

*Electronic Supplementary Information for*

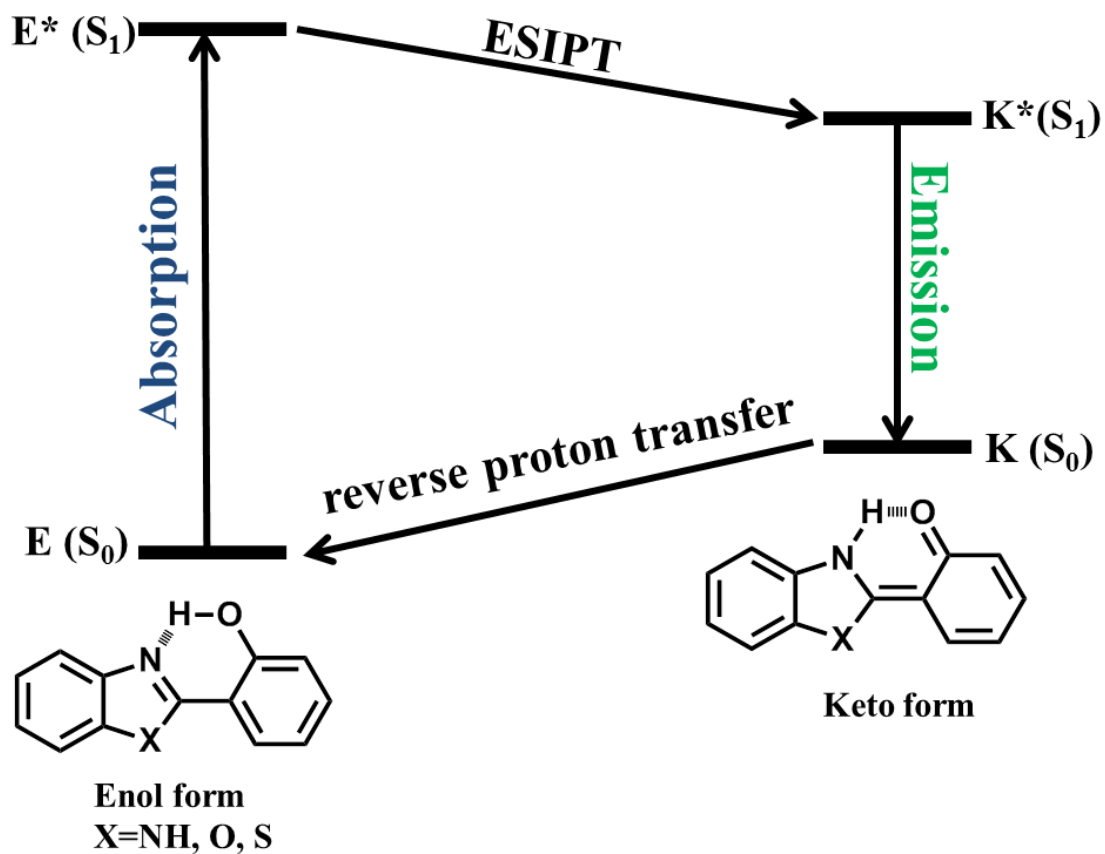
**An ESIPT fluorescent dye based on HBI with high quantum yield and large stokes shift for selective detection of Cys**

**Ying Zhang,<sup>a, b</sup> Jun-Hao Wang,<sup>b</sup> Wenjie Zheng,<sup>a</sup> Tianfeng Chen,<sup>a</sup>  
Qing-Xiao Tong\*<sup>b</sup> and Dan Li\*<sup>b</sup>**

