

Supporting Information

A Water Soluble Fluorescent Sensor for the Reversible Detection of Tin (IV) Ion and Phosphate Anion

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Determination of quantum yields

The quantum yield of DQS (Φ_0) and DQS-Sn⁴⁺ (Φ_1 , in the present of 5 equiv of Sn⁴⁺ ions) were determined according to the literature.¹

$$\Phi_{Sample} = \frac{\Phi_{QS} \cdot A_{QS} \cdot F_{Sample} \cdot \lambda_{exQS} \cdot \eta_{Sample}^2}{A_{Sample} \cdot F_{QS} \cdot \lambda_{exSample} \cdot \eta_{QS}^2}$$

Where Φ is quantum yield; A is absorbance at the excitation wavelength; F is integrated area under the corrected emission spectra; λ_{ex} is the excitation wavelength; η is the refractive index of the solution; the Sample and QS refer to the sample and the standard, respectively. We chose quinine sulfate in 0.1N H₂SO₄ as standard, which has the quantum yield of 0.546.²

Other Photophysical properties of DQS

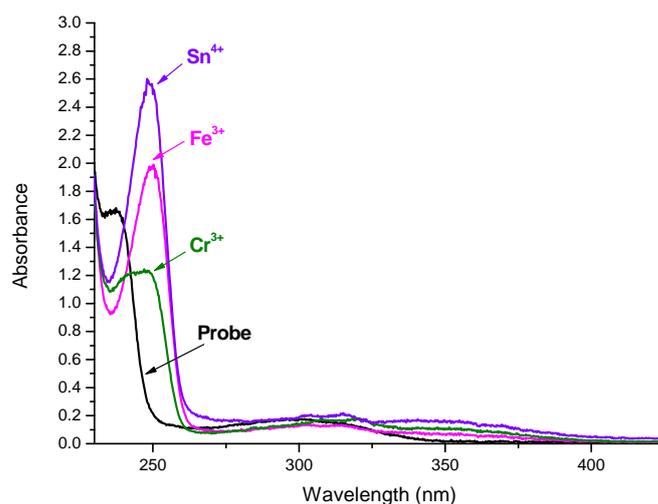


Figure S1. Absorption spectra of DQS (10 μM) in water solution in the present of Sn⁴⁺, Fe³⁺, and Cr³⁺ (1 equiv), respectively.

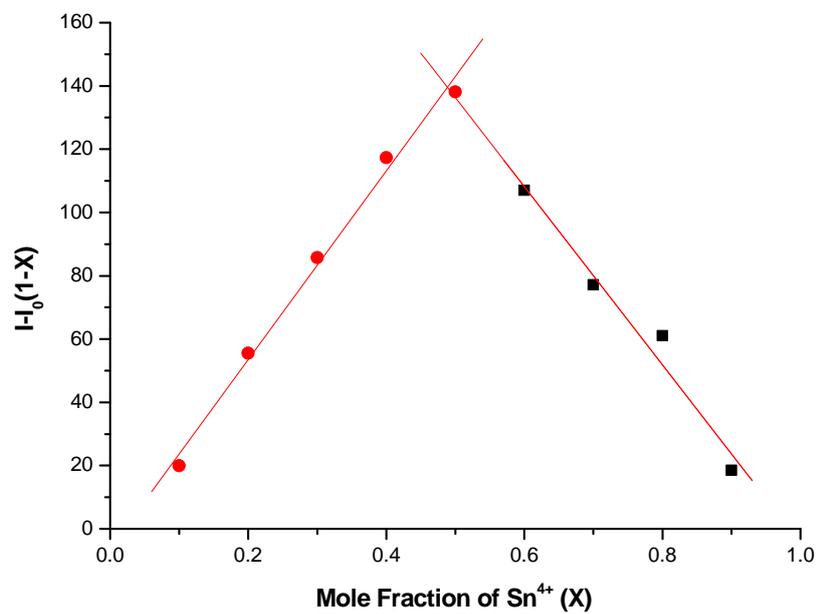


Figure S2. Job's plot of sensor **DQS**, the total concentration of the sensor and Sn^{4+} is $25.0 \mu\text{M}$.

