Supporting information

A near-infrared fluorescent probe with improved Stokes shift by tuning the donor-acceptor-donor character of rhodamine skeleton and its applications

Jin Gong,[†,‡] Chang Liu,[†] Xiaojie Jiao,[†] Song He,[†] Liancheng Zhao,[†,‡] and Xianshun Zeng[*,†,‡]

[†] Tianjin Key Laboratory for Photoelectric Materials and Devices, School of Materials Science & Engineering, Tianjin University of Technology, Tianjin, 300384, China

[‡] School of Materials Science and Engineering, Harbin Institute of Technology, Harbin, 150001, China

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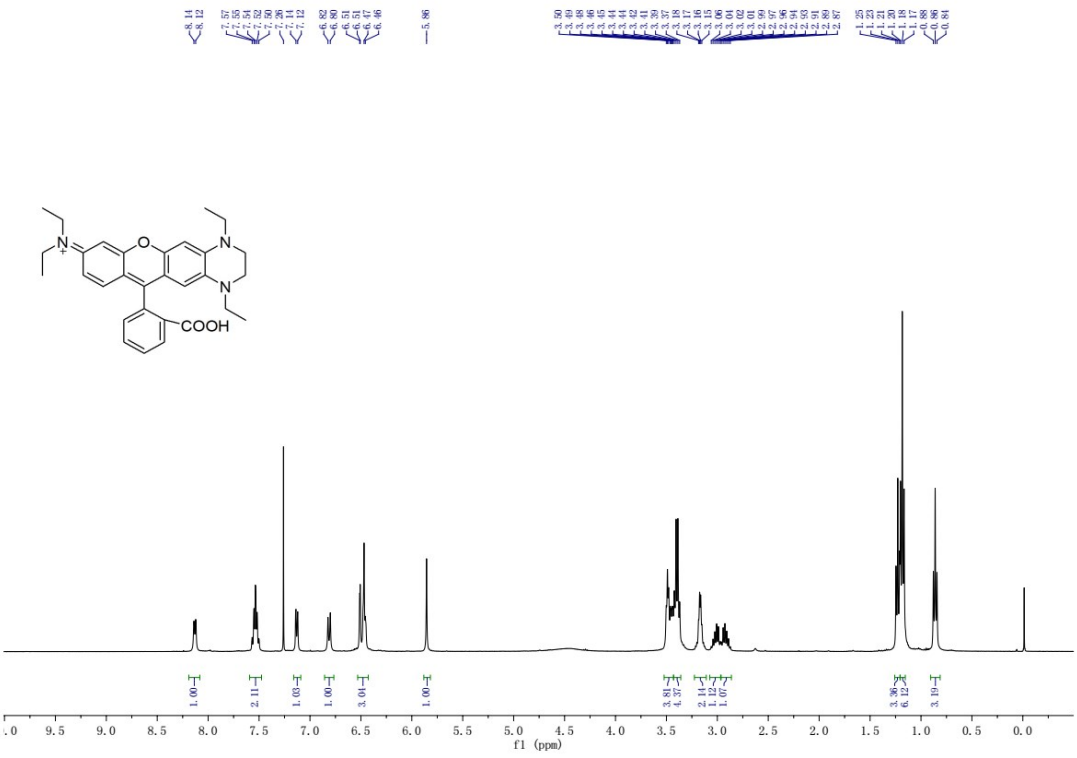


