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Electronic Supplementary Information

Thiophene-based pyridine derivatives: Synthesis, crystal structures, two-photon absorption properties and bio-imaging application in Near-IR region

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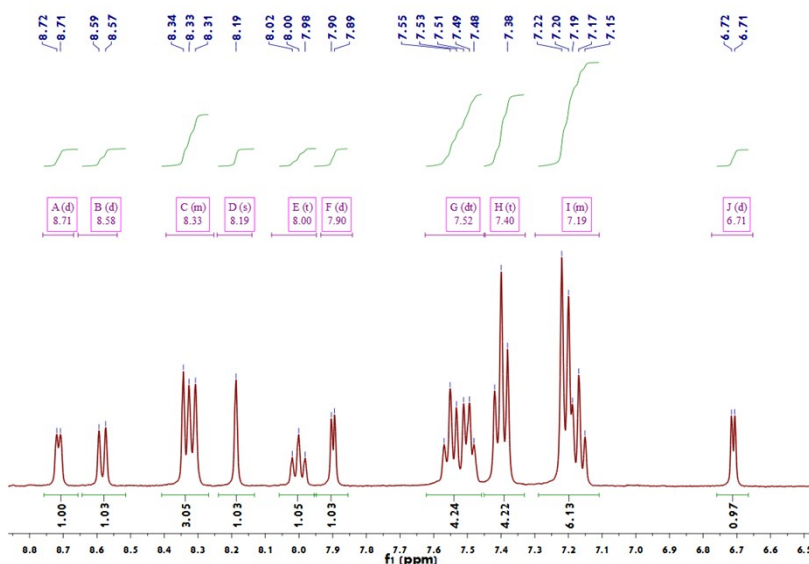


Fig. S1 ¹H-NMR of dye1.

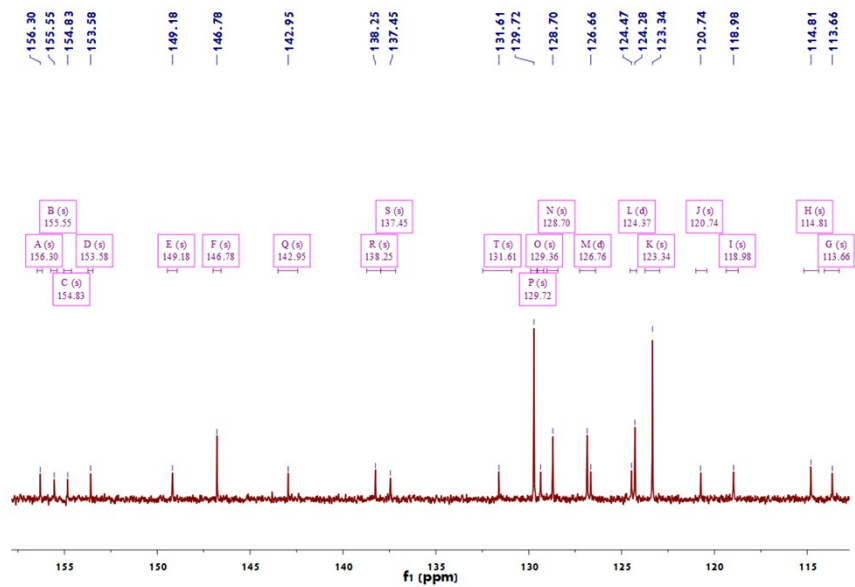


Fig. S2 ^{13}C -NMR of dye2.

