Supplementary Information

A Mitochondria-Targeting ICT Probe for Dual-Functional Peroxynitrite Sensing: From Live-Cell Imaging to Serum Model and Plasma-Activated Water Monitoring

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Contents

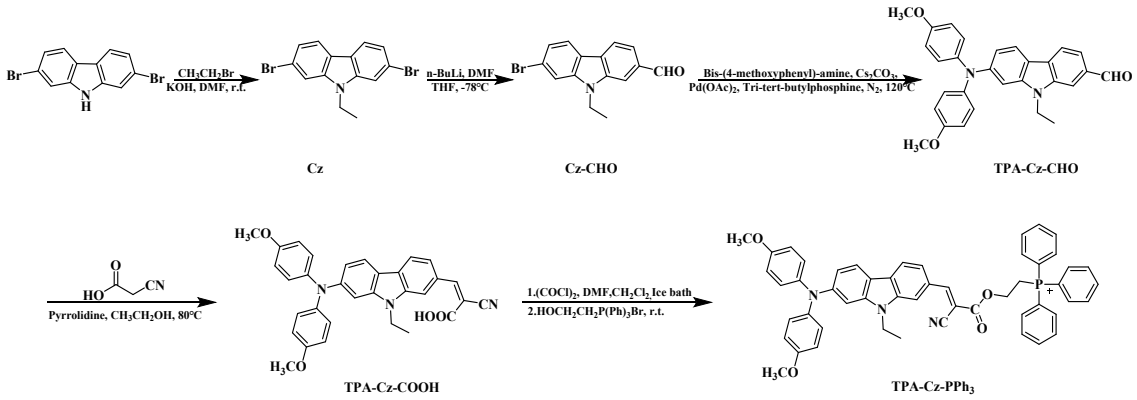
S1 Instruments and reagents

The following instruments were used in this study: an Avance NEO 400 MHz NMR spectrometer (Bruker, Germany); a Q Exactive hybrid quadrupole-Orbitrap mass spectrometer (Thermo Fisher Scientific, USA); a T10CS UV–Vis spectrophotometer (Purkinje General, China); a Varian Cary Eclipse fluorescence spectrophotometer (Varian, USA); a FluoroMax Plus fluorescence spectrometer (HORIBA, Japan); a Tech X-4 melting point apparatus (Beijing Tech Instrument Co., Ltd., China); an SU3800 scanning electron microscope (SEM) (Hitachi High-Tech, Japan); a CB160 CO_2 incubator (BINDER, Germany); a Microplate reader (Thermo Fisher Scientific, USA); a Ti2-A inverted fluorescence microscope (Nikon, Japan); and a plasma-activated water (PAW) generation system (Chongqing Zixian Technology Co., China).

2-Cyanoacetic acid, (2-hydroxyethyl)triphenylphosphonium bromide, oxalyl chloride, 2,7-dibromocarbazole, bromoethane, bis(4-methoxyphenyl)amine, n-butyllithium, tri-tert-butylphosphine, cesium carbonate, palladium acetate, pyrrolidine, acetic acid (CH_3COOH), potassium hydroxide (KOH), absolute ethanol (EtOH), tetrahydrofuran (THF), N,N-dimethylformamide (DMF), dimethyl sulfoxide (DMSO) and MitoTracker Red were purchased from Shanghai Titan Scientific Co., Ltd., all with analytical purity. L929 cell-specific media was obtained from Wuhan Procell Life Science & Technology Co., Ltd. The water used in the experiments was distilled water, further purified by the SZ-97 automatic triple-distillation water purification system (from Shanghai Yarong).

S2 Synthesis and characterization

The synthetic route for the probe TPA-Cz-PPh_3 is illustrated in **Scheme 1.**



Scheme 1 Synthetic route of the probe TPA-Cz-PPh_3

S2.1 Synthesis method of Cz.

2,7-Dibromocarbazole (5.02 g, 15.45 mmol), potassium hydroxide (30.13 g, 535.00 mmol), and N,N-dimethylformamide (100 mL) were sequentially added to a 250 mL three-necked round-bottom flask. The reaction mixture was stirred magnetically for 40 minutes. Subsequently, bromoethane (10 mL, 134.00 mmol) was added dropwise using a constant-pressure dropping funnel, and the reaction was maintained at room temperature with continuous stirring for 18 hours. Upon completion of the reaction, the mixture was slowly poured into 1000 mL of deionized water, yielding a white flocculent precipitate. The solid product was collected by vacuum filtration through a Büchner funnel and washed with anhydrous ethanol (3 × 20 mL) to remove residual impurities. After drying, a white product (5.37 g) was obtained with a yield of 98.3%, melting point 139–141 °C. ^{1}H NMR(400 MHz，$CDCl_3$，298 K)δ: 7.88 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 1.7 Hz, 2H), 7.35–7.33 (m, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H).

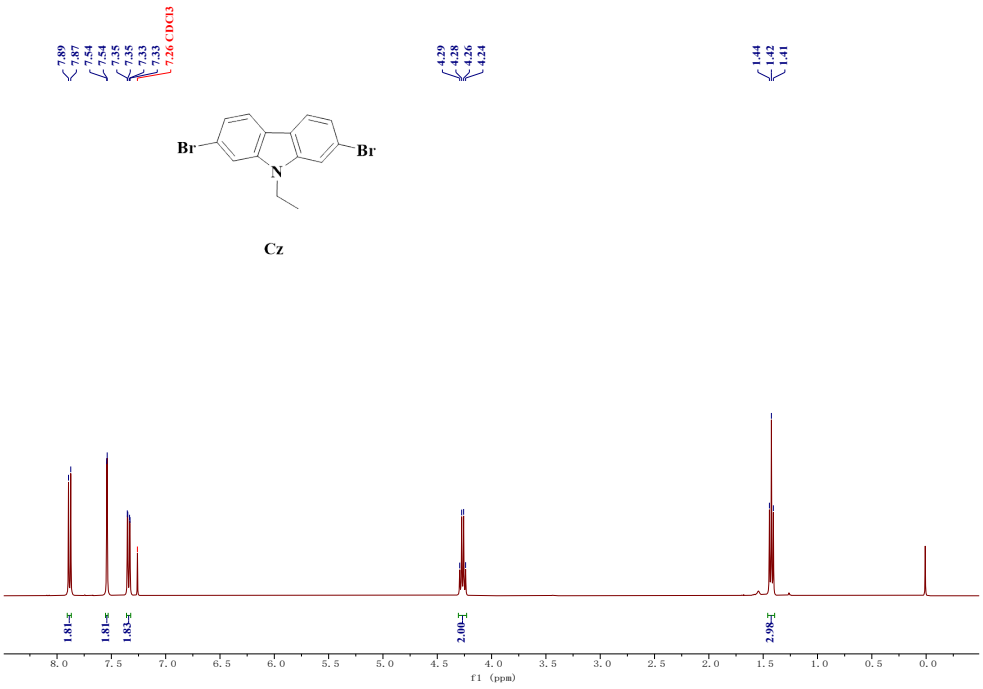


Figure S1 The ^{1}H NMR spectrum of Cz in $CDCl_3$

S2.2 Synthesis method of Cz-CHO.