Figure S1. ^{1}H NMR spectra of **RQ** in $CDCl_3$

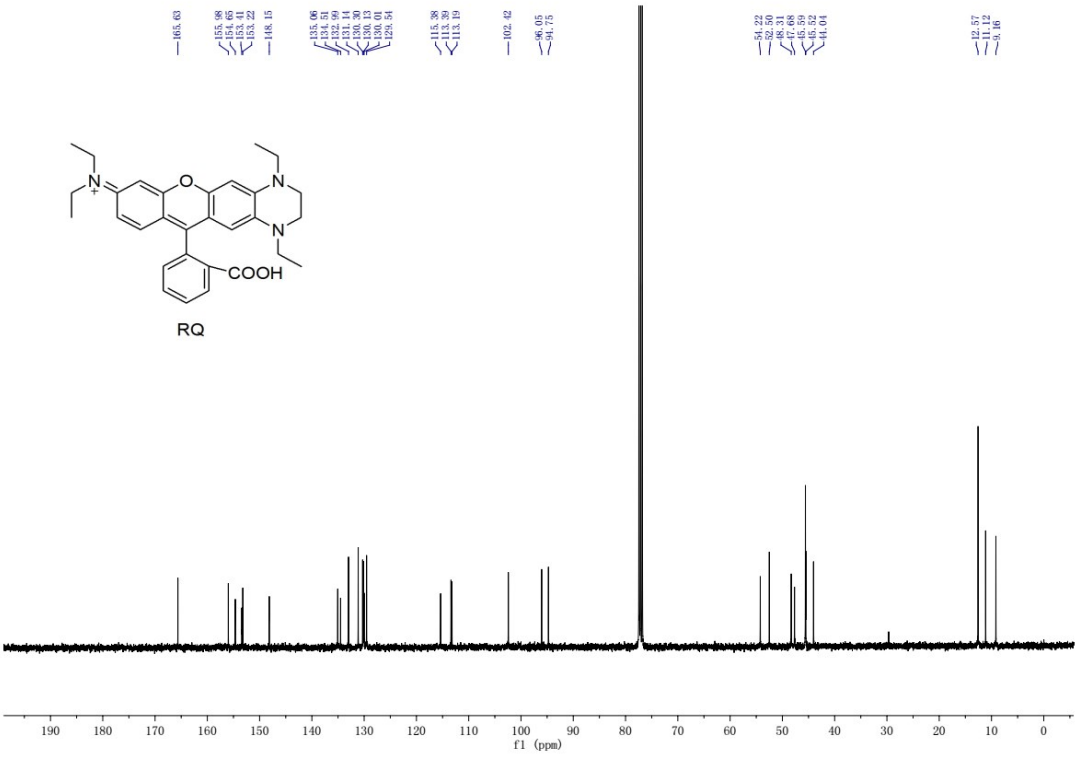


Figure S2. ^{13}C NMR spectra of **RQ** in $CDCl_3$

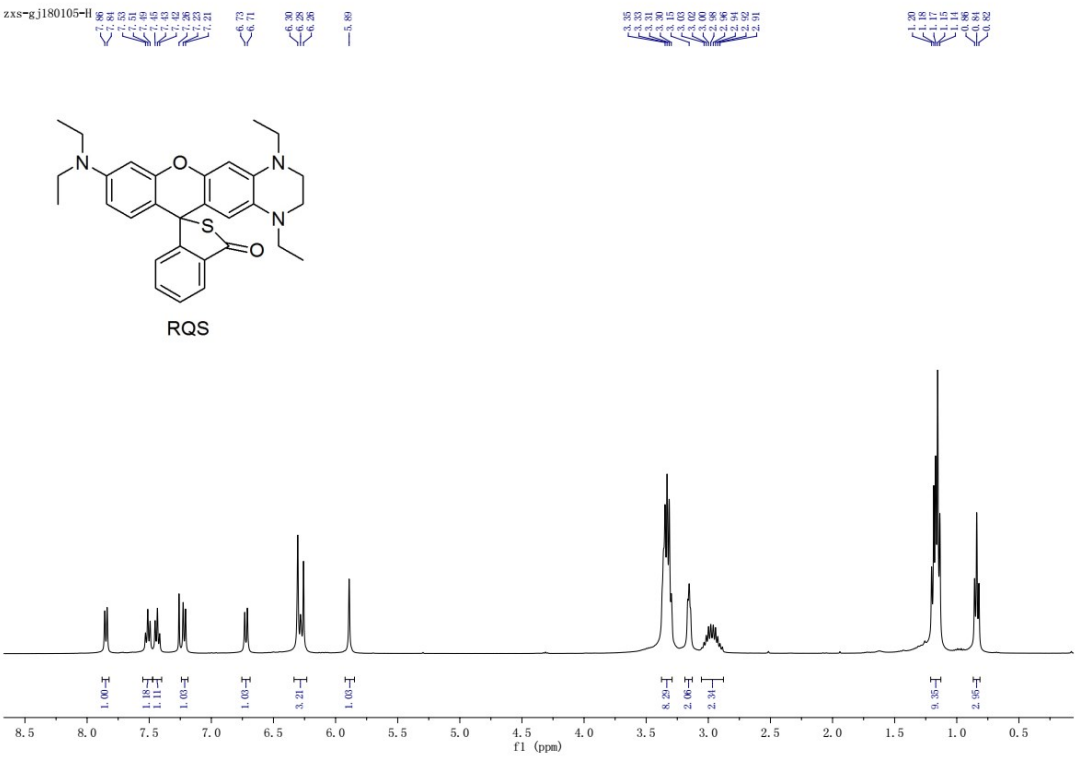