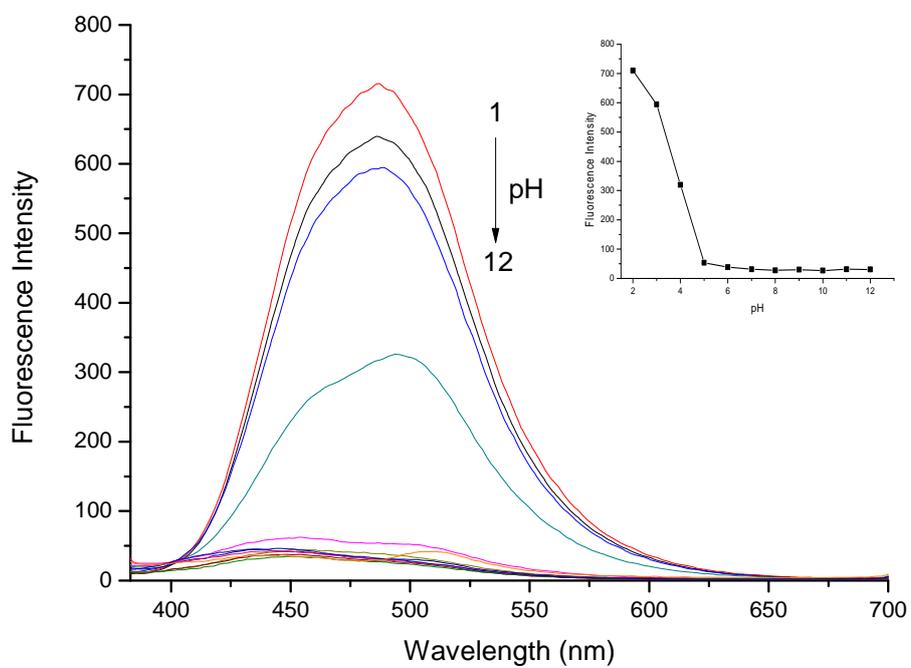


Figure S3. Effect of the pH on the fluorescence emission of **DQS** ($5.0 \mu\text{M}$).

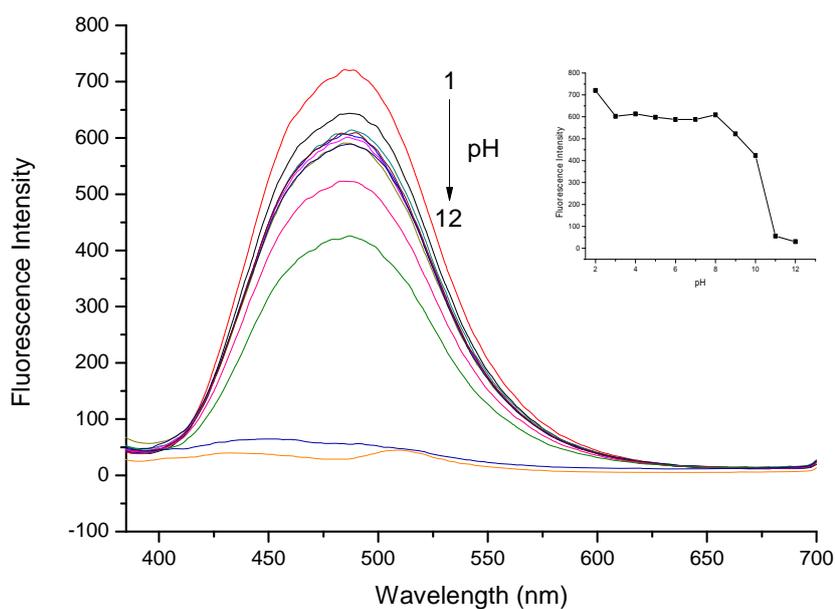


Figure S4. Effect of the pH on the fluorescence emission of **DQS-Sn⁴⁺** complex (5.0 μM of **DQS** in the present of 20 equiv of **Sn⁴⁺**).

