

Supporting information

A novel near-infrared fluorescent probe with improved Stokes shift for specific detection of Hg²⁺ in mitochondria

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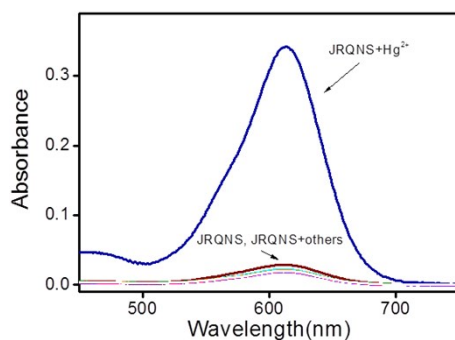


Fig. S1. Absorption spectra of **JRQNS** (10 μM) in response to 1 equiv. various analytes (Al^{3+} , Cr^{3+} , Fe^{3+} , Cd^{2+} , Co^{2+} , Mg^{2+} , Cu^{2+} , Fe^{2+} , Ca^{2+} , Pd^{2+} , Zn^{2+} , Pd^{2+} , Pb^{2+} , Ni^{2+} , Mn^{2+} , **JRQNS**, K^+ , Ag^+ , Li^+ , Na^+ , Hg^{2+}) in HEPES/ CH_3CN (8:2, v/v).

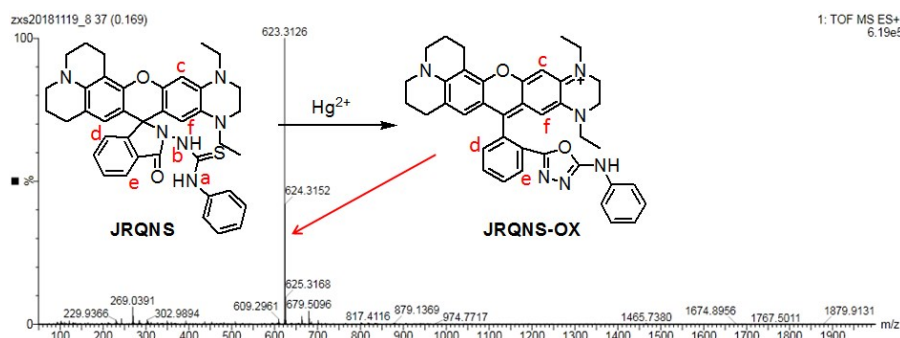


Fig. S2. HRMS spectra of **JRQNS** upon addition of Hg^{2+} (1.0 equiv.).

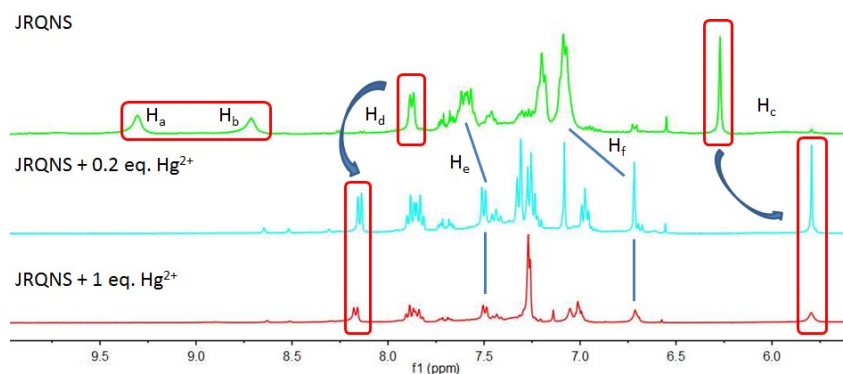


Fig. S3. ^1H NMR spectra changes of **JRQNS** upon addition of Hg^{2+} in DMSO-d_6 .

