

Supplementary Table 1: Summary of the Wavenumbers in (cm⁻¹) and Assignments of the Main IR Bands of Free Adenine and its Zn²⁺ and Cd²⁺ Complexes at pH~ 2

Free adenine	Adenine-Zn	Adenine-Cd	Assignment
		3432	v (NH ₂)
	3370	3334	v (NH ₂)
3282			v (NH ₂)
	3165	3145	v (NH ₂)
3101			v (NH ₂)
2970	2996		v (N-9-H)
2979			v (C-H)
2684			v (C-H)
2593			v (C-H)
2064			Not assigned
		1982	
1893	1865		Not assigned
		1697	
1669	1662	1661	δ (NH ₂)
	1617		δ (N-9-H))
1598	1602	1604	δ (N-9-H))
		1588	δ (N-9-H))
	1563		
1502	1519	1519	v (C=N), v(C=C)
	1487	1484	
1449	1438	1433	v (imidazole ring)
1417	1417	1414	δ(N=CH)
1365	1397	1371	δ(C-8-H), δ(C-2-H)
1332	1337	1333	v(C-N), v(C=N)
1306	1304	1318	v(C-N), v(C=N)
	1288		
1250	1270	1242	v(C-NH ₂)
1154	1216	1143	δ(CH)
	1160		
1124	1140	1111	δ(C-2-N-1=C-6), v(C-5-N-7=C-8)
1021	1036	1018	δ(C-N-C)
	994		
	954		
938	937	957	δ(N-C=N)
910	914	914	r(NH ₂)
866		869	ω(N-9-H)
843			skeletal mode
796	787	787	v(C-C)
	776		
	742		
722	724	726	v(C-C),v(C-N)
	683	678	
636	631		
619		619	δ(N-C-C)

Supplementary Table 2: Potentiometric Titrations of Zn²⁺:Adenine in Various Ratios

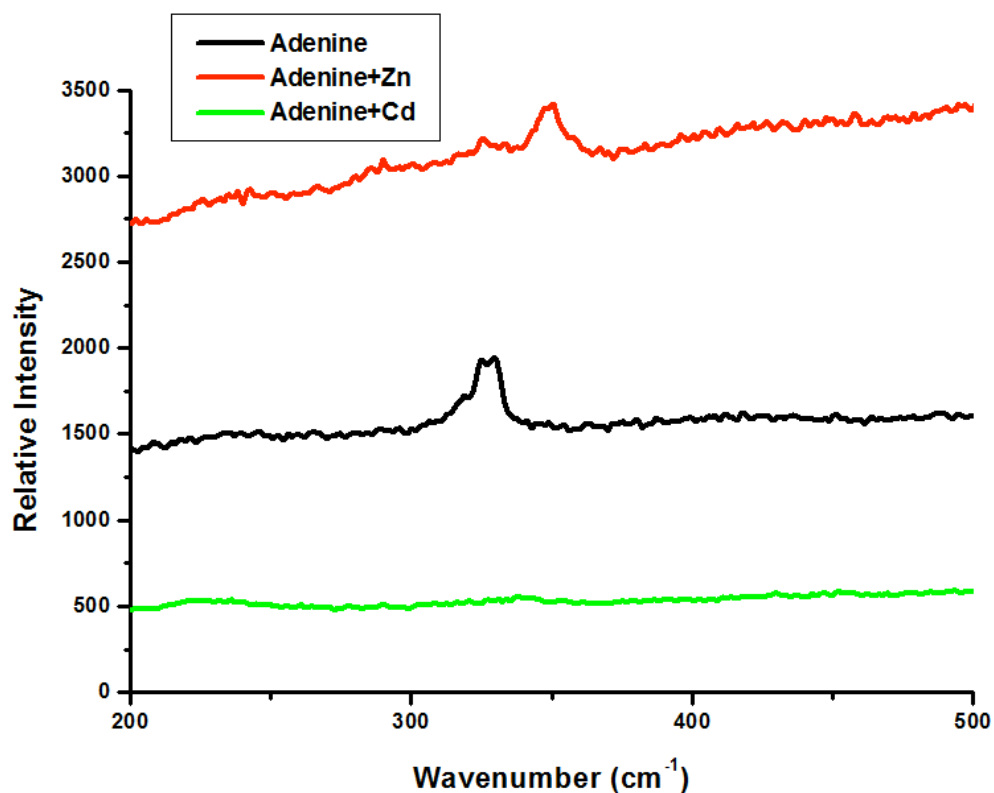
	Adenine	Zn ²⁺	Zn ²⁺ :Adenine 1:1	Zn ²⁺ :Adenine 1:2	Zn ²⁺ :Adenine 1:3
Run #1	1.010	2.184	2.105	1.843	1.668
Run #2	1.010	2.272	2.105	1.930	1.668
Run #3	1.073	2.272	2.105	1.843	1.756
Run #4	1.010				
Run #5	1.010				
Average	1.023	2.243	2.105	1.872	1.697
SD	0.0282	0.0508	0.0000	0.0502	0.0508

Supplementary Table 3: Summary of all Potentiometric Titrations of Cd²⁺:Adenine in Various Ratios

