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Supplementary information

Probing the Binding Interaction between Cadmium (II) Chloride and Lysozyme

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Paper Summary

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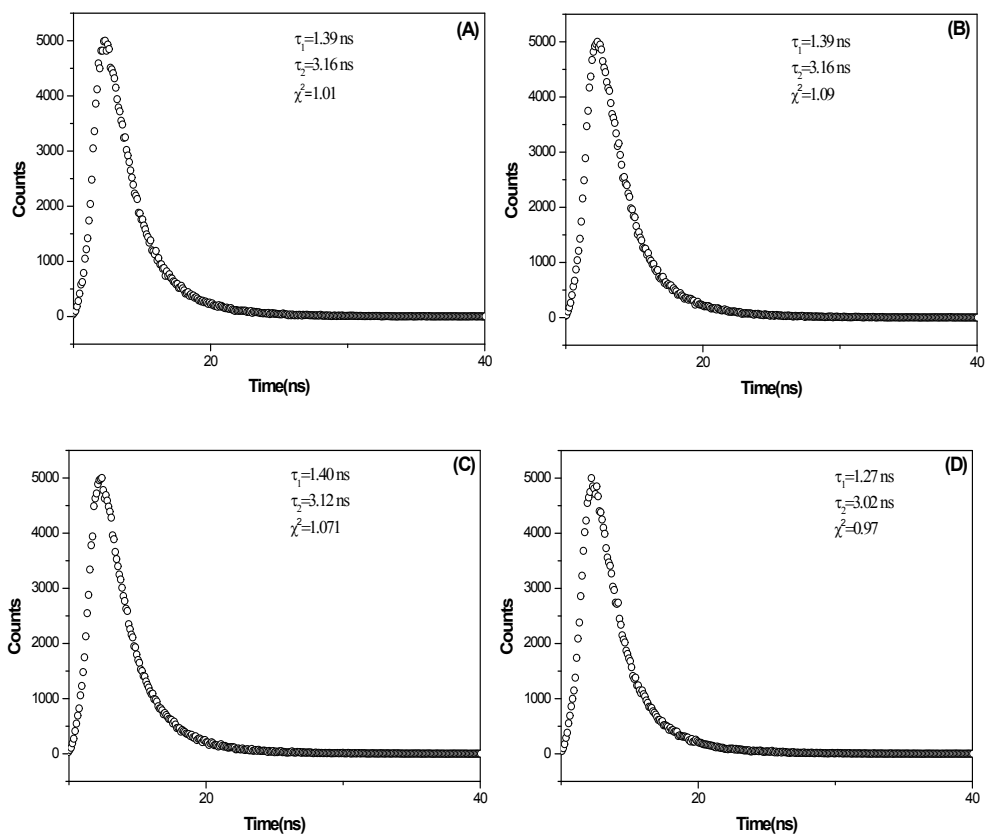


Fig. S1 Time-resolved fluorescence decay profile of CdCl₂-lysozyme system. Conditions: T= 298K, pH=7.4, c (lysozyme) = 5×10^{-6} M, c (CdCl₂) (10^{-4} M) A-D: 0, 1,5,10.

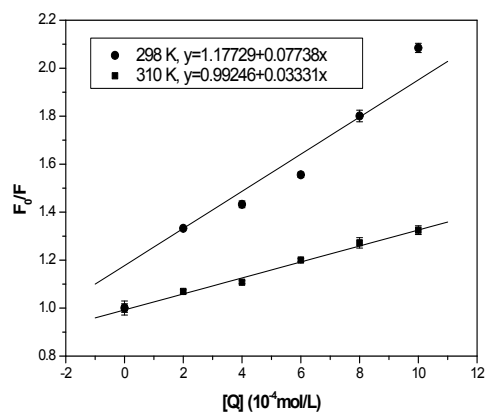


Fig. S2 Stern-Volmer plots for the quenching of lysozyme (5×10^{-6} M) by different concentration of CdCl_2 ($\times 10^{-4}$ M) (0, 2, 4, 6, 8, 10) at 298 K and 310 K at pH 7.4.

