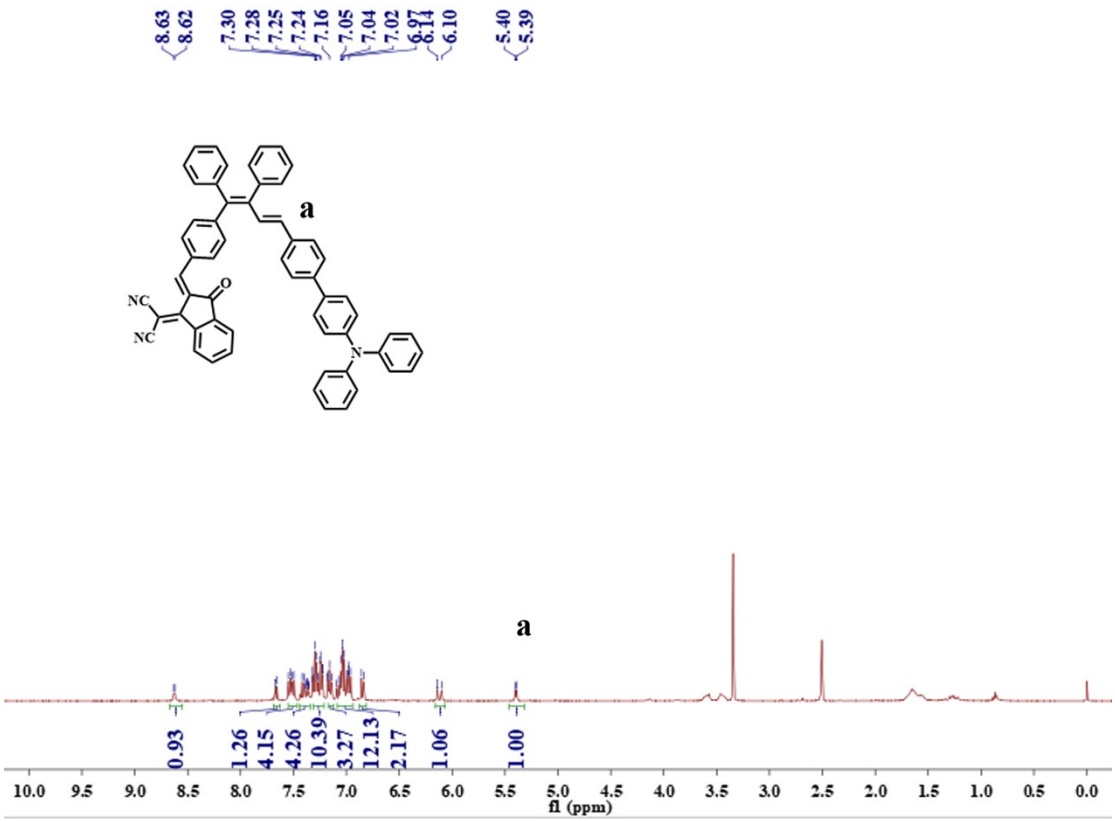

Figure S10. ^{1}H NMR spectrum of Z-TPB-OIY in DMSO-d6.

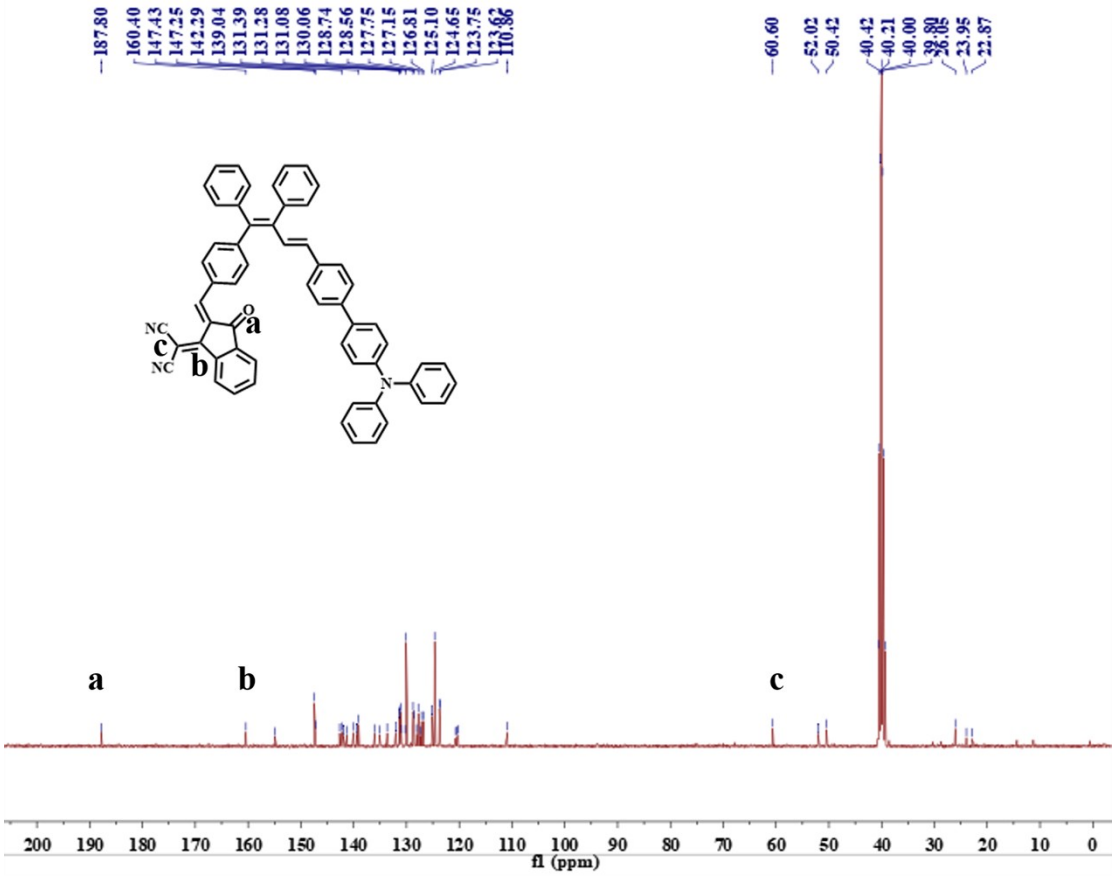

Figure S11. ^{13}C NMR spectrum of Z-TPB-OIY in DMSO-d6.

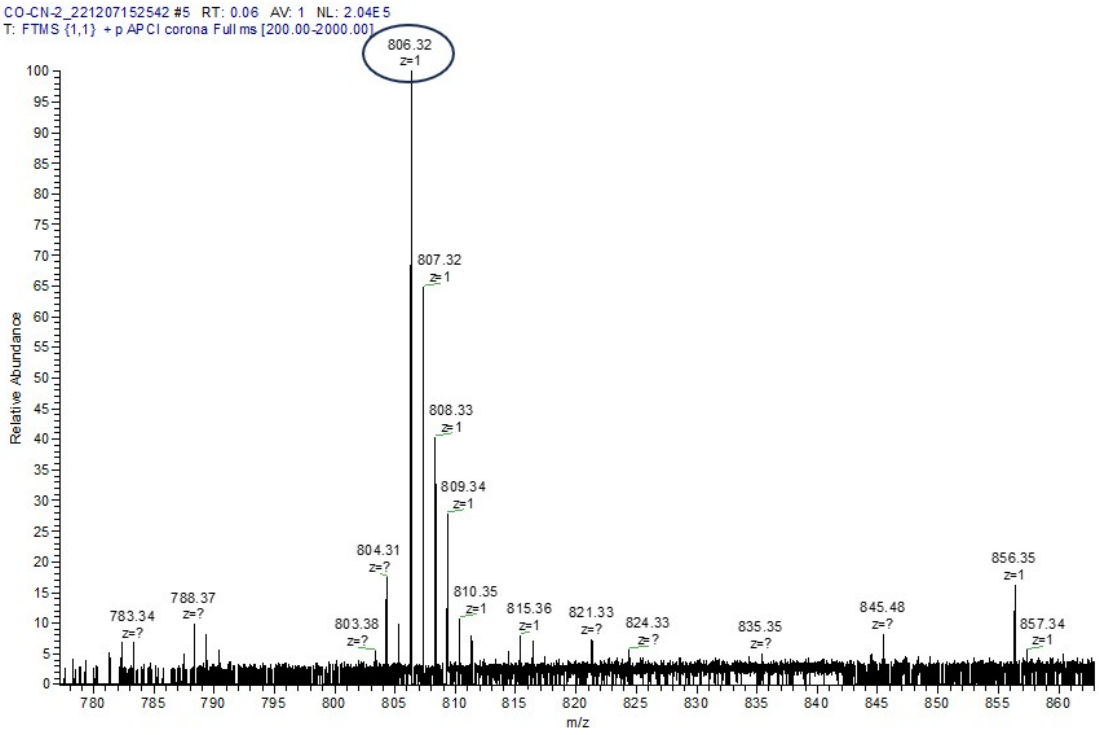

Figure S12. MS spectrum of Z-TPB-OIY.

