Supporting Information

A smartphone-integrated AIE probe for multimodal and real-time detection of peroxynitrite in plasma-activated water

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Contents

1. The Preparation Method of Sample Solution

1.1 Preparation of Probe CNBT-TPE-BOH Stock Solution

Accurately weigh 18.72 mg of the probe **CNBT-TPE-BOH** into a vial. Dissolve it by stirring in 5 mL of DMSO to prepare a fluorescent probe stock solution with a concentration of 5.0×10^{-3} M for future use.

1.2 Preparation of Reactive Oxygen Species, Metal Cations, and Anion Solutions

Under ice-bath conditions, add 2.00 mL of HCl (0.60 M) and 2.00 mL of an aqueous H_2O_2 solution (0.70 M) to a reaction flask and mix by stirring for 20 min. Then, add 2.00 mL of NaOH solution (3.00 M) and 2.00 mL of a sodium nitrite solution (0.60 M) and continue the reaction for 1 min to obtain a slightly yellow $ONOO^-$ stock solution. Determine its concentration as 9.8 mM by measuring the absorbance at 302 nm. Weigh 149.00 mg (0.5 mM) of sodium nitroprusside and dissolve it in 10.00 mL of distilled water to prepare a 0.05 M NO^- solution. The TBHP solution is prepared by diluting a commercially available TBHP solution (70% aqueous solution) with distilled water to a concentration of 0.05 M. A 0.05 M TBO^- solution is prepared by mixing equal volumes of a 0.05 M TBHP solution and a 0.05 M ferrous sulfate solution. Dilute the H_2O_2 solution with distilled water to obtain a 0.05 M H_2O_2 stock solution. Weigh 41.13 mg (2.5 mM) of sodium hypochlorite pentahydrate and dissolve it in 50 mL of distilled water to prepare a 0.05 M ClO^- stock solution. A 0.05 M ·OH stock solution is prepared by mixing equal volumes of a 0.05 M ferrous sulfate aqueous solution and a 0.50 M H_2O_2 aqueous solution. A 0.05 M $^1O_2$ stock solution is prepared by mixing equal volumes of a 0.05 M sodium molybdate solution and a 0.50 M H_2O_2 aqueous solution. Weigh 34.50 mg (0.5 mM) of $NaNO_2$ and dissolve it in 10.00 mL of distilled water to prepare a 0.05 M NO_2^- solution.

Prepare aqueous solutions of the corresponding metal cations (0.01 M) of $LiCl\cdot H_2O$, $FeCl_3\cdot H_2O$, $Mg(NO_3)_2\cdot 6H_2O$, $Cu(NO_3)_2\cdot 3H_2O$, KNO_3, $NaNO_3$, $AgNO_3$, $Pb(NO_3)_2$, $Co(NO_3)_2\cdot 6H_2O$, $Zn(NO_3)_2\cdot 4H_2O$, $Ni(NO_3)_2\cdot 6H_2O$, $Al(NO_3)_3\cdot 9H_2O$, $Ca(NO_3)_2\cdot 6H_2O$, $HgCl_2$, $MnCl_2\cdot 4H_2O$, $Cr(NO_3)_3\cdot 9H_2O$, $BaCl_2\cdot 2H_2O$, and $Cd(NO_3)_2\cdot 4H_2O$ respectively.

Prepare aqueous solutions of the corresponding anions (0.01 M) of KF, K_2SO_4, KBr, KCl, KI, KH_2PO_4, KNO_3, $K_2C_2O_4$, and $NaClO_2$ respectively.

The chemical reagents used above are all analytically pure.

