

Supporting information

Novel rhodamine dye with large stokes shifts by fusing the 1,4-diethylpiperazine moiety and its applications in fast detection of Cu^{2+}

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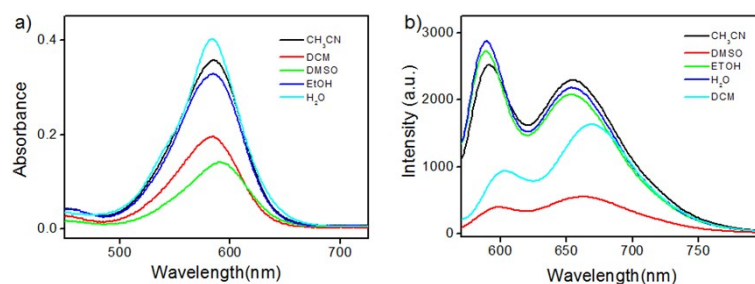


Fig. S1 Absorption a) and fluorescence b) spectra of **JRQ** in different solvents.

Table S1. Photophysical properties of **JRQ** in different solvents.

Solvent	λ_{Abs} (nm)	λ_{em} (nm)	λ_{ex} (nm)	ϵ_{b} ($\text{M}^{-1} \text{cm}^{-1}$)	Stocks Shift (nm)	Φ^a
DCM	585	668	613	19500	55	0.54
CH ₃ CN	585	654	593	35700	61	0.05
H ₂ O	583	654	585	42000	69	0.18
DMSO	590	662	600	14200	62	0.20
EtOH	585	655	592	32800	63	0.09

^a Relative fluorescence quantum yield estimated by using Nile Blue ($\Phi_{\text{B}} = 0.27$ in ethanol) as a fluorescence standard.

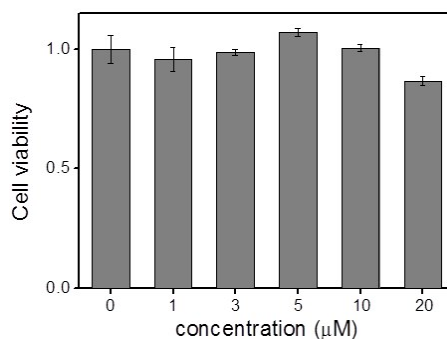


Fig. S2 MTT assay of **JRQ**.

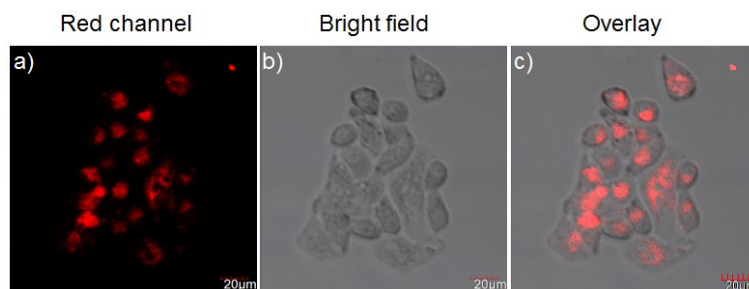


Fig. S3 Fluorescent images of HeLa cells incubated with **JRQ** (1 μM) for 30 min. $\lambda_{\text{ex}} = 559 \text{ nm}$, $\lambda_{\text{em}} = 618\text{--}718 \text{ nm}$.

Table. S2 Overlap coefficients and Pearson's coefficients of commercial targeting reagents and **JRQ**

Reagents	Overlap	Pearson's
Mito-Tracker Green	0.92	0.91
Lyso-Tracker Green	0.80	0.78
ER-Tracker Green	0.73	0.72
Golgi-Tracker Green	0.80	0.79

