Supporting Information

A Highly Sensitive and Selective Fluorescent Chemosensor for Pb^{2+} Ion in Aqueous Solution

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Photophysical properties of the sensors

Table S1. Photophysical properties of the sensors.

entry	$\lambda_{ab\ (nm)}$	$\lambda_{em\ (nm)}$	Φ_0[a]	Φ_1[a]	ε / M^{-1} cm^{-1}
LS3	497	508	0.005	0.005	28150
LS2	497	508	0.006	0.014[b]	34820
LS1	497	510	0.006	0.112[c]	40380

(a) The quantum yield of the sensor (Φ_0) and the sensor-Pb^{2+} (Φ_1) were determined according to the literature.[2] (b) Φ_1 was determined in the present of 100 equiv of Pb^{2+} ions. (c) Φ_1 was determined in the present of 2 equiv of Pb^{2+} ions.

$$\Phi_S = \frac{\Phi_B I_S A_B \lambda_{exB} \eta_S}{I_B A_S \lambda_{exS} \eta_B}$$

Where Φ is quantum yield; I is integrated area under the corrected emission spectra; A is absorbance at the excitation wavelength; λ_{ex} is the excitation wavelength; η is the refractive index of the solution; the S and B refer to the sample and the standard, respectively. We chose fluorescein in 0.1 M NaOH as standard, which has the quantum yield of 0.95.[1]

Emission spectra, competition experiment, and Job's plot of sensor LS2

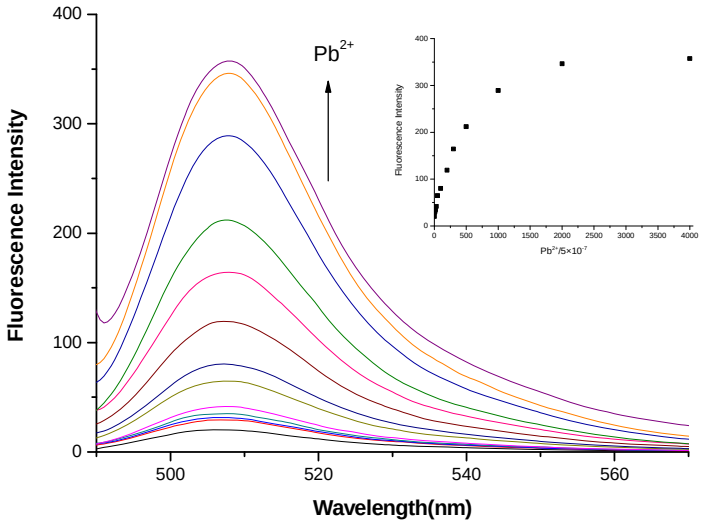


Figure S1. Emission spectra (λ_{ex} = 470 nm) of **LS2** (0.5 μM) in phosphate (0.1 M) solution (pH = 7.2) in the presence of different concentrations of Pb^{2+} ions. The up-arrow indicates the increase of [Pb^{2+}] from 0 to 3 mM. Inset: Binding isotherm between **LS2** and Pb^{2+} with emission intensity at 510 nm.

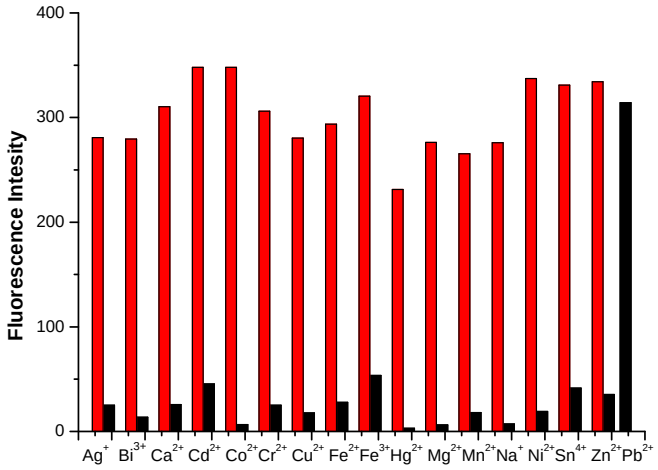


Figure S2. Fluorescence responses of **LS2** to various metal ions (0.1 M PBS, pH 7.2). Black bars represent the addition of 5.0 equiv of the appropriate metal ion to a 5 μM solution of **LS2**. Red bars represent the addition of 5.0 equiv of Pb^{2+} to the solutions containing **LS2** and the appropriated metals.

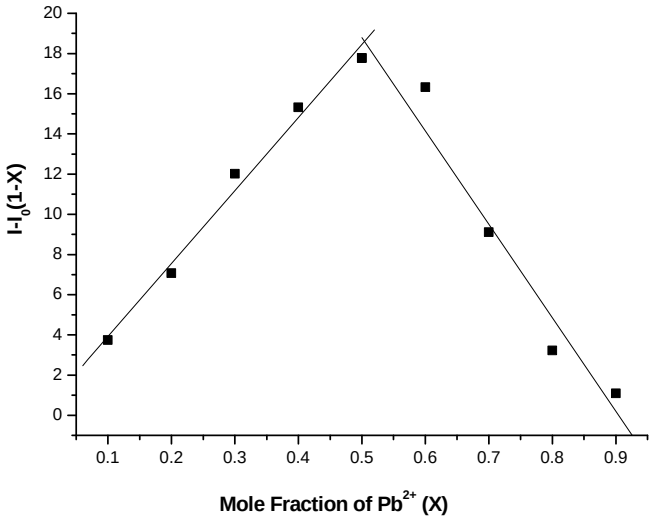


Figure S3. Job's plot of sensor **LS2** in 0.1 M phosphate buffered water solution (pH = 7.2). The total concentration of the sensor and Pb^{2+} is 5.0 μM.