2. The ^{1}H NMR, ^{13}C NMR, MS (ESI) spectra

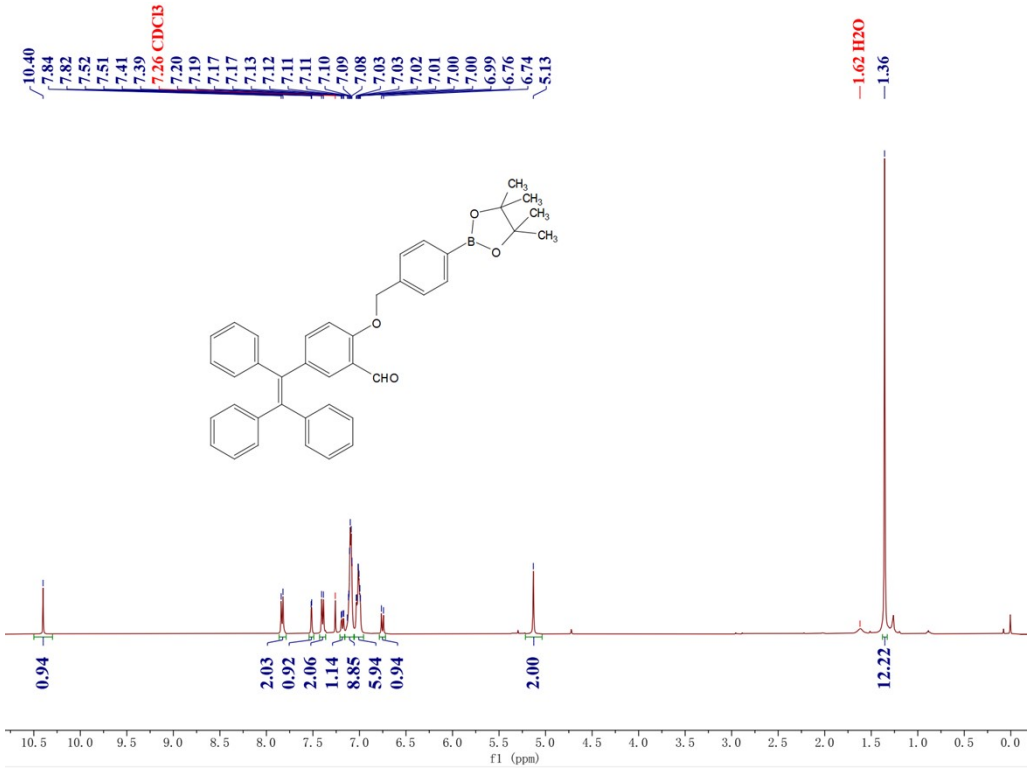

Fig. S1. The ^{1}H NMR spectrum of **CHO-TPE-BOH** in $CDCl_3$.

