

Analysis

The data collection for this project can be divided into four parts: [AR94] selection, fluorescence vs. $[\text{Pb}^{2+}]$, selectivity and sensitivity, and complex structure.

For the [AR94] selection procedure, the fluorescence intensity difference for the five pairs of solutions are shown in the graph below, such that the sample pairs number matches the number of the numbered vial in the corresponding pair.

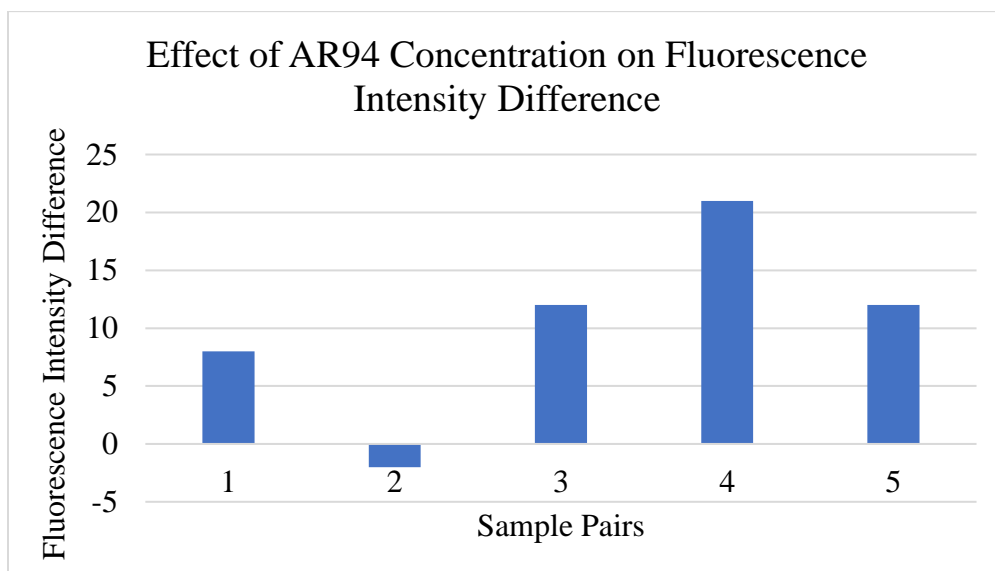


Figure 3: Data used to select [AR94]

The fluorescence spectra measured on the first and third lab days were then related to $[\text{Pb}^{2+}]$ using Stern-Volmer plots fitted with linear, exponential, and quadratic models. For the exponential and quadratic models, the data was linearized then then fitted with a straight line. An example Stern-Volmer plot is shown below. It is from Lab Day 3 and is fitted with a linearized exponential model

