Supporting information

A near-infrared fluorescent probe based on a novel rectilinearly π-extended rhodamine derivative and its applications

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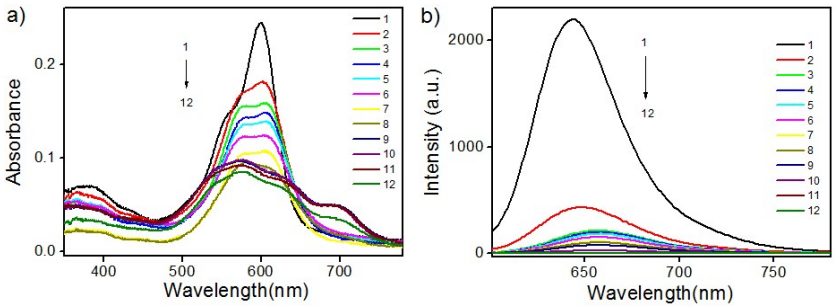
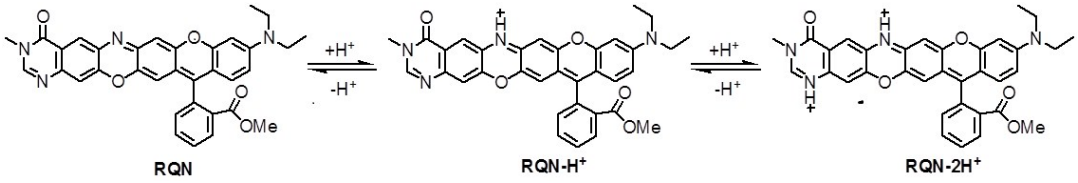


Figure S1. Absorption a) and fluorescence spectra b) of **RQN** (10 mM) in water under different pH conditions. λ_{ex}: 580 nm, slit: 5/5 nm



Scheme S1. Proposed conversions of **RQN** in water under different pH conditions.

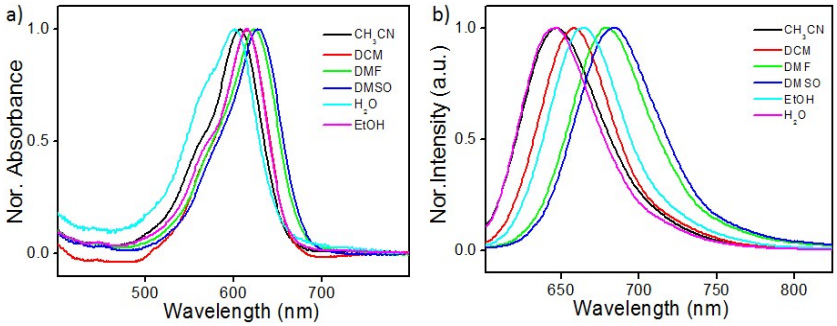


Figure S2. Normalized UV–Vis absorption a) and fluorescence b) spectra of **RQN** in different solvents in the presence of TFA (1%).

Table S1. Photophysical properties of **RQN** in different solvents in the presence of TFA (1%).

Dyes	Solvent	λ_{Abs} (nm)	λ_{em} (nm)	ε_b (M^{-1} cm^{-1})	Stocks Shift (nm)	Φ [a]
RQN	DCM	615	658	25400	43	0.117
	CH_3CN	607	647	28300	40	0.096
	H_2O	600	648	10900	48	0.116
	DMF	623	681	29000	58	0.086
	DMSO	627	683	26600	56	0.106
	EtOH	613	664	32800	51	0.071
Rh B	EtOH	553	572	11700	19	0.53

[a] Relative fluorescence quantum yield estimated by using Nile Blue (Φ_B = 0.27 in ethanol)[1] as a fluorescence standard.

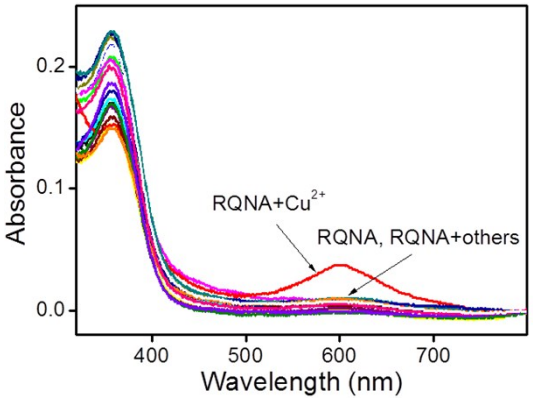


Figure S3. Absorption spectra response of **RQNA** (10 μM) upon addition of different species (50 μM). 1) Ag^{+}; 2) Al^{3+}; 3) Ca^{2+}; 4) Cd^{2+}; 5) Co^{2+}; 6) Cr^{3+}; 7) Cu^{2+}; 8) Fe^{2+}; 9) Fe^{3+}; 10) K^{+}; 11) Li^{+}; 12) Mg^{2+}; 13) Mn^{2+}; 14) Na^{+}; 15) Ni^{2+}; 16) Pb^{2+}; 17) Pd^{2+}; 18) Zn^{2+}.

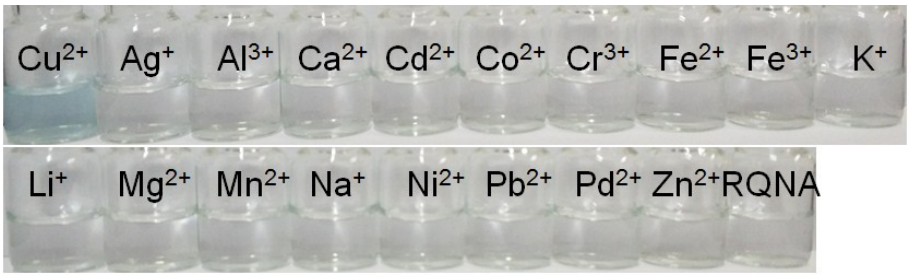


Figure S4. Color changes of **RQNA** towards various metal ions.