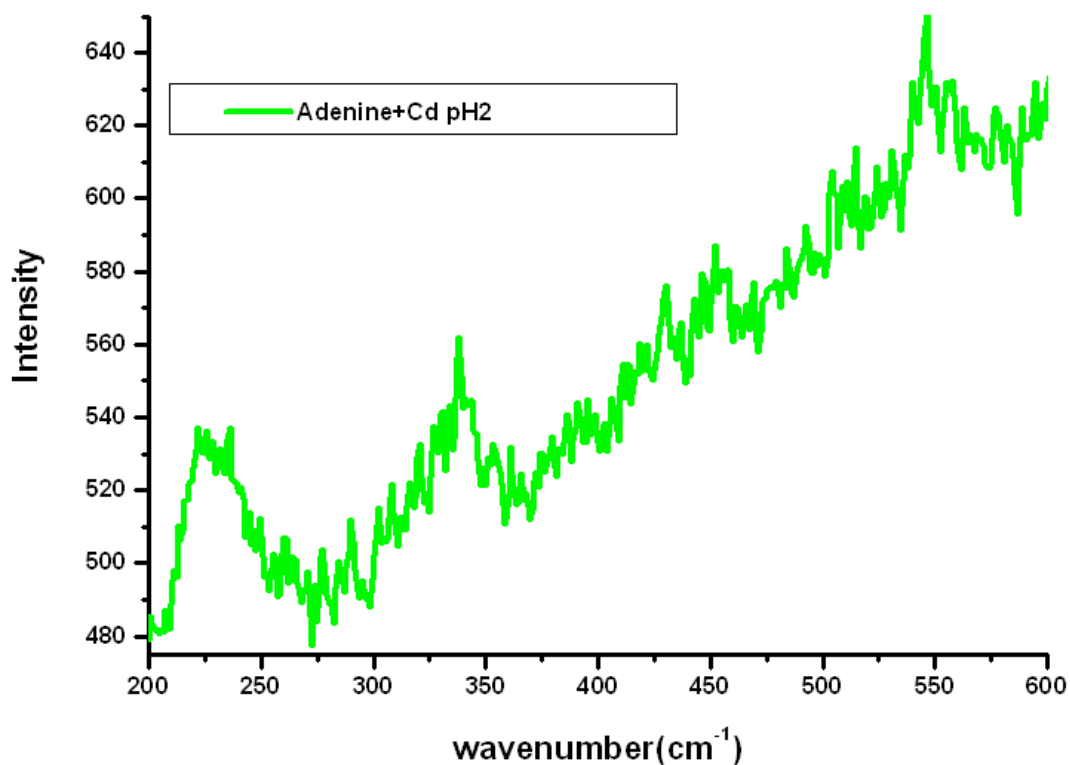
	Adenine	Cd ²⁺	Cd ²⁺ :Adenine 1:1	Cd ²⁺ :Adenine 1:2	Cd ²⁺ :Adenine 1:3
Run #1	1.010	2.000	2.088	2.088	2.088
Run #2	1.010	2.000	2.088	2.088	2.088
Run #3	1.073	2.000	2.262	2.088	2.175
Run #4	1.010				
Run #5	1.010				
Average	1.023	2.000	2.146	2.088	2.117
SD	0.0282	0.0000	0.1005	0.0000	0.0502

Supplementary TABLE 4: Summary of all Potentiometric Titrations of Hg²⁺:Adenine in Various Ratios. Potentiometric titration data compiled in the above Tables showing the number of equivalents of protons titrated from each titration ratio for the metal reacted with adenine in this study