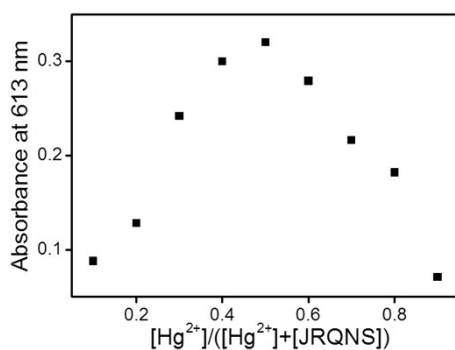


Fig. S4. Job's plot of **JRQNS** and Hg^{2+} . The total concentration of **JRQNS** and Hg^{2+} was kept at a fixed 20 μM .

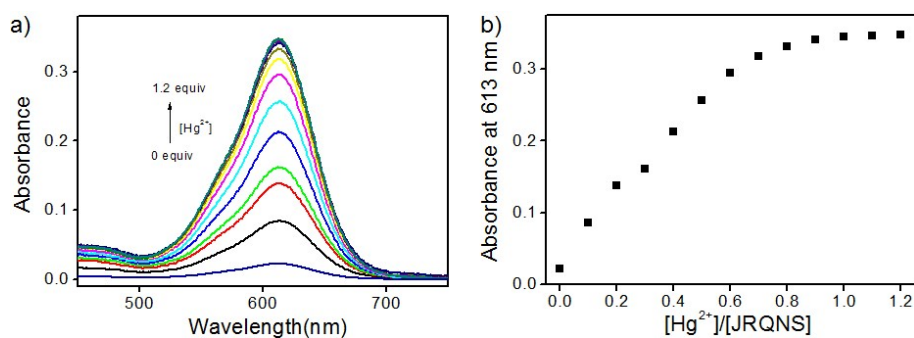
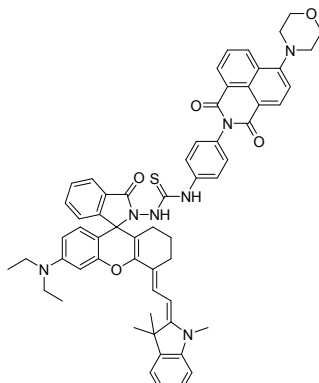
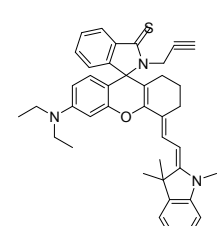
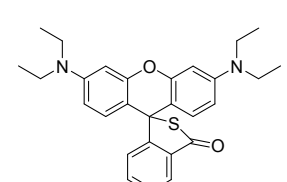
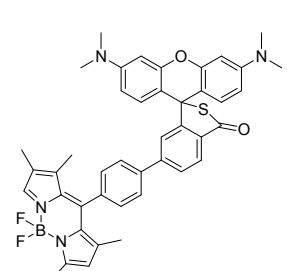
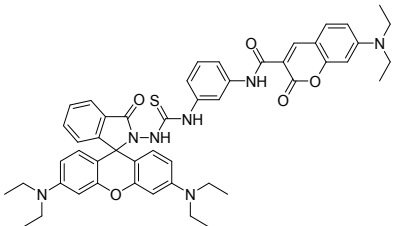
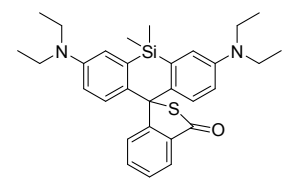
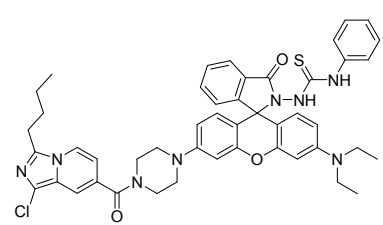
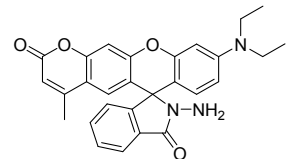
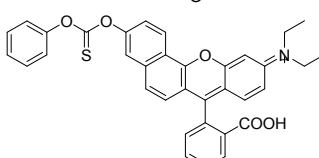
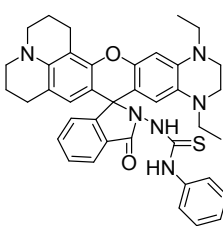


Fig. S5. a) Absorption spectra of **JRQNS** (10 μM) upon the addition of Hg^{2+} (0-1.2 equiv.) in HEPES/ CH_3CN (8:2, v/v). b) Plot of absorption intensity changes at 613 nm of **JRQNS** with Hg^{2+} (0-1.2 equiv.).