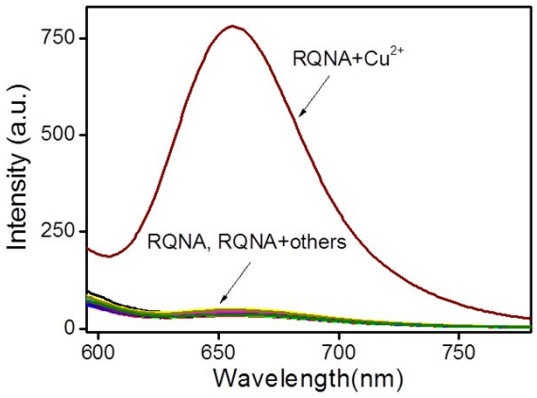
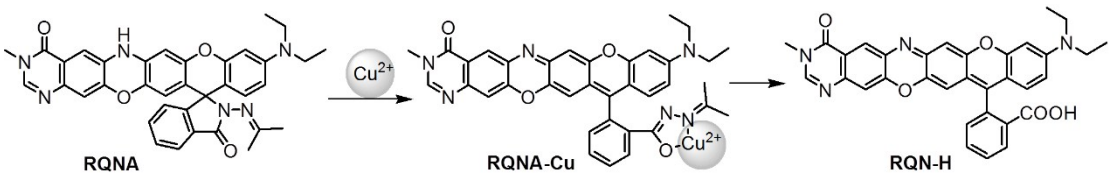


Figure S5. Fluorescence emission responses of **RQNA** (10 μM) upon addition of ROS and RNS (50 μM); 1) $^1O_2$; 2) H_2O_2; 3) ClO^{-}; 4) NO; 5) NO_2^{-}; 6) NO_3^{-}; 7) Cu^{2+}; 8) $O_2^{\bullet-}$; 9) •OH; 10) $ONOO^{-}$; 11) TBHP. The conditions: HEPES buffer (10 mM, pH = 7.4, containing 20% CH_3CN), λ_{ex} = 575 nm, slit = 10/10 nm.



Scheme S2. Mechanism of **RQNA** reacts with Cu^{2+}.

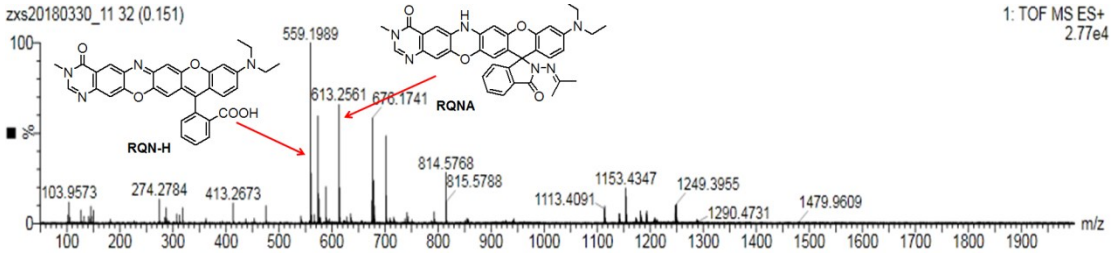


Figure S6. HRMS of **RQNA** in the presence of Cu^{2+}.

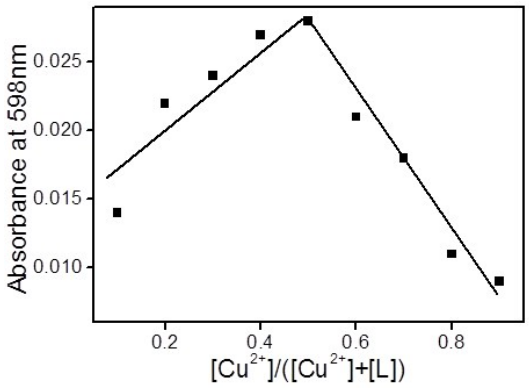


Figure S7. Job's plot of **RQNA** and Cu^{2+}. The total concentration of **RQNA** and Cu^{2+} was kept at a fixed 20 μM.

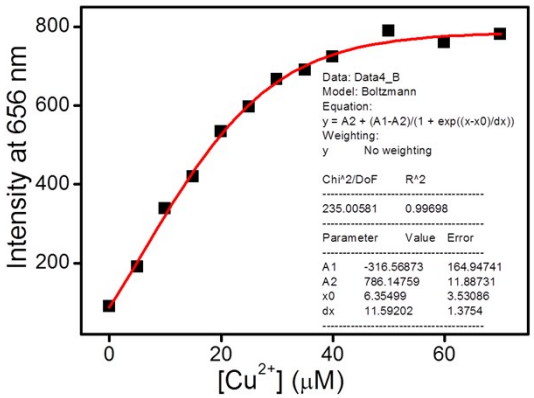


Figure S8. The fluorescence dissociation constant (K_d) of **RQNA** for Cu^{2+} was calculated based on 1:1 stoichiometry.

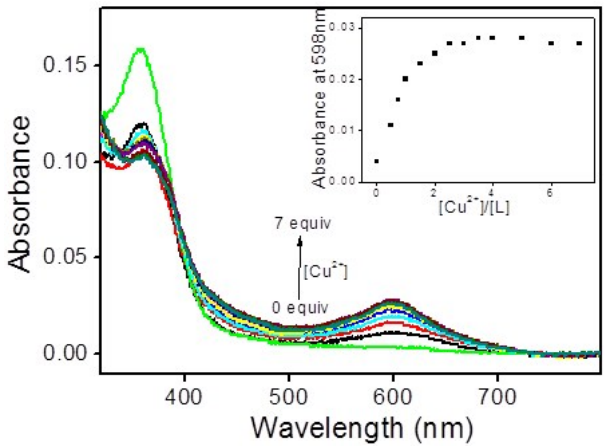


Figure S9. The absorption spectra changes of **RQNA** (10 μM) treated with increasing concentrations of Cu^{2+} (0–70 μM). Inset: The plot of the absorption intensities at 598 nm versus the equivalents of Cu^{2+}.

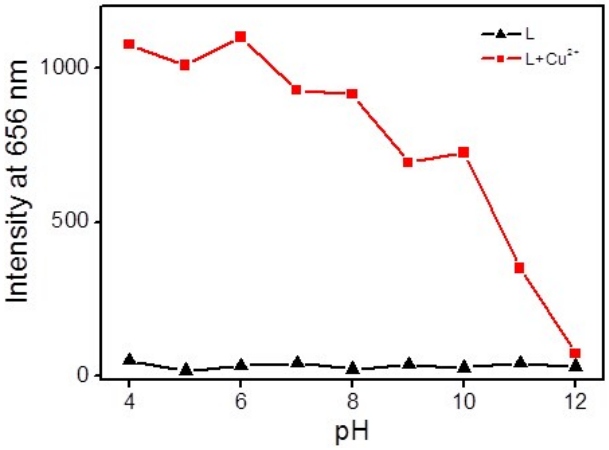


Figure S10. Effect of pH on the fluorescence intensity of **RQNA** (10 μM) in the absence (black line) and presence (red line) of Cu^{2+} (50 μM).