Determination of the association constant

The association constant K_S were determined by a nonlinear least-squares analysis of *I* versus c_M using the following equation:[2]

$$I = \frac{I_0 + c_M \Phi K_{11}[M] + I_{lim} K_S[M]^2}{1 + K_{11}[M] + K_S[M]^2}$$

Where $K_S = K_{11}K_{21}$

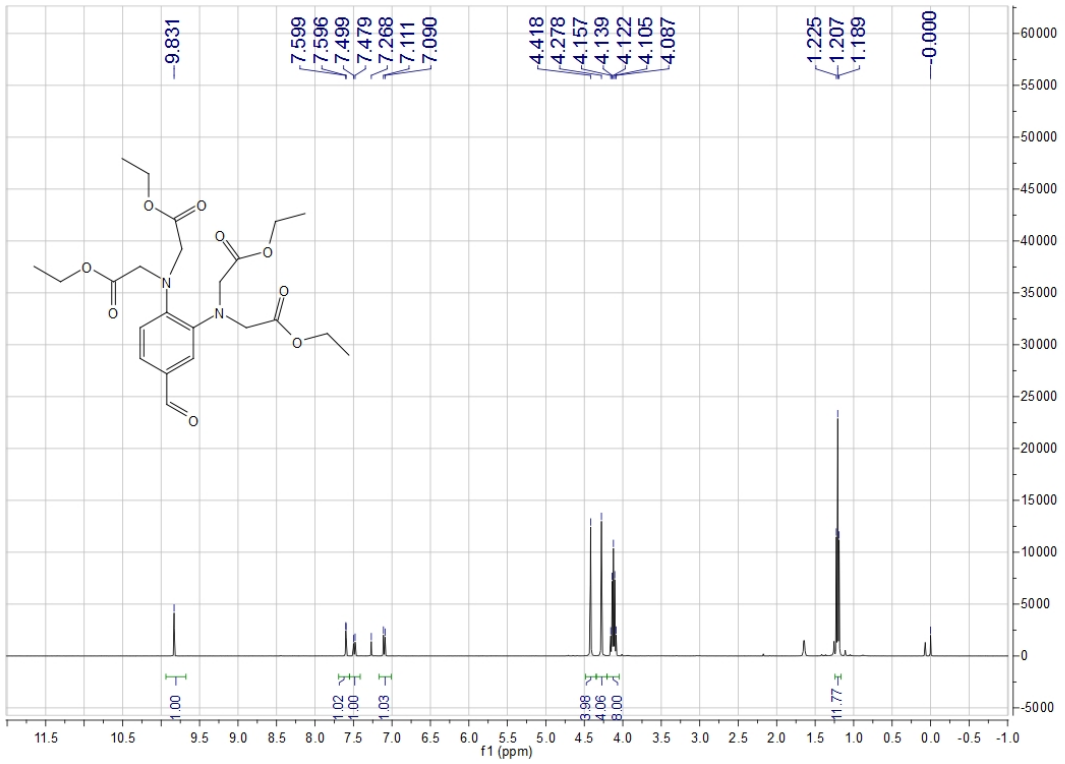
$$K_{11} = \frac{[LS1 \cdot Pb^{2+}]}{[LS1][Pb^{2+}]} \qquad LS1 + Pb^{2+} \rightleftharpoons LS1{\bullet}Pb^{2+}$$

$$K_{21} = \frac{[LS1 \cdot Pb^{2+}{}_2]}{[LS1 \cdot Pb^{2+}][Pb^{2+}]} \qquad LS1{\bullet}Pb^{2+} + Pb^{2+} \rightleftharpoons LS1{\bullet}Pb^{2+}{}_2$$

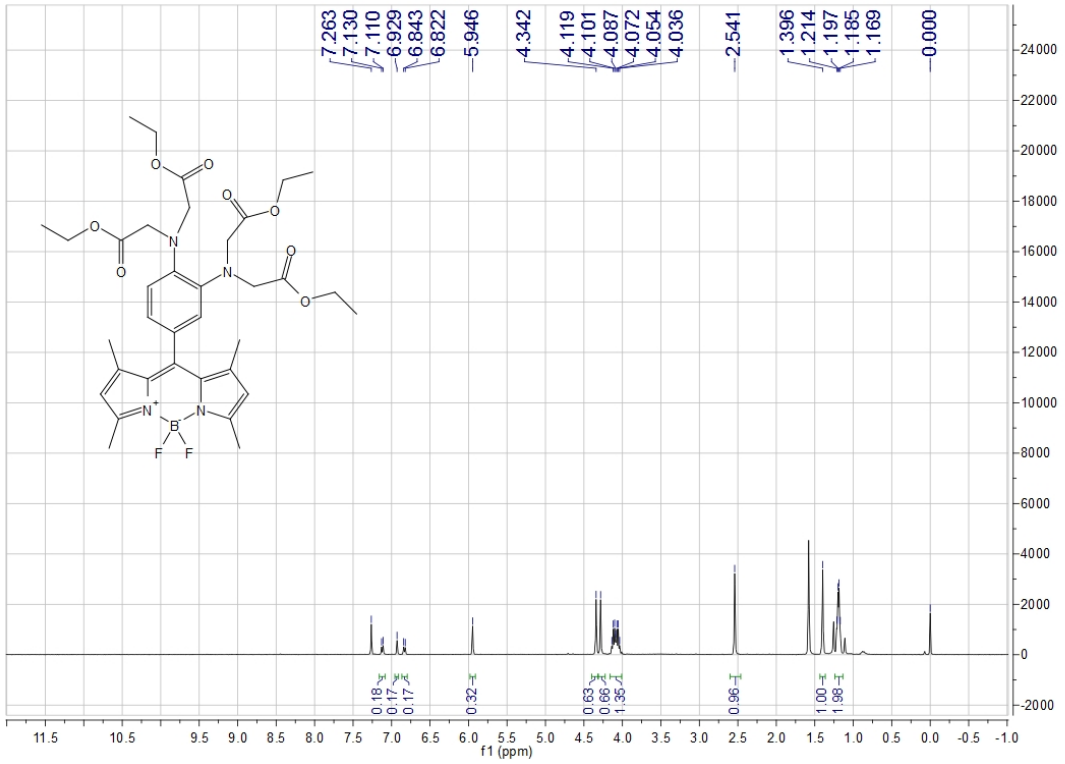
$[M] \approx c_M$ is Pb^{2+} ion concentration, I_0 or *I* is integrated emission in the absence or presence of Pb^{2+} ions, Φ is approximately substituted by 0.014, the quantum yield of the 1:1 **LS2**-Pb^{2+} complex, since the quantum yield of the 1:1 **LS1**-Pb^{2+} complex could not be precisely determined.

