

Supporting Information

A highly selective A- π -A' "turn-on" fluorescent probe for hypochlorite in tap

water

Wenshuai Cheng, Chunping Ren, Shuang Liu, Wenshuo Jiang, Xiuna Zhu, Wenxuan Jia, Jianbo Cheng and Zhenbo Liu*

College of Chemistry and Chemical Engineering, Yantai University, Yantai 264005,
People's Republic of China

*Corresponding author: zhenboliu@foxmail.com

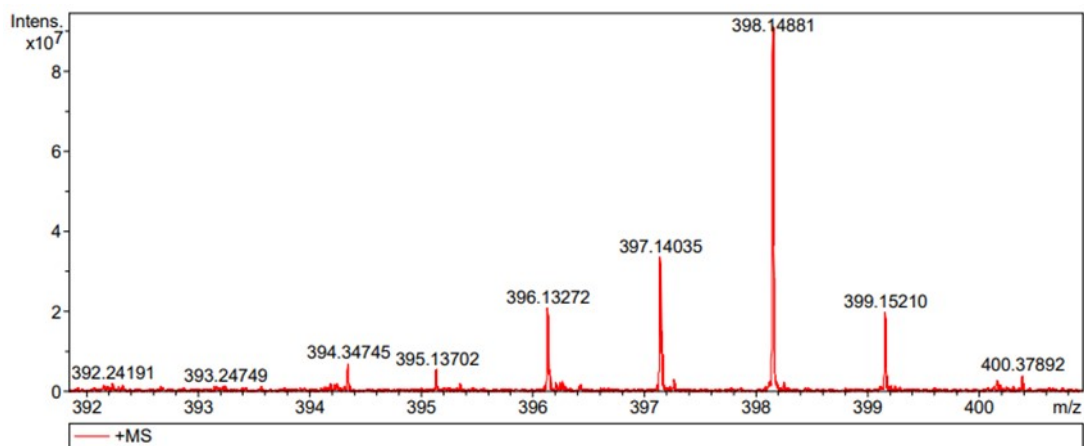


Fig. S1 MS data of **BODIPY-CHO**

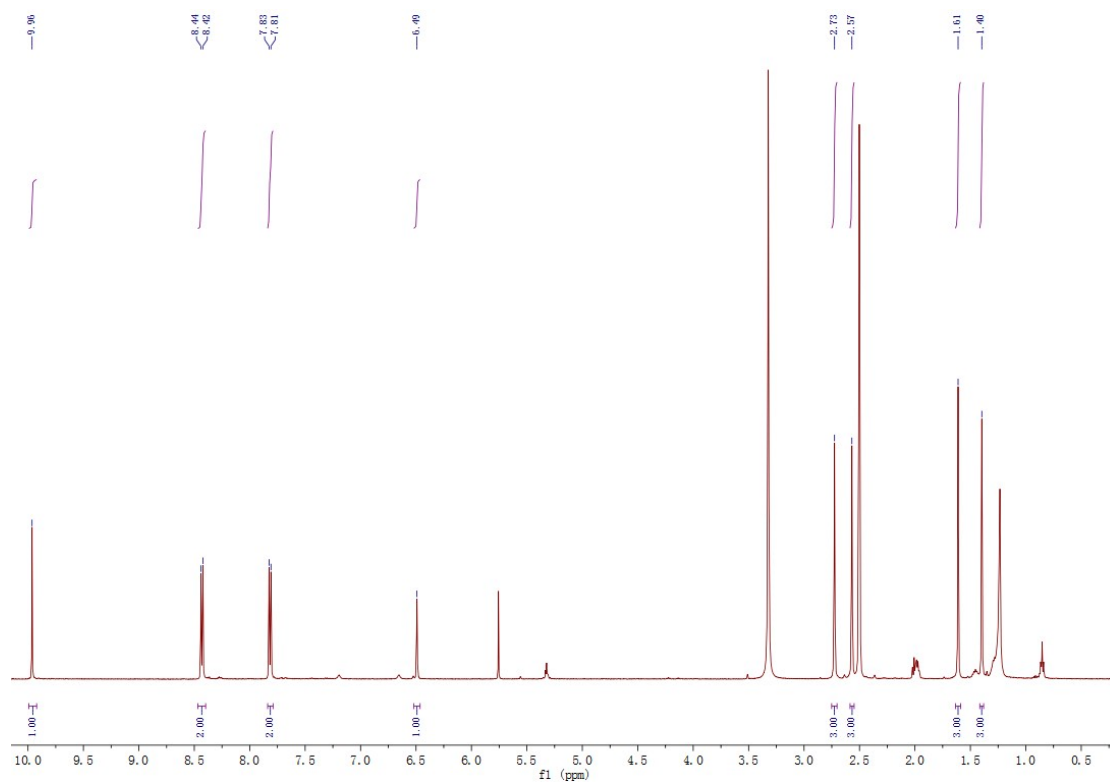


Fig. S2 ¹H-NMR data of **BODIPY-CHO**

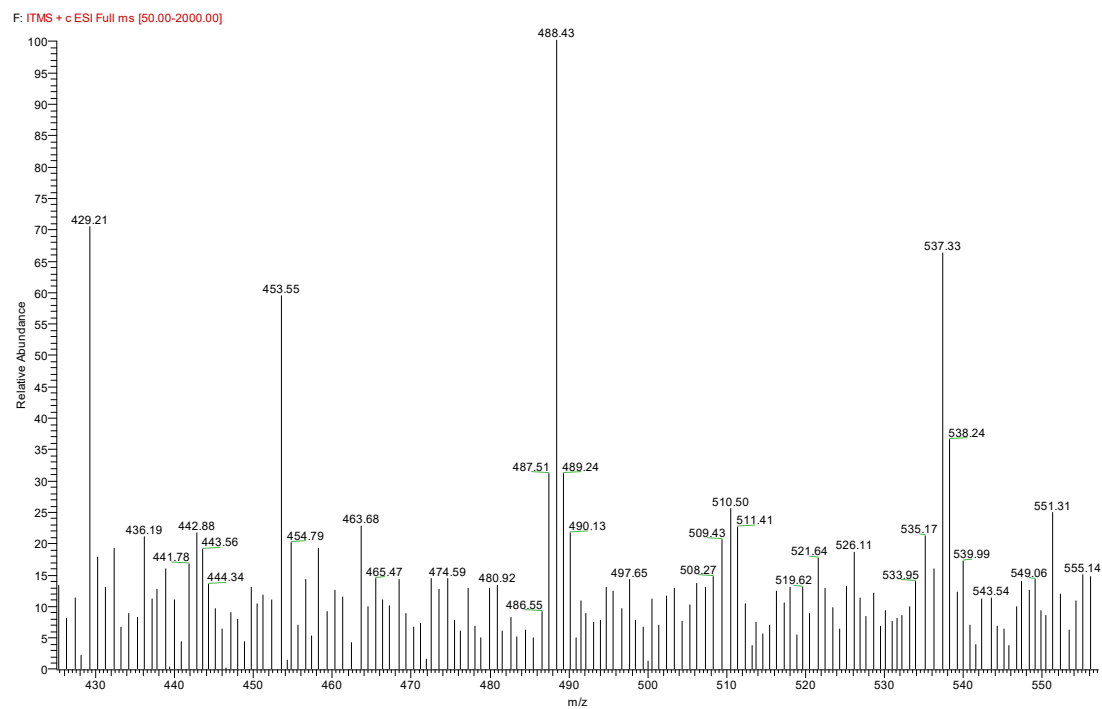


Fig. S3 MS data of the probe **BON**

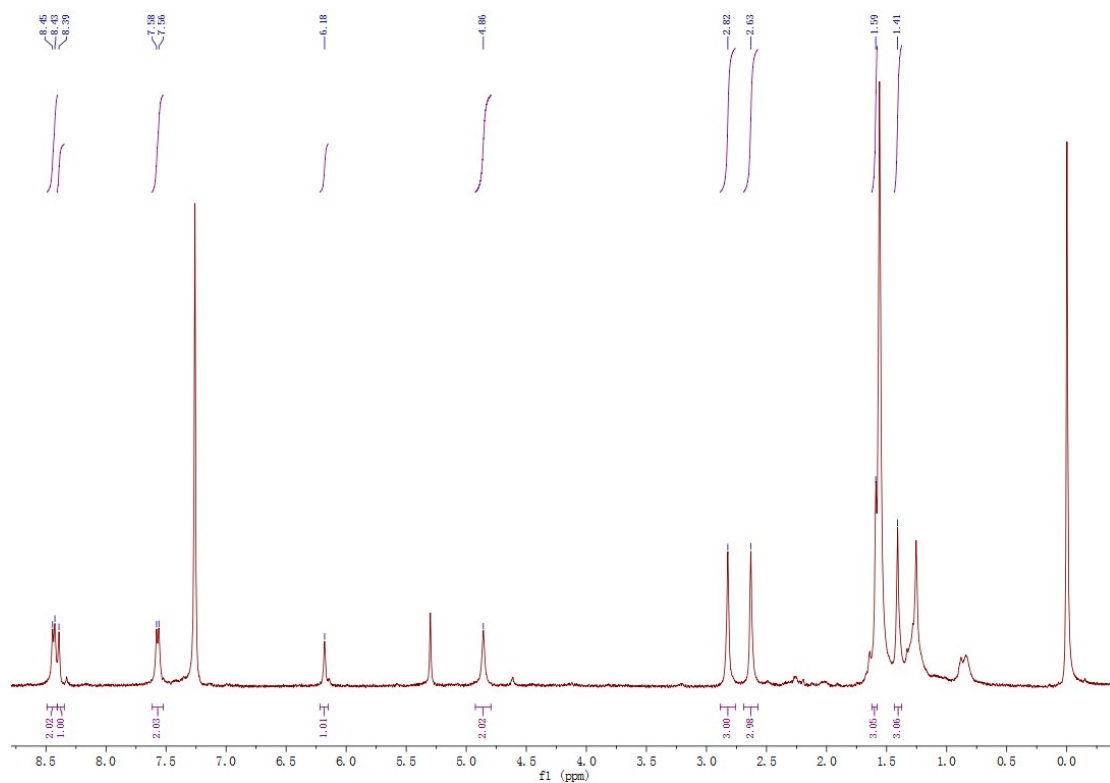


Fig. S4 $^1\text{H-NMR}$ data of the probe **BON**