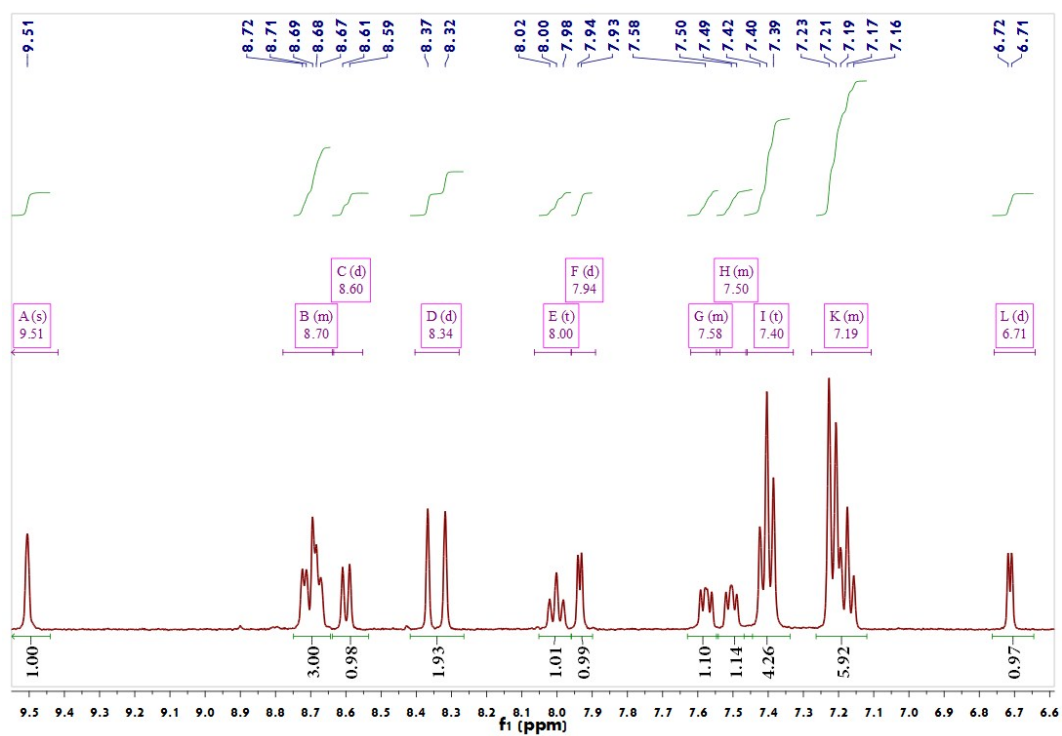


Fig. S3 ^1H -NMR of dye2.

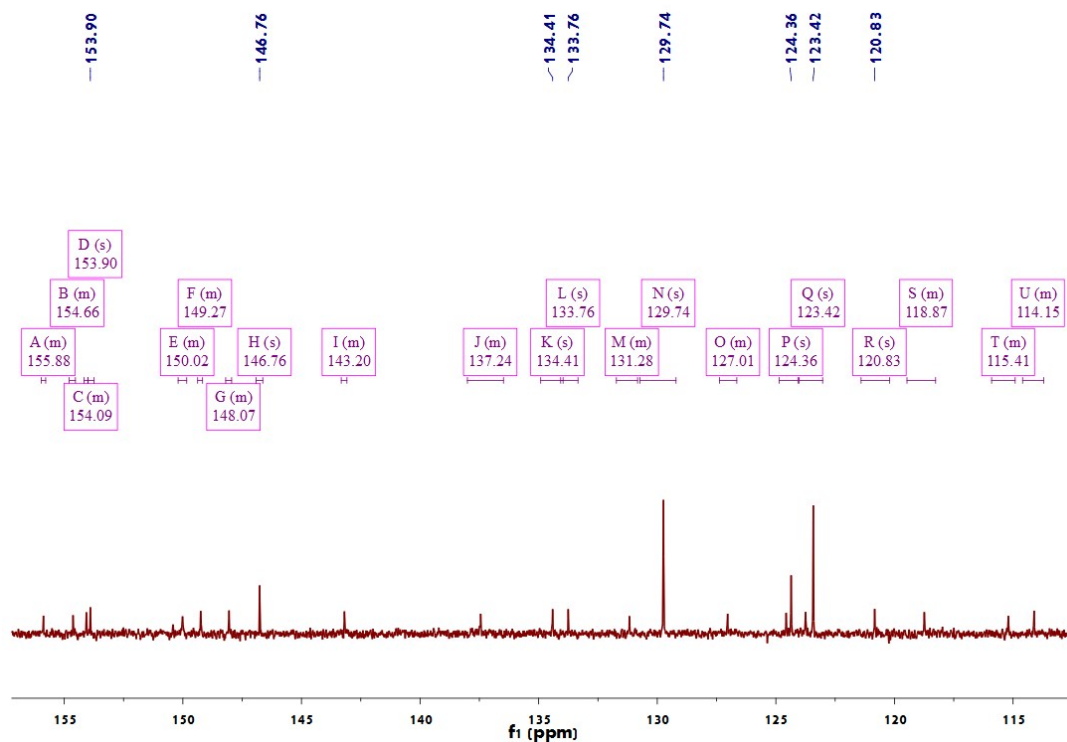


Fig. S4 ^{13}C -NMR of dye2.