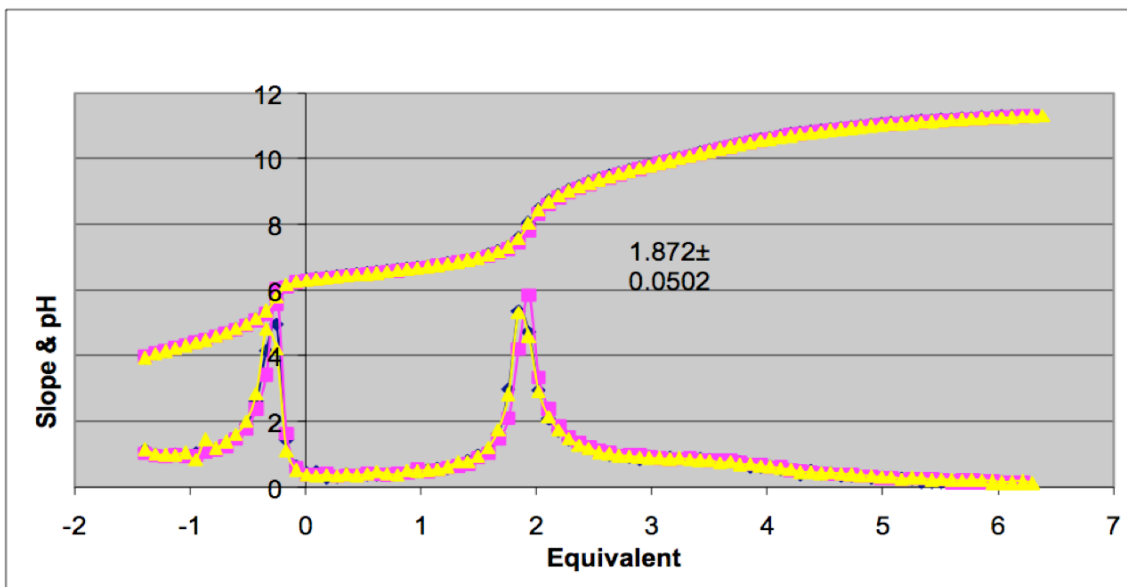
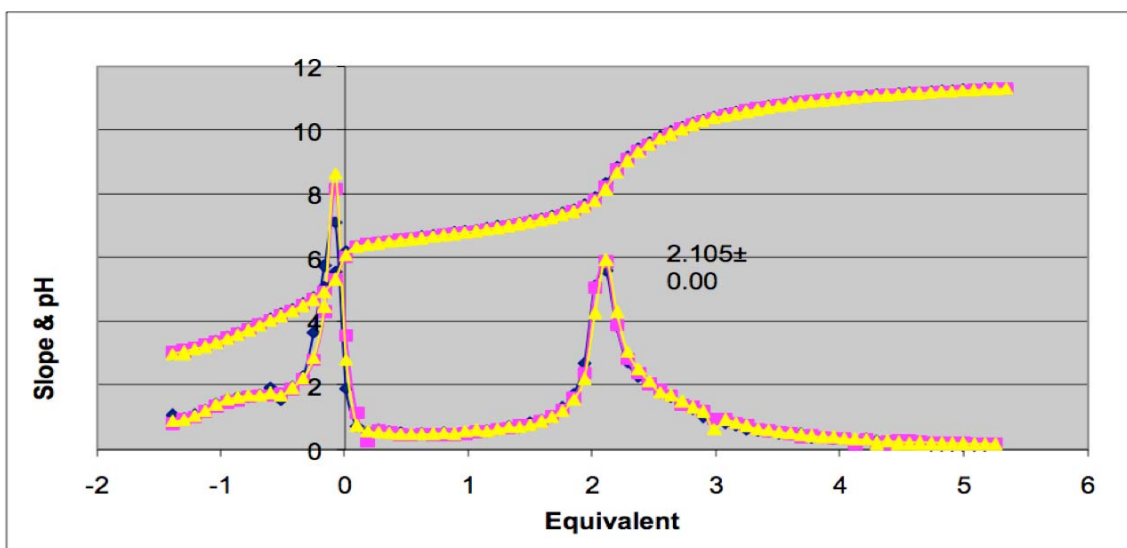
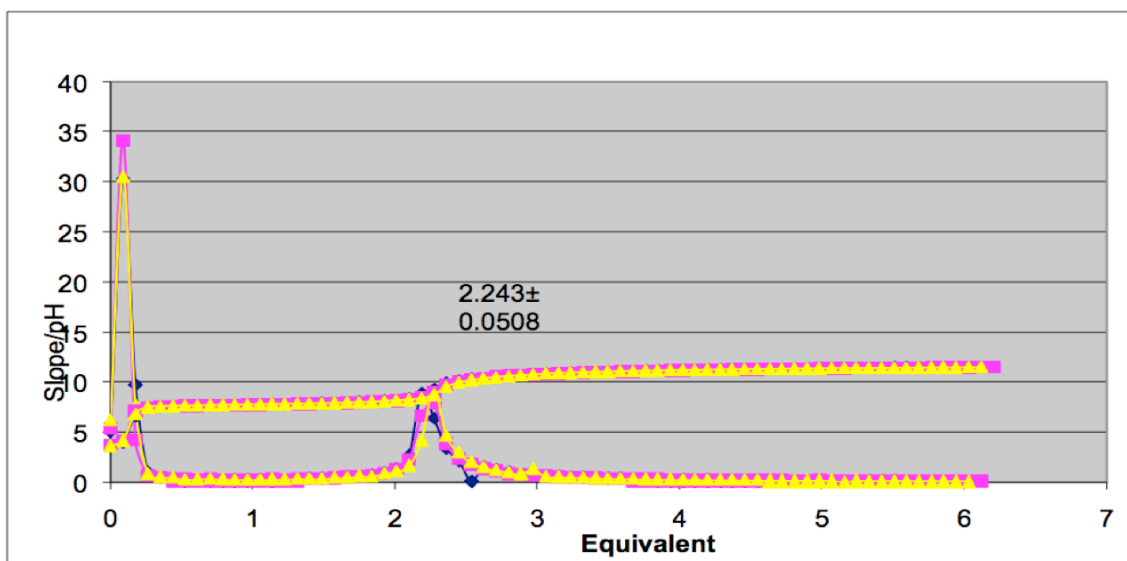
	Adenine	Hg ²⁺	Hg ²⁺ :Adenine 1:1	Hg ²⁺ :Adenine 1:2	Hg ²⁺ :Adenine 1:3
Run #1	1.010	2.026	2.166		
Run #2	1.010	1.948	2.194		
Run #3	1.073	1.948	2.166		
Run #4	1.010				
Run #5	1.010				
Average	1.023	1.974	2.175		
SD	0.0282	0.0450	0.0162		



