Supporting Information

Cationic AIE-active photosensitizer for high-efficient photodynamic eradication of drug-resistant bacteria

Yuewen Yu, [†a] Yubo Liu, [†a] Yitao Chen, [a] Jinke Chen, [a] Guangxue Feng, [*a] Ben Zhong Tang[*b]

[a] State Key Laboratory of Luminescent Materials and Devices, Guangdong Provincial Key Laboratory of Luminescence from Molecular Aggregates, School of Materials Science and Engineering, AIE Institute, South China University of Technology, Guangzhou, 510640, China

[b] Shenzhen Institute of Aggregate Science and Technology, School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, 2001 Longxiang Boulevard, Longgang District, Shenzhen City, Guangdong 518172, China

*Corresponding author.

E-mail: fenggx@scut.edu.cn (G. Feng). tangbenz@cuhk.edu.cn (B. Z. Tang)

† These authors contributed equally to this work.

Materials and methods

1. Materials

All solvents were of analytical grade in this work. Malononitrile, 4-bromotriphenylamine, 4-bromopuinoline, methyl iodide and quinoline-4-boronic acid were purchased from Energy Chemical Co., Ltd. 4-(Diphenylamino)phenylboronic acid was obtained from Soochiral Chemical Science & Technology Co., Ltd. 9',10'-anthracenediyl-bis(methylene)-dimalonic acid (ABDA) and 2', 7'-dichlorodihydrofluorescein diacetate (DCFH-DA) were offered from Aladdin Co., Ltd. Dihydrorhodamine 123 (DHR 123) and hydroxyphenyl fluorescein (HPF)were offered from Sigma-Aldrich, and Shanghai Maokang Biotechnology Co., Ltd, respectively. Phosphate buffered saline (PBS) was offered by Thermo Fisher Scientific. *Escherichia coli* (*E. coli*), *Staphylococcus aureus* (*S. aureus*, ATCC 6538) as well as *Methicillin-resistant S. aureus* (*MRSA*, ATCC43300) were purchased from China General Microbiological Culture Collection Center.

2. Instruments

^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker AV 500 spectrometer. High resolution mass spectra (HRMS) were obtained using an Agilent1290/Bruker maXis impact mass spectrometer. Shimadzu UV-2600 spectrophotometer was employed to measure the UV-vis absorption spectra. PL spectra was measured on a Horiba Fluoromax-4 spectrofluorometer. Hamamatsu absolute PL quantum yield spectrometer (C11347 Quantaurus QY) was used to recorded the fluorescence quantum yields of solution. The absolute quantum yield in solid powder was carried out by photoluminescence spectrometer FLS1000 (Edinburgh). Particle size analysis and the scanning electron microscopy (SEM) images were obtained on a Malvern Zetasizer Nano-S90 and Phenom Pro X (Netherlands), respectively. Confocal laser scanning microscopy (CLSM) images were obtained on a Zeiss LSM7 DUO Laser Scanning Confocal Microscope. An automated cell counter (Countess II, Invitrogen) was utilized for cell counting. The white light irradiation experiment was performed by xenon lamp device (CXE-350, Beijing).

3. Synthesis

3.1 Synthesis of compound TPAQ

4-Bromopuinoline (0.42 g, 2 mmol), 4-(diphenylamino)phenylboronic acid (0.87 g, 3 mmol) and tetrakis (triphenylphosphine)palladium (0) (50 mg) were dissolved in Toluene/THF mixture (10 mL) in two-neck round-bottom flask. 6 mL saturated potassium carbonate solution (2 M) was then added to the reaction mixture under stirring. The reaction was carried out at 100 °C under N_2 atmosphere for 24 h. After the mixture was cooled down, the solvent was removed under reduced pressure. The residue dissolved in DCM (50 mL) was extracted three times with brine and water (3×50 mL). The organic layer was separated and dried over anhydrous Na_2SO_4. The residue was purified *via* flash column chromatography on silica gel to get the product as off-white solid with the yield of 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (d, J = 4.4 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 8.06 (d, J = 8.3 Hz, 1H), 7.71 (dd, J = 11.2, 4.0 Hz, 1H), 7.52 (t, J = 7.3 Hz, 1H), 7.38 (d, J = 8.5 Hz, 2H), 7.34-7.28 (m, 5H), 7.19 (d, J = 8.0 Hz, 6H), 7.08 (t, J = 7.3 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.95, 148.74, 148.32, 147.44, 131.20, 130.50, 129.83, 129.48, 129.33, 126.84, 126.53, 126.00, 124.99, 123.54, 122.62, 121.18.

3.2 Synthesis of compound TPAQ-PF_6

To a stirred solution of compound **TPAQ** (0.15 g, 0.4 mmol) in acetonitrile (10 mL) under nitrogen atmosphere, iodomethane (0.5 mL) was added and then heated to reflux for 16 h. The mixture was poured into diethyl ether to get the precipitates, then the precipitates were filtered and redissolved in 20 mL methanol, followed by adding saturated KPF_6 solution (2 mL). After stirring for 2 h, evaporated the solvent and filtered the residue again, the residue was purified *via* flash column chromatography on silica gel (DCM: CH_3OH, 10:1, v/v) to get the product as red solid with the yield of 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (d, J = 6.2 Hz, 1H), 8.42 (dd, J = 12.1, 9.0

Hz, 2H), 8.23-8.18 (m, 1H), 7.91 (t, J = 6.4 Hz, 2H), 7.45 (d, J = 8.7 Hz, 2H), 7.37 (t, J = 7.8 Hz, 4H), 7.23 (d, J = 7.6 Hz, 4H), 7.20-7.16 (m, 4H), 4.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.05, 151.04, 148.64, 146.27, 139.31, 135.50, 131.46, 129.81, 129.70, 129.28, 127.64, 126.29, 126.07, 125.00, 121.44, 120.72, 118.80, 45.98. HRMS (MALDI): m/z ($[C_{28}H_{23}N_2]^+$): 387.1856; found: 387.1852.

3.3 Synthesis of compound 1

4-Bromotriphenylamine (1.62 g, 5 mmol) was dissolved in 8 mL dry DMF, and stirred in the ice bath at 0 ℃. Subsequently, the solution of $POCl_3$ (7.5 mL) was added dropwise, and then stirred for 30 min. After refluxing at 80 ℃ for 2 hours until the reaction was completed (monitored by TLC), 50 mL water was slowly added into the reaction solution, and then adjusted the pH of the solution to 7-8 to get the yellow solid and filtrate it. The residue was further purified *via* silica column chromatography (petroleum ether: ethyl acetate = 10/1, v/v) to afford the pure product **1** with the yield of 89%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.83 (s, 1H), 7.71-7.68 (m, 2H), 7.45-7.42 (m, 2H), 7.35 (dd, 2H), 7.20-7.14 (m, 3H), 7.05-7.02 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.42, 152.86, 145.84, 145.38, 132.78, 131.34, 129.88, 129.65, 127.42, 126.27, 125.40, 119.92, 117.72.

3.4 Synthesis of CHO-TPAQ

Compound 1 (1.27 g, 3.6 mmol), quinoline-4-boronic acid (0.76 g, 4.4 mmol), tetrakis (triphenylphosphine)palladium (0) (125 mg) and tetrabutylammonium bromide (0.6 eq.) were dissolved in 10 mL of dry ethanol in two-neck round-bottom flask. 6 mL saturated potassium carbonate solution (2 M) was then added to the reaction mixture under stirring. The reaction was carried out at 80 °C under N_2 atmosphere for 24 h. The solvent was removed under reduced pressure after the mixture was cooled down. The residue dissolved in DCM (50 mL) was extracted three times with brine and water (3×50 mL). The organic layer was separated and dried over anhydrous Na_2SO_4. The

residue was purified by flash column chromatography on silica gel to obtain the product as yellow solid with the yield of 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.85 (d, *J* = 2.1 Hz, 1H), 8.20 (t, *J* = 5.8 Hz, 1H), 8.02 (t, *J* = 5.9 Hz, 1H), 7.77-7.73 (m, 1H), 7.56 (dd, *J* = 8.3, 7.0 Hz, 1H), 7.50-7.46 (m, 1H), 7.43-7.37 (m, 1H), 7.33-7.30 (m, 1H), 7.26 (dt, *J* = 5.5, 1.8 Hz, 1H), 7.22 (s, 1H), 7.18-7.14 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.47, 153.02, 149.77, 148.52, 147.92, 146.66, 146.02, 133.89, 131.37, 130.89, 129.97, 129.78, 129.53, 126.78, 126.67, 126.63, 125.74 125.57, 125.36, 121.24, 120.34.

3.5 Synthesis of CN-TPAQ

A solution of malononitrile (0.09 g, 1.35 mmol) in acetonitrile (25 mL) was added to a mixture of piperidine (0.25 mL, 2.5 mmol) and **CN-TPAQ** (0.4 g, 1 mmol). The solution was stirred at 40 ℃ for 1 h. After cooling to room temperature, the residue dissolved in DCM (50 mL) was extracted three times with brine and water (3×50 mL). The organic layer was separated and dried over anhydrous Na_2SO_4. The residue was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate, 10:1, v/v) to get the product as orange solid with the yield of 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, *J* = 4.4 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.04-8.00 (m, 1H), 7.83 (d, *J* = 9.0 Hz, 2H), 7.80-7.75 (m, 1H), 7.61-7.53 (m, 4H), 7.49-7.45 (m, 2H), 7.40-7.36 (m, 3H), 7.32 (td, *J* = 7.7, 1.3 Hz, 3H), 7.12 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.94, 153.15, 149.88, 148.63, 147.55, 145.61, 145.07, 135.16, 133.03, 131.11, 130.21, 129.92, 129.58, 127.03, 126.89, 126.51, 126.12, 125.63, 123.40, 121.29, 119.28, 115.05, 113.99, 76.32.

3.6 Synthesis of CN-TPAQ-PF_6

The synthetic process was similar with **TPAQ-PF_6** except for the change of starting

materials. Pure **CN-TPAQ-PF$_6$** was isolated as red powder with the yield of 83%. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.51 (d, J = 6.2 Hz, 1H), 8.58 (d, J = 8.9 Hz, 1H), 8.40-8.37 (m, 1H), 8.35-8.30 (m, 2H), 8.17 (d, J = 6.1 Hz, 1H), 8.08 (t, J = 7.7 Hz, 1H), 7.92 (d, J = 9.0 Hz, 2H), 7.75 (d, J = 8.5 Hz, 2H), 7.54 (t, J = 7.8 Hz, 2H), 7.47 (d, J = 8.5 Hz, 2H), 7.37 (dd, J = 13.7, 7.4 Hz, 3H), 7.12 (d, J = 8.9 Hz, 2H), 4.66 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.91, 157.32, 152.65, 149.51, 147.73, 145.05, 139.36, 135.51, 133.48, 132.28, 131.49, 130.82, 130.61, 128.77, 127.77, 127.41, 127.22, 125.98, 124.52, 122.34, 120.05, 115.64, 114.73, 45.70。HRMS (MALDI): m/z ($[C_{32}H_{23}N_4]^+$): 463.1917; found: 463.1911.

4. ROS Generating Ability Test

4.1 General ROS detection

2', 7'-Dichlorodihydrofluorescein (DCFH) was employed as a probe to examine the generation of general ROS (λ_{ex} = 480 nm, λ_{em} = 525 nm). Initially, 0.01 M NaOH was used to hydrolyze the acetate-protected DCFH-DA. Subsequently, PBS buffer solution containing DCFH (50 μM) was added with 10 μM PSs. The PL spectrum of DCFH that was mixed with various PBs was recorded under white light irradiation (20 mWcm^{-2}). The fluorescence intensity at 514 nm was recorded to indicate the general ROS generation rate.

4.2 Superoxide anion radical ($O_2^{\bullet-}$) detection

Dihydrorhodamine 123 (DHR 123) was used as a probe to examine the generation of superoxide anion radical (λ_{ex} = 480 nm, λ_{em} = 525 nm), which can be converted to Rhodamine 123 in the presence of $O_2^{\bullet-}$. PBS buffer solution containing 20 μM DHR 123 was added with 10 μM PSs. The PL spectrum of DHR 123 that was mixed with various PBs was recorded under white light irradiation (20 mWcm^{-2}). The fluorescence intensity at 525 nm was recorded to indicate the $O_2^{\bullet-}$ generation rate.

4.3 Hydroxyl radical ($OH^{\bullet-}$) detection

Hydroxyphenyl fluorescein (HPF) was used as a probe to examine the generation of hydroxyl radical (λ_{ex} = 480 nm, λ_{em} = 514 nm), PBS buffer solution containing 10 μM

HPF (stock solution: 5 mM in DMF) was added with 10 μM PSs. The PL spectrum of HPF that was mixed with various PBs was recorded under white light irradiation (20 $mWcm^{-2}$). The fluorescence intensity at 514 nm was recorded to indicate the $OH^{\bullet-}$ generation rate.

4.4 Singlet oxygen ($^1O_2$) detection

PBS buffer solution containing 50 μM ABDA was added with 10 μM PSs. After irradiating the mixture by white light irradiation (20 $mWcm^{-2}$), subsequently, the absorption spectra were monitored. The decrease in absorbance relative to the initial value was recorded at 380 nm to indicate the rate of decomposition of ABDA ($^1O_2$ generation rate).

5. Theoretical Calculation

The S_1 state geometries in gas phase was optimized using time-dependent density function theory (TD-DFT) method with B3LYP functional at the basis set level of 6-31G(d,p), using the Gaussian 16 package. The ΔE_{ST} values were vertical energy between the S_1 and T_1 states obtained at the level of B3LYP/6-31G(d,p).

6. Antibacterial experiments

6.1 Bacteria culture

Individual colonies of S. aureus and MRSA on Nutrient Broth solid agar plates were transferred to 5-10 mL Nutrient Broth liquid medium and grown at 37°C for a certain time (8-24 h). Bacteria were harvested *via* centrifugation (7100 rpm, 3 min) and washed three times with phosphate buffered saline (PBS). The supernatant was removed and the remaining S. aureus or MRSA was resuspended in PBS and its OD_{600} value was adjusted to 1 (approximate to 1×10^9 CFU mL^{-1}).