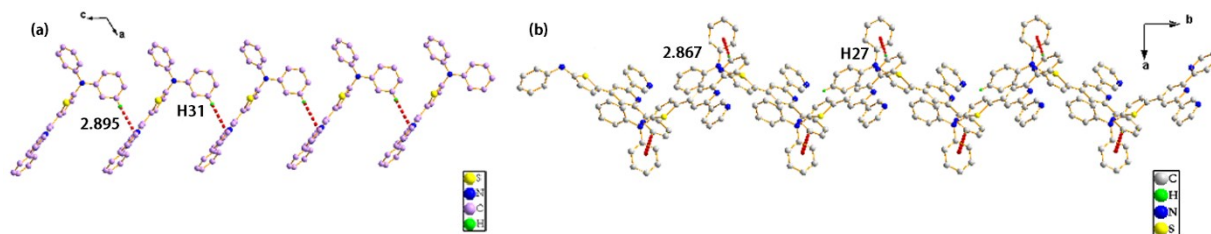


Fig. S5 The molecular packing diagrams of dye1 (left) and dye2 (right).

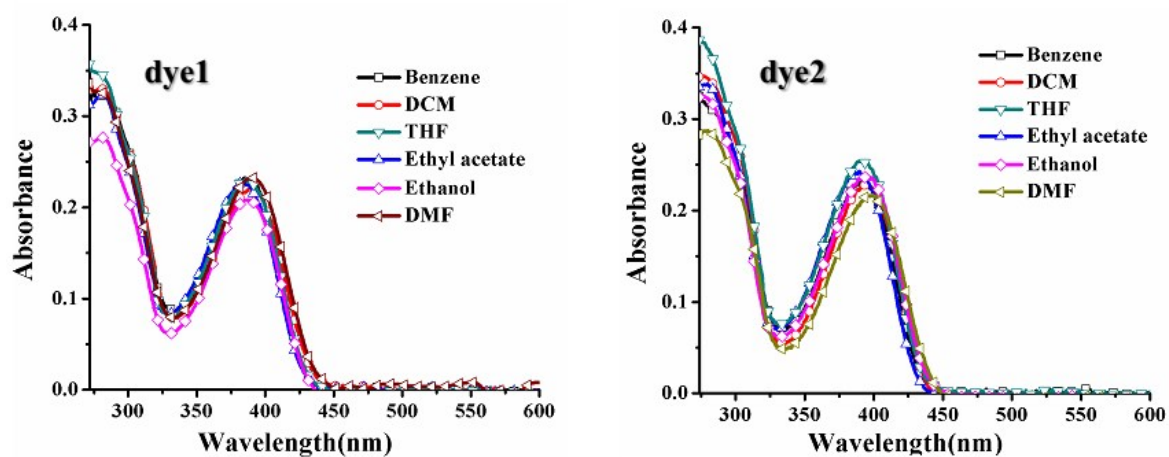


Fig. S6 Linear absorption spectra of dye1 and dye2 in six solvents with a concentration of 1×10^{-5} mol L⁻¹, respectively.