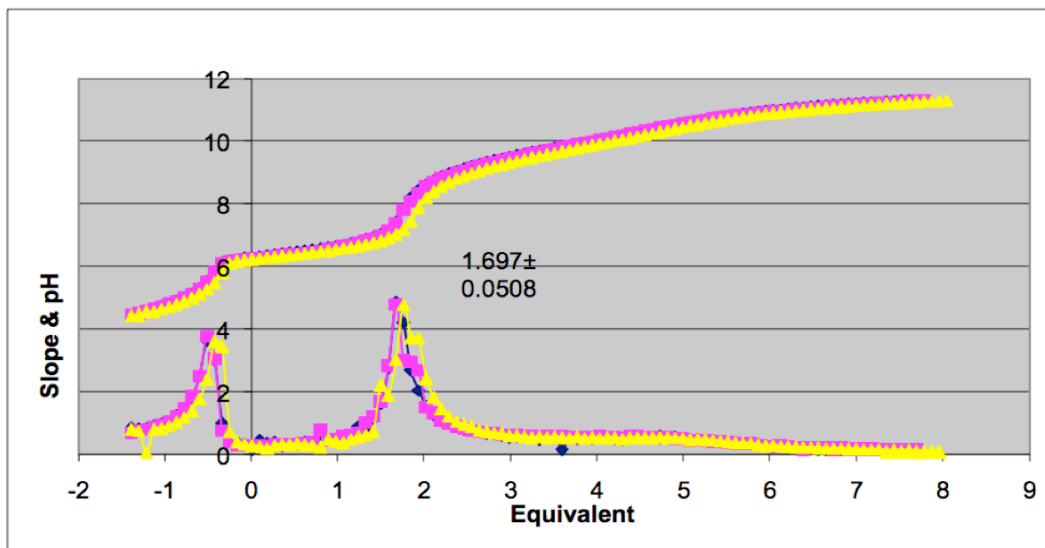
Supplementary Figure 1: Raman spectra of adenine with its complexes of Cd^{2+} and Zn^{2+} at pH 2.



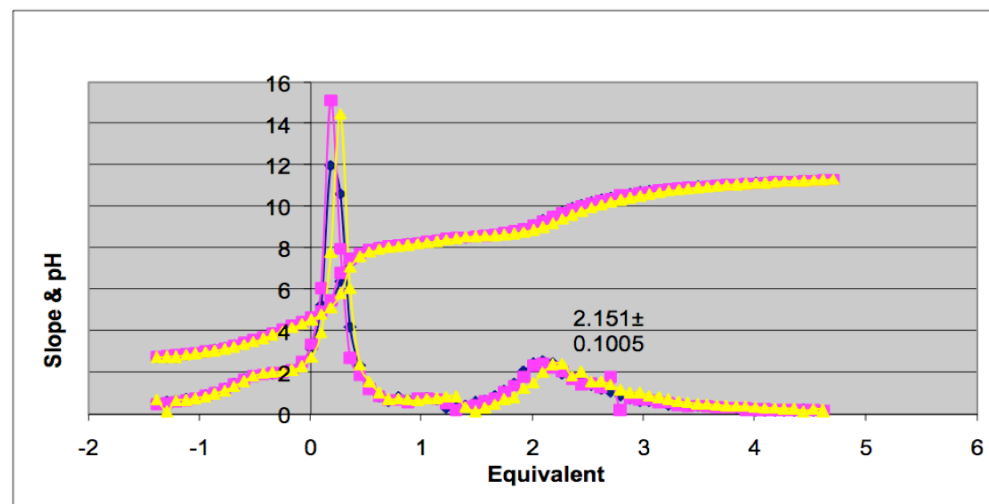
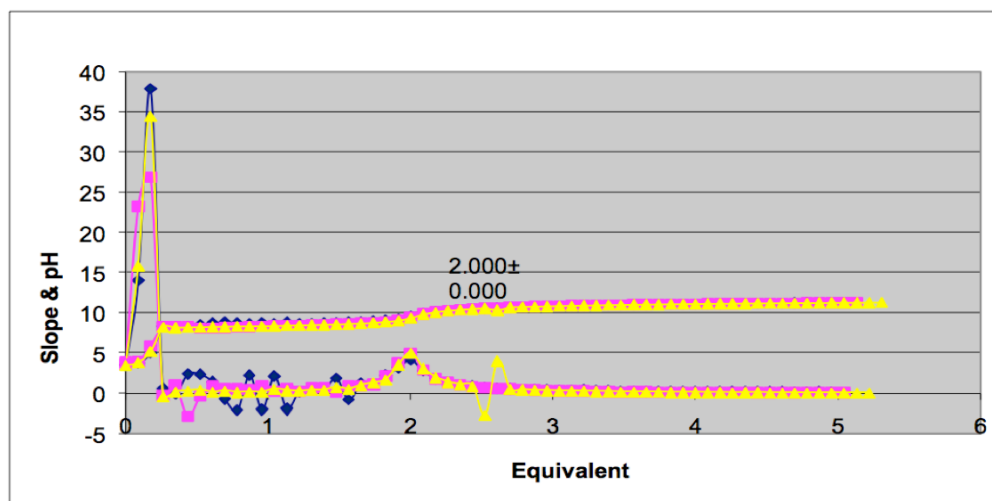
Supplementary Figure 2: Raman spectra of adenine with its complexes of Cd^{2+} at pH 2. See the next second derivative figure.