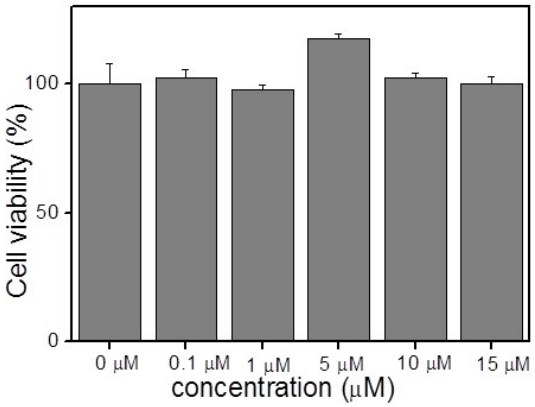


Figure S11. MTT assay of **RQNA**.

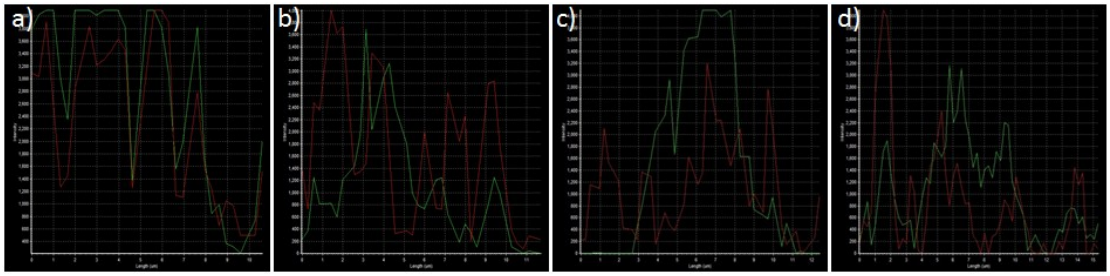


Figure S12. Intensity profiles of respective tracker-probe with **RQNA** within the linear regions of interest across the cells. a) Costained with Mito-Tracker Green; b) Costained with Lyso-Tracker Green, c) Costained with Golgi-Tracker Green; d) Costained with ER-Tracker Green**.**