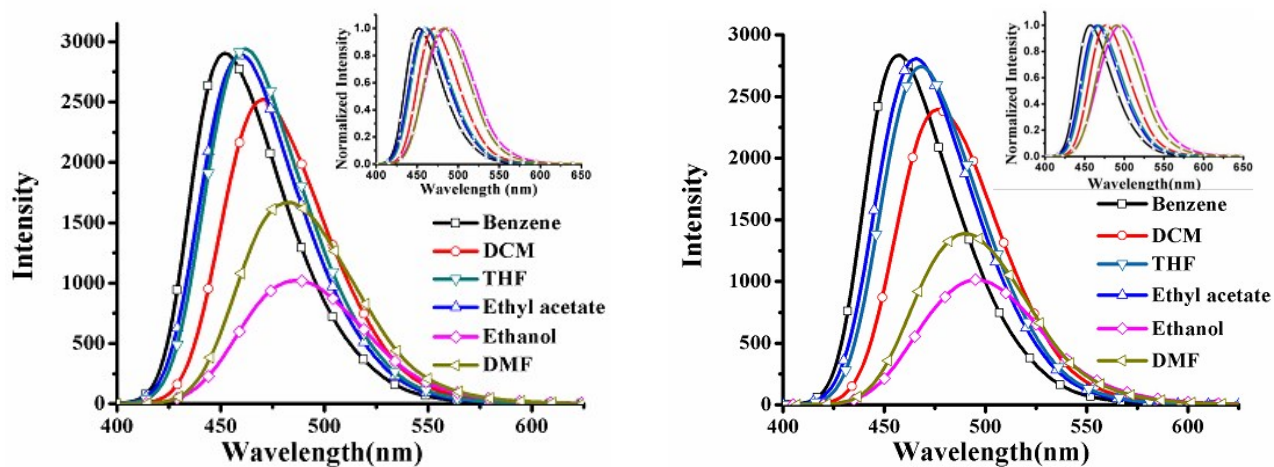


Fig. S7 Single-photon fluorescence spectra of dye1 (left) and dye2 (right) in six solvents with a concentration of 1×10^{-5} mol L⁻¹, respectively.

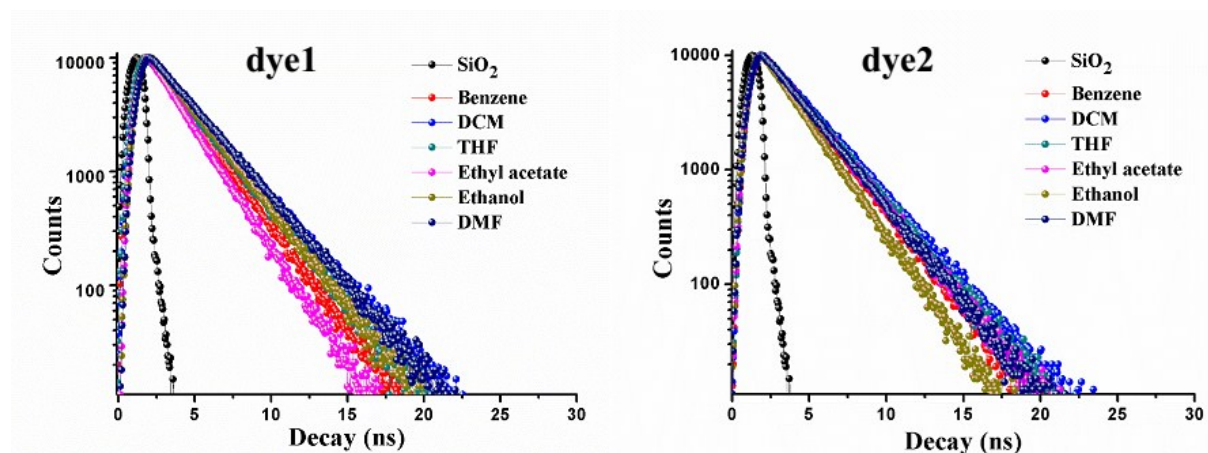


Fig. S8 Time-resolved fluorescence curves of dye1 and dye2 in six solvents, respectively.

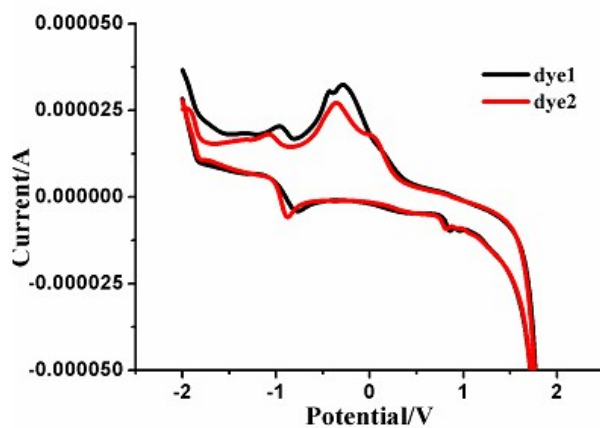


Fig. S9. Cyclic voltammetry spectrum of dye1 and dye2.

