Electronic Supplementary Material (ESI) for Analyst.

Alizarins-based molecular probes for the detection of hydrogen peroxide and peroxynitrite

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Materials and apparatus

All chemistry reagents are analytical grade without further purification. All aqueous solutions were prepared using deionized water from a Milli-Q water purification system (Millipore, Bedford, MA, USA). Absorption spectra were measured on a Lambda 365 spectrophotometer (PerkinElmer, U.K.). Fluorescence spectra were performed on a spectrophotometer (Varian Cary Eclipse). The pH was adjusted using a Phs-3c pH meter (Germany Sartorius).

Electrochemical measurements

Electrochemical measurements were conducted on the CHI660E electrochemical workstation purchased from Chenhua (Instrument Company, Shanghai, China) at room temperature with a traditional three-electrode system. In this system, the Pt wire was used as the auxiliary electrode, the Ag/AgCl was used as the reference electrode and the glassy carbon electrode (GCE) as a working electrode (Φ=3.0 mm). Differential pulse voltammetry (DPV): increment potential, 0.004 V; pulse amplitude, 0.05 V; pulse width, 0.05 s; pulse period, 0.5 s; quiet time, 2 s. The GCE was hand-polished repeatedly with Al_2O_3, successively rinsed with ultrapure water and ethanol, and dry under room temperature prior to experimentation.

Table S1. Comparison of reaction-based IDA method and other method.

probes	Method	Synthesis step	Synthesis time	media
Ref.[1]	Reaction-based probe	Three steps	>24 h	phosphate buffer
Ref.[2]	Reaction-based probe	Three steps	>6 h	8% DMSO
Ref.[3]	Reaction-based probe	Two steps	>12 h	1% DMSO
Ref.[4]	Reaction-based probe	Two steps	>12 h	50% DMSO
Ref.[5]	Reaction-based probe	Two steps	>12 h	50% DMSO
This work	Reaction-based indicator displacement assay	One step	10 min	phosphate buffer

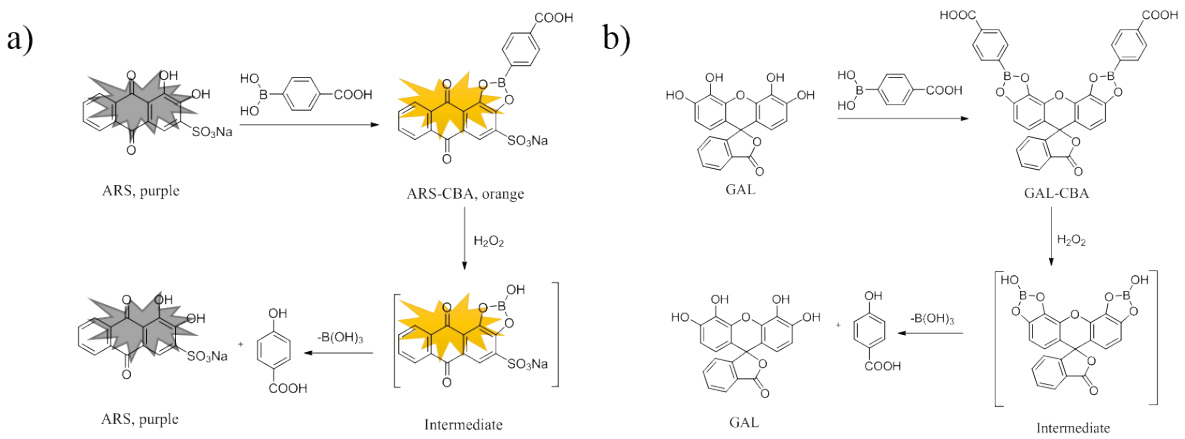


Fig. S1 Design strategy of ARS-CBA and GAL-CBA for H_2O_2 in neutral aqueous buffer with CTAB.

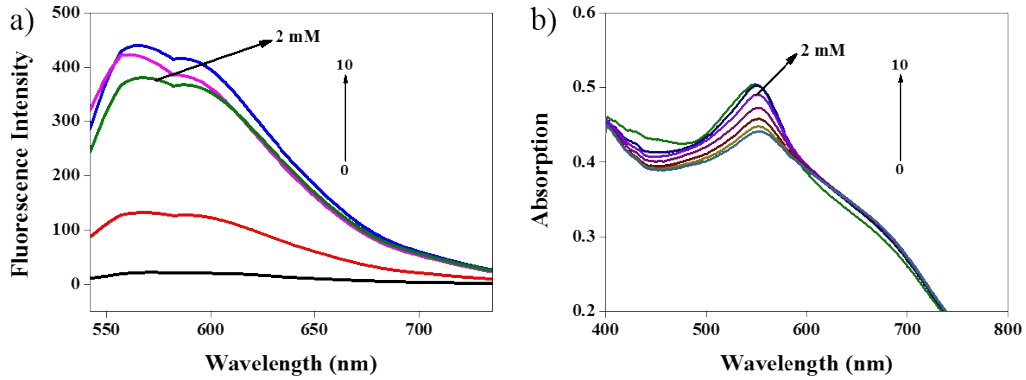


Fig. S2 (a) Fluorescence spectra of **ARS-CBA** (**ARS**: 50 μM, **CBA**: 200 μM) with different concentrations of CTAB (0 mM, 1 mM, 2 mM, 5 mM, 10 mM). (b) UV-Vis response of **ARS-CBA** (**ARS**: 50 μM, **CBA**: 400 μM) with different concentrations of CTAB (0 mM, 0.5 mM, 1 mM, 1.5 mM, 2 mM, 5mM, 10 mM).

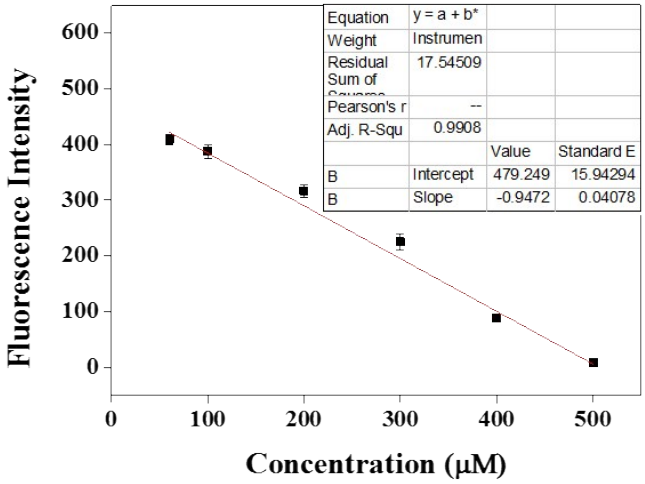


Fig. S3 Linear correlation between the fluorescence intensity of ARS-CBA at 568 nm and H_2O_2 concentration (60-500 μM). Slit: 10/10

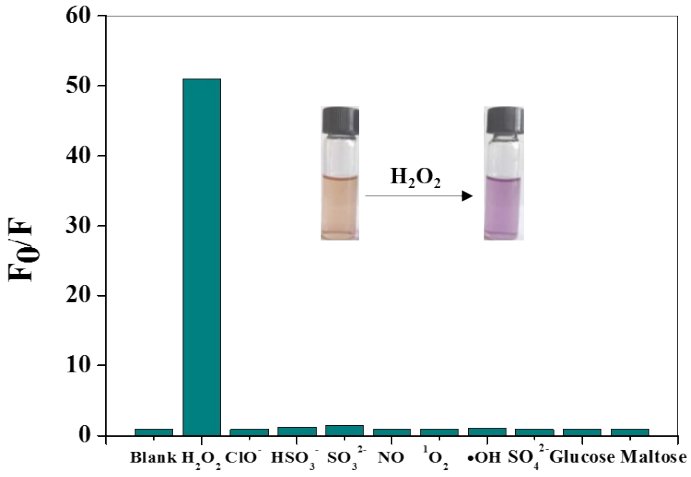


Fig. S4 Fluorescence response of ARS-CBA toward various reactive oxygen species and some typical physiological nucleophiles.

Table S2. Determination of hydrogen peroxide in disinfectant samples.

Disinfectant	Content (mM)	Added (mM)	Detected (mM)	RSD (%,N=6)	Recovery (%)
1	0.10	0.2	0.31	3.56	105
2	0.30	0.2	0.49	2.12	95
3	0.50	0.2	0.705	1.30	102.5

Table S3. Determination of hydrogen peroxide in disinfectant samples.

Disinfectant	Content (mM)	Added (mM)	Detected (mM)	RSD (%,N=6)	Recovery (%)
1	0.10	0.2	0.29	2.16	95
2	0.30	0.2	0.503	3.12	101.5
3	0.50	0.2	0.695	2.30	97.5

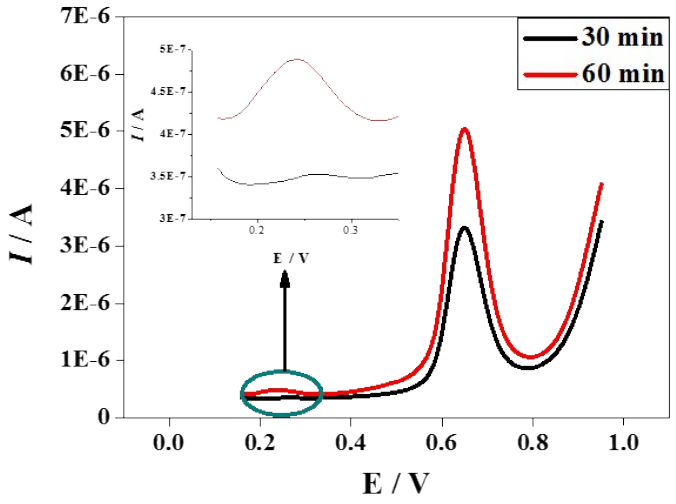


Fig. S5 Differential pulse voltammograms of ARS-CBA (ARS, 50 μM; CBA, 200 μM) in the presence of H_2O_2 (500 μM, 30 and 60 min).

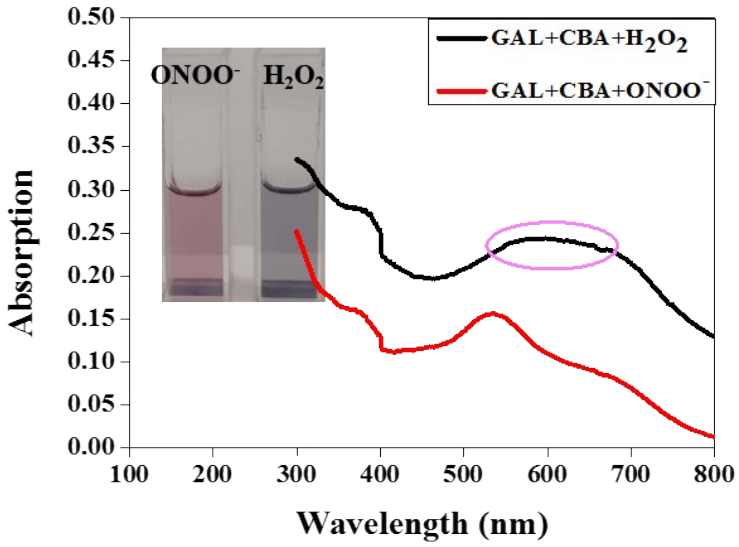


Fig. S6 UV-Vis absorption spectra of GAL-CBA in the present of H_2O_2 and $ONOO^-$.

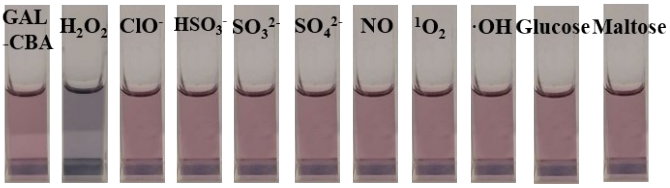


Fig. S7 Optical photographs of GAL-CBA toward various reactive oxygen species and some typical physiological nucleophiles under ambient light after leaving them overnight.

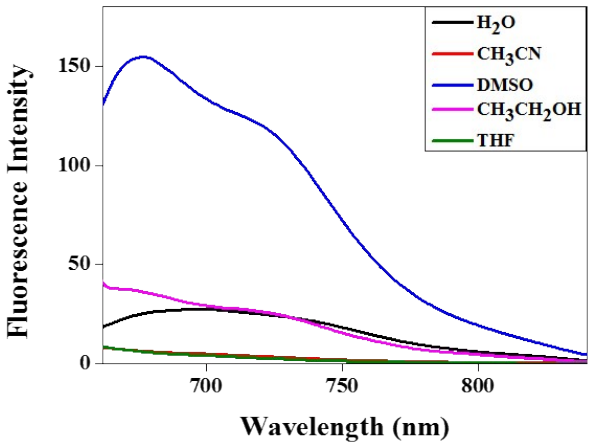


Fig. S8 The fluorescence response of ABS in various solvents.

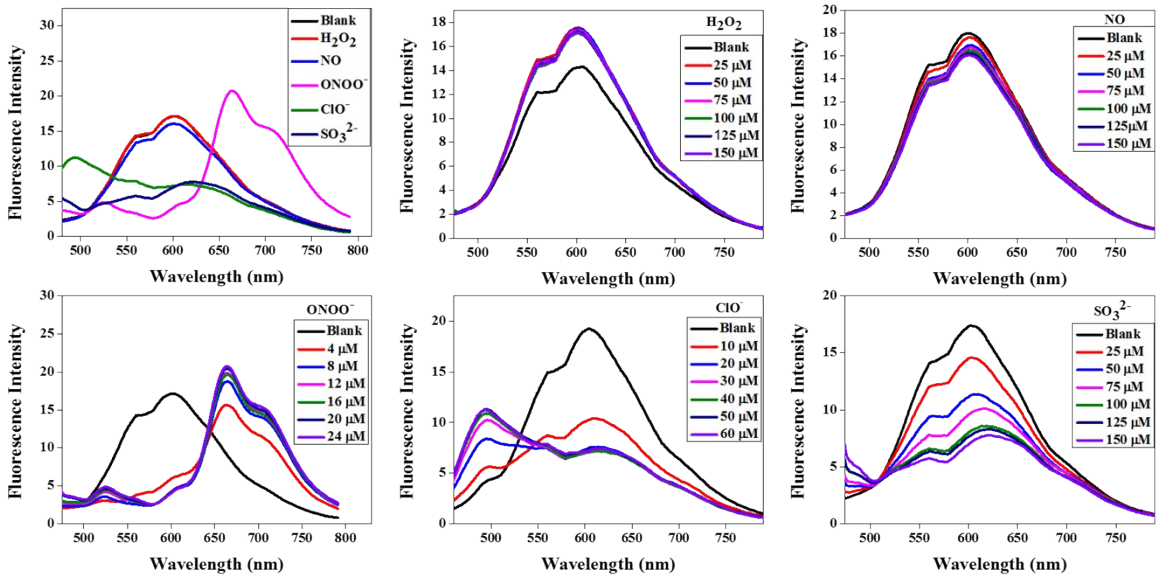


Fig. S9 Fluorescence titration spectra of ARS (50 μM) after treated with various agents in DMSO. Slit:10/10.

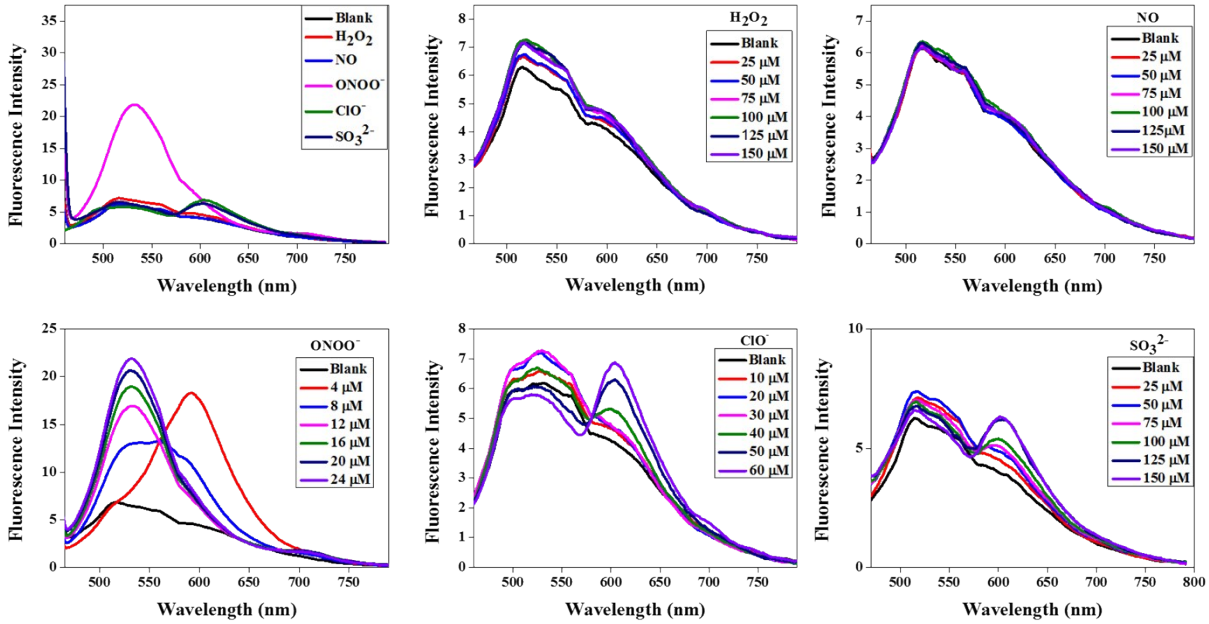


Fig. S10 Fluorescence titration spectra of GAL (50 μM) after treated with various agents in DMSO. Slit:10/10.

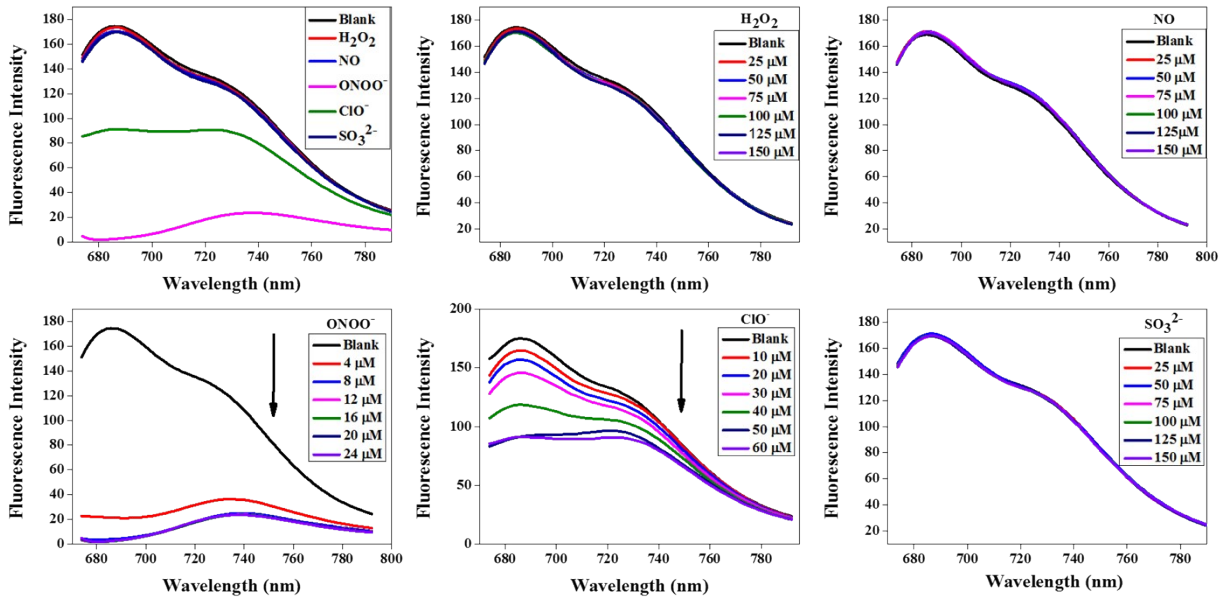


Fig. S11 Fluorescence titration spectra of ABS (50 μM) after treated with various agents in DMSO. Slit:10/10.

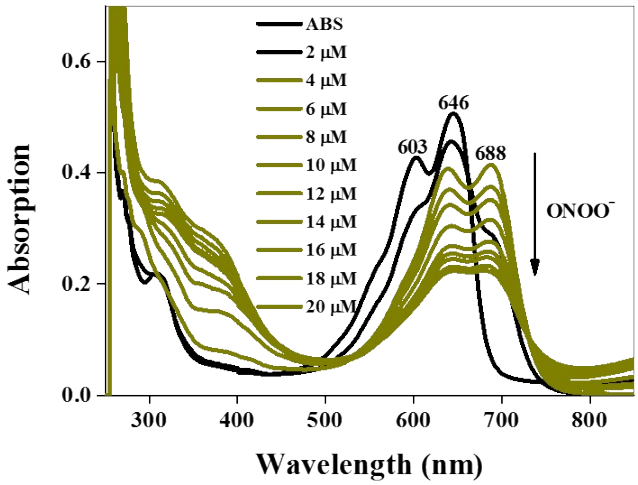
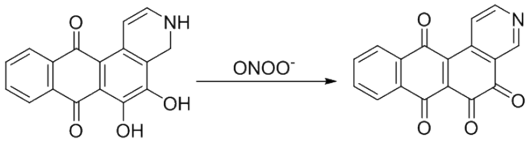


Fig. S12 UV-Vis titration for ABS (50 μM) in the presence of various concentrations of $ONOO^-$ (0-20 μM) in DMSO.



Scheme S1 Reaction of ABS with $ONOO^-$.

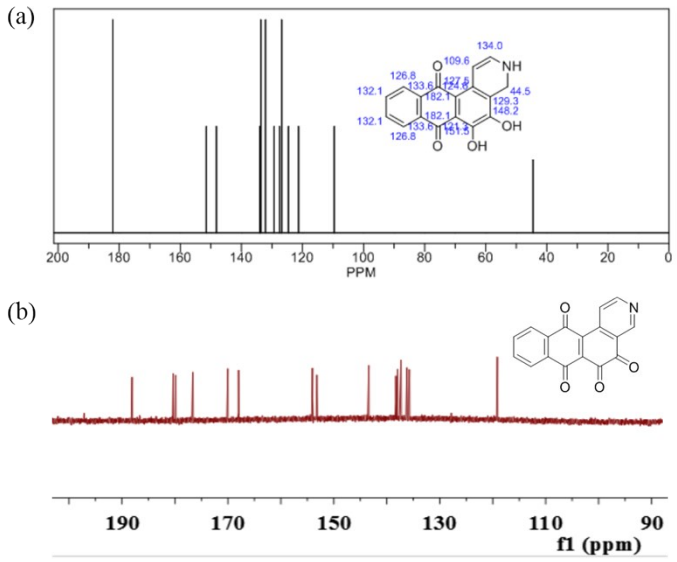


Fig. S13 The ^{13}C NMR spectra of (a) ABS and (b) ABS with $ONOO^-$.

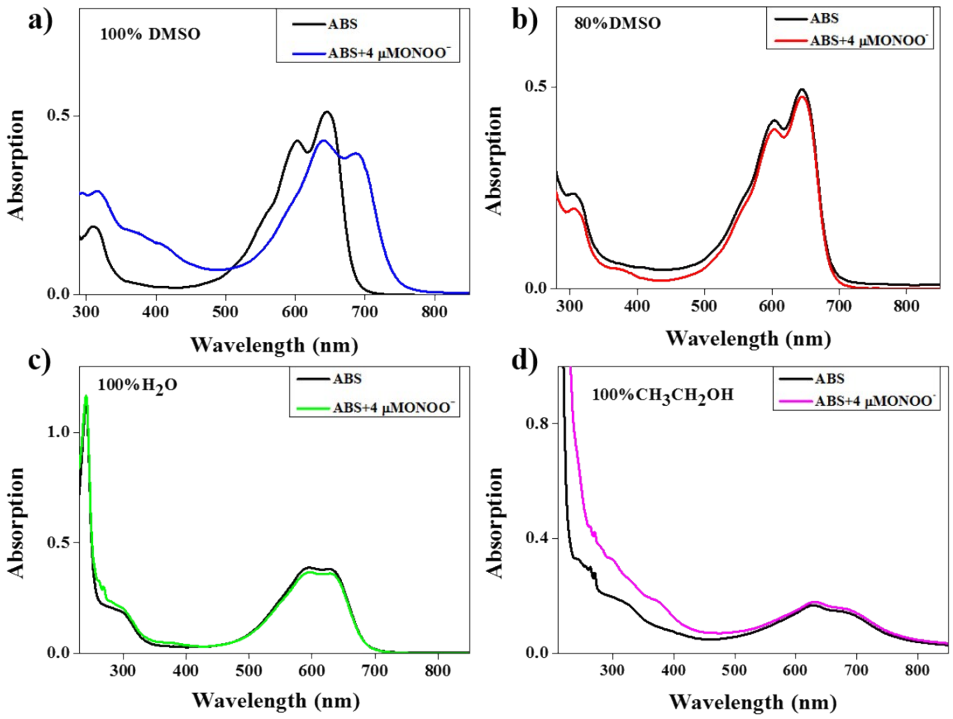


Fig. S14 Absorption spectra of ABS (50 μM) in the absence and presence of 4 μM $ONOO^-$ in different solvents.

References

1 H. Y. Li, X. H. Li, X. F. Wu, W. Shi and H. M. Ma, *Anal. Chem.,* 2017, **89**, 5519.

2 L. L. Wu, Y. Wang, M. Weber, L. Y. Liu, A. C. Sedgwick, S. D. Bull, C. Huang and T. D. James, *Chem. Commun.,* 2018, **54**, 9953.

3 X. L. Xie, F. Y. Tang, G. Z. Liu, Y. Li, X. X. Su, X. Y. Jiao, X. Wang and B. Tang, *Anal.*

Chem., 2018, **90**, 11629.

4 Y. Q. Wu, A. P. Shi, Y. Y. Li, H. Zeng, X. Y. Chen, J. Wu and X. L. Fan, *Analyst,* 2018, **143**, 5512.

5 Y. S. Fu, H. L. Nie, R. B. Zhang, F. Y. Xin, Y. Tian, J. Jing and X. L. Zhang, *RSC Adv.,* 2018, **8**, 1826.