Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Theoretical exploration on binding selectivity of inhibitors to BRD7 and BRD9 with multiple short molecular dynamics simulations

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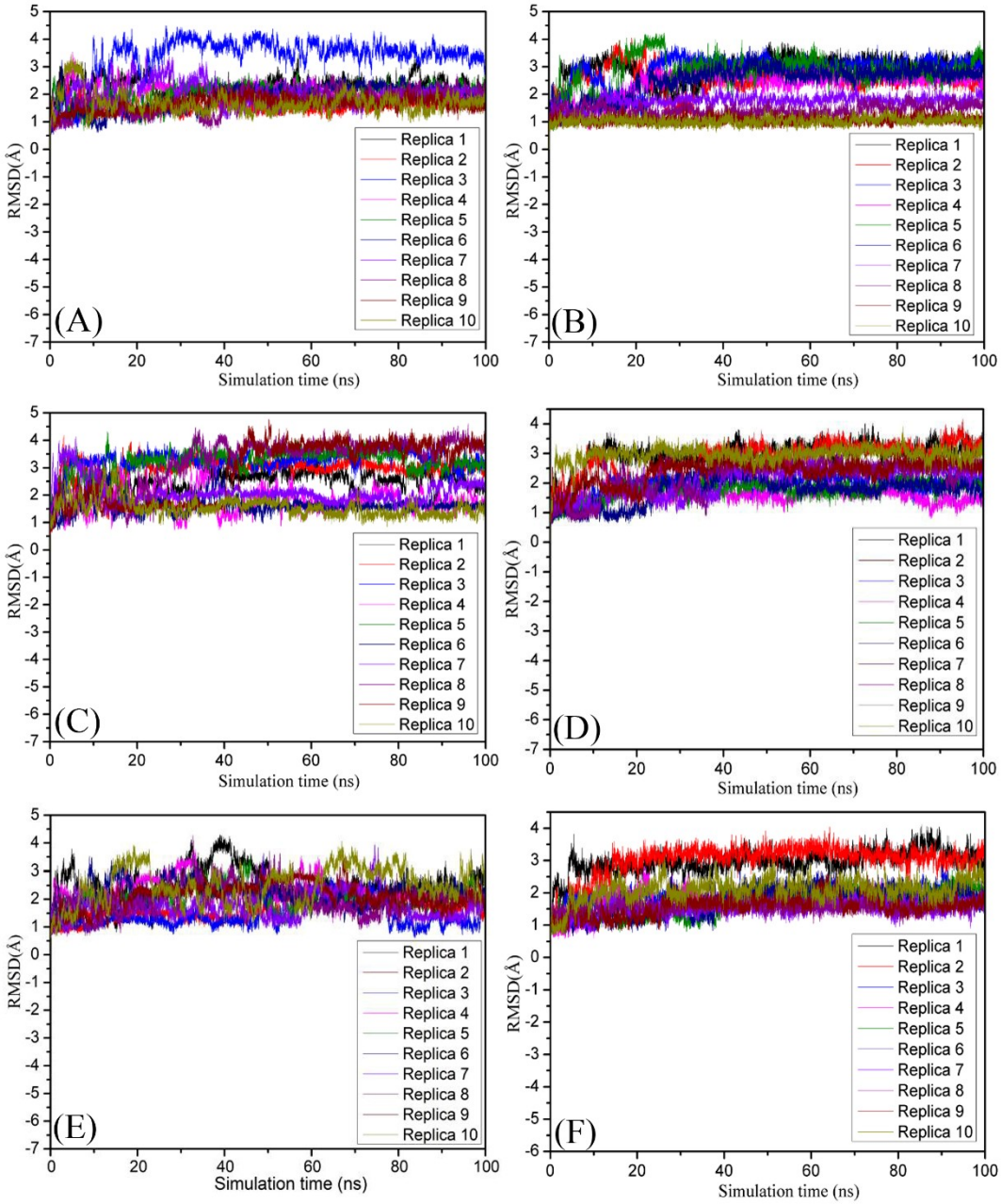

Fig. S1 Root-mean-square deviations (RMSDs) of backbone atoms in BRD7 and BRD9 calculated by using MSMD trajectories of ten replicas: (A) the 4L2-BRD7 complex, (B) the 4L2-BRD9 complex, (C) the 5U6-BRD7 complex, (D) the 5U6-BRD9 complex, (E) the 6KT-BRD7 complex and (F) the 6KT-BRD9 complex.