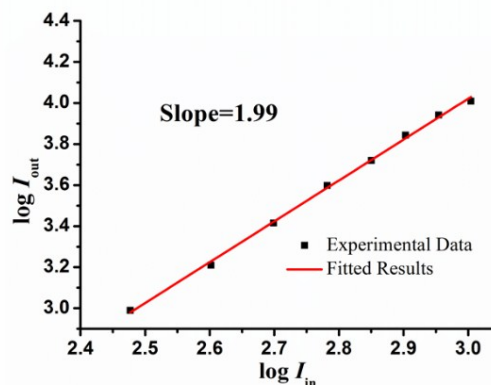
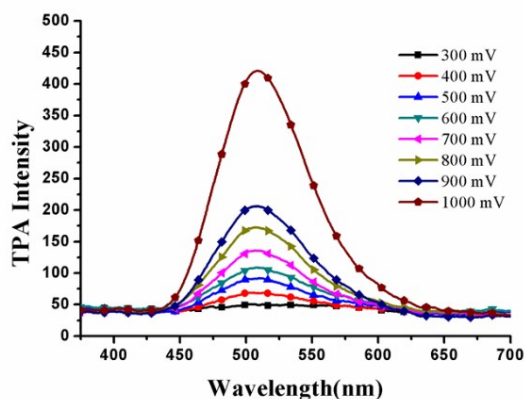


Fig. S10. TPAF spectra of **dye1** under different pumped powers at 770 nm, with $c = 1.0 \times 10^{-3} \text{ mol L}^{-1}$ in DMF (Left); Output fluorescence (I_{out}) vs. the square of input laser power (I_{in}) for **dye1** (Right).

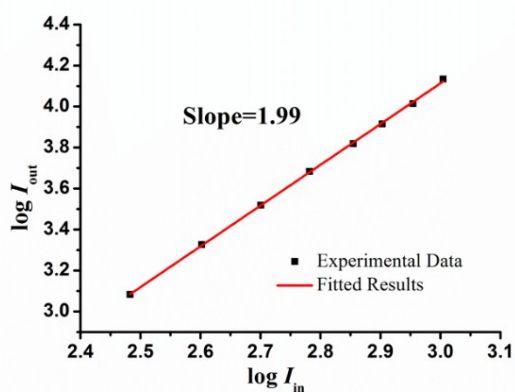
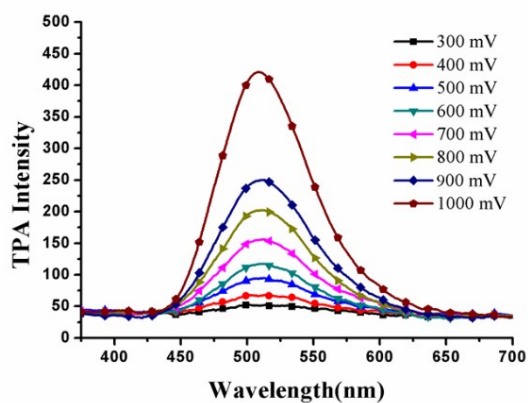


Fig. S11. TPAF spectra of **dye2** under different pumped powers at 770 nm, with $c = 1.0 \times 10^{-3} \text{ mol L}^{-1}$ in DMF (Left); Output fluorescence (I_{out}) vs. the square of input laser power (I_{in}) for **dye2** (Right).

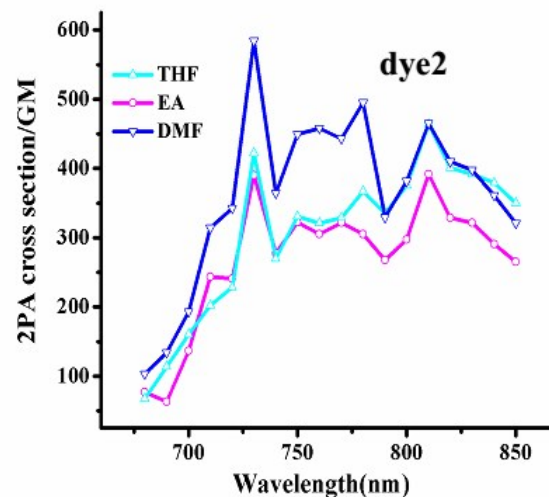
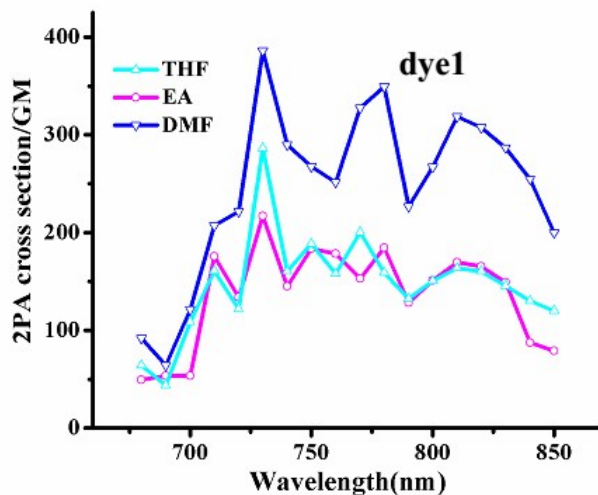