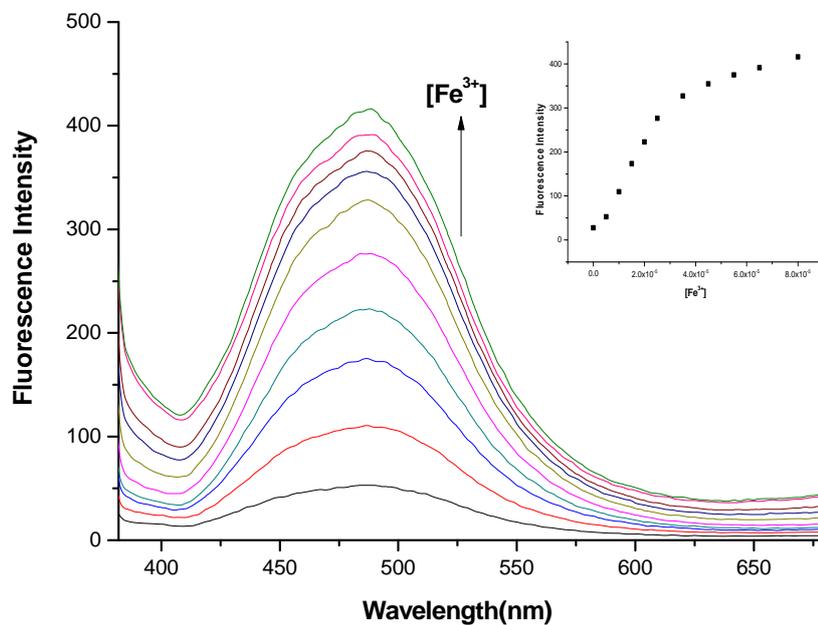


Figure S5. Fluorescence spectra of **DQS** (5 μM) in water in the presence of different concentrations of Fe^{3+} (0-90 μM) ($\lambda_{\text{ex}} = 360 \text{ nm}$). Inset: fluorescence intensity changes as a function of Fe^{3+} concentration.

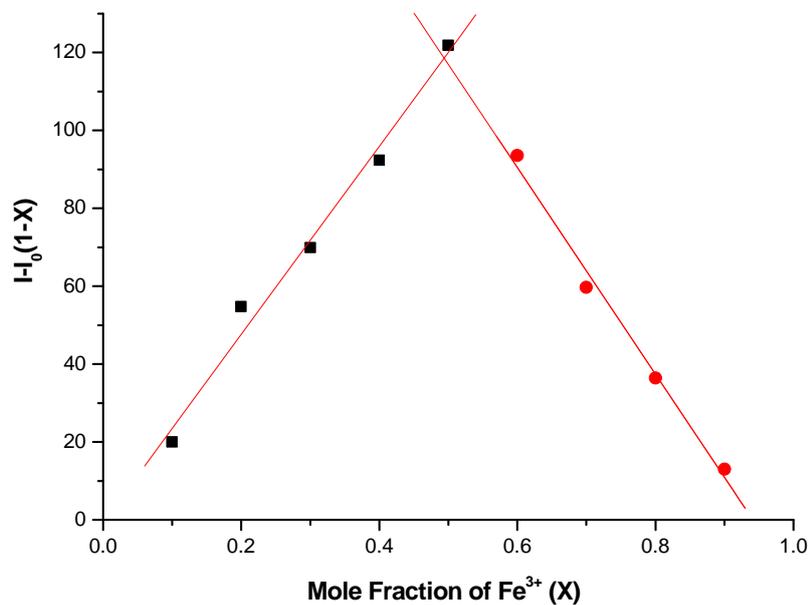


Figure S6. Job's plot of sensor **DQS**, the total concentration of the sensor and Fe^{3+} is $25.0 \mu\text{M}$.

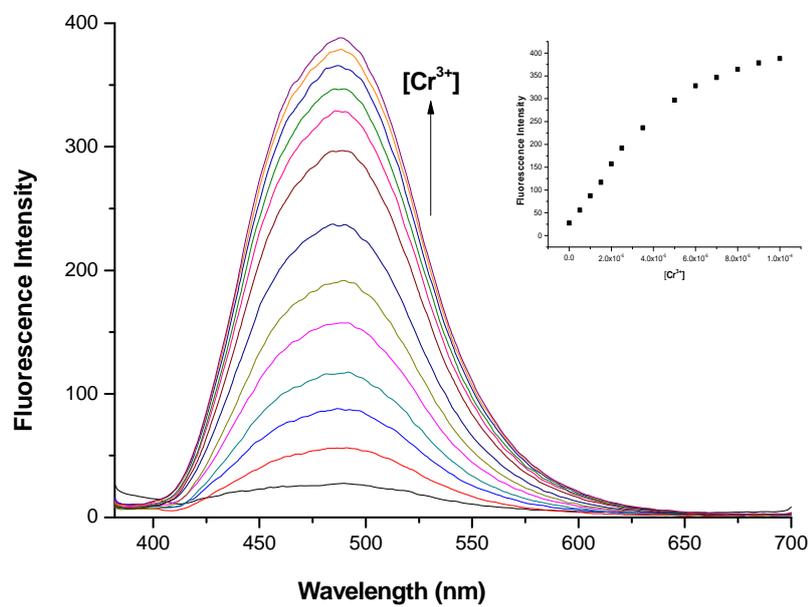


Figure S7. Fluorescence spectra of **DQS** ($5 \mu\text{M}$) in water in the presence of different concentrations of Cr^{3+} (0-100 μM) ($\lambda_{\text{ex}} = 360 \text{ nm}$). Inset: fluorescence intensity changes as a function of Cr^{3+} concentration.