The characterization data of all compounds

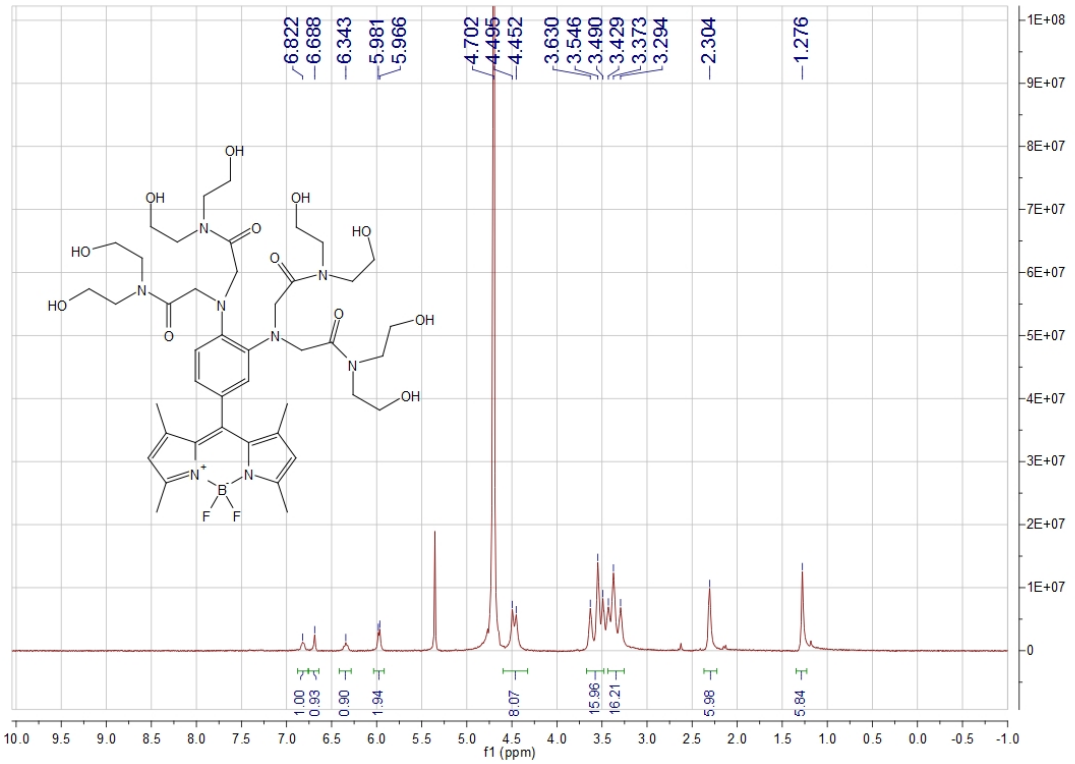
^{1}H NMR of compound **3**



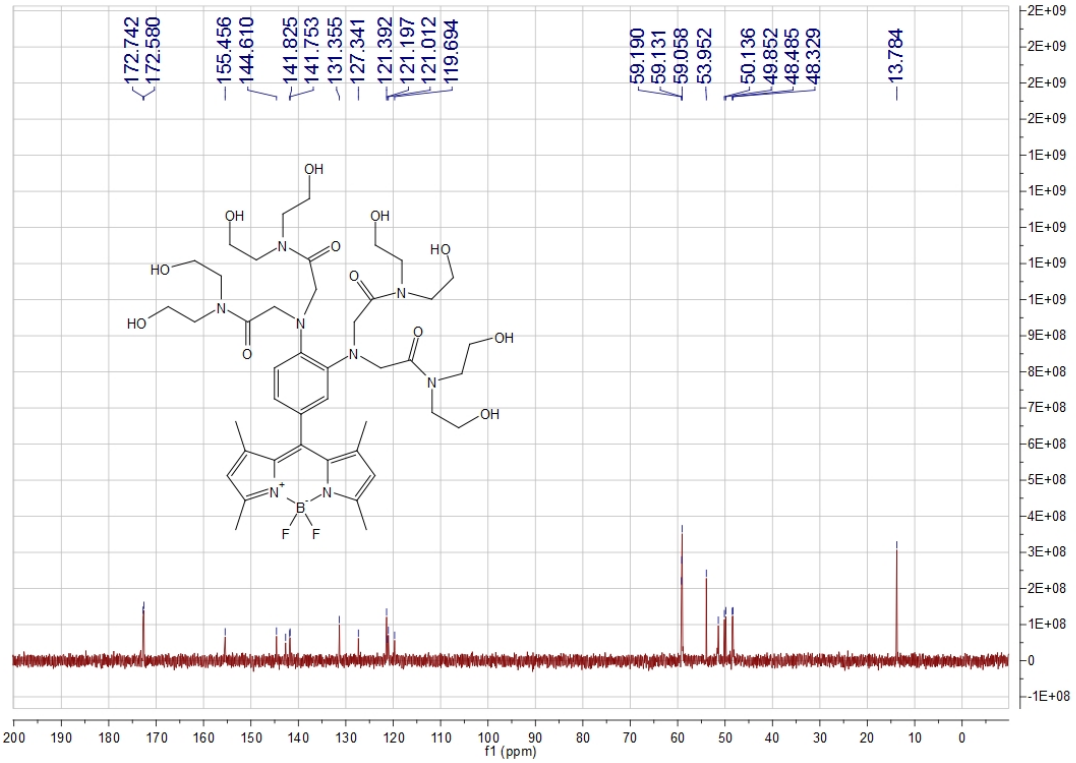
^{1}H NMR of compound **4**



