Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting information

Highly selective and sensitive optical probe for Fe^{3+} base on a well water-soluble squarylium dye

Zongguang Xu[a], Mengying Jiang[b], Chen Zhang[a], Jinfeng Mei[c], Zhongyu Li[a,b,c*], Song Xu[a], Liping Wang[c*]

[a] *Jiangsu Key Laboratory of Advanced Catalytic Materials and Technology, School of Petrochemical Engineering, Changzhou University, Changzhou 213164, PR China*

[b] *Advanced Catalysis and Green Manufacturing Collaborative Innovation Center, Changzhou University, Changzhou 213164, PR China*

[c] *School of Environmental and Safety Engineering, Changzhou University, Changzhou 213164, PR China*

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* Corresponding author. Tel.: +86-519-86334771; Fax: +86-519-86334771

E-mail address: zhongyuli@mail.tsinghua.edu.cn; wlp@cczu.edu.cn

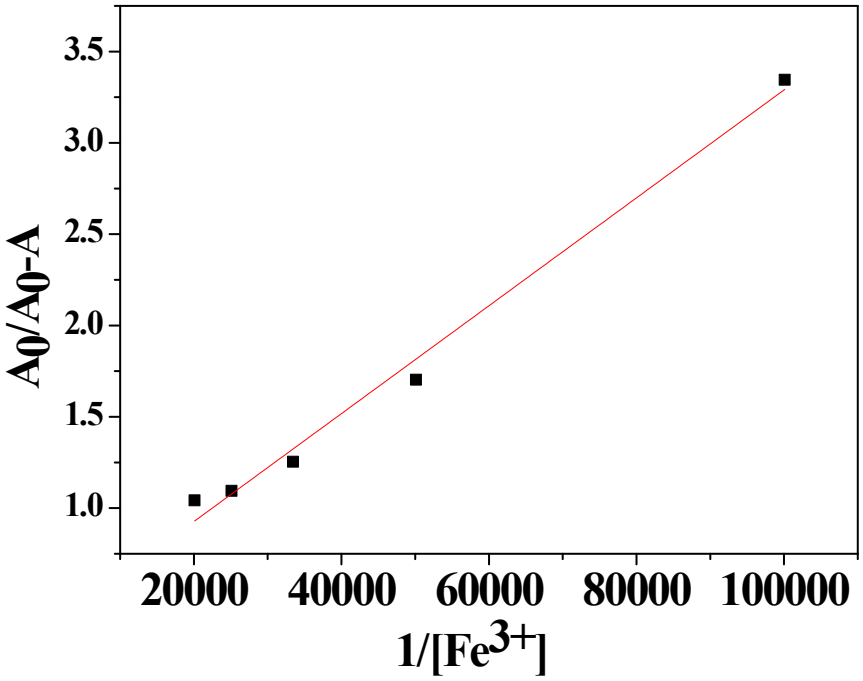


Fig. S1. Benesi-Hildebrand plot (absorbance at 636 nm) derived from $[A_0/(A_0-A)]$ as a function of the $1/[Fe^{3+}]$.

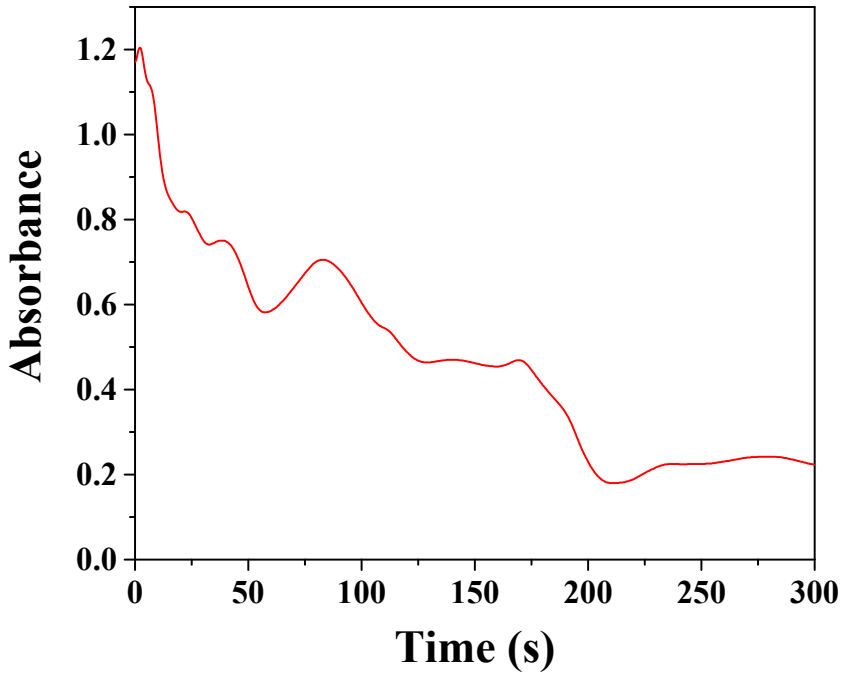


Fig. S2. Absorbance of **SQ** at 636 nm (1ml, 2.0×10^{-5} M) in deionized water upon the