Table S1. Comparison of detection limits of various probes for detecting Hg^{2+}

Structure	λ_{em} (nm)	Stokes shift (nm)	Time	LOD (nM)	Ref.
	746	16	80 s	191	New J Chem 2017;41:13495- 13503
	760	40	<1 min	870	Sens Actuators B 2017;245:462-469
	585	25	1 min	20	Chem Commun 2008;0:1856-1858
	585	22	5min	ppm scale	Chem Eur J 2011;17:3179-3191

	587	19	1 min	3.2	Dyes Pigments 2015;120:208-212
	687	28	<1 min	81	Dyes Pigments 2017;137:601-607
	584	20	5 min	0.93	Dyes Pigments 2017;146:136-142
	576	73	5 min	5.5	Dyes Pigments 2017;142:437-446
	625	105	30 min	3.6	Analyst 2019;144:1426-1432
	691	78	3 min	1.5	This work

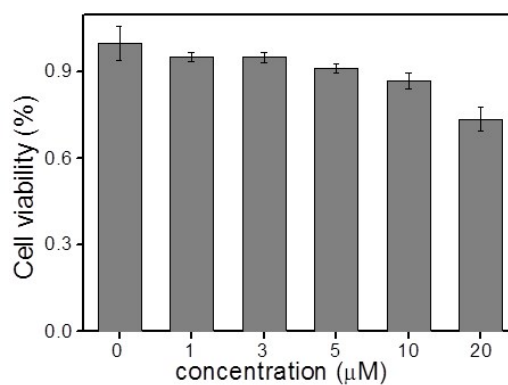


Fig. S6. MTT assay of JRQNS.