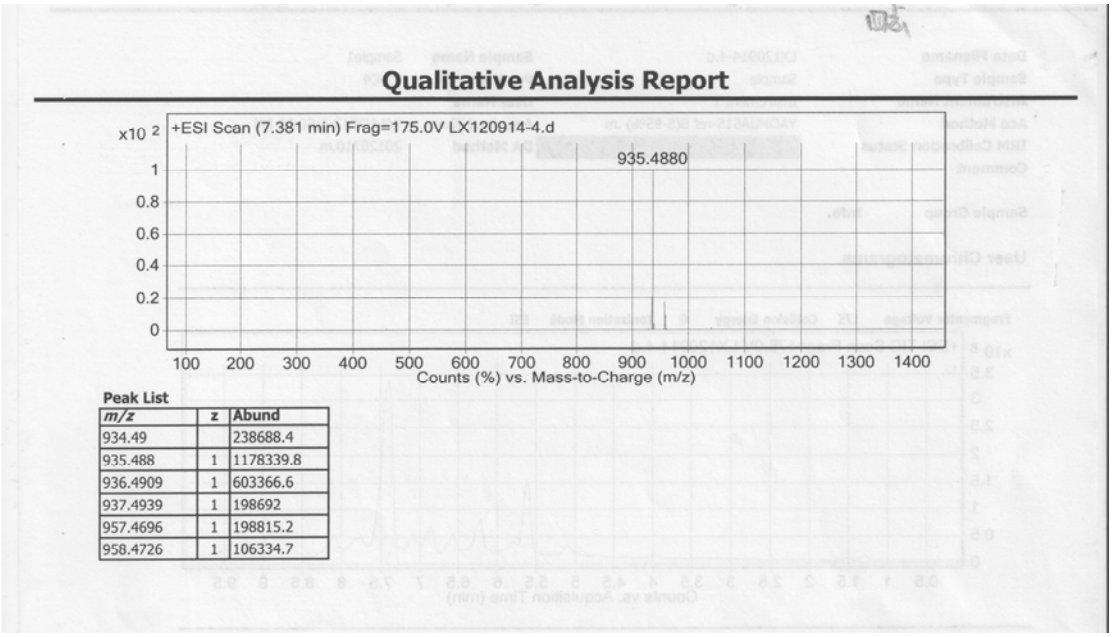
^{1}H NMR of compound **5** (**LS1**)



^{13}C NMR of compound **5** (**LS1**)



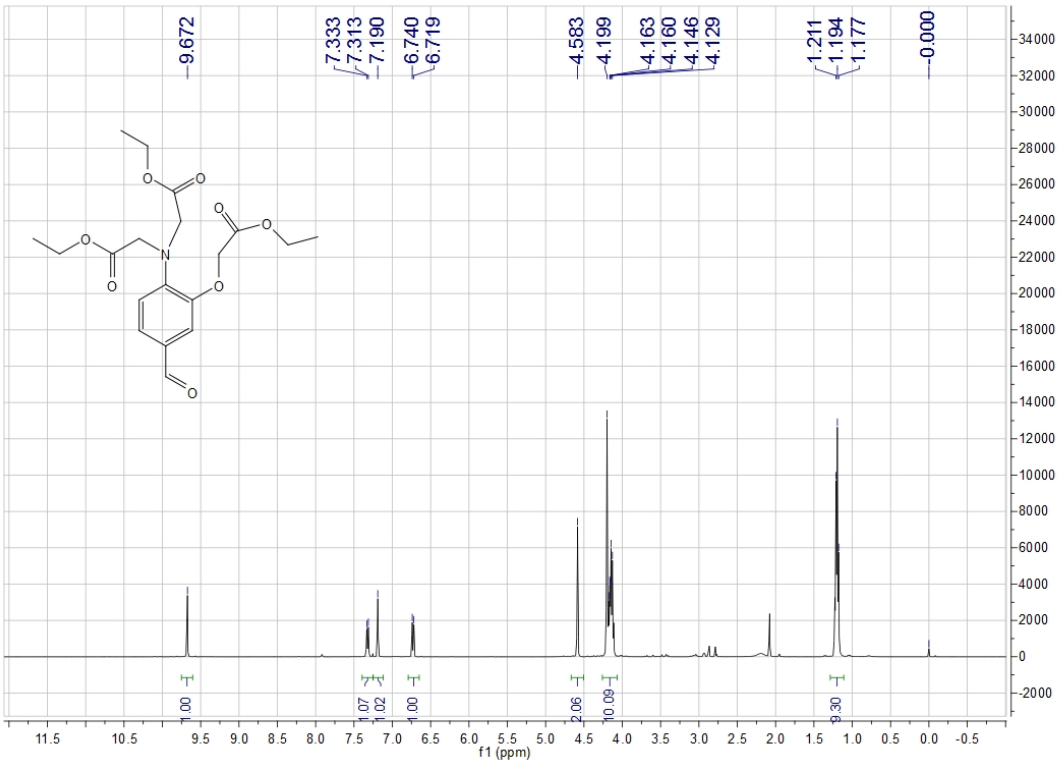
HRMS of compound **5** (**LS1**)



