

# AIE-active luminogens as highly efficient free-radical ROS photogenerator for image-guided photodynamic therapy

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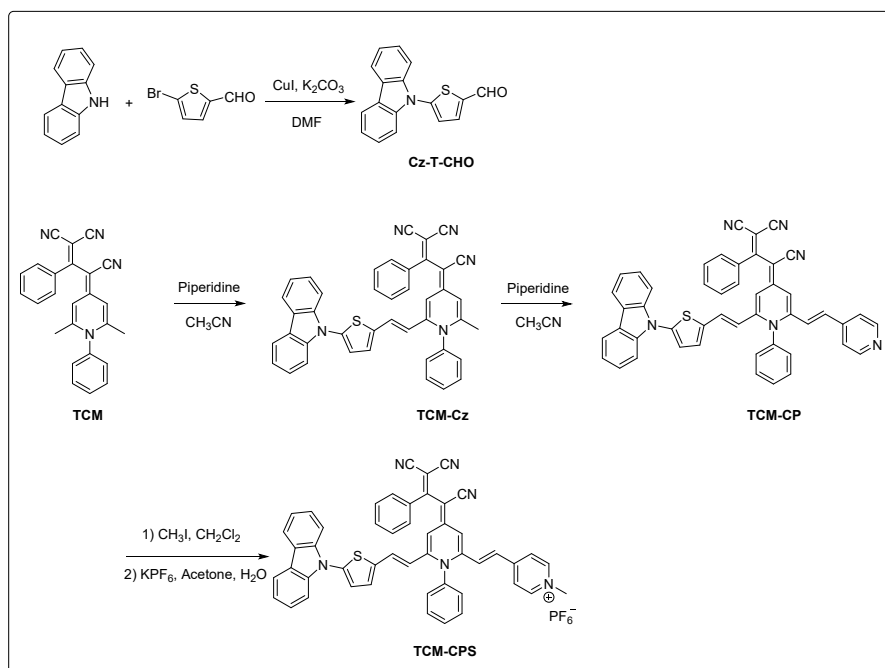
## 1. Experimental section

### 1.1 Materials and general methods

All solvents and starting reactants were purchased from commercial suppliers in analytical grade and used without purification unless special noted. All reagents were weighed by analytical balance (METTLER TOLEDO, ME204E/02). The NMR spectra ( $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^1\text{H}$ - $^1\text{H}$  COSY) were obtained from Bruker AM 400 spectrometer, using TMS ( $\delta = 0$ ) as internal standard. Waters LCT premier XE spectrometer was used to obtain high resolution mass spectrometry (HRMS) data of the products. UV-Vis absorption spectra and fluorescence spectra were obtained from Agilent Cary 60 UV-Vis spectrophotometer and Agilent Cary Eclipse fluorescence spectrophotometer, respectively. Dynamic light scattering (DLS) experiments were performed on Zetasizer Nano ZSE. The viscosity of solution was measured by TA Instruments DISCOVERY HR-2 Hybrid Rheometer. Transmission electron microscopy (TEM) images were taken on JEOL JEM-1400 instrument. The electron paramagnetic resonance (EPR) signal was obtained with Bruker EMX-8/2.7. Scanning electron microscope images of bacteria were taken on ZEISS GeminiSEM 500 and Hitachi S-3400N. Cell imaging was performed on Lecia TCS SP8 laser scanning confocal microscopy.

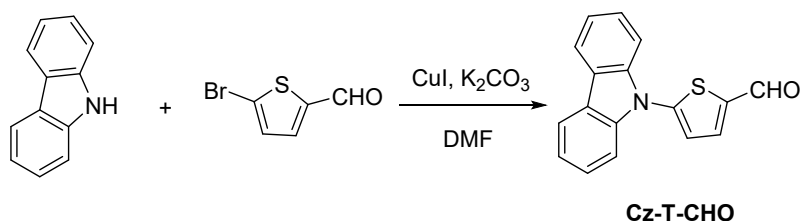
### 1.2 Synthesis route of TCM-CP and TCM-CPS

The important intermediate **TCM** was synthesized according to our previous work.<sup>1</sup>



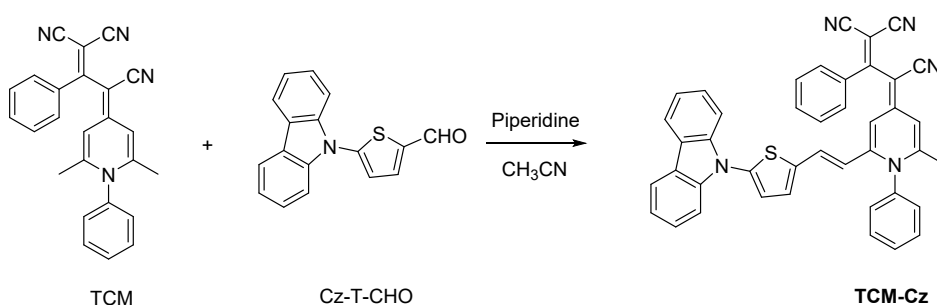
**Scheme S1.** The synthetic route of **TCM-CP** and **TCM-CPS**.

### 1.3 Synthesis of Cz-T-CHO



Carbazole (5000 mg, 29.90 mmol), 5-bromo-2-thiophenecarbaldehyde (6858 mg, 35.90 mmol), cuprous iodide (570 mg, 2.99 mmol), anhydrous potassium carbonate (6199 mg, 44.85 mmol) and dry DMF (25 mL) were added to a dry 100 mL three-necked flask in sequence. The mixture was heated at 140 °C under nitrogen atmosphere for 24 h. After cooling to room temperature, the mixture was poured into 100 mL sodium chloride aqueous solution, and the crude product was obtained by extracting three times with dichloromethane (100 mL\*3). The organic phase was dried with anhydrous sodium sulfate. After removing the solvent under reduced pressure, the crude product was further purified by silica gel chromatography with petroleum ether/dichloromethane (v/v, 5:1) to afford faint yellow solid (3520 mg, 42% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm), δ: 9.95 (s, 1H, -CHO), 8.11 (d, 2H, *J* = 7.7 Hz, Ar-H), 7.88 (d, 1H, *J* = 4.0 Hz, thiophene-H), 7.67 (d, 2H, *J* = 8.2 Hz, Ar-H), 7.51-7.44 (m, 2H, Ar-H), 7.39-7.31 (m, 3H, Ar-H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm), δ: 182.84, 148.63, 140.55, 139.71, 136.10, 126.71, 124.25, 123.67, 121.71, 120.46, 110.34. Mass spectrometry (ESI positive ion mode for [M+H]<sup>+</sup>): Calcd. for C<sub>17</sub>H<sub>12</sub>NOS: 278.0640; found: 278.0616.