6.2 Bacteria staining

To get a *MRSA* bacterial suspension with bacterial amount of 1×10^8 CFU mL^{-1}, 100 μL Bacterial suspensions (1×10^9 CFU mL^{-1}) was added to PBS solution (900 μL). Then 2 μL **CN-TPAQ/CN-TPAQ-PF$_6$** (1 mM in DMSO) was added to 1 mL 1×10^8

CFU mL^{-1} bacterial suspension and incubated for 30 min on a shaking incubator (170 rpm) at 37 ℃. Then the bacteria were harvested *via* centrifuging (7100 rpm for 2 min) and resuspended in PBS (10 μL). 2 μL suspension was placed in drops on a clean glass slide, and then covered with a coverslip to immobilize the bacteria. The specimens were then observed and taken photographs by CLSM. The fluorescence photograph of **CN-TPAQ /CN-TPAQ-PF_6** was highlighted in red (For **CN-TPAQ/CN-TPAQ-PF_6**, λ_{ex} = 488 nm, λ_{em} = 500-700 nm).

6.3 Colocalization assay

S. aureus or *MRSA* bacterial suspension (1×10^8 CFU mL^{-1}, 1 mL) were incubated with **CN-TPAQ/CN-TPAQ-PF_6** (2 μM) and Hoechst 33342 (5 μg mL^{-1}) simultaneously for 30 min in 37 ℃. Then the bacteria were harvested *via* centrifuging (7100 rpm for 2 min) and resuspended in 10 μL of PBS. 2 μL suspension was placed in drops on a clean glass slide, and then covered with a coverslip, subsequently, imaged by CLSM at channel mode (For Hoechst 33342, λ_{ex} = 405 nm, λ_{em} = 430-500 nm; and for **CN-TPAQ/CN-TPAQ-PF_6**, λ_{ex} = 488 nm, λ_{em} = 600-700 nm).

6.4 Bacterial ROS measurements

MRSA bacterial suspension (OD_{600} = 0.1) was incubated with DCFH-DA (20 μM) for 2 hours. Then incubated with 2 μM **CN-TPAQ/CN-TPAQ-PF_6** at 37 °C for 30 min. The suspension was subsequently irradiated with white light (40 $mWcm^{-2}$) for 5 min. Then the bacteria were harvested *via* centrifuging (7100 rpm for 2 min) and resuspended in PBS (10 μL). 2 μL suspension was placed in drops on a clean glass slide, and then covered with a coverslip to immobilize the bacteria. Fluorescence intensity of DCFH solution was recorded at 500-550 nm with the excitation wavelength of 488 nm.

6.5 Co-staining of dead bacteria

S. aureus or *MRSA* bacterial suspension (1×10^8 CFU mL^{-1}, 1 mL) were incubated with **CN-TPAQ/CN-TPAQ-PF_6** (2 μM) for 30 min in 37℃ and then treated in dark or white light irradiation (40 mW cm^{-2}, 30 min). Then SYTOX™ Blue (5 μg mL^{-1}) was added

to the bacterial suspension. After incubating the mixture at room temperature for 5 min, the bacteria were harvested *via* centrifuging (7100 rpm for 2 min) and re-suspended in PBS (10 μL). 2 μL suspension was placed in drops on a clean glass slide, and then covered with a coverslip to immobilize the bacteria. The specimens were then taken photographs by CLSM (For SYTOX^{TM} Blue, λ_{ex} = 405 nm, λ_{em} = 500-650 nm; and for **CN-TPAQ/CN-TPAQ-PF$_6$**, λ_{ex} = 488 nm, λ_{em} = 600-700 nm).

6.6 Antibacterial Experiments.

S. aureus or *MRSA* bacterial suspension (1×10^8 CFU mL^{-1}, 1 mL) were incubated with certain concentration **CN-TPAQ /CN-TPAQ-PF$_6$** for 30 min in 37 ℃ and then treated in dark or with white light irradiation (40 mW cm^{-2}, 30 min). And then the suspension was serially diluted with suitable folds (10^4,10^3,10^2,10^1) or without diluted. Then 100 μL suspension was spread on NB agar plate and incubation at 37 °C for 24 h (each group with three parallel independent plates). Then the number of colony-forming units was counted. The number of survived bacterial in suspension before dilute is calculate according to following equation: $C = C_{plate} \times 10^A$ (Where C is the actual CFU of colony number before dilute, C_{plate} is the average number of colony-forming units on agar plate, and A is diluted magnitude).

6.7 SEM characterization

S. aureus or *MRSA* bacterial suspension (1×10^8 CFU mL^{-1}, 1 mL) were incubated with certain concentration of **CN-TPAQ/CN-TPAQ-PF$_6$** for 30 min at 37 ℃ and then treated in dark or with white light irradiation (40 mW cm^{-2}, 30 min). Then the bacteria suspension was harvested *via* centrifuging (7100 rpm for 2 min) and re-suspended in glutaraldehyde (0.5%) in PBS for overnight. Under room temperature, gradient dehydration was operated with 20, 40, 60, 70, 80, 90, 95, 99 and 100% ethanol aqueous solution in sequence with each incubation time of 10 min. Finally, the bacterial was resuspended with 50 μL ethanol and 10 μL was dropped onto silicon wafers (5∗5 mm) and wait for 10 min after drying. The samples were then covered by metal spraying and viewed by SEM.

6.8 Determination of minimum inhibitory concentrations (MICs)

The bacterial suspensions were diluted into 5×10^5 CFU mL^{-1} in PBS and incubated with different concentrations of **CN-TPAQ/CN-TPAQ-PF_6**, and then transfered to a 96 well plate. The 96 well plates were shaken (170 rpm) at 37 °C for 30 min and then treated in dark or with white light irradiation (40 mW cm^{-2}, 30 min). After cultured 16 h on a shaking incubator (170 rpm) at 37 ℃, the OD_{600} value was measured the absorbance at 600 nm using Microplate Reader. MICs were detected at the concentration that no growth was observed.

6.9 Lake water sterilization

The natural water of western lake of SCUT was collected and incubated with **CN-TPAQ-PF_6** (2 μM) for 30 min in 37℃. Subsequently, the suspension was treated in dark or with white light irradiation (40 mW cm^{-2}, 30 min). Without further dilution, 100 μL suspension was laid on NB agar plate and incubation at 37 °C for 24 h. Then the colony-forming units was counted and photographed.

7. Statistical analysis

Statistical analysis was carried out by GraphPad Prism 5 software. All dates are expressed as mean ± standard deviation (SD) with n = 3, unless otherwise stated. Differences between groups were identified by Student' s t-test or one-way analysis of variance (ANOVA). $^{**}P < 0.01$, and $^{***}P < 0.001$ were statistically significant.

Supplementary Figures and Tables

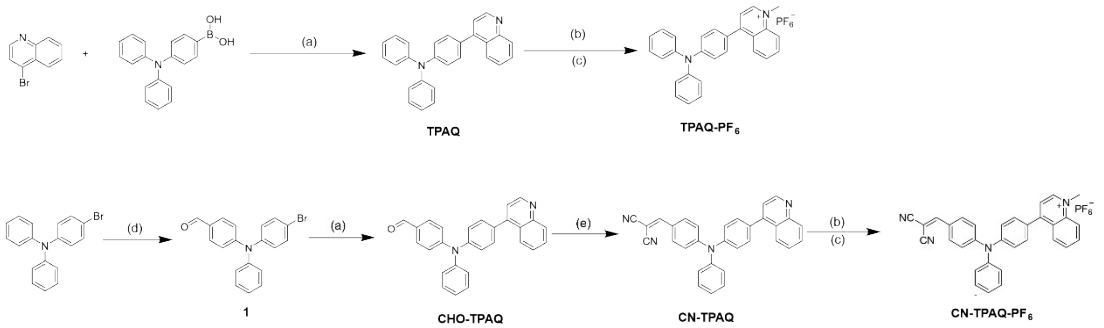

Figure S1. Synthetic routes of **TPAQ**, **TPAQ-PF_6**, **CN-TPAQ**, **CN-TPAQ-PF_6**. Reagents and conditions: (a) $Pd(PPh_3)_4$, toluene, THF, K_2CO_3, tetrabutylammonium bromide. (b) Iodomethane, acetonitrile, diethyl ether. (c) KPF_6. (d) $POCl_3$, DMF, 80 ℃. (e) Malononitrile, acetonitrile, piperidine.

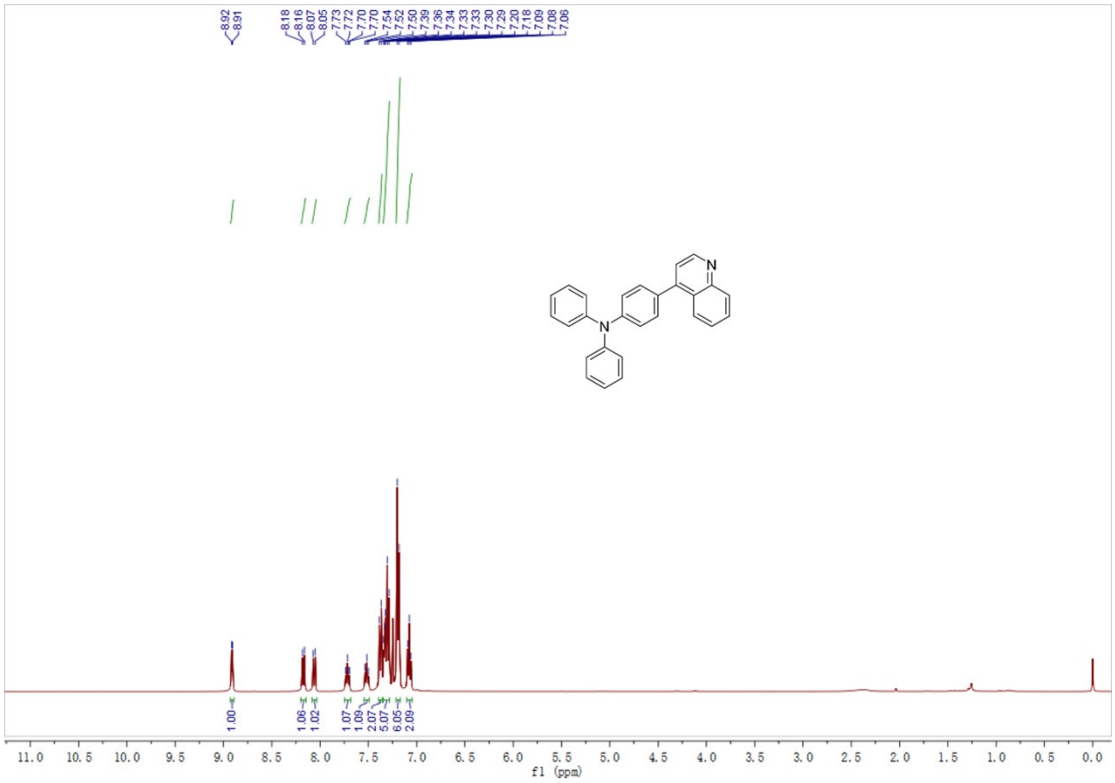

Figure S2. ^1H NMR spectrum of **TPAQ** in $CDCl_3$.

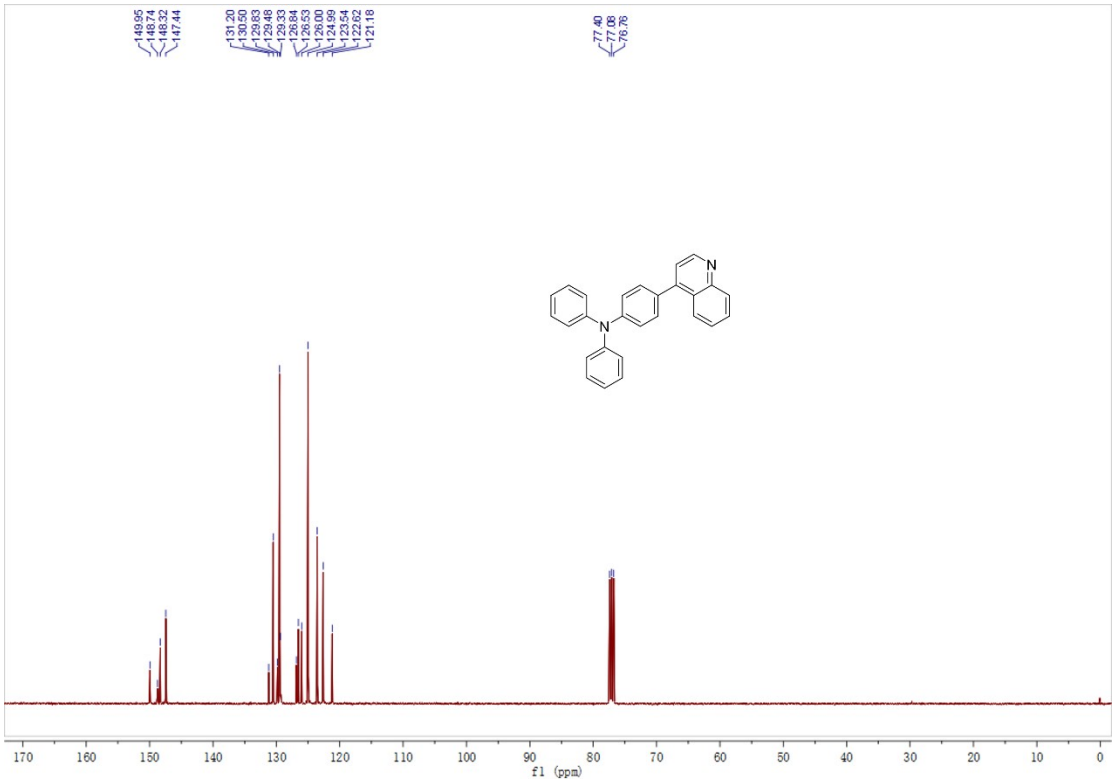

Figure S3. ^{13}C NMR spectrum of **TPAQ** in $CDCl_3$.