Under a nitrogen atmosphere, 2,7-dibromo-9-ethylcarbazole (2.84 g, 8.04 mmol) was dissolved in anhydrous tetrahydrofuran (25 mL) and cooled to –78 °C in a low-temperature reactor with constant temperature control. A hexane solution of n-butyllithium (4.02 mL, 8.04 mmol) was added dropwise via syringe, with the addition rate controlled to maintain the reaction temperature at –78 °C. After stirring for 1 h, anhydrous N,N-dimethylformamide (0.92 mL, 11.93 mmol) was introduced into the system via syringe. The reaction was continued for an additional 2 h under maintained low-temperature conditions before removing the cooling bath to allow the system to warm to room temperature. The reaction was quenched by the slow addition of 20 mL of aqueous hydrochloric acid solution (2 M), followed by extraction with dichloromethane (3 × 50 mL). The organic phase was dried over anhydrous magnesium sulfate, filtered, and concentrated to yield a brownish-yellow crude product. Purification by column chromatography (eluent: petroleum ether/ethyl acetate = 80:1, v/v) afforded a pale yellow solid (1.32 g, yield 54.3%), with a melting point of 171–172 °C. ^{1}H NMR(400

MHz，$CDCl_3$，298 K)δ: 10.15 (s, 1H), 8.22–8.11 (m, 1H), 7.99–7.94 (m, 2H), 7.76–7.73 (m, 1H), 7.60 (d, *J* = 1.7 Hz, 1H), 7.39–7.36 (m, 1H), 4.36 (t, *J* = 7.3 Hz, 2H), 1.48–1.44 (m, 3H).

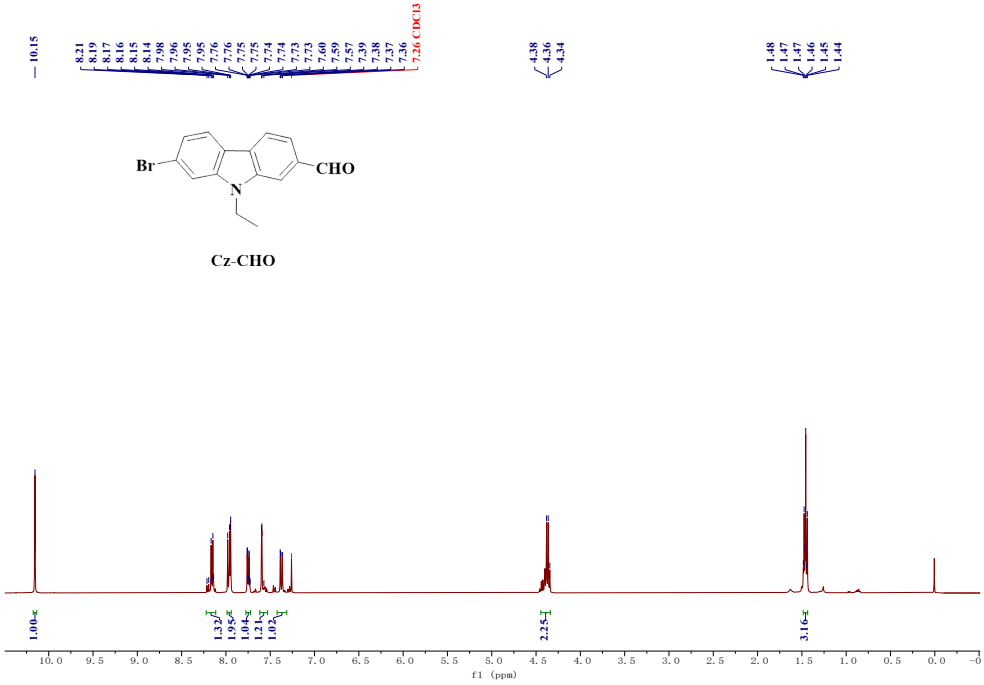


Figure S2 The ^{1}H NMR spectrum of Cz-CHO in $CDCl_3$

S2.3 Synthesis method of TPA-Cz-CHO.

Cz-CHO (0.31 g, 1.03 mmol), bis(4-methoxyphenyl)amine (0.59 g, 2.56 mmol), and cesium carbonate (0.84 g, 2.56 mmol) were sequentially added to a 50 mL three-necked round-bottom flask containing 5 mL of toluene. The system was purged with nitrogen three times to establish an inert atmosphere and stirred thoroughly to form a homogeneous suspension. Subsequently, palladium acetate (0.012 g, 0.051 mmol) and tri-tert-butylphosphine (241 μL, 0.10 mmol) were added as the catalytic system. The reaction mixture was heated to 120 °C and stirred continuously at this temperature for 24 h. After cooling to room temperature, the reaction was quenched by slowly adding 20 mL of aqueous hydrochloric acid (1 M), followed by extraction with dichloromethane (3 × 30 mL). The combined organic phases were dried over anhydrous magnesium sulfate, filtered, and concentrated to afford a brownish-yellow crude product. Column

chromatography (eluent: petroleum ether/ethyl acetate = 50:1, v/v) was employed to isolate the target compound as an orange-yellow solid (0.22 g, yield 47.6%), m.p. 155–156 °C. ^{1}H NMR(400 MHz，$CDCl_3$，298 K)δ: 10.10 (s, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 9.8 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 8.9 Hz, 4H), 6.87 (d, *J* = 6.6 Hz, 5H), 6.65 (d, *J* = 4.2 Hz, 1H), 4.22 (q, *J* = 7.2 Hz, 2H), 3.82 (s, 6H), 1.34 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$，298 K)δ: 192.70, 156.19, 149.61, 143.37, 141.23, 140.05, 132.69, 128.93, 126.89, 123.02, 122.19, 122.00, 119.39, 115.90, 114.90, 114.83, 108.74, 100.03, 55.66, 37.68, 13.94.

