Supporting Information

Binding Selectivity of Inhibitors toward Bromodomains BAZ2A and BAZ2B Uncovered by Multiple Short Molecular Dynamics Simulations and MM-GBSA Calculations

Lifei Wang[a*], Yan Wang[a], Zhiyong Yang[b*] , Shuobo Xu[c] , and Hongyun Li[a]

[a]School of Science, Shandong Jiaotong University, Jinan, 250357, China

[b]Department of Physics, Jiangxi Agricultural University, Nanchang, 330045, China

[c]School of Information Science and Electrical Engineering, Shandong Jiaotong University, Jinan, 250357, China

[*]Corresponding Authors:

Lifei Wang, Email: fisherwang@126.com;wanglf@sdjtu.edu.cn (L. Wang).

Zhiyong Yang，Email：zhiyongyang2009@163.com (Z. Yang).

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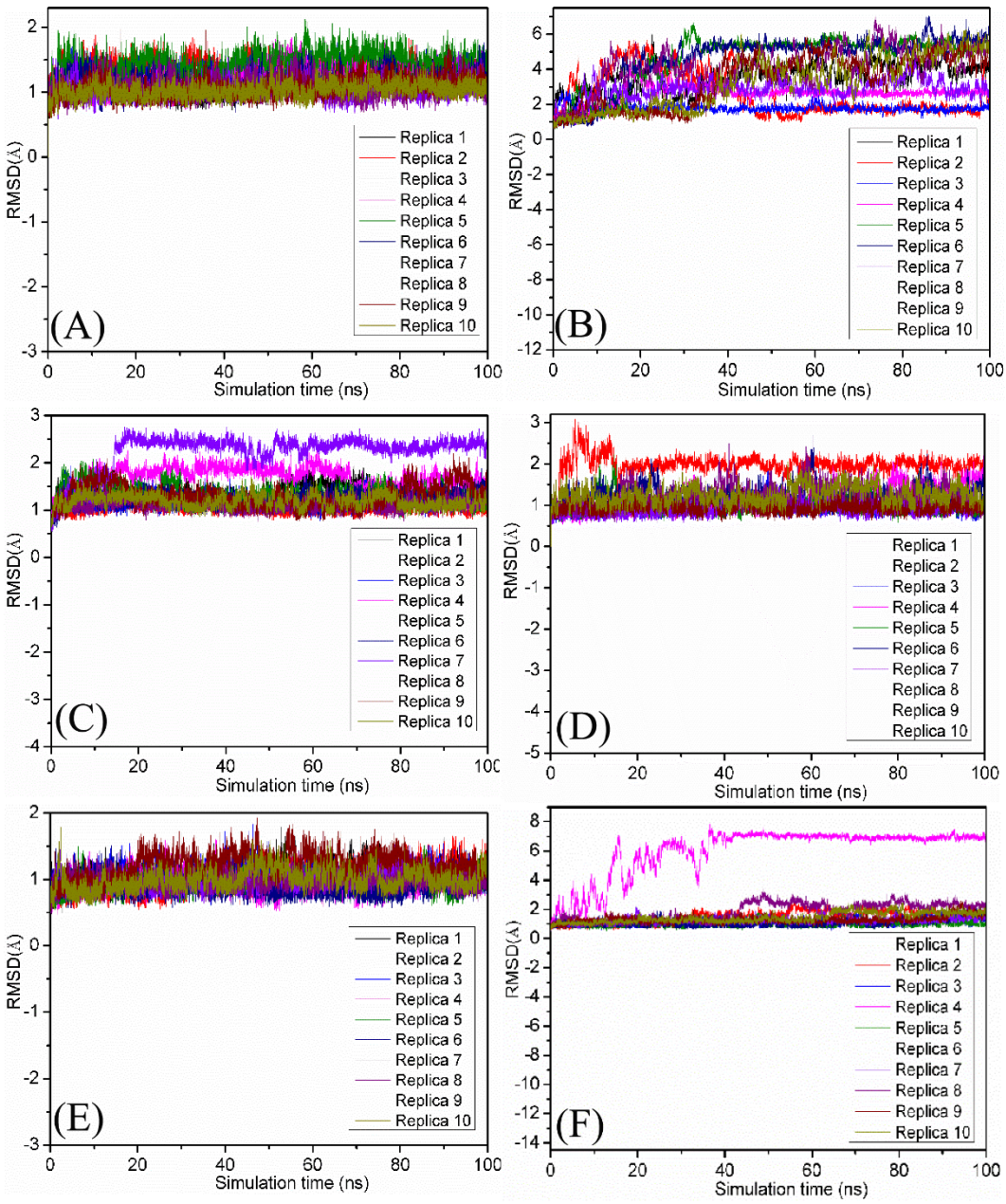

Figure S1. Root-mean-square deviations (RMSDs) of backbone atoms in BAZ2A and BAZ2B calculated by using MSMD trajectories of ten replicas: (A) the D8Q-BAZ2A complex, (B) the D8Q-BAZ2B complex, (C) the D9T-BAZ2A complex, (D) the D9T-BAZ2B complex, (E) the UO1-BAZ2A complex and (F) the UO1-BAZ2B complex.