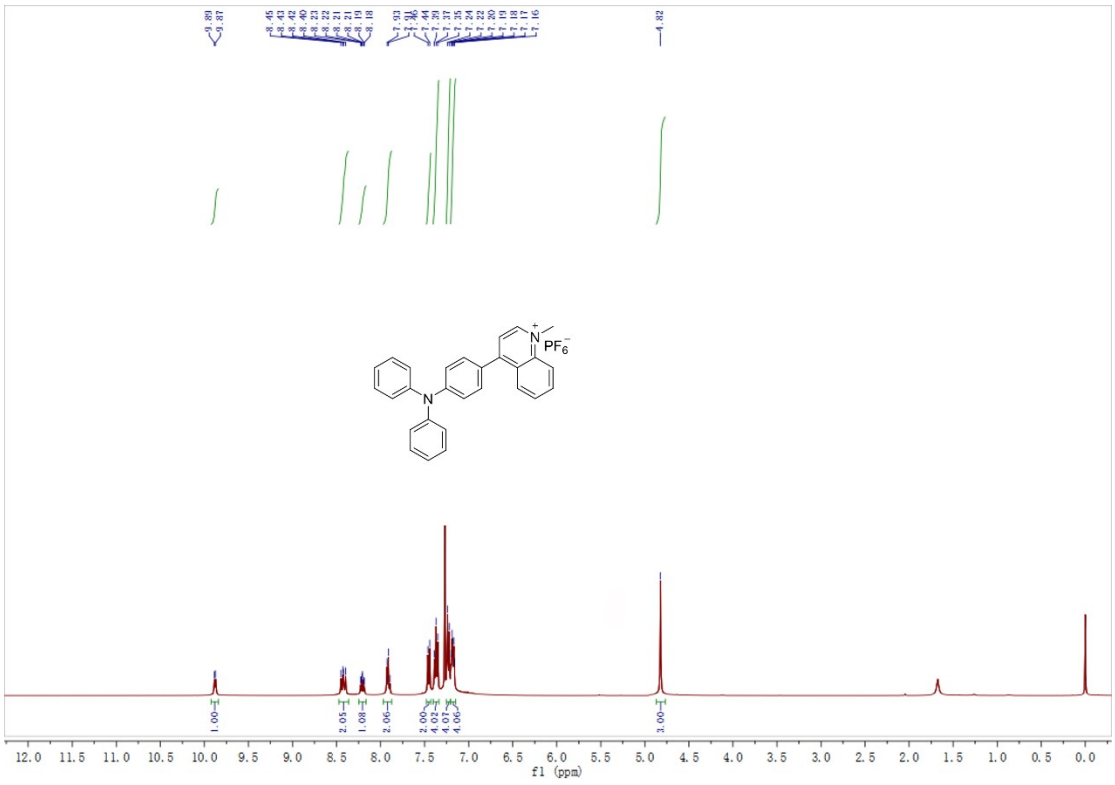

Figure S4. ^{1}H NMR spectrum of **TPAQ-PF$_6$** in $CDCl_3$.

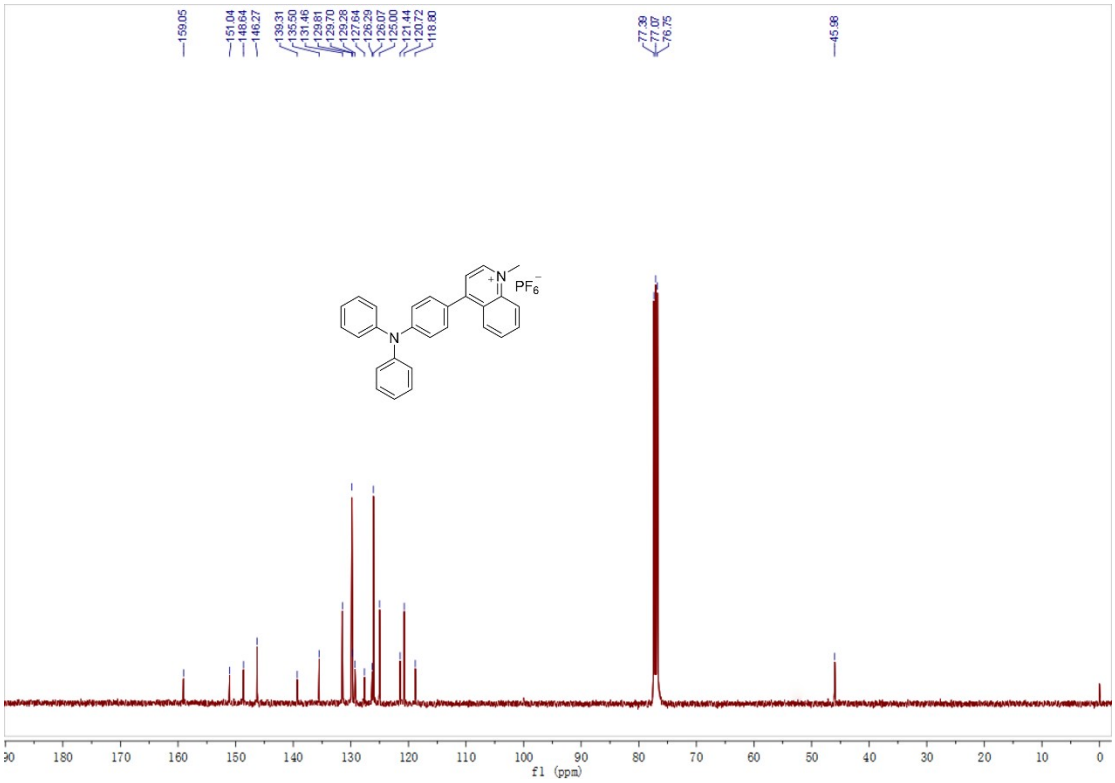

Figure S5. ^{13}C NMR spectrum of **TPAQ-PF$_6$** in $CDCl_3$.

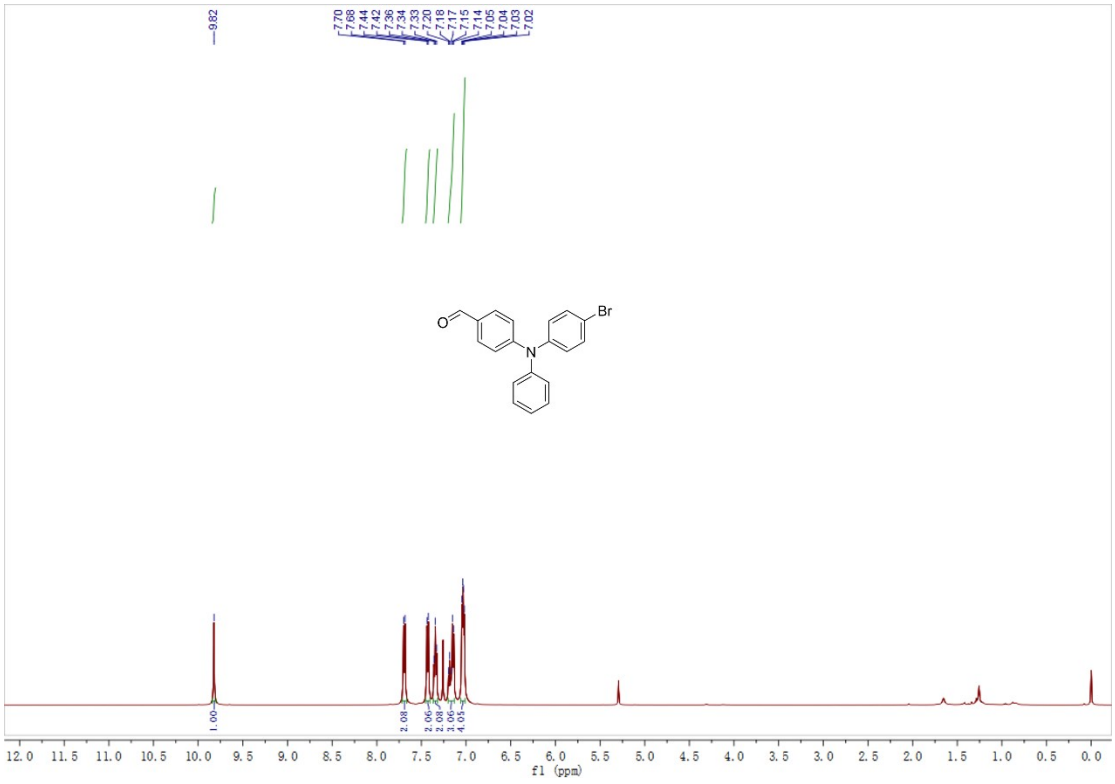

Figure S6. ^{1}H NMR spectrum of **1** in $CDCl_3$.

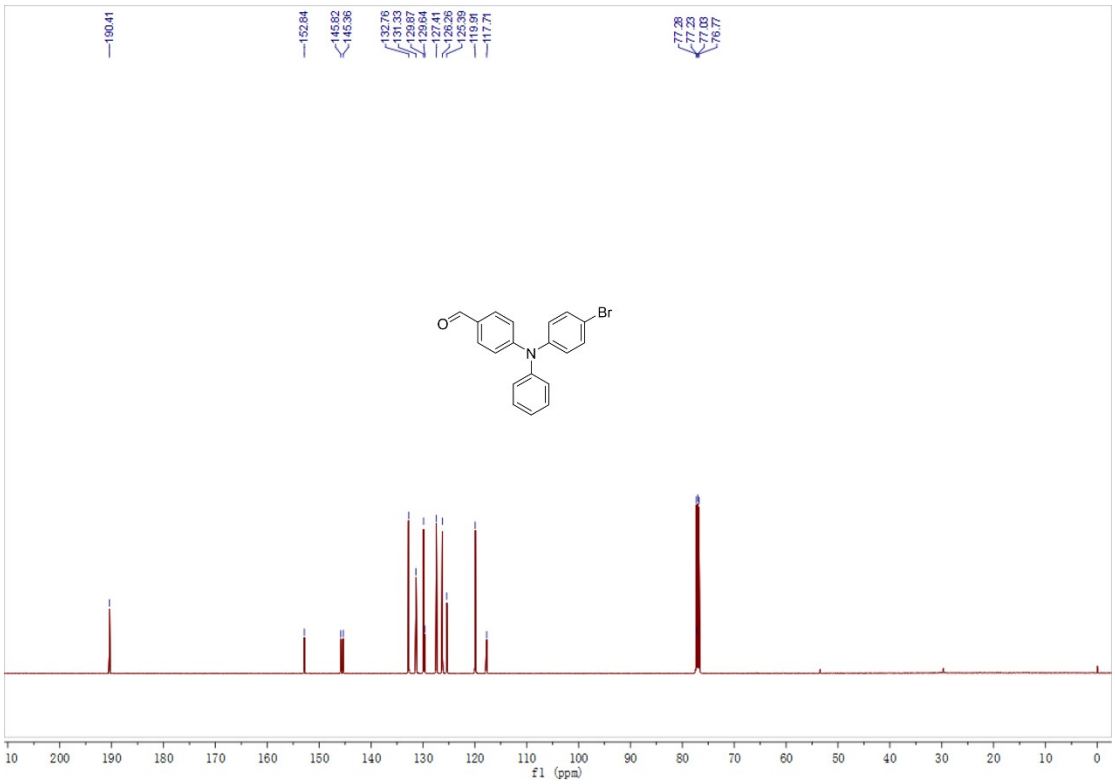

Figure S7. ^{13}C NMR spectrum of **1** in $CDCl_3$.

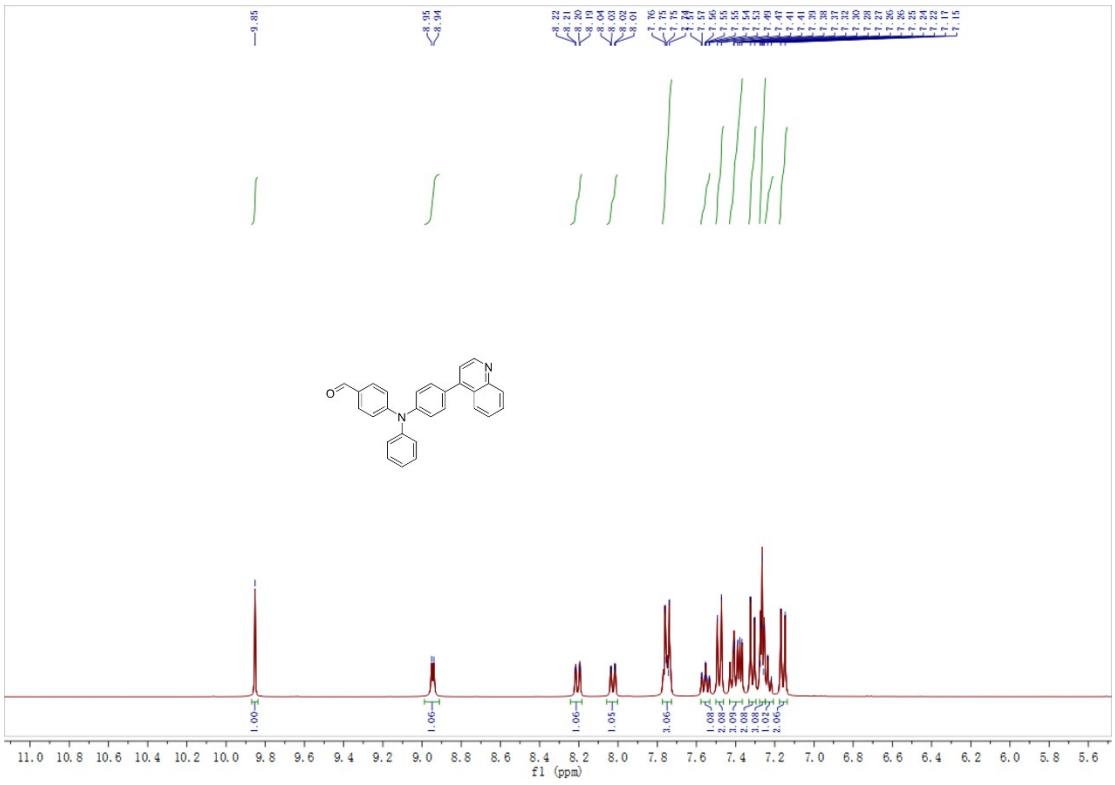

Figure S8. ^{1}H NMR spectrum of **CHO-TPAQ** in $CDCl_3$.