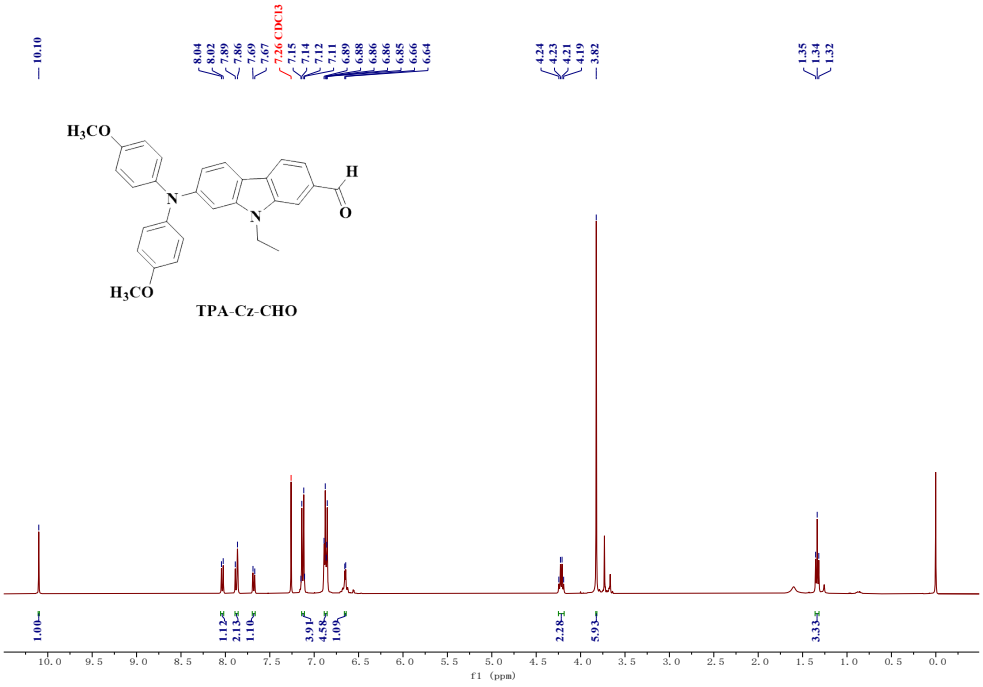


Figure S3 The ^{1}H NMR spectrum of TPA-Cz-CHO in $CDCl_3$

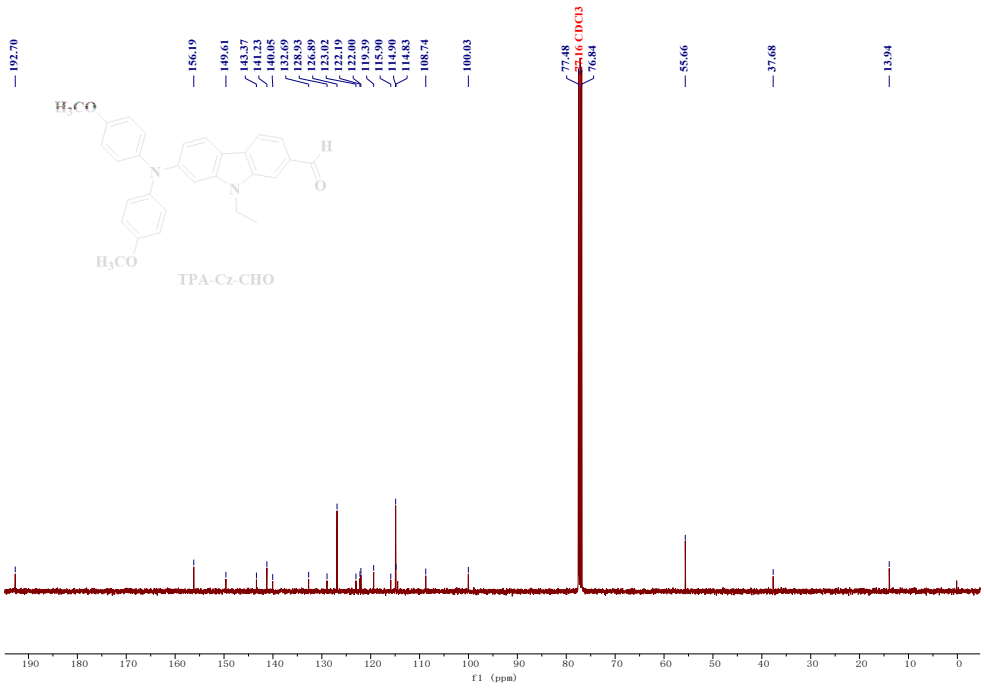


Figure S4 The ^{13}C NMR spectrum of TPA-Cz-CHO in $CDCl_3$

S2.4 Synthesis method of TPA-Cz-COOH.

TPA-Cz-CHO (0.50 g, 1.11 mmol), 2-cyanoacetic acid (0.19 g, 2.22 mmol), and ethanol (20 mL) were added to a 50 mL round-bottom flask. Pyrrolidine (0.10 mL) was then added dropwise. The mixture was heated under reflux at 80 °C for 3 h. After completion of the reaction, the mixture was allowed to cool to room temperature. The product was extracted with dichloromethane (3 × 30 mL). The combined organic phases were dried over anhydrous magnesium sulfate, filtered, and concentrated to afford a crude red product. The red solid (0.53 g, 74.9% yield) was isolated by column chromatography (eluent: dichloromethane/methanol, 50:1 v/v). Mp: 149–151 °C. ^1H NMR(400 MHz，$CDCl_3$，298 K)δ: 8.44 (s, 1H), 8.20 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 4H), 6.87 (d, *J* = 9.8 Hz, 6H), 4.28–4.17 (m, 2H), 3.83 (s, 6H), 1.26 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$，298 K)δ: 156.35, 143.79, 140.84, 140.53, 140.10, 139.91, 126.69, 122.33, 122.32, 119.55, 119.50, 114.94, 111.00, 110.71, 55.65, 38.12, 30.11, 13.86.