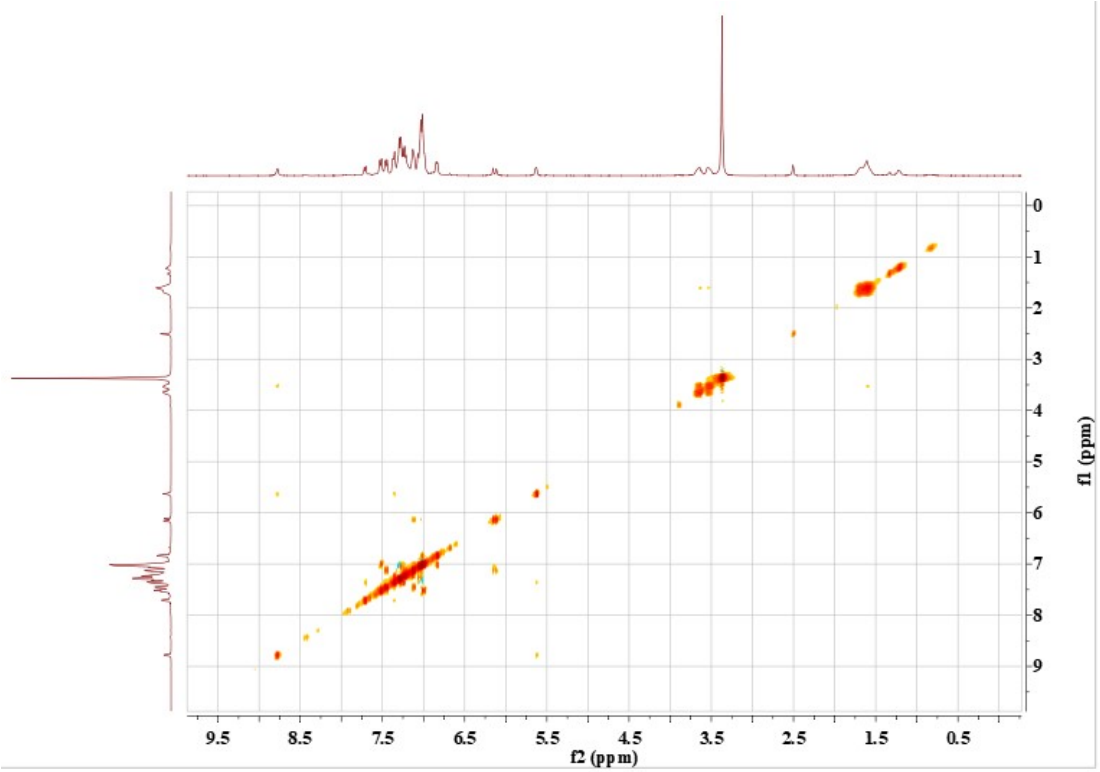

Figure S13. NOESY spectrum of E-TPB-OIY.

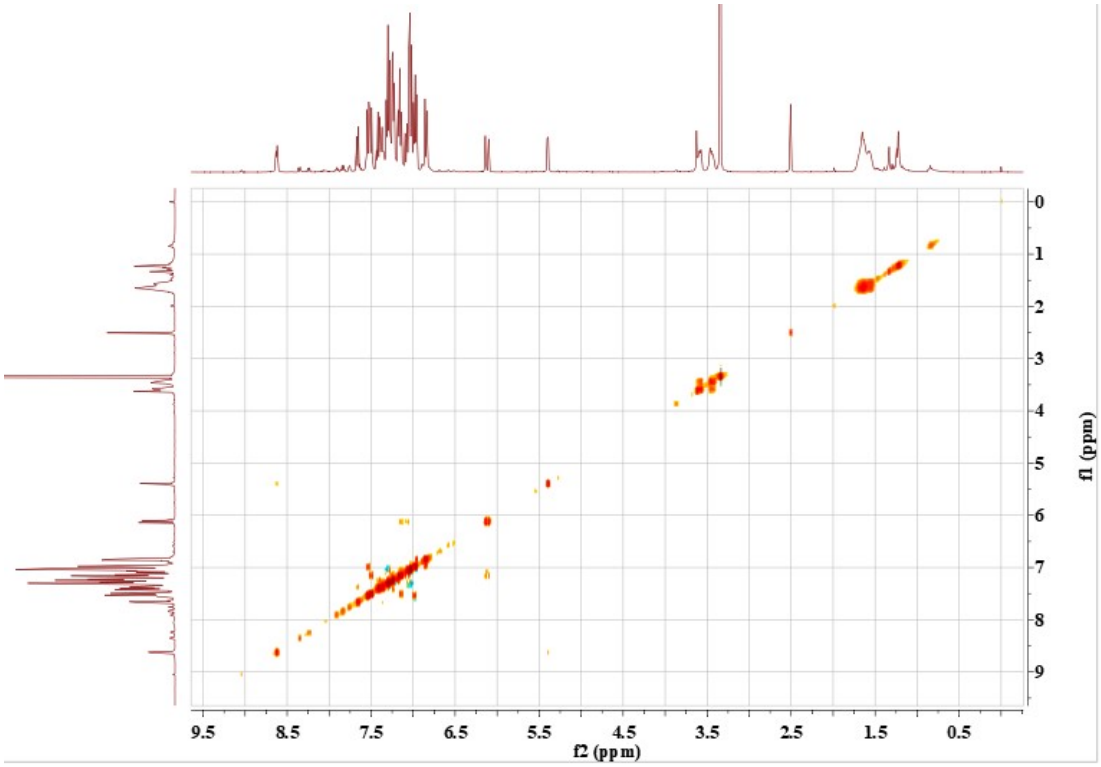

Figure S14. NOESY spectrum of Z-TPB-OIY.

Synthesis of E/Z-TPB-CTY: Following a similar synthetic procedure to that described for E/Z-TPB-OIY, and only using 2-(3-Cyano-4,5,5-trimethylfuran-2-ylidene)propanedinitrile instead of 2-(3-Oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile. E-TPB-CTY was obtained with 15% yield, and Z-TPB-CTY was obtained with 8% yield.

E-TPB-CTY**:** ^{1}H NMR (400 MHz, DMSO): δ (ppm): 7.95 (d, *J* = 3.7 Hz, 1H), 7.92 (d, *J* = 4.3 Hz, 1H), 7.51 (dd, *J* = 8.4, 5.5 Hz, 4H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.24 (dt, *J* = 17.7, 7.7 Hz, 10H), 7.16-7.10 (m, 3H), 7.05-6.91 (m, 12H), 6.84 (dd, *J* = 7.4, 2.0 Hz, 2H), 6.19 (d, *J* = 15.9 Hz, 1H), 1.77 (s, 6H). ^{13}C NMR (101 MHz, DMSO): δ (ppm): 177.6, 175.5, 147.4, 147.3, 146.4, 142.5, 142.1, 140.2, 140.0, 139.3, 135.9, 134.1, 133.6, 133.3, 132.1, 131.5, 131.1, 130.5, 130.1, 129.9, 128.6, 128.1, 127.8, 127.6, 127.4, 146.9, 124.7, 123.8, 123.6, 116.1, 113.2, 112.3, 111.4, 100.0, 99.9, 55, 25.6. MS (APCl, *m/z*) Calcd for $C_{58}H_{42}N_4O$ $[M+H]^+$: 811.34, found: 811.34. Z-TPB-CTY**:** ^{1}H NMR (400 MHz, DMSO): δ (ppm): 7.78 (d, *J* = 16.4 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.56 (t, *J* = 7.3 Hz, 4H), 7.50-7.40 (m, 3H), 7.36-7.20 (m, 12H), 7.17-6.76 (m, 13H), 6.23 (d, *J* = 16.0 Hz, 1H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, DMSO): δ (ppm): 177.6, 175.5, 147.4, 147.3, 142.1, 141.8, 140.4, 139.9, 139.3, 135.9, 133.6, 133.2, 132.9, 131.9, 131.5, 131.3, 130.7, 130.1, 129.2, 128.9, 128.8, 128.5, 127.8, 127.4, 126.9, 124.7, 123.8, 123.6, 115.6, 113.2, 112.3, 111.3, 99.8, 99.6, 54.8, 25.5. MS (APCl, *m/z*) Calcd for $C_{58}H_{42}N_4O$ $[M+H]^+$: 811.34, found: 811.34.

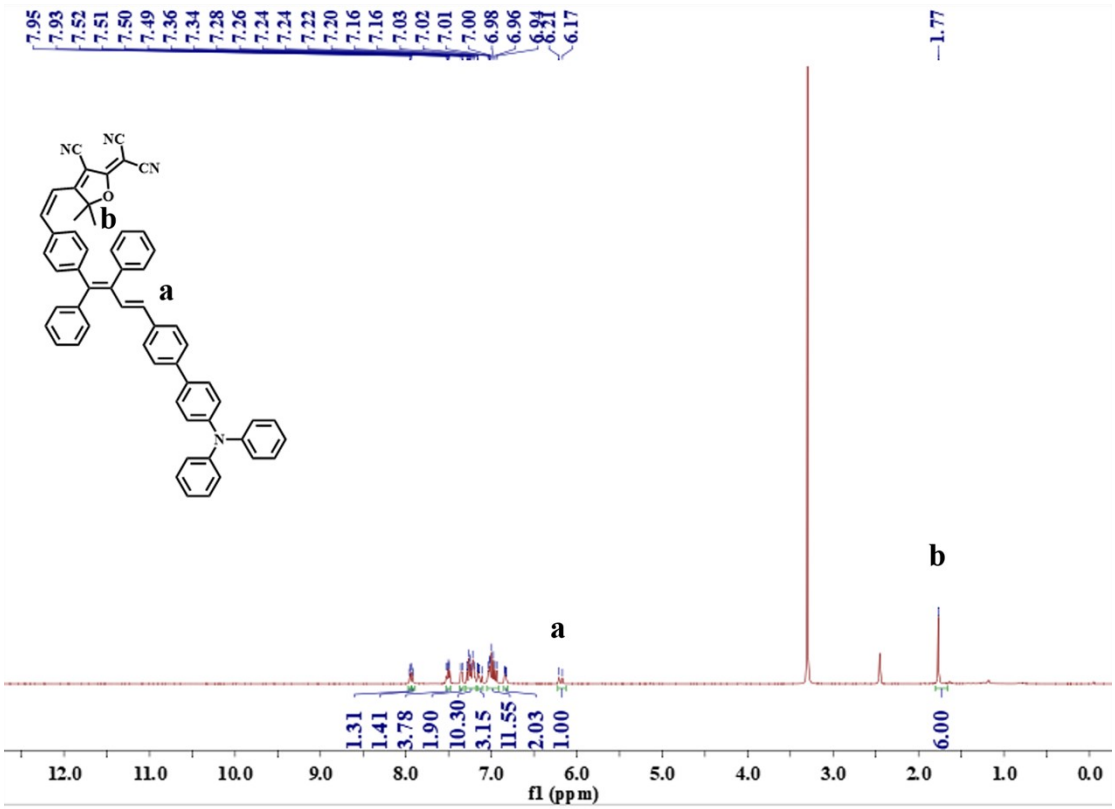

Figure S15. [1]H NMR spectrum of E-TPB-CTY in DMSO-d6.