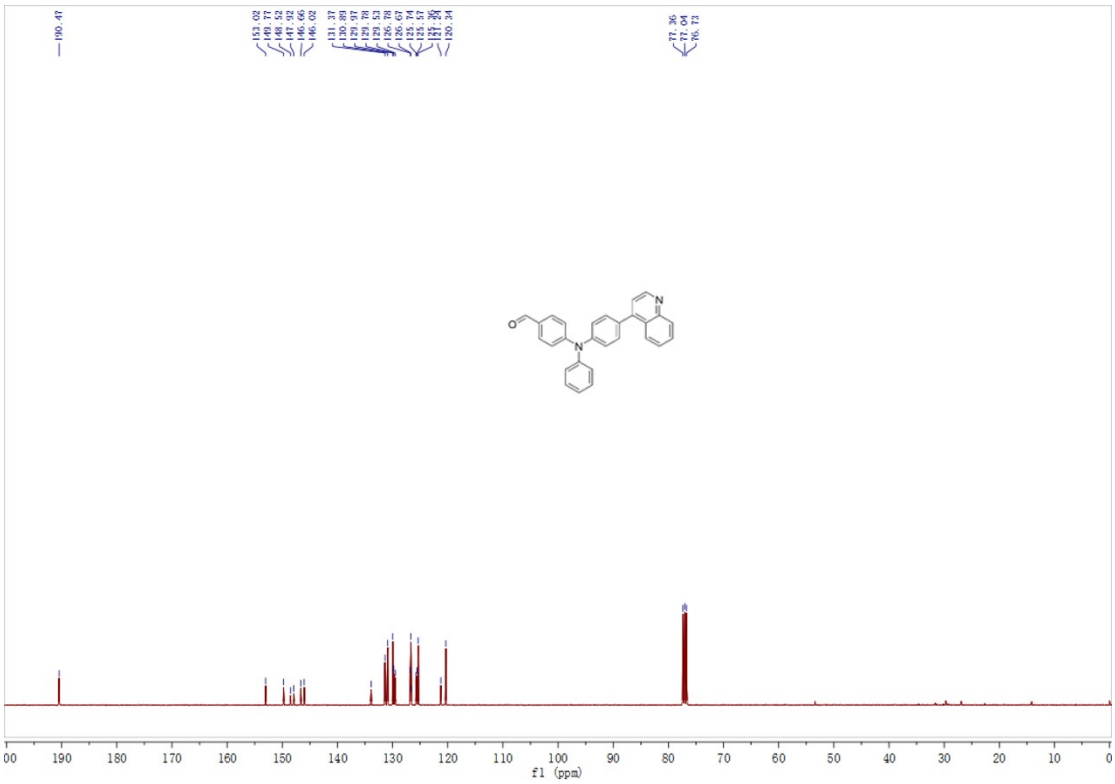

Figure S9. ^{13}C NMR spectrum of **CHO-TPAQ** in $CDCl_3$.

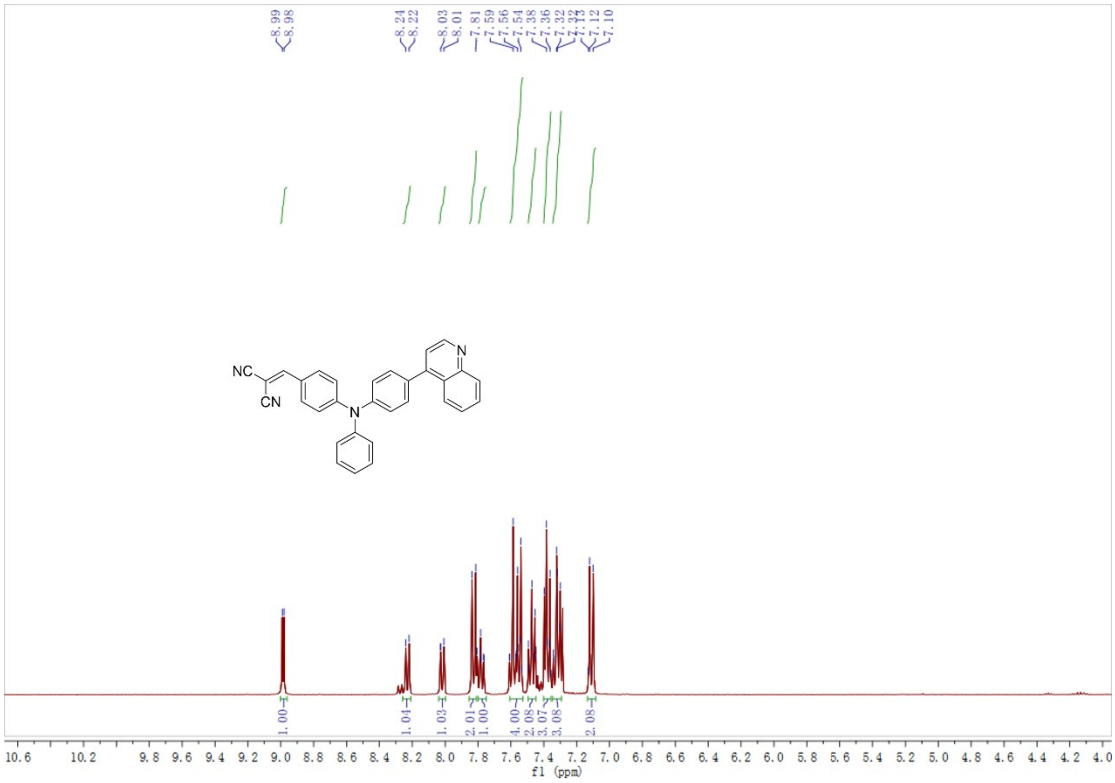

Figure S10. ^{1}H NMR spectrum of **CN-TPAQ** in $CDCl_3$.

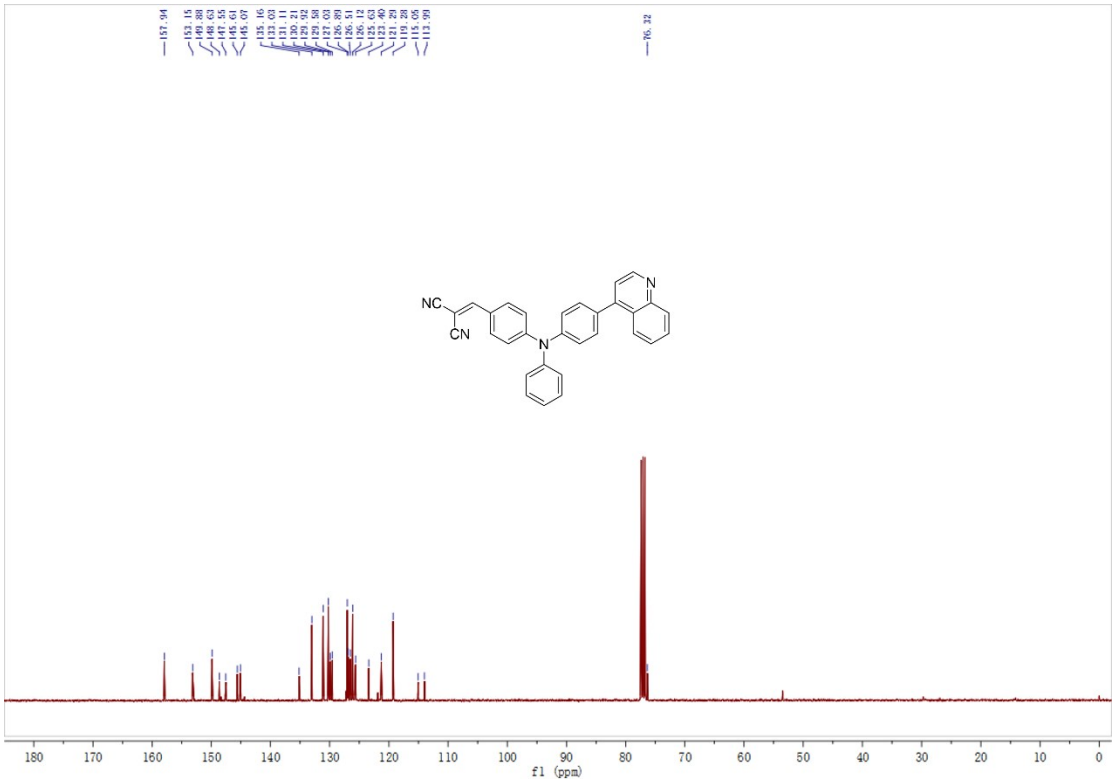

Figure S11. ^{13}C NMR spectrum of **CN-TPAQ** in $CDCl_3$.

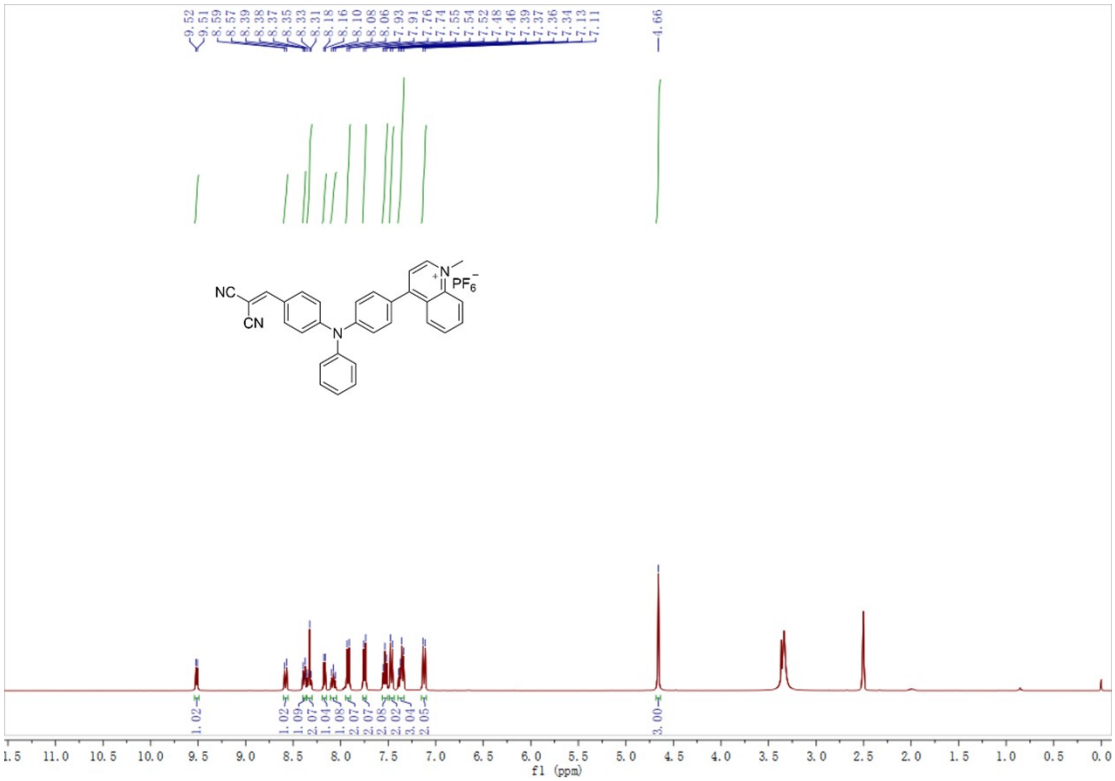

Figure S12. ^{1}H NMR spectrum of **CN-TPAQ-PF$_6$** in DMSO-d_6.

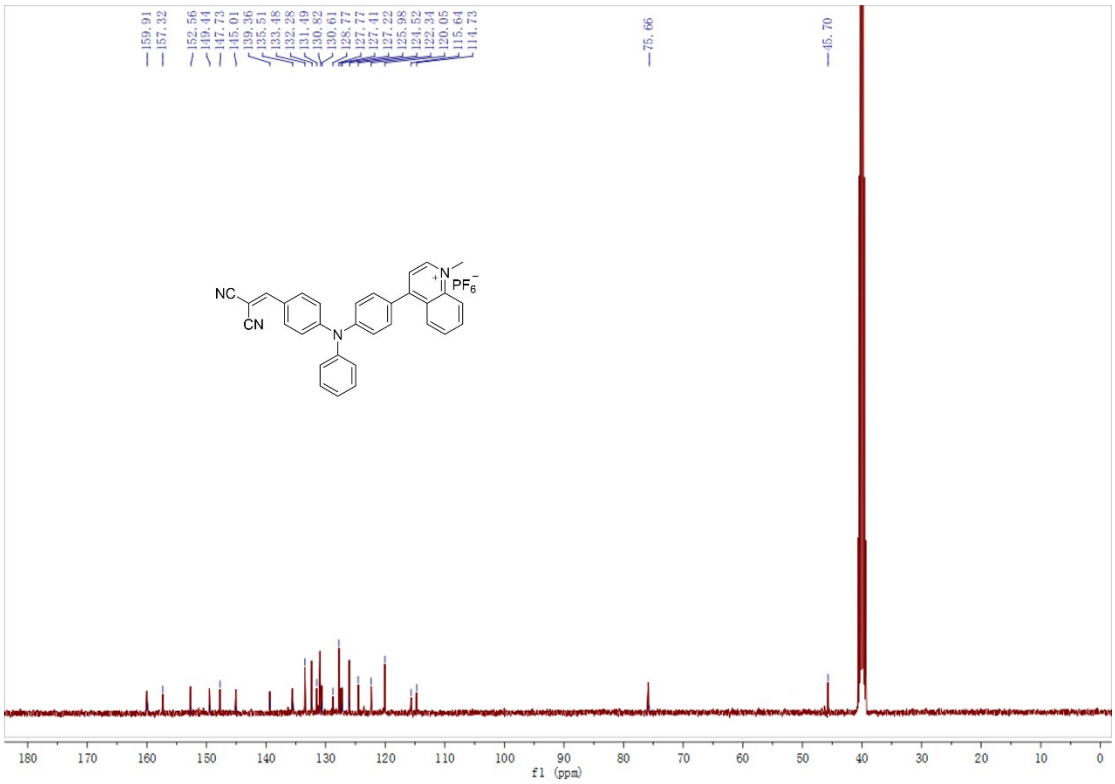

Figure S13. ^{13}C NMR spectrum of **CN-TPAQ-PF$_6$** in DMSO-d_6.