Figure S3. ^{1}H NMR spectra of **RQS** in $CDCl_3$

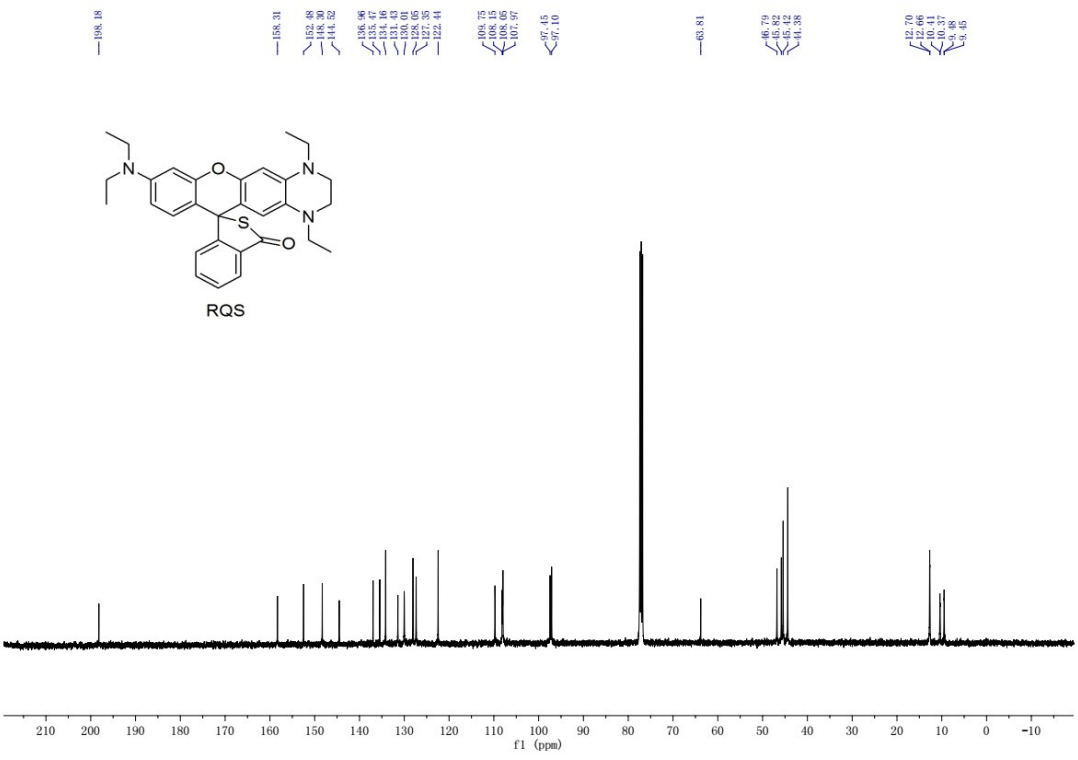


Figure S4. ^{13}C NMR spectra of **RQS** in $CDCl_3$

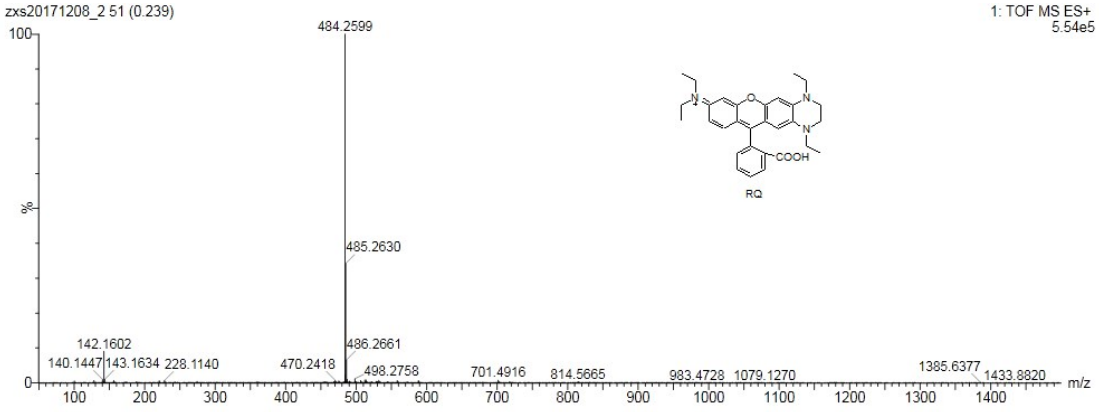


Figure S5. HRMS of **RQ**