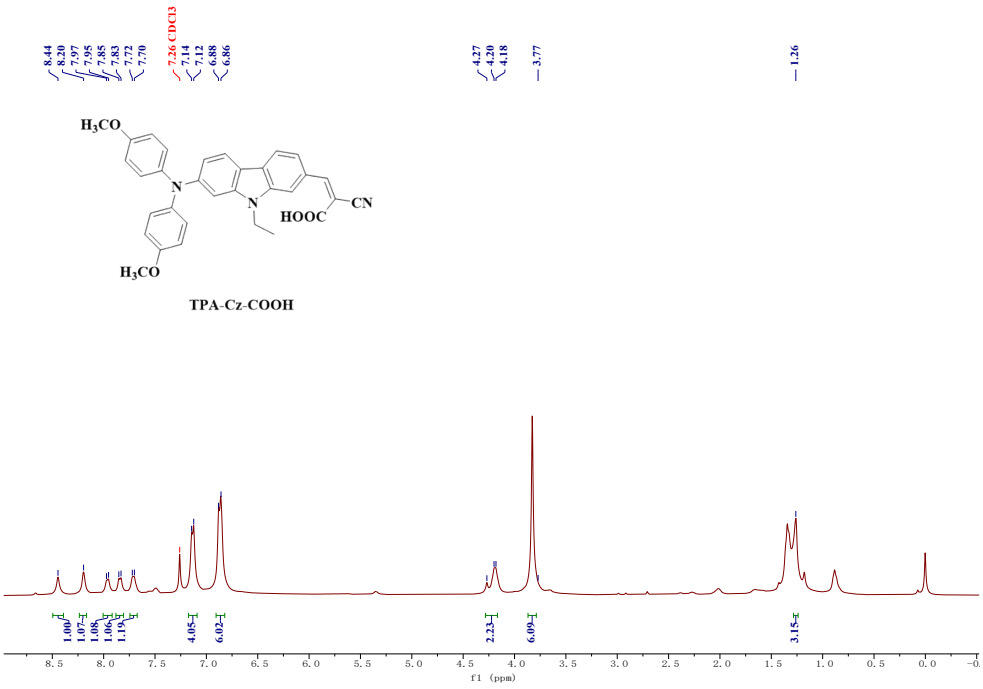


Figure S5 The ^{1}H NMR spectrum of TPA-Cz-COOH in $CDCl_3$

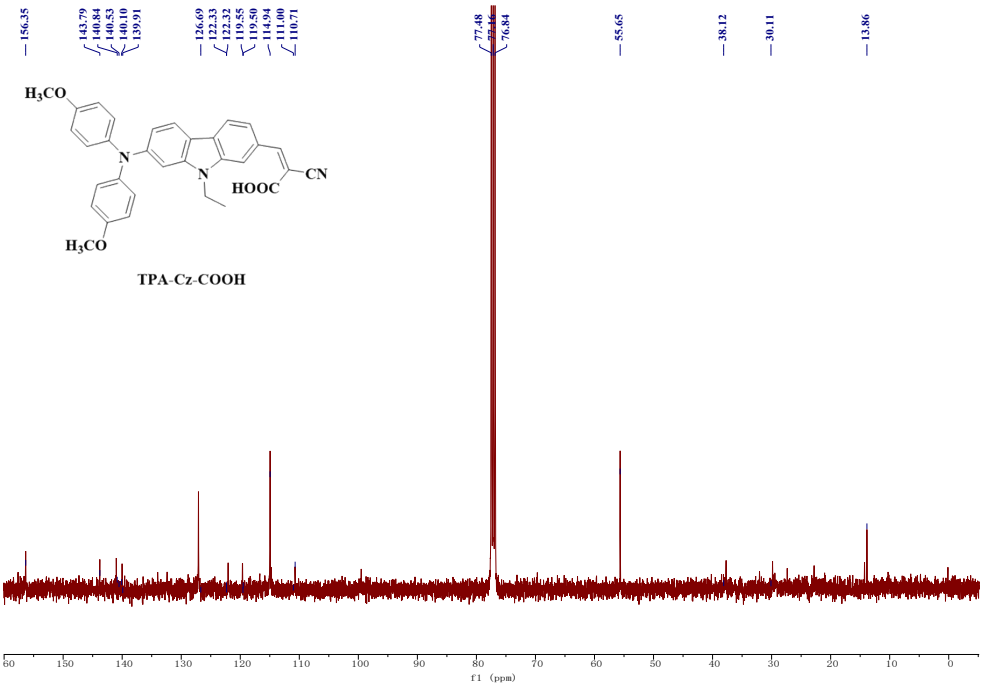


Figure S6 The ^{13}C NMR spectrum of TPA-Cz-COOH in $CDCl_3$

S2.5 Synthesis and Characterization of TPA-Cz-PPh_3.

TPA-Cz-COOH (0.30 g, 0.58 mmol) and anhydrous dichloromethane (10 mL) were added to a 25 mL round-bottom flask. The mixture was stirred until complete

dissolution of the solid. Under ice-bath conditions, oxalyl chloride (0.10 mL) and two drops of DMF were added dropwise, and the mixture was stirred for 10 minutes while maintaining the low temperature. The reaction flask was then warmed to room temperature, and stirring was continued for 2 hours. Subsequently, (2-hydroxyethyl)triphenylphosphonium bromide (0.45 g, 1.16 mmol) was added to the reaction mixture, and the reaction proceeded for 4 hours. The mixture was extracted using dichloromethane (3 × 30 mL). The combined organic phases were dried over anhydrous magnesium sulfate, filtered, and concentrated to yield a red crude product. Finally, purification by column chromatography using a dichloromethane:methanol (100:1) eluent yielded a purple-red solid (0.28 g, with a 60.0% yield). m.p.103–104 °C. ^{1}H NMR(400 MHz，$CDCl_3$，298 K) δ (ppm): 8.43 (s, 1H), 8.29 (d, *J* = 10.7 Hz, 2H), 7.84–7.68 (m, 19H), 7.52 (s, 1H), 7.40 (s, 2H), 7.13 (s, 2H), 6.91–6.85 (m, 3H), 4.34 (s, 1H), 4.26 (s, 1H), 4.07 (s, 4H), 3.95 (s, 3H), 3.82 (s, 3H), 1.34 (t, *J* = 5.3 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d6, 298 K) δ (ppm): 161.94, 156.59, 155.96, 149.43, 145.31, 142.96, 140.08, 139.17, 135.27, 135.03, 134.80, 134.77, 134.60, 134.57, 134.05, 133.95, 133.80, 133.77, 133.70, 133.66, 130.46, 130.33, 130.20, 130.09, 130.00, 129.88, 127.32, 126.91, 126.38, 122.37, 119.59, 118.74, 118.48, 117.62, 117.04, 115.01, 112.61, 98.47, 97.42, 55.26, 54.50, 25.13, 24.63, 13.44. HRMS (ESI): Cal. for $C_{52}H_{45}N_3O_4P^+$ [M] 806.314; Found, 806.314.