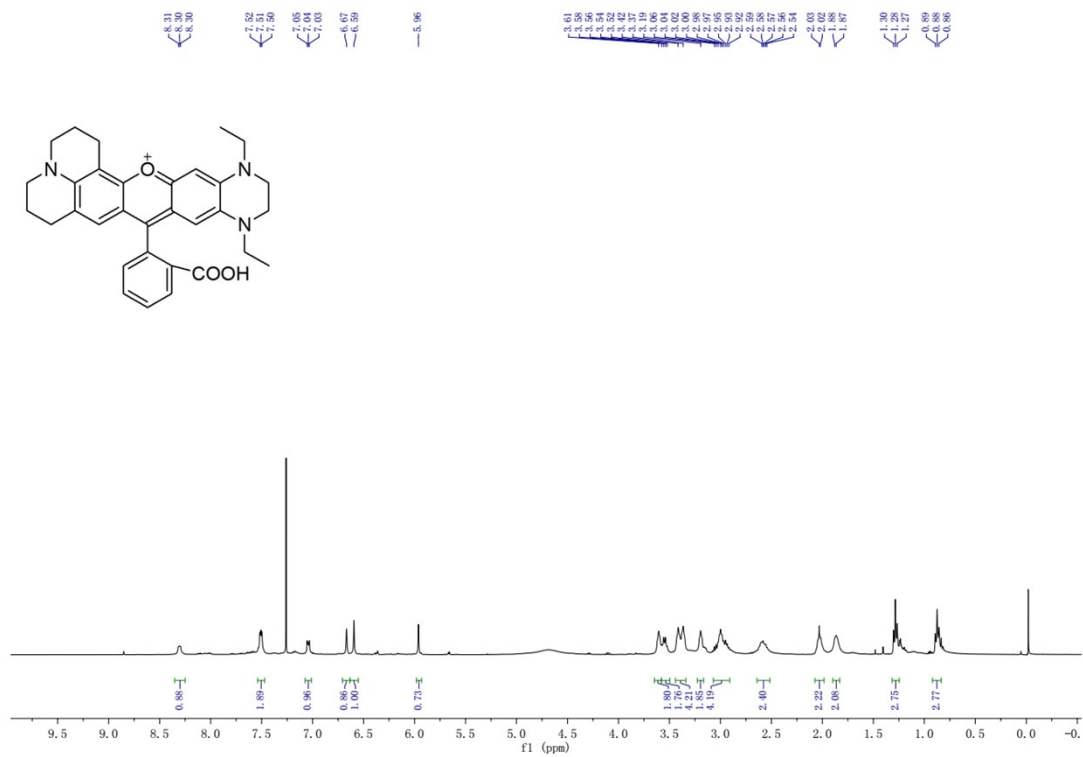


Fig. S7. ¹H NMR spectra of JRQ in CDCl₃

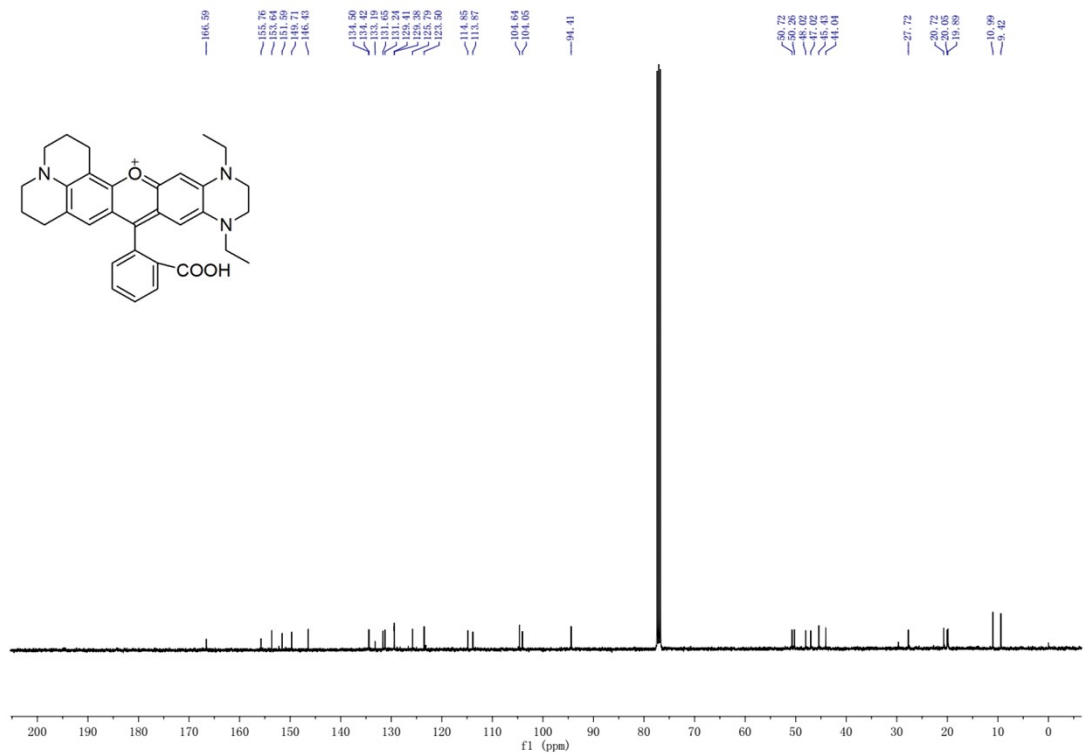


Fig. S8. ¹³C NMR spectra of JRQ in CDCl₃