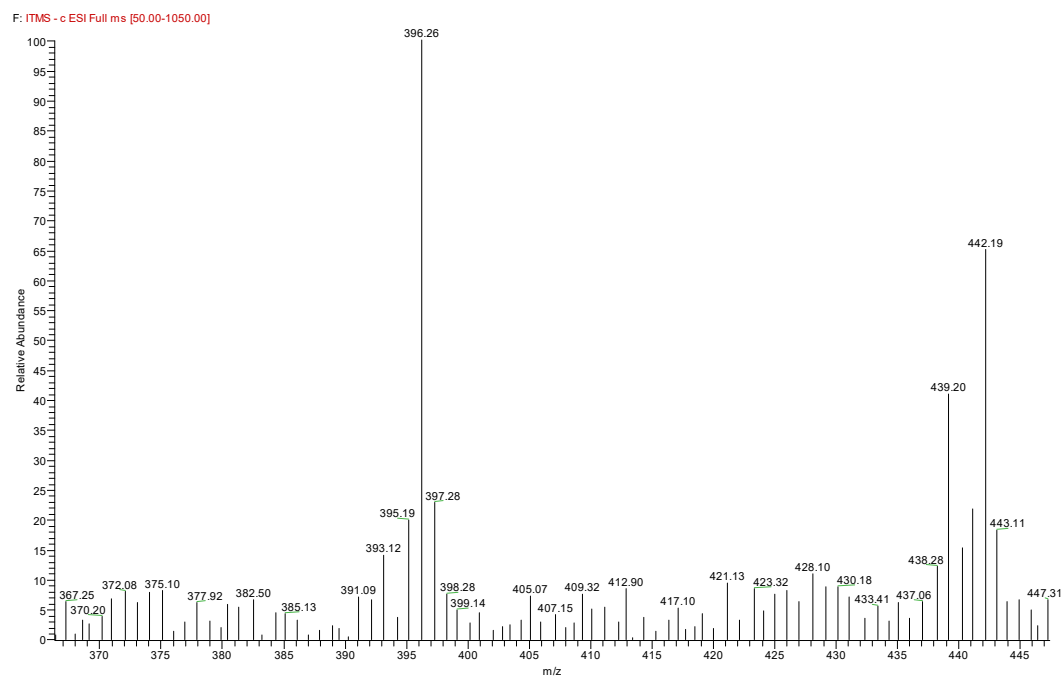


Fig. S5 MS data of **BON** with ClO^-

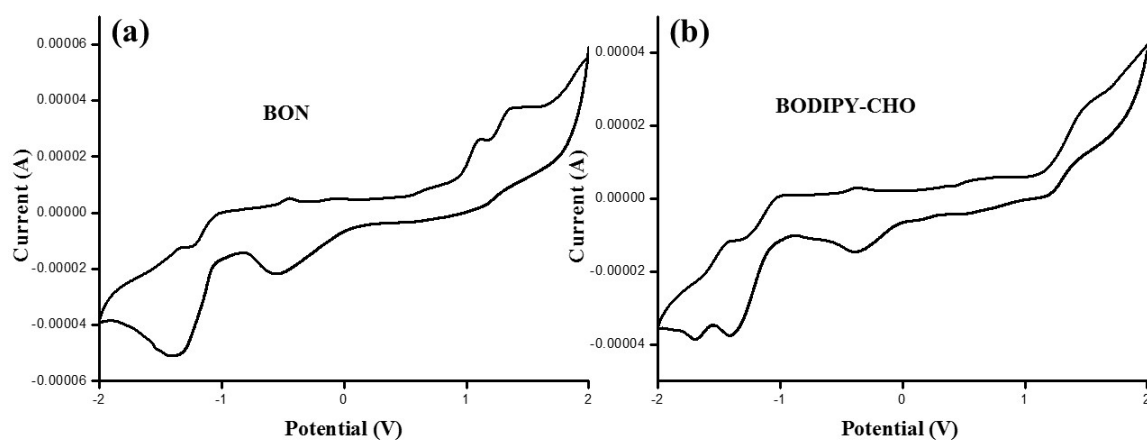


Fig. S6 Cyclic voltammograms of 1 mM **BON** (a) and **BODIPY-CHO** (b) measured in dichloromethane solution, containing 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF_6) as the supporting electrolyte at room temperature. The glassy carbon electrode as the working electrode. The Ag/Ag^+ electrode as the reference electrode. The platinum wire as the counter electrode.

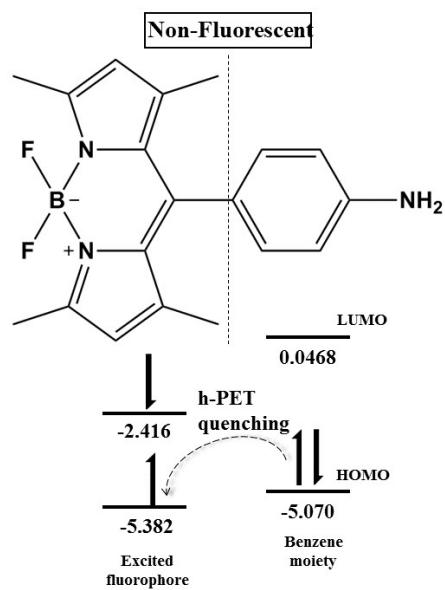


Fig. S7 Photoinduced electron transfer (PET) mechanism between BODIPY moiety and phenylamino.

Tab. S1 Quantum yields of **BODIPY-CHO** in different solvents.

Solvents	EtOH	DCM	Toluene
(ϕ)	8.9%	21.4%	35.6%