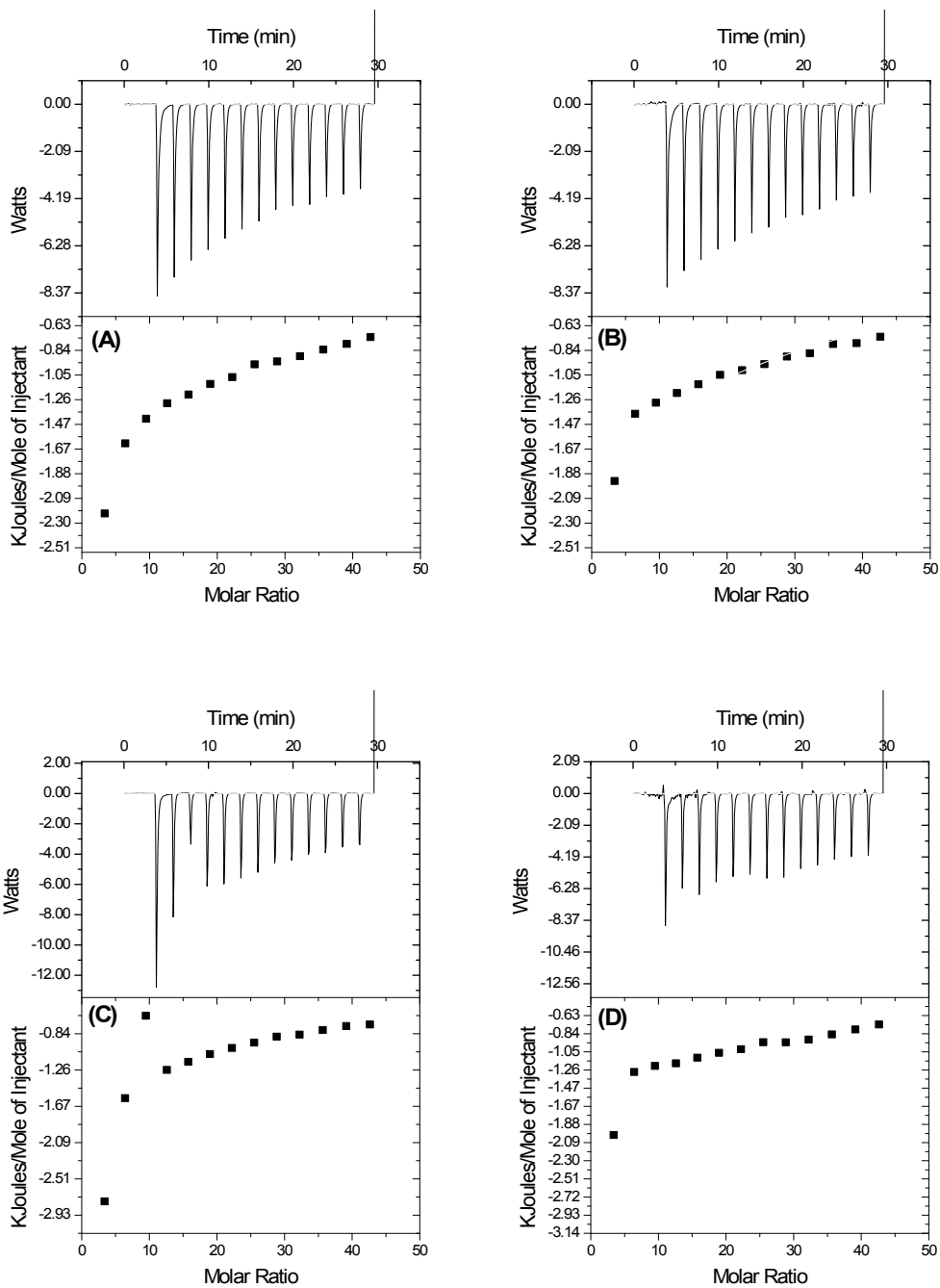


Fig. S3 ITC profiles of the interaction between lysozyme and CdCl₂ at 298.15 K and 310.15 K. (A) Sequential titration of CdCl₂ solution into buffer solution at 298.15 K. (B) Sequential titration of CdCl₂ solution into lysozyme solution at 298.15 K. (C) Sequential titration of CdCl₂ solution into buffer solution at 310.15 K. (D) Sequential titration of CdCl₂ solution into lysozyme solution at 310.15 K. Conditions: c(lysozyme)=100 μM, c(CdCl₂)=20 mM. Tris-HCl buffer (0.02 M, pH=7.4)