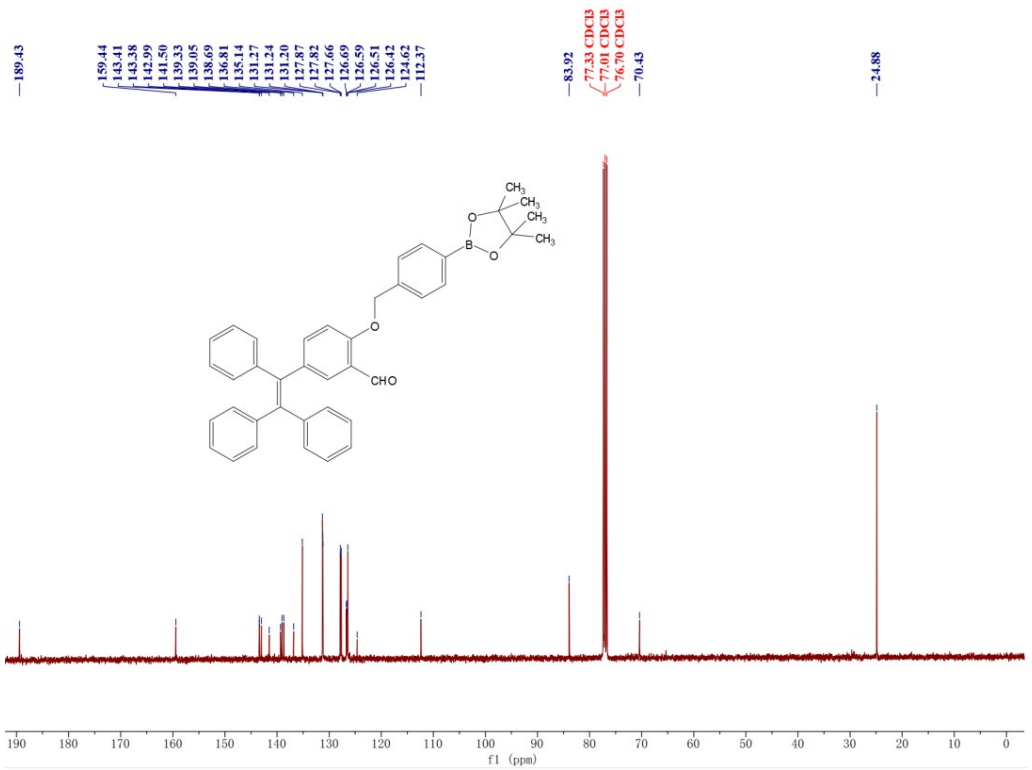

Fig. S2. The ^{13}C NMR spectrum of **CHO-TPE-BOH** in $CDCl_3$

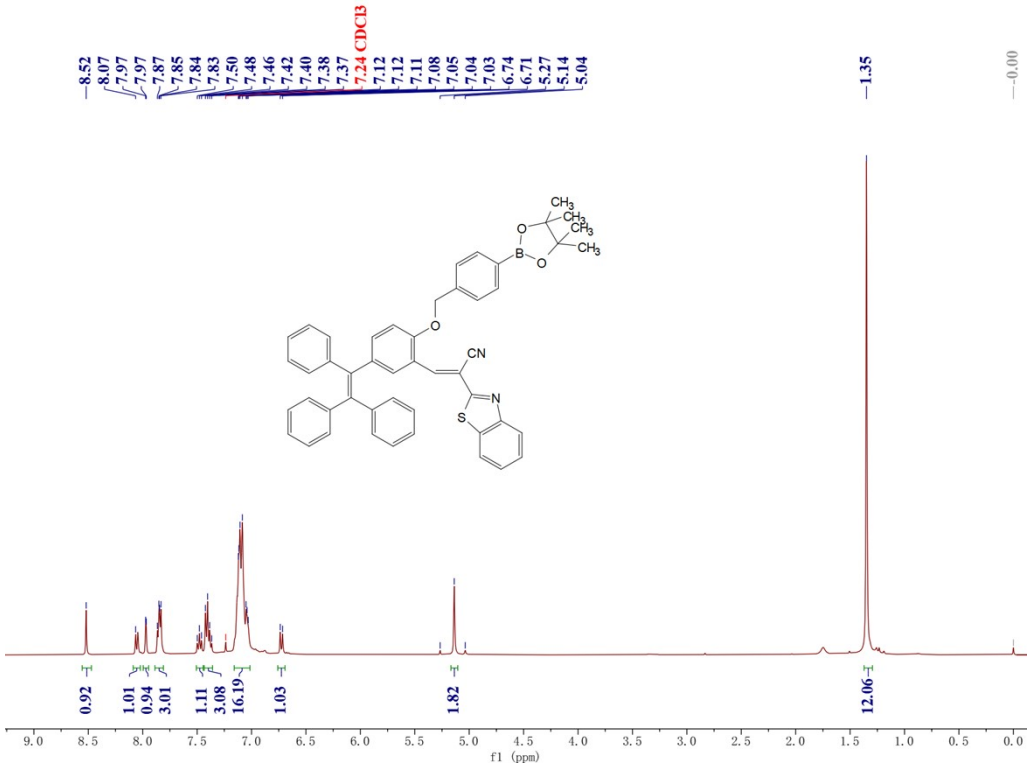

Fig. S3. The ^{1}H NMR spectrum of **CNBT-TPE-BOH** in $CDCl_3$.

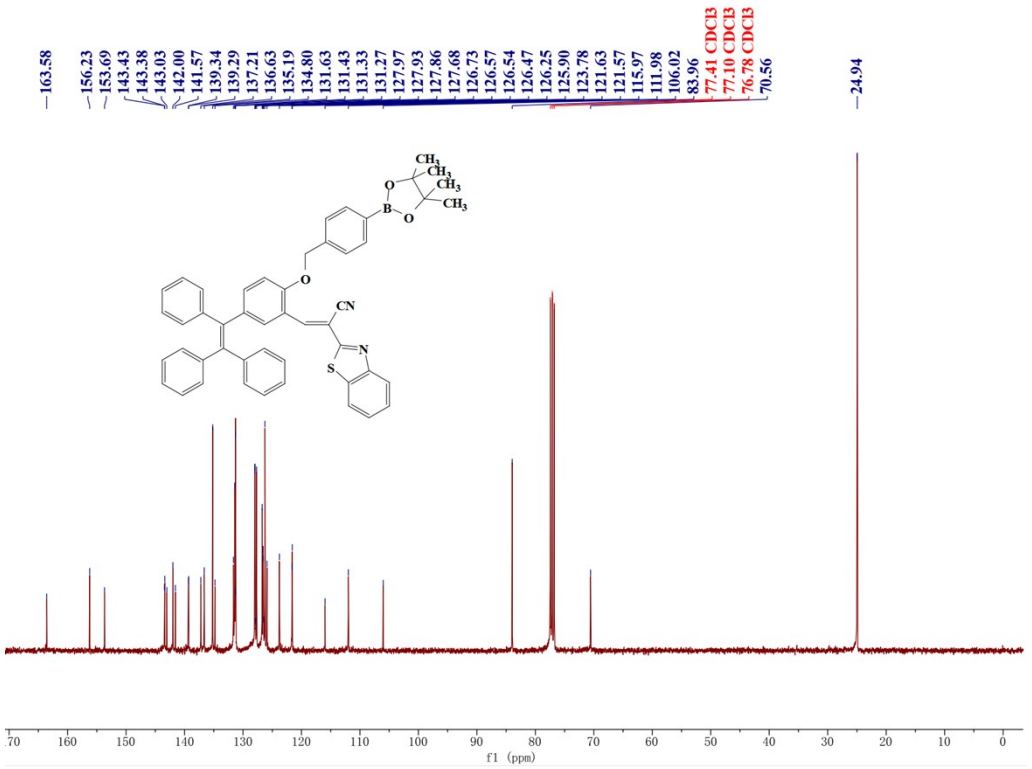

Fig. S4. The ^{13}C NMR spectrum of **CNBT-TPE-BOH** in $CDCl_3$.