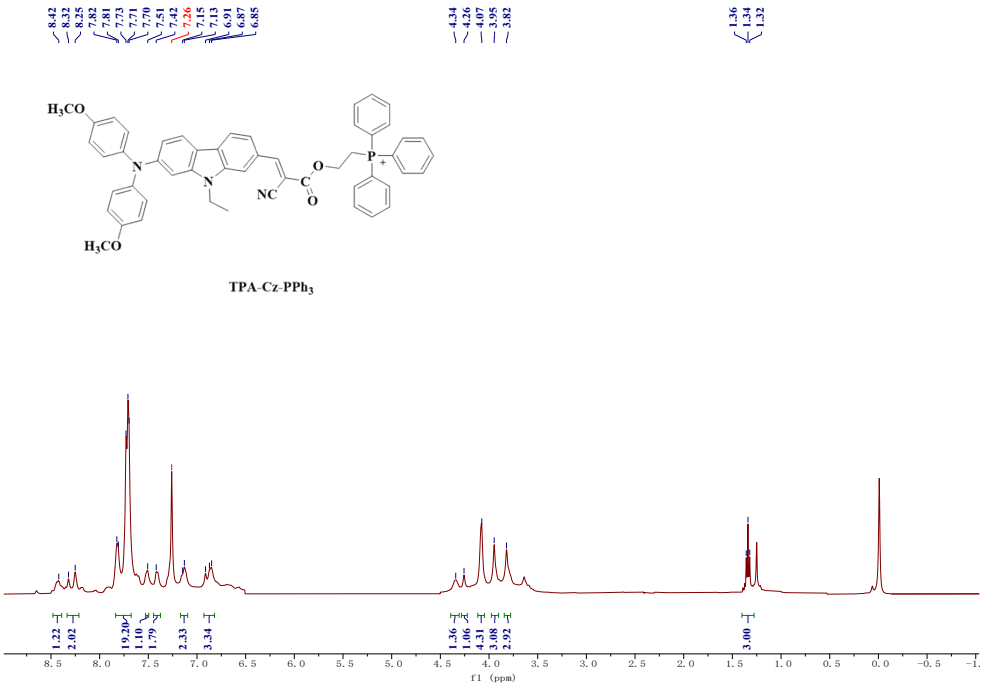


Figure S7 The ^{1}H NMR spectrum of TPA-Cz-PPh_3 in $CDCl_3$

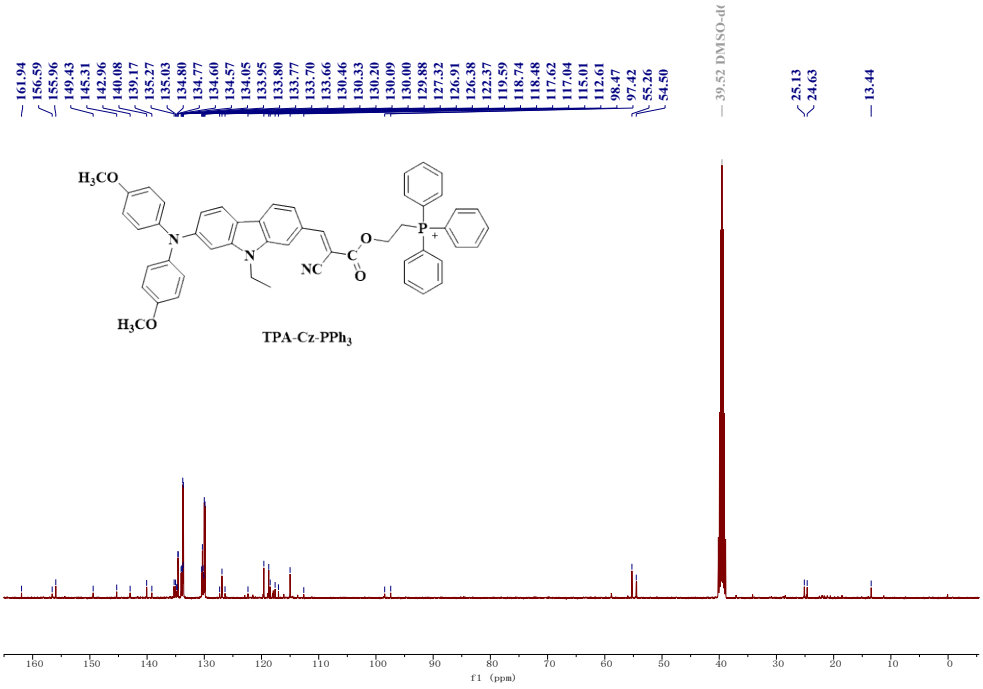


Figure S8 The ^{13}C NMR spectrum of TPA-Cz-PPh_3 in DMSO-d6

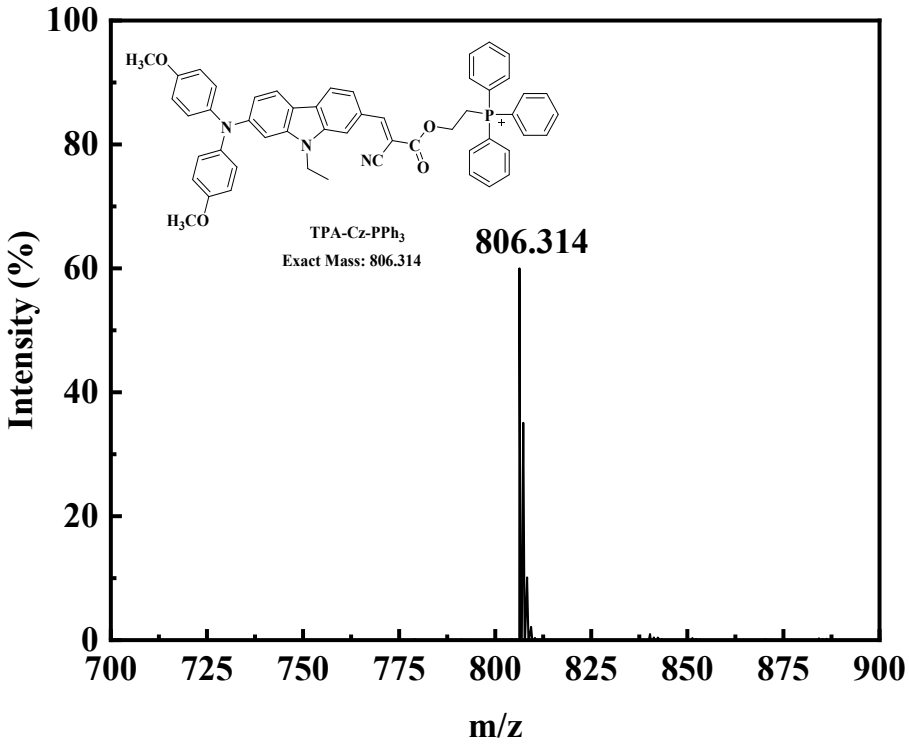


Figure S9 The HRMS (ESI) spectrum of TPA-Cz-PPh_3

S3 Spectroscopic and Biological Assays

S3.1 Preparation of Reactive Oxygen/Nitrogen Species, Metal Ions, Anions, other nucleophiles，and Quinine Sulfate Solutions

According to the literature procedure[1], 2.00 mL of hydrochloric acid (0.60 M) and 2.00 mL of hydrogen peroxide solution (0.70 M) were added under ice-bath conditions. After stirring for 20 minutes, 2.00 mL of sodium hydroxide solution (3.00 M) and 2.00 mL of sodium nitrite solution (0.60 M) were added and allowed to react for 1 minute to yield a pale yellow $ONOO^-$ stock solution. Its concentration was determined to be 1.19 mM by UV absorption at 302 nm. A 0.05 M NO^- solution was prepared by dissolving 149.00 mg (0.5 mmol) of sodium nitroprusside in 10.00 mL of distilled water. The TBHP solution was obtained by diluting a commercial 70% TBHP aqueous solution with distilled water to 0.05 M. Equal volumes of 0.05 M TBHP and 0.05 M ferrous sulfate solutions were mixed to prepare a 0.05 M TBO^- solution. A 30% hydrogen peroxide solution was diluted with distilled water to obtain a 0.05 M H_2O_2 stock solution. A 0.05 M ClO^- stock solution

was prepared by dissolving 41.13 mg (2.5 mmol) of sodium hypochlorite pentahydrate in 50 mL of distilled water. Following the method reported in the reference[2], equal volumes of 0.05 M ferrous sulfate solution and 0.50 M hydrogen peroxide solution were mixed to yield a 0.05 M ·OH stock solution. A 0.05 M $^1O_2$ stock solution was prepared by mixing equal volumes of 0.05 M sodium molybdate and 0.50 M hydrogen peroxide solutions.