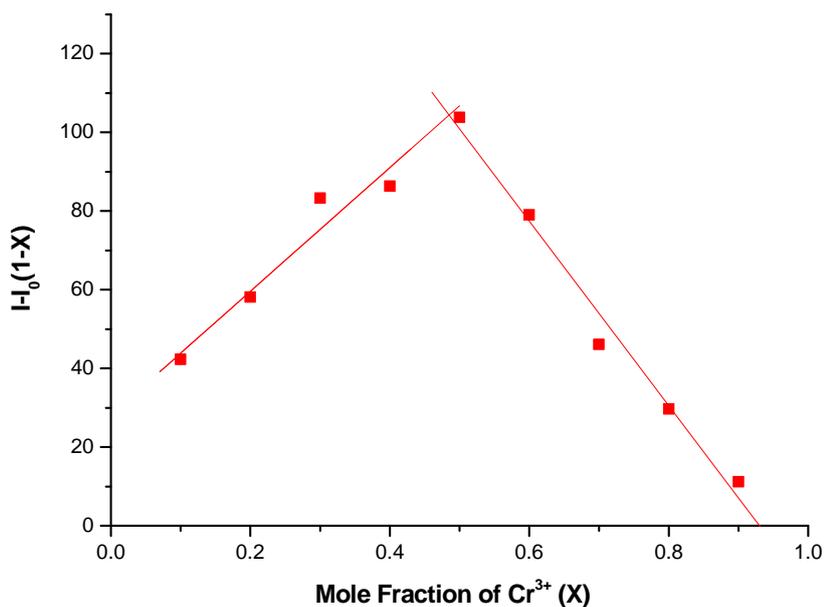


Figure S8. Job's plot of sensor **DQS**, the total concentration of the sensor and Cr^{3+} is $25.0 \mu\text{M}$.

Determination of the binding constant

The apparent binding constant (K_S) of **DQS** with Sn^{4+} was determined using the nonlinear least-squares analysis base on a 1:1 complex expression:³

$$\frac{F}{F_0} = 1 + \left(\frac{F_{\max}}{2F_0} - \frac{1}{2} \right) \left[1 + \frac{C_M}{C_L} + \frac{1}{K_S C_L} - \sqrt{\left(1 + \frac{C_M}{C_L} + \frac{1}{K_S C_L} \right)^2 - 4 \frac{C_M}{C_L}} \right]$$

Where F_0 or F is the fluorescence emission intensities in the absence or presence of Sn^{4+} ions, C_M and C_L are the concentrations of Sn^{4+} and **DQS**, and K_S is the stability constant.