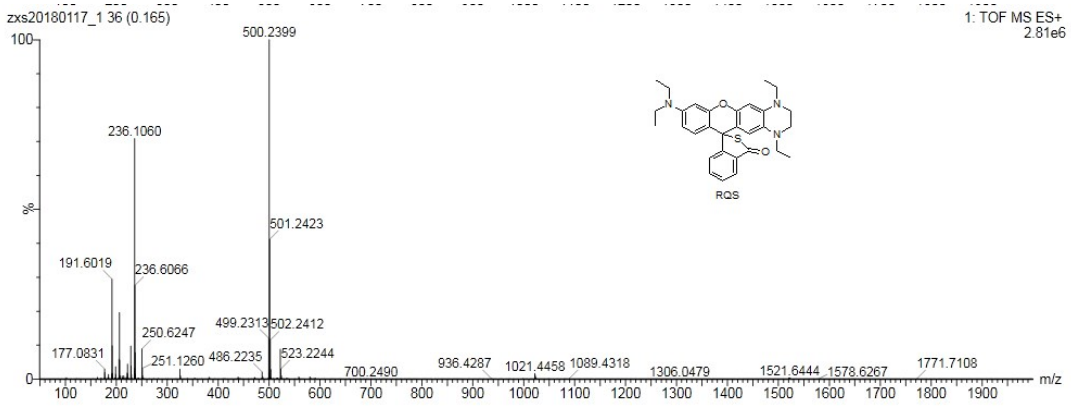


Figure S6. HRMS of **RQS**

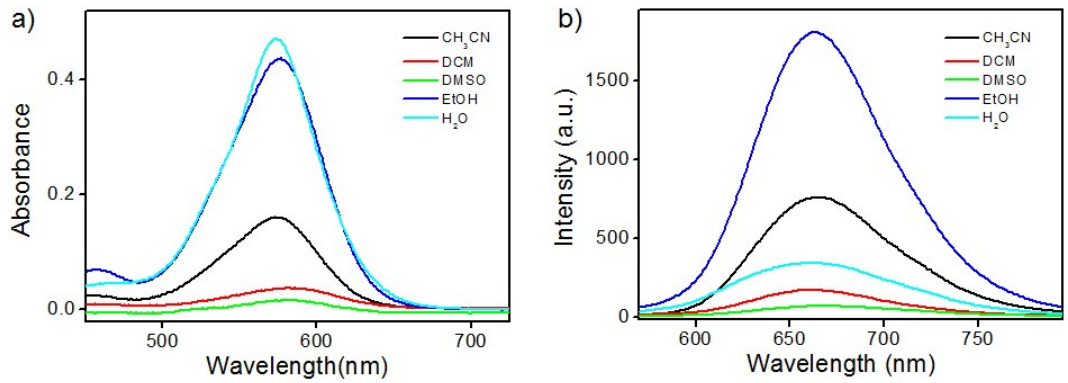


Figure S7. Absorption and fluorescence spectra of **RQ** in different solvents.