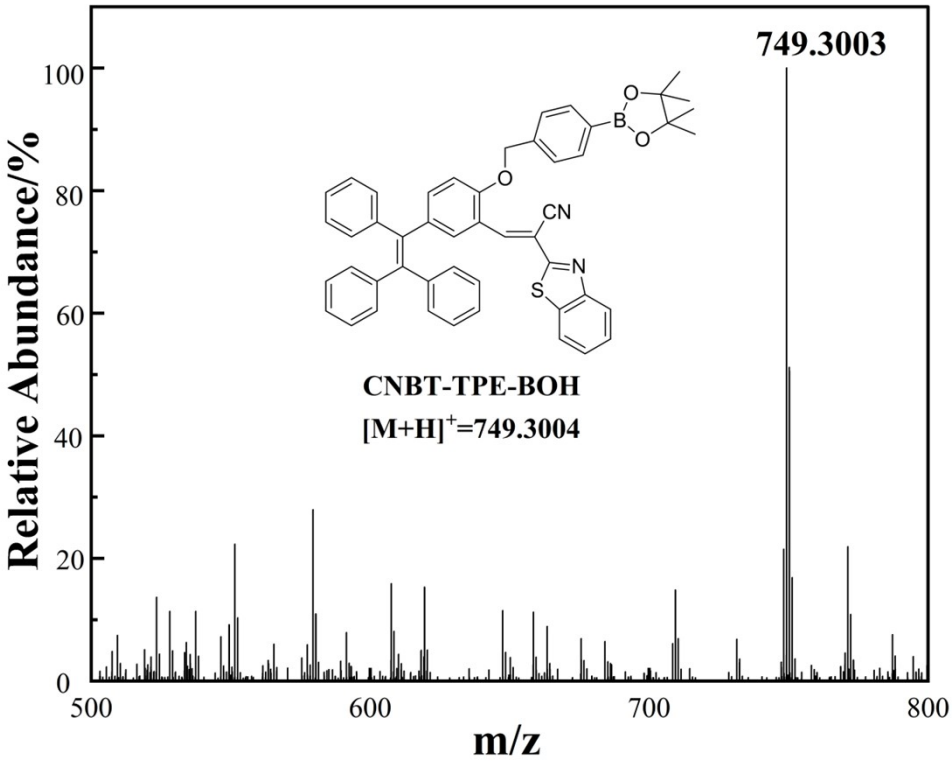

Fig. S5. The HRMS (ESI) spectrum of **CNBT-TPE-BOH.**

3.Results and Discussion

3.1 Effect of Water Volume Fraction on Probe Response Performance

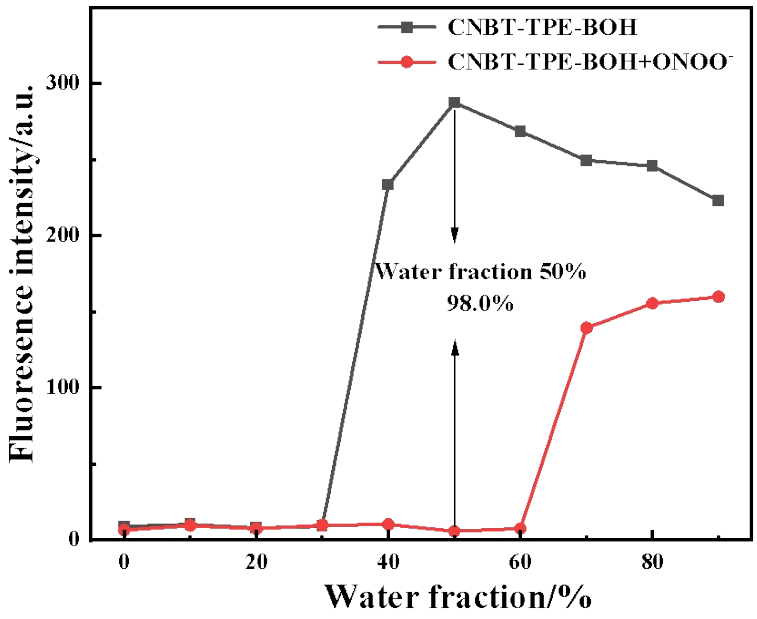

Fig. S6. $ONOO^-$-fluorescence response of probe **CNBT-TPE-BOH** to water volume fraction 0-90% (DMSO/H_2O) (10μM, λ_{ex} = 329 nm).

3.2 Optimization of Composite Solution Concentration

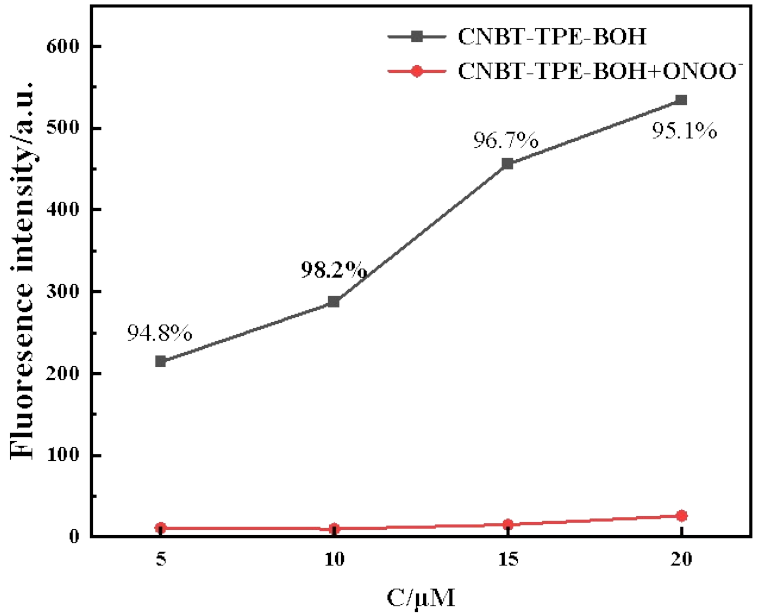

Fig. S7. Fluorescence spectra of probe **CNBT-TPE-BOH** (at varying concentrations) in DMSO/H_2O (1:1 v/v) upon addition of $ONOO^-$ (10 equiv.) (λ_{ex} = 329 nm)