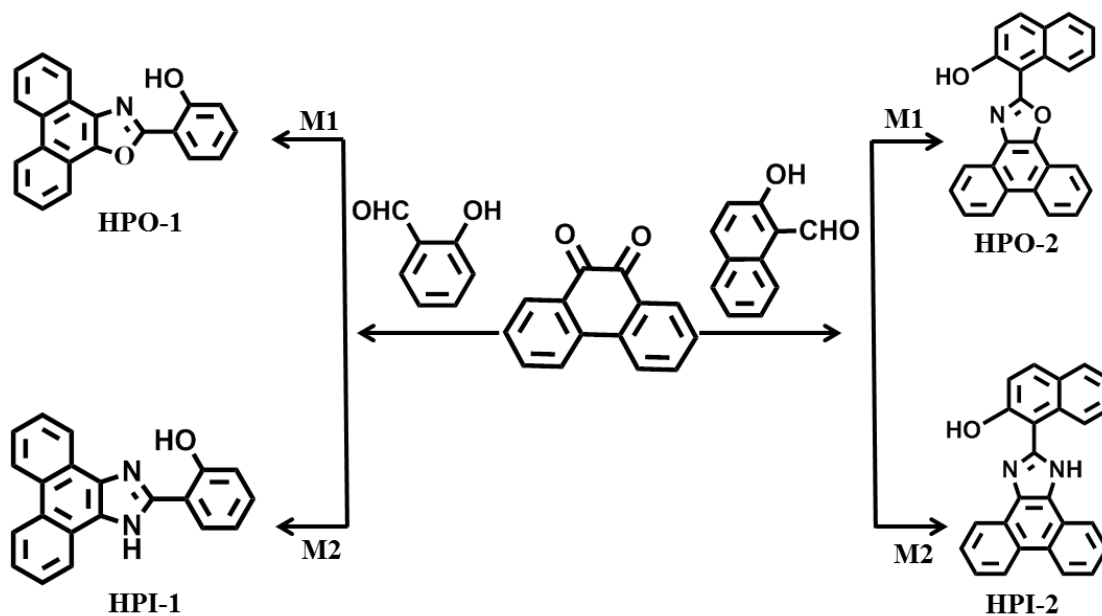
<sup>a</sup> *Department of Chemistry, School of Life Science and Technology, Jinan University, Guangzhou 510632, China.*

<sup>b</sup> *Department of Chemistry and Research Institute for Biomedical and Advanced Materials, Shantou University, Guangdong 515063, China.*

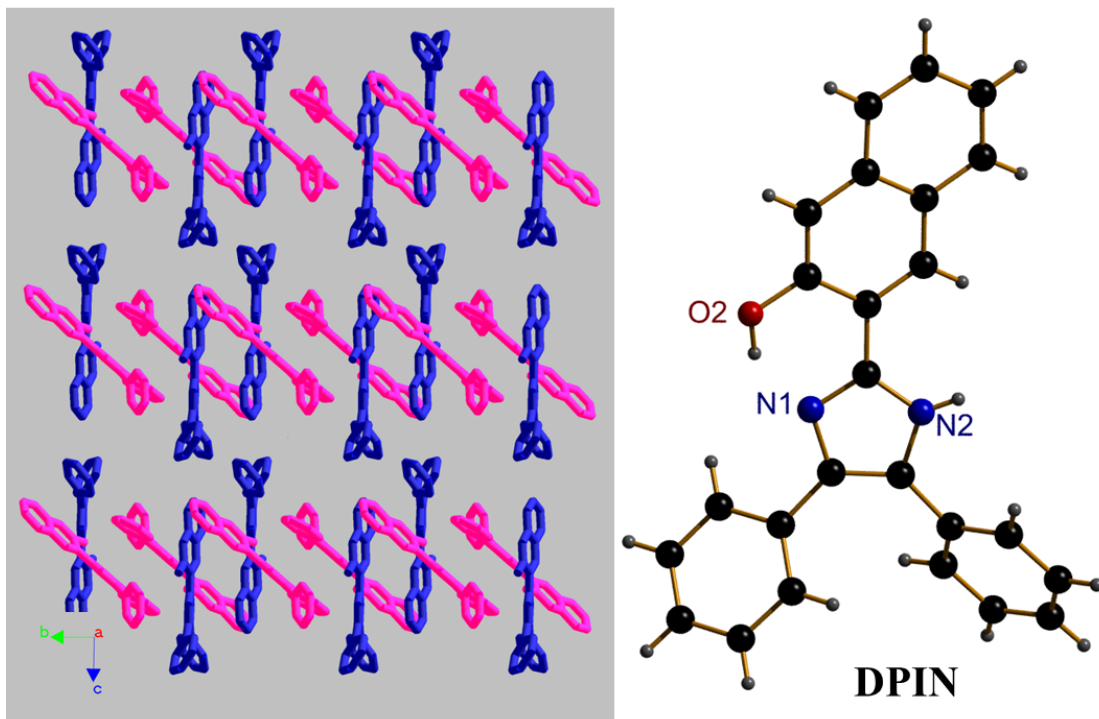
\*E-mail: [qxtong@stu.edu.cn](mailto:qxtong@stu.edu.cn); [dli@stu.edu.cn](mailto:dli@stu.edu.cn)



Scheme S1. Schematic representation of the ESIPT photocycle.