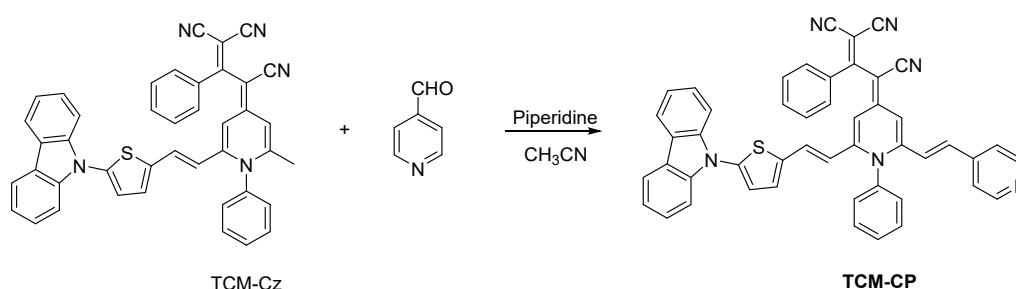
### 1.4 Synthesis of TCM-Cz



Piperidine (0.25 mL) was added dropwise to 50 mL two-necked flask containing the mixture of TCM (1215 mg, 3.24 mmol), Cz-T-CHO (300 mg, 1.08 mmol) and acetonitrile (15 mL), followed by refluxing at 95 °C under nitrogen atmosphere for 12 h. The mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The solid was further purified by silica gel chromatography with petroleum ether/dichloromethane (v/v, 1:4) to afford red solid (302 mg, 44%

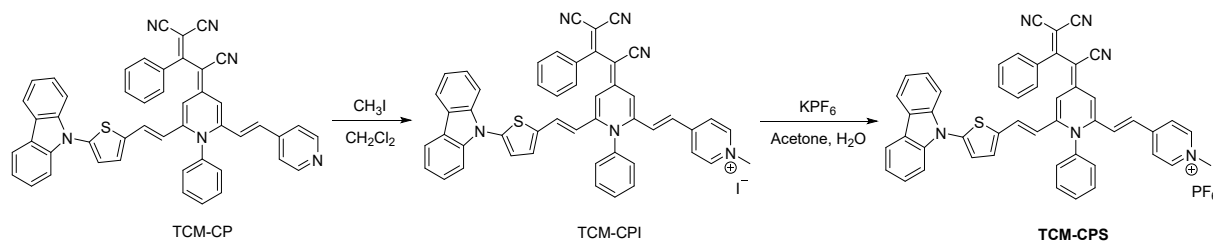
yield).  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , ppm),  $\delta$ : 8.23 (d, 2H,  $J = 7.7$  Hz, carbazole-H), 7.73-7.55 (m, 8H, Ar-H), 7.55-7.43 (m, 6H, Ar-H), 7.41 (s, 2H, Ar-H), 7.37-7.29 (m, 2H, Ar-H), 7.21 (s, 1H, Ar-H), 7.11-6.98 (m, 2H, Ar-H), 5.88 (d, 1H,  $J = 15.8$  Hz, alkene-H), 2.14 (s, 3H,  $-\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , ppm),  $\delta$ : 166.22, 152.60, 151.06, 147.87, 140.49, 139.56, 137.57, 137.38, 136.47, 131.35, 130.82, 130.70, 130.62, 130.47, 130.28, 129.27, 127.25, 126.76, 126.22, 123.08, 121.25, 120.59, 119.22, 118.64, 118.12, 116.45, 115.09, 110.02, 79.99, 61.25, 21.37. Mass spectrometry (ESI positive ion mode for  $[\text{M}+\text{H}]^+$ ): Calcd. for  $\text{C}_{42}\text{H}_{28}\text{N}_5\text{S}$ : 634.2065; found: 634.2061.

## 1.5 Synthesis of TCM-CP



Piperidine (0.25 mL) was added dropwise to 50 mL two-necked flask containing the mixture of TCM-Cz (200 mg, 0.32 mmol), 4-pyridinecarboxaldehyde (684 mg, 6.39 mmol) and acetonitrile (15 mL), followed by refluxing at 95 °C under nitrogen atmosphere for 12 h. The mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The solid was further purified by silica gel chromatography with dichloromethane/methanol (v/v, 100:1) to afford red solid (112 mg, 49% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , ppm),  $\delta$ : 8.54 (d, 2H,  $J = 6.0$  Hz, pyridine-H), 8.22 (d, 2H,  $J = 7.7$  Hz, carbazole-H), 7.78-7.70 (m, 1H, Ar-H), 7.70-7.57 (m, 7H, Ar-H), 7.54-7.43 (m, 7H, Ar-H), 7.41 (d, 1H,  $J = 3.9$  Hz, thiophene-H), 7.38-7.30 (m, 3H, Ar-H), 7.28 (s, 1H, Ar-H), 7.23 (d, 2H,  $J = 6.0$  Hz, pyridine-H), 7.19 (s, 1H, Ar-H), 6.97 (d, 1H,  $J = 15.9$  Hz, alkene-H), 6.56 (d, 1H,  $J = 16.0$  Hz, alkene-H), 5.97 (d, 1H,  $J = 15.8$  Hz, alkene-H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , ppm),  $\delta$ : 166.37, 152.53, 150.41, 148.32, 147.88, 141.55, 140.47, 139.74, 137.43, 136.98, 136.21, 135.44, 131.50, 131.46, 130.96, 130.52, 130.36, 129.43, 127.84, 126.77, 126.17, 124.02, 123.09, 121.27, 121.21, 120.60, 118.94, 117.91, 116.22, 115.52, 110.04, 80.51, 62.32. Mass spectrometry (ESI positive ion mode for  $[\text{M}+\text{H}]^+$ ): Calcd. for  $\text{C}_{48}\text{H}_{31}\text{N}_6\text{S}$ : 723.2331; found: 723.2330.

## 1.6 Synthesis of TCM-CPS



$\text{CH}_3\text{I}$  (80 mg, 0.56 mmol) was added dropwise to 50 mL two-necked flask containing the mixture of TCM-CP (30 mg, 0.04 mmol), and dichloromethane (6 mL), followed by stirring at room temperature for 24 h. The solvent was removed under reduced pressure, and the solid was further purified by silica gel chromatography with dichloromethane/methanol (v/v, 15:1) to afford black solid TCM-CPI (23 mg, 64% yield).

The pure intermediate compound TCM-CPI (21 mg, 0.02 mmol) was dissolved in 5 mL acetone, and 5 mL saturated  $\text{KPF}_6$  aqueous solution was poured into the acetone solution. The mixture was stirred at room temperature for 12 h, and solids were precipitated out of the solution. After filtering and washing with n-hexane, the black green solid (14 mg) was obtained with the yield of 65%.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , ppm),  $\delta$ : 8.85 (d, 2H,  $J = 5.3$  Hz, pyridinium salt-H), 8.24 (d, 2H,  $J = 7.2$  Hz, carbazole-H), 8.03 (d, 2H,  $J = 5.2$  Hz, pyridinium salt-H), 7.76-7.59 (m, 8H, Ar-H), 7.57-7.51 (m, 2H, Ar-H), 7.51-7.41 (m, 6H, Ar-H), 7.39-7.21 (m, 6H, Ar-H and alkene-H), 7.01 (d, 1H,  $J = 16.0$  Hz, alkene-H), 5.97 (d, 1H, alkene-H,  $J = 15.7$  Hz), 4.24 (s, 3H,  $-\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , ppm),  $\delta$ : 166.47, 152.47, 149.35, 148.42, 147.27, 145.79, 140.45, 139.85, 137.37, 136.82, 136.15, 132.18, 131.68, 131.60, 131.09, 130.52, 130.36, 129.41, 127.94, 126.79, 126.27, 124.74, 123.10, 121.31, 120.64, 119.01, 117.74, 117.03, 116.16, 115.88, 110.04, 80.72, 63.04, 47.41.  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO}-d_6$ , ppm),  $\delta$ : -70.12 ( $J = 711$  Hz). Mass spectrometry (ESI positive ion mode for  $[\text{M}-\text{PF}_6]^+$ ): Calcd. for  $\text{C}_{49}\text{H}_{33}\text{N}_6\text{S}$ : 737.2487; found: 737.2485.