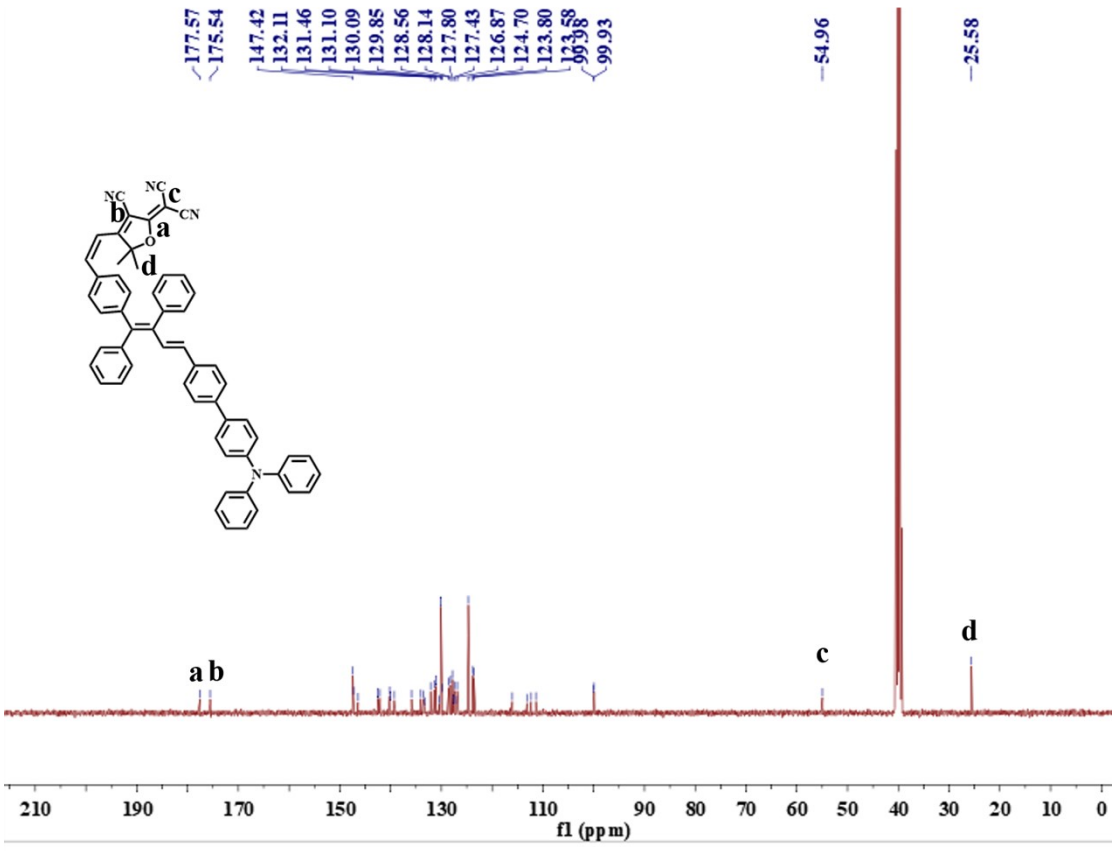

Figure S16. [13]C NMR spectrum of E-TPB-CTY in DMSO-d6.

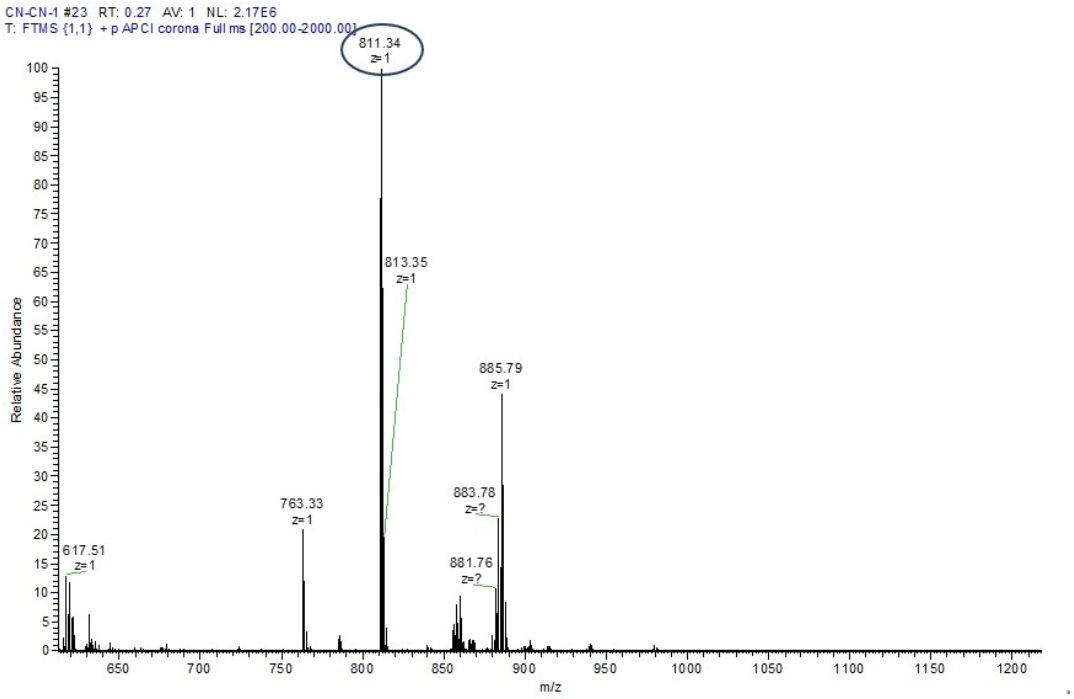

Figure S17. MS spectrum of **E-TPB-CTY**.

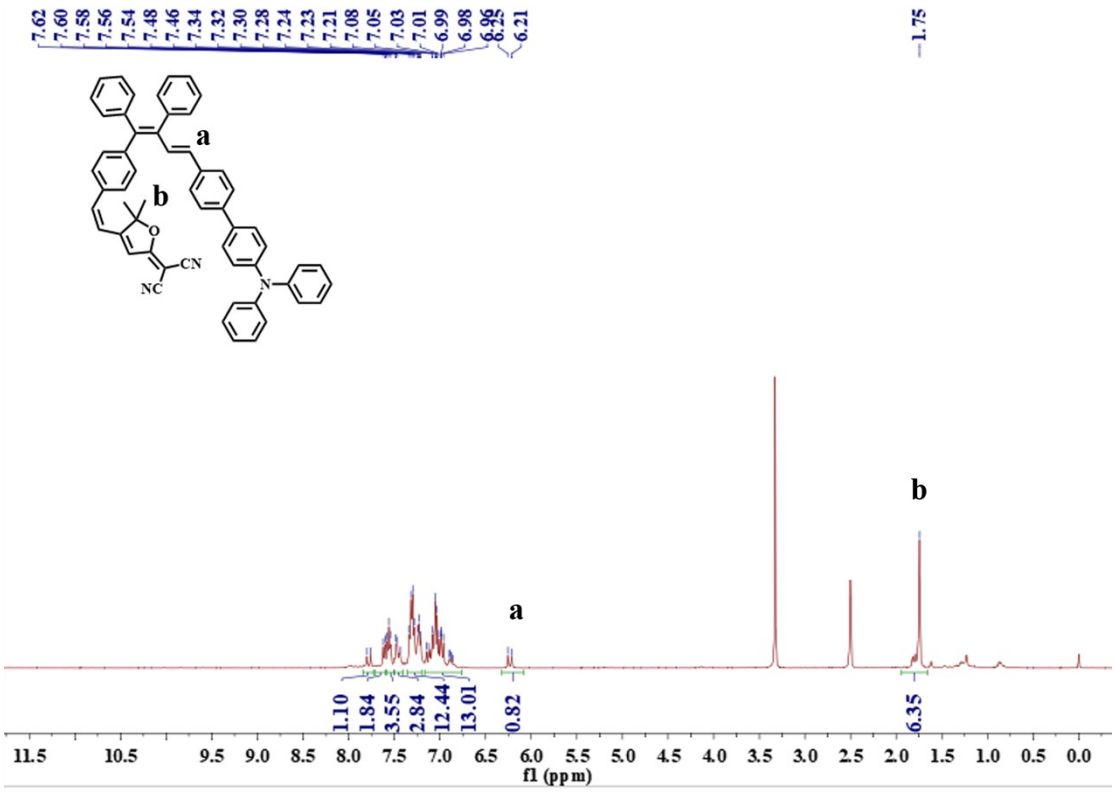

Figure S18. ^{1}H NMR spectrum of Z-TPB-CTY in DMSO-d6.