Scheme S2. Synthetic routes of the HBIs and HBOs for comparison. M1:  $\text{NH}_4\text{Ac}/\text{HAc}/\text{reflux}$ . M2:  $\text{CH}_2\text{Cl}_2/\text{Ethanol}/\text{HAc}/\text{reflux}$ .



**Fig. S1** Intermolecular stacking of **DPIN** viewed from *a* direction and the single Crystal structure of **DPIN**.

**Table S1** Data of selected dihedral angles and weak interactions of **DPIN** (see also Fig. 1)

Dihedral angle (°)			
A-C	51.87	A'-C'	43.97
B-C	16.46	B'-C'	34.50
D-C	17.81	D'-C'	17.70
Weak interaction (Å)			
bond Molecule	N-H...O	C-H... $\pi$	O-H...N
M-1	2.04	3.29	1.74
		3.08	
M-2	2.01	3.27	1.75
		3.11	

**Table S2** Crystal data and structure refinement for **DPIN**

Parameters	DPIN
Formula	C <sub>25</sub> H <sub>18</sub> N <sub>2</sub> O
<i>M<sub>r</sub></i>	362.14
Temp (K)	298(2)
Cryst system	Triclinic
Space group	<i>p</i> -1
<i>a</i> (Å)	12.0614(10)
<i>b</i> (Å)	12.2502(10)
<i>c</i> (Å)	14.7645(13)
<i>α</i> (deg)	87.449(7)
<i>β</i> (deg)	85.384(7)
<i>γ</i> (deg)	72.203(7)
<i>V</i> (Å <sup>3</sup> )	2069.9(3)
<i>Z</i>	2
<i>D<sub>calcd</sub></i> (g cm <sup>-3</sup> )	1.296
<i>μ</i> (mm <sup>-1</sup> )	1.777
Reflns collcd	14791
Unique reflns	8119
<i>R<sub>int</sub></i>	0.0832
<i>R</i> 1[ <i>I</i> >2σ( <i>I</i> )] <sup>a</sup>	0.0720
<i>wR</i> 2[ <i>I</i> >2σ( <i>I</i> )] <sup>a</sup>	0.2514
<i>R</i> 1(all data)	0.0832
<i>wR</i> 2(all data)	0.2817
GOOF	1
<sup>a</sup> $R_1 = \sum( F_o  -  F_c ) / \sum  F_o $ ; $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$	

