Supporting information.

Deciphering the functional mechanism of zinc ions of PARP1 binding with single-strand breaks and double strand-strand breaks.

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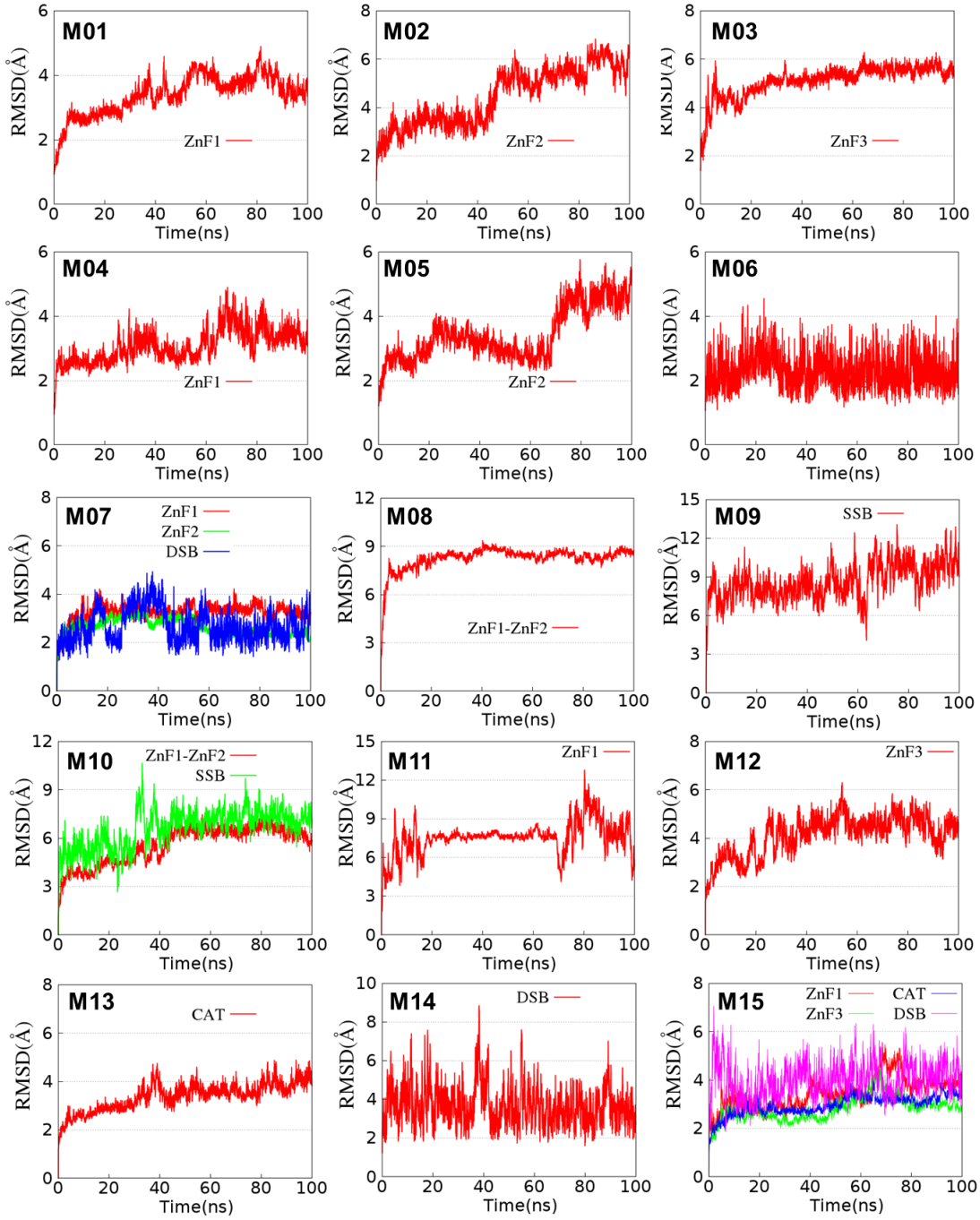

Fig S1. RMSDs of all system in Table 1.

