Molecular Mechanism of the Effects of Salt and pH on the Affinity between Protein A and Human Immunoglobulin G1 Revealed by Molecular Simulations

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Supporting Information

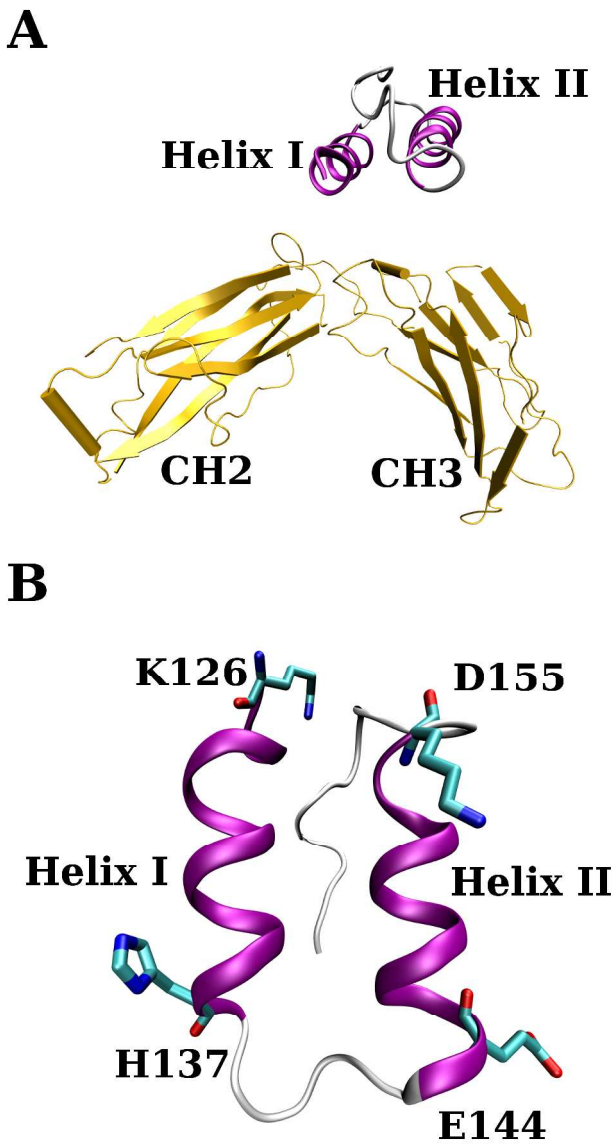

Figure S1. (A) Initial conformation of the SpA-hIgG1 complex. (B) Structure of the B domain of SpA.

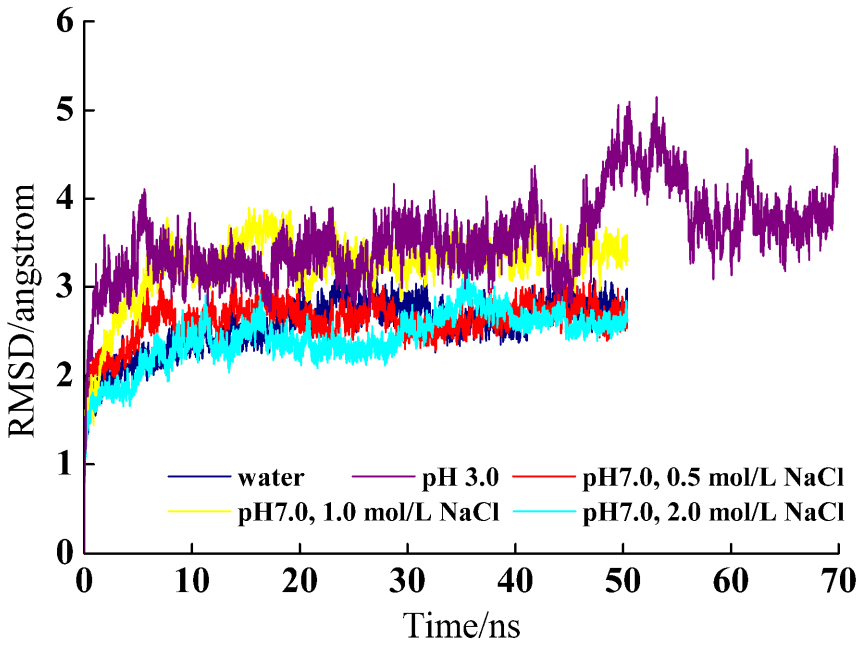

Figure S2. RMSD profiles of the six MD systems, calculated based on heavy atoms of SpA.

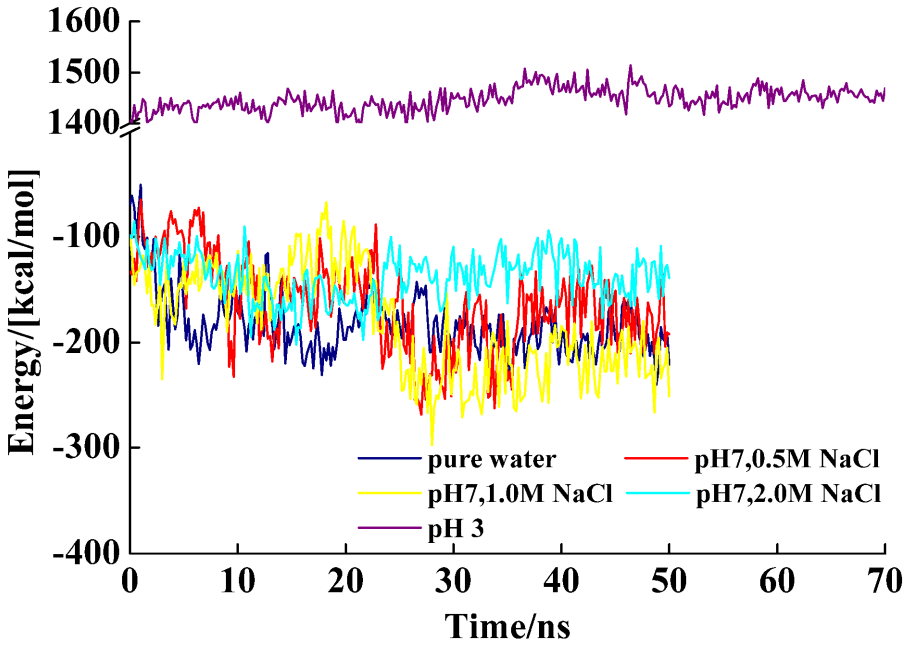

Figure S3. Time evolutions of the intermolecular potential energy between SpA and hIgG1 in different solutions.