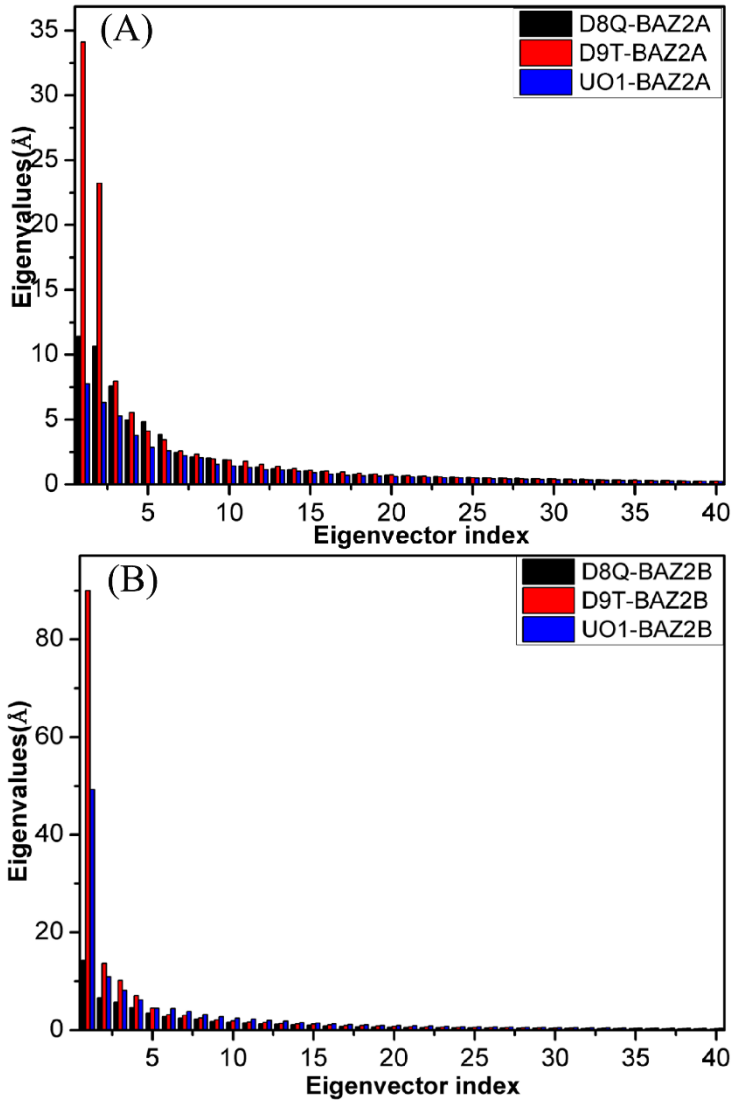

Figure S2. The function of eigenvalues versus eigenvector index stemming from PC analysis based on the single joined MSMD trajectory: (A) BAZ2A and (B) BAZ2B complexed with three inhibitors D8Q, D9T, and UO1.