**Table S3** Selected Bond lengths (Å) and bond angles (°) for DPIN

Bond lengths (Å)				Bond angles (°)			
C(40)-N(1)	1.331(3)	C(17)-O(1)	1.364(3)	N(1)-C(40)-N(2)	110.51(17)	N(3)-C(15)-C(16)	123.95(18)
C(40)-N(2)	1.345(3)	C(17)-C(18)	1.364(3)	N(1)-C(40)-C(41)	124.11(17)	N(4)-C(15)-C(16)	125.64(18)
C(40)-C(41)	1.462(3)	C(7)-C(8)	1.377(3)	N(2)-C(40)-C(41)	125.36(17)	C(5)-C(4)-C(3)	118.0(2)
C(41)-C(42)	1.371(3)	C(7)-N(3)	1.383(3)	C(42)-C(41)-C(50)	118.59(18)	C(5)-C(4)-C(7)	122.6(2)
C(41)-C(50)	1.431(3)	C(7)-C(4)	1.472(3)	C(42)-C(41)-C(40)	122.37(18)	C(3)-C(4)-C(7)	119.3(2)
C(42)-C(43)	1.410(3)	C(43)-C(44)	1.415(3)	C(50)-C(41)-C(40)	119.03(17)	C(28)-C(29)-C(30)	119.1(2)
C(16)-C(25)	1.368(3)	C(33)-N(2)	1.372(3)	C(41)-C(42)-C(43)	122.07(19)	C(28)-C(29)-C(32)	121.5(2)
C(16)-C(17)	1.425(3)	C(33)-C(32)	1.380(3)	C(41)-C(42)-H(42)	119.0	C(30)-C(29)-C(32)	119.4(2)
C(16)-C(15)	1.462(3)	C(33)-C(34)	1.476(3)	C(43)-C(42)-H(42)	119.0	N(1)-C(32)-C(33)	109.34(17)
C(50)-O(2)	1.358(3)	C(15)-N(3)	1.324(3)	C(25)-C(16)-C(17)	118.67(19)	N(1)-C(32)-C(29)	119.64(18)
C(50)-C(49)	1.367(3)	C(15)-N(4)	1.345(3)	C(25)-C(16)-C(15)	122.48(18)	C(33)-C(32)-C(29)	130.96(19)
C(24)-C(19)	1.411(3)	C(4)-C(5)	1.390(3)	C(17)-C(16)-C(15)	118.85(18)	C(16)-C(25)-C(24)	121.8(2)
C(24)-C(25)	1.415(3)	C(4)-C(3)	1.393(3)	O(2)-C(50)-C(49)	119.77(19)	C(16)-C(25)-H(25)	119.1
C(24)-C(23)	1.418(3)	C(29)-C(28)	1.389(4)	O(2)-C(50)-C(41)	119.88(18)	C(24)-C(25)-H(25)	119.1
C(49)-C(48)	1.406(3)	C(29)-C(30)	1.392(4)	C(49)-C(50)-C(41)	120.35(19)	N(4)-C(8)-C(7)	105.62(18)
C(48)-C(43)	1.420(3)	C(29)-C(32)	1.474(3)	C(19)-C(24)-C(25)	118.5(2)	N(4)-C(8)-C(9)	117.65(18)
C(48)-C(47)	1.420(3)	C(32)-N(1)	1.375(3)	C(19)-C(24)-C(23)	119.2(2)	C(7)-C(8)-C(9)	136.6(2)
C(8)-N(4)	1.375(3)	C(8)-C(9)	1.479(3)	C(25)-C(24)-C(23)	122.3(2)	C(17)-C(18)-C(19)	120.6(2)
C(18)-C(19)	1.411(3)	C(34)-C(35)	1.389(3)	C(50)-C(49)-C(48)	121.27(19)	C(17)-C(18)-H(18)	119.7
C(34)-C(39)	1.392(3)	C(19)-C(20)	1.428(3)	C(50)-C(49)-H(49)	119.4	C(19)-C(18)-H(18)	119.7
C(35)-C(36)	1.384(4)	C(47)-C(46)	1.352(4)	C(48)-C(49)-H(49)	119.4	C(35)-C(34)-C(39)	118.3(2)
C(44)-C(45)	1.369(4)	C(5)-C(6)	1.387(4)	C(49)-C(48)-C(43)	119.02(19)	C(35)-C(34)-C(33)	120.8(2)
C(9)-C(10)	1.378(4)	C(9)-C(14)	1.397(4)	C(49)-C(48)-C(47)	123.1(2)	C(39)-C(34)-C(33)	120.7(2)
C(23)-C(22)	1.358(4)	C(30)-C(31)	1.383(4)	C(43)-C(48)-C(47)	117.8(2)	C(24)-C(19)-C(18)	119.4(2)
C(36)-C(37)	1.361(5)	C(39)-C(38)	1.382(4)	O(1)-C(17)-C(18)	119.35(19)	C(24)-C(19)-C(20)	118.6(2)
C(46)-C(45)	1.394(5)	C(6)-C(1)	1.375(5)	C(49)-C(48)-C(47)	123.1(2)	C(35)-C(34)-C(33)	120.8(2)
C(28)-C(27)	1.401(4)	C(20)-C(21)	1.368(4)	C(43)-C(48)-C(47)	117.8(2)	C(39)-C(34)-C(33)	120.7(2)
C(21)-C(22)	1.389(5)	C(10)-C(11)	1.401(5)	O(1)-C(17)-C(18)	119.35(19)	C(24)-C(19)-C(18)	119.4(2)
C(2)-C(1)	1.385(5)	C(14)-C(13)	1.379(4)	O(1)-C(17)-C(16)	119.84(19)	C(24)-C(19)-C(20)	118.6(2)
C(38)-C(37)	1.384(5)	C(13)-C(12)	1.383(6)	C(18)-C(17)-C(16)	120.8(2)	C(18)-C(19)-C(20)	122.0(2)
C(12)-C(11)	1.352(7)	C(27)-C(26)	1.367(7)	C(8)-C(7)-N(3)	108.76(18)	C(36)-C(35)-C(34)	120.5(3)
C(31)-C(26)	1.358(7)	C(51)-Cl(2)	1.678(10)	C(8)-C(7)-C(4)	132.0(2)	C(36)-C(35)-H(35)	119.8
C(51)-Cl(1)	1.693(9)			N(3)-C(7)-C(4)	119.19(18)	C(34)-C(35)-H(35)	119.8
				C(42)-C(43)-C(44)	122.1(2)	C(46)-C(47)-C(48)	121.3(3)
				C(42)-C(43)-C(48)	118.63(19)	C(46)-C(47)-H(47)	119.3
				C(44)-C(43)-C(48)	119.3(2)	C(48)-C(47)-H(47)	119.3
				N(2)-C(33)-C(32)	105.36(17)	C(45)-C(44)-C(43)	120.6(3)
				N(2)-C(33)-C(34)	120.16(17)	C(45)-C(44)-H(44)	119.7
				C(32)-C(33)-C(34)	134.44(19)	C(6)-C(5)-C(4)	120.7(2)
				N(3)-C(15)-N(4)	110.39(18)	C(6)-C(5)-H(5)	119.6