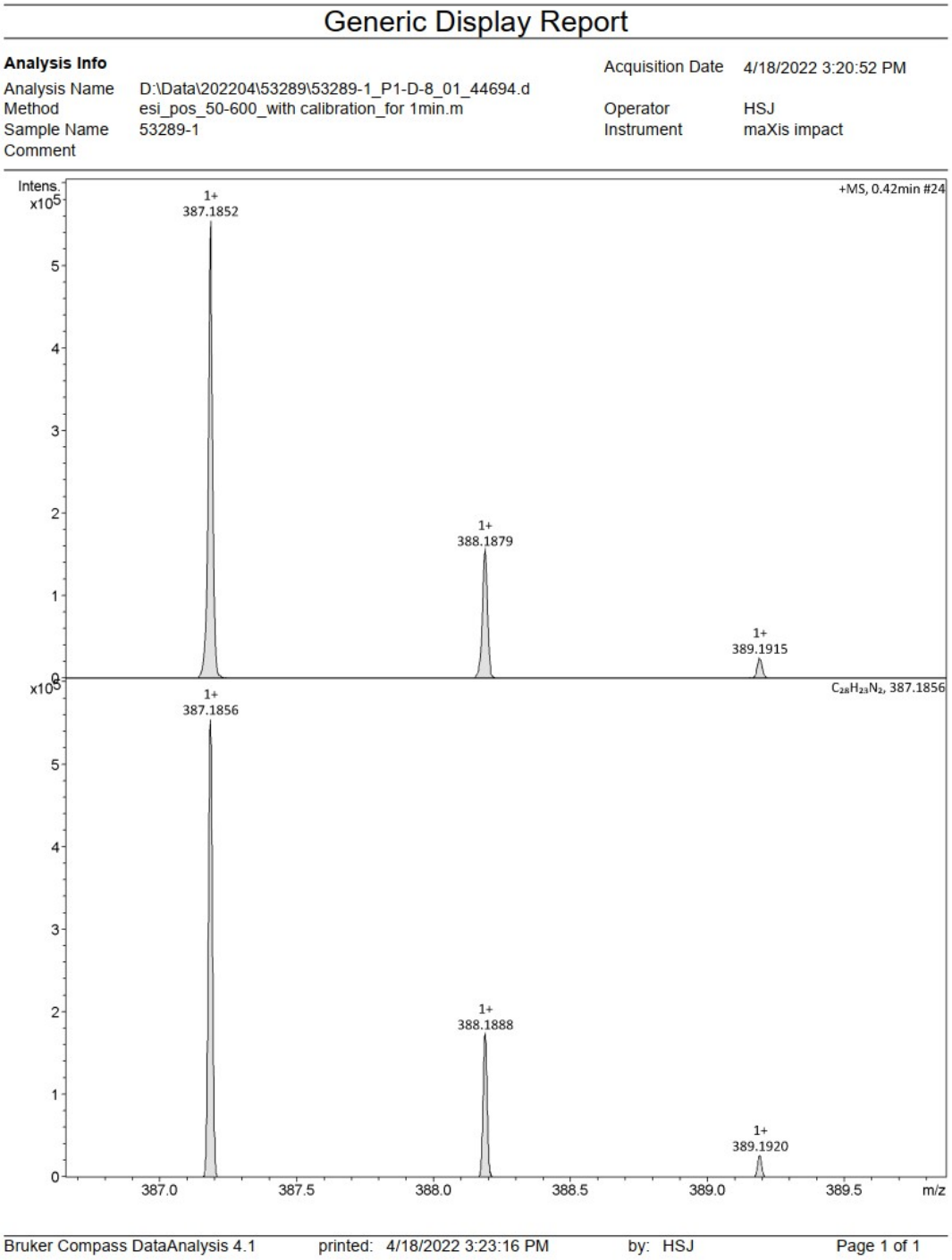

Figure S14. HRMS of **TPAQ-PF_6**.

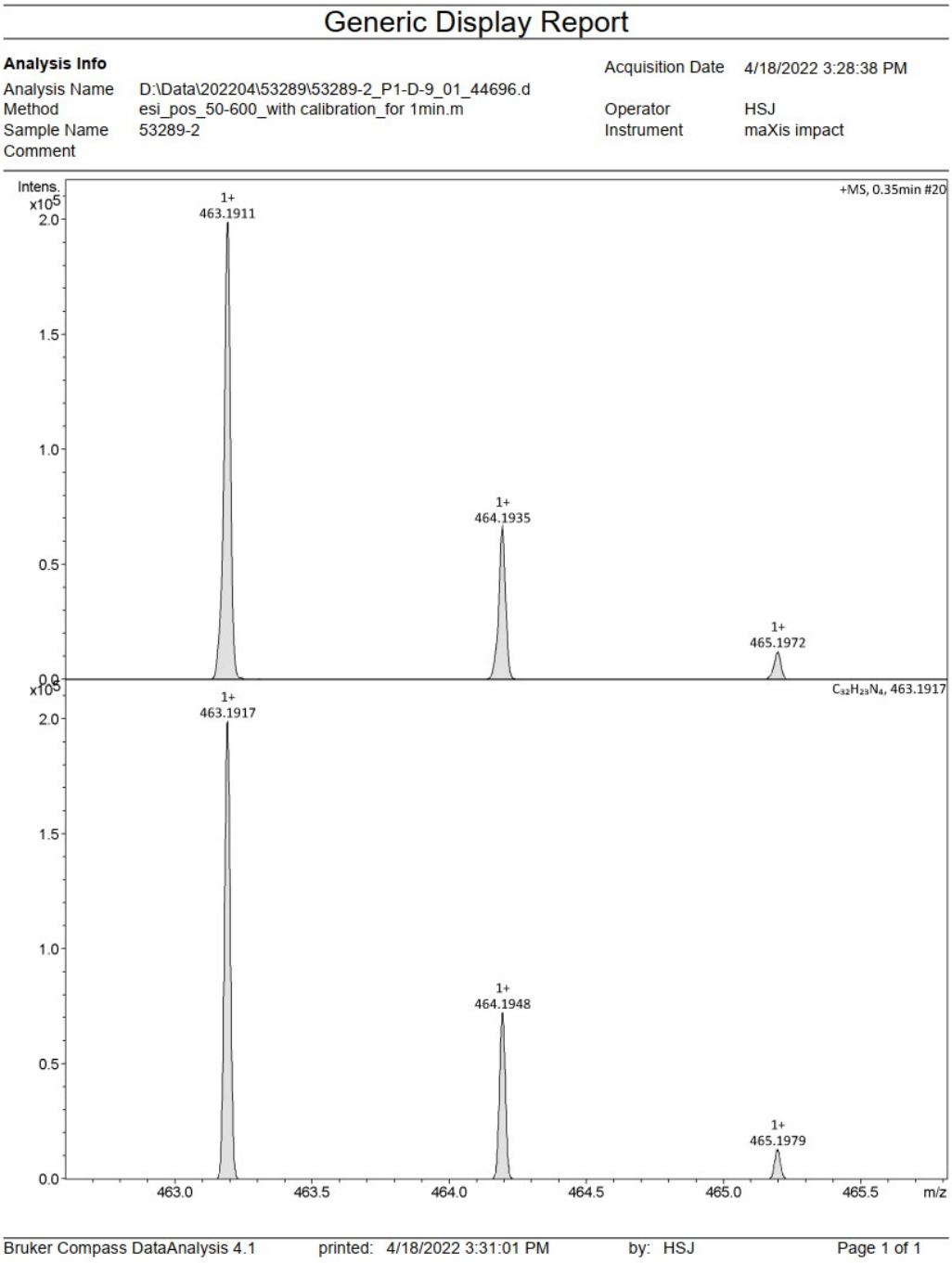

Figure S15. HRMS of **CN-TPAQ-PF$_6$**.

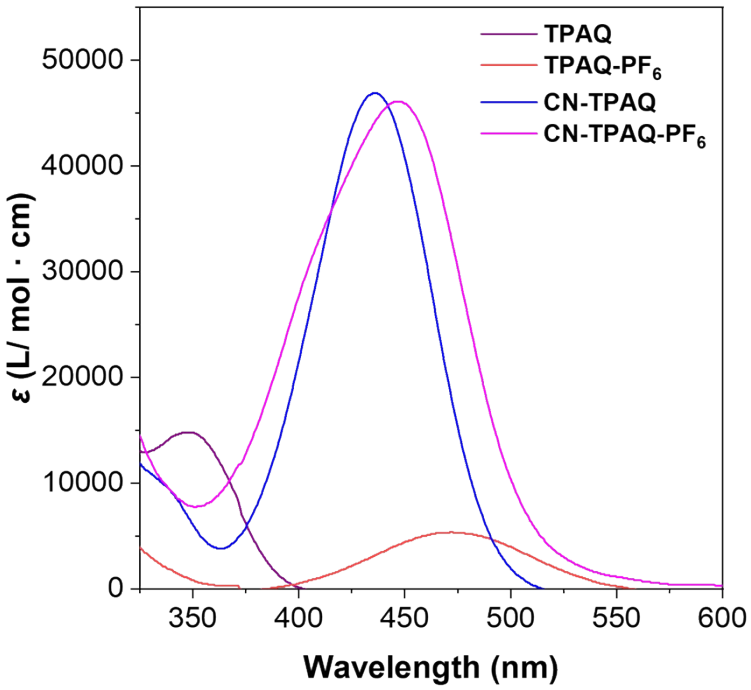

Figure S16. Absorption spectra of these four AIE PSs in THF solution (concentration: 10 μM).

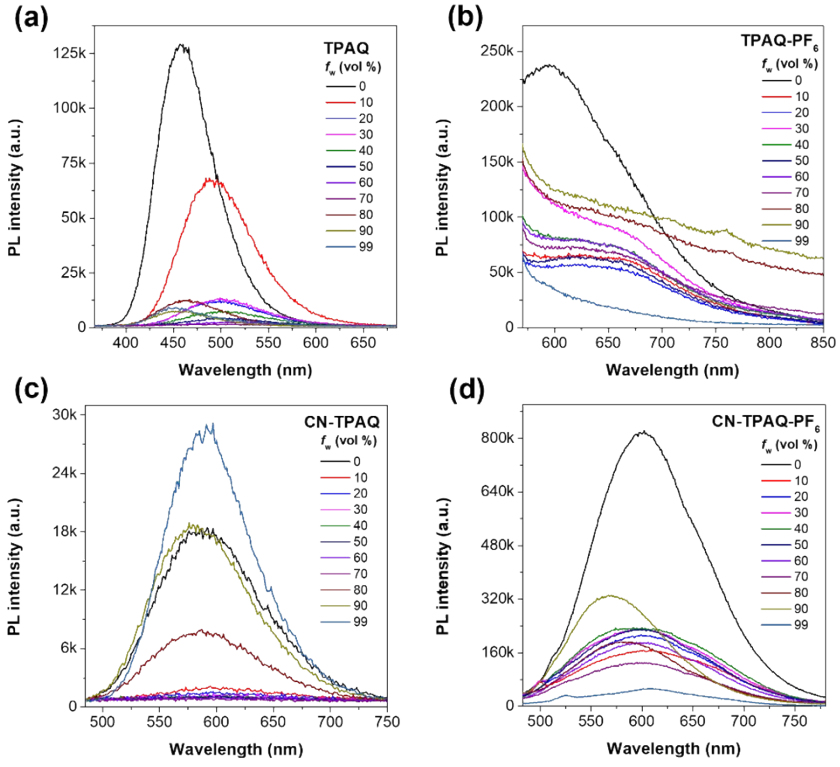

Figure S17. Plot of PL intensity versus water fraction of these four PSs in the THF/H_2O mixtures.

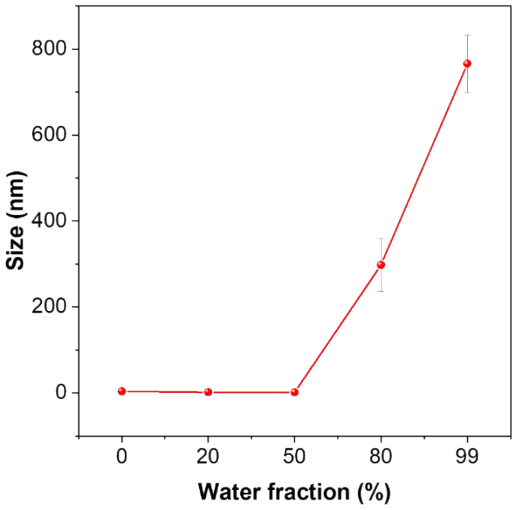

Figure S18. Average hydrodynamic size of **CN-TPAQ-PF$_6$** at different water fraction.

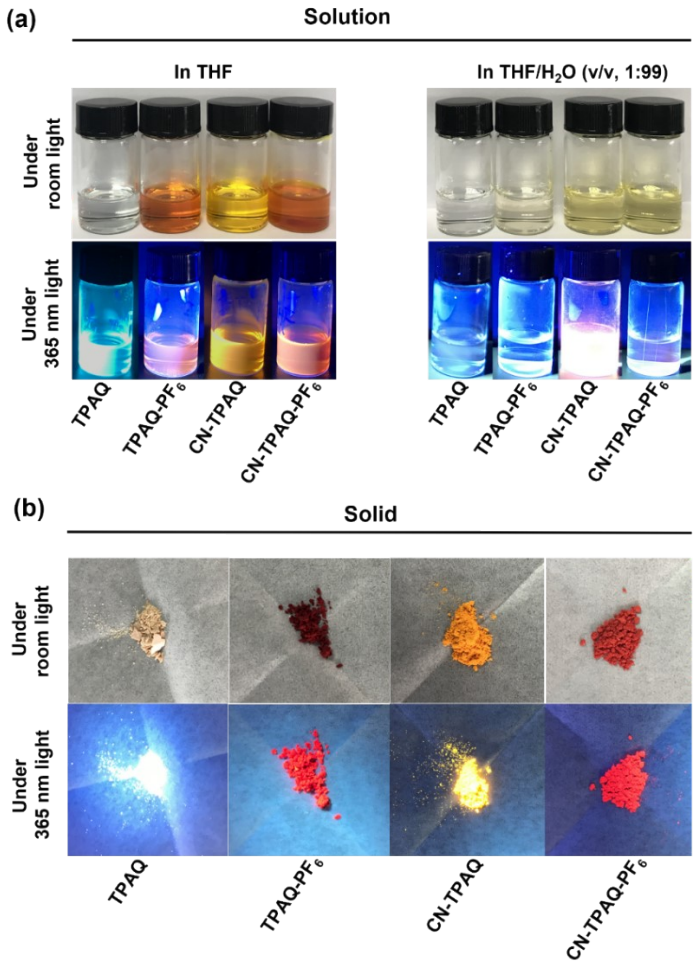

Figure S19. (a) Photos of these four AIE PSs in different solution system under room light and 365 nm light; (b) Photos of these four AIE PSs in solid state under room light and 365 nm light.