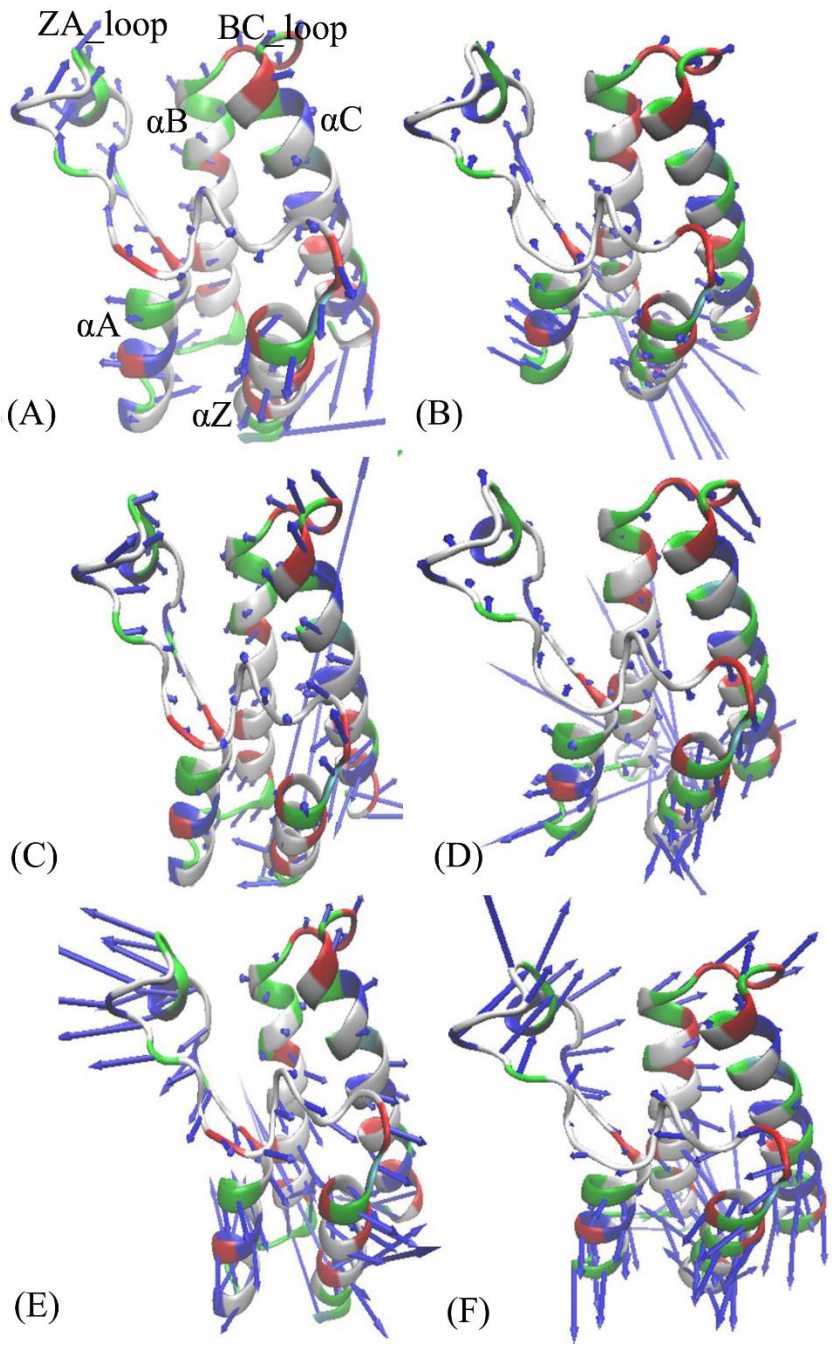

Figure S3. Collective motions corresponding to the first component PC1 obtained from principal component (PC) analysis based on the single joined trajectories: (A) the D8Q-BAZ2A complex, (B) the D8Q-BAZ2B complex, (C) the D9T-BAZ2A complex, (D) the D9T-BAZ2B complex, (E) the UO1-BAZ2A complex and (F) the UO1-BAZ2B complex.

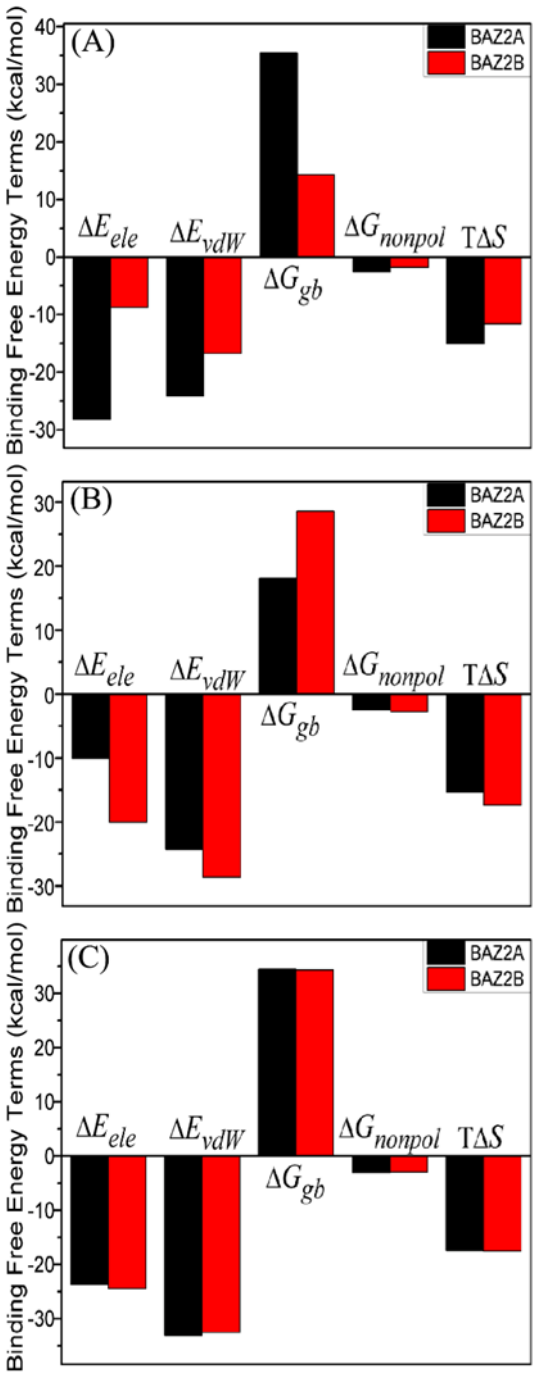

Figure S4. Comparisons between binding free energy terms of BAZ2A and BAZ2B, (A) D8Q, (B) D9T and (C) UO1.