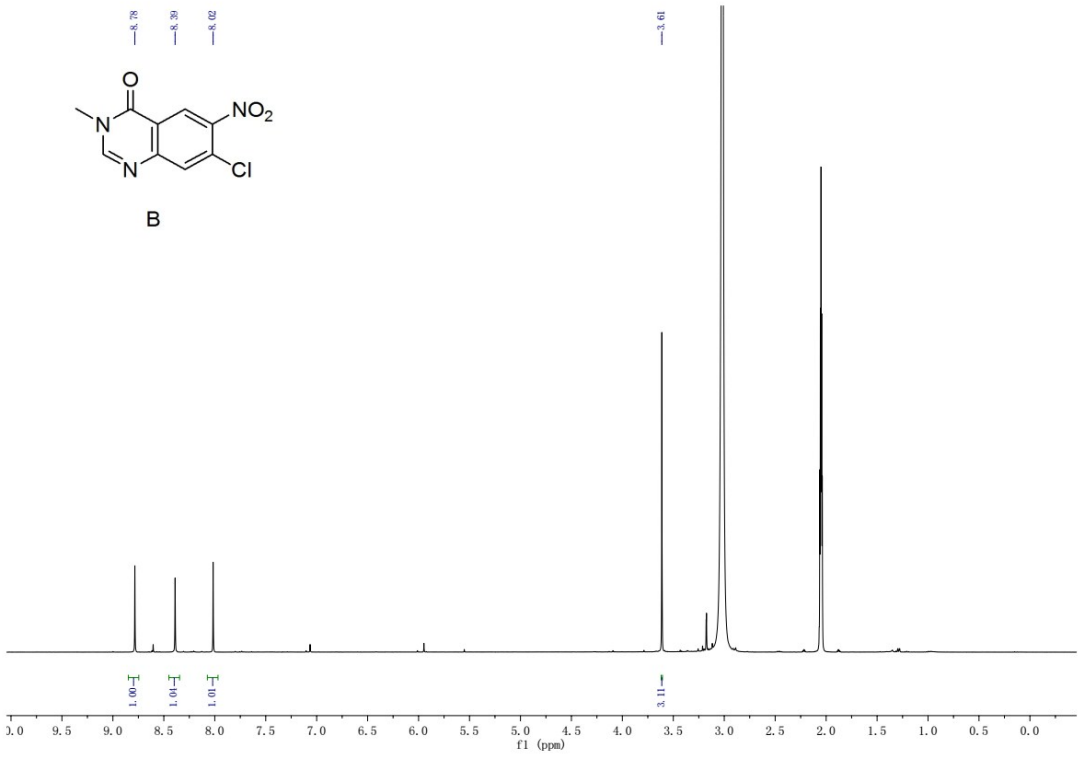


Figure S13. ^{1}H NMR spectra of **B** in $(CD_3)_2CO$

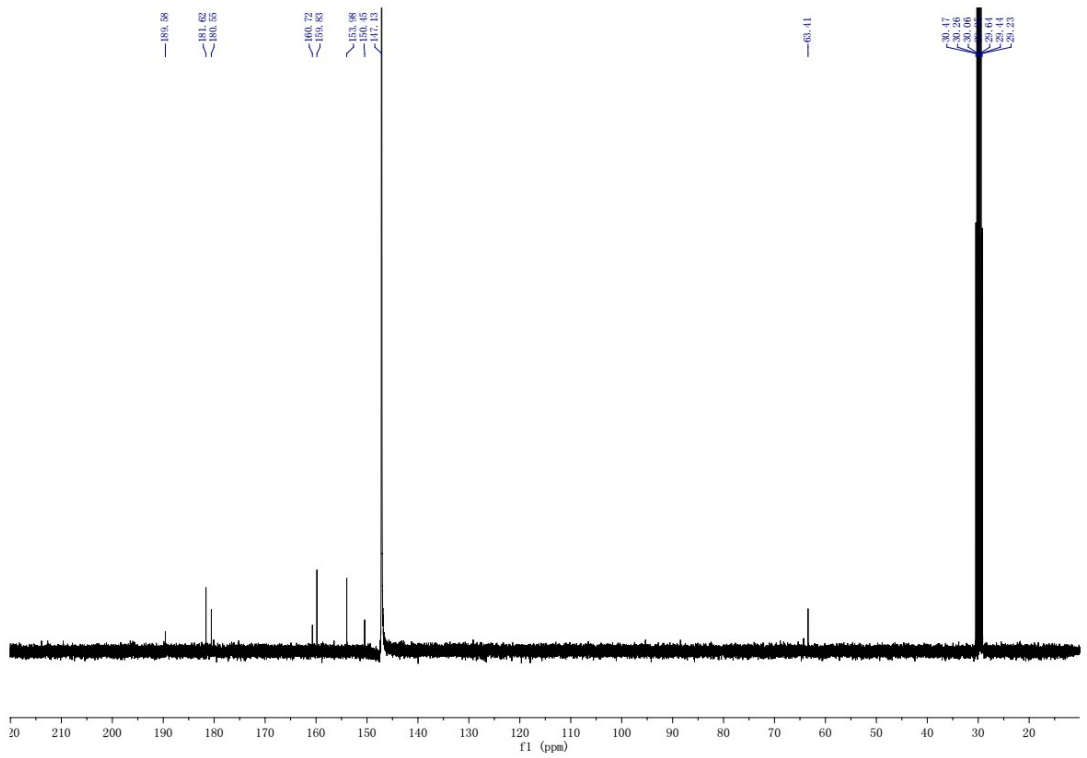


Figure S14. ^{13}C NMR spectra of **B** in $(CD_3)_2CO$

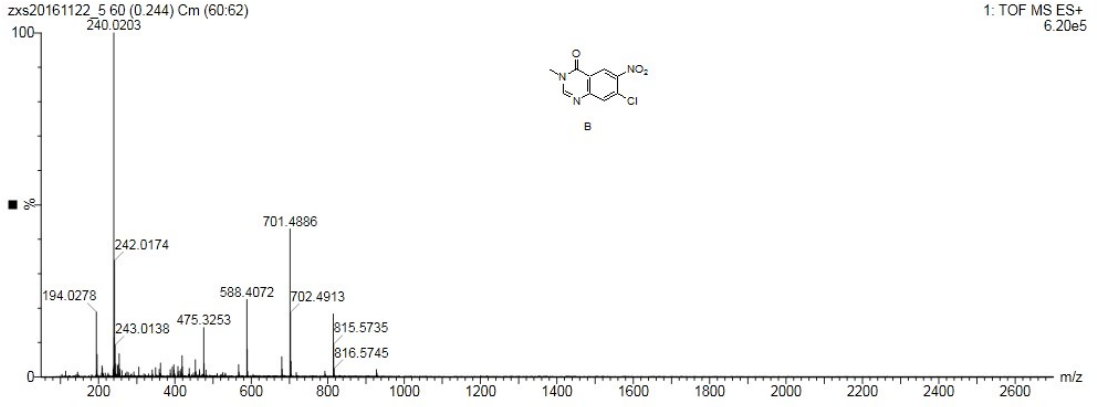


Figure S15. HRMS spectra of **B**