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

Sol.	λ_{Abs} (nm)	λ_{em} (nm)	ε_b ($M^{-1}cm^{-1}$)	Stocks shift (nm)	Φ_f
CH_3CN	573	666	16100	93	0.11
DCM	580	661	3800	81	0.33
EtOH	576	664	43700	88	0.09
H_2O	573	662	47100	89	0.03
DMSO	581	670	1700	89	0.07

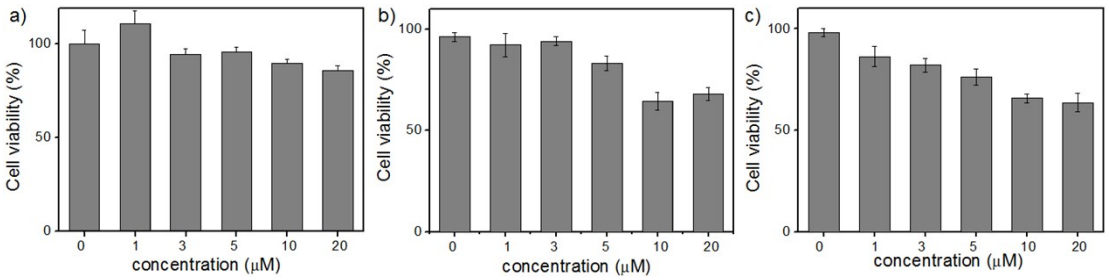


Figure S8. MTT assay of **RQ**. a) 24 h; b) 48 h; c) 72 h.

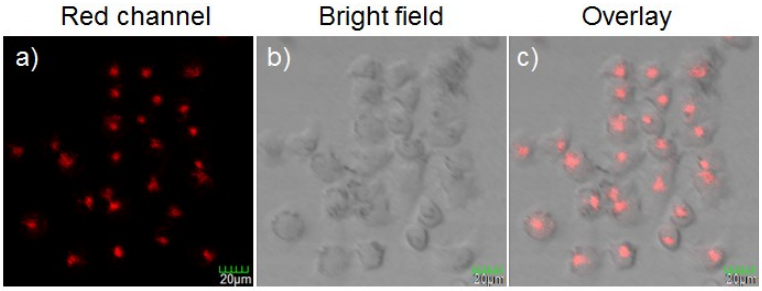
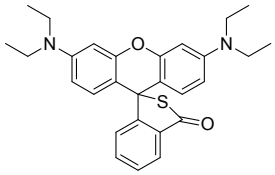
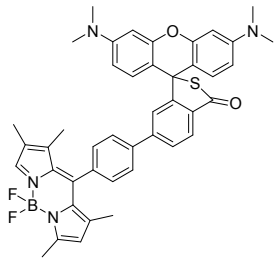
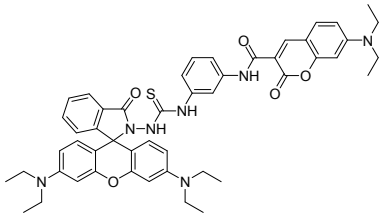
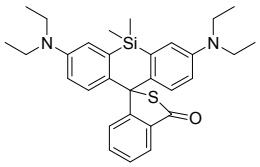
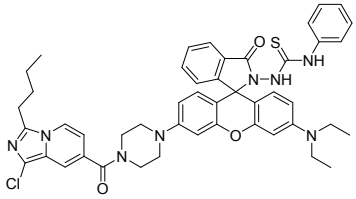
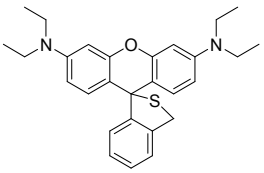
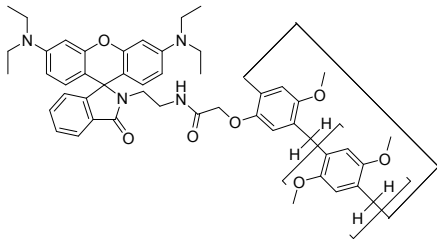
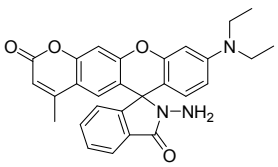
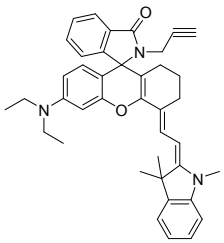
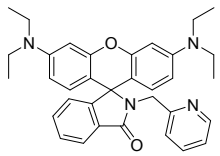
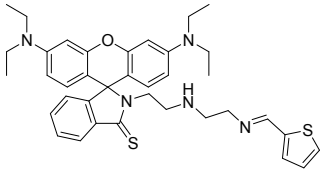
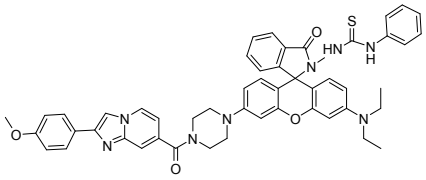
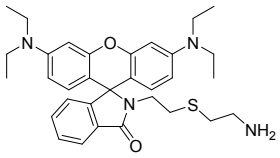
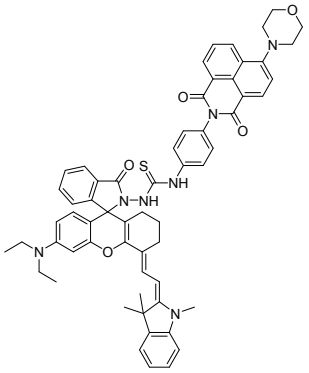