## 1.7 Transmission electron microscopy imaging of TCM-CP and TCM-CPS

10  $\mu\text{L}$  TCM-CP or TCM-CPS (10  $\mu\text{M}$  in 99% water) was added onto a carbon-coated copper grid, followed by drying overnight at room temperature. The TEM imaging was performed on JEOL JEM-1400 with an accelerating bias voltage of 100 kV.

## 1.8 Cell culture

Human epithelioid cervical carcinoma (HeLa) cells were purchased from the Institute of Cell Biology (Shanghai, China). Cells were propagated in cell culture flask at 37 °C under humidified 5% CO<sub>2</sub> atmosphere. Dulbecco's modified eagle medium (DMEM, GIBCO/Invitrogen, Camarillo, CA, USA) was supplemented with 1% penicillin-streptomycin (10,000 U mL<sup>-1</sup> penicillin, and 10 mg mL<sup>-1</sup> streptomycin, Solarbio life science, Beijing, China) and 10% fetal bovine serum (FBS, Biological Industry, Kibbutz Beit Haemek, Israel).

## 1.9 Intracellular ROS Detection

The HeLa cells were seeded onto glass bottom cell culture dish (Φ 20 mm, NEST). After reaching 80% confluence, the cells were incubated with TCM-CPS (10 μM) for 6 h, followed by incubating with dichlorofluorescein diacetate (DCFH-DA, 20 μM) for 20 min. After light irradiation (40 mW cm<sup>-2</sup>, 400-650 nm) for 5 min or in the dark, the cells were imaging by Leica TCS SP8. The **PSs+light+vitamin C** group: After incubation with TCM-CPS, the cells were treating with DCFH-DA/vitamin C mixtures (50 mM for vitamin C) for 20 min, then irradiated by light before imaging. Green channel:  $\lambda_{\text{ex}} = 488 \text{ nm}$ ,  $\lambda_{\text{em}} = 505\text{-}560 \text{ nm}$ .

## 1.10 Cell ablation study

The viabilities of HeLa cells were evaluated by methylthiazolyldiphenyltetrazolium bromide (MTT) assays. Briefly, the cells were seeded onto 96-well plates at the density of  $8 \times 10^3$  cells per well and cultured for 12 h. The cells were divided into three groups: in the dark, light irradiation for 7.5 min, and light irradiation for 15 min. Then, the cells were incubated with various concentration of TCM-CPS for 6 h, followed by replacing the TCM-CPS solution with fresh DMEM. After light irradiation (40 mW cm<sup>-2</sup>) for different time (7.5 min and 15 min) or in the dark, the cells were further cultured for 12 h. 10 μL MTT solution (5 mg mL<sup>-1</sup>) was added into each well, and further cultured for 4 h. After removing liquid supernatant, 100 μL DMSO was added into each well to dissolve the crystals. The cell viability was accessed by means of MTT absorbance at 600 nm recorded by a microplate reader (BioTek Synergy H4), and cells incubated with culture medium only in each group were designated as cells with 100% cell viability.

## 1.11 Live/dead cell staining

The cells were seed onto glass bottom cell culture dish (Φ 20 mm, NEST). After reaching 80% confluence, the cells were incubated with TCM-CPS (10 μM) or fresh DMEM for 6 h. The selected

cells were irradiated by white light ( $40 \text{ mW cm}^{-2}$ , 400-650 nm) for 15 min, and further cultured for 12 h. The cells were stained with Calcein-AM/PI mixtures ( $2 \mu\text{M}$  for Calcein-AM,  $4.5 \mu\text{M}$  for PI), followed by imaging with Leica TCS SP8. Green channel from Calcein:  $\lambda_{\text{ex}} = 488 \text{ nm}$ ,  $\lambda_{\text{em}} = 495\text{-}540 \text{ nm}$ , red channel from PI:  $\lambda_{\text{ex}} = 561 \text{ nm}$ ,  $\lambda_{\text{em}} = 590\text{-}650 \text{ nm}$ .

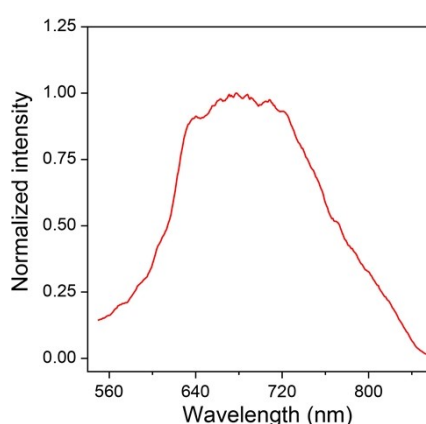
### 1.12 Bacterial culture and staining

A single colony of bacteria was incubated with LB medium in shaking table ( $37^\circ\text{C}$ , 200 r/min). Briefly, the bacteria with an optical density (OD) 0.5 at 600 nm were diluted 100 times in PBS, and incubated with TCM-CMS ( $10 \mu\text{M}$ ) for various time (15 min, 30 min, and 60 min) in shaking table ( $37^\circ\text{C}$ , 200 r min<sup>-1</sup>). After incubation, the bacteria were washed with PBS, and concentrated by centrifuge. Then, the bacteria solution ( $10 \mu\text{L}$ ) was added onto a glass slide with a coverslip, and imaged by confocal laser scanning microscope (Leica TCS SP8). Red channel from TCM-CPS:  $\lambda_{\text{ex}} = 514 \text{ nm}$ ,  $\lambda_{\text{em}} = 650\text{-}750 \text{ nm}$ .

### 1.13 Killing the bacteria

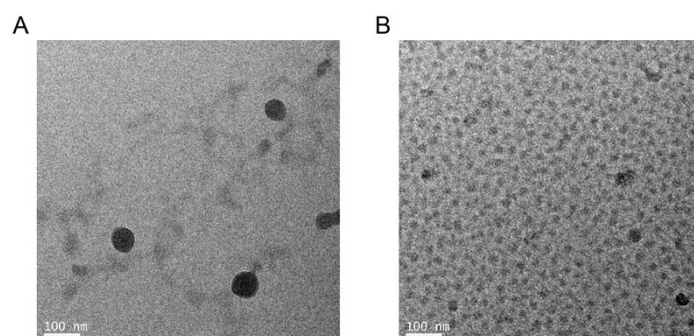
The antibacterial activity of TCM-CPS was determined by plate count method. Briefly, the bacterial suspensions were incubated with TCM-CMS ( $2.5$ ,  $5$ , and  $10 \mu\text{M}$ ) for 30 min in shaking table ( $37^\circ\text{C}$ , 200 r/min). Then, the bacterial suspensions were either exposed to light ( $40 \text{ mW cm}^{-2}$ ) for 15 min or under the dark. The bacterial suspensions ( $30 \mu\text{L}$ ) were transferred onto an agar plate (1.5% agar + LB medium), and further cultured for 12 h, followed by imaging.

## 2. Normalized fluorescence spectrum of TCM-CPS in water



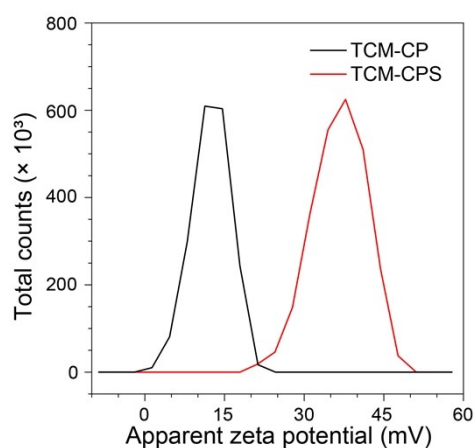
**Figure S1** Normalized fluorescence intensity of TCM-CPS in 99% water,  $\lambda_{\text{ex}} = 520 \text{ nm}$ .