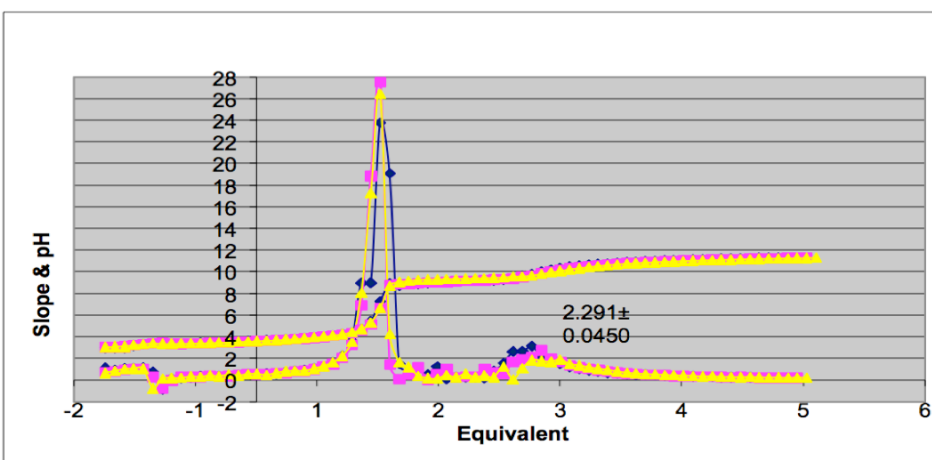
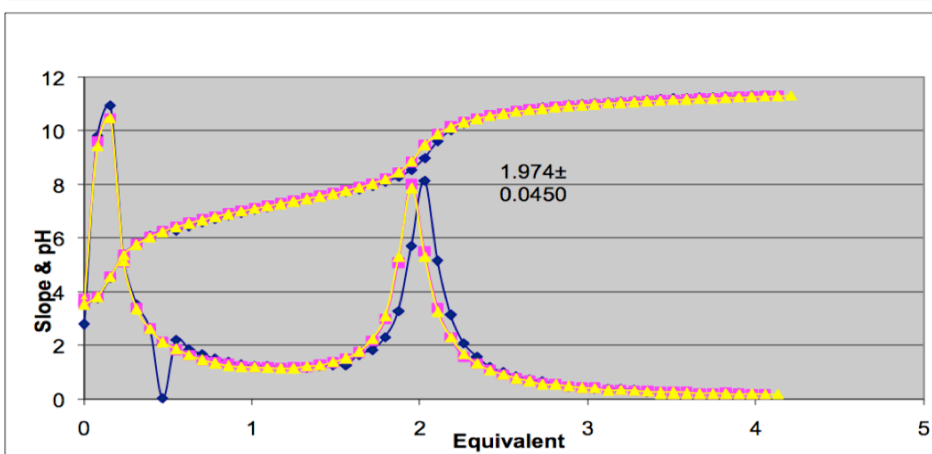
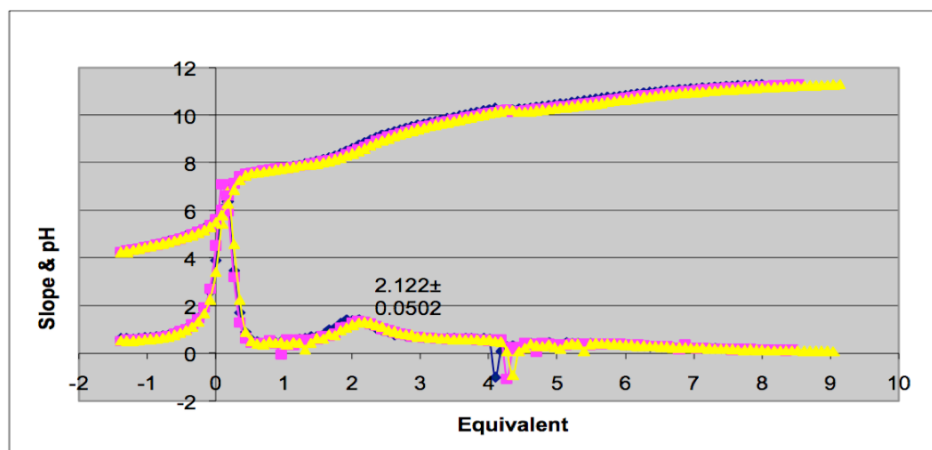
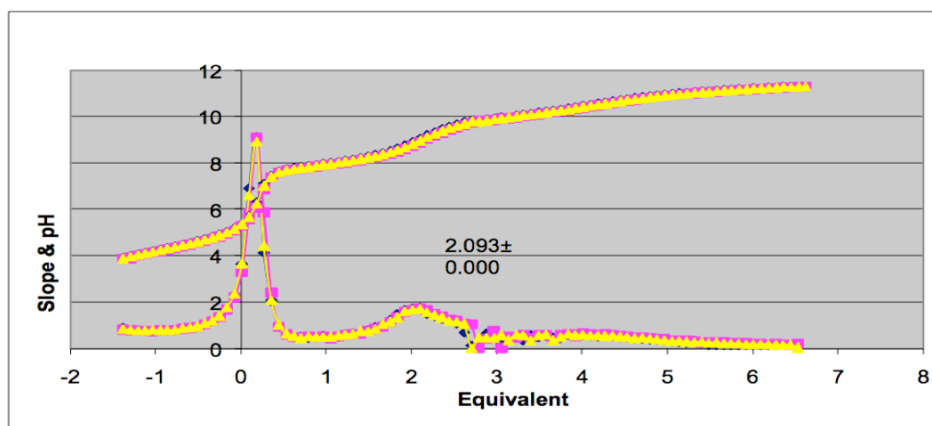