Bond angles (°)					
C(4)-C(5)-H(5)	120.9(3)	C(4)-C(3)-H(3)	119.5	C(10)-C(9)-C(14)	118.2(2)
C(2)-C(3)-H(3)	119.5	C(10)-C(9)-C(8)	121.9(2)	C(14)-C(9)-C(8)	119.5(2)
C(24)-C(23)-H(23)	119.7	C(22)-C(23)-C(24)	120.6(3)	C(22)-C(23)-H(23)	119.7
C(31)-C(30)-C(29)	120.3(3)	C(31)-C(30)-H(30)	119.8	C(29)-C(30)-H(30)	119.8
C(35)-C(36)-H(36)	119.7	C(37)-C(36)-H(36)	119.7	C(37)-C(36)-C(35)	120.5(3)
C(35)-C(36)-H(36)	119.7	C(38)-C(39)-C(34)	120.9(3)	C(38)-C(39)-H(39)	119.6
C(34)-C(39)-H(39)	119.6	C(47)-C(46)-C(45)	120.9(2)	C(47)-C(46)-H(46)	119.6
C(45)-C(46)-H(46)	119.6	C(1)-C(6)-C(5)	120.8(3)	C(1)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6	C(29)-C(28)-C(27)	119.1(4)	C(29)-C(28)-H(28)	120.5
C(27)-C(28)-H(28)	120.5	C(21)-C(20)-C(19)	119.9(3)	C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0	C(20)-C(21)-C(22)	121.0(2)	C(20)-C(21)-H(21)	119.5
C(22)-C(21)-H(21)	119.5	C(9)-C(10)-C(11)	120.0(3)	C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0	C(3)-C(2)-C(1)	120.5(3)	C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8	C(6)-C(1)-C(2)	119.0(2)	C(6)-C(1)-H(1)	120.5
C(13)-C(14)-H(14)	119.5	C(13)-C(14)-C(9)	121.0(3)	C(2)-C(1)-H(1)	120.5
C(9)-C(14)-H(14)	119.5	C(23)-C(22)-C(21)	120.6(3)	C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7	C(39)-C(38)-C(37)	119.6(3)	C(39)-C(38)-H(38)	120.2
C(37)-C(38)-H(38)	120.2	C(44)-C(45)-C(46)	120.1(2)	C(44)-C(45)-H(45)	120.0
C(46)-C(45)-H(45)	120.0	C(14)-C(13)-C(12)	120.0(4)	C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0	C(36)-C(37)-C(38)	120.1(3)	C(36)-C(37)-H(37)	119.9
C(38)-C(37)-H(37)	119.9	C(11)-C(12)-C(13)	119.5(3)	C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2	C(26)-C(27)-C(28)	120.9(4)	C(26)-C(27)-H(27)	119.6
C(28)-C(27)-H(27)	119.6	C(12)-C(11)-C(10)	121.1(4)	C(12)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4	C(26)-C(31)-C(30)	120.6(4)	C(26)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7	C(31)-C(26)-C(27)	120.1(3)	C(31)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0	Cl(2)-C(51)-Cl(1)	115.0(5)	C(40)-N(1)-C(32)	106.29(16)
C(15)-N(3)-C(7)	106.73(16)	C(40)-N(2)-C(33)	108.49(16)	C(40)-N(2)-H(2A)	122(2)
C(33)-N(2)-H(2A)	129(2)	C(15)-N(4)-C(8)	108.49(17)	C(15)-N(4)-H(4)	127.0(18)
C(50)-O(2)-H(2B)	112(2)	C(17)-O(1)-H(1A)	103(3)		