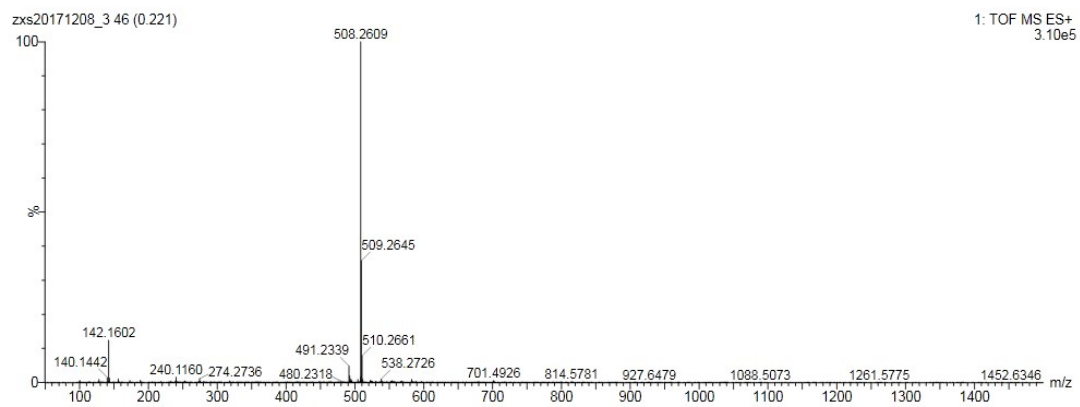


Fig. S9. HRMS spectra of **JRQ**

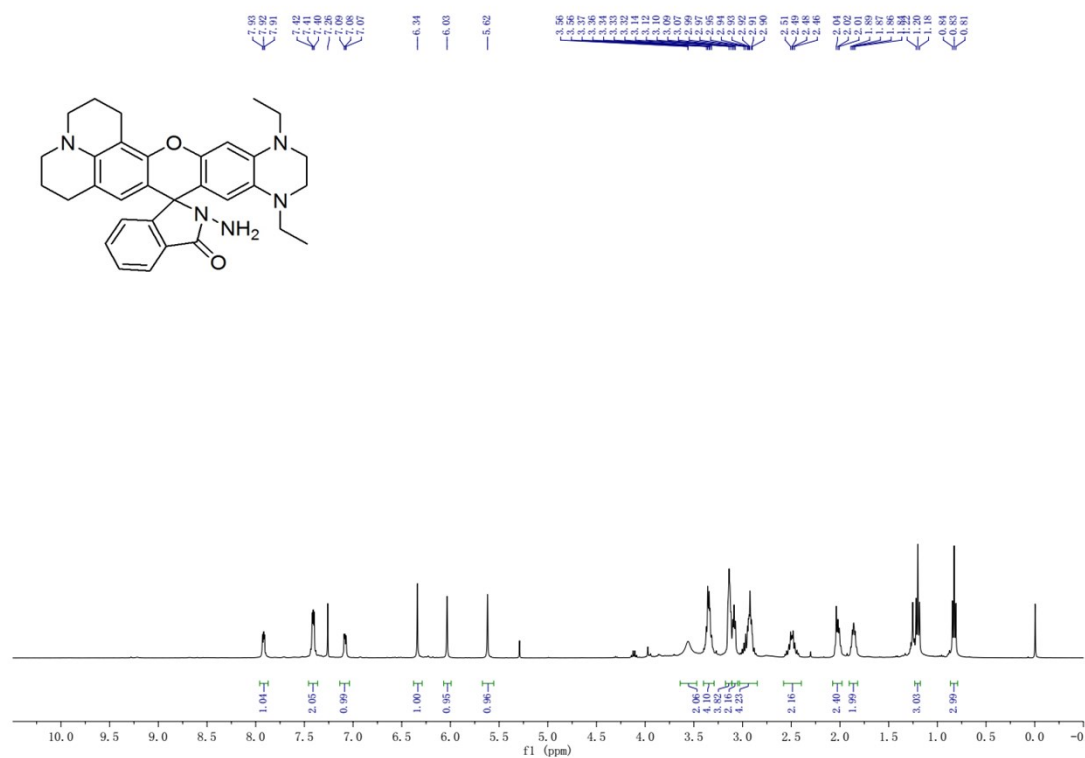