addition of Fe^{3+} (9.98 μM) after a period of time.

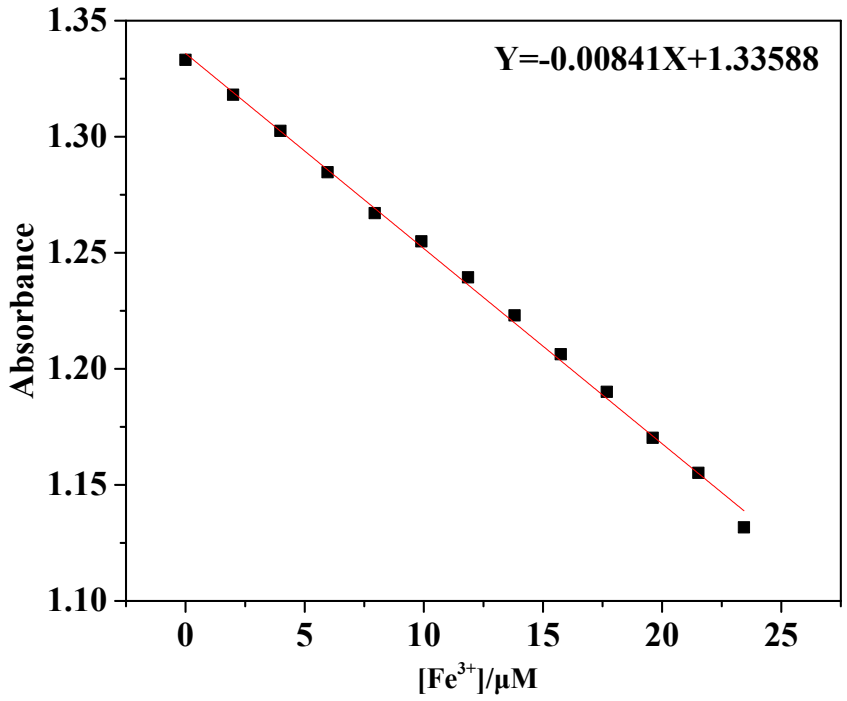


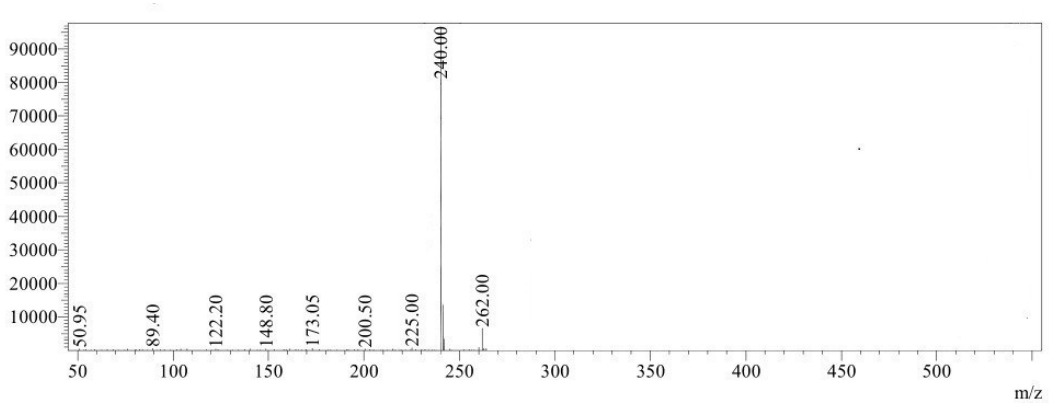
Fig. S3. Plot of the absorbance of SQ +Fe^{3+} at 636 nm in deionized water with Fe^{3+} ranging from 0 to 23.4375 μM

The result of the analysis as follows:

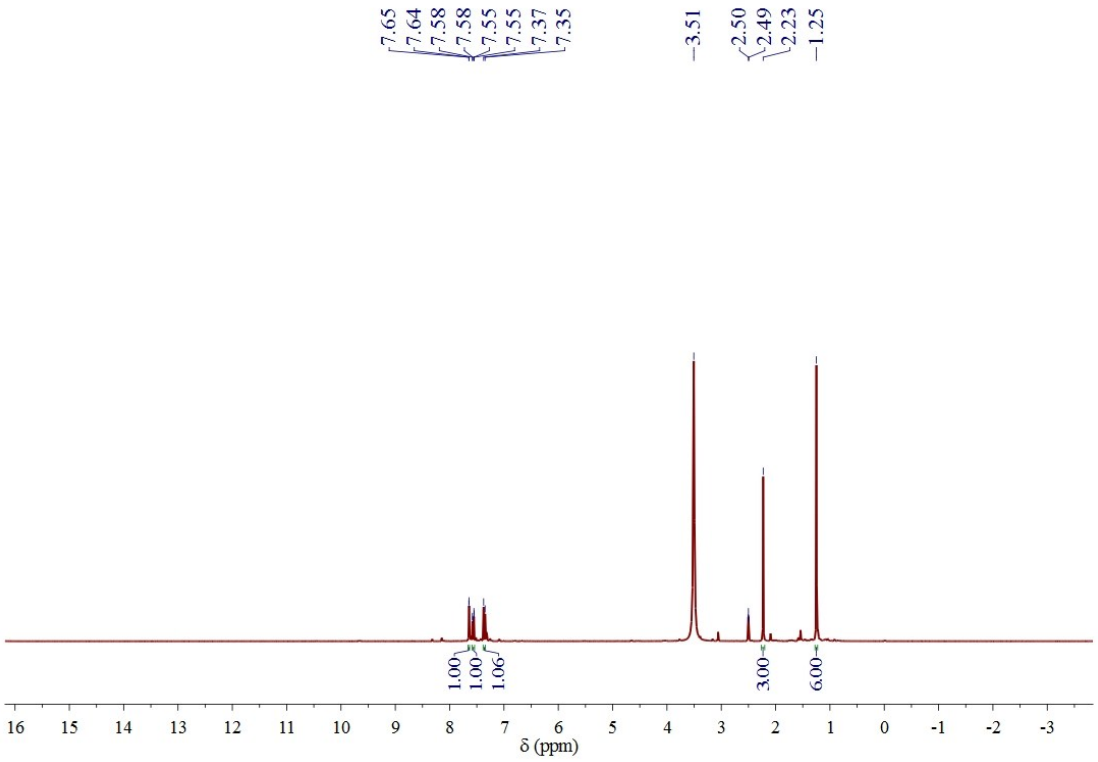
Linear Equation: Y= -0.00841×X+1.33588 R = 0.99912

$\delta=\sqrt{\frac{\sum\left(A_0-\overline{A_0}\right)^2}{N-1}}$ = 0.011398 (N=20) K=3