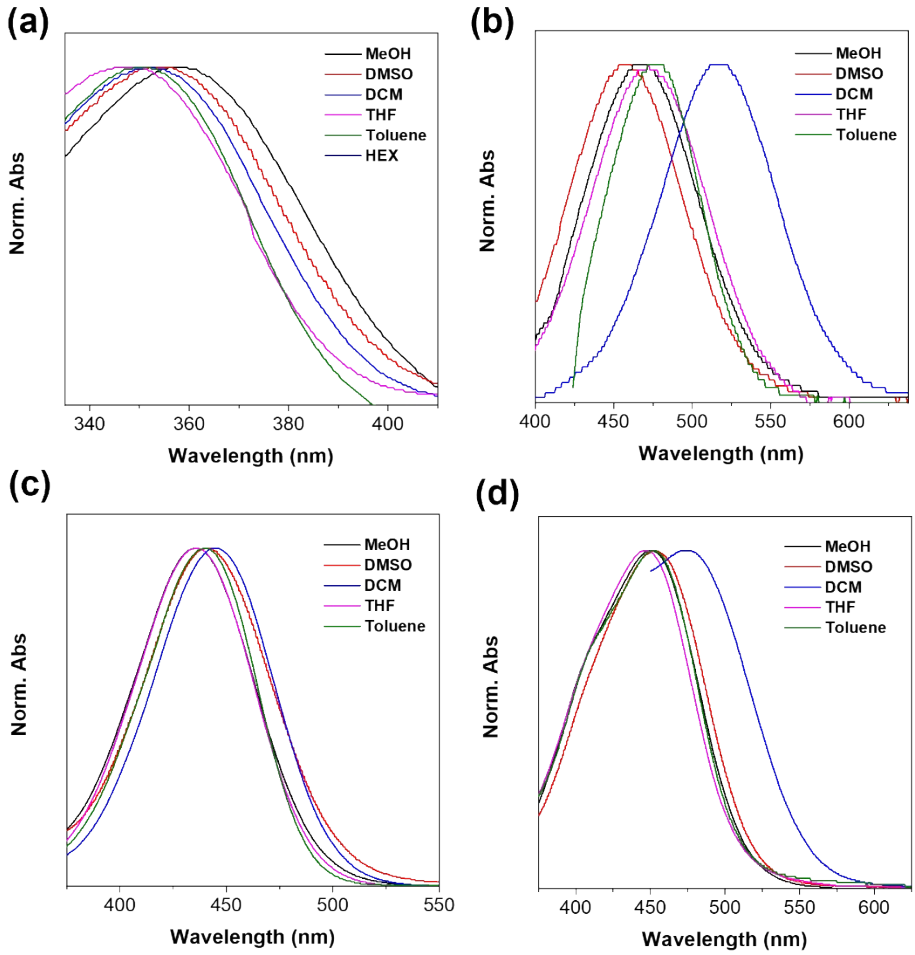

Figure S20. Normalized UV spectra of **TPAQ**, **TPAQ-PF$_6$**, **CN-TPAQ** and **CN-TPAQ-PF$_6$** in different solvents with various polarities.

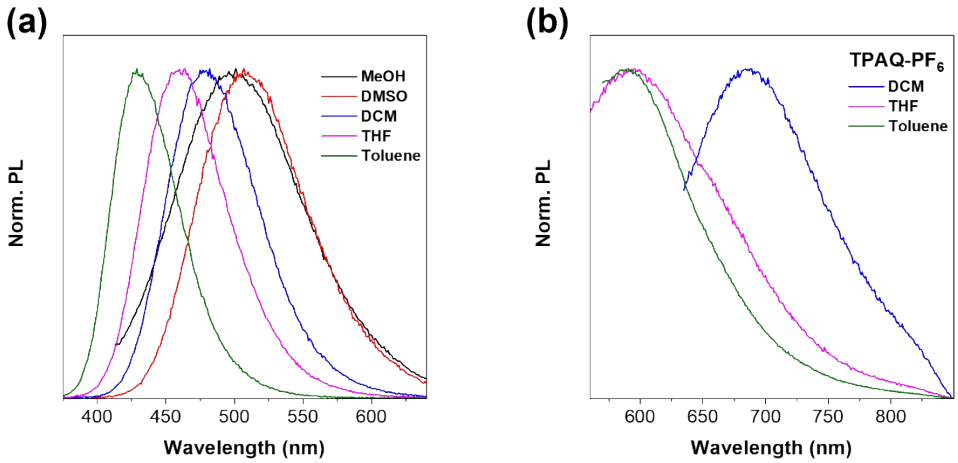

Figure S21. Normalized PL spectra of **TPAQ** and **TPAQ-PF$_6$** in different solvents with various polarities.

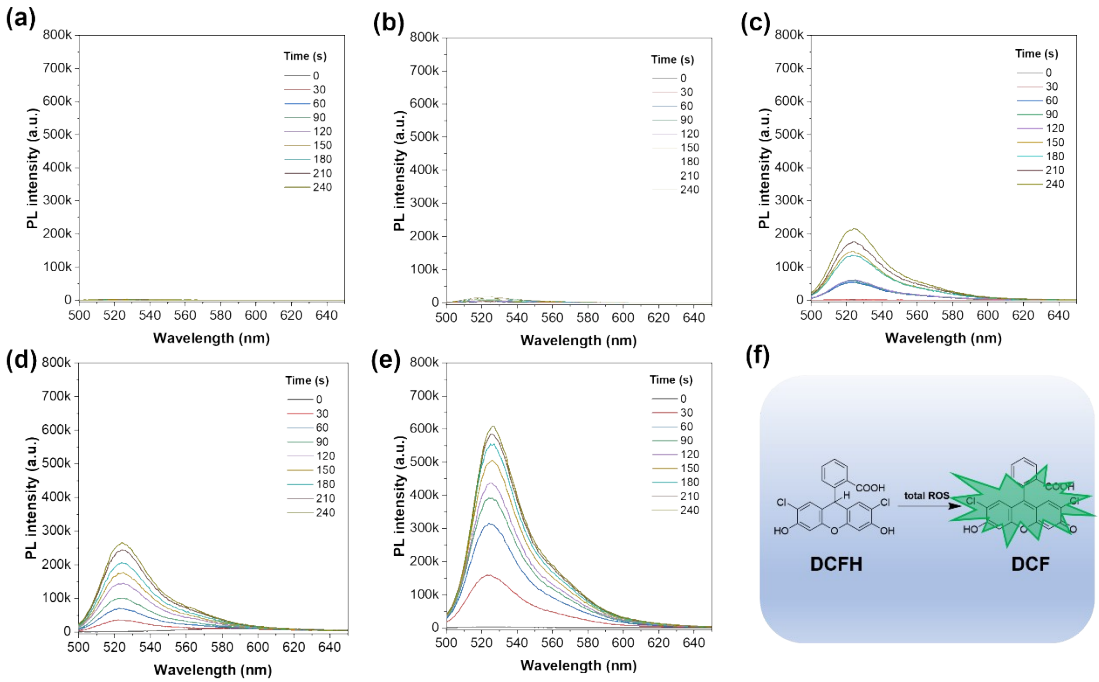

Figure S22. PL spectra of DCFH in the presence of (a) blank, (b) **TPAQ**, (c) **TPAQ-PF$_6$**, (d) **CN-TPAQ** and (e) **CN-TPAQ-PF$_6$** in DMSO/PBS (v/v = 1: 99) mixture under the different irradiation time. (f) Detection mechanism of DCFH for total ROS. [AIE PSs] = 10 μM, [DCFH] = 50 μM;

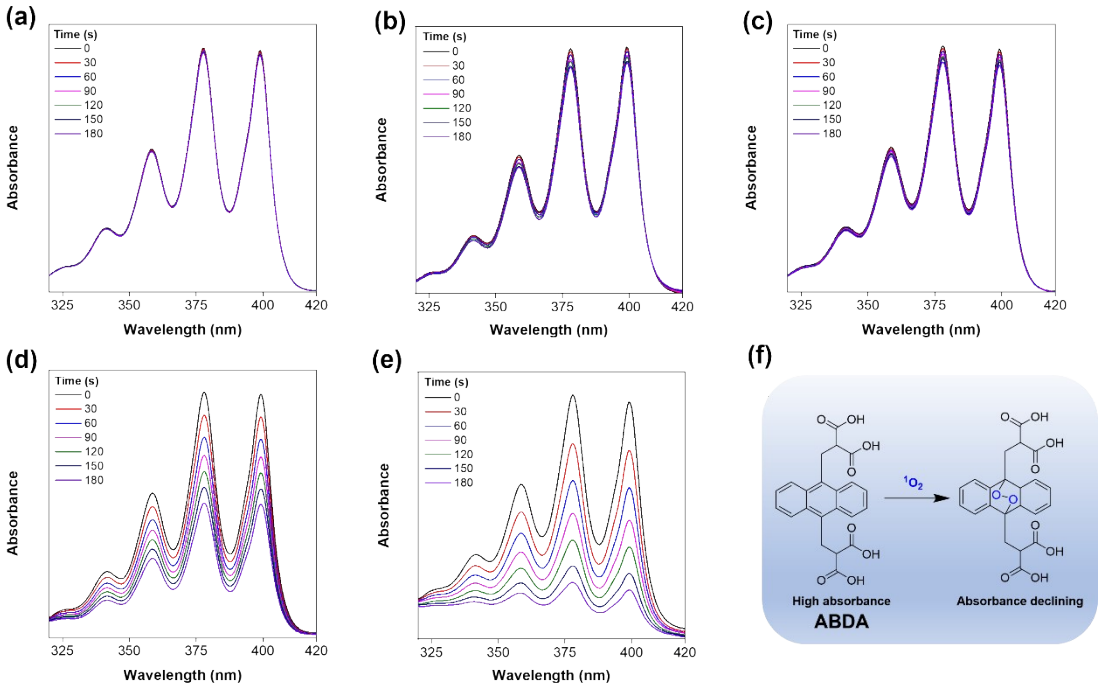

Figure S23. Absorption spectra of ABDA in the presence of (a) blank, (b) **TPAQ**, (c) **TPAQ-PF$_6$**, (d) **CN-TPAQ** and (e) **CN-TPAQ-PF$_6$** under white light irradiation (20 mWcm^{-2}). (f) Detection mechanism of ABDA for $^1O_2$. [AIE PSs] = 10 μM and [ABDA] = 50 μM.

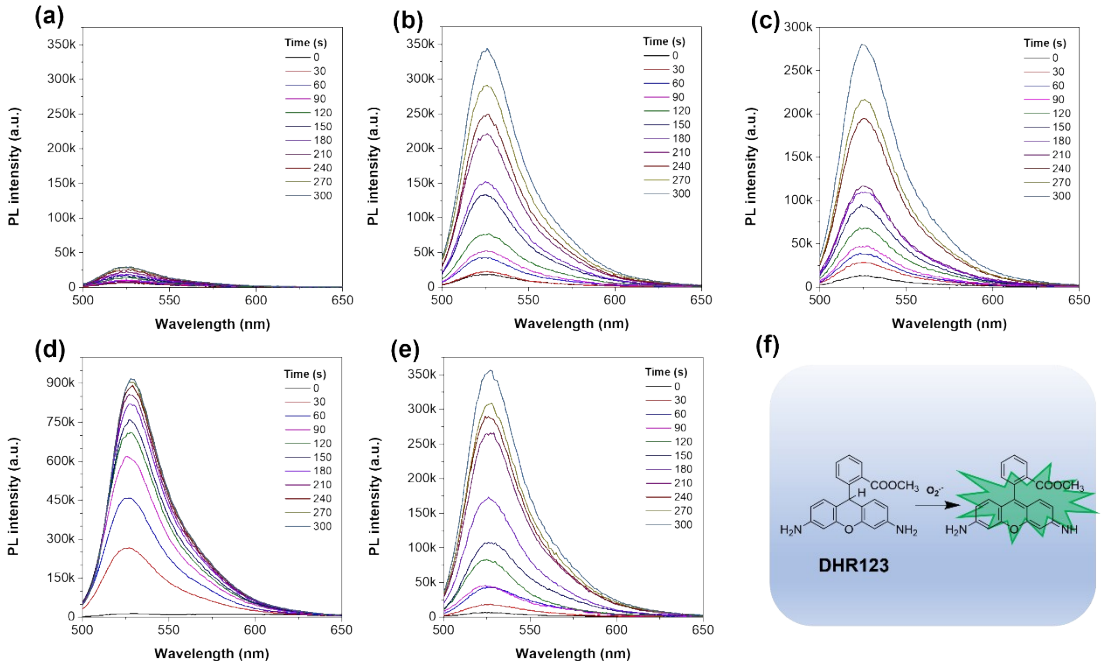

Figure S24. PL spectra of DHR123 in the presence of (a) blank, (b) **TPAQ**, (c) **TPAQ-PF$_6$**, (d) **CN-TPAQ** and (e) **CN-TPAQ-PF$_6$** in DMSO/PBS (v/v = 1: 99) mixture under the different irradiation time. (f) Detection mechanism of DHR123 for $O_2^{\cdot-}$. [AIE PSs] = 10 μM, [DHR 123] = 20 μM.

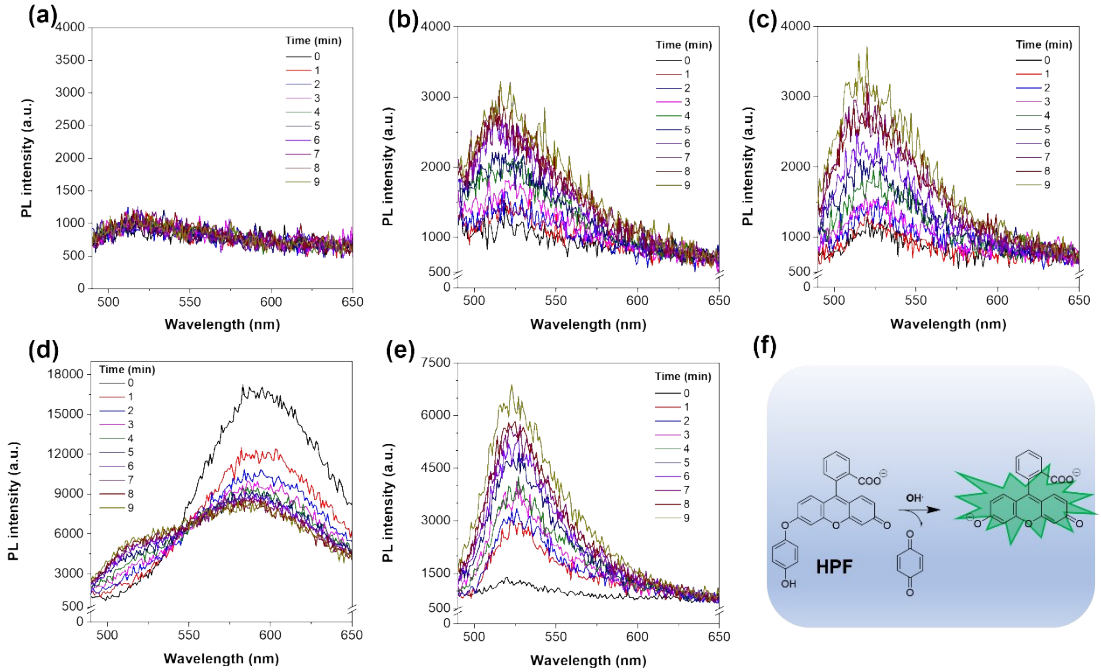

Figure S25. PL spectra of HPF in the presence of (a) blank, (b) **TPAQ**, (c) **TPAQ-PF$_6$**, (d) **CN-TPAQ** and (e) **CN-TPAQ-PF$_6$** in DMSO/PBS (v/v = 1: 99) mixture under the different irradiation time. (f) Detection mechanism of HPF for $OH^{\cdot}$. [AIE PSs] = 10 μM, [HPF] = 10 μM.