Fig. S10. ^1H NMR spectra of **JRQN** in CDCl_3

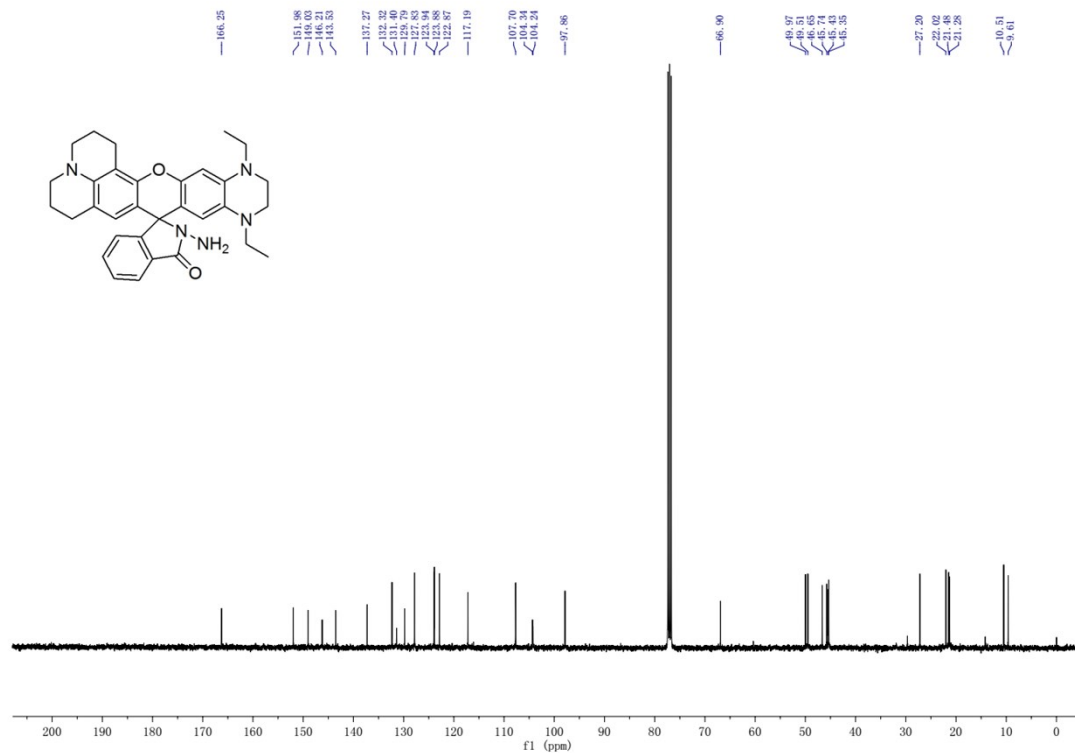


Fig. S11. ¹³C NMR spectra of JRQN in CDCl₃

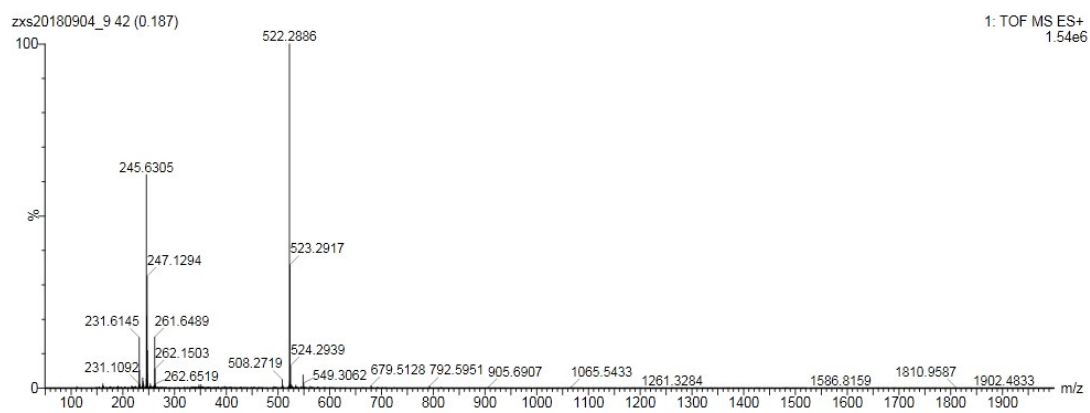