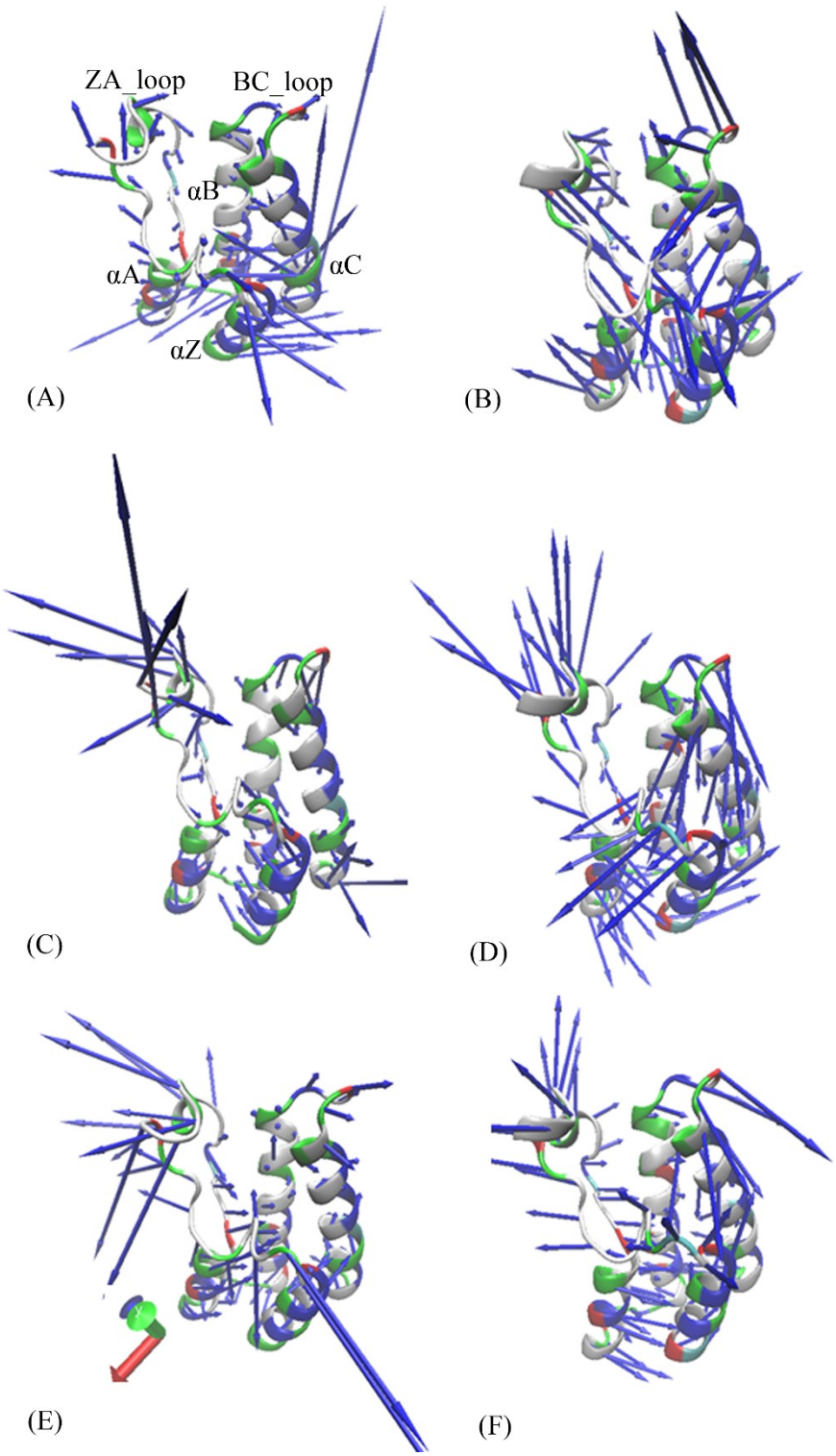

Fig. S2 Collective motions corresponding to the first component PC1 obtained from principal component (PC) analysis based on the single joined MSMD trajectories: (A) the 4L2-BRD7 complex, (B) the 4L2-BRD9 complex, (C) the 5U6-BRD7 complex, (D) the 5U6-BRD9 complex, (E) the 6KT-BRD7 complex and (F) the 6KT-BRD9 complex.