### 3. TEM images of TCM-CP and TCM-CPS in water



**Figure S2** TEM images of (A) TCM-CP and (B) TCM-CPS in 99% water. All images share scale bar of 100 nm.

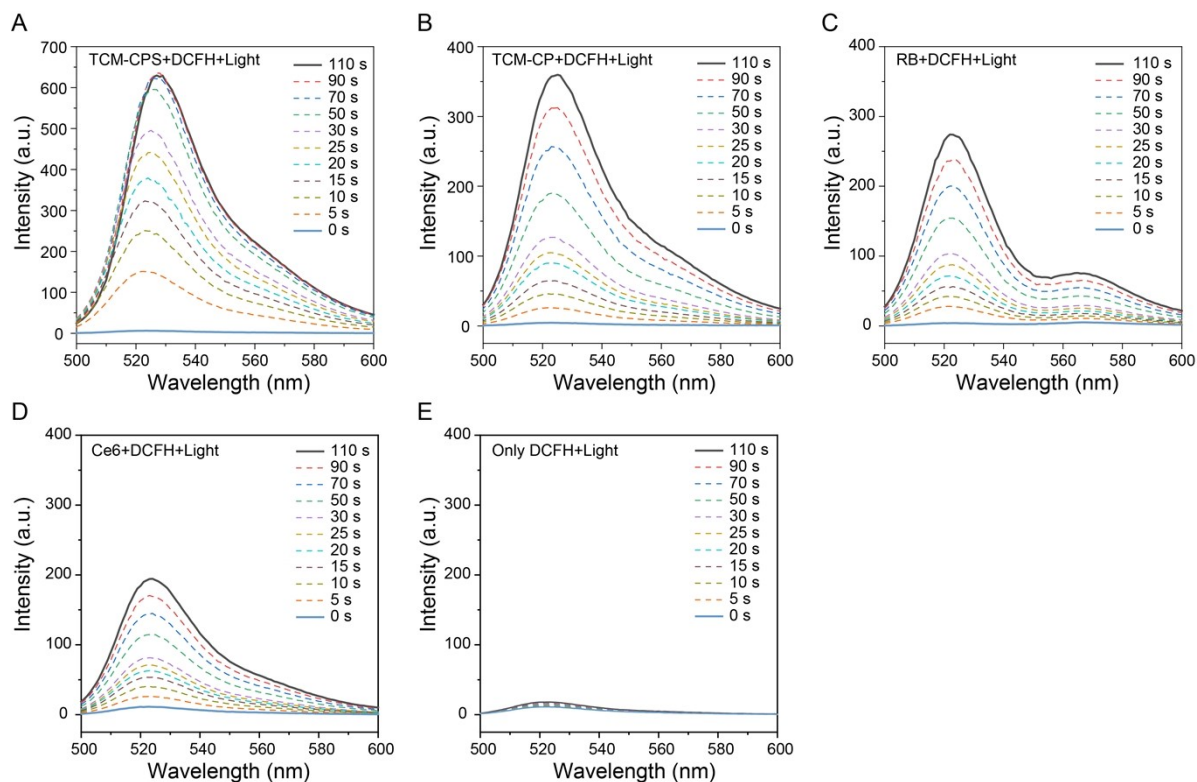
### 4. Zeta potential distribution of TCM-CP and TCM-CPS in water



**Figure S3** Zeta potential distribution of TCM-CP and TCM-CPS in 99% water.



## 5. Total ROS generation of TCM-CPS, TCM-CP, RB and Ce6



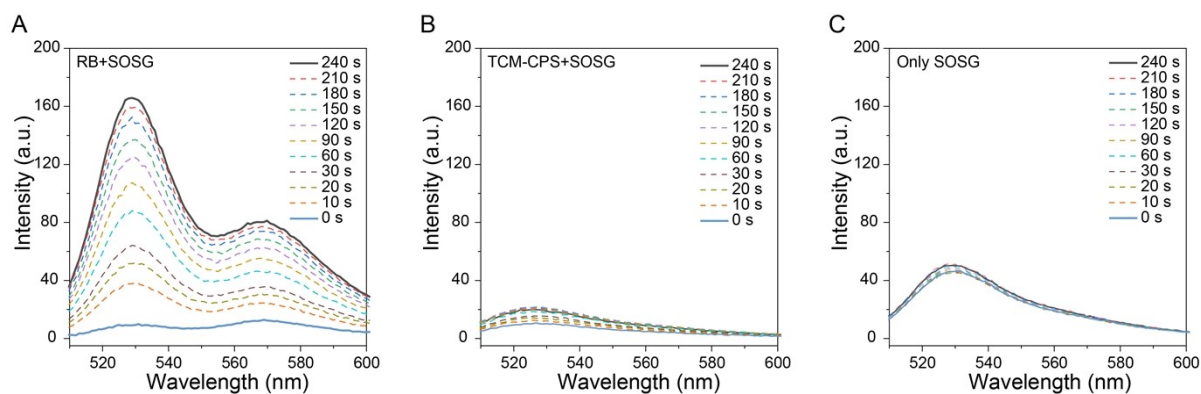
**Figure S4** Total ROS generation of (A) TCM-CPS, (B) TCM-CP, (C) RB, and (D) Ce6 (10  $\mu$ M) upon white light irradiation using DCFH (40  $\mu$ M) as an indicator. (E) The change of solution' fluorescence without photosensitizer upon white light irradiation.  $\lambda_{ex}$  = 488 nm.

## 6. Calculated energy of the singlet and triplet excited states

**Table S1** Calculated energy of the singlet (S) and triplet (T) excited states (Gaussian/B3LYP/6-311G(d))

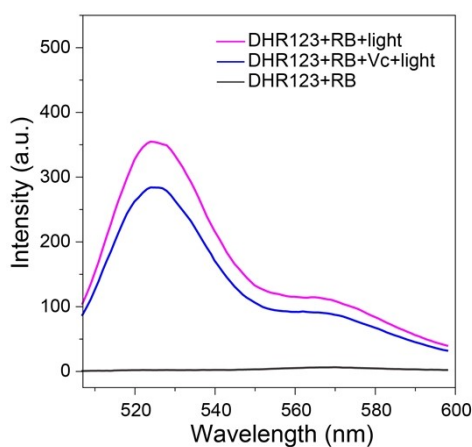
		1	2	3	4	5	6	7	8	9	10
TCM-CP	S	2.3418	2.3804	2.6554	2.8605	3.0752	3.0977	3.3214	3.3286	3.5191	3.5436
	T	1.5550	1.8896	2.1713	2.4053	2.5590	2.7891	2.9370	3.0369	3.0416	3.1915
TCM-CPS	S	0.5354	0.9665	0.9822	1.6635	1.9728	2.0031	2.0789	2.2203	2.3349	2.3562
	T	0.3147	0.5551	0.9656	1.4387	1.6593	1.8310	1.9733	1.9996	2.0792	2.2449

## 7. Singlet oxygen generation of RB and TCM-CPS



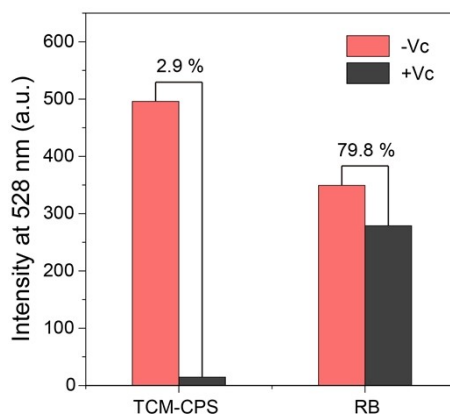
**Figure S5** Singlet oxygen generation of (A) RB and (B) TCM-CPS (10  $\mu\text{M}$ ) upon light irradiation using SOSG (10  $\mu\text{M}$ ) as an indicator. (C) The change of solution' fluorescence without photosensitizer upon white light irradiation.  $\lambda_{\text{ex}} = 500 \text{ nm}$ .