3.3 Solvent System Optimization of CNBT-TPE-BOH Composite Solution

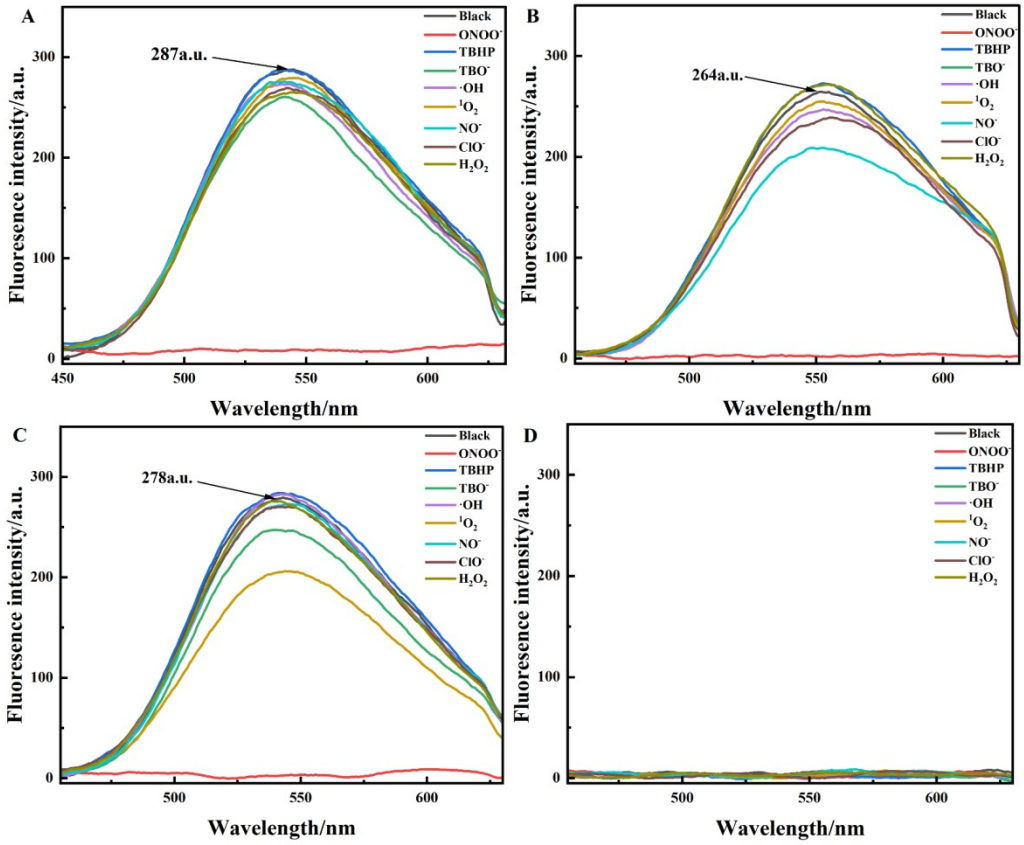

Fig. S8. Fluorescence spectra of probe **CNBT-TPE-BOH** (10 μM) in (A) DMSO/H_2O (1:1 v/v), (B) CH_3OH/H_2O (1:1 v/v), (C) DMF/H_2O (1:1 v/v), and (D) CH_3CH_2CN/H_2O (1:1 v/v) solutions upon addition of various reactive oxygen/nitrogen species (ROS/RNS) (λ_{ex} = 329 nm).

3.4 Selectivity Detection of CNBT-TPE-BOH for $ONOO^-$

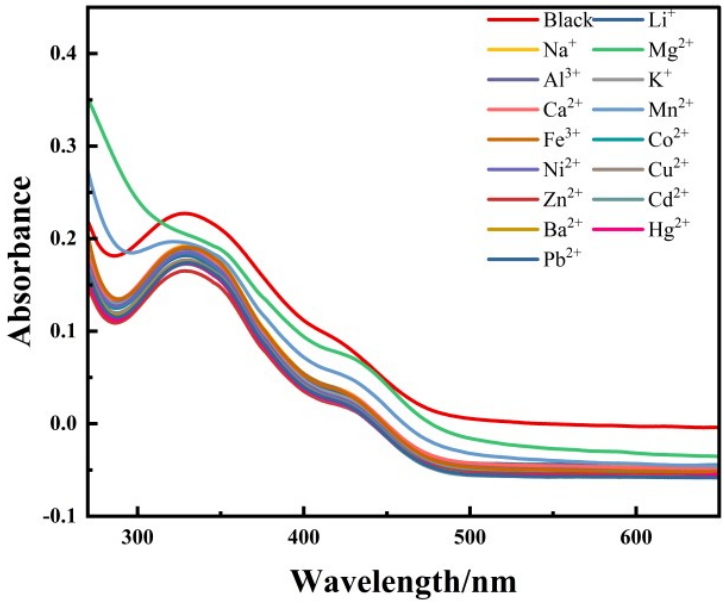

Fig. S9. UV-vis absorption spectra of **CNBT-TPE-BOH** in DMSO/H_2O solution (10 μM, 1:1 v/v, pH 7.4) after the addition of 10 equiv. of cations (Li^+, Na^+, Mg^{2+}, Al^{3+}, K^+, Ca^{2+}, Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Ba^{2+}, Hg^{2+}, Pd^{2+}).