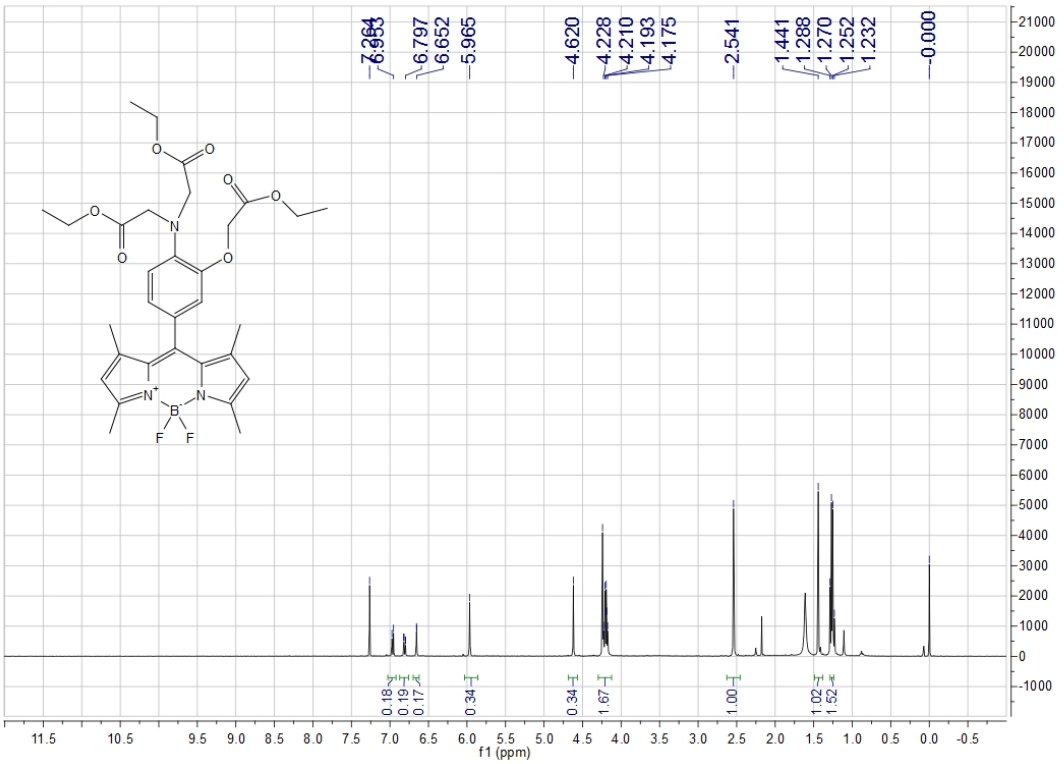
Peak List

m/z	z	Abund
934.49		238688.4
935.488	1	1178339.8
936.4909	1	603366.6
937.4939	1	198692
957.4696	1	198815.2
958.4726	1	106334.7