The probe stock solution (5 mM) was prepared by dissolving TPA-Cz-PPh_3 in THF.

The analytes (0.01 M) required for the selectivity experiments were prepared with ultrapure water, including $LiCl·H_2O$, $FeCl_3·H_2O$, $Mg(NO_3)_2·6H_2O$, $Cu(NO_3)_2·3H_2O$, KNO_3, $NaNO_3$, $AgNO_3$, $Pb(NO_3)_2$, $Co(NO_3)_2·6H_2O$, $Zn(NO_3)_2·4H_2O$, $Ni(NO_3)_2·6H_2O$, $Al(NO_3)_3·9H_2O$, $Ca(NO_3)_2·6H_2O$, $MnCl_2·4H_2O$, $HgCl_2$, $Cr(NO_3)_3·9H_2O$, $BaCl_2·2H_2O$, $Cd(NO_3)_2·4H_2O$, KF, K_2SO_4, KBr, KCl, KI, KH_2PO_4, $NaHCO_3$, KNO_3, KC_2O_4, glutathione, cysteine, Na_2S, Na_2SO_3. On this basis, it was then diluted with ultrapure water to achieve the desired concentration of ionic solutions.

0.0030 g of quinine sulfate was accurately weighed, dissolved in 0.05 M sulfuric acid solution, and diluted to 250 mL to obtain a 12 mg/L quinine sulfate solution (fluorescence quantum yield, Φ = 0.54).

S3.2 Detailed Fluorescence Property Test Method

To a DMSO stock solution of TPA-Cz-PPh_3 (500 μM, 40 μL), gradually add 0–100 μL of an $ONOO^-$ solution (10 mM), and supplement with DMSO, distilled water, and PBS buffer (10 mM) to a final volume of 5 mL, resulting in a final $ONOO^-$ concentration of 0–200 μM. The final concentration of the probe in a DMSO/H_2O solution (volume ratio 9:1, pH 7.4) is 40 μM. Allow the mixed solution to stand at room temperature for 5 minutes. Set the fluorescence spectrophotometer to an excitation wavelength of 307 nm, a lamp voltage of 600 V, and a slit width of 5 mm to measure the fluorescence emission spectrum, recording the fluorescence intensity at 480 nm. Investigate the fluorescence signal of the TPA-Cz-PPh_3 probe solution in the presence of varying concentrations of

$ONOO^-$ and 200 μM of various anions ($C_2O_4^{2-}$、Br^-、F^-、HCO_3^-、I^-、$H_2PO_4^-$、Cl^-、NO_3^-), metal cations (K^+、Li^+、Ag^+、Na^+、Hg^{2+}、Mg^{2+}、Cd^{2+}、Pb^{2+}、Mn^{2+}、Ni^+、Co^{2+}、Ba^{2+}、Ca^{2+}、Cu^{2+}、Zn^{2+}、Cr^{3+}、Al^{3+}、Fe^{3+}), other ROS/RNS ($^1O_2$、TBO^-、TBHP、NO^-、H_2O_2、·OH、ClO^-) and other nucleophiles (glutathione, cysteine, H_2S, SO_2) using the aforementioned method.

S3.3 Determination and Calculation of Fluorescence Quantum Yield

Weigh 12 mg of quinine sulfate and transfer it to a beaker. Dissolve the compound by adding the minimal volume of 0.05 M sulfuric acid solution required. Quantitatively transfer the solution to a 1 L volumetric flask and dilute to the mark with 0.05 M H_2SO_4 to prepare a 12 mg/L quinine sulfate stock solution. Dilute this stock solution to 0.6 mg/L. Measure its UV-vis absorption spectrum and record the absorbance at 350 nm. Subsequently, using an excitation wavelength of 350 nm, acquire the fluorescence emission spectrum from 360 to 650 nm and record the integrated fluorescence intensity. Dilute a 500 μM TPA-Cz-PPh_3 DMSO stock solution to prepare a 10 μM TPA-Cz-PPh_3 DMSO solution, repeat the procedure, and record the absorbance at 350 nm and the integrated fluorescence peak area for the 10 μM TPA-Cz-PPh_3 DMSO solution. The fluorescence quantum yield is calculated using **Formula (1)** as follows:

$$\Phi_x = \Phi_s(I_x/I_s)(A_s/A_x)(n_x/n_s)^2 \quad (1)$$

Where A represents the ultraviolet absorbance value, I denotes the fluorescence integral area, n signifies the refractive index of the solvent (n_s = 1.33 and n_x = 1.43), Φ indicates the quantum yield (Φ_s = 0.54), and the subscripts s and x refer to quinine sulfate and the probe TPA-Cz-PPh_3, respectively.

S3.4 Cytotoxicity Test (CCK-8) Protocol

The cytotoxicity of TPA-Cz-PPh_3 was assessed using the CCK-8 assay on mouse skin fibroblasts (L929, Cell line number: PC-H2025030527). L929 cells (1×10^4 cells/well, 100 μL) were seeded in a 96-well plate and incubated at 37°C with 5% CO_2 and 95% humidity for 12 hours to facilitate cell adhesion. TPA-Cz-PPh_3 was sterilized under UV light for 30

minutes and subsequently dissolved in MEM medium to prepare sample stock solutions at varying initial concentrations (ranging from 20 to 70 μM). The culture medium was replaced with an equal volume of sample solution (200 μL of the probe stock was added to 1 mL of culture medium, resulting in a final exposure concentration approximately one-sixth of the initial stock concentration), and the cells were incubated for an additional 24 hours. MEM medium served as the blank control, and co-cultures were maintained for 1, 3, 5, and 7 days. After incubation, 10 μL of CCK-8 reagent was added to each well, followed by a 2-hour incubation period. Absorbance (OD value) was measured at 450 nm using a microplate reader. Each experiment was performed in triplicate, and the mean value was used as the final result. The relative cell viability of the TPA-Cz-PPh_3 probe was calculated using **Formula (2)**:

$$M(\%) = OD\ Sample / OD\ Control \times 100\% \quad (2)$$

In the formula, M represents cell viability (expressed as a percentage, %), OD denotes the optical density value of the sample group, and OD Control corresponds to the optical density.