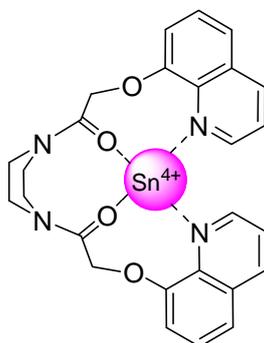
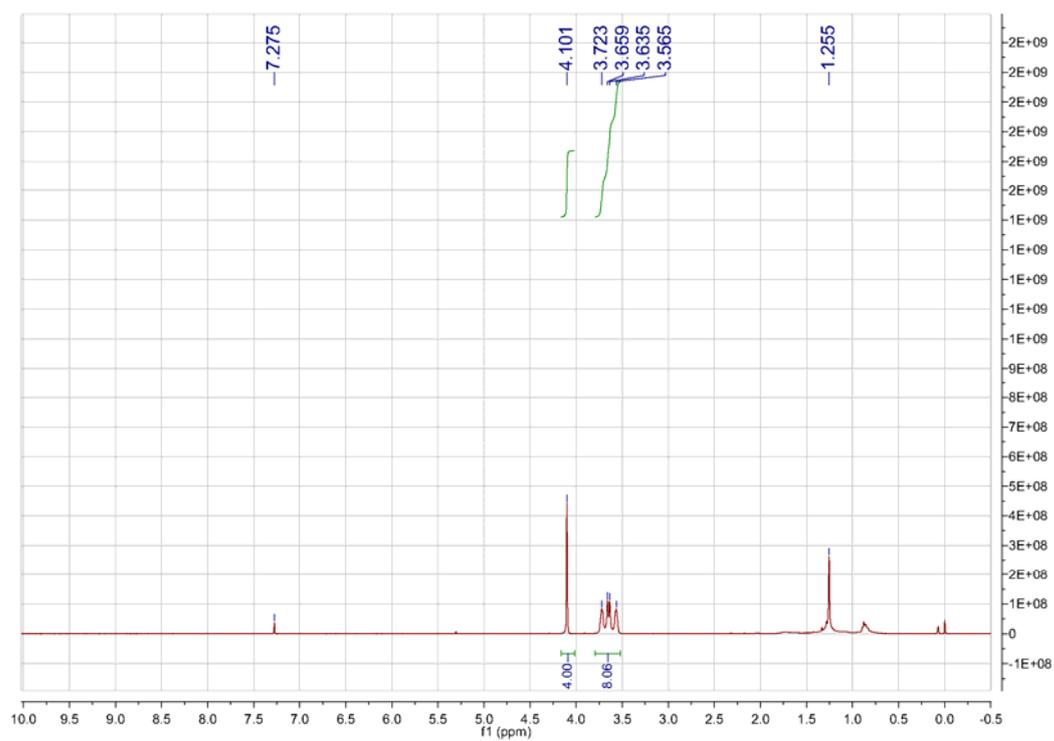


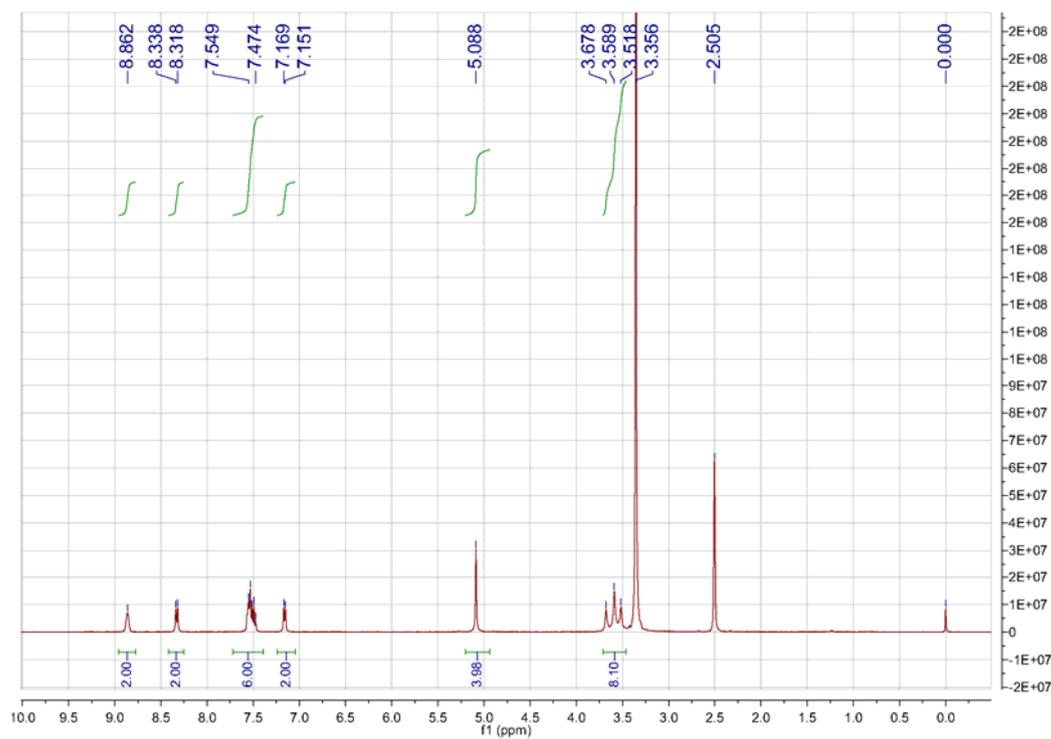
Figure S9. A proposed structure of **DQS-Sn⁴⁺** complex.