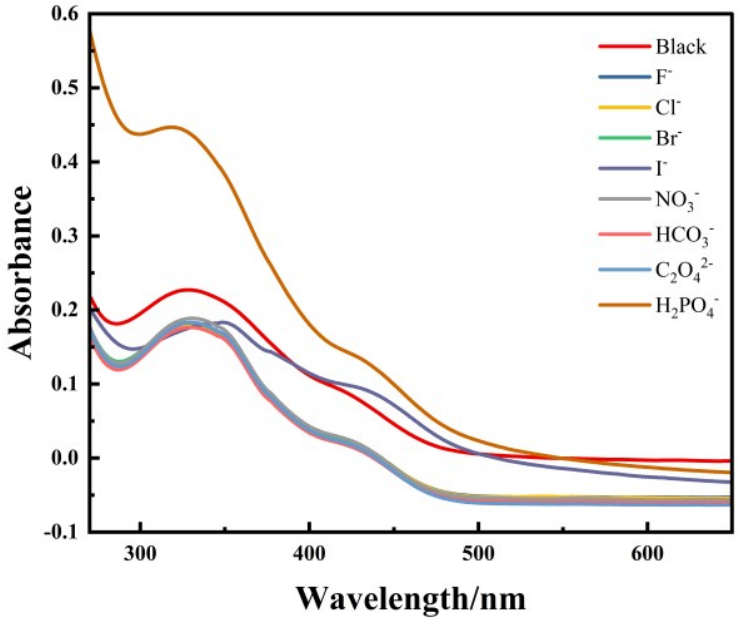

Fig. S10. UV-vis absorption spectra of **CNBT-TPE-BOH** in DMSO/H_2O solution (10 μM, 1:1 v/v, pH 7.4) after the addition of 10 equiv. of anions (F^-, Cl^-, Br^-, I^-, NO_3^-, HCO_3^-, $H_2PO_4^-$ and $C_2O_4^{2-}$).

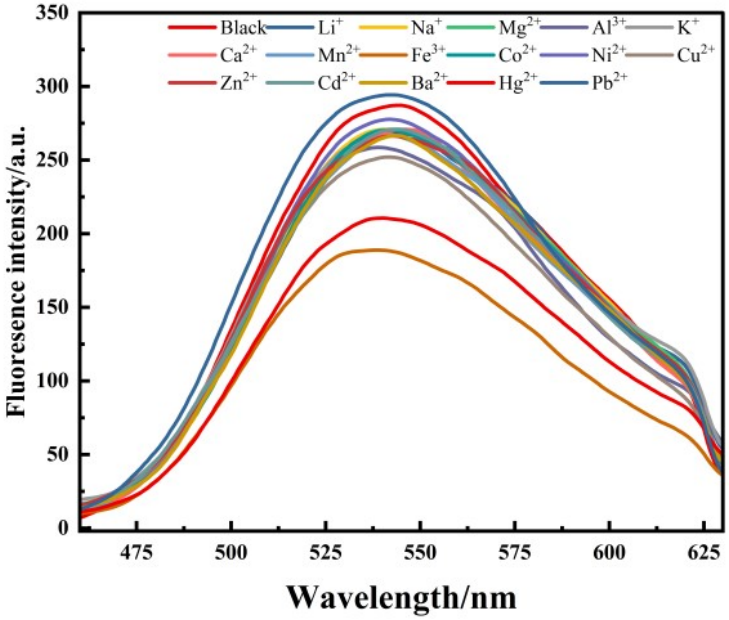

Fig. S11. Fluorescence spectra of **CNBT-TPE-BOH** in DMSO/H_2O solution (10 μM, 1:1 v/v, pH 7.4) after the addition of 10 equiv. of cations (Li^+, Na^+, Mg^{2+}, Al^{3+}, K^+, Ca^{2+}, Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Ba^{2+}, Hg^{2+}, Pd^{2+}).

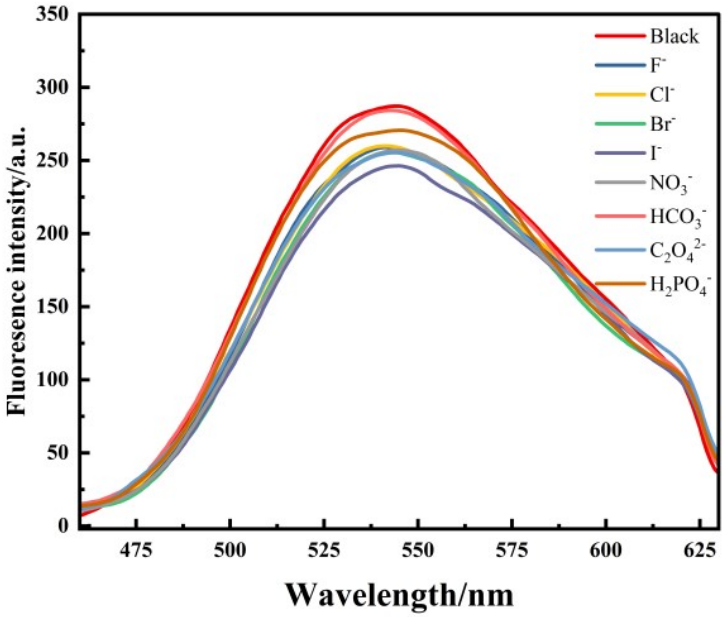

Fig. S12. Fluorescence spectra of **CNBT-TPE-BOH** in DMSO/H_2O solution (10 μM, 1:1 v/v, pH 7.4) after the addition of 10 equiv. of anions (F^-, Cl^-, Br^-, I^-, NO_3^-, HCO_3^-, $H_2PO_4^-$ and $C_2O_4^{2-}$).