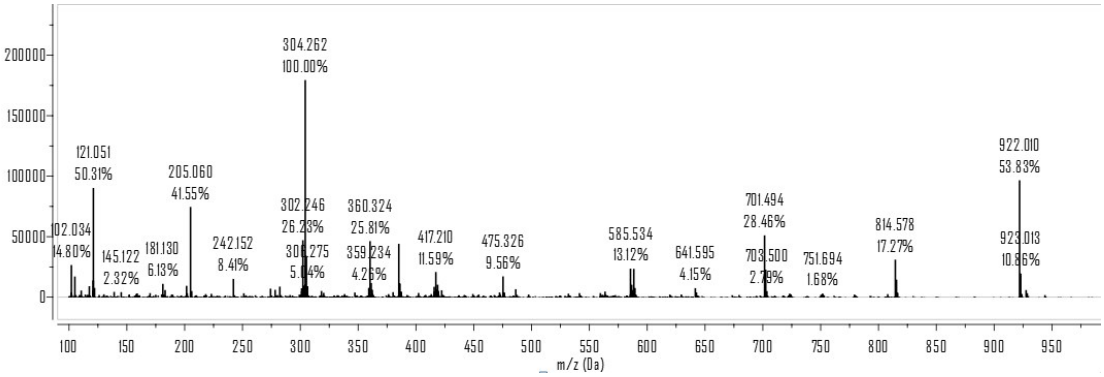
LOD = K × δ / S = 4.03×10^{-6} M



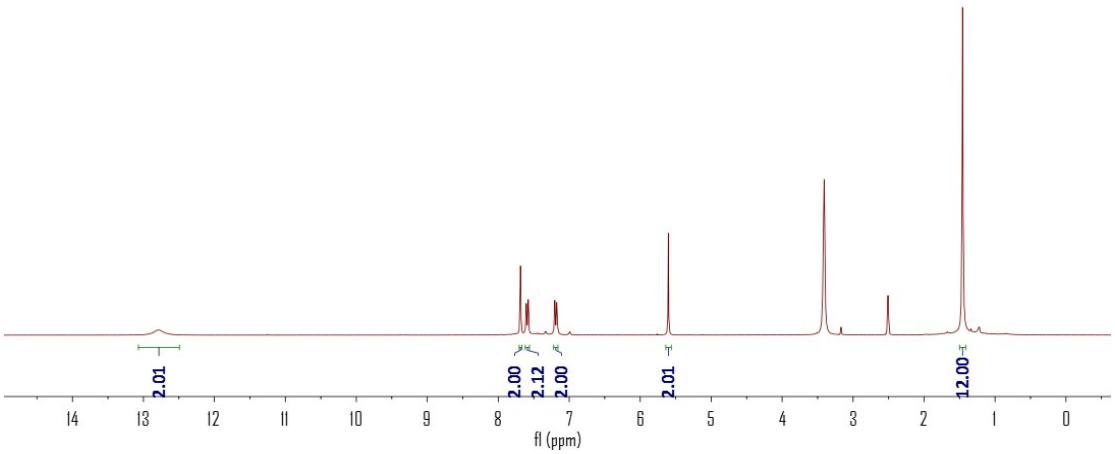
ESI-MS spectrum of **Compound 1**



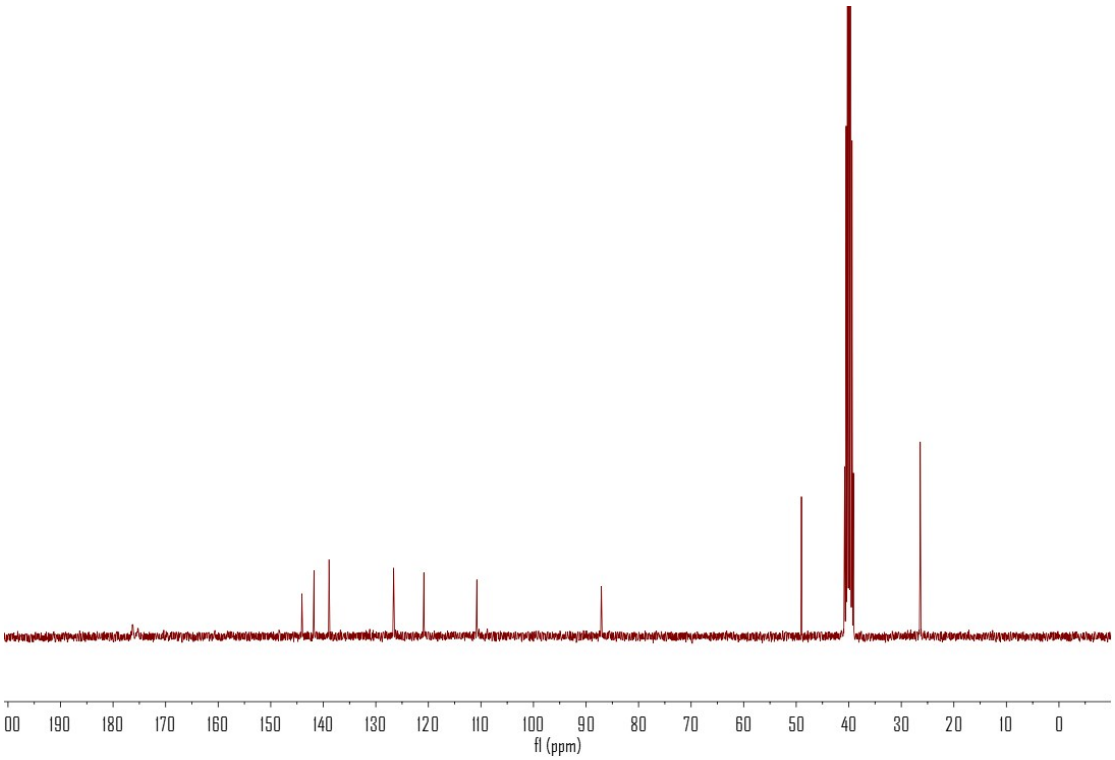
^{1}H NMR spectrum of **Compound 1**



HRMS spectrum of **Compound 2** (**SQ**)