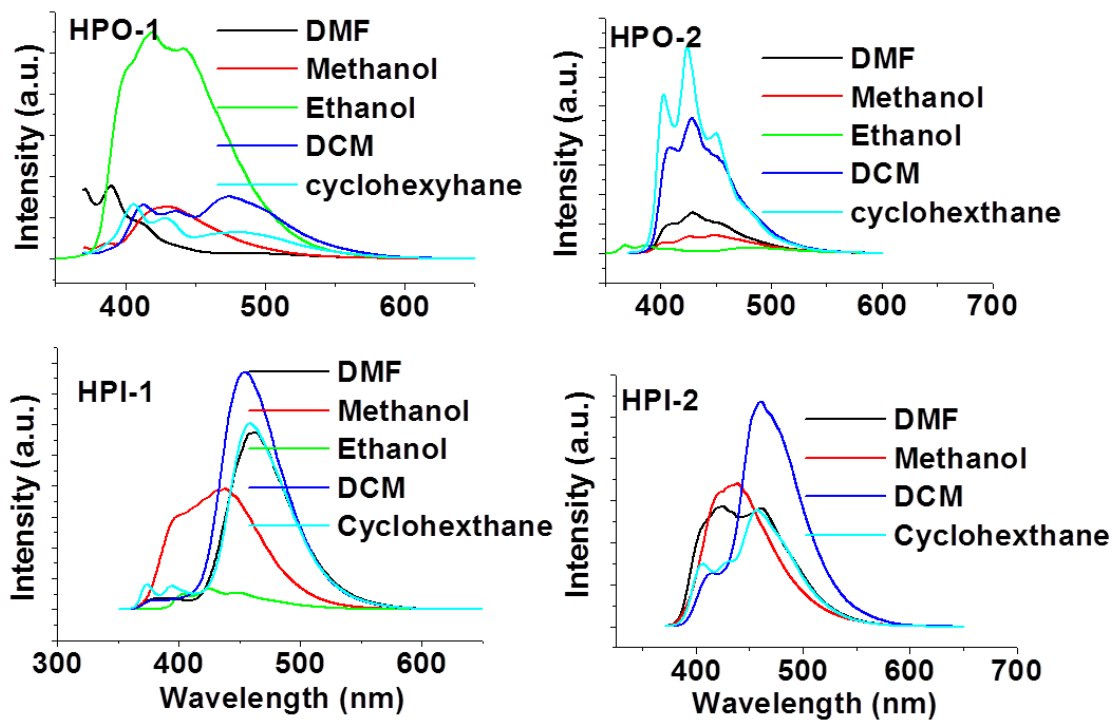


Fig. S2 Fluorescent emission of HPI-1, HPI-2, HPO1, HPO-2 in different solvent. All the concentration is 10  $\mu$ M.