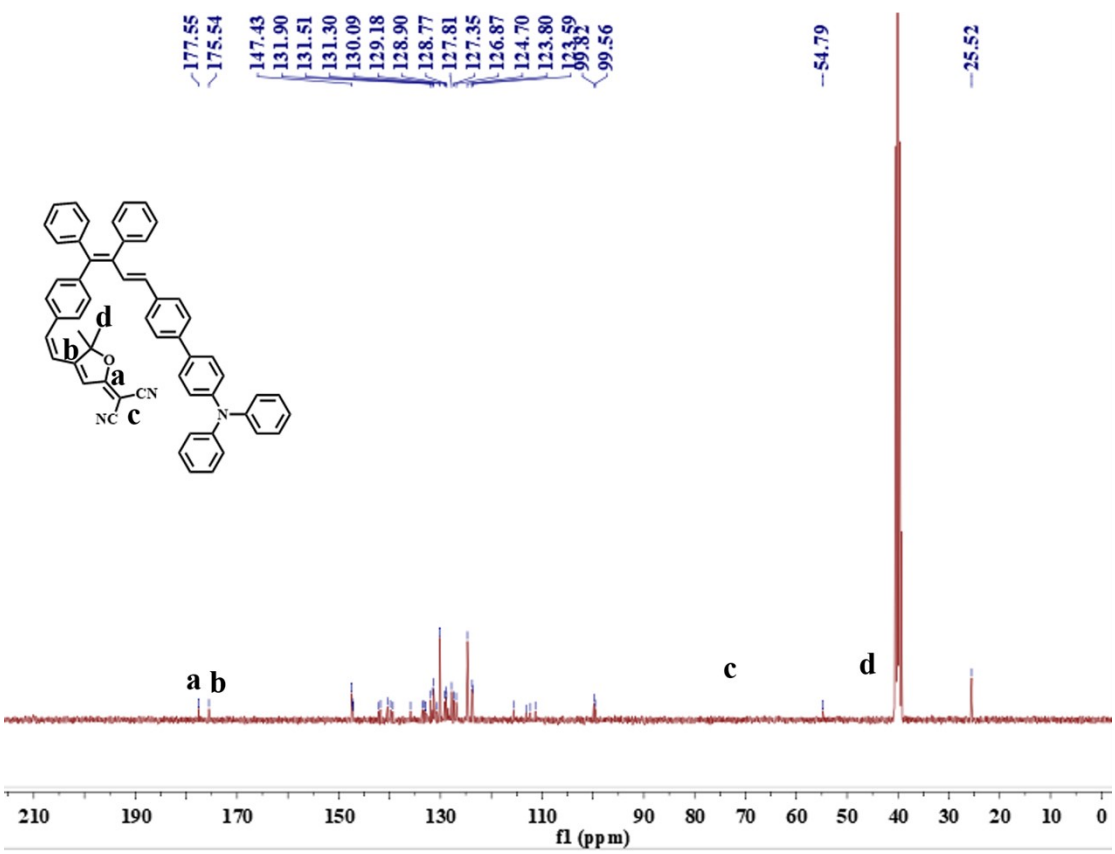

Figure S19. ^{13}C NMR spectrum of Z-TPB-CTY in DMSO-d6.

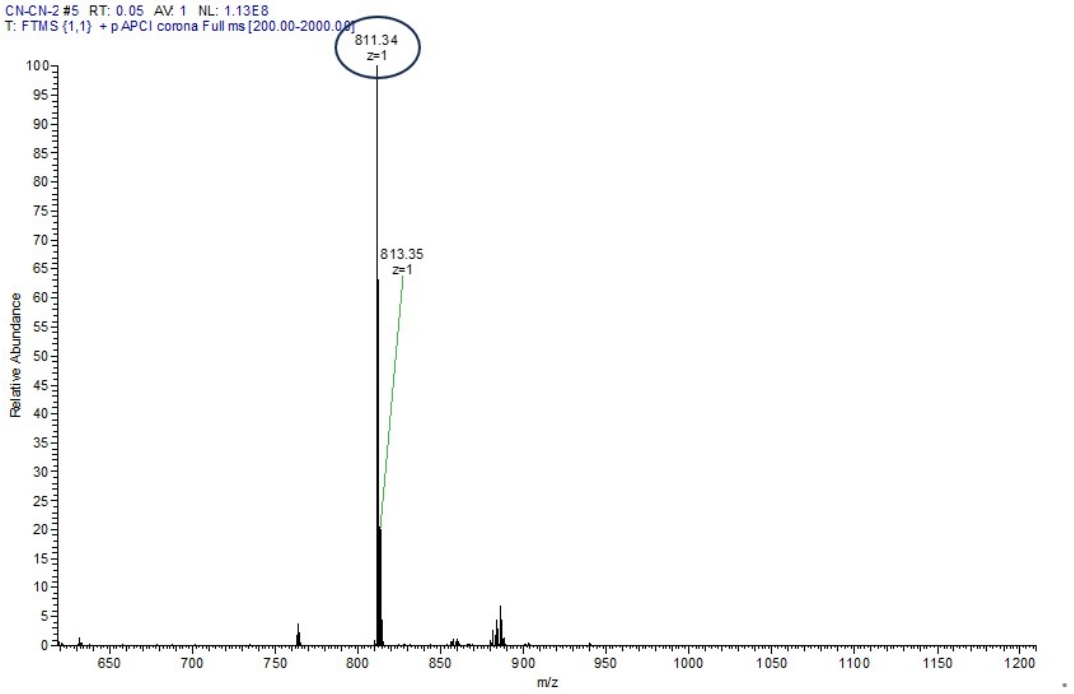

Figure S20. MS spectrum of Z-TPB-CTY.

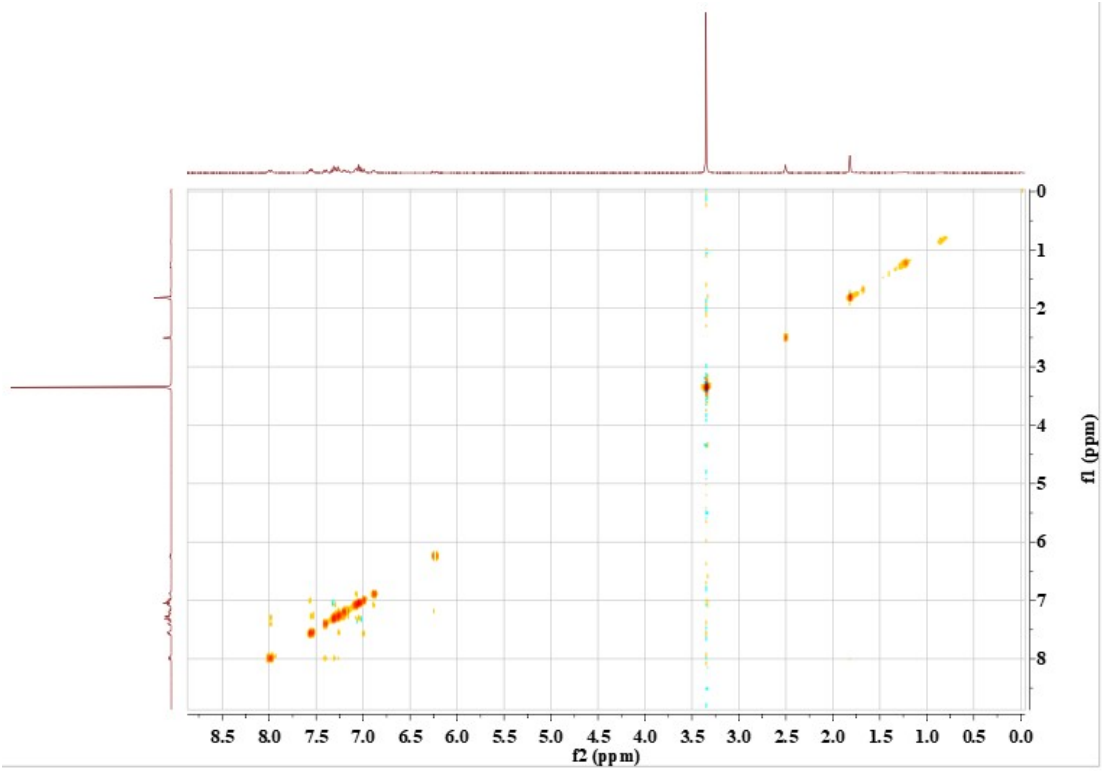

Figure S21. NOESY spectrum of E-TPB-CTY.

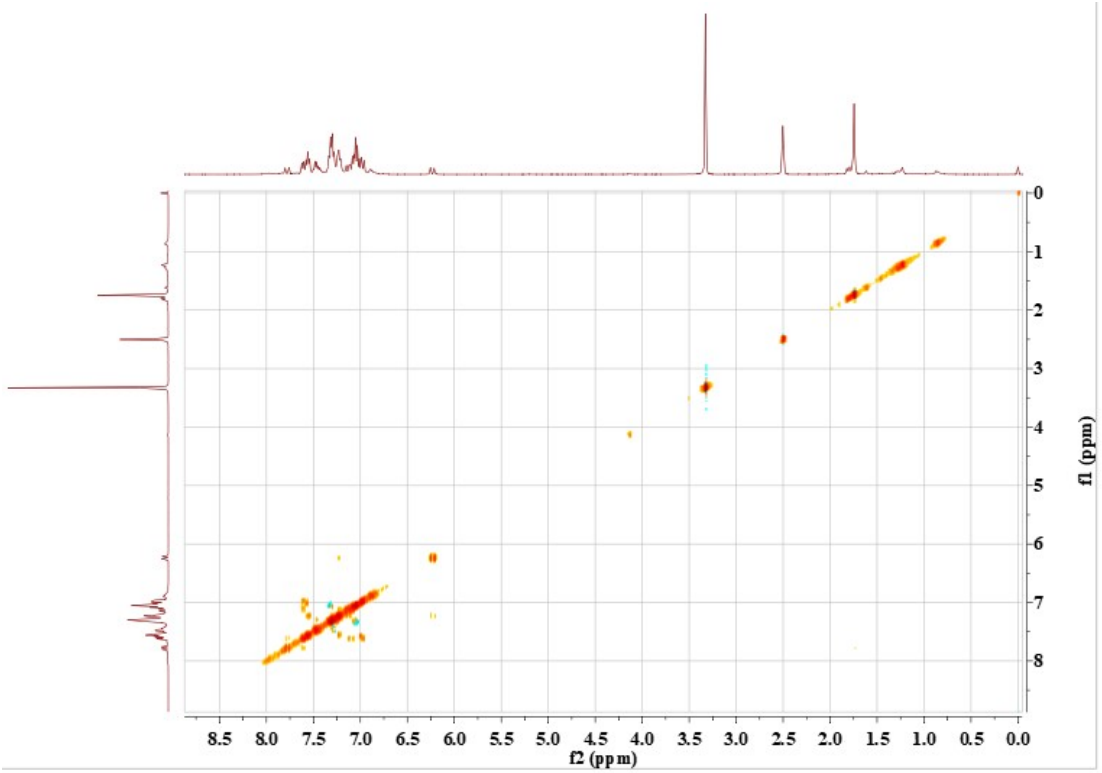

Figure S22. NOESY spectrum of Z-TPB-CTY.