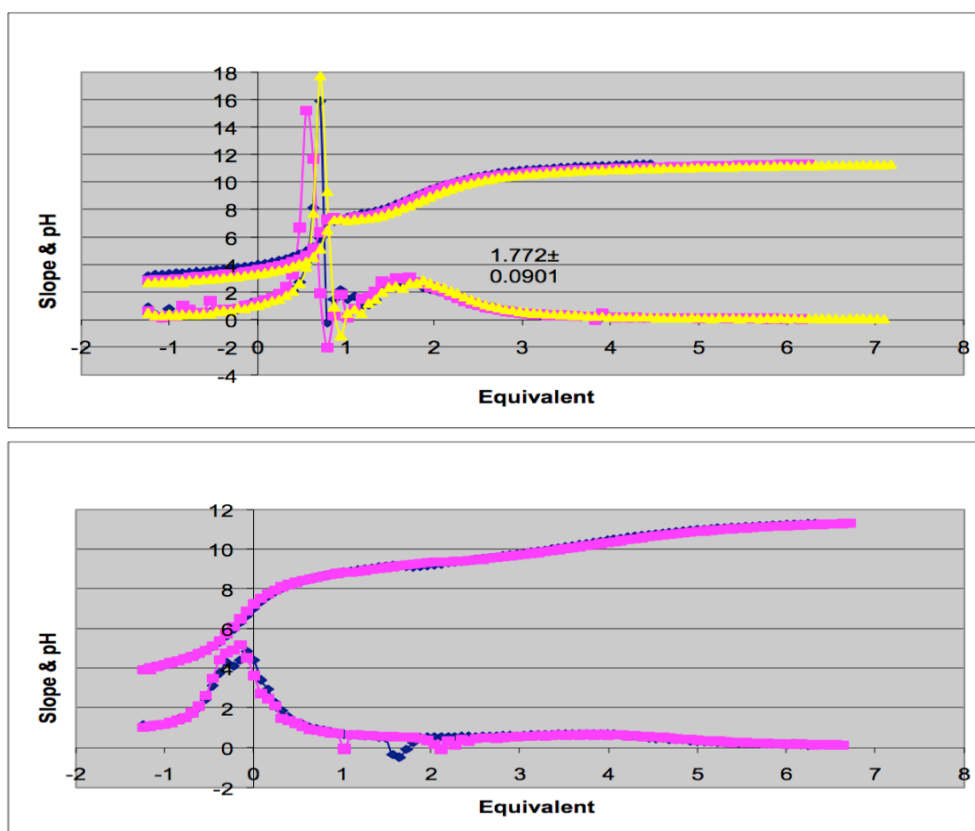
(Supplementary Figure 3). Continued



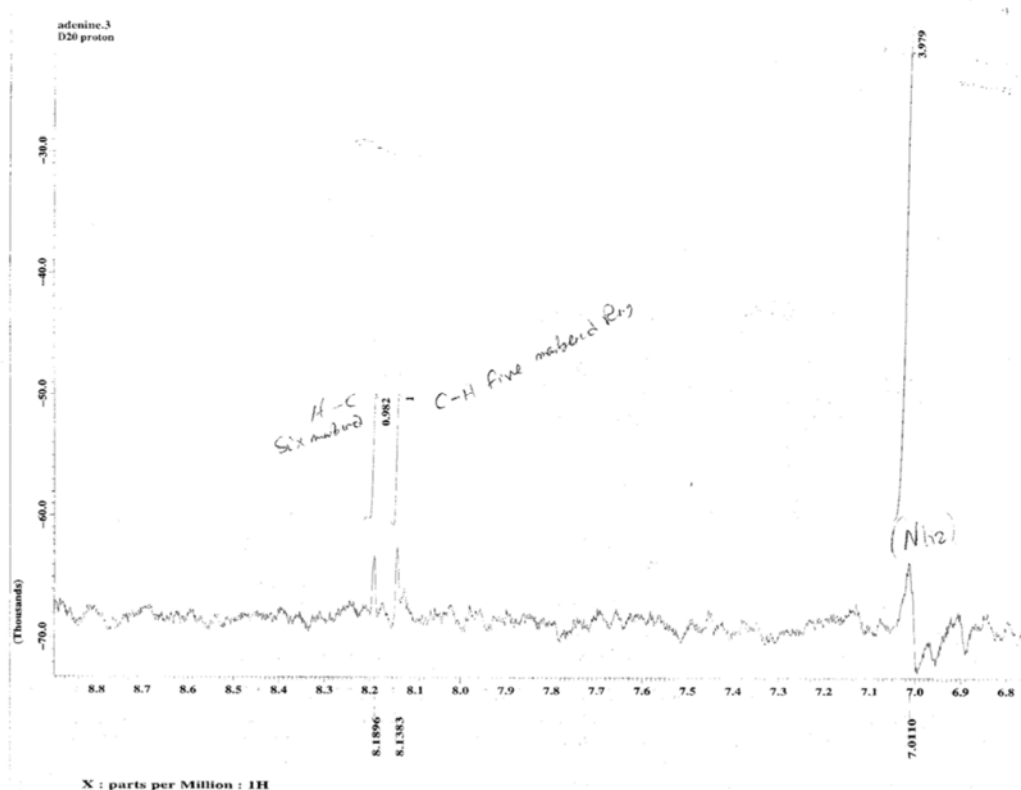
Supplementary Figure 3: Potentiometric titration graphs for adenine with Zn^{2+} . All plots were superimposed indicating the consistency of the titrations. The equivalent on the x-axis is defined as the number of mill-moles of titrant per milli-moles of adenine. If the metal ion is present the equivalent is defined as the number of milli-moles of titrant per milli-moles metal ion (Zn^{2+} , Cd^{2+} , or Hg^{2+} in this case). Supplementary Tables 2, 3, and 4 are the summary of all runs of Zn^{2+} , Cd^{2+} , and Hg^{2+} . See the next series of figures for Cd^{2+} and Hg^{2+} .