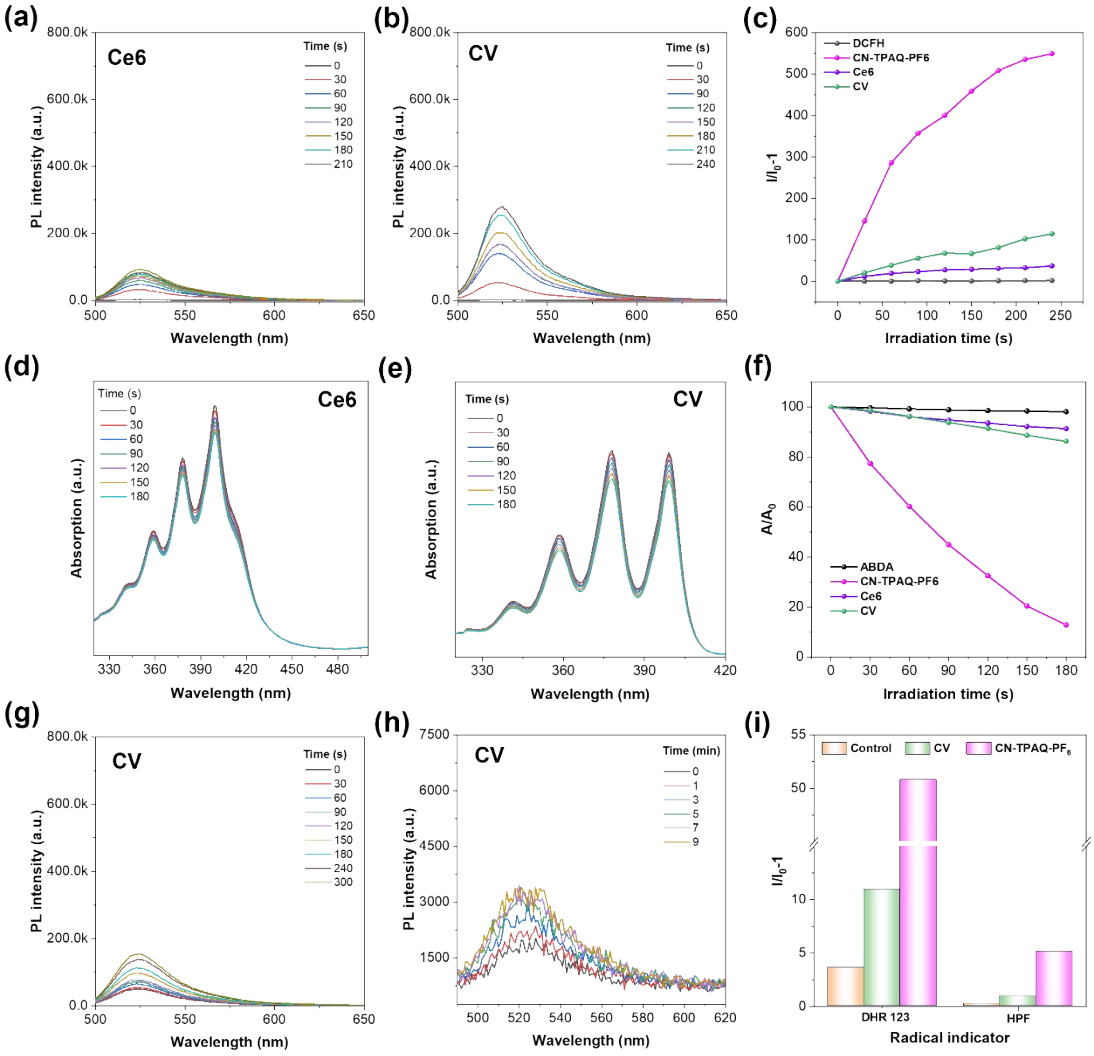

Figure S26. PL spectra of DCFH in the presence of (a) Ce6 and (b) CV in DMSO/PBS: (v/v = 1: 99) mixture under the irradiation with different time; (c) Time-course plots of DCFH fluorescence enhancement versus irradiation time; Absorption spectra of ABDA in the presence of (d) Ce6 and (e) CV under white light irradiation (20 mWcm^{-2}); (f) Time-course plots of ABDA decomposition versus irradiation time; (g) PL spectra of DHR123 in the presence of CV; (h) PL spectra of HPF in the presence of CV; (i) $O_2^{\bullet-}$ and $OH^{\bullet-}$ generation of CV and **CN-TPAQ-PF$_6$**. [PSs] = 10 μM, [DCFH] = 50 μM, [ABDA] = 50 μM, [DHR123] = 20 μM and [HPF] = 10 μM.

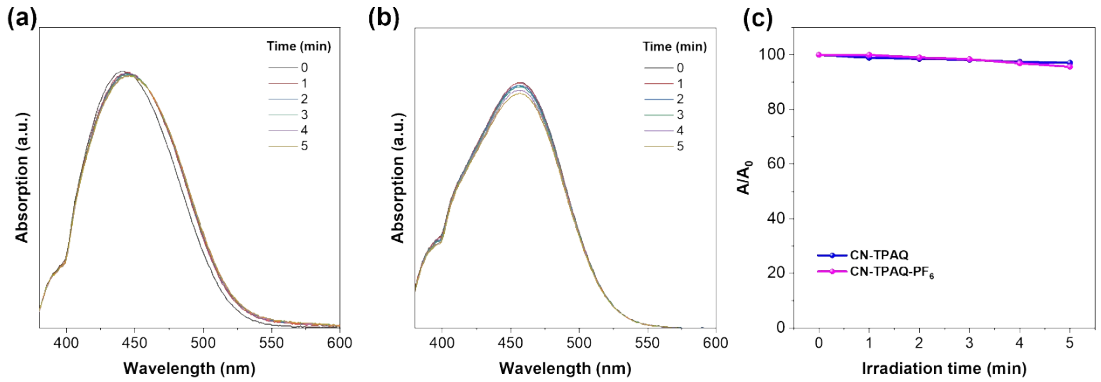

Figure S27.The absorption changes of **CN-TPAQ** (10 μM) and **CN-TPAQ-PF$_6$** (10 μM) before and after white light irradiation (20 mWcm^{-2}, 5 min) in water.

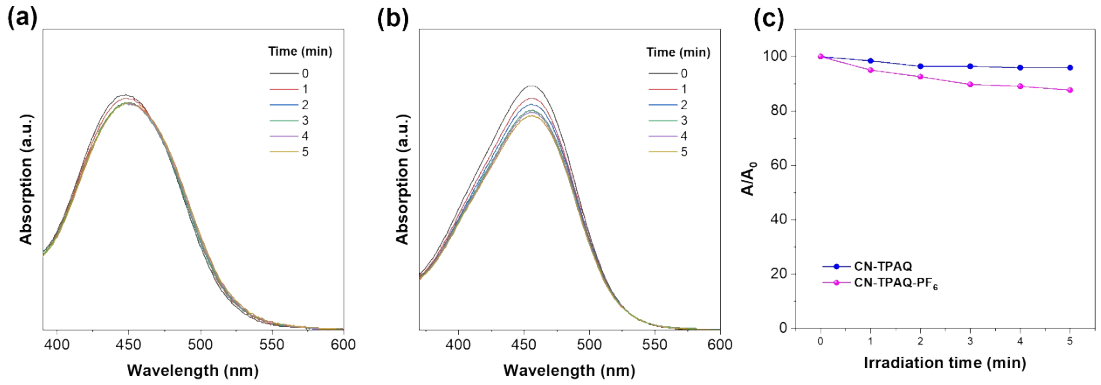

Figure S28.The absorption changes of **CN-TPAQ** (10 μM) and **CN-TPAQ-PF$_6$** (10 μM) before and after white light irradiation (20 mWcm^{-2}, 5 min) in 1 × PBS.

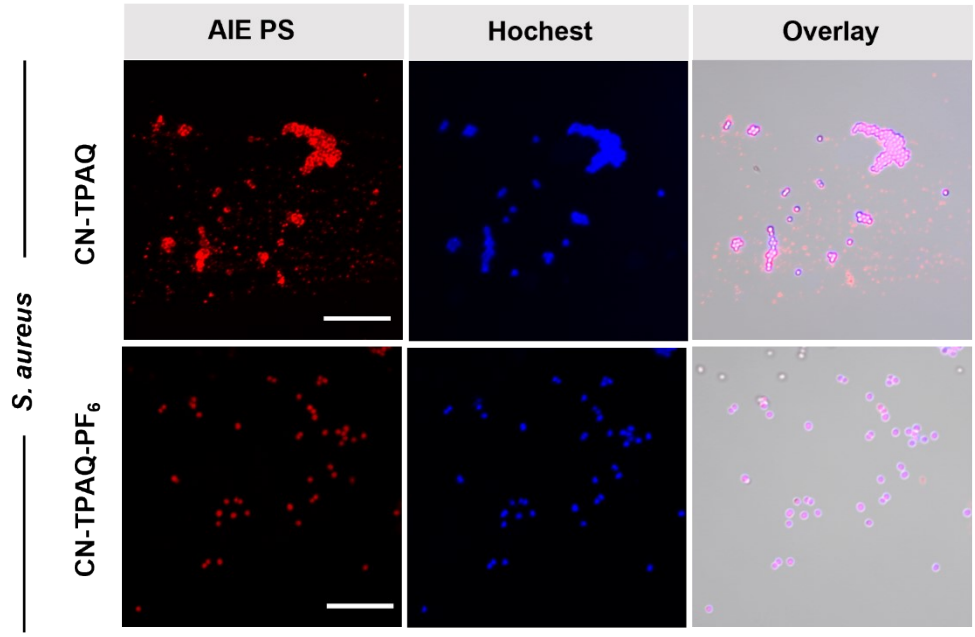

Figure S29. CLSM images of *S. aureus* incubated with **CN-TPAQ** and **CN-TPAQ-PF$_6$** for 30 min. [AIE PSs] = 2 μM, [Hochest33342] = 10 μM, scale bar = 10 μm.

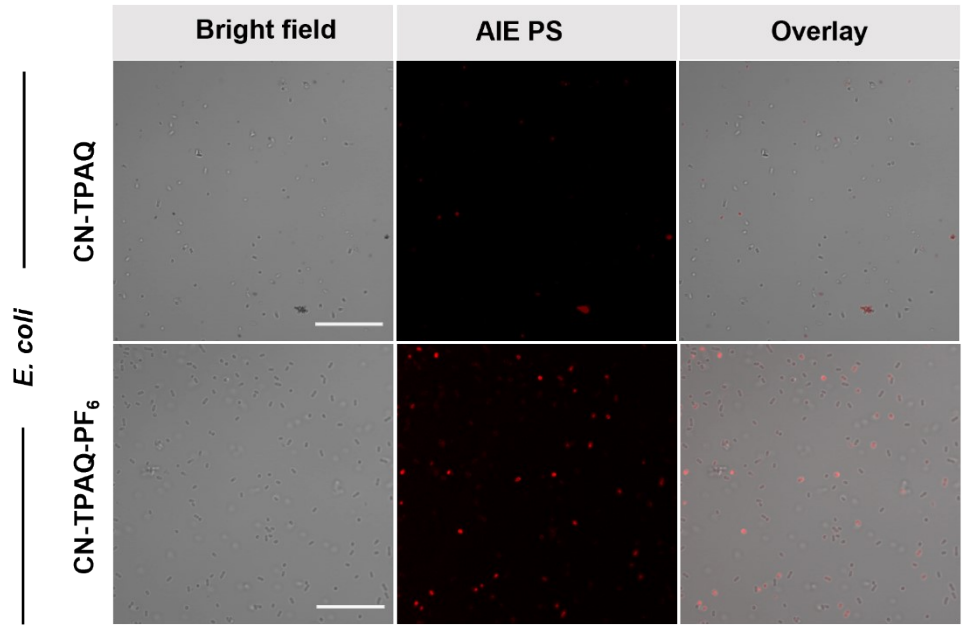

Figure S30. CLSM images of *E. coli* incubated with **CN-TPAQ** (a) and **CN-TPAQ-PF$_6$** (b) for 30 min. [AIE PSs] = 2 μM, scale bar = 10 μm.

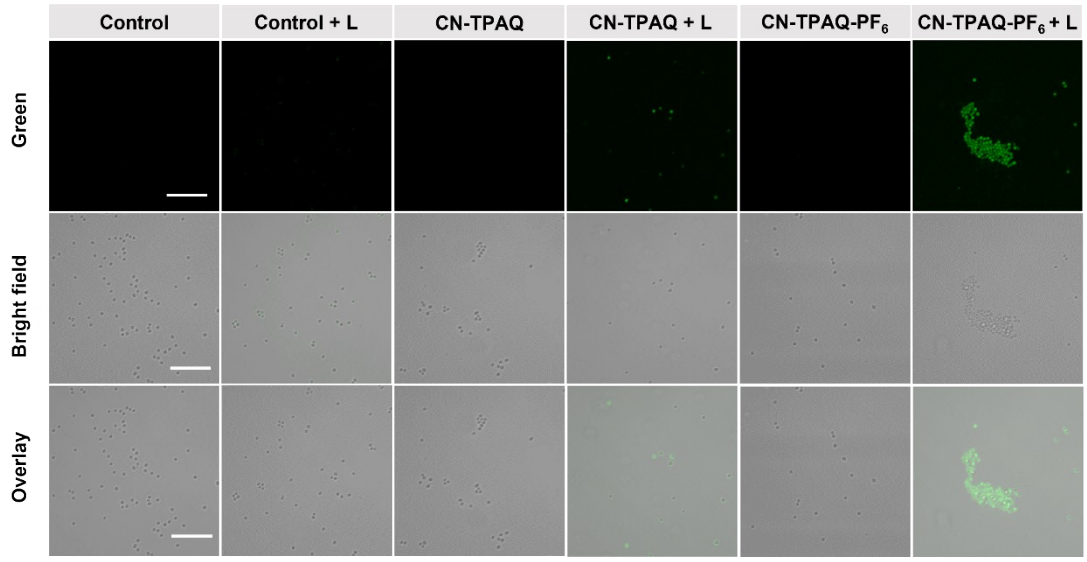

Figure S31. CLSM images of bacterial ROS detection inside **CN-TPAQ** and **CN-TPAQ-PF$_6$** treated *MRSA* for 30 min, accessed by DCFH-DA. [AIE PSs] = 2 μM, [DCFH] = 30 μM, scale bar = 10 μm.