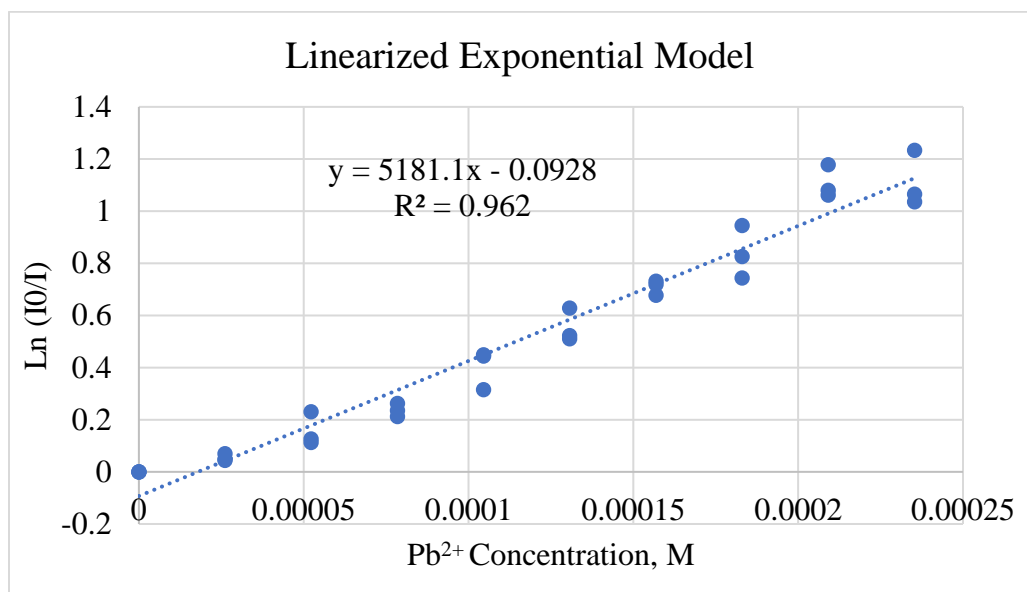


Figure 4: Modified Stern-Volmer Plot

For the selectivity part of the data collection, the AR94 soaked filter paper strips dipped in metal solution other than the $Pb^{2+}_{(aq)}$ solution had the same reaction as one dipped in dI water, whereas the paper strip dipped in lead solution changed color from pink to purple. Regarding the sensitivity section, the strips exhibited a more pronounced pink to purple color change for higher $[Pb^{2+}]$. The procedure previously described for calculating detection limit were performed twice and yielded the results shown in the table below.

Table 1: Detection Limit Calculation (EPA Action Level $\approx 7.24\text{E-}08\text{ M}$)

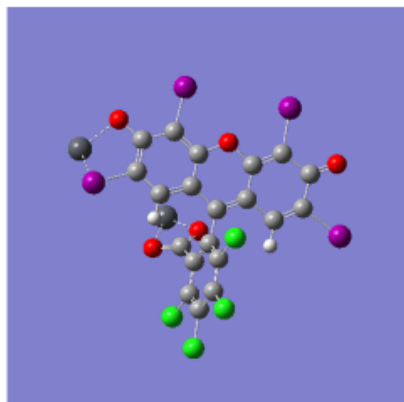
Trials	Lab Day 2	Lab Day 3
	$I_0/(I_0^*)$	$I_0/(I_0^*)$
1	1.040	0.983
2	1.048	0.987
3	1.046	0.981
4	1.045	0.981
5	1.036	0.979
6	1.035	0.981
7	1.021	0.986
8	1.019	0.977
9	1.018	0.981
10	1.021	0.976
Average Ratio	1.033	0.981
Standard Deviation (σ)	0.012	0.003
Average Stern-Volmer Plot Slope (s)	4438	5181
Limit of Detection (M)	8.12E-06	2.02E-06

Finally, the complex structure part of the data collection resulted in the Job plot data shown below in Figure 5, where X_{AR94} represents the mole fraction of Acid Red 94 and ΔI is the difference in the fluorescence emission intensity of AR94 (I_0) and the fluorescence emission intensity of AR94 in the presence of increasing concentration of lead ions (I). The maximum on the Job plot occurs at the mole fraction of 0.33 of AR94, suggesting that the most stable complex occurs at the mole ratio of 1:2 for the AR94:Pb²⁺ complex as proposed in Figure 6.

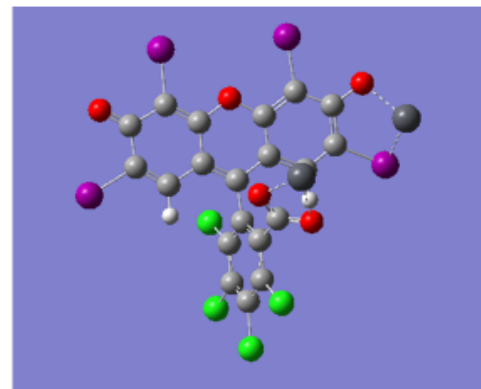
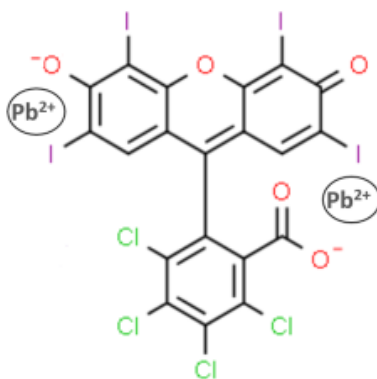


Figure 5: Job plot for AR94 to Pb^{2+} complexation molar ratio determination.

AR94 and Pb^{2+} Complex Proposed Structure



3D Molecular Structure of the Complex (front view)



3D Molecular Structure of the Complex (back view)

Figure 6: Chemical structure of AR94- Pb^{2+} complex