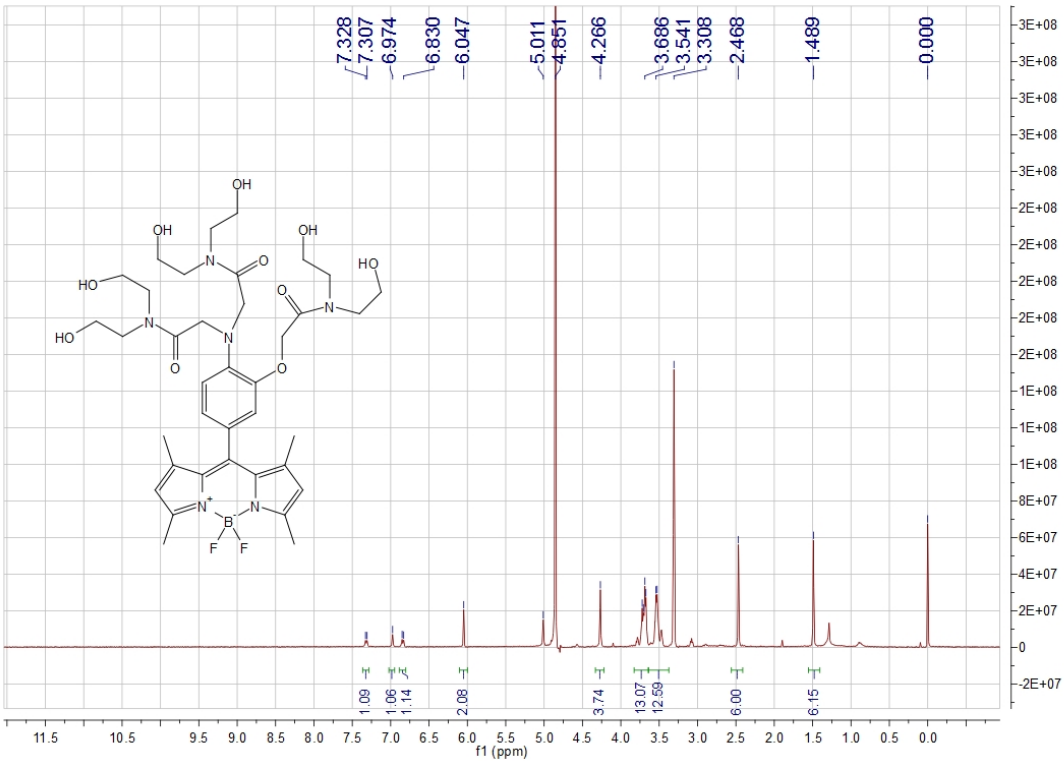
^{1}H NMR of compound **6**



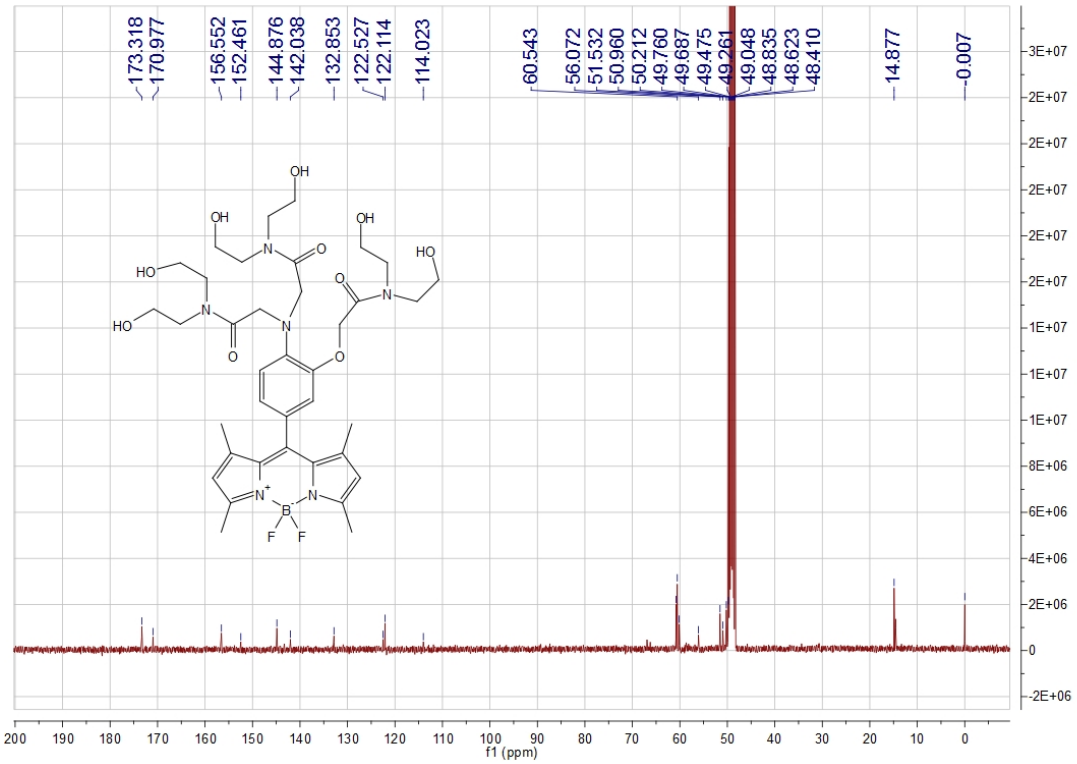
^{1}H NMR of compound **7**



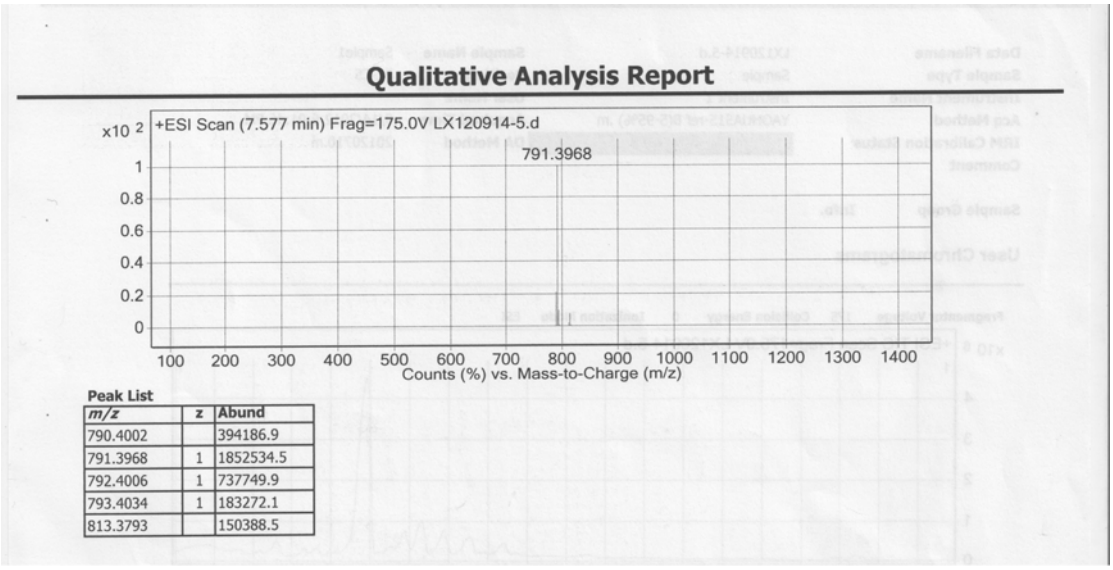
^{1}H NMR of compound **8** (**LS2**)