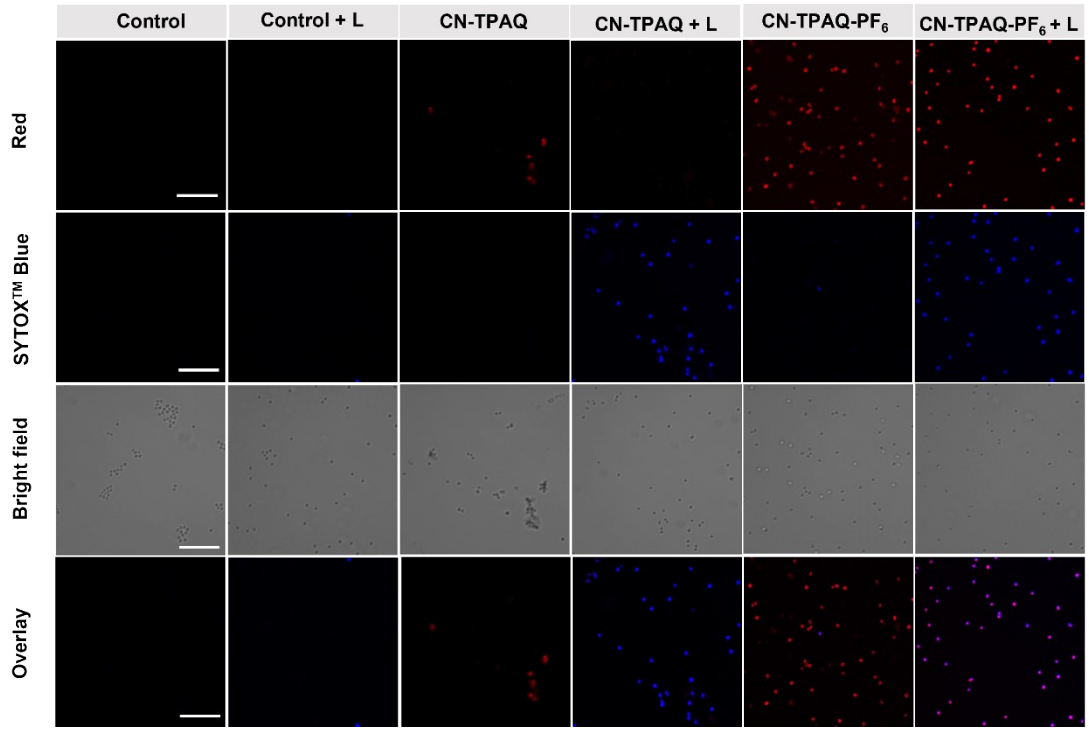

Figure S32. Dead bacterial staining using SYTOX™ Blue (blue emission for dead bacteria) assays after different treatments for 30 min. [AIE PSs] = 2 μM, [Hochest33342] = 10 μM, [SYTOX™ Blue] = 10 μM, scale bar = 10 μm.

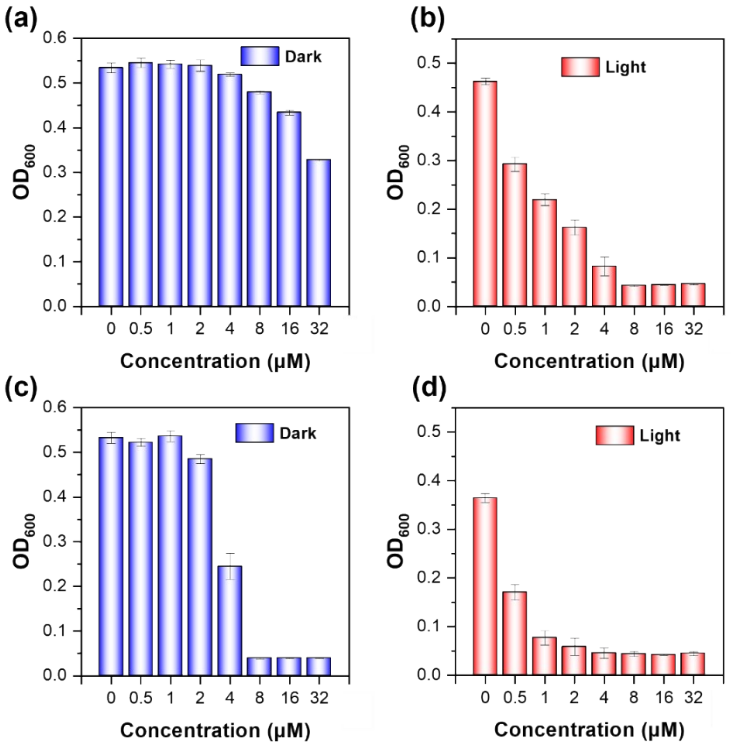

Figure S33. (a) and (b) are the growth of *MRSA* after treatment with **CN-TPAQ** against *MRSA* strain under dark and light condition, respectively; (c) and (d) are the growth of *MRSA* after

treatment with **CN-TPAQ-PF$_6$** under dark and light condition, respectively; White light: 40 mWcm^{-2}, 30 min.

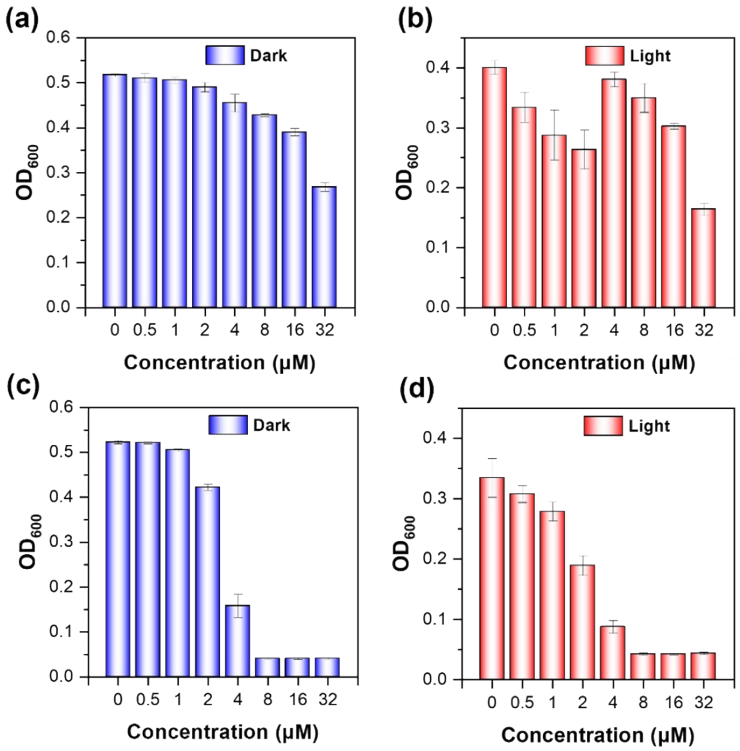

Figure S34. (a) and (b) are the growth of *S. aureus* after treatment with **CN-TPAQ** under dark and light condition, respectively; (c) and (d) are the growth of *S. aureus MRSA* after treatment with **CN-TPAQ-PF$_6$** under dark and light condition, respectively; White light: 40 mWcm^{-2}, 30 min.

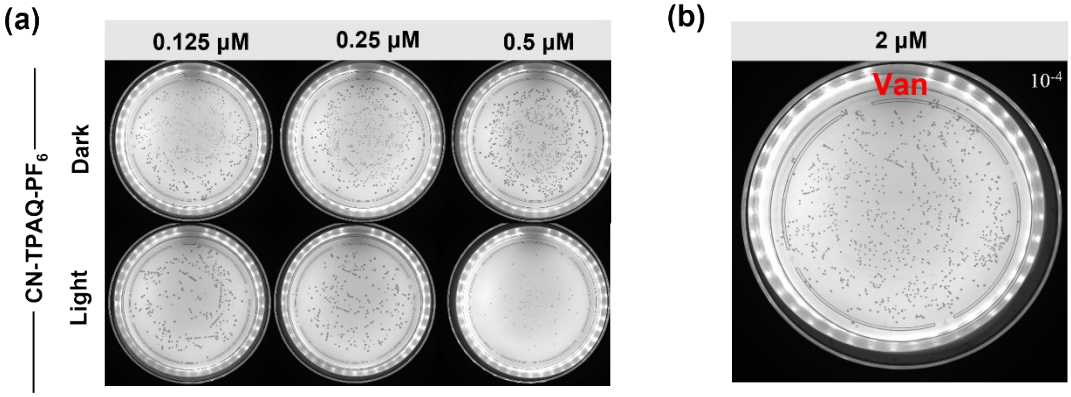

Figure S35. (a) *MRSA* treated by **CN-TPAQ-PF$_6$** with different concentration on the agar plates under dark and light condition. (b) Antibacterial effect of *MRSA* treated by Van.

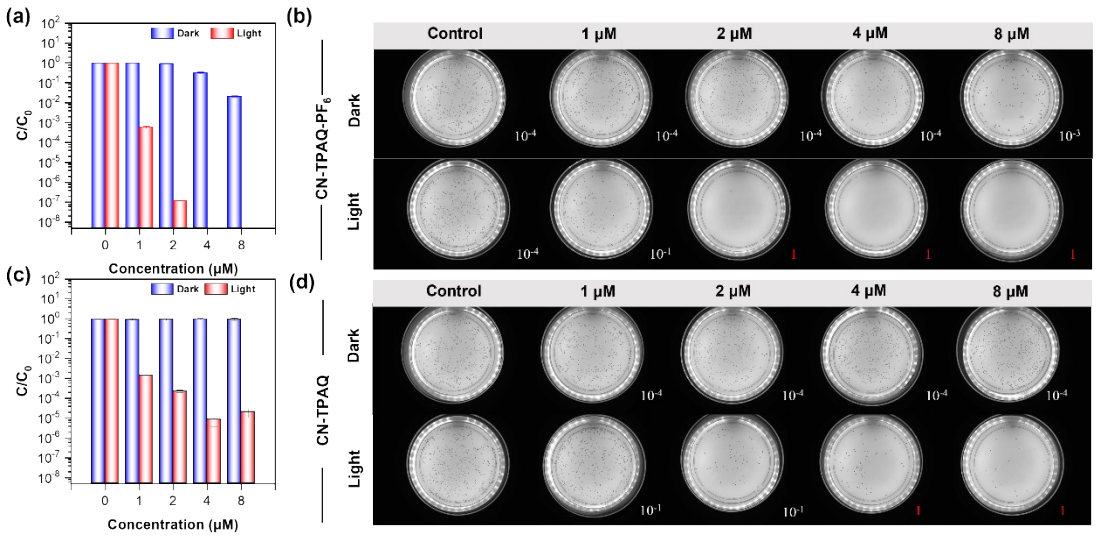

Figure S36. (a) and (c) are inactivation of *S. aureus* in the presence of **CN-TPAQ-PF$_6$** and **CN-TPAQ**, respectively. (b) and (d) are *S. aureus* treated by **CN-TPAQ-PF$_6$** and **CN-TPAQ** with different concentrations on the agar plates under dark and light condition, respectively.

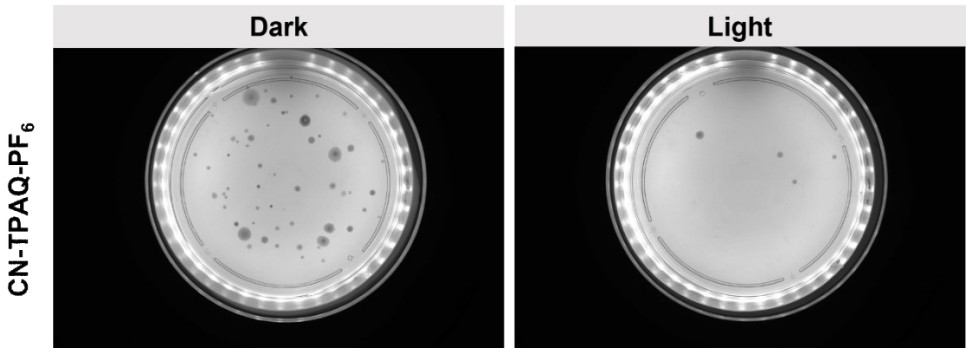

Figure S37. Light sterilization of natural lake water from the West District of South China University of Technology (SCUT).

Table S1. The optical properties and theory calculated properties of **TPAQ**, **TPAQ-PF$_6$**, **CN-TPAQ** and **CN-TPAQ**.

Compd	λ_{abs}[a,b] (nm)	ε[b,c] ($\times 10^4$ M^{-1}cm^{-1})	λ_{em}[a,b] (nm)	Stokes shift (nm)	η[a,d] (%)	η[d,c] (%)	ΔE_{ST} (eV)	ABDA decom-position (%)	DCF enhance factor	DHR 123 enhance factor	HPF enhance factor
TPAQ	350	1.48	464	114	85.3	4.8	/	7.30	13.5	14.2	1.51
TPAQ-PF$_6$	472	0.53	594	122	0.97	18.1	/	6.60	196.8	20.0	1.88
CN-TPAQ	437	4.69	590	153	11	64.3	0.9342	45.3	216.0	66.1	1.37
CN-TPAQ-PF$_6$	448	4.61	602	154	2.4	10.8	0.5320	87.3	549.3	50.8	5.15

[a] In THF. [b] Measured in solution 10 μM. [c] Molar absorptivity. [d] Absolute fluorescence quantum yield determined using a calibrated integrating sphere. [e] In solid state.