Fig. S12. Two-photon absorption cross-section of **dye1** and **dye2** in three solvents with concentration of 1.0×10^{-3} mol L⁻¹.

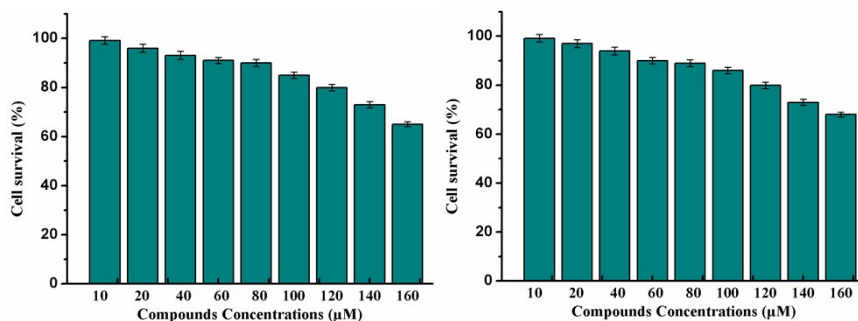


Fig. S13. MTT assay of HepG2 cells treated with dye1 (Left) and dye2 (Right) at different concentrations for 24 h.

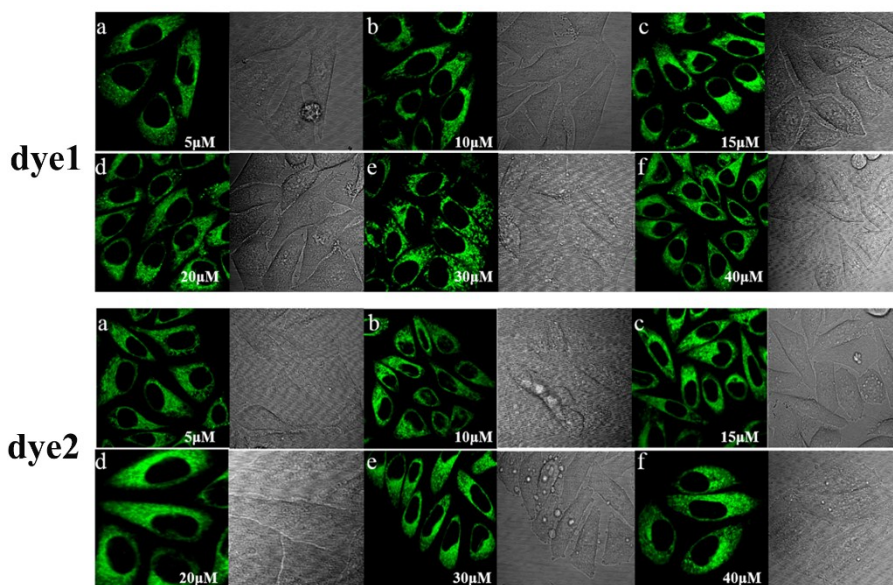


Fig. S14. Confocal microscopy images of HepG2 cells incubated with different concentration of **dye1** (up) and **dye2** (down) after 30min of incubation (emission wavelength from 450 nm to 550 nm).

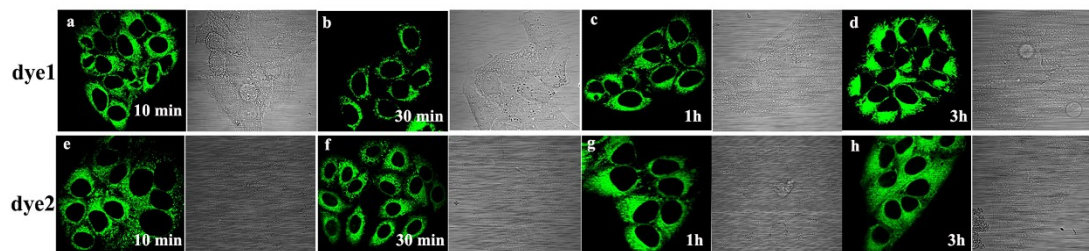


Fig. S15. Confocal microscopy images of HepG2 cells with 10 μM **dye1** (up) and **dye2** (down) after different incubation time (emission wavelength from 450 nm to 550 nm).