Figure S9. Fluorescent images of HeLa cells incubated with **RQ** (1 μM) for 30 min. λ_{ex}= 559 nm, λ_{em} = 618−718 nm.

Table S2. Comparison of detection limits of various probes for detecting Hg^{2+}.[1-14]

No.	Sensor structures	LOD (nM)	λ_{Abs} (nm)	λ_{em} (nm)	Stocks shift (nm)
1		20	560	585	25

2		ppm scale	557	585	28
3		3.2	568	587	29
4		81	659	687	28
5		0.93	564	584	20
6		2.5	565	576	11
7		28.5	556	573	17
8		5.5	503	576	73
9		870	720	760	40

10		10	545	575	30
11		195	560	575	15
12		9.1	565	590	25
13		140	561	578	17
14		191	730	746	16
15	**This work**	**2**	**680**	**584**	**96**

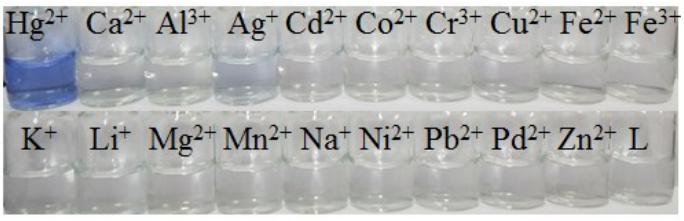


Figure S10. Color change of **RQS** with metal ions.