The characterization data of all compounds

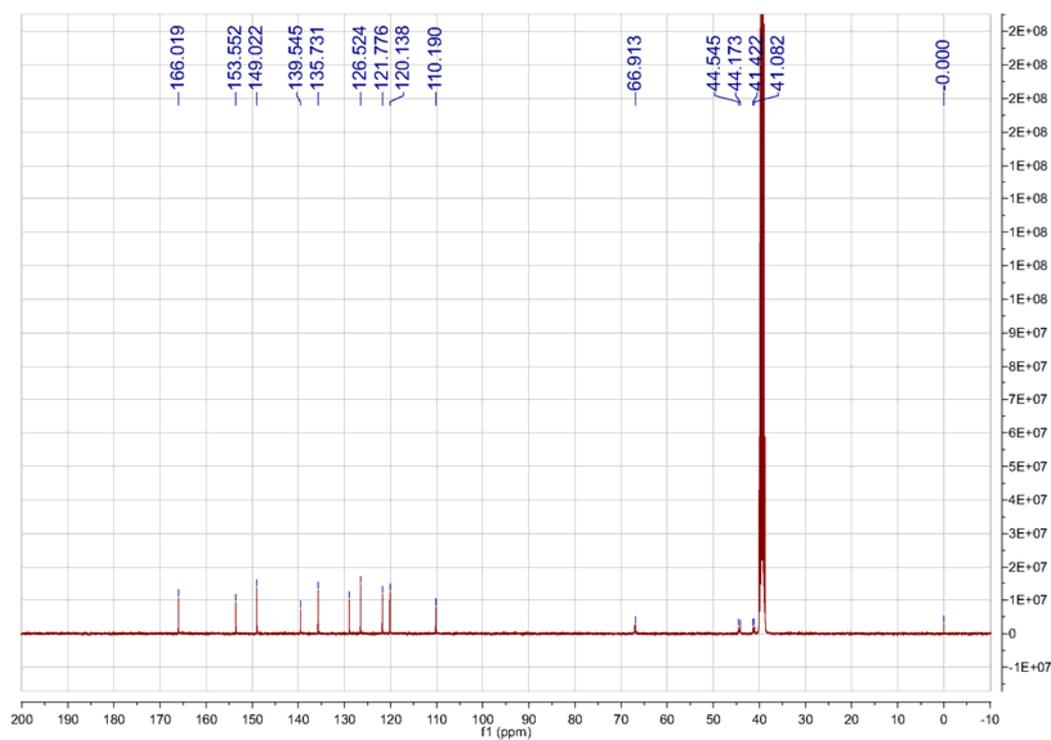
¹H NMR of compound **1**



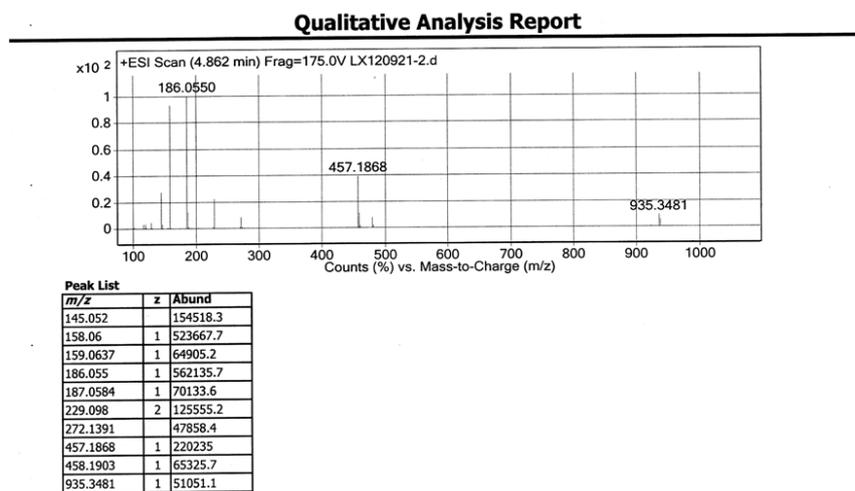
^1H NMR of compound **2** (DQS)



^{13}C NMR of compound **2** (DQS)



HRMS of compound 2 (DQS)



References

- (1) Velapoldi, R. A.; Tønnesen, H.; *H. J. Fluoresc.* **2004**, *14*, 465-472.
- (2) Eaton, D. F. *Pure Appl. Chem.* **1988**, *60*, 1107-1114.
- (3) Valeur, B. *Molecular Fluorescence Principle and Applications*; Wiley-VCH Verlag GmbH: New York, 2001.