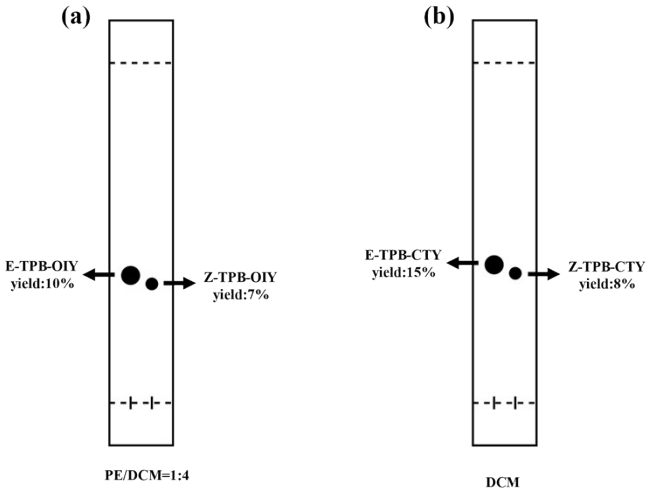

Figure S23. TLC of (a)E/Z-TPB-OIY and (b)E/Z-TPB-CTY.

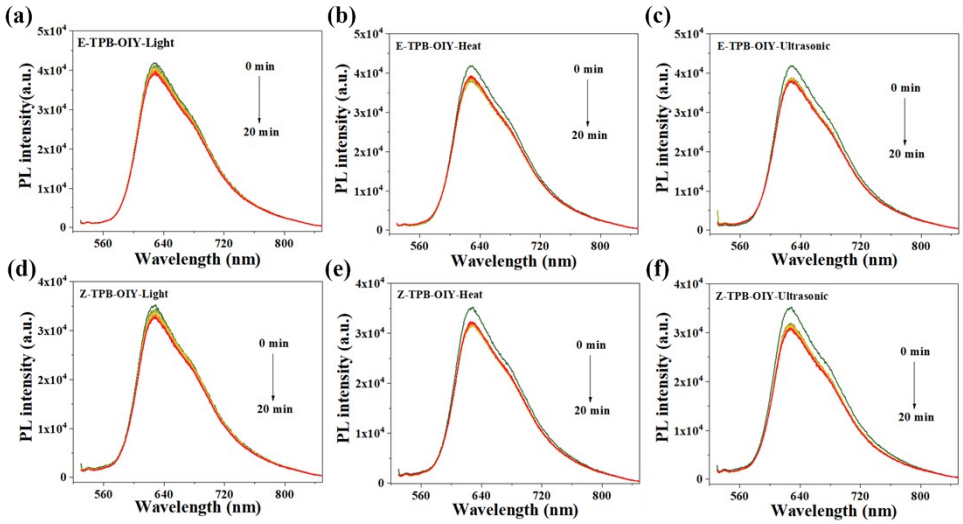

Figure S24. Stability test of E/Z-TPB-OIY. (a) and (d) fluorescence spectra of E/Z-TPB-OIY light treatment for 20 min. (b) and (e) fluorescence spectra of E/Z-TPB-OIY heating treatment for 20 min. (c) and (f) fluorescence spectra of E/Z-TPB-OIY ultrasonic treatment for 20 min.

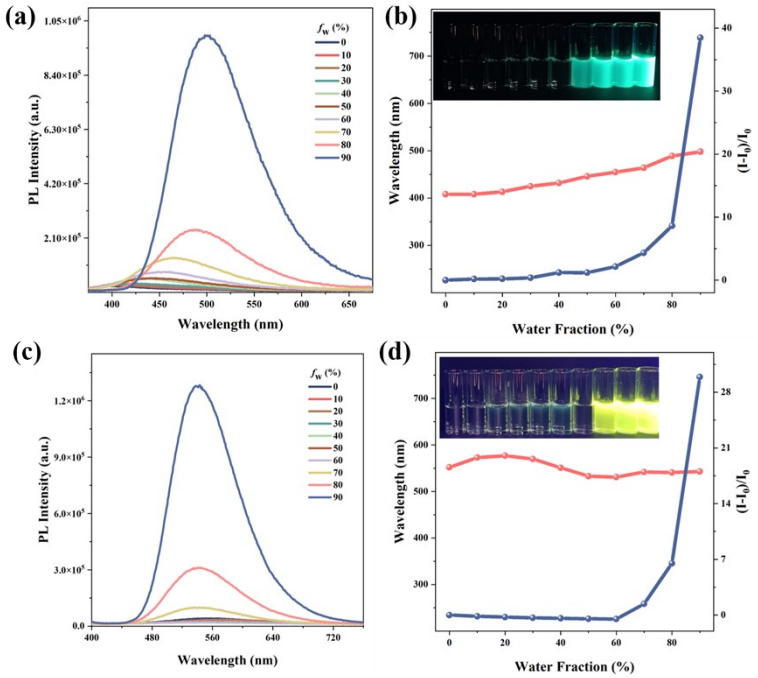

Figure S25. (a) PL spectra of TPB-Br-CHO in DMSO/water mixtures. (b) Correlation between the net change in PL intensity $[(I-I_0)/I_0]$, and the wavelength of TPB-Br-CHO with different water fractions. Inset: fluorescence photographs of solutions or suspensions of TPB-Br-CHO with different fractions of water. (c) PL spectra of TPB-TPA-CHO in DMSO/water mixtures. (d) Correlation between the net change in PL intensity $[(I-I_0)/I_0]$, and the wavelength of TPB-TPA-CHO with different water fractions. Inset: fluorescence photographs of solutions or suspensions of TPB-TPA-CHO with different fractions of water. [TPB-Br-CHO] = [TPB-TPA-CHO] = 1.0×10^{-5} mol L^{-1}. (λ_{ex} = 360 nm)

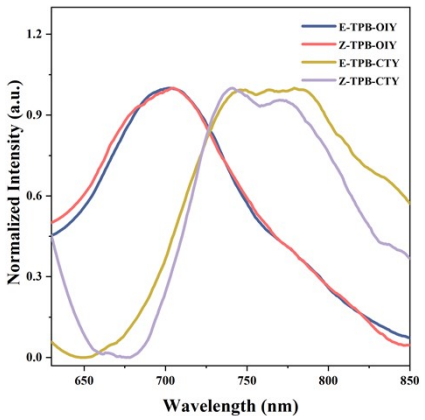

Figure S26. Normalized PL of E/Z-TPB-OIY and E/Z-TPB-CTY in solid.

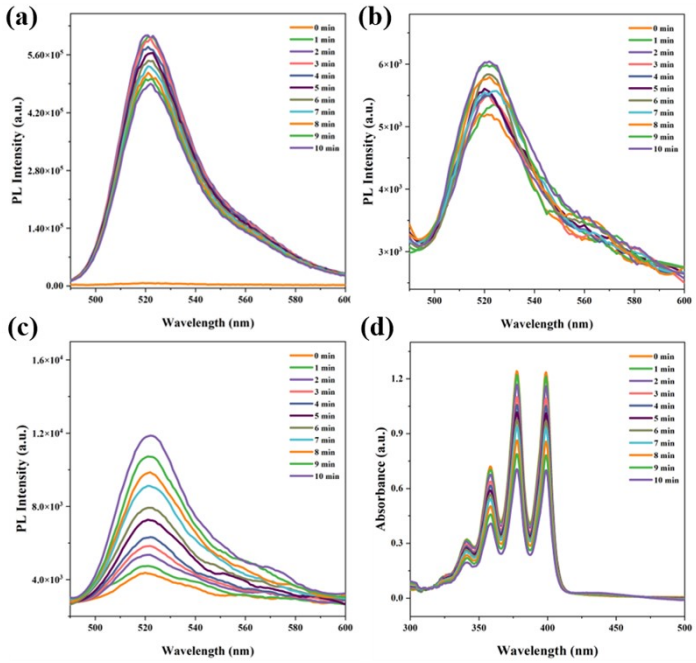

Figure S27. PL spectra of (a) E-TPB-OIY with DCFH in PBS solution under white light irradiation (2 mW cm^{-2}), (b) E-TPB-OIY with DCFH in PBS solution at dark and (c) only DCFH in PBS solution under white light irradiation (2 mW cm^{-2}). (d) UV absorption spectra of E-TPB-OIY with ABDA in PBS solution under white light irradiation (2 mW cm^{-2}).