Fig. S12. HRMS spectra of JRQN

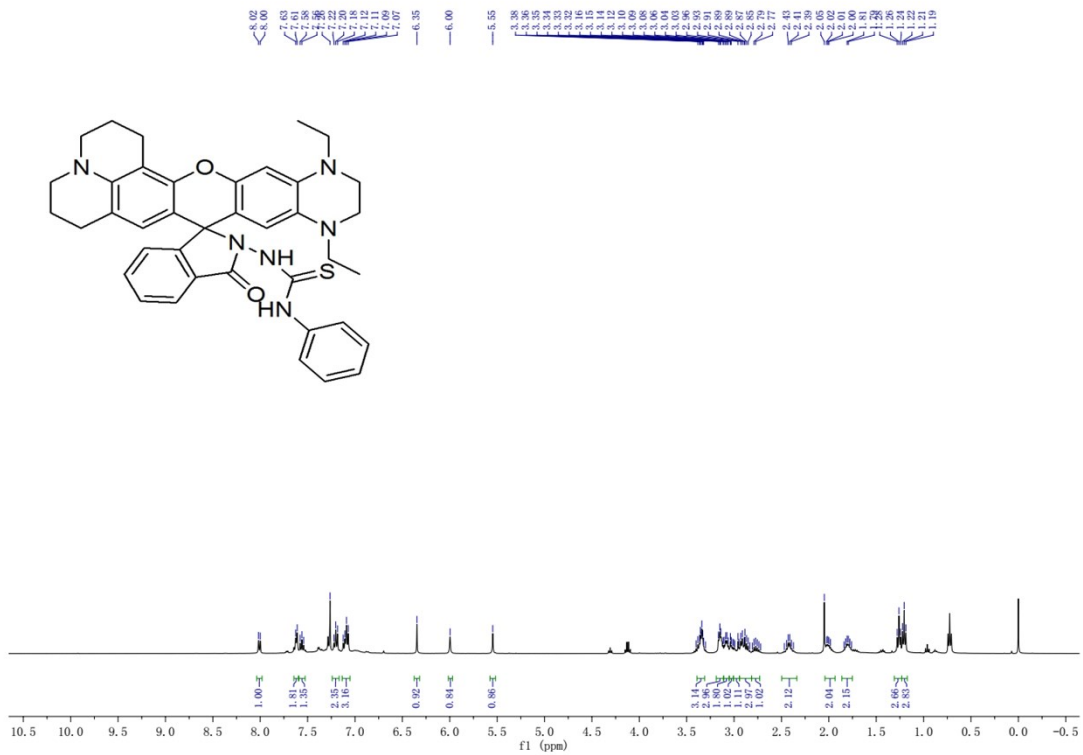


Fig. S13. ^1H NMR spectra of JRQNS in CDCl_3