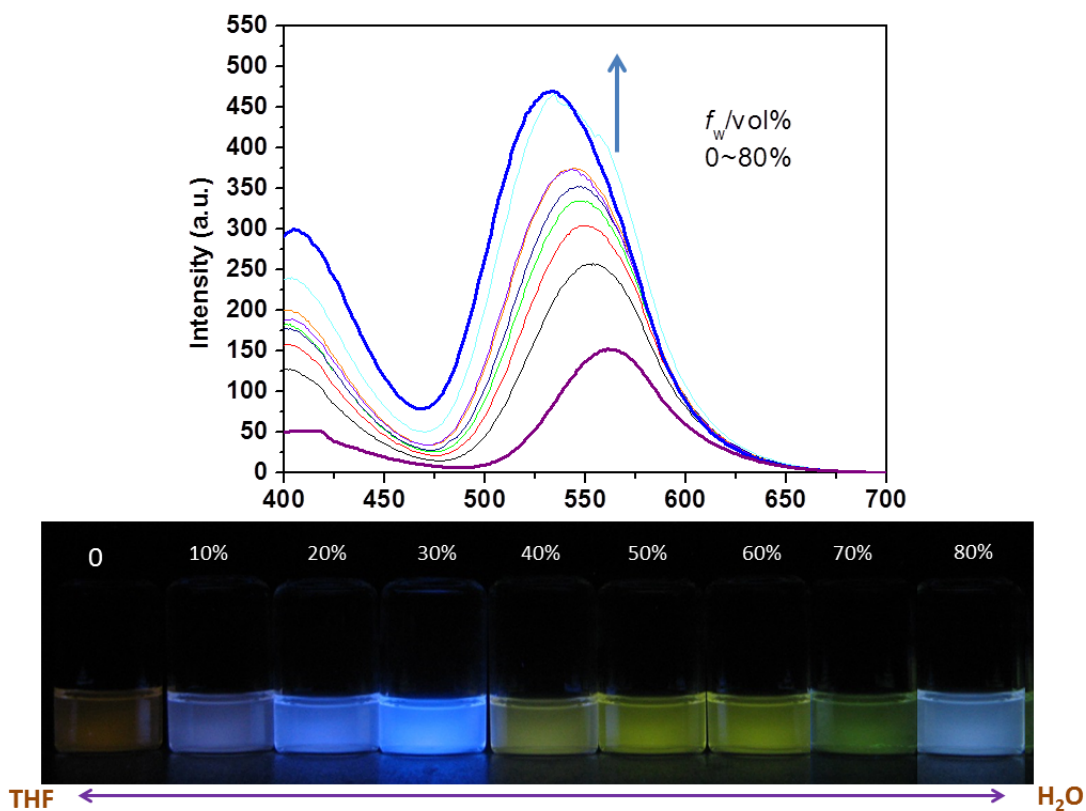


Fig. S3. Fluorescent performance of DPIN (10  $\mu$ M) in THF with different proportion of H<sub>2</sub>O from 0 to 80%.