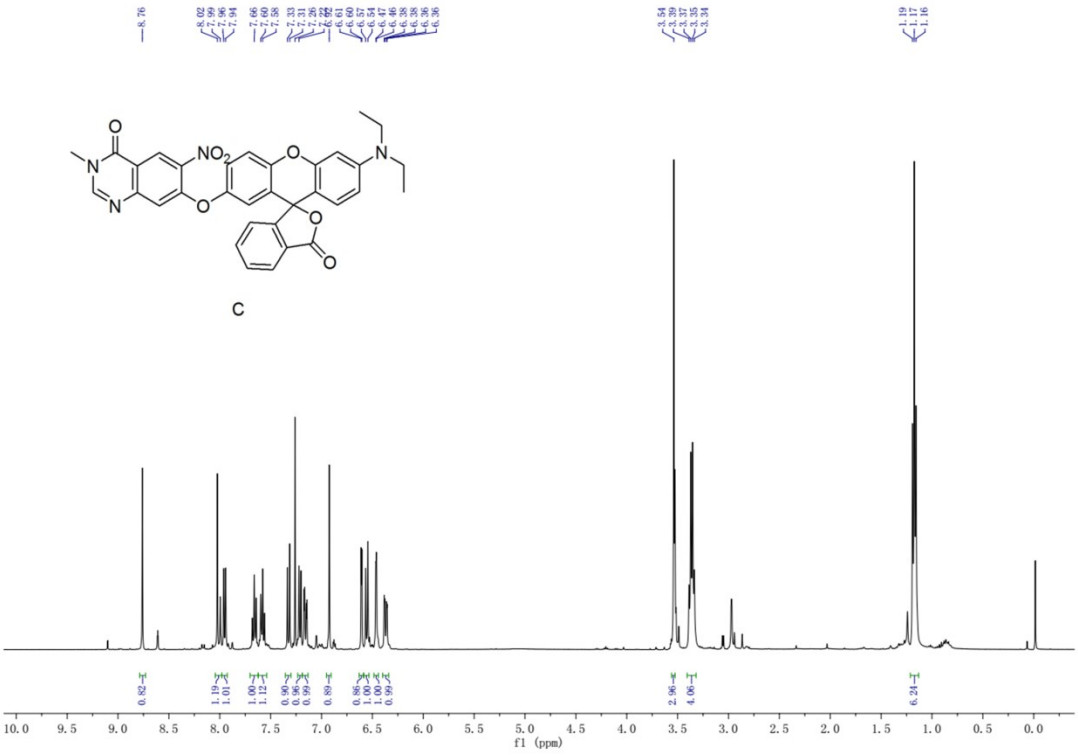


Figure S16. ^{1}H NMR spectra of **C** in $CDCl_3$

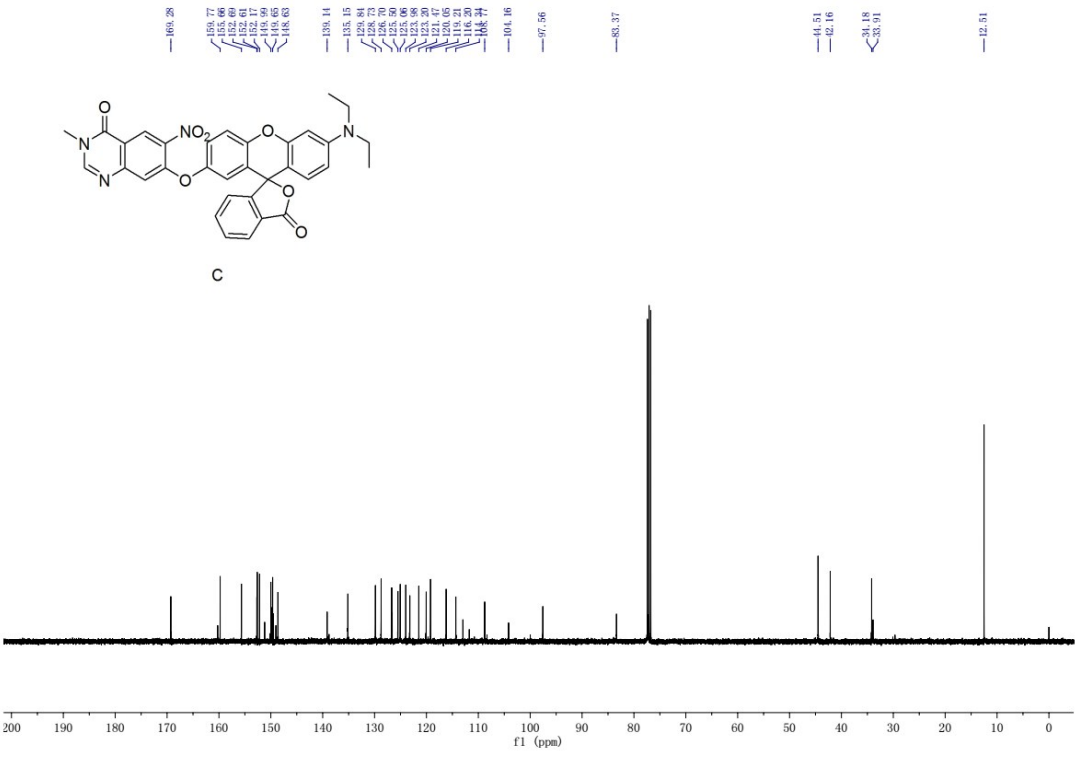


Figure S17. ^{13}C NMR spectra of **C** in $CDCl_3$

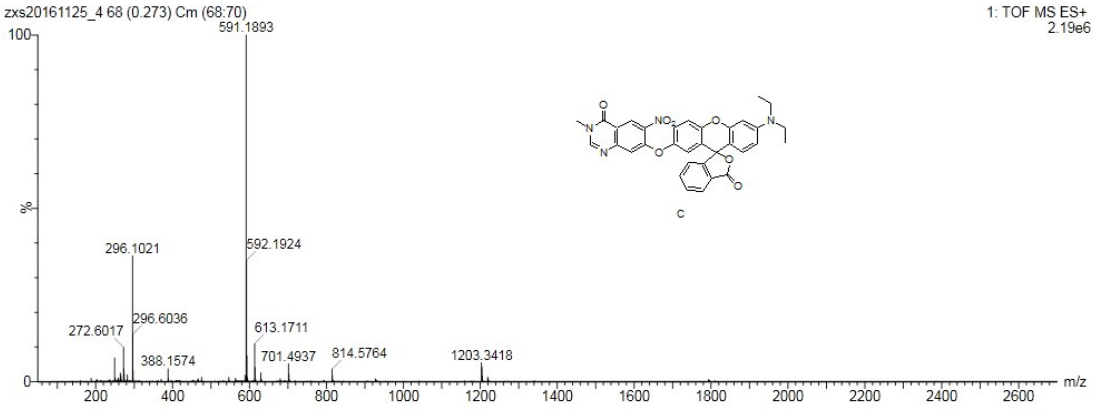


Figure S18. HRMS spectra of **C**

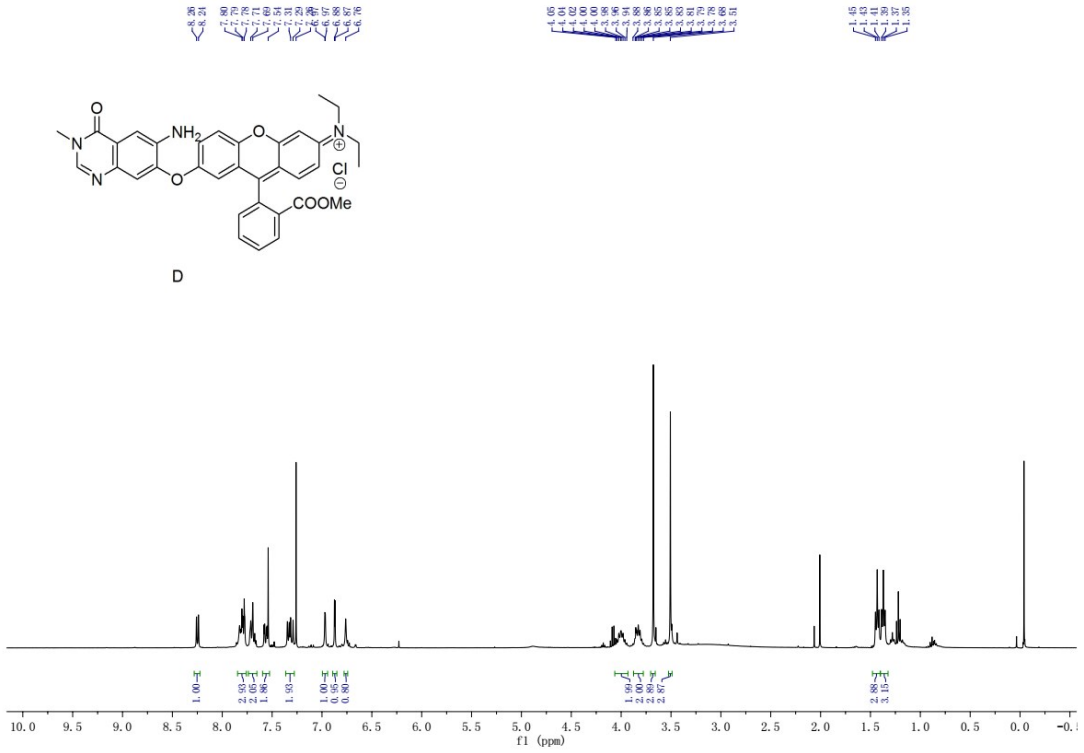