Tab. S2. Electrochemical data acquired at 50 mV/s, and HOMO-LUMO Gaps determined from spectroscopy of dyes **BON**, **BODIPY-CHO**.^a

dye	$E_{\text{red}}^{\text{onset}}$	$E_{\text{ox}}^{\text{onset}}$	LUMO	HOMO	E_{g}^{e}
	(V)	(V)	(eV)	(eV)	(eV)
BON	-1.383	1.356	-3.027	-5.766	2.739
BODIPY-CHO	-1.404	1.523	-3.006	-5.906	2.927

^a $E_{\text{red}}^{\text{onset}}$ = the onset reduction potentials; $E_{\text{ox}}^{\text{onset}}$ = the onset oxidation potentials; $E_{\text{LUMO}} = -e(E_{\text{red}}^{\text{onset}} - E_{\text{Fc}/\text{Fc}^+} + 4.80)$;

By assuming the energy level of ferrocene/ferrocenium (Fc/Fc^+) to be 4.8 eV below the vacuum level¹, $E_{\text{Fc}/\text{Fc}^+}$ is

the potential of Fc/Fc^+ against the Ag/Ag^+ reference electrode which is measured to be 0.39 eV²; $E_{\text{HOMO}} = -$

$e(E_{\text{ox}}^{\text{onset}} - E_{\text{Fc}/\text{Fc}^+} + 4.80)$; E_{g}^{e} = bandgap, obtained from the intercept of the electrochemical data; $E_{\text{g}}^{\text{e}} = E_{\text{LUMO}} -$

E_{HOMO} .

Tab. S3 Results of spiked recovery of hypochlorite in tap water

Water samples	ClO⁻ spiked (μM)	Recovered (μM)	Recovery (%)
Tap water sample 1	1	1.8±0.02	91.0
Tap water sample 2	2	2.7±0.01	90.5
Tap water sample 3	3	3.7±0.02	93.6

References

1. M. Soltani, R. Minakar, H. R. Memarian and H. Sabzyan, *J. Phys. Chem. A*, 2019, **123**, 2820-2830.
2. M. X. Lu, W. Wang, L. Y. Liang, S. H. Yan and Q. D. Ling, *Polym. Bull.*, 2017, **74**, 603-614.