Supporting Information

A novel colorimetric and ratiometric fluorescent probe for targeting detection of hypochlorous acid based on HClO-mediated anthracene-hydrazone to anthracene-triazole transformation

Chen Jiang[a], Yuewei Yao[a], Chuilian Kong[a], Jiaqi Du[b], Jingjing Meng*[c], Cheng Yao**[a]

[a] *College of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, China.*

[b] *College of Chemical Engineering, Nanjing Tech University, Nanjing 211816 (China)*

[c] *College of Biotechnology and Pharmaceutical Engineering, Nanjing Tech University, Nanjing 211816 (China)*

*Corresponding author: C. Yao, E-mail: yaochengnjut@126.com

**Corresponding author: J. J. Meng, E-mail: jjmeng@njtech.edu.cn

Fig. S1

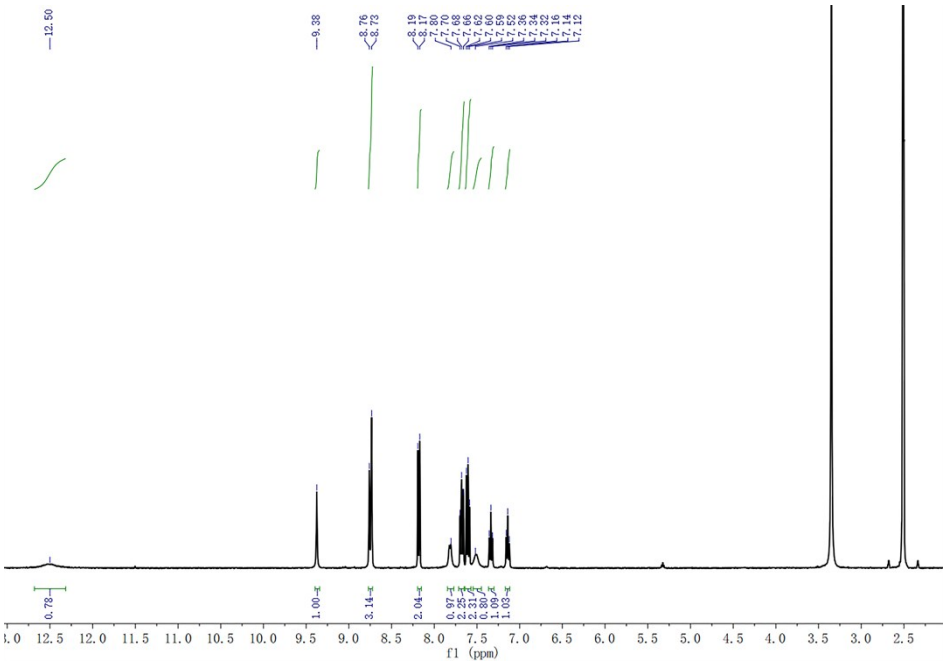


Fig. S1 ^{1}H NMR of probe **B-ClO** in DMSO-d_6;

Fig. S2

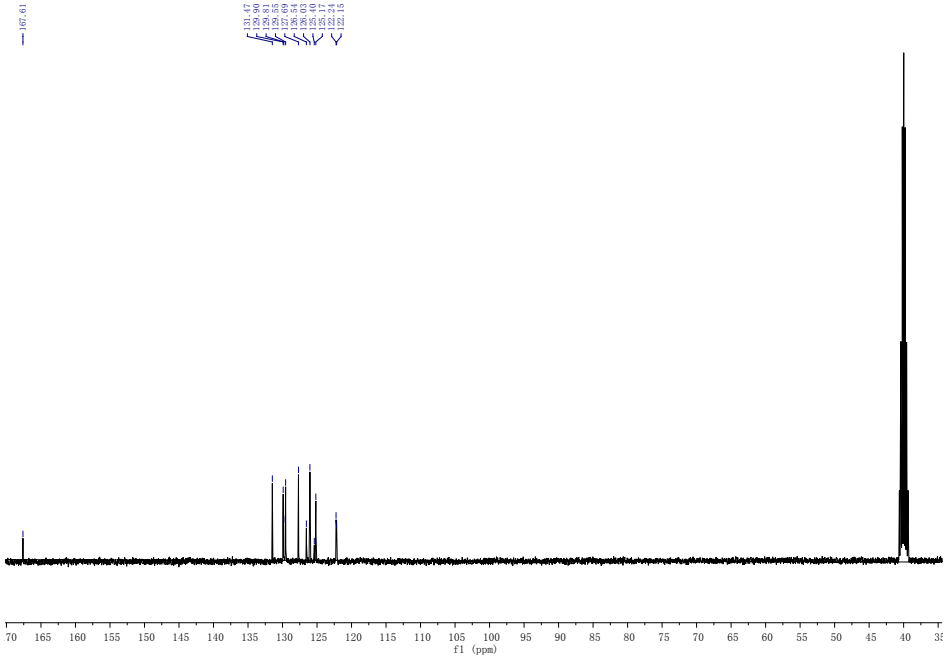


Fig. S2 ^{13}C NMR of probe **B-ClO** in DMSO-d_6;