S3.5 Intracellular $ONOO^-$ fluorescence imaging experiment

L929 cells were seeded at a density of 5×10^4 cells/well in a 12-well plate and allowed to adhere for 24 hours. After adhesion, the cells were incubated with 20 μM (initial stock concentration, final exposure concentration: 3.3 μM) TPA-Cz-PPh_3 for 60 minutes at 37°C and washed three times. Following treatment with 100 μM (initial stock concentration; 100 μL of this stock was added to 1 mL of culture medium, resulting in a final exposure concentration of 9.1 μM) $ONOO^-$ for 30 minutes, the cells were fixed, and the samples were imaged using an inverted fluorescence microscope.

S3.6 Experimental method of mitochondrial co-location

L929 cells were seeded at a density of 5×10^4 cells/well in a 12-well plate and allowed to adhere for 24 hours. After incubation with TPA-Cz-PPh_3 (20 μM) for 4 hours, the medium was aspirated, and the cells were washed three times with cold phosphate-

buffered saline (PBS, pH 7.4). The cells were fixed with 4% paraformaldehyde (300 μL) at room temperature for 20 minutes, followed by three rinses with PBS.The cells were subsequently co-stained with 2 μL of Mito-Detector Red (500 nM) for 30 minutes at 37°C, washed three times with serum-free medium, and then treated with peroxynitrite ($ONOO^-$, 100 μM) for 30 minutes to activate TPA-Cz-PPh_3. Finally, the samples were imaged using an inverted fluorescence microscope, and the fluorescence intensity was analyzed using ImageJ software.

S3.7 Analysis of $ONOO^-$ in PAW and fetal bovine serum

A 10 mM PBS solution (pH 7.4, 2 L), a 25 mM $NaHCO_3$ solution (pH 8.34, 2 L), and a 1 mM NaOH solution (pH 11, 2 L) were separately treated in a plasma-activated water preparation system (220 V, 50 Hz, 500 W) for 10 minutes at room temperature under dark conditions to produce PAW. Additionally, to obtain protein-free serum samples, fetal bovine serum(FBS) was mixed with an equal volume of acetonitrile to precipitate proteins, followed by centrifugation at 4000 rpm for 40 minutes. The supernatant was collected and acetonitrile was removed by rotary evaporation to obtain protein-free fetal bovine serum. The serum was then diluted 10-fold with PBS buffer and stored at 4°C for subsequent use.

The test solution was prepared as described in Section 3.2, using PAW or FBS instead of PBS. Different volumes of the $ONOO^-$ stock solution (1.19×10^{-3} M) were then added to achieve final $ONOO^-$ concentrations of 60, 100 ,140and 180 μM. The solutions were immediately tested according to section 3.2. All experiments were conducted in triplicate, and mean values are reported. The spike recovery was calculated using **Formula (3)**:

$$Recovery = {}^{c_{Found}}/_{c_{Added}} \times 100\% \quad (3)$$

Where cFound is the measured concentration and cAdded is the spiked concentration.

S3.8 Optimization of Experimental Conditions

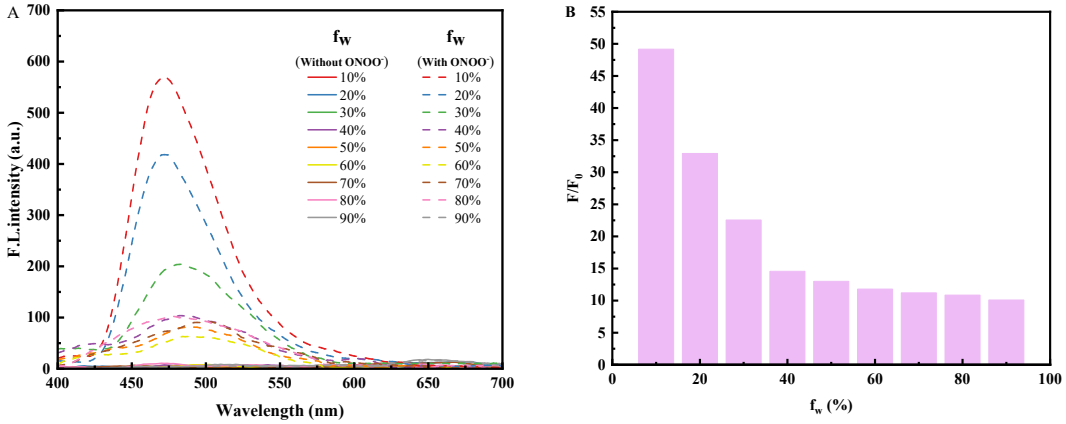


Figure S10 (A) The probe TPA-Cz-PPh_3 (20 μM in DMSO/H_2O) shows its recognition effect toward $ONOO^-$ under different aqueous fractions; (B) The corresponding plot displays the fluorescence enhancement fold before and after the reaction with $ONOO^-$.

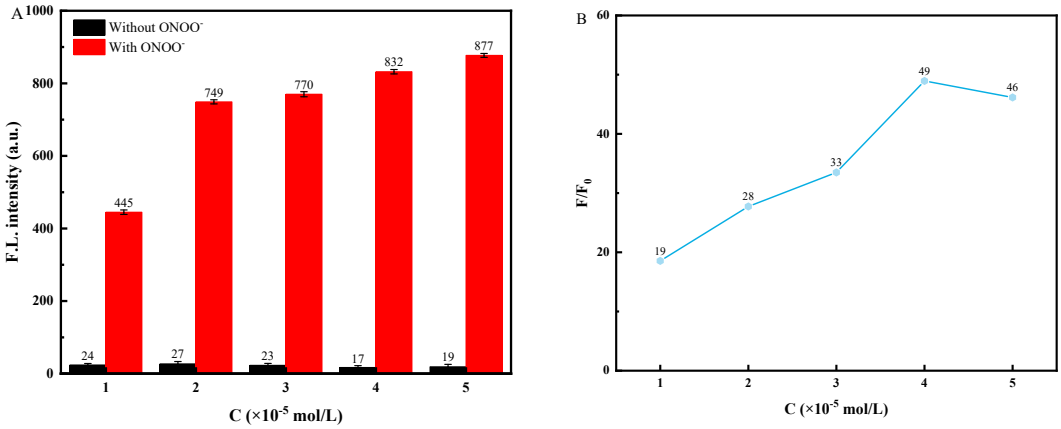


Figure S11 (A) The probe TPA-Cz-PPh_3 (in DMSO/H_2O, 9:1 v/v) shows its recognition effect toward $ONOO^-$ at different concentrations; (B) The corresponding plot displays the fluorescence enhancement fold before and after the reaction with $ONOO^-$.