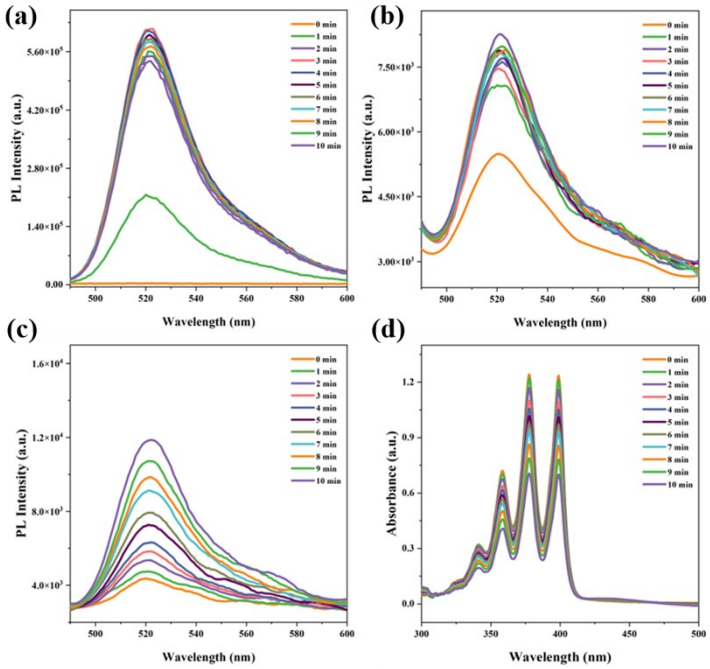

Figure S28. PL spectra of (a) Z-TPB-OIY with DCFH in PBS solution under white light irradiation (2 mW cm^{-2}), (b) Z-TPB-OIY with DCFH in PBS solution at dark and (c) only DCFH in PBS solution under white light irradiation (2 mW cm^{-2}). (d) UV absorption spectra of Z-TPB-OIY with ABDA in PBS solution under white light irradiation (2 mW cm^{-2}).

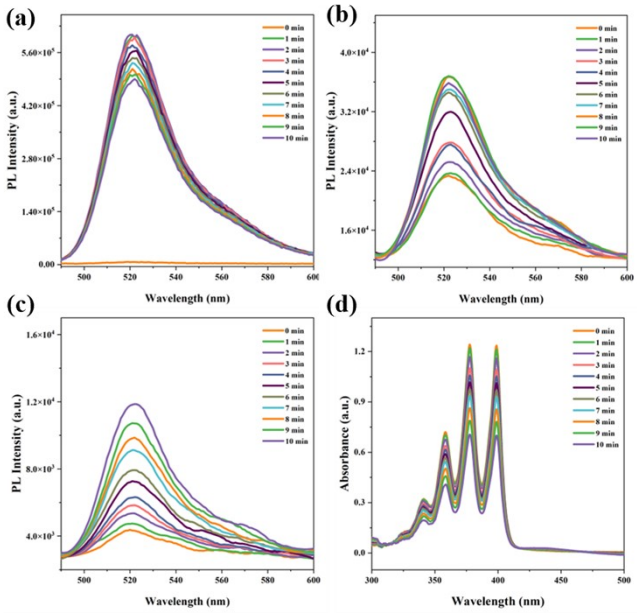

Figure S29. PL spectra of (a) E-TPB-CTY with DCFH in PBS solution under white light irradiation (2 mW cm^{-2}), (b) E-TPB-CTY with DCFH in PBS solution at dark and (c) only DCFH in PBS solution under white light irradiation (2 mW cm^{-2}). (d) UV absorption spectra of E-TPB-CTY with ABDA in PBS solution under white light irradiation (2 mW cm^{-2}).

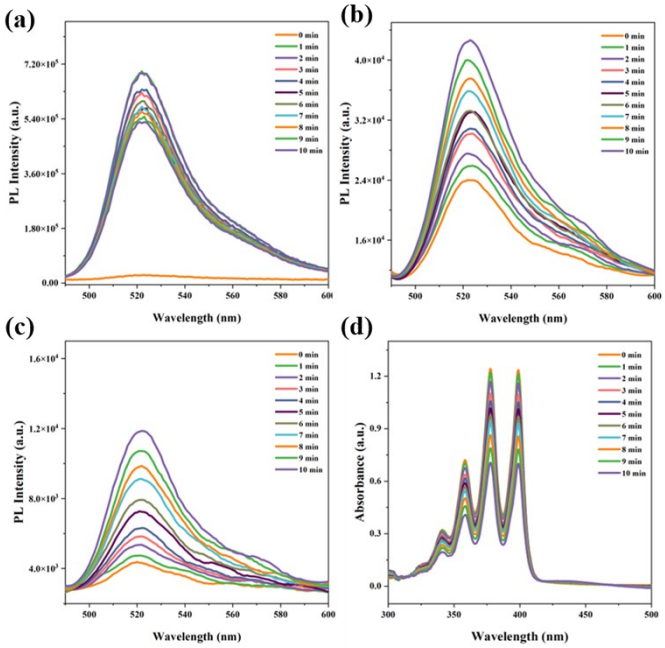

Figure S30. PL spectra of (a) Z-TPB-CTY with DCFH in PBS solution under white light irradiation (2 mW cm^{-2}), (b) Z-TPB-CTY with DCFH in PBS solution at dark and (c) only DCFH in PBS solution under white light irradiation (2 mW cm^{-2}). (d) UV absorption spectra of Z-TPB-CTY with ABDA in PBS solution under white light irradiation (2 mW cm^{-2}).

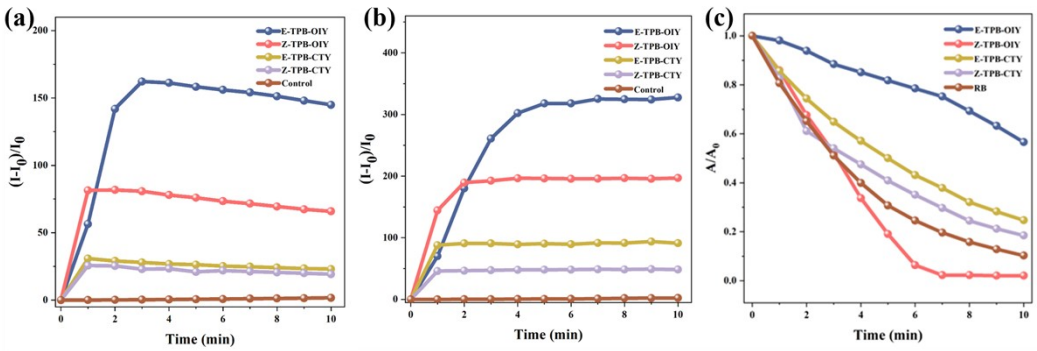

Figure S31. Fluorescence intensity net change $[(I-I_0)/I_0]$ (a) at 532 nm for the DCFH indicator and (b) at 530 nm for the DHR123 indicator with E/Z-TPB-OIY and E/Z-TPB-CIY upon white light irradiation (2 mW cm^{-2}). (c) Absorbance intensity change (A/A_0) for the ABDA indicator with E/Z-TPB-OIY and E/Z-TPB-CIY upon white light irradiation (2 mW cm^{-2})

Table S1. The ROS ($^1O_2$) quantum yield of **E/Z-TPB-OIY**

Probe	K_{Probe}	A_{Probe}	Φ_{Probe}
E-TPB-OIY	**0.05**	**3.09**	**0.57**
Z-TPB-OIY	**0.43**	**3.05**	**4.67**
RB	**0.23**	**10.1**	**0.75**

$$\Phi_{probe} = \Phi_{Rose\ Bengal} \times \frac{K_{probe} \times A_{Rose\ Bengal}}{K_{Rose\ Bengal} \times A_{Rose\ Bengal}}$$

K_{Probe}: The slope of the linear fitting equation of the compound; $K_{Rose\ Bengal}$: The slope of the linear fitting equation for Rose Bengal; A_{Probe} : UV absorption spectrum peak area of E-TPB-OIY and Z-TPB-OIY; $A_{Rose\ Bengal}$: Rose Bengal UV absorption spectrum peak area

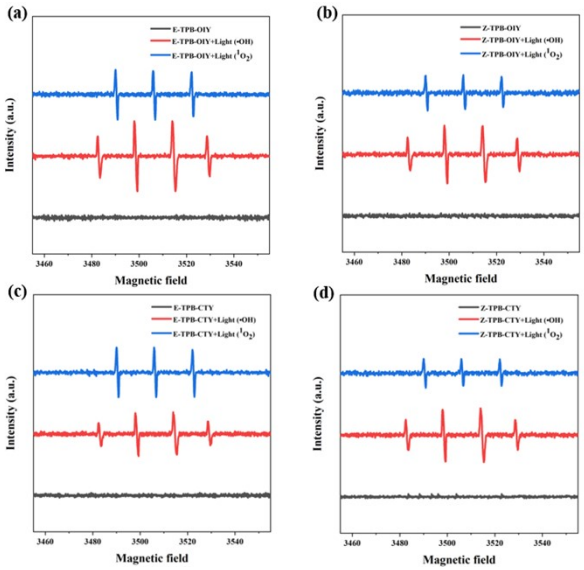

Figure S32. ESR spectra of DMPO/•OH and DMPO/$^1O_2$ for (a)(b) E/Z-TPB-OIY and (c)(d) E/Z-TPB-CIY.

Table S2. Energy levels and energy gaps of E-TPB-OIY and Z-TPB-OIY.

	LUMO (eV)	HOMO (eV)	Eg (eV)
E-TPB-OIY	-3.076	-4.950	1.874
Z-TPB-OIY	-3.133	-4.907	1.774

Table S3. Based on the optimized S_0 structure, the energy levels and oscillator strengths of E/Z-TPB-OIY were calculated by TD-DFT.