Figure S19. ^{1}H NMR spectra of **D** in $CDCl_3$

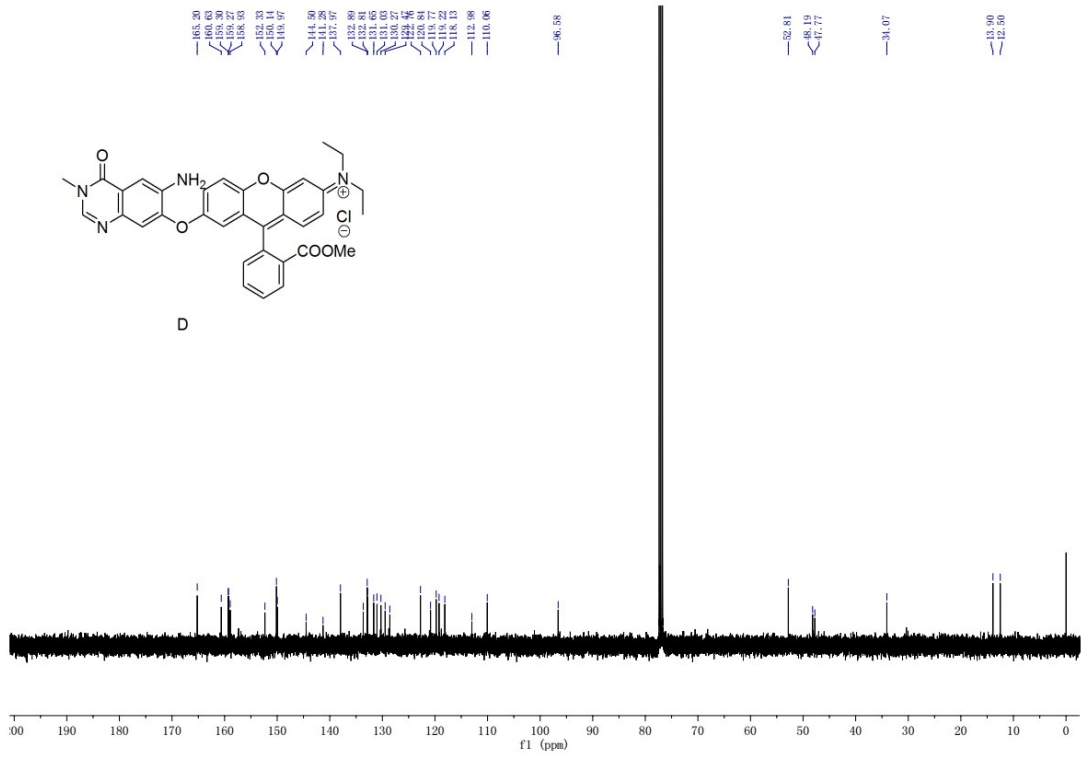


Figure S20. ^{13}C NMR spectra of **D** in $CDCl_3$

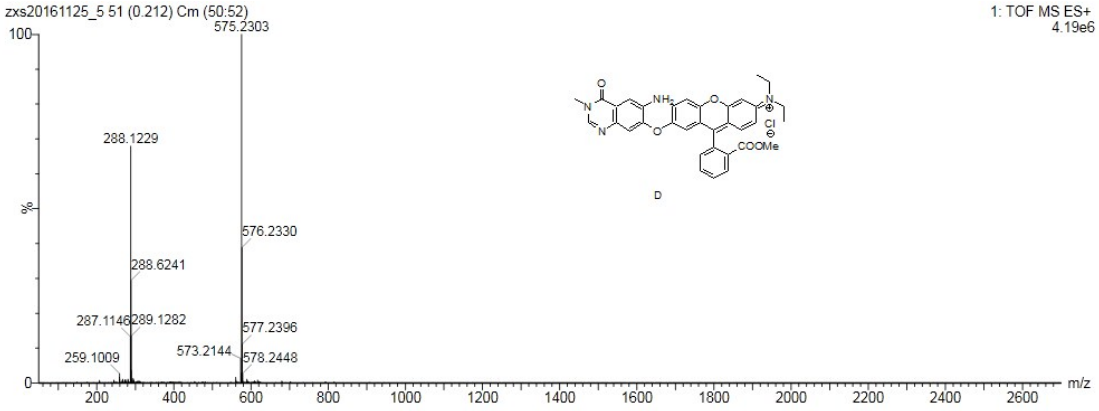


Figure S21. HRMS spectra of **D**

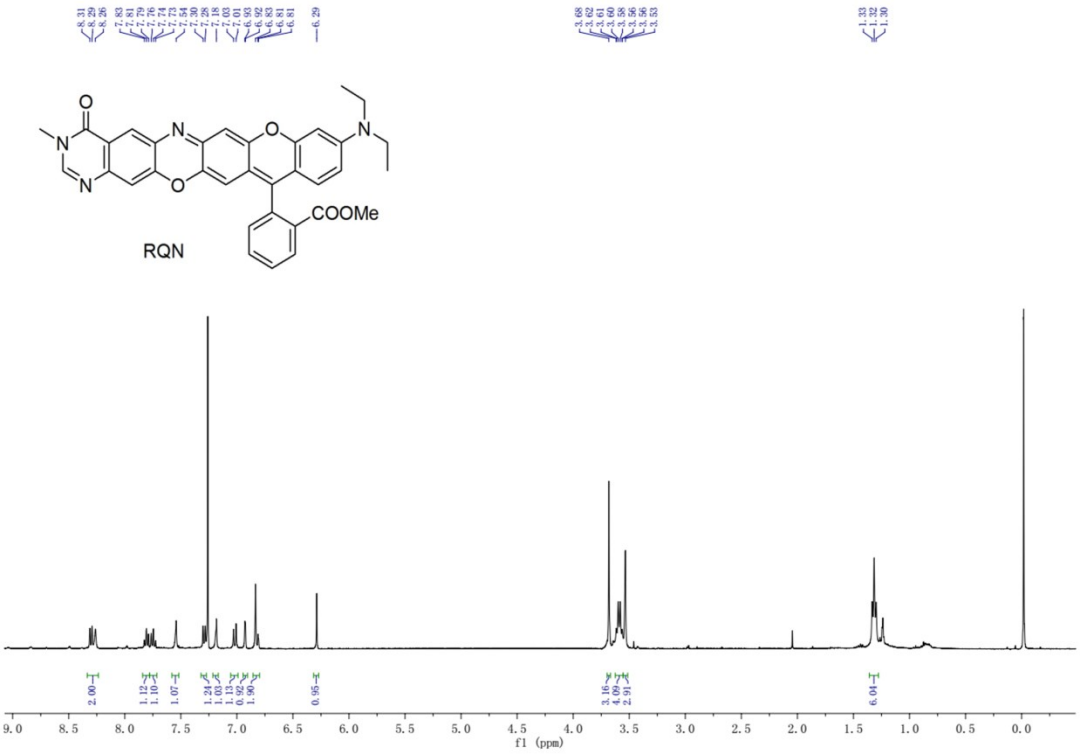