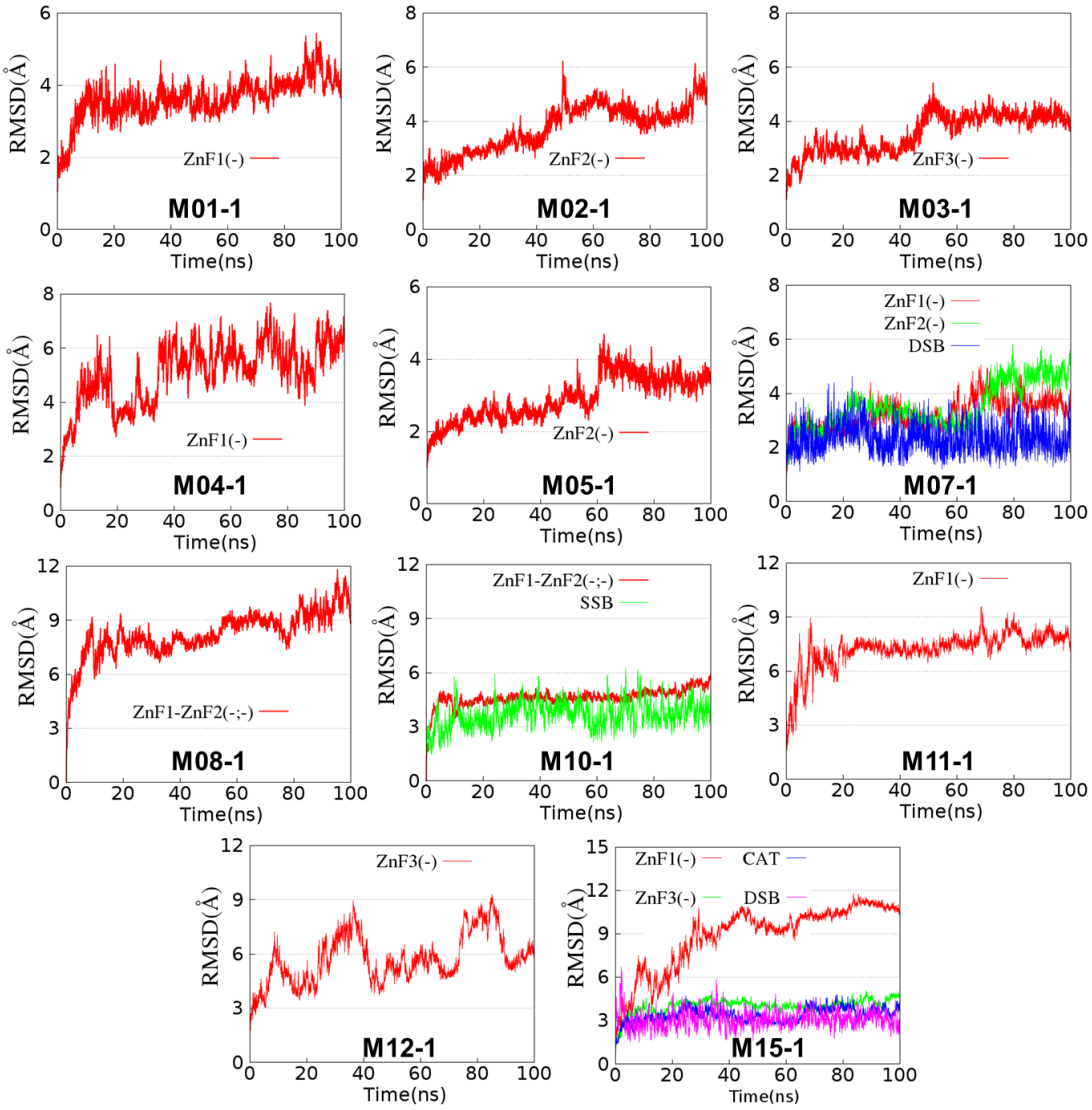

Fig S2. RMSDs of all system of Table 2.

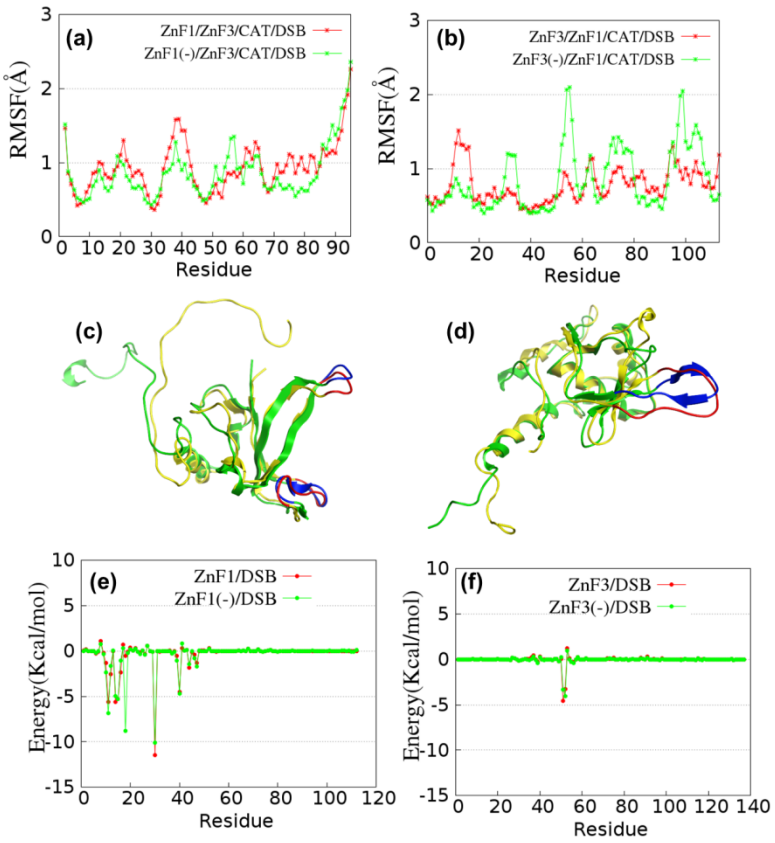

Fig S3. The binding interaction analysis between ZnF1(-)/ZnF3(-) and DSB. (a) Comparison of RMSF values of ZnF1 between ZnF1/DSB and ZnF1(-)/DSB complex. (b) Comparison of RMSF values of ZnF3 between ZnF3/DSB and ZnF3(-)/DSB complex. (c-d) The Comparison of 3D structures of ZnF1 and ZnF3 or ZnF1(-) and ZnF3(-) binding with DSB after 100 ns MD simulation. The green cartoon model is ZnF1 or ZnF3 in the system of ZnF1/ZnF3/DSB, and the yellow one is ZnF1(-) or ZnF3(-) in ZnF1(-)/ZnF3(-)/DSB. Blue and red cartoon correspond to the loop area of L_1 or L_2 in ZnF1/ZnF3/DSB and ZnF1(-)/ZnF3(-)/DSB, respectively. (e-f) The per-residue energy decomposition of ZnF1 in ZnF1/DSB and ZnF1(-) in ZnF1(-)/DSB and the per-residue energy decomposition of ZnF3 in ZnF3/DSB and ZnF3(-) in ZnF3(-)/DSB.