	States	Energy (eV)	Oscillator strengths	States	Energy (eV)
E-TPB-OIY	S_1	1.8778	1.4685	T_1	0.9506
	S_2	2.7620	0.0729	T_2	1.8777
	S_3	2.8517	0.1493	T_3	2.3204
	S_4	2.9702	0.0776	T_4	2.4862
	S_5	3.1661	0.1243	T_5	2.5664
Z-TPB-OIY	S_1	2.0862	1.1544	T_1	1.2817
	S_2	2.8584	0.2805	T_2	1.9778
	S_3	2.9673	0.2829	T_3	2.4366
	S_4	3.0916	0.3360	T_4	2.6146
	S_5	3.3818	0.2907	T_5	2.6714

Table S4. SOC constants (ξ) between singlet and triplet states of E/Z-TPB-OIY.

	Energy levels	SOC constants
E-TPB-OIY	ξ (S_1-T_1)	0.059 cm^{-1}
	ξ (S_1-T_2)	0.471 cm^{-1}
	ξ (S_1-T_3)	0.590 cm^{-1}
	ξ (S_1-T_4)	0.214 cm^{-1}
	ξ (S_1-T_5)	0.352 cm^{-1}
Z-TPB-OIY	ξ (S_1-T_1)	0.095 cm^{-1}
	ξ (S_1-T_2)	0.770 cm^{-1}
	ξ (S_1-T_3)	0.162 cm^{-1}
	ξ (S_1-T_4)	0.150 cm^{-1}
	ξ (S_1-T_5)	0.251 cm^{-1}

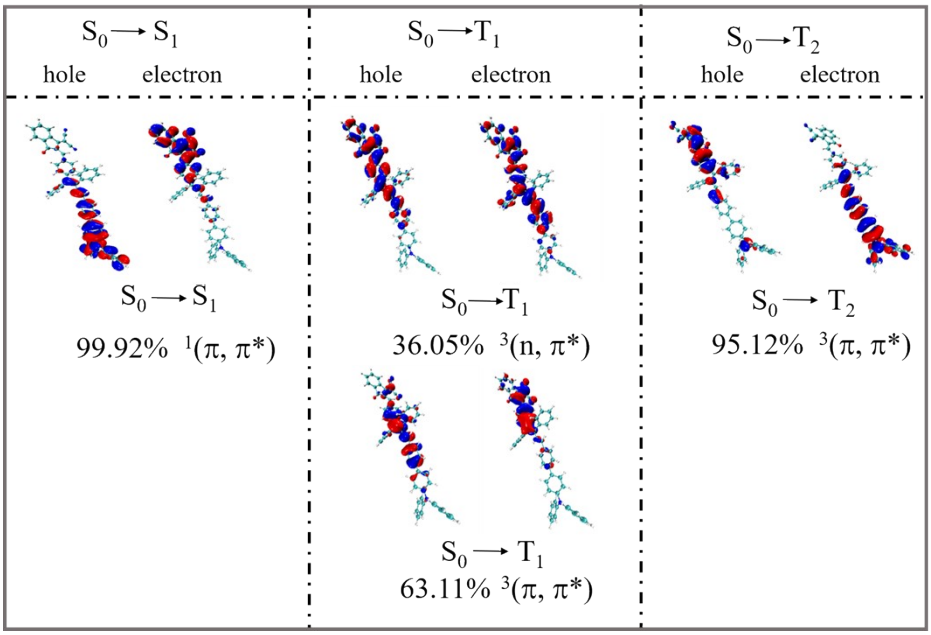

Figure S33. Natural transition orbital (NTO) distributions of S_1, lower-lying T_1, and T_2 for E-TPB-OIY.

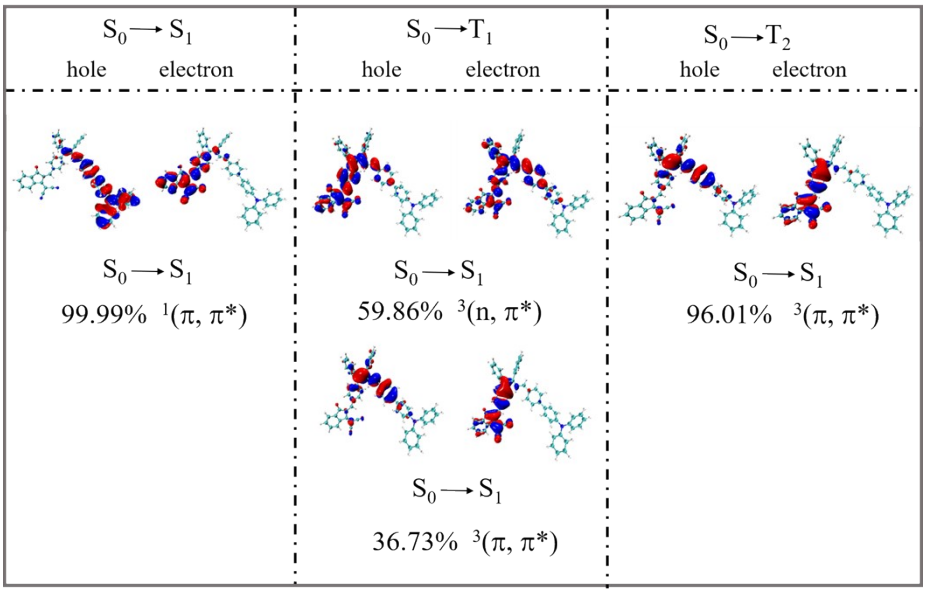

Figure S34. NTO distributions of S_1, lower-lying T_1, and T_2 for Z-TPB-OIY.

Table S5. Geometry Data for E-TPB-OIY

	X	Y	Z
C	-5.92723	-0.47665	0.261976
C	-4.54838	-0.34601	0.244431
C	-3.91863	0.909658	0.107112
C	-4.74906	2.045754	0.000802
C	-6.12672	1.921911	-0.0039
C	-6.76131	0.66009	0.132917
C	-8.20687	0.688628	0.111729
C	-2.44376	1.064182	0.13527
C	-1.94344	2.214702	0.945597
C	-1.5794	0.220226	-0.52931
C	-2.06963	-0.76769	-1.53976
C	-0.14234	0.277222	-0.28432
C	0.816365	-0.28466	-1.06098
C	2.256498	-0.26187	-0.82395
C	-2.38254	2.397386	2.269595
C	-1.93306	3.474187	3.030723
C	-1.0473	4.403216	2.479942
C	-0.61361	4.244871	1.163049
C	-1.05627	3.161656	0.403996
C	-1.78143	-2.13736	-1.41436
C	-2.24055	-3.05212	-2.36091
C	-2.97979	-2.61284	-3.46112
C	-3.25711	-1.2529	-3.60702
C	-2.80747	-0.33948	-2.65443
C	3.112296	-0.84828	-1.7766
C	4.491422	-0.8559	-1.61022
C	5.090415	-0.2754	-0.4786

C	4.2362	0.31093	0.47645
C	2.858955	0.31733	0.312005
C	7.434104	-0.17218	-1.39107
C	8.81396	-0.18581	-1.22666
C	9.381113	-0.29354	0.054462
C	8.517151	-0.39437	1.158015
C	7.138817	-0.39524	0.980313
C	6.559066	-0.28062	-0.29566
N	10.78733	-0.30024	0.228913
C	11.3836	-1.14646	1.205451
C	11.6121	0.538296	-0.57229
C	11.24333	1.868828	-0.82705
C	12.05242	2.682722	-1.61721
C	13.24733	2.194354	-2.14943
C	13.62131	0.874591	-1.88907
C	12.80979	0.047209	-1.11558
C	12.41839	-0.66738	2.024303
C	13.00875	-1.50238	2.970686
C	12.56886	-2.81782	3.13044
C	11.53415	-3.29422	2.322957
C	10.95006	-2.47277	1.360973
C	-9.21451	-0.23481	0.262233
C	-9.11738	-1.68449	0.619754
C	-10.5042	-2.16126	0.821164
C	-11.4145	-1.11962	0.576509
C	-10.6548	0.091242	0.177099
O	-8.12367	-2.38735	0.749904
C	-11.2406	1.273093	-0.23799
C	-10.906	-3.43531	1.20083
C	-12.2721	-3.67535	1.347641
C	-13.194	-2.64667	1.114311
C	-12.7856	-1.36763	0.727782
C	-10.5297	2.426575	-0.69672
N	-10.0055	3.39336	-1.08239
C	-12.6563	1.474526	-0.27799
N	-13.8005	1.688104	-0.32551
H	-6.37968	-1.45077	0.384751
H	-3.93677	-1.23399	0.352892
H	-4.29847	3.027848	-0.09512
H	-6.74012	2.811798	-0.11707
H	-8.5597	1.698807	-0.05741
H	0.158228	0.828264	0.600806
H	0.510262	-0.80267	-1.96671
H	-3.07518	1.681833	2.702332
H	-2.27588	3.589483	4.054874
H	-0.70258	5.24636	3.071241
H	0.065897	4.968244	0.721764
H	-0.72333	3.047911	-0.62286

H	-1.20343	-2.48275	-0.56258
H	-2.02072	-4.1088	-2.23892
H	-3.33427	-3.3251	-4.20029
H	-3.82424	-0.90108	-4.46384
H	-3.02648	0.717331	-2.77025
H	2.678641	-1.3132	-2.65835
H	5.113578	-1.34357	-2.35441
H	4.665735	0.791718	1.350084
H	2.24339	0.786241	1.073155
H	7.027571	-0.06152	-2.39174
H	9.461926	-0.10333	-2.09243
H	8.933221	-0.48168	2.155754
H	6.49935	-0.50109	1.851363
H	10.3231	2.257008	-0.40357
H	11.75225	3.709751	-1.80445
H	13.8787	2.83381	-2.75845
H	14.54482	0.478637	-2.30171
H	13.09774	-0.98146	-0.92662
H	12.75447	0.357957	1.912381
H	13.80837	-1.11571	3.596014
H	13.02648	-3.46317	3.873785
H	11.18673	-4.31782	2.430083
H	10.15647	-2.85176	0.725823
H	-10.161	-4.20512	1.37417
H	-12.6253	-4.65813	1.644345
H	-14.2549	-2.84306	1.23559
H	-13.5304	-0.60278	0.559261
H	-12.6253	-4.65813	1.644345
H	-14.2549	-2.84306	1.23559
H	-13.5304	-0.60278	0.559261

Table S6. Geometry Data for Z-TPB-OIY.