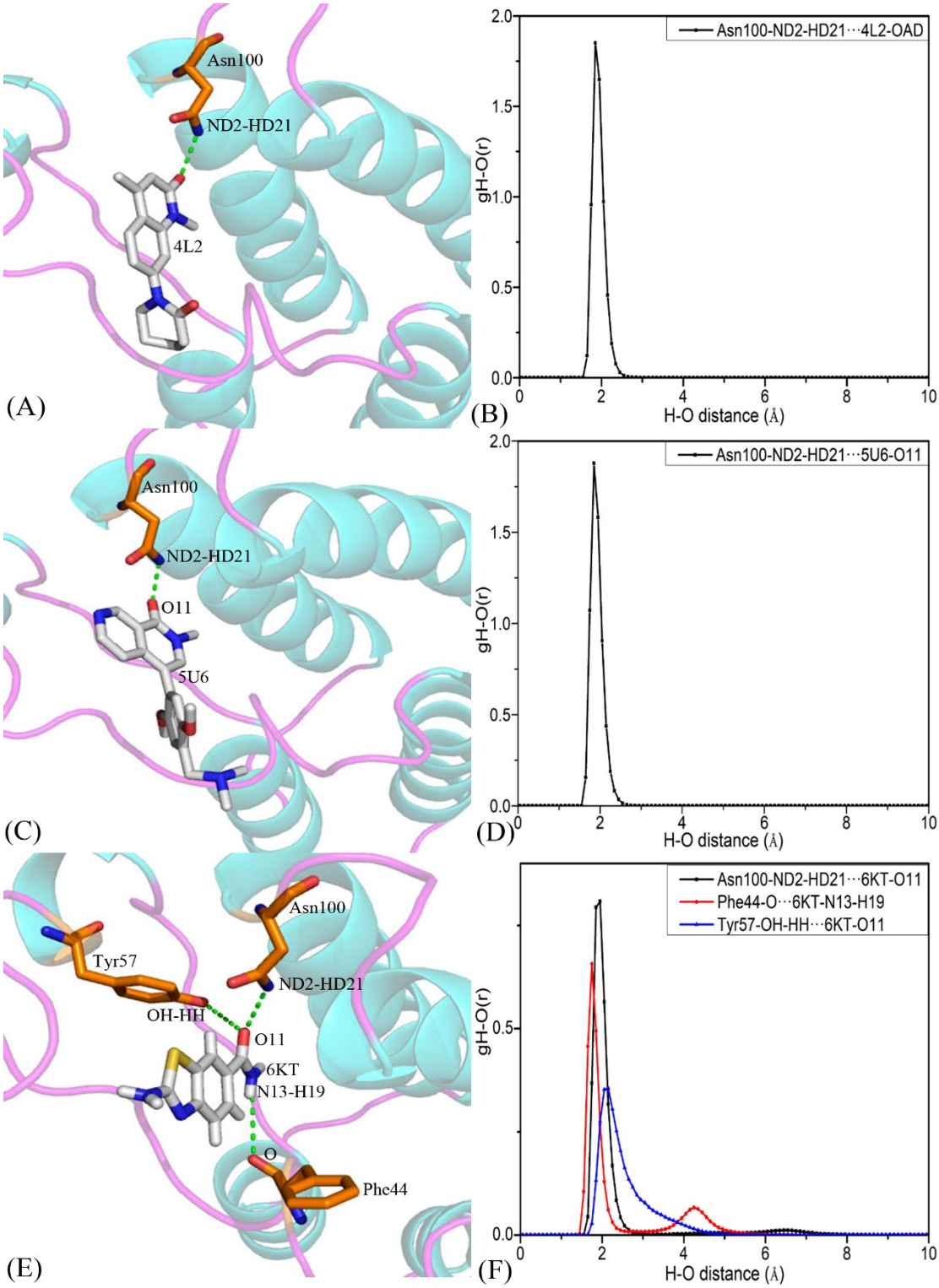

Fig. S3 Hydrogen bonds and the corresponding radial distribution function (RDF) of H-O distance between three inhibitors and key residues of BRD9: (A) the 4L2-BRD9 complex, (B) RDF of H-O distance between 4L2-OAD and Asn100-ND2-HD21, (C) the 5U6-BRD9 complex, (D) RDF of H-O distance between 5U6-O11 and Asn100-ND2-HD21, (E) the 6KT-BRD9 complex and (F) RDF of H-O distances between 6KT-O11 and Asn100-ND2-HD21, 6KT-N13-H19 and Phe44-O, and 6KT-O11 and Tyr57-OH-HH.