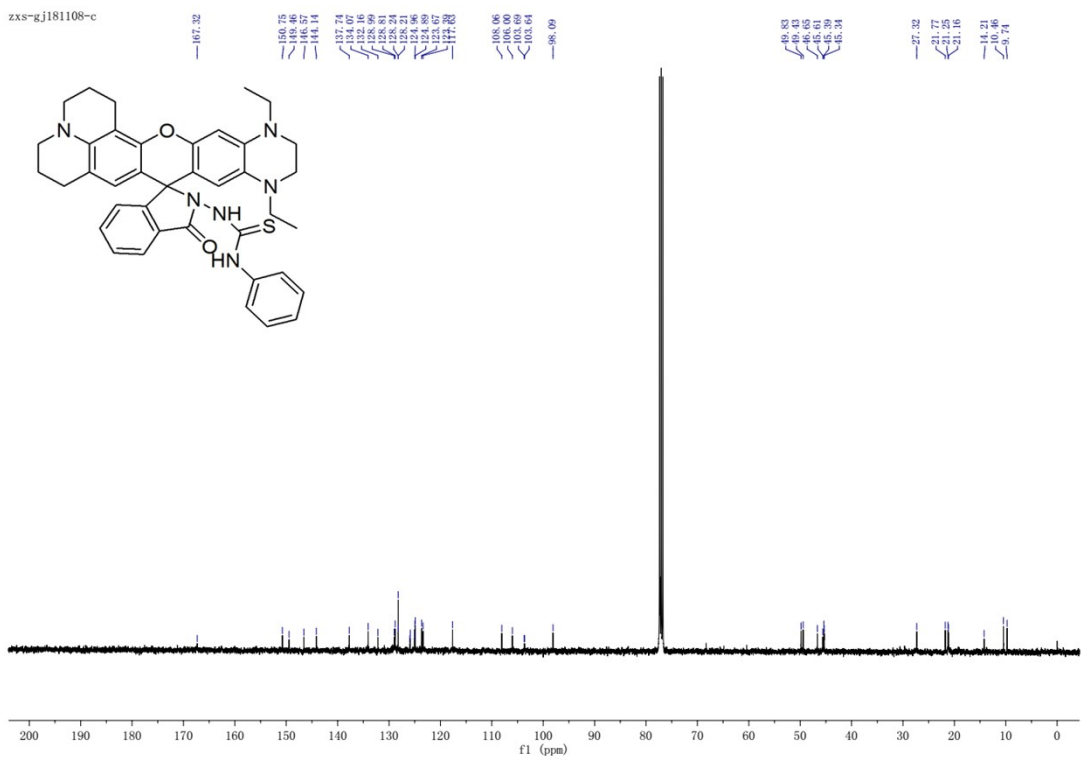


Fig. S14. ^{13}C NMR spectra of JRQNS in CDCl_3

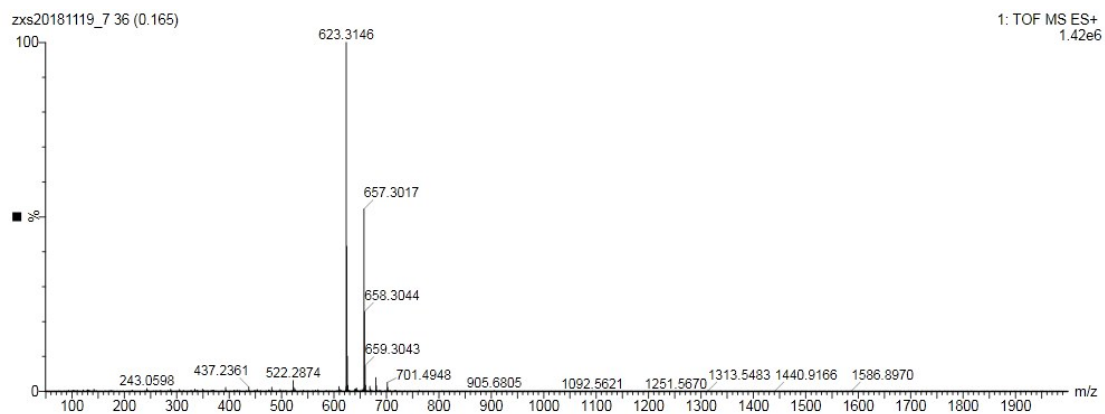


Fig. S15. HRMS spectra of JRQNS