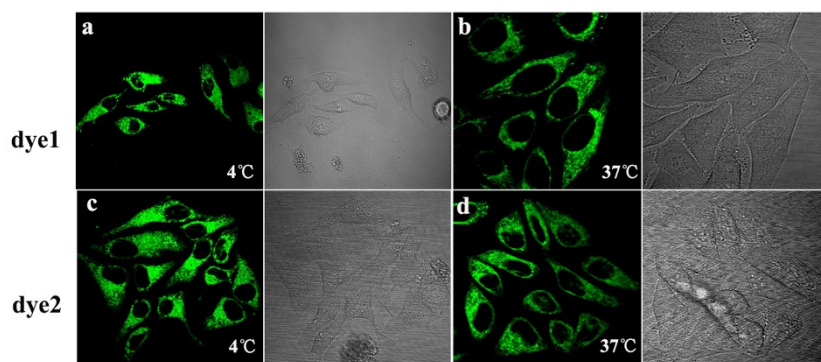


Fig. S16. Confocal microscopy images of HepG2 cells incubated with 10 μ M of **dye1** (up) and **dye2** (down) at 4°C and 37°C (emission wavelength from 450 nm to 550 nm).

Table S1 Crystal data and structure refinements for **dye1** and **dye 2**.

Compound	dye1	dye2
Empirical formula	C ₆₄ H ₄₄ N ₆ S ₂	C ₃₁ H ₂₂ N ₄ S ₁
Formula weight	963.19	482.59
Temperature	273(2) K	273(2) K
Wavelength	0.71069 Å	0.71069 Å
Crystal system	P2 ₁ /c	P2 ₁ /n
Space group	Monoclinic	Monoclinic
a /Å	15.423(5)	9.148(6)
b /Å	41.104(5)	14.095(6)
c /Å	9.126(5)	18.970(13)
β (°)	120.433 (5)	91.97 (10)
V/ Å ³	4988(3)	2445(3)
Z	4	4
D _c /Mg m ⁻³	1.283	1.311
μ /mm ⁻¹	0.160	0.160
F(000)	2016	1008
Goodness-of-fit on F ²	0.923	0.958
Final R indices	R ₁ =0.055, wR ₂ =0.216	R ₁ =0.054, wR ₂ = 0.079
CCDC	912390	1465317

Table S2 Selected bond distances (Å) and angles (°) for **dye1** and **dye2**.

dye1			
C(21)-N(3)	1.429(3)	C(13)-C(6)	1.482(4)
C(27)-N(3)	1.415(3)	C(7)-C(12)	1.482(4)
C(20)-N(3)	1.411(4)	C(27)-N(1)-C(21)	122.3(2)
C(17)-S(1)	1.722(3)	C(20)-N(1)-C(21)	117.7(2)
C(19)-C(20)	1.343(4)	C(27)-N(1)-C(20)	119.5(3)
C(19)-C(18)	1.413(4)	C(14)-C(13)-N(1)	122.0(3)
C(17)-C(18)	1.354(4)	C(7)-C(12)-N(1)	115.8(3)
C(17)-C(16)	1.479(4)		
dye2			
C(1)-N(1)	1.429(3)	C(17)-C(23)	1.489(4)
C(13)-N(1)	1.408(3)	C(21)-C(31)	1.490(4)
C(7)-N(1)	1.419(4)	C(13)-N(1)-C(7)	119.0(3)
C(13)-S(1)	1.734(1)	C(13)-N(1)-C(1)	119.1(3)
C(13)-C(14)	1.346(4)	C(1)-N(1)-C(7)	121.6(3)
C(14)-C(15)	1.415(3)	C(23)-C(17)-N(2)	115.3(3)
C(15)-C(16)	1.354(4)	C(21)-C(31)-N(3)	117.4(3)
C(1)-C(19)	1.463(4)		