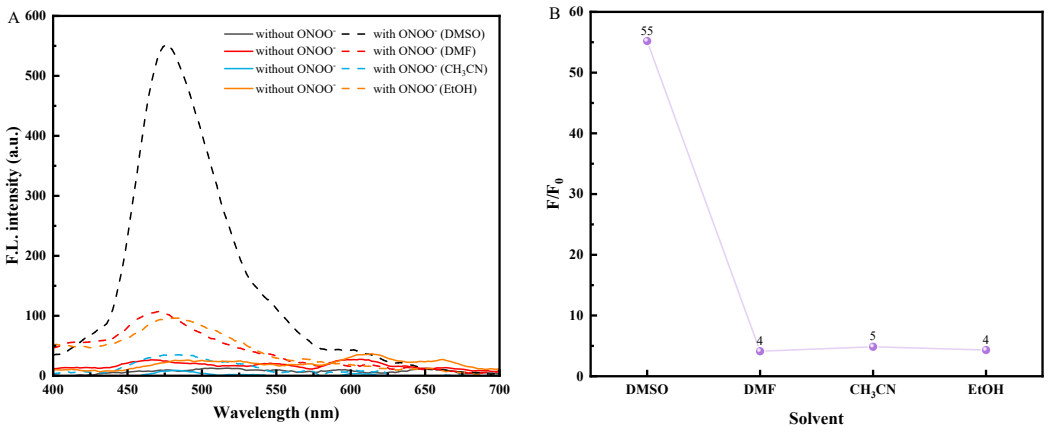


Figure S12 (A) The probe TPA-Cz-PPh_3 (40 μM, solvents/H_2O, 9:1 v/v) shows its recognition effect toward $ONOO^-$ in different solvents; (B) The corresponding plot displays the fluorescence enhancement fold before and after the reaction with $ONOO^-$.

S4 Supplementary Validation of the Aggregation-Induced Emission Mechanism for the Reaction Product TPA-Cz-CHO

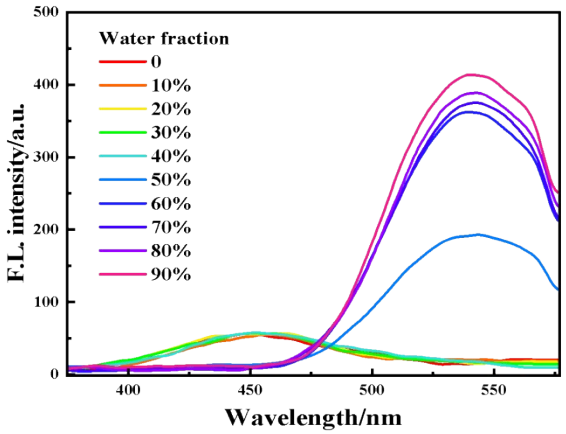


Figure S13. Fluorescence spectra of the reaction product TPA-Cz-CHO at varying water fractions

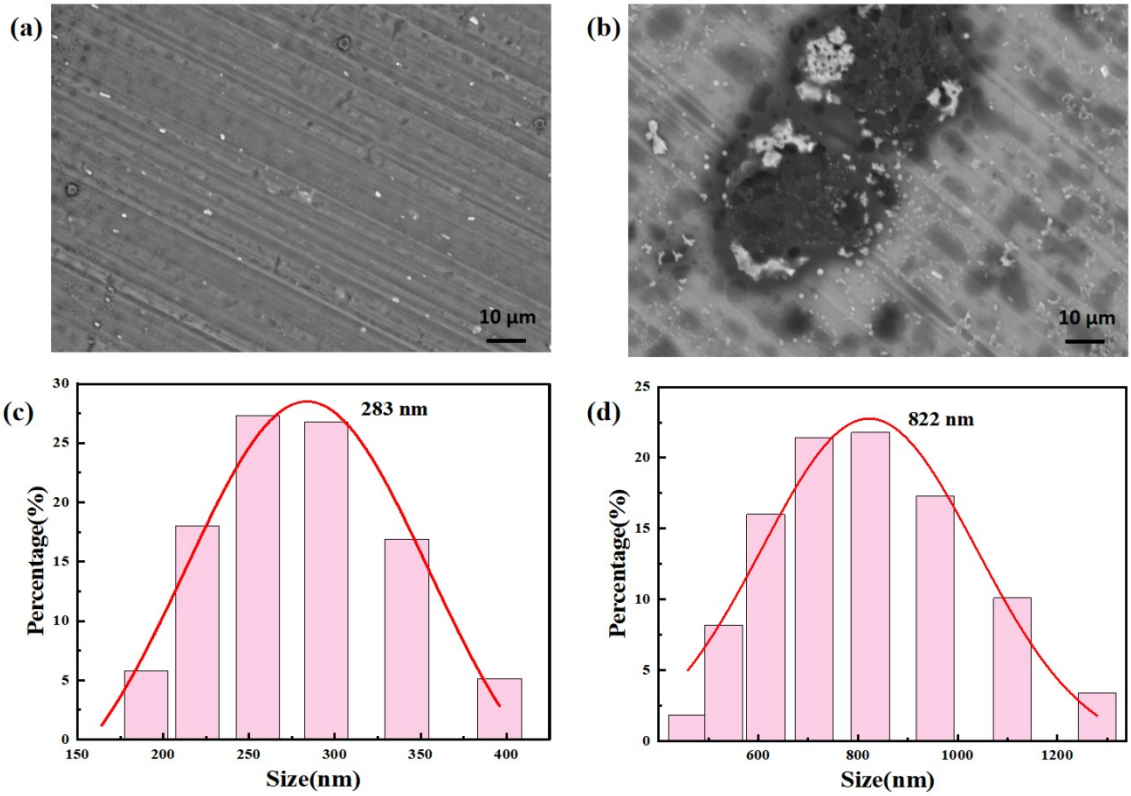


Figure S14. SEM images of TPA-Cz-CHO in DMSO/H_2O (40 μM, 9:1 v/v) solution (a) and DMSO/H_2O (40 μM, 1:9 v/v) solution (b); Particle size distribution of TPA-Cz-CHO in DMSO/H_2O (40 μM, 9:1 v/v) solution (c) and DMSO/H_2O (40 μM, 1:9 v/v) solution(d).

S5 Theoretical calculation method

The geometric structures of the compounds TPA-Cz-PPh_3 and TPA-Cz-CHO were optimized using Gaussian 09 software, with calculations performed at the B3LYP/6-31G level. The electron density distribution and molecular orbital diagrams were generated using Multiwfn[3–5] and VMD software[6].

S6 Spike Recovery of $ONOO^-$ in PAW in the Presence of High-Concentration ROS/RNS

Table S1 Spike Recovery Results of $ONOO^-$ in PAW Under Various Interference Conditions

Sample	Added (μM)	Found (μM)	Recovery (%)	RSD (%) (n = 3)
PAW+H_2O_2	100	99.80	99.80	1.25
PAW+NO_2^-	100	100.26	100.26	2.78
PAW+ClO^-	100	100.51	100.51	1.63
PAW+$^1O_2$	100	100.14	100.14	2.15

PAW+·OH	100	99.99	99.99	0.94
PAW+NO^-	100	100.38	100.38	2.41
PAW+TBO·	100	99.84	99.84	1.87
PAW+TBHP	100	101.03	101.03	2.09

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