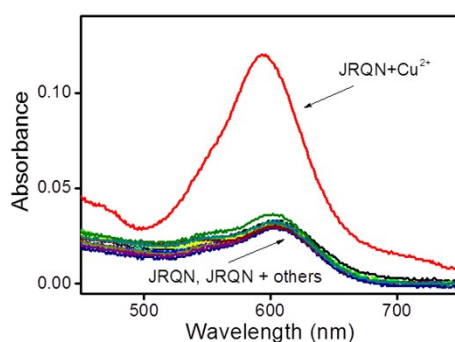


Fig. S4 Absorption spectra response of **JRQ** (10 μ M) upon addition of different species (100 μ M). 1) Ag^+ ; 2) Al^{3+} ; 3) Ca^{2+} (10 mM); 4) Cd^{2+} ; 5) Co^{2+} ; 6) Cr^{3+} ; 7) Cu^{2+} ; 8) Fe^{2+} ; 9) Fe^{3+} ; 10) Pd^{2+} ; 11) K^+ (10 mM); 12) Li^+ (10 mM); 13) Mg^{2+} (10 mM); 14) Mn^{2+} ; 15) Na^+ ; 16) Ni^{2+} ; 17) Zn^{2+} .

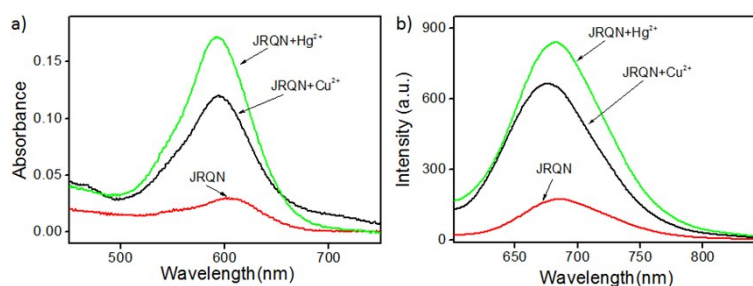


Fig. S5 Absorption and emission spectra response of **JRQ** (10 μ M) upon addition of Hg^{2+} (100 μ M).

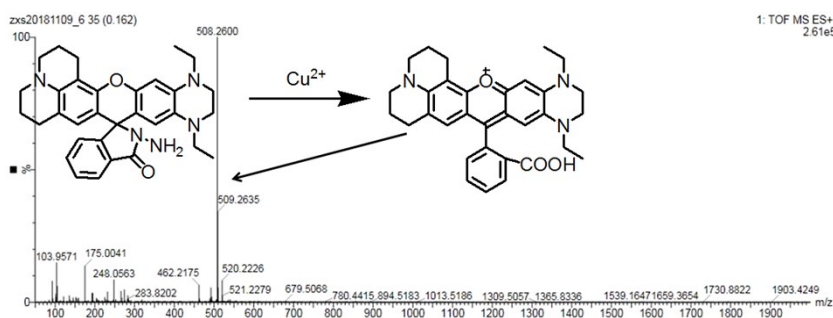


Fig. S6 HRMS of **JRQ** in the presence of Cu^{2+} .

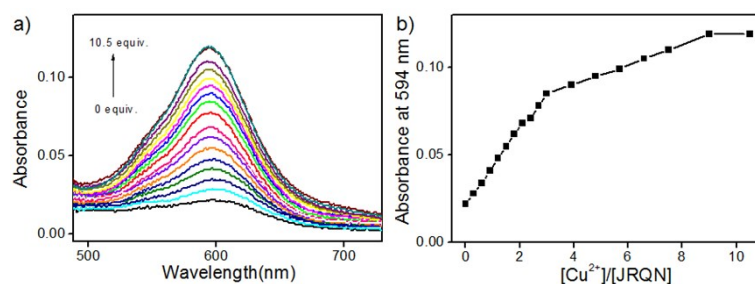


Fig. S7 a) The absorption spectra changes of **JRQN** (10 μM) treated with increasing concentrations of Cu^{2+} (0–105 μM); b) The plot of the absorption intensities at 594 nm versus the equiv. of Cu^{2+} .