3.5 Detection Mechanism of CNBT-TPE-BOH for $ONOO^-$

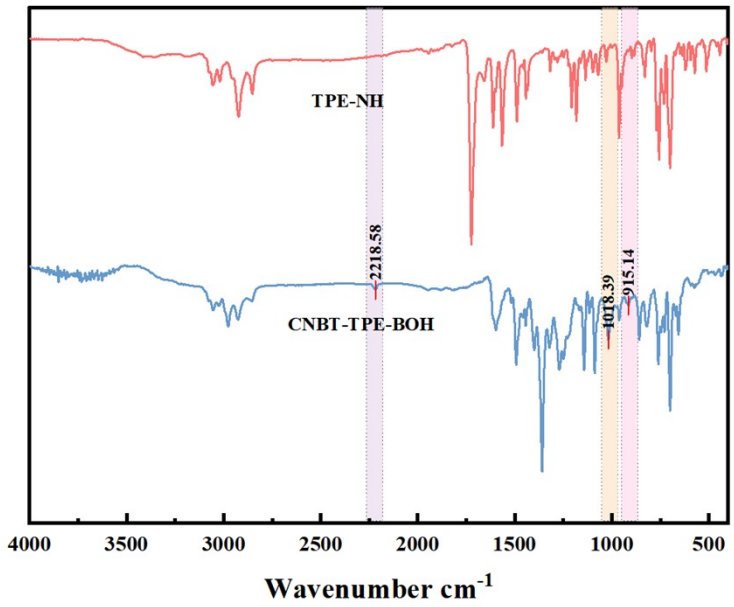

Fig. S13. FT-IR spectra of **CNBT-TPE-BOH** and **TPE-NH.**

3.6 Comprehensive Data for Smartphone-Based Detection under Different Conditions

Table S1. G value, detection limit, and LOD of **CNBT-TPE-BOH** after reaction with $ONOO^-$ under different mobile phones and lighting conditions.

mobile phone	lighting condition	G value							Linear Equation	R^2	LOD/ μM
		20	30	40	50	60	70	80			
Huawei P40 Pro	indoor light	179	170	165	157	146	140	134	$y = –7.9108 \times 10^5x + 195.6247$	0.9940	0.92
Xiaomi 14	indoor light	178	170	164	155	145	140	133	$y = -7.6429 \times 10^5x + 193.2143$	0.9949	1.04
iPhone 14 Pro	indoor light	180	172	163	158	146	138	133	$y = –8.0714 \times 10^5x + 196.07129$	0.9928	0.99
Huawei P40 Pro	LED light box	177	169	163	156	147	141	135	$y = –7.0714 \times 10^5x + 190.7857$	0.9975	1.13
Huawei P40 Pro	natural	179	171	164	156	144	140	133	$y = –7.8571 \times 10^5x + 194.5714$	0.9915	1.02

3.7 CNBT-TPE-BOH Fluorescence Lifetime after $ONOO^-$ Recognition

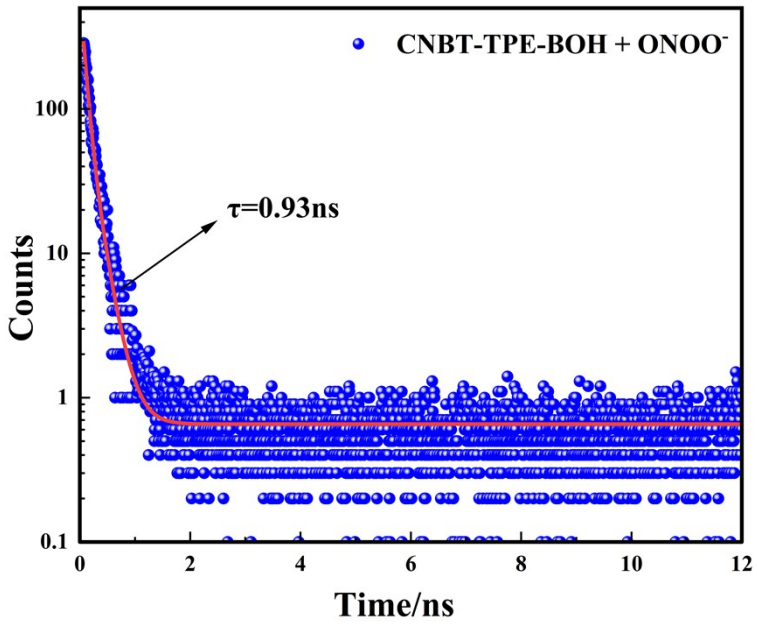

Fig. S14. Fluorescence lifetime of **CNBT-TPE-BOH** after the addition of $ONOO^-$.