Figure S22. ^{1}H NMR spectra of **RQN** in $CDCl_3$

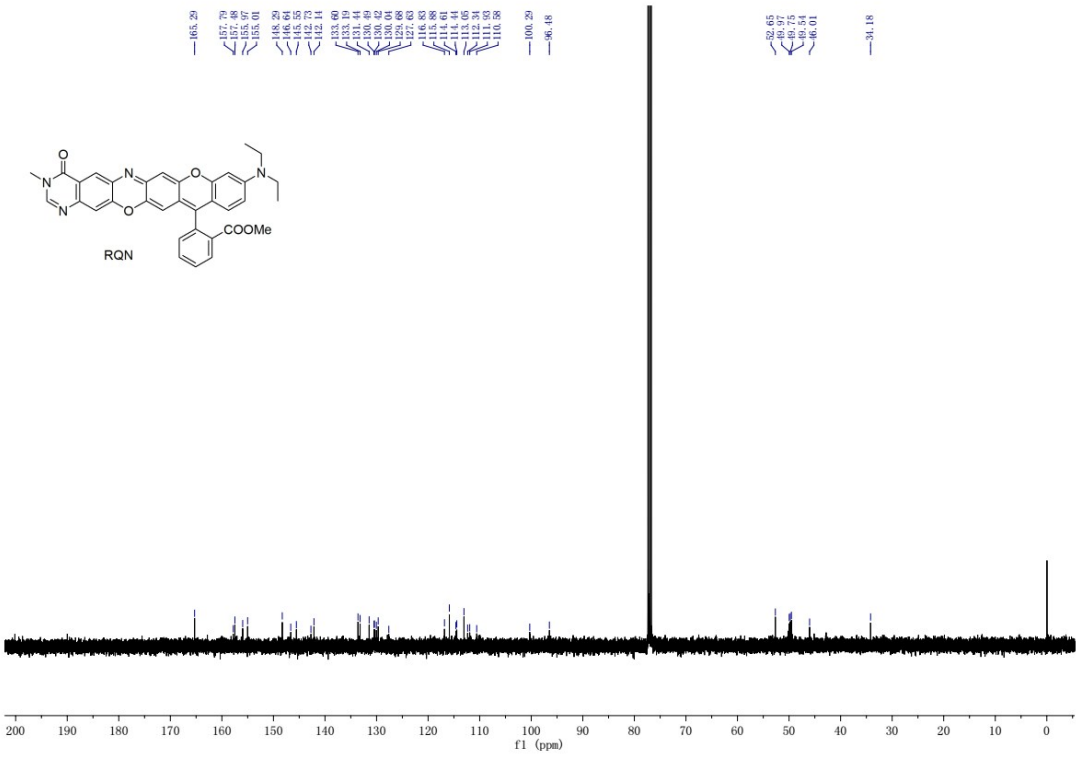


Figure S23. ^{13}C NMR spectra of **RQN** in $CDCl_3$

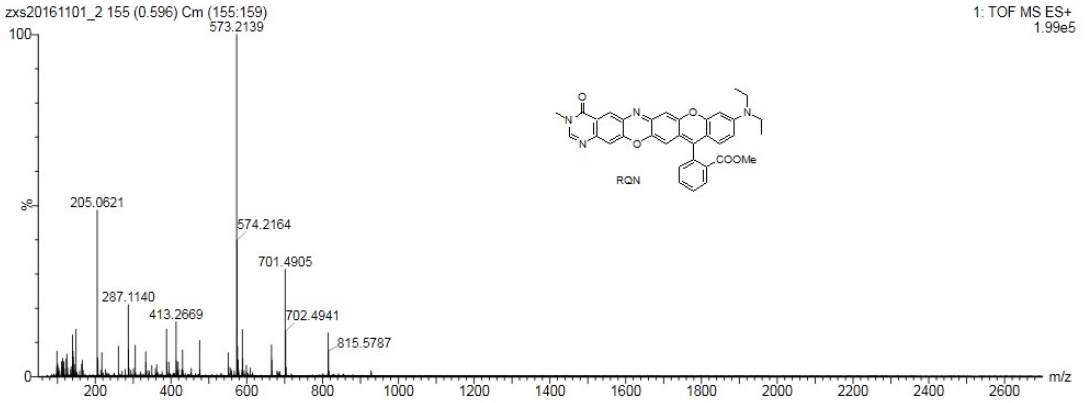


Figure S24. HRMS spectra of **RQN**

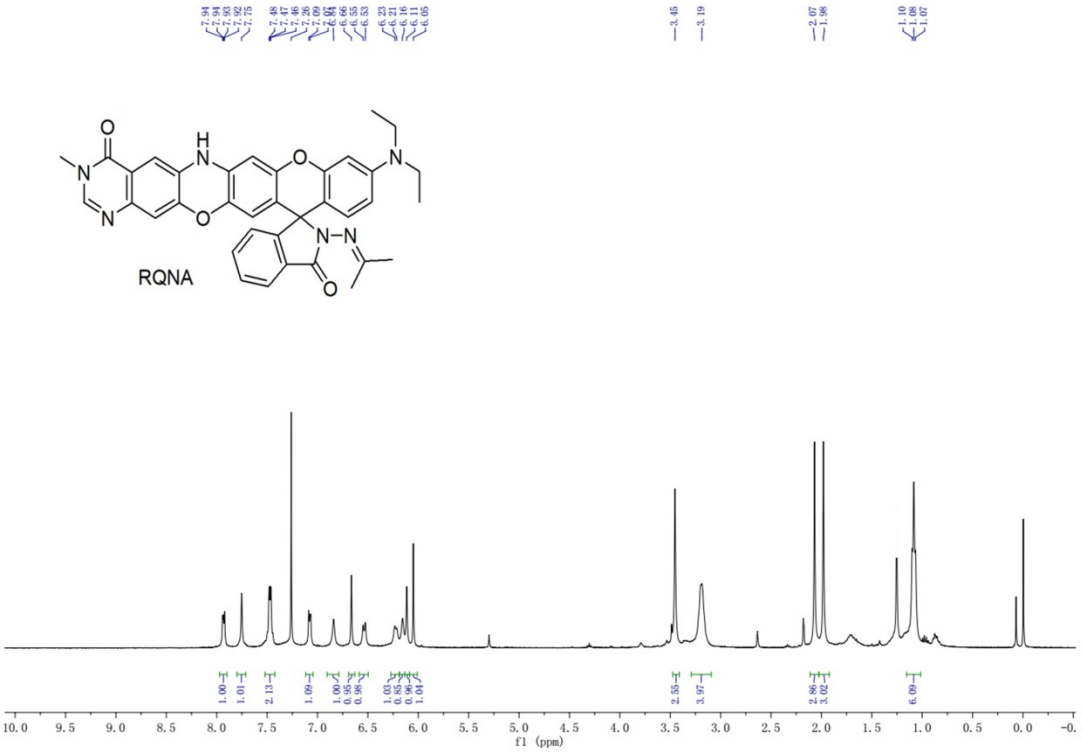