^{1}H NMR spectrum of **Compound 2 (SQ)**



^{13}C NMR spectrum of **Compound 2 (SQ)**

Table 1. Fluorescence Quantum Yields at Their Excitation Wavelengths

sample	A/λ_{max} (nm)	Fluorescence intensity/emission wavelength (nm)	F/emission wavelength (nm)	Y/fluorescence quantum yield
RhB	0.0989 / 554	175 / 573	8218 / 573	0.31
SQ	0.0878 / 636	431 / 659	18183 / 659	0.7726

The calculation for a sample that needs to be measured is

$$Y_u = Y_s (F_u/F_s) (A_s/A_u)$$

The value of the fluorescence quantum yield of **SQ** is 0.7726 by calculating.

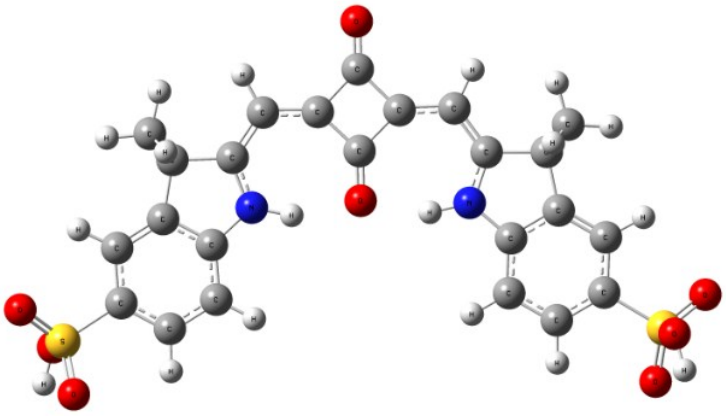


Fig. S4. B3LYP optimized geometries of **SQ**.

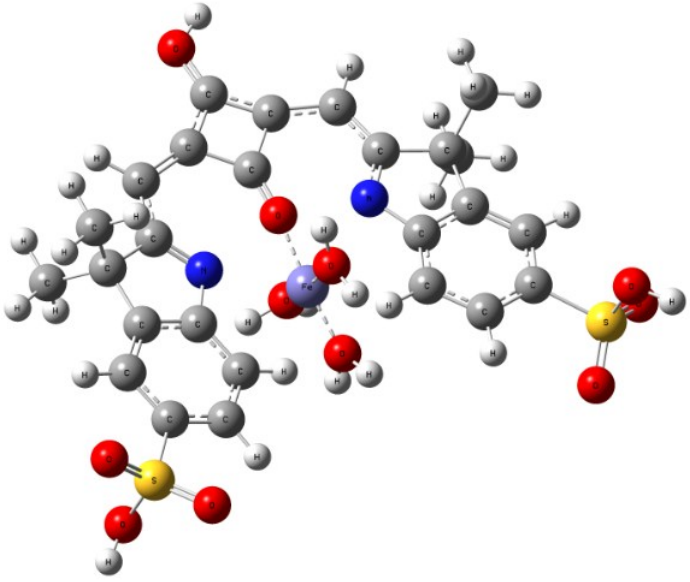


Fig. S5. B3LYP optimized geometries of [**SQ**-Fe^{3+}] complex.

Table 2. Absorbance and fluorescence emission of **SQ** in aqueous solution according to the density functional calculation, together with the experimental values.

Absorbance	**Excitation[a] (coeff)**	E_{nm} **(eV)**	**Oscillator**	**Exptl (nm)[b]**
S_1	H→L (0.70)	574 (2.15)	1.2374	636
S_3	H-2→L (0.54)	364 (3.39)	0.0079	
S_4	H→L+1 (0.53)	340 (3.63)	0.3217	
S_5	H-3→L (0.58)	331 (3.73)	0.0095	
S_7	H→L+3 (0.67)	321 (3.85)	0.0732	
Emission	L→H (0.70)	668 (1.85)	1.3334	659

Table 3. Absorbance of (**SQ-**Fe^{3+}**)** in aqueous solution according to the density functional calculation, together with the experimental values.

Absorbance	**Excitation[a] (coeff)**	E_{nm} **(eV)**	**Oscillator**	**Exptl (nm)[b]**
S_1	H-1→L (0.87)	537 (2.30)	0.8152	636

As shown in Table 3, the UV absorption wavelength was calculated to be 537 nm, and the fluorescence emission has not been successfully optimized due to the complex coordination structure between the compound (**SQ**) and the Fe^{3+}.