## 8. Free radical generation of RB



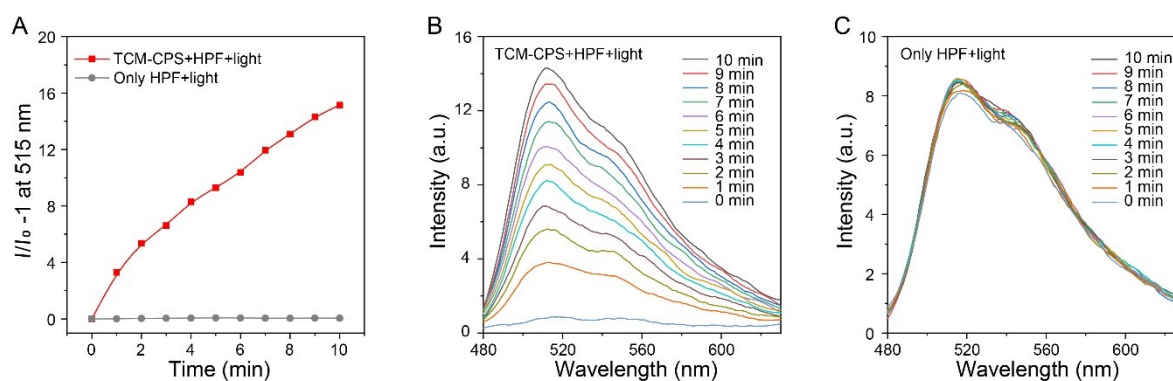
**Figure S6** Fluorescence spectra of the DHR123 probe for detecting free-radical ROS generated by RB in the presence of Vc (100  $\mu\text{M}$ ) under light irradiation for 10 min.  $\lambda_{\text{ex}} = 495 \text{ nm}$ . The concentration of RB is 10  $\mu\text{M}$ .

## 9. Comparison of DHR123's fluorescence intensity with or without Vc



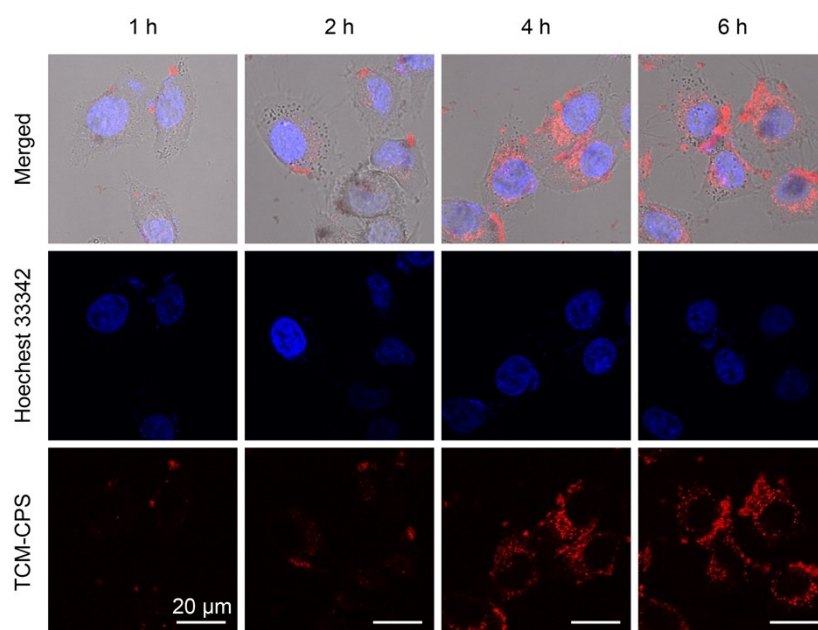
**Figure S7** Comparison of DHR123's fluorescence intensity with or without Vc.

## 10. Hydroxyl radical generation of TCM-CPS



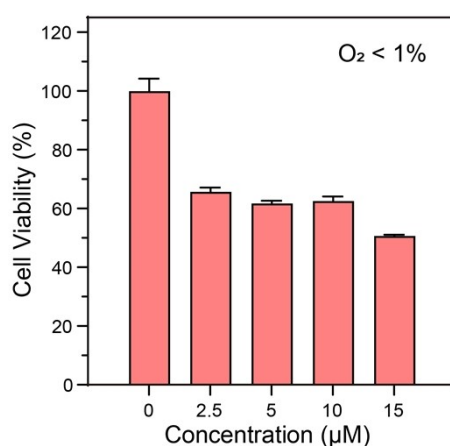
**Figure S8** (A) The hydroxyl radical generation of TCM-CPS (10  $\mu$ M) upon white light irradiation (80 mW  $\text{cm}^{-2}$ , 400-650 nm) using HPF (10  $\mu$ M) as an indicator.  $I_0$  is the fluorescence of mixtures before light irradiation. The change of fluorescence spectra of mixtures (B) with or (C) without TCM-CPS as photosensitizer upon white light irradiation.  $\lambda_{\text{ex}} = 460$  nm.

## 11. Confocal images of cells with different incubation time



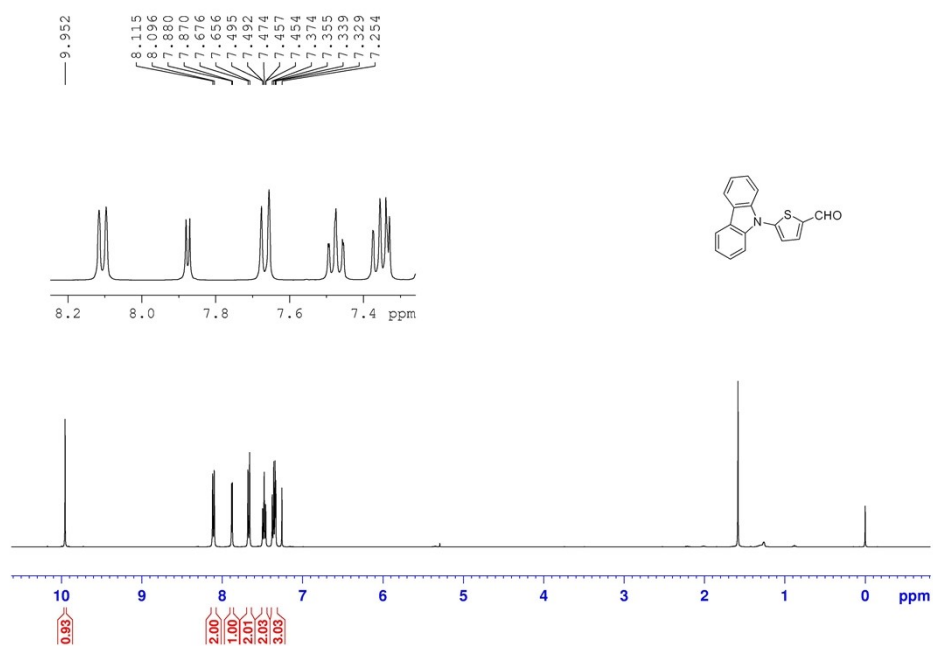
**Figure S9** Confocal images of HeLa cells incubated with 10  $\mu\text{M}$  TCM-CPS for different time, followed by incubated with 5  $\mu\text{g mL}^{-1}$  Hoechst 33342 for 15 min. Red channel from TCM-CPS:  $\lambda_{\text{ex}} = 514 \text{ nm}$ ,  $\lambda_{\text{em}} = 630\text{-}750 \text{ nm}$ , blue channel from Hoechst 33342:  $\lambda_{\text{ex}} = 405 \text{ nm}$ ,  $\lambda_{\text{em}} = 415\text{-}460 \text{ nm}$ . Scale bar: 20  $\mu\text{m}$ .