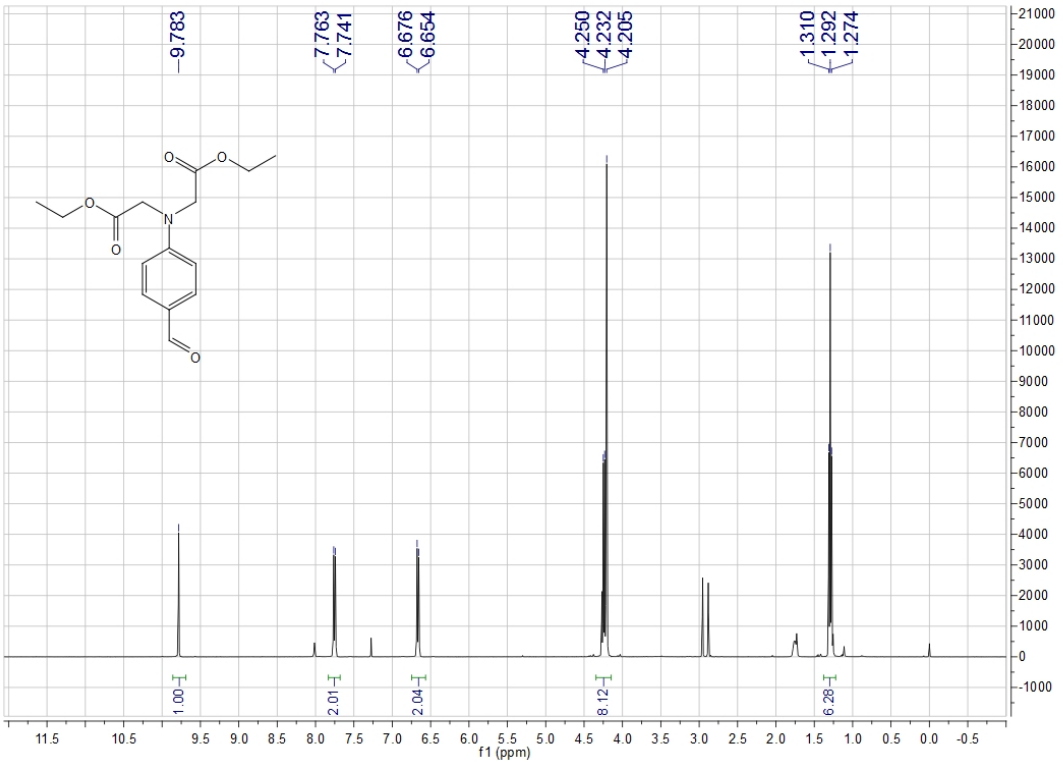
^{13}C NMR of compound **8** (**LS2**)



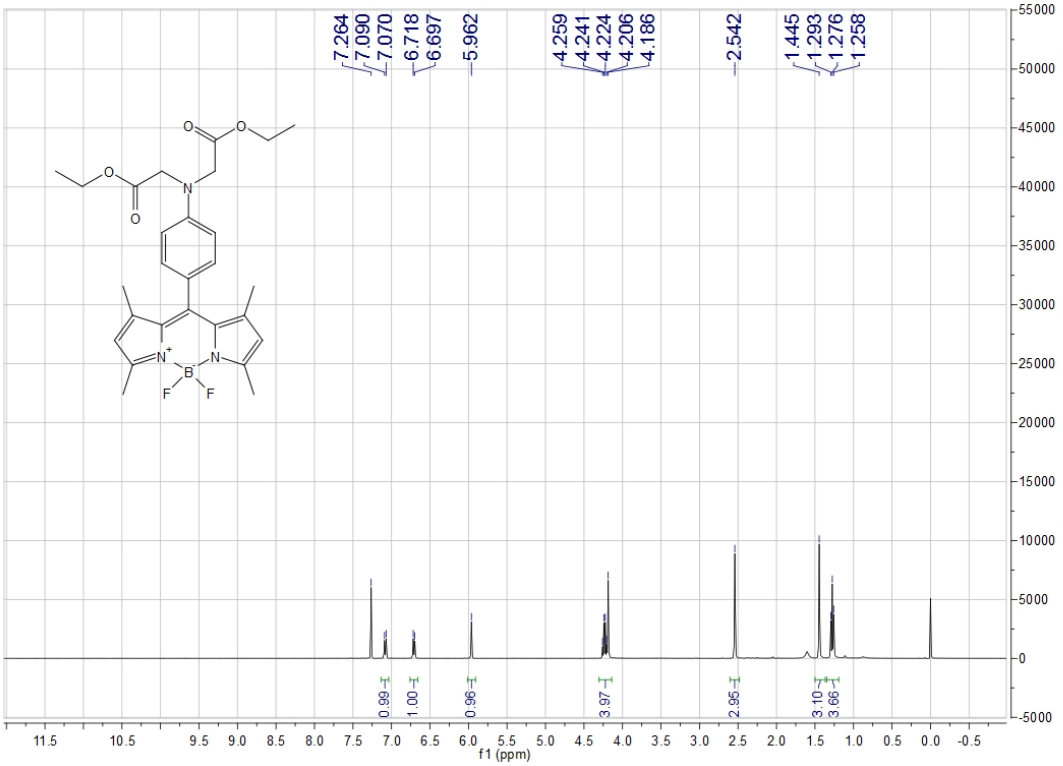
HRMS of compound **8** (**LS2**)