Figure S25. ^{1}H NMR spectra of **RQNA** in $CDCl_3$

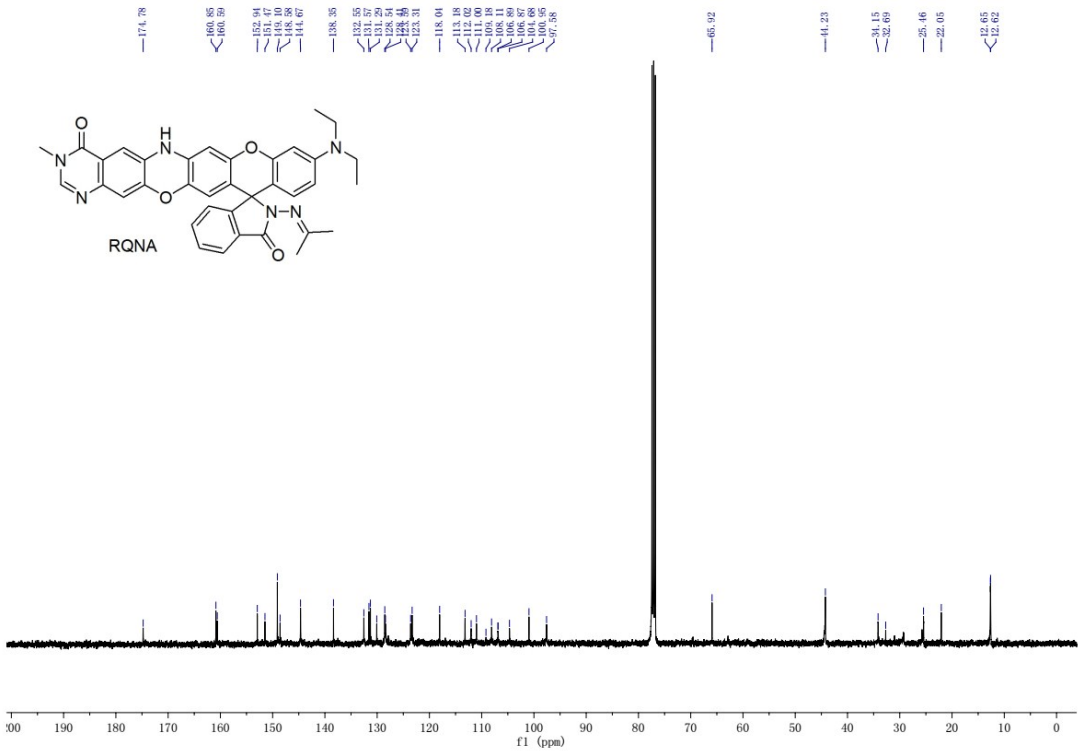


Figure S26. ^{13}C NMR spectra of **RQNA** in $CDCl_3$

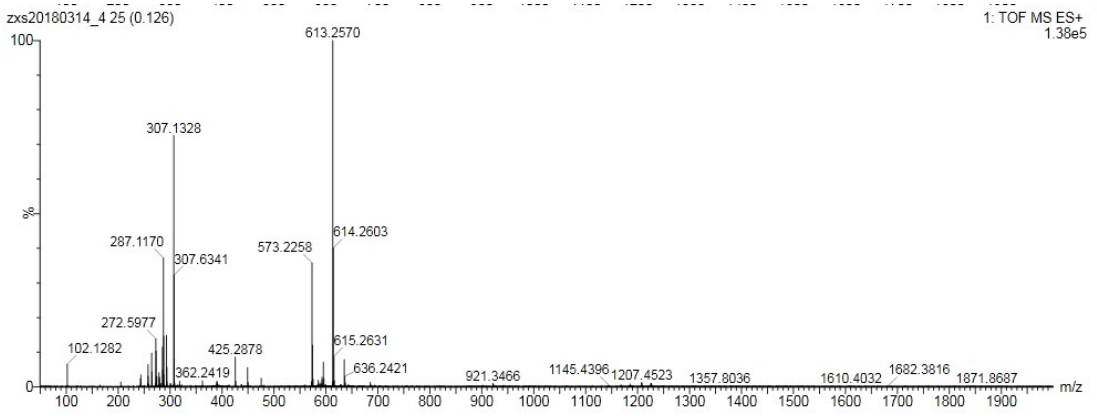


Figure S27. HRMS of **RQNA**

Reference:

1. R. Sens, K. H. Drexhage, *J. Luminesc.*, 1981, **24**, 709.