3.8 The stability of the probe during long-term storage in PAW

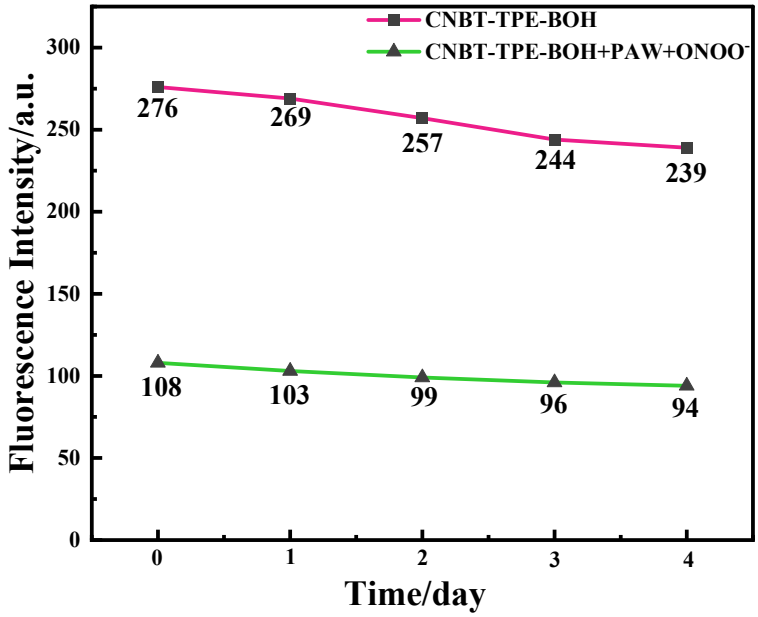

Fig.S15 Long-term stability of the CNBT-TPE-BOH probe in a PAW environment containing 60 μM $ONOO^-$(10μM, λ_{ex} = 329 nm).

3.9 The photobleaching performance of the probe during use in PAW

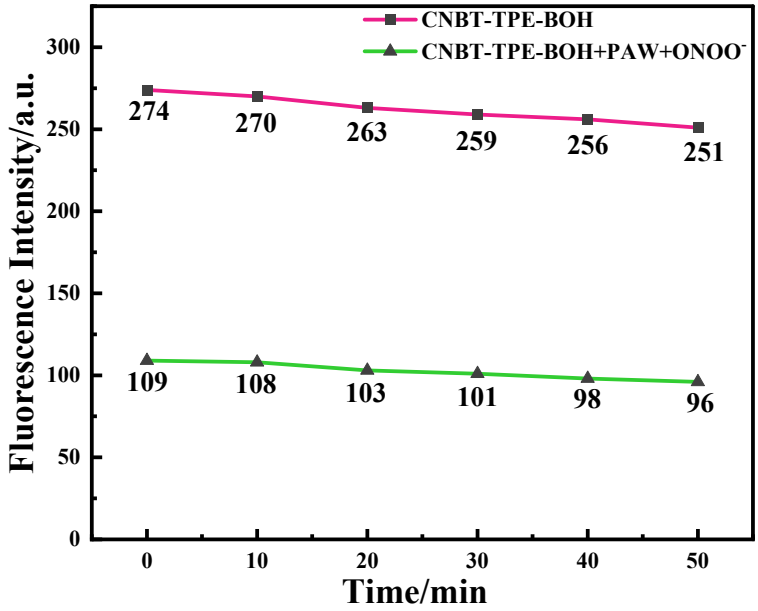

Fig.S16 Photostability assessment of the CNBT-TPE-BOH probe under 365 nm UV irradiation in a PAW environment containing 60 μM $ONOO^-$(10μM, λ_{ex} = 329 nm).

3.10 Comparison with Previously Reported $ONOO^-$ Detection Strategies

Table S2. Comparison of analytical performance of this method with $ONOO^-$ detection methods in literature

Fluorescent probe	response time	Stokes shift	LOD	Detection Mode	pH Range	Application	Refs.
NA-DP	15 min	130 nm	0.31 μM	UV-vis FL	4.0-10.0	Cell Imaging	1
PNDP	20 min	175 nm	119 nM	FL	6.5-8.5	Mouse Imaging	2
Rod-Br	3 min	53 nm	27.9 nM	FL	5.0-9.0	Mouse Imaging	3
Cou-BN	120 s	107 nm	30.2 nM	FL	3.0-10.0	Mouse Imaging	4
BDP-NIR-ONOO	80 s	80 nm	25 nM	FL	7.0-10.0	Mouse Imaging	5
HN-ONOO	1 min	102 nm	1.117 μM	FL	5.0-9.0	Cell Imaging	6
W-3a	10 min	97 nm	85 nM	FL	5.0-10.0	Mouse Imaging	7
CNBT-TPE-BOH	**8 s**	**215 nm**	**UV-vis: 11.80 μM FL: 0.62 μM Colorimetric: 0.92 μM**	**UV-vis FL Colorimetric**	**0.8-11.9**	**PAW**	**This work**

References

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