## 12. In vitro cytotoxicity of TCM-CPS under hypoxia

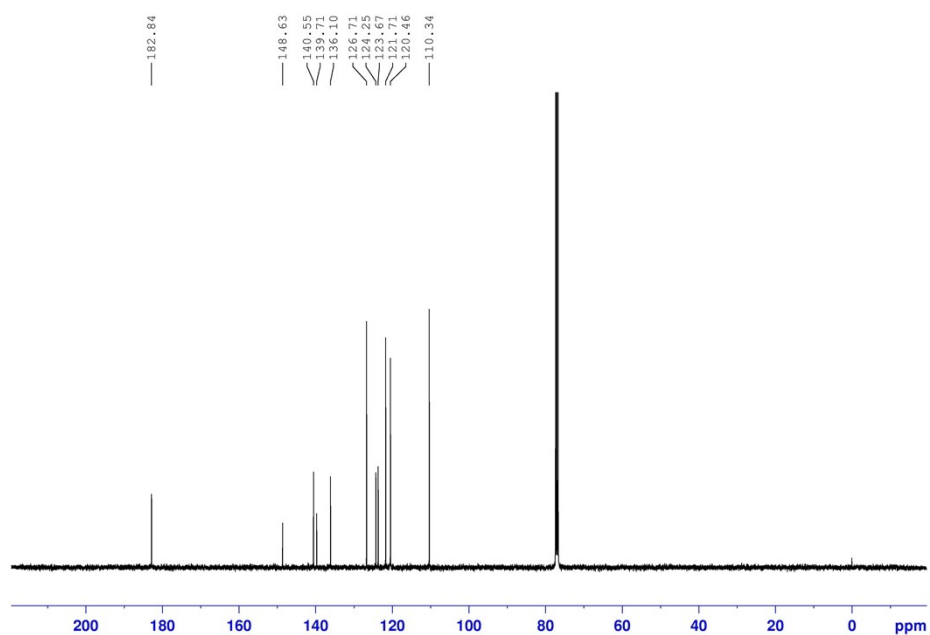


**Figure S10** In vitro cytotoxicity of TCM-CPS under extreme hypoxia environment (Oxygen concentration < 1%). The cells were seeded onto 96-well plate at the density of  $8 \times 10^3$  cells per well and cultured for 12 h. Then, the cells were incubated with various concentration of TCM-CPS for 6 h, followed by replacing the TCM-CPS solution with fresh DMEM. The 96-well plate was put into sealed bag (Hopebio), the oxygen in the bag was consumed by anaerobic gas producing bag (Hopebio) for 2 h. After light irradiation ( $40 \text{ mW cm}^{-2}$ ) for 15 min, the cells were further cultured

for 12 h. 10  $\mu\text{L}$  MTT solution (5 mg  $\text{mL}^{-1}$ ) was added into each well, and further cultured for 4 h. After removing liquid supernatant, 100  $\mu\text{L}$  DMSO was added into each well to dissolve the crystals. The cell viability was accessed by means of MTT absorbance at 600 nm recorded by a microplate reader (BioTek Synergy H4), and cells incubated with culture medium only were designated as cells with 100% cell viability.



**Figure S11** <sup>1</sup>H NMR spectrum of **Cz-T-CHO** in CDCl<sub>3</sub>.



**Figure S12** <sup>13</sup>C NMR spectrum of **Cz-T-CHO** in CDCl<sub>3</sub>.

### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-17 H: 0-12 N: 0-1 O: 0-1 S: 0-1

WH-ZHU

ZW-LZX-122 101 (1.143) Cm (100:108)

1: TOF MS ES+  
2.86e+003

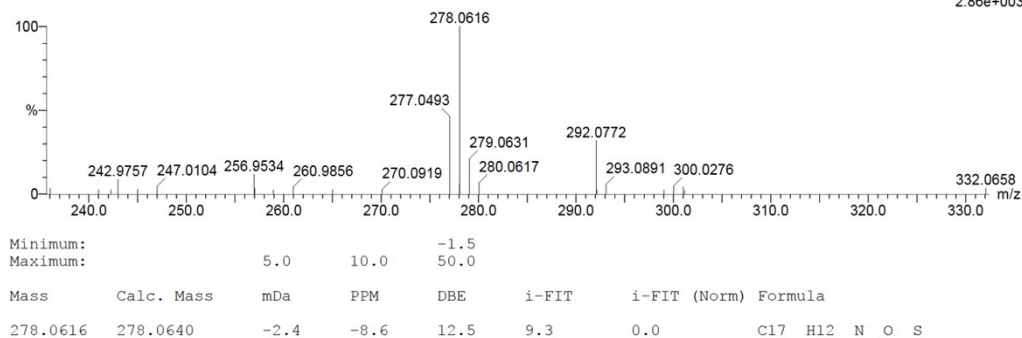


Figure S13 HRMS spectrum of Cz-T-CHO.