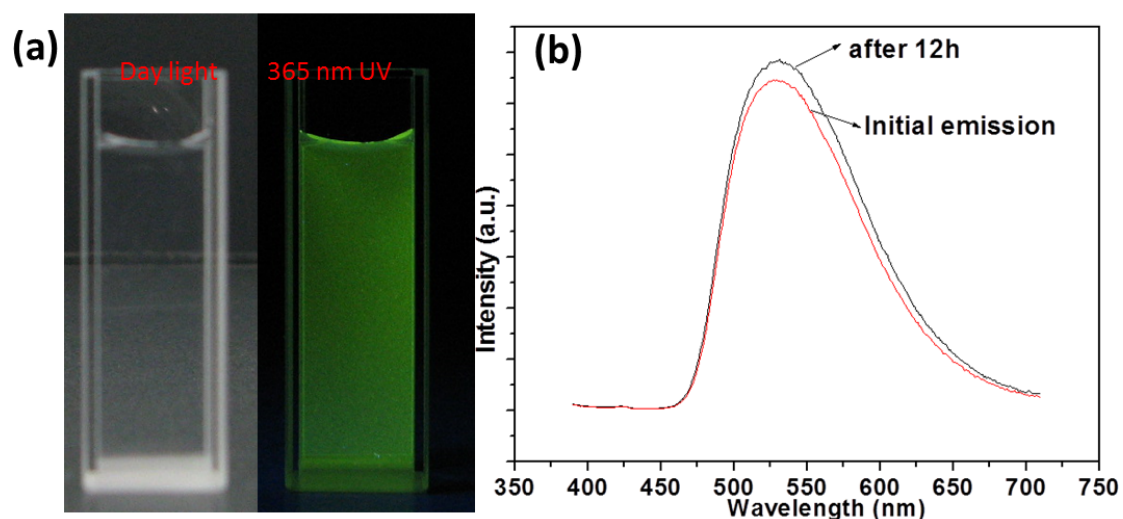


Fig. S4. (a), DPIN solution in pure water (10  $\mu$ M) standing for 12h. left: under daylight. Right: under 365nm excitation. (b), Emission spectra of DPIN in pure water (10  $\mu$ M) at initial state and after standing for 12h.

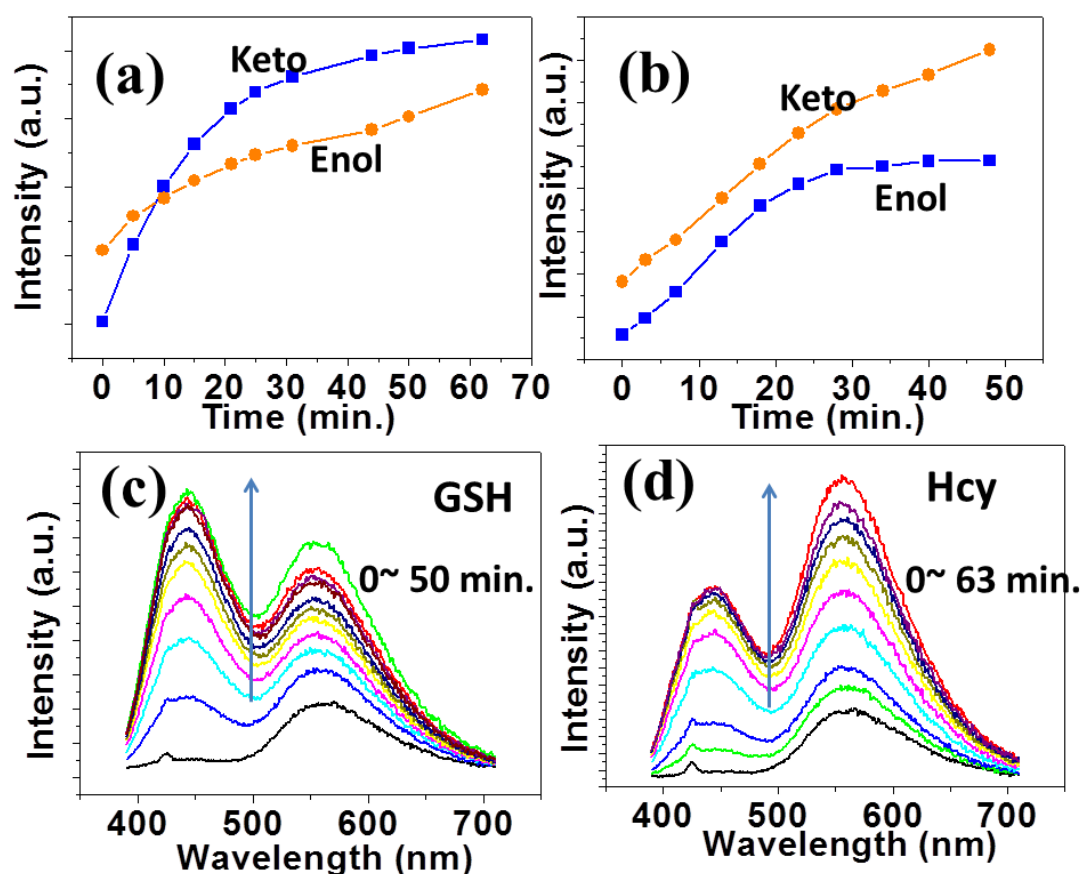


Fig. S5. Intensity of Keto emission and Enol emission towards time. (a), GSH, (b), Hcy. Emission spectra of probe in PBS buffer (20 mM, pH, 7.2) towards GSH (c) and Hcy (d) with time increasing.