	X	Y	Z
C	6.862799	-5.54559	1.227972
C	5.649853	-4.86793	1.114136
C	5.434008	-3.94748	0.075931
C	6.477625	-3.71669	-0.83692
C	7.688129	-4.39928	-0.72775
C	7.885267	-5.31688	0.305821
C	4.14192	-3.20454	-0.04024
C	4.23249	-1.7361	-0.04751
C	2.928956	-3.86316	-0.12541
C	2.868751	-5.34246	-0.33656
C	1.660851	-3.15661	-0.00709
C	0.460798	-3.61829	-0.44232
C	-0.82591	-2.94242	-0.33211
C	3.276521	-0.89799	-0.62174

C	3.299969	0.463704	-0.66647
C	4.415671	1.145794	-0.0893
C	5.419682	0.346496	0.512312
C	5.32999	-1.0363	0.5276
C	3.495749	-5.93609	-1.44361
C	3.419109	-7.31189	-1.65379
C	2.720667	-8.12214	-0.75706
C	2.089442	-7.54482	0.346244
C	2.15407	-6.16707	0.548683
C	-1.97098	-3.56748	-0.86409
C	-3.22311	-2.97054	-0.79731
C	-3.39801	-1.71355	-0.19158
C	-2.25402	-1.08725	0.343043
C	-1.00331	-1.6819	0.275963
C	-5.90206	-1.83197	0.035326
C	-7.15536	-1.23504	0.096023
C	-7.28715	0.162113	0.019905
C	-6.12143	0.933328	-0.12621
C	-4.87447	0.324754	-0.20016
C	-4.72903	-1.07169	-0.11814
N	-8.56148	0.776787	0.087826
C	-8.85105	1.915447	-0.71621
C	-9.56067	0.262313	0.960651
C	-10.891	0.146662	0.527319
C	-11.87	-0.34442	1.388565
C	-11.54	-0.74439	2.684917
C	-10.2161	-0.63798	3.115712
C	-9.23331	-0.13076	2.2682
C	-9.53513	3.0136	-0.17183
C	-9.82817	4.121292	-0.96467
C	-9.4308	4.162129	-2.3025
C	-8.74296	3.074432	-2.84408
C	-8.46182	1.954373	-2.06443
C	4.368913	2.587177	-0.17176
C	5.206259	3.619623	0.180482
C	6.606386	3.559553	0.705387
C	7.117971	4.948847	0.692453
C	6.116024	5.829246	0.25032
C	4.883943	5.048071	-0.02012
O	7.256538	2.58939	1.071775
C	3.660429	5.607849	-0.339
C	8.389738	5.378646	1.048304
C	8.672786	6.740986	0.9497
C	7.688392	7.631894	0.502614
C	6.407846	7.196239	0.152034
C	2.443434	4.874416	-0.5045
N	1.423476	4.328223	-0.644
C	3.463871	7.013943	-0.51236

N	3.25668	8.149794	-0.6672
H	7.00982	-6.25093	2.040752
H	4.859111	-5.04941	1.834742
H	6.331911	-3.00138	-1.6412
H	8.477792	-4.21346	-1.45005
H	8.829488	-5.84611	0.394002
H	1.69982	-2.18258	0.469958
H	0.431146	-4.58413	-0.94137
H	2.498416	1.031957	-1.13251
H	6.269278	0.835413	0.968577
H	6.118718	-1.60845	1.004898
H	4.042118	-5.3109	-2.14202
H	3.905458	-7.75093	-2.52001
H	2.665578	-9.1947	-0.91857
H	1.543506	-8.16706	1.049532
H	1.654514	-5.72108	1.403222
H	-1.86563	-4.53464	-1.34902
H	-4.07509	-3.47155	-1.24636
H	-2.35607	-0.12855	0.841936
H	-0.15431	-1.16277	0.709074
H	-5.83262	-2.91197	0.122918
H	-8.04131	-1.84967	0.21208
H	-6.1993	2.013083	-0.19027
H	-3.99653	0.948161	-0.33888
H	-11.1493	0.444549	-0.48328
H	-12.8945	-0.42705	1.037214
H	-12.3042	-1.13299	3.350788
H	-9.94569	-0.93713	4.124363
H	-8.20892	-0.03569	2.612357
H	-9.83356	2.991272	0.870891
H	-10.3578	4.963055	-0.52782
H	-9.65384	5.030241	-2.91492
H	-8.43383	3.089034	-3.88527
H	-7.93942	1.105627	-2.49294
H	3.445093	2.909439	-0.63739
H	9.126144	4.657848	1.388592
H	9.656248	7.115162	1.21702
H	7.921259	8.689478	0.4249
H	5.67791	7.916637	-0.1894

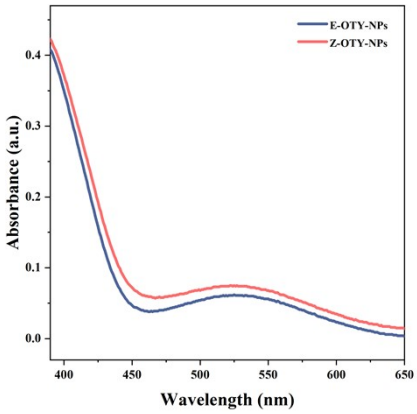

Figure S35. UV absorption spectra of E/Z-OIY-NPs.

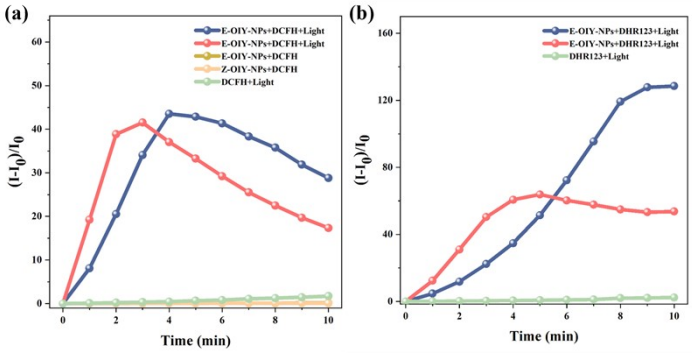

Figure S36. Fluorescence intensity net change [$(I-I_0)/I_0$] (a) at 532 nm for the DCFH indicator and (b) at 530 nm for the DHR123 indicator with E/Z-OIY-NPs upon white light irradiation (2 mW cm^{-2}).

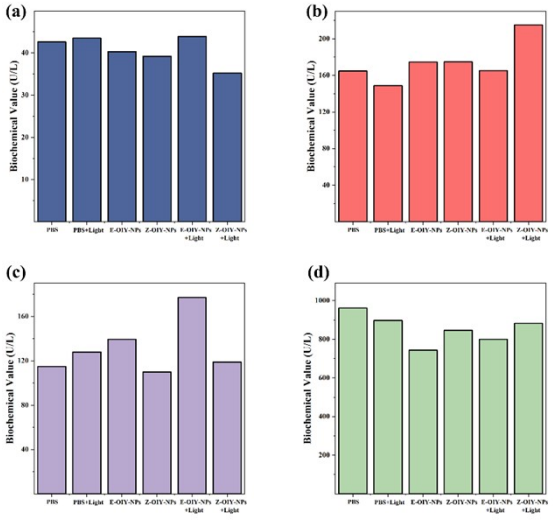

Figure S37. Serum biochemical parameters analyzed with the specimens collected from the animals received various treatments. The levels of (a) aspartate alanine aminotransferase (ALT), (b) aminotransferase (AST), (c) alkaline phosphatase (ALP), and (d) lactate dehydrogenase (LDH) by an automated analyzer.

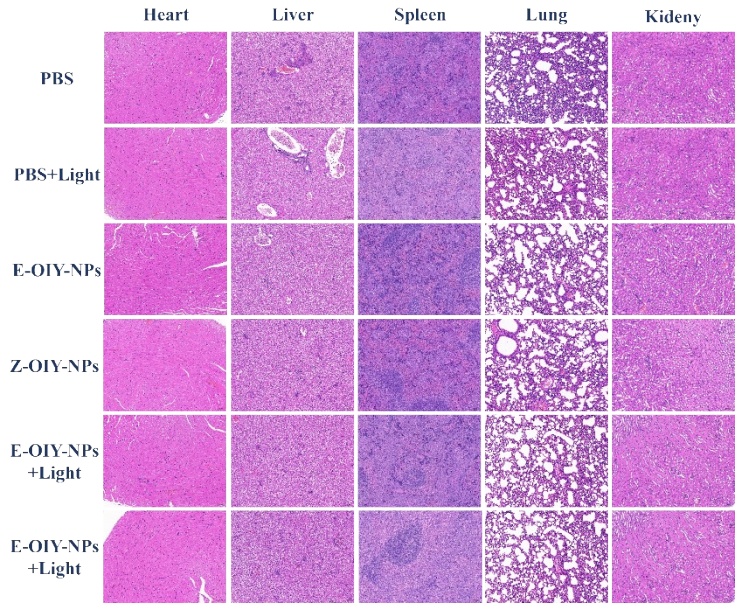

Figure S38. Histological H&E staining for different organs collected from mice in group vi on the 14th day after the treatment.