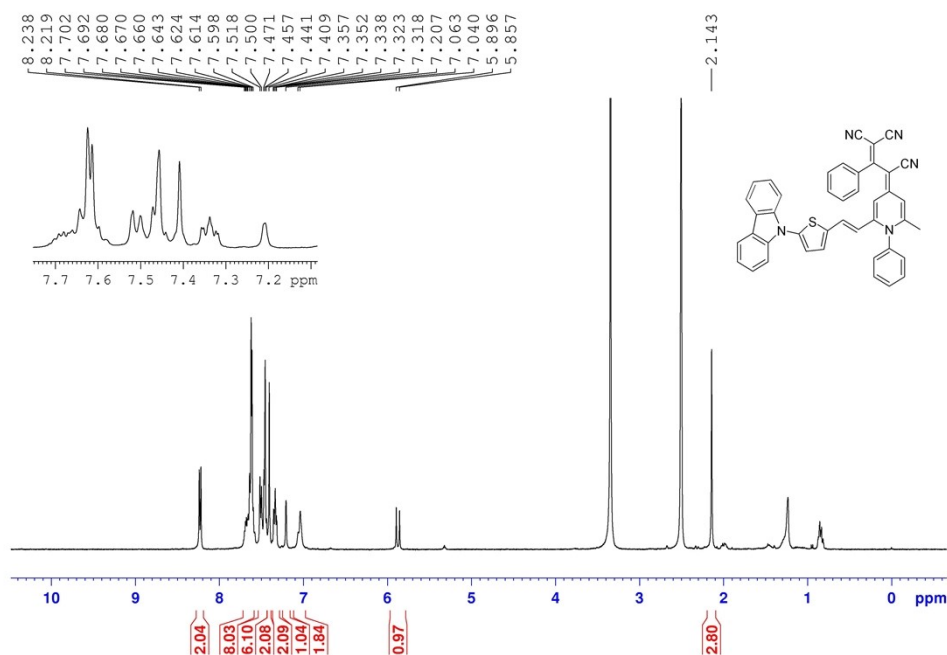
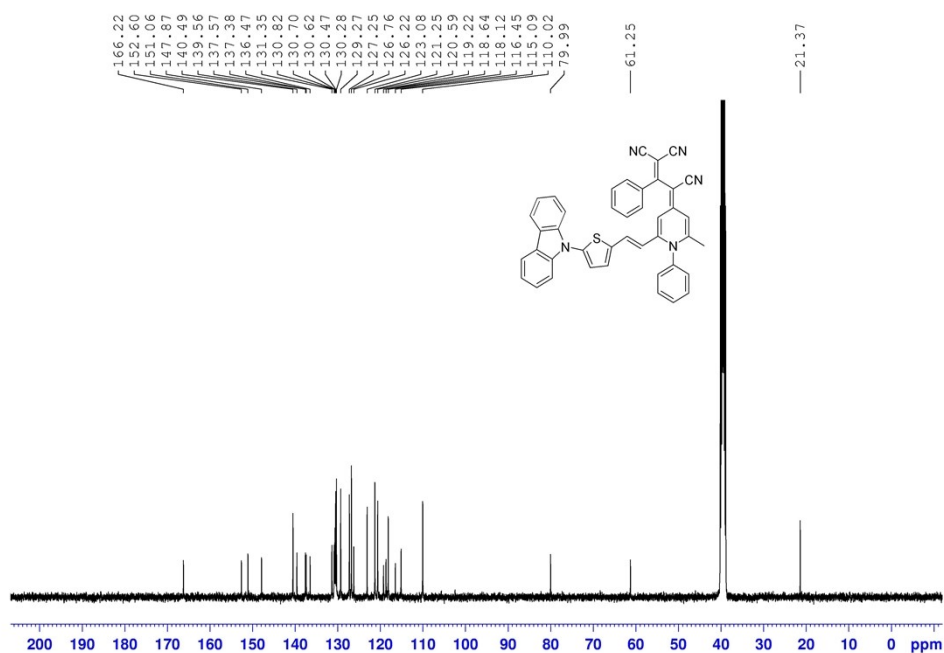


Figure S14  $^1\text{H}$  NMR spectrum of TCM-Cz in  $\text{DMSO}-d_6$ .



**Figure S15**  $^{13}\text{C}$  NMR spectrum of TCM-Cz in  $\text{DMSO-}d_6$ .

#### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

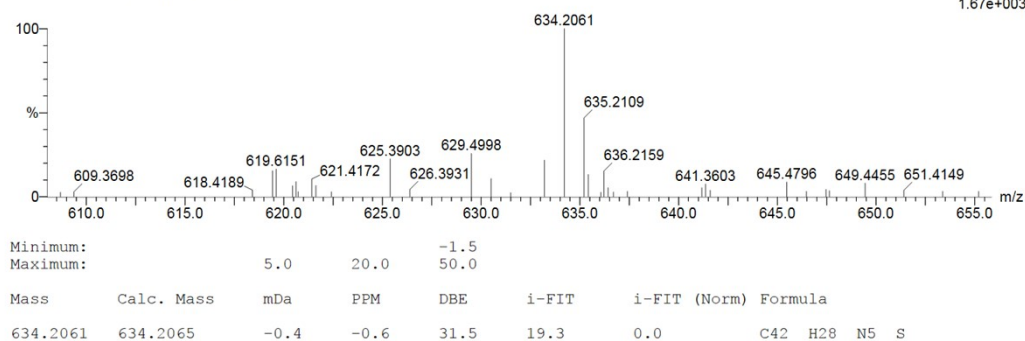
Elements Used:

C: 0-42 H: 0-35 N: 0-5 S: 0-1

WH-ZHU

ZW-LZX-207 96 (1.086) Cm (94:97)

1: TOF MS ES+  
1.67e+003



**Figure S16** HRMS spectrum of TCM-Cz.





### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 48-48 H: 0-52 N: 0-6 S: 0-2

WH-ZHU

ZW-LZX-224 20 (0.212) Cm (16:21)

1: TOF MS ES+  
4.27e+003

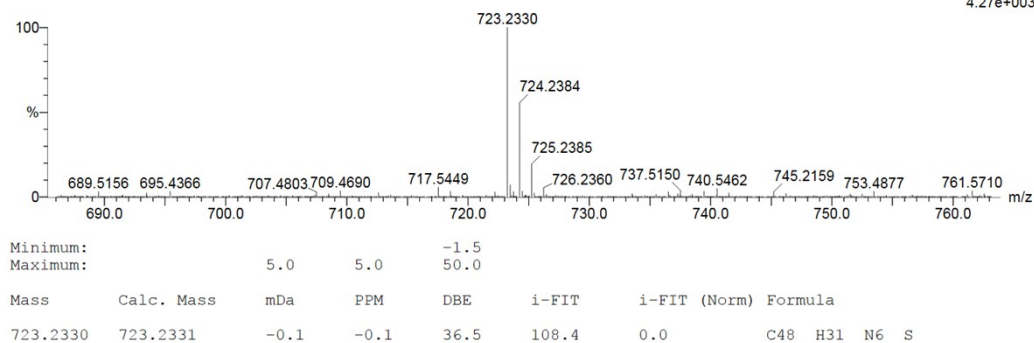
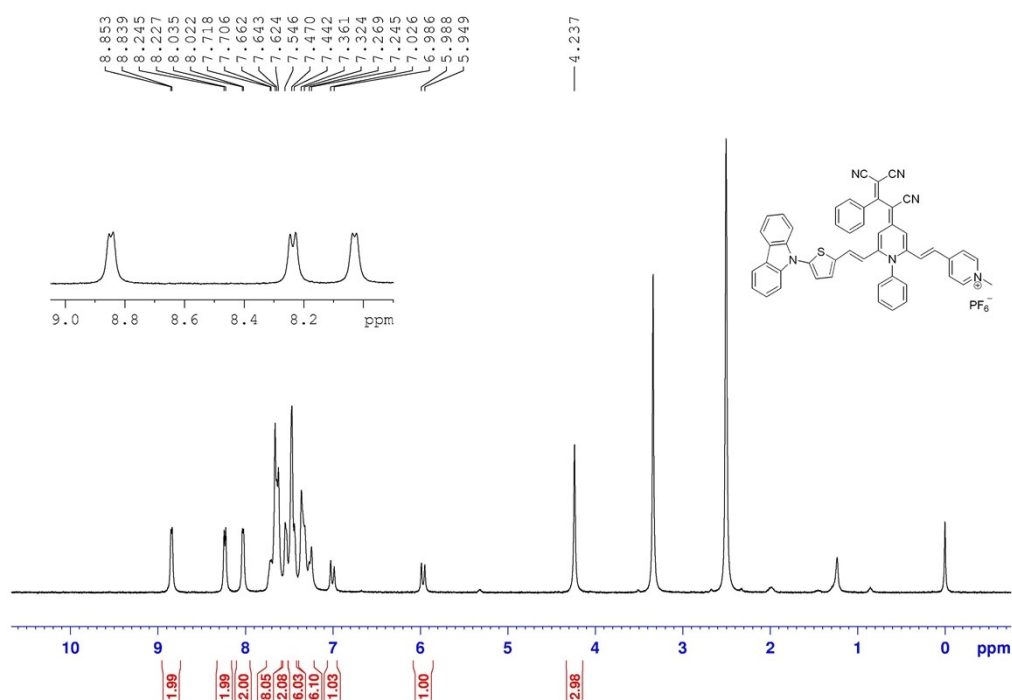
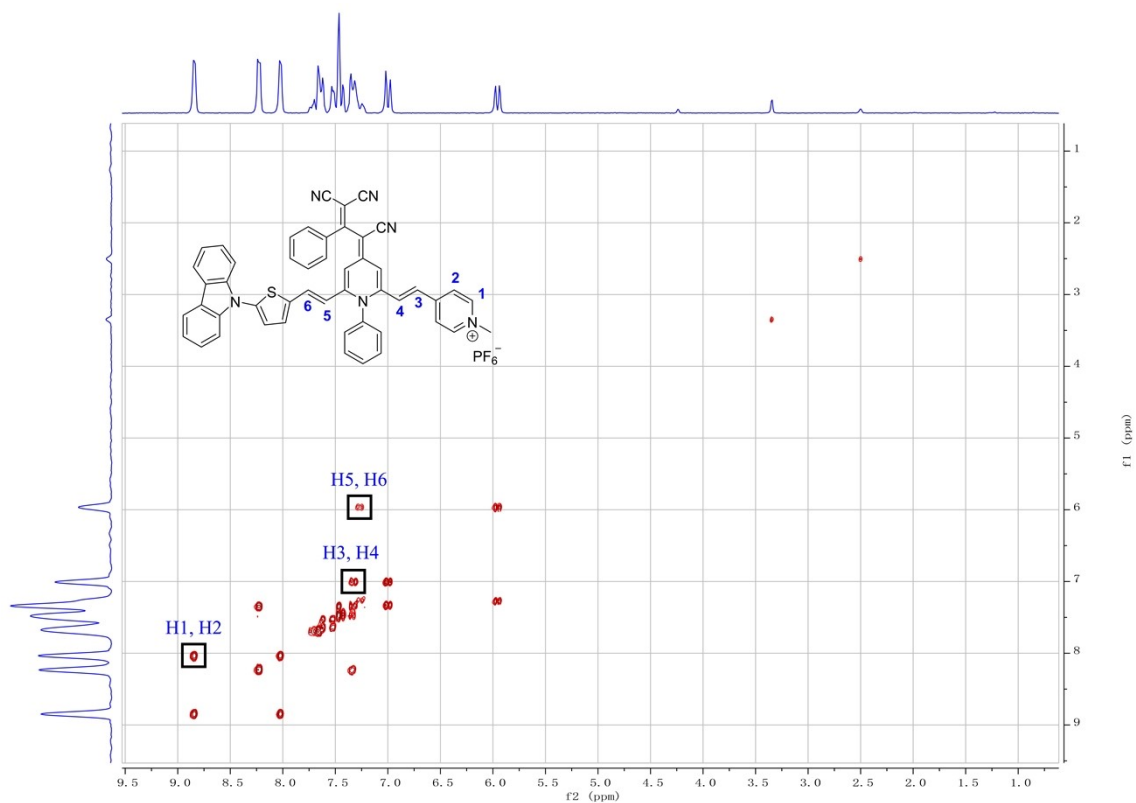
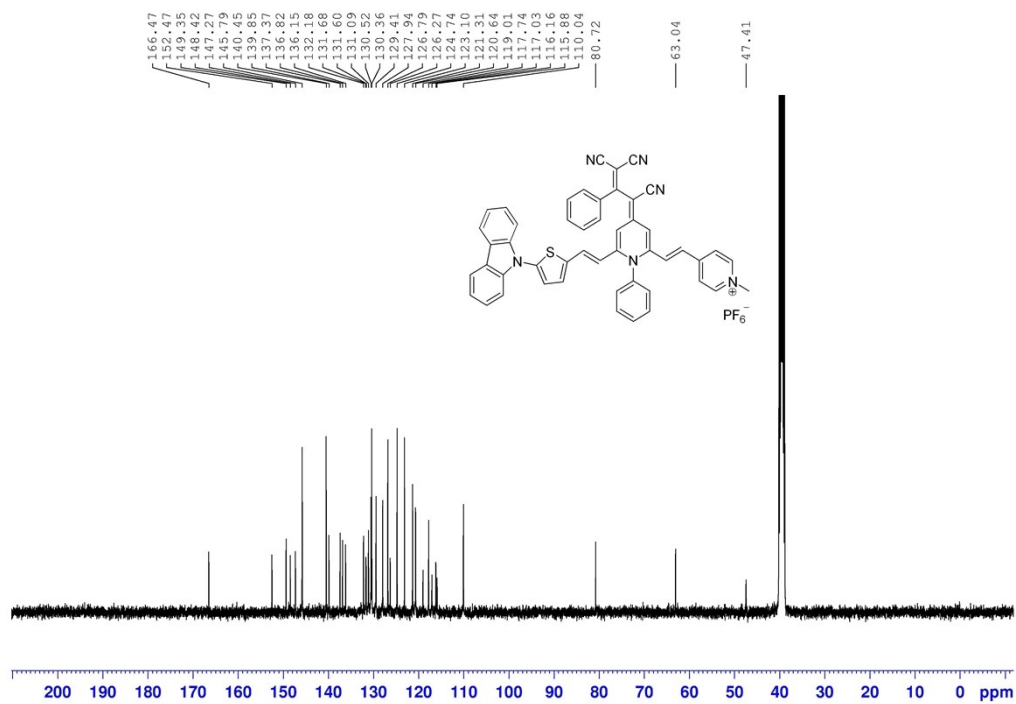


Figure S19 HRMS spectrum of TCM-CP.





**Figure S21** Two-dimensional  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of TCM-CPS in  $\text{DMSO-}d_6$ .



**Figure S22**  $^{13}\text{C}$  NMR spectrum of TCM-CPS in  $\text{DMSO-}d_6$ .



**Figure S23**  $^{19}\text{F}$  NMR spectrum of TCM-CPS in  $\text{DMSO-}d_6$ .

#### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

7 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

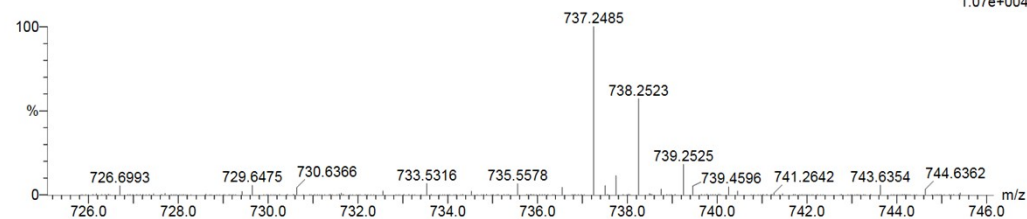
Elements Used:

C: 0-49 H: 0-50 N: 0-6 S: 0-1

WH-ZHU

ZW-LZX-307 66 (0.748) Cm (66.71)

1: TOF MS ES+  
1.07e+004



Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
737.2485	737.2487	-0.2	-0.3	36.5	142.4	0.0	C49 H33 N6 S	

**Figure S24** HRMS spectrum of TCM-CPS.

#### Reference

1. Z. Liu, Q. Wang, Z. Zhu, M. Liu, X. Zhao and W.-H. Zhu, *Chem. Sci.*, 2020, **11**, 12755-12763.