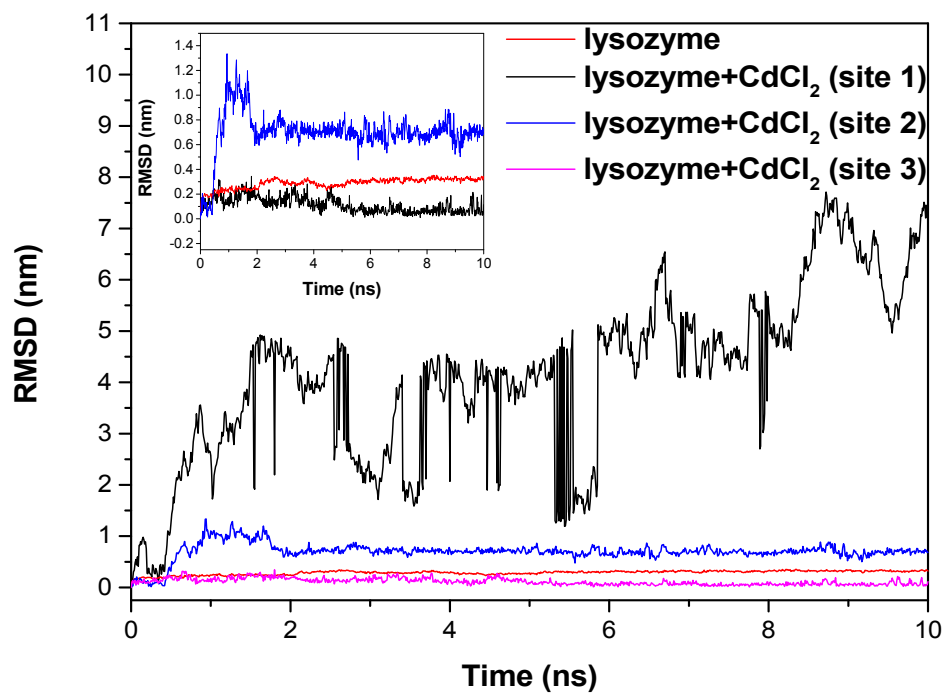


Fig. S4. Time dependence of RMSD values of lysozyme and lysozyme-CdCl₂ complexes during 10 ns MD simulation.

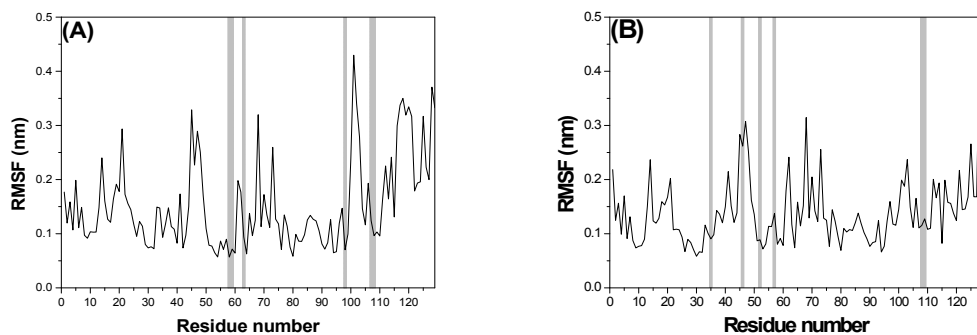


Fig.S5 RMSF values of lysozyme and lysozyme-CdCl₂ complexes were plotted against residue numbers. The residues located in the site are highlighted by gray bars. (A) Site 2. (B) Site 3.

Table S1. Energy ranked conformers through docking with CdCl₂, CdCl⁺, Cd²⁺ and Cl⁻ from low to high.

Species	Energy(kcal/mol)
CdCl ₂	-35.76
CdCl ₂	-10.26
CdCl ₂	-9.02
CdCl ⁺	-8.03
CdCl ⁺	-8.0
CdCl ⁺	-7.86
Cd ²⁺	-0.76
Cl ⁻	>0