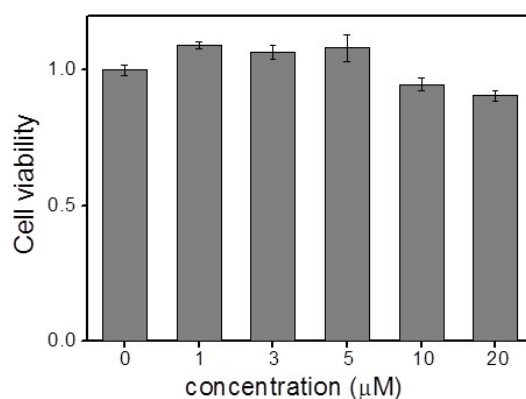


Fig. S8 MTT assay of **JRQN**.

Table. S3 Overlap coefficients and Pearson's coefficients of commercial targeting reagents and **JRQN**

Reagents	Overlap	Pearson's
Mito-Tracker Green	0.93	0.92
Lyso-Tracker Green	0.84	0.83
ER-Tracker Green	0.65	0.64
Golgi-Tracker Green	0.60	0.59



Fig. S9 ¹H NMR spectra of JRQ in CDCl₃

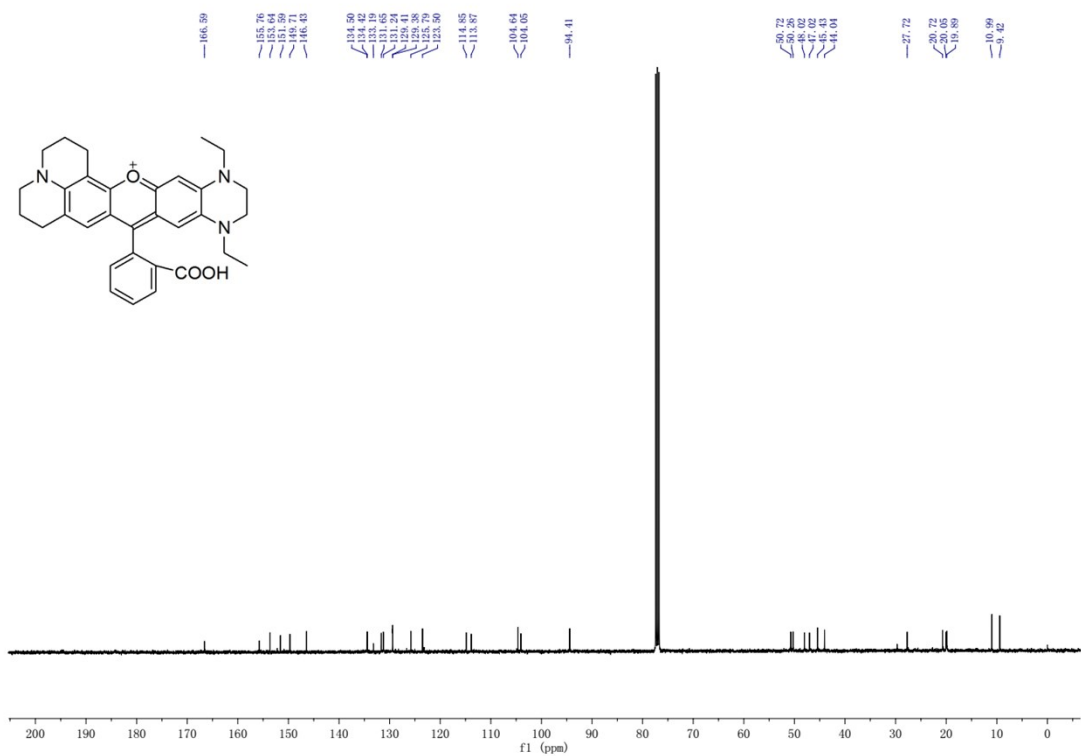


Fig. S10 ¹³C NMR spectra of JRQ in CDCl₃

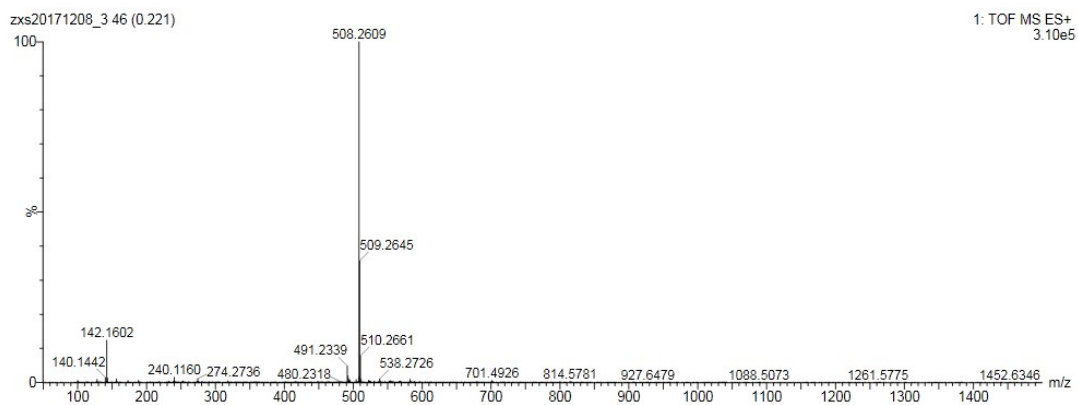


Fig. S11 HRMS spectra of JRQ