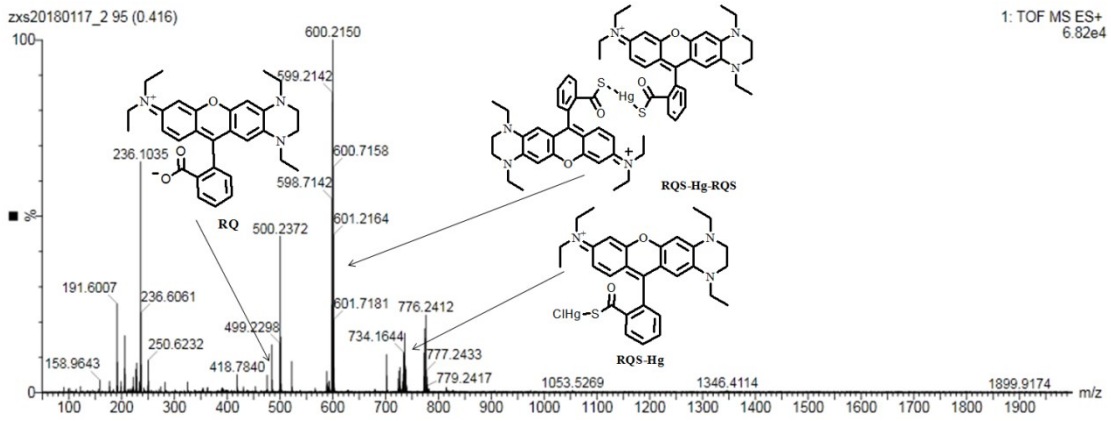


Figure S11. HRMS of the reaction products of **RQS** with 2 equiv of Hg^{2+}**.**

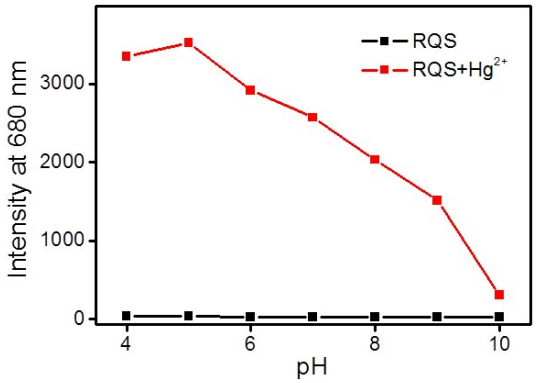


Figure S12. Effect of pH on the fluorescence intensity of **RQS** (10 μM) in the absence (black line) and presence of 100 μM Hg^{2+} (red line).

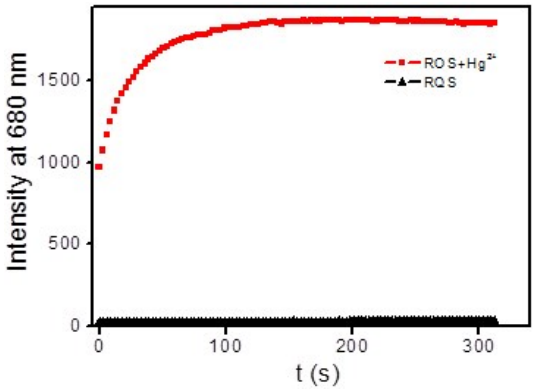


Figure S13. Time-dependence of the fluorescence intensity at 680 nm of **RQS** (10 μM) with 100 μM Hg^{2+}.

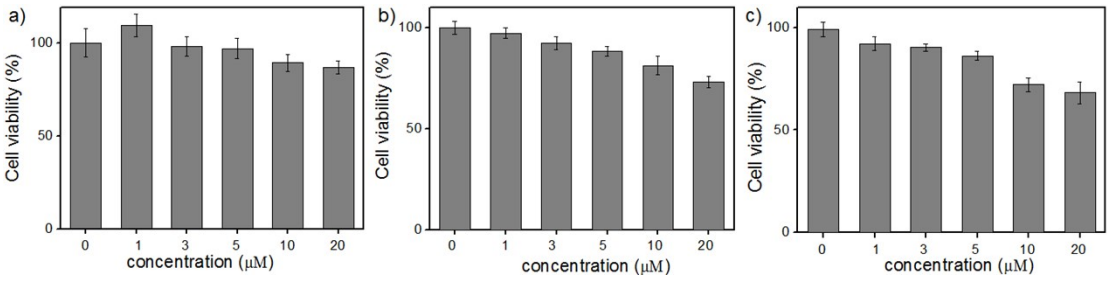


Figure S14. MTT assay of **RQS**. a) 24 h; b) 48 h; c) 72 h.

References

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