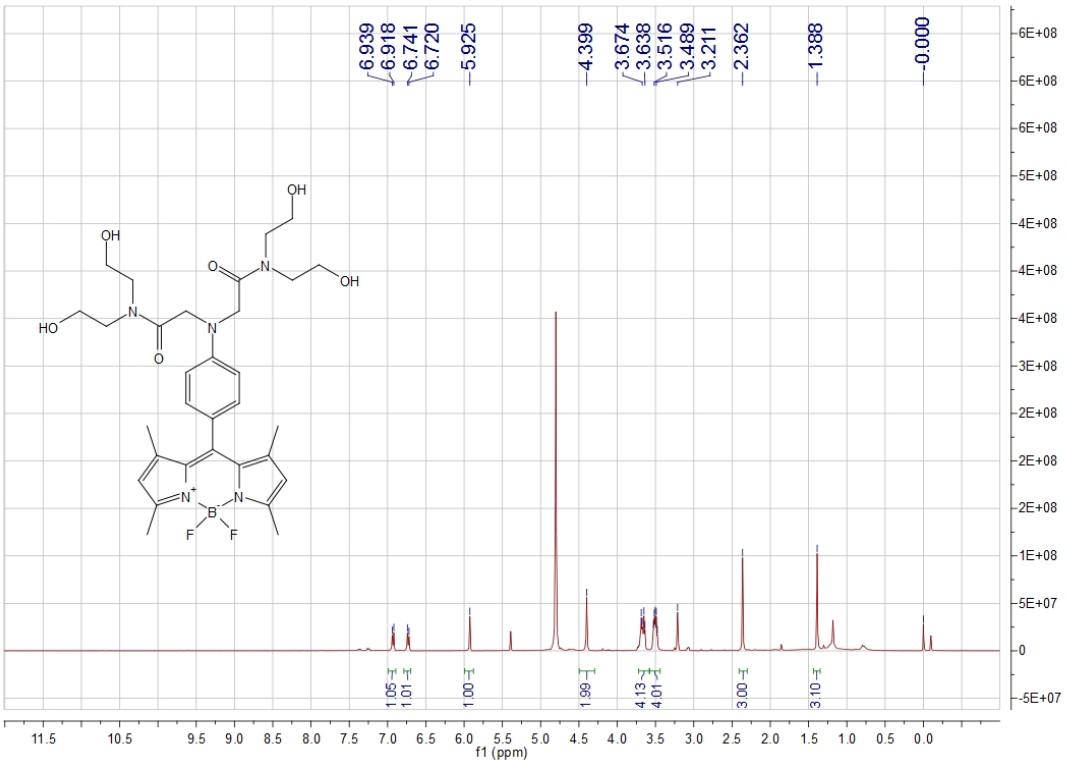
^{1}H NMR of compound **9**



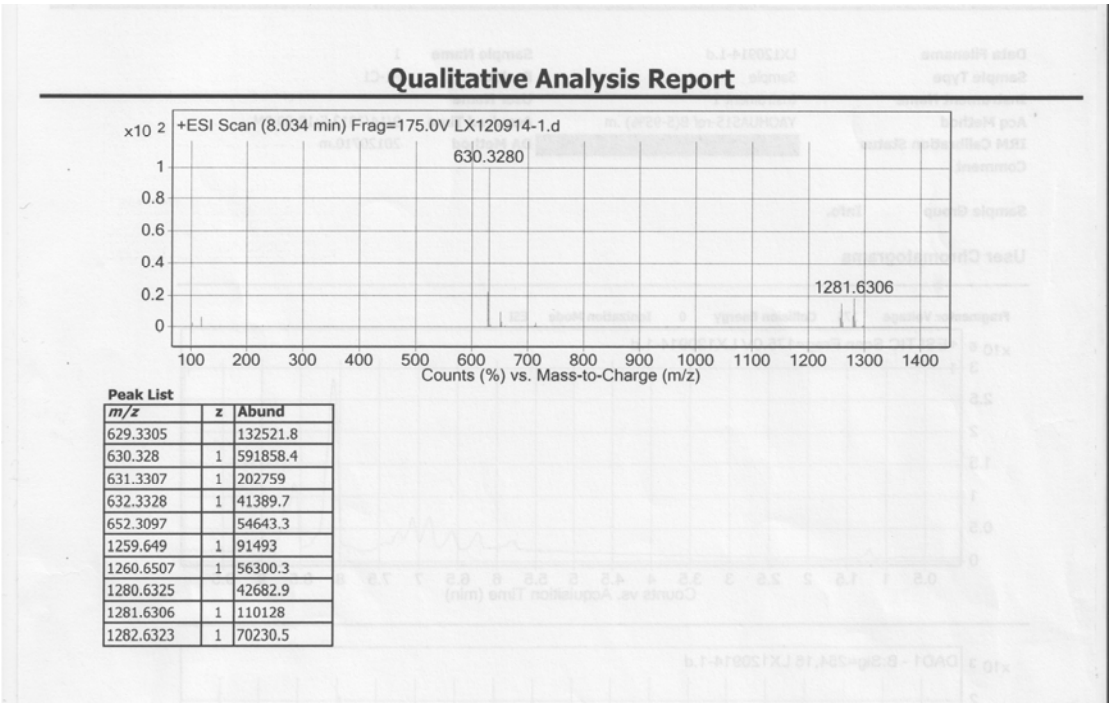
^{1}H NMR of compound **10**



^{1}H NMR of compound **11** (**LS3**)



HRMS of compound **11** (**LS3**)



Peak List

m/z	z	Abund
629.3305		132521.8
630.328	1	591858.4
631.3307	1	202759
632.3328	1	41389.7
652.3097		54643.3
1259.649	1	91493
1260.6507	1	56300.3
1280.6325		42682.9
1281.6306	1	110128
1282.6323	1	70230.5

References

(1) Velapoldi, R. A.; Tønnesen, H.; H. *J. Fluoresc.* **2004**, *14*, 465-472.

(2) Valeur, B. *Molecular Fluorescence: Principles and Applications*; Wiley-VCH, Weinheim, Germany, 2002.