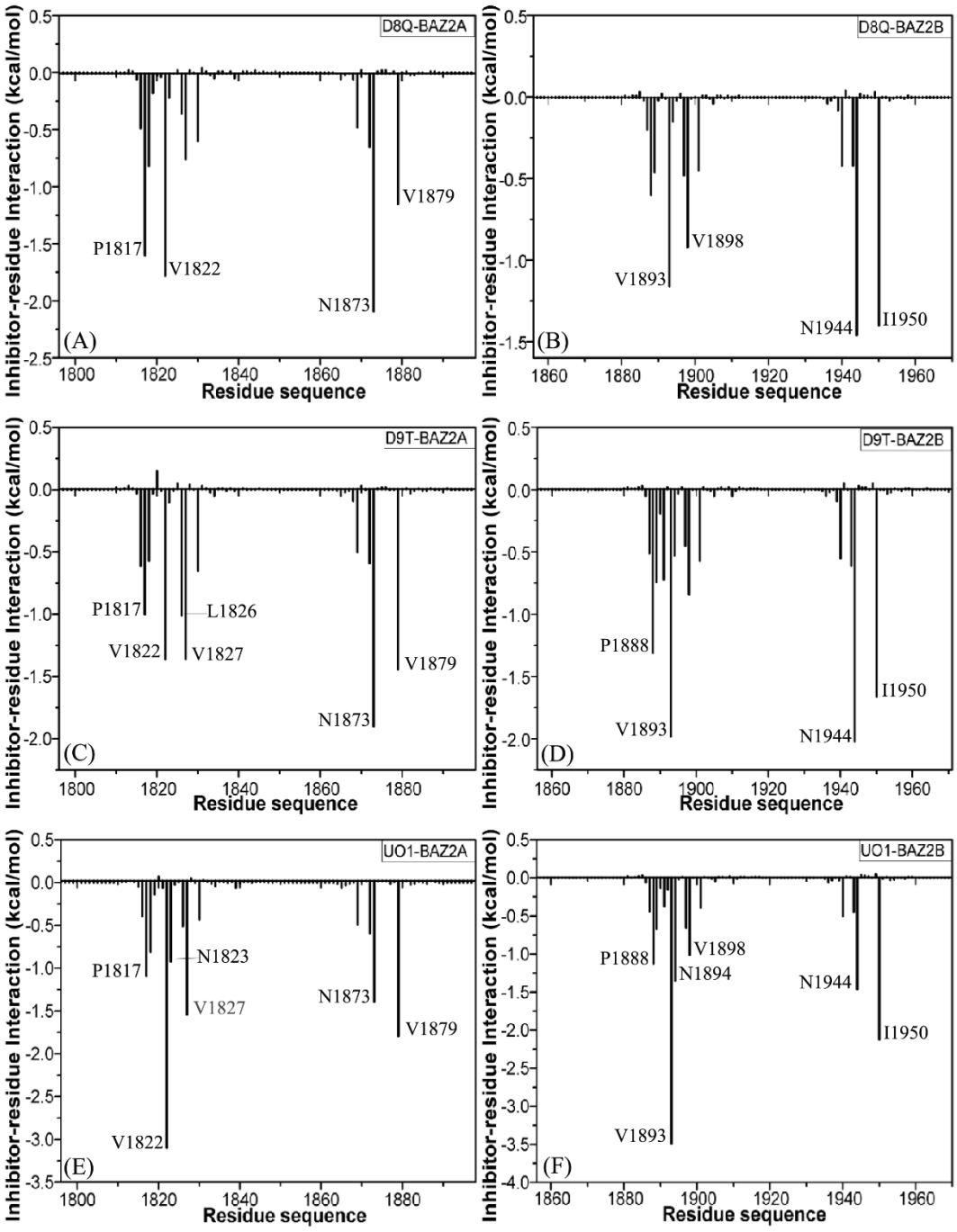

Figure S5. Inhibitor-Residue interactions computed by using residue-based free energy decomposition method, only residues stronger than 0.9 kcal/mol were labeled: (A) the D8Q-BAZ2A complex, (B) the D8Q-BAZ2B complex, (C) the D9T-BAZ2A complex, (D) the D9T-BAZ2A complex, (E) the UO1-BAZ2A complex and (F) the UO1-BAZ2B complex.