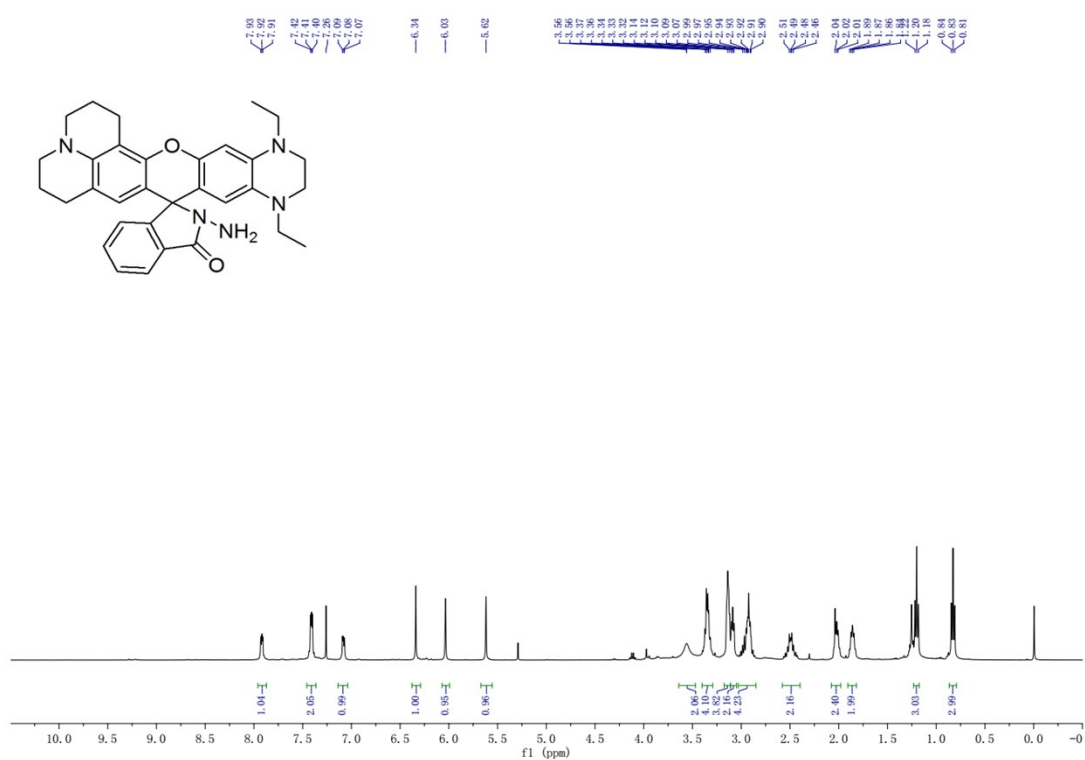


Fig. S12 ^1H NMR spectra of JRQ in CDCl_3

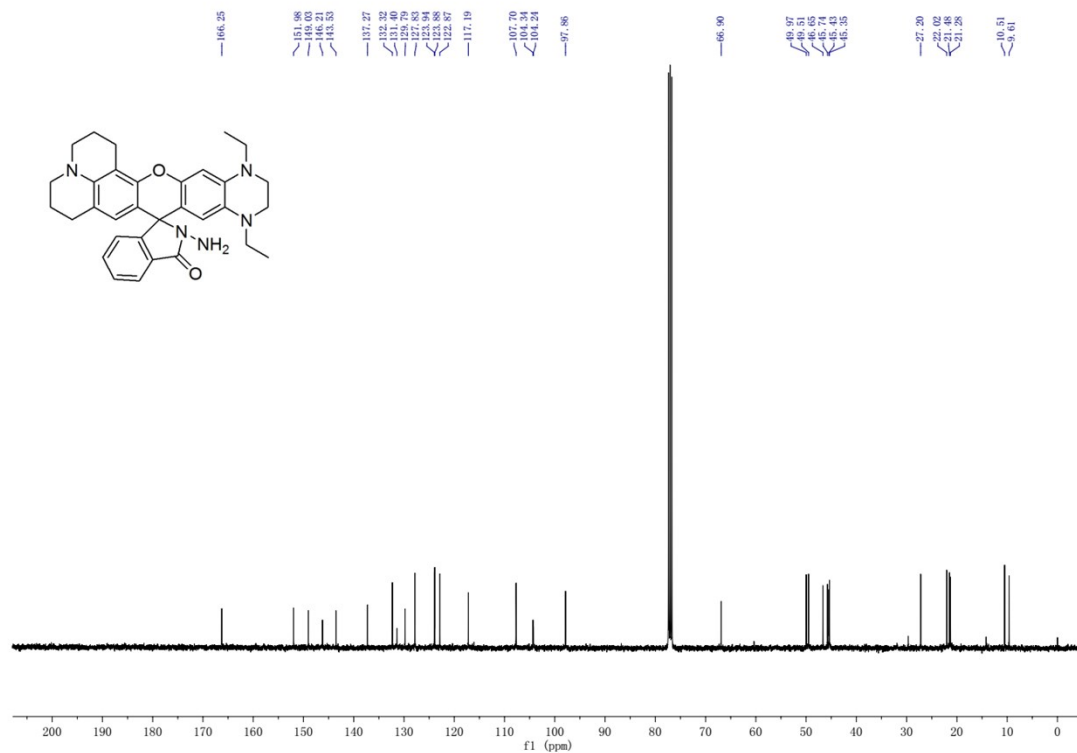


Fig. S13 ¹³C NMR spectra of JRQN in CDCl₃

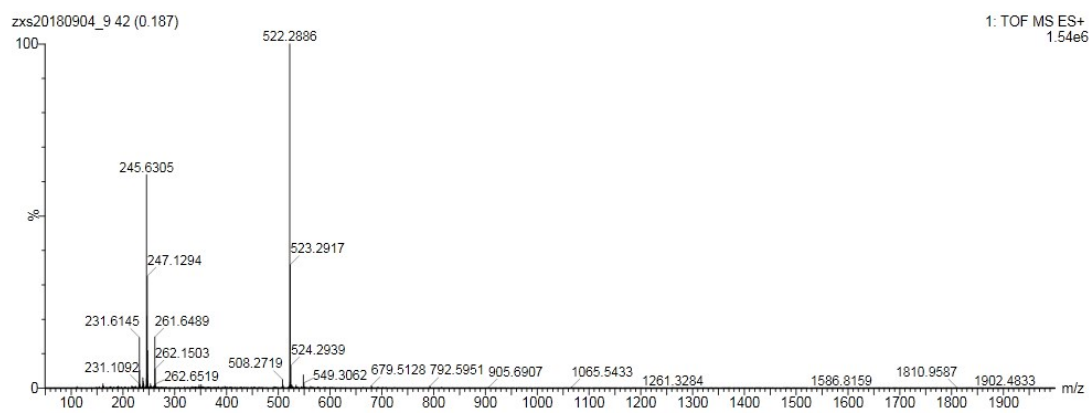


Fig. S14 HRMS spectra of JRQN