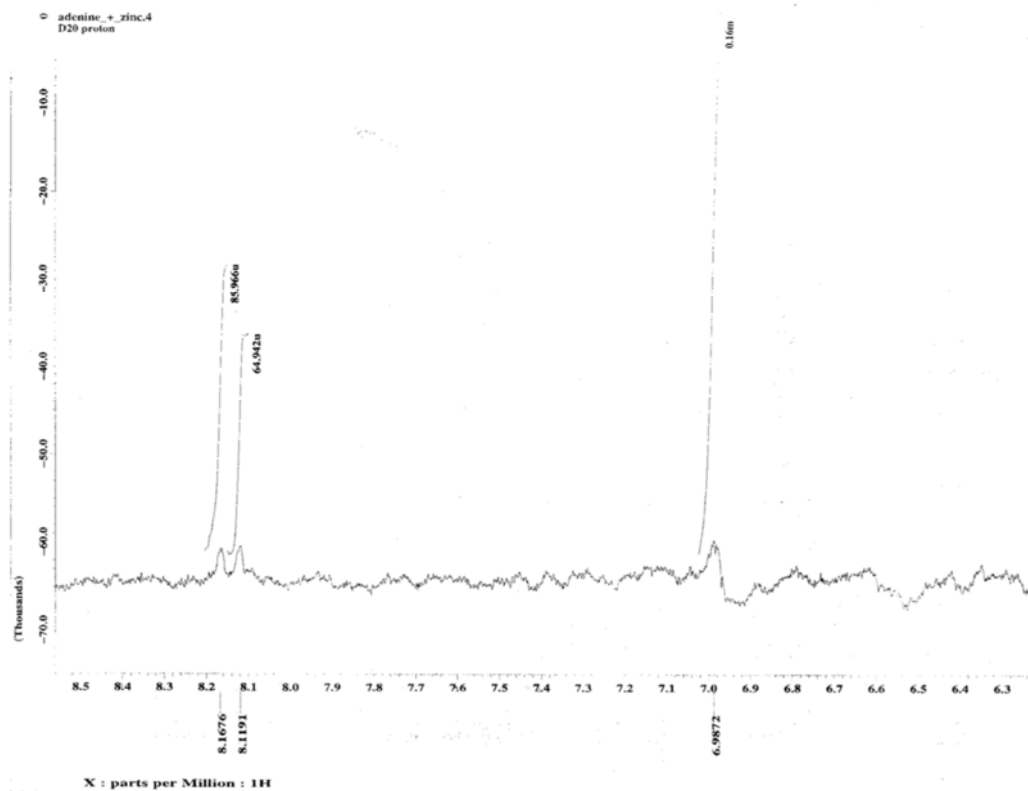




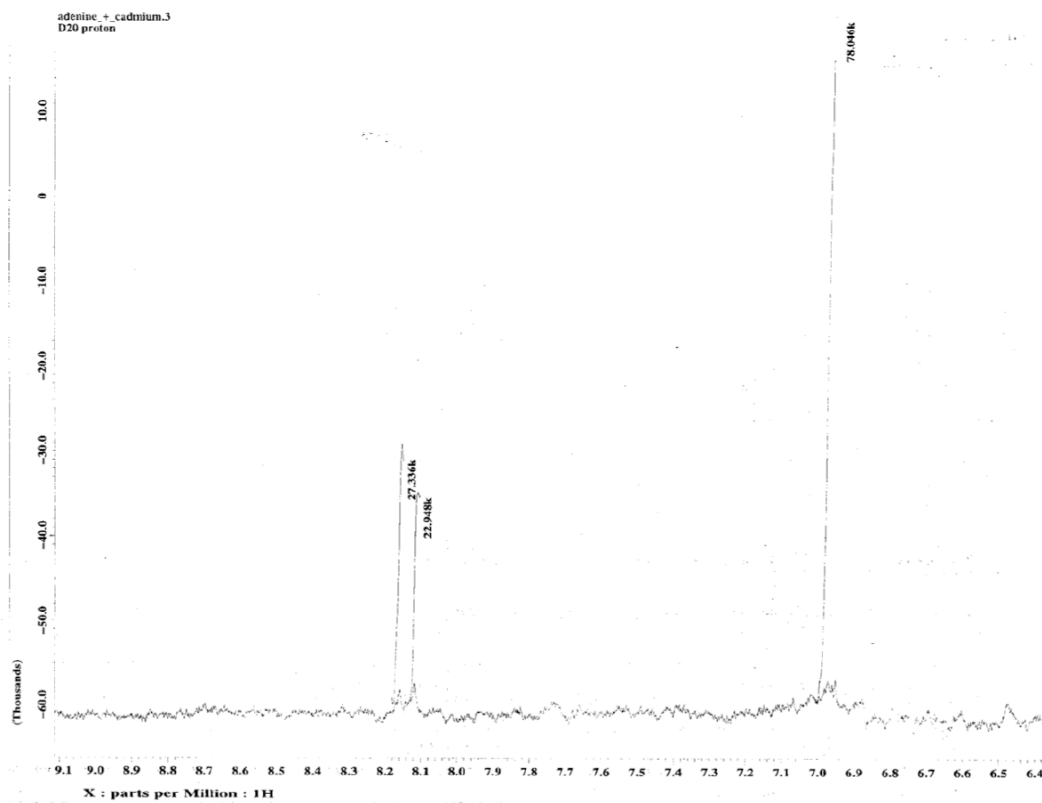
Supplementary Figure 4: The inflection points (the point of the highest slope) for all of the above potentiometric titration graphs of the free adenine along with that of adenine:(Ml)²⁺ are summarized in Tables 2-4.



