**Binding modes and conformational changes of FK506-binding protein 51 induced by inhibitor bindings: insight into molecular mechanisms based on multiple simulation technologies**

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Figure S1. Root-mean-square deviations (RMSDs) of backbone atoms in four systems calculated by using MSMD trajectories of ten replicas: (A) the *apo* FKBP51, (B) the 3JP-FKBP51 complex, (C) the 3JR-FKBP51 complex and (D) the 3JQ-FKBP51 complex.



Figure S2. Time evolution of the secondary structure of FKBP51: (A) the *apo* FKBP51, (B) the 3JP-FKBP51 complex, (C) the 3JR-FKBP51 complex and (D) the 3JQ-FKBP51 complex..



Figure S3. The function of the eigenvalues as the eigenvector indices arising from the covariance matrix constructed using the equilibrated MSMD trajectories.



Figure S4. Interactions of inhibitors with separate residues of FKBP51: (A) residues involved in significant contributions to inhibitor-FKBP51 bindings, (B) inhibitor-residue interactions between 3JP and FKBP51, (C) inhibitor-residue interactions of 3JR with FKBP51 and (D) inhibitor-residue interactions between 3JQ and FKBP51.



Figure S5. Hydrogen bonding interactions of inhibitors with key residues of FKBP51: (A) 3JP, (B) 3JR and (C) 3JQ.

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