Fig. S3

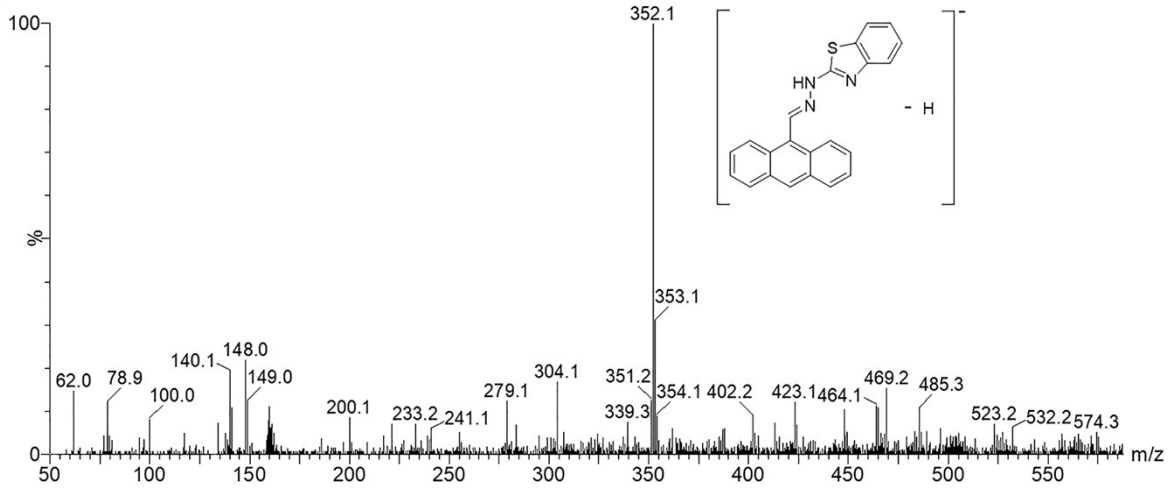
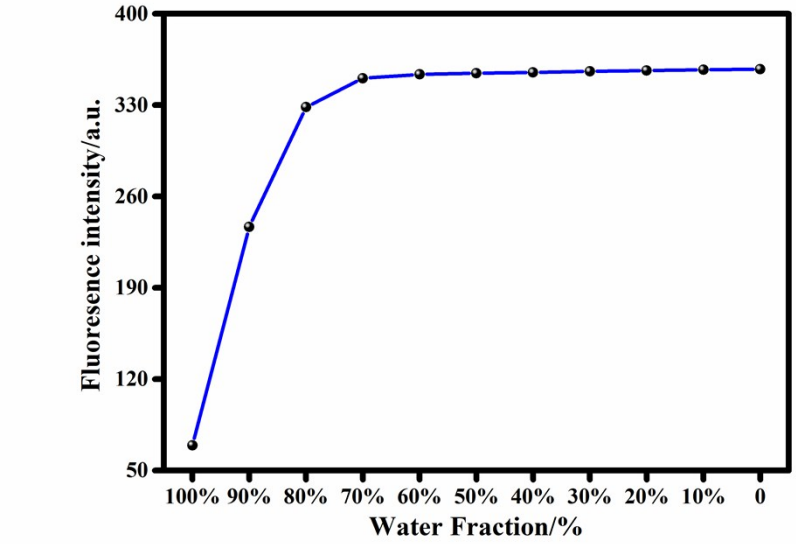


Fig. S3 MS of probe **B-ClO**;

Fig. S4
(a)



(b)

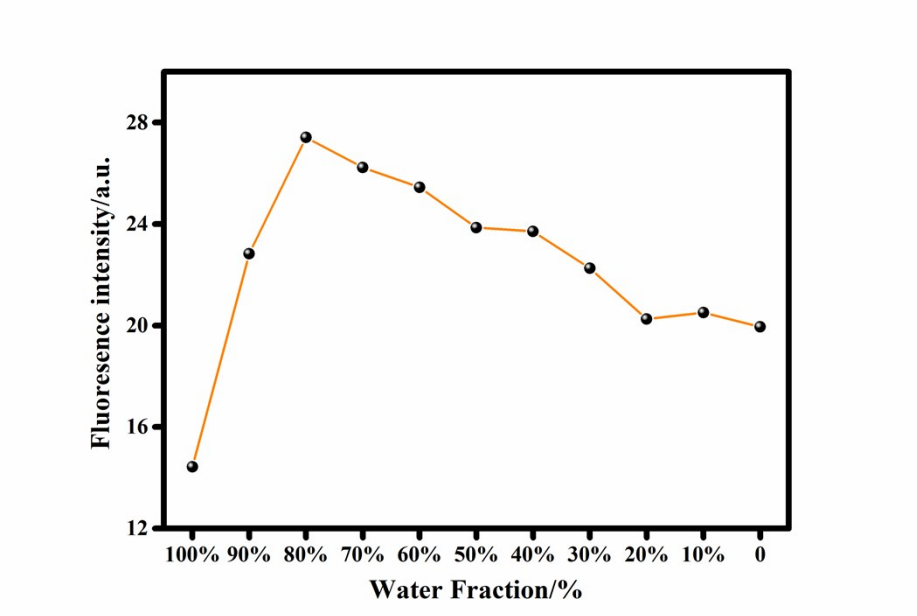


Fig. S4 Fluorescent spectra of compound **C-ClO** (a) and probe **B-ClO** (b) in DMF/H_2O (v/v) mixtures with different water fraction (f_w) at λ_{ex} = 336 nm.

Fig. S5

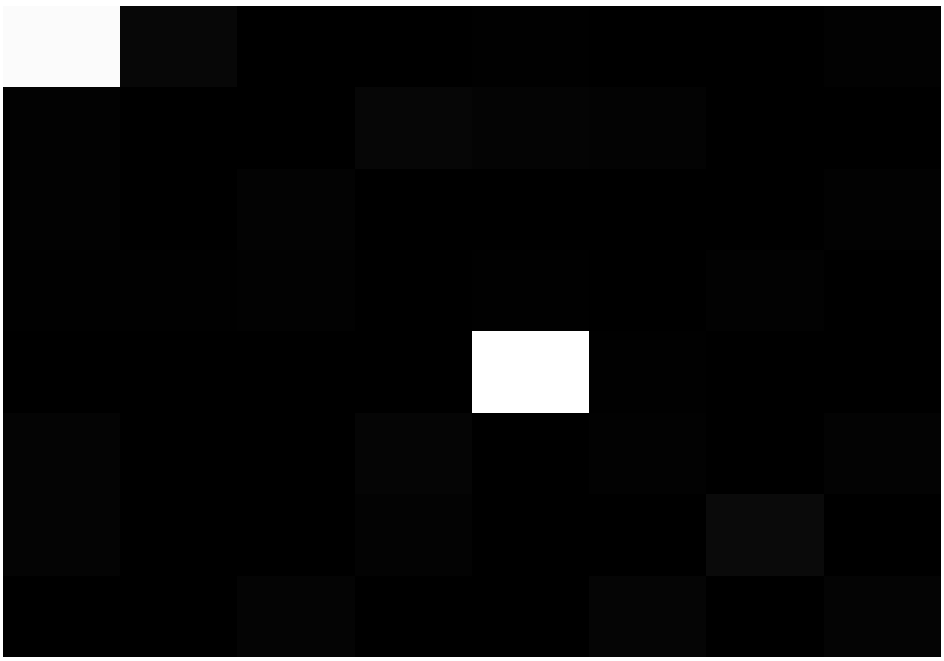


Fig. S5 ^1H NMR (400 MHz) spectra of **B-ClO** (black) in DMSO-d_6 and **C-ClO** (red) in $CDCl_3$;

Fig. S6

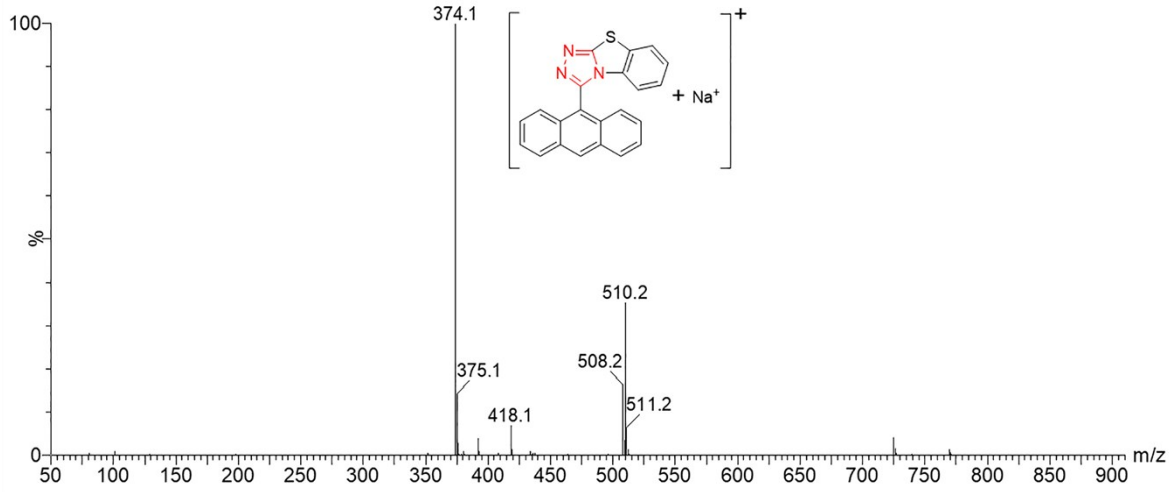


Fig. S6 MS of probe **C-ClO**;

Fig. S7

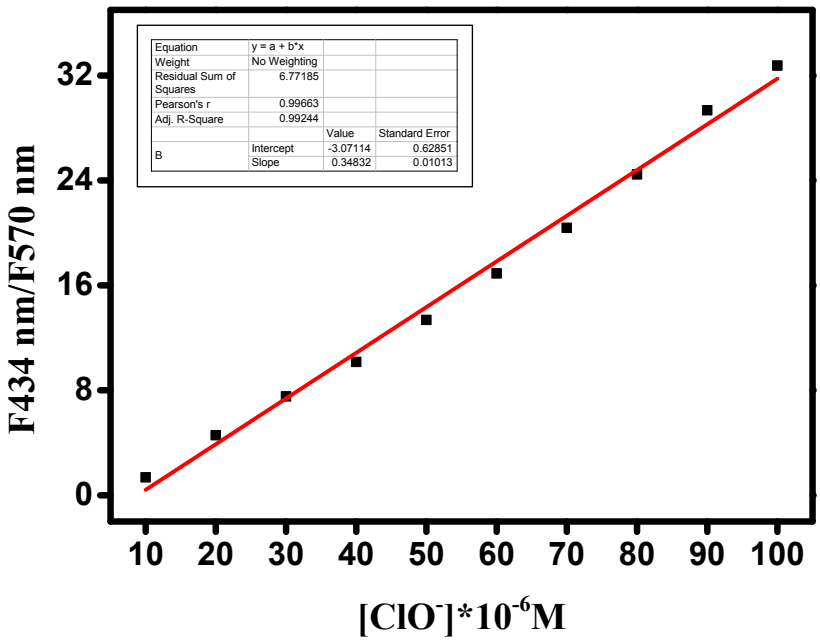


Fig. S7 Plot of the fluorescence intensity at $F_{434\ nm}/F_{570\ nm}$ against NaClO concentrations.

Table S1

	electronic transitions	DFT//B3LYP/6-311+G(d,p)				
		excitation energy (eV)	λ (nm)	f	composition	CI
Probe	S0→S1	2.7876 eV	444.77 nm	f=0.3441	HOMO→LUMO	0.70290
	S0→S2	3.4659 eV	357.72 nm	f=0.0177	HOMO-1→LUMO	0.65415
					HOMO→LUMO+1	0.25035
	S0→S3	3.6636 eV	338.43 nm	f=0.1155	HOMO-3→LUMO	-0.31440
					HOMO-1→LUMO	-0.21772
					HOMO→LUMO+1	0.51988
					HOMO→LUMO+3	0.26849
	S0→S4	3.6926 eV	335.76 nm	f=0.0790	HOMO-3→LUMO	0.41682
					HOMO-1→LUMO	-0.12611
					HOMO→LUMO+1	0.38910
					HOMO→LUMO+3	-0.37893

(a)

	electronic transitions	DFT//B3LYP/6-311+G(d,p)				
		excitation energy (eV)	λ (nm)	f	composition	CI
Probe+ClO^-	S0→S1	3.0643 eV	404.61 nm	f=0.1073	HOMO→LUMO	0.69962
	S0→S2	3.5654 eV	347.74 nm	f=0.0023	HOMO-1→LUMO	0.70161
	S0→S3	3.7783 eV	328.15 nm	f=0.0020	HOMO-2→LUMO	0.49106
					HOMO→LUMO+1	-0.25917
					HOMO→LUMO+2	0.15862
					HOMO→LUMO+3	0.40246
	S0→S4	3.9105 eV	317.05 nm	f=0.0078	HOMO-2→LUMO	0.14548
					HOMO→LUMO+1	0.64719
					HOMO→LUMO+2	0.13785
					HOMO→LUMO+3	0.18462

(b)

Table S1 Selected electronic excitation energies (eV) and oscillator strengths (f), configurations of the low-lying excited states of (a) the probe **B-ClO** and (b) the compound **C-ClO**