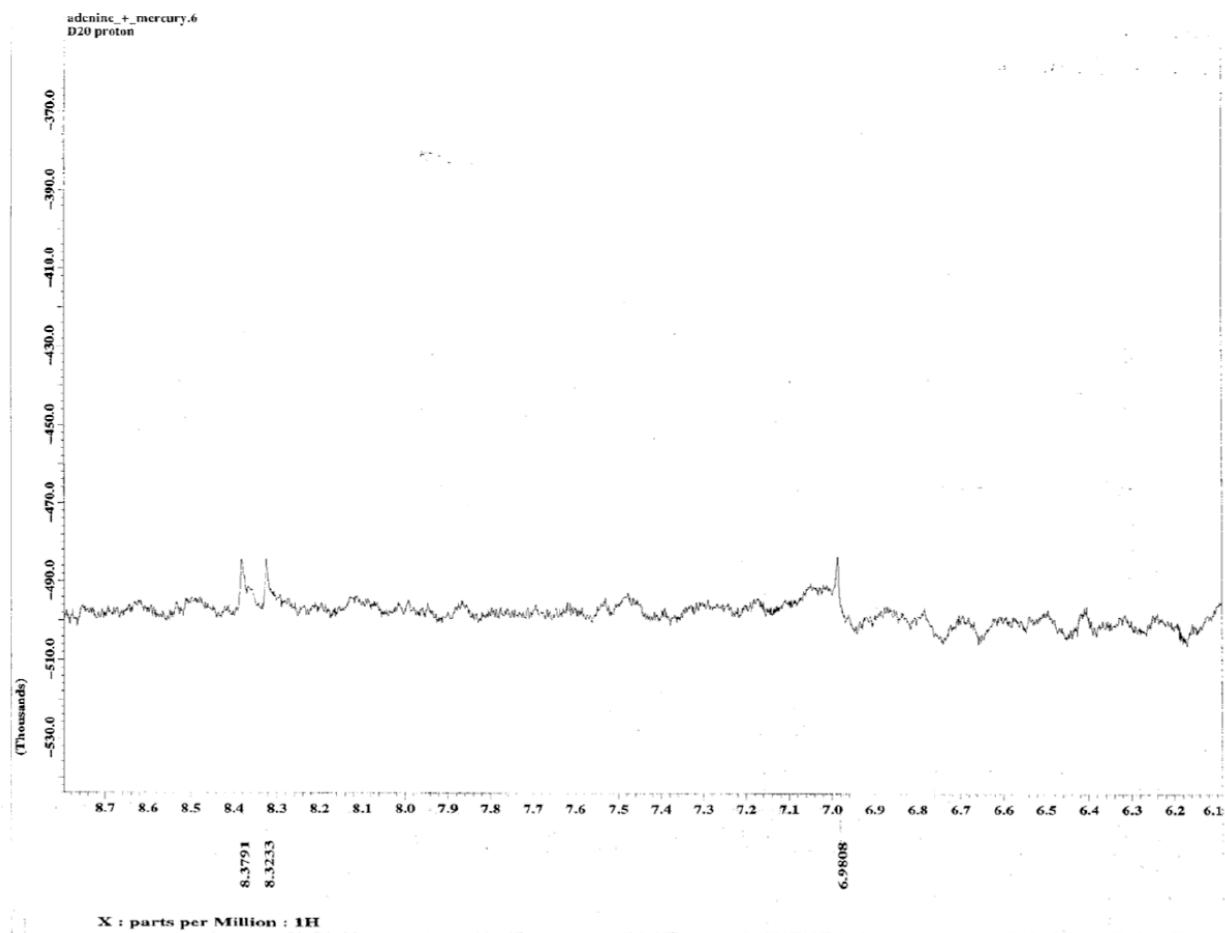
Supplementary Figure 5: ¹H-NMR- of free adenine in D₂O at pH ~ 3.5.



Supplementary Figure 6: $^1\text{H-NMR}$ of Zn^{2+} :adenine in D_2O in 1:1 ratio at pH ~ 3.5.



Supplementary Figure 7: $^1\text{H-NMR}$ of Cd^{2+} :adenine in D_2O in 1:1 ratio at pH ~ 3.5.



Supplementary Figure 8: 1H -NMR of Hg^{2+} :adenine in D_2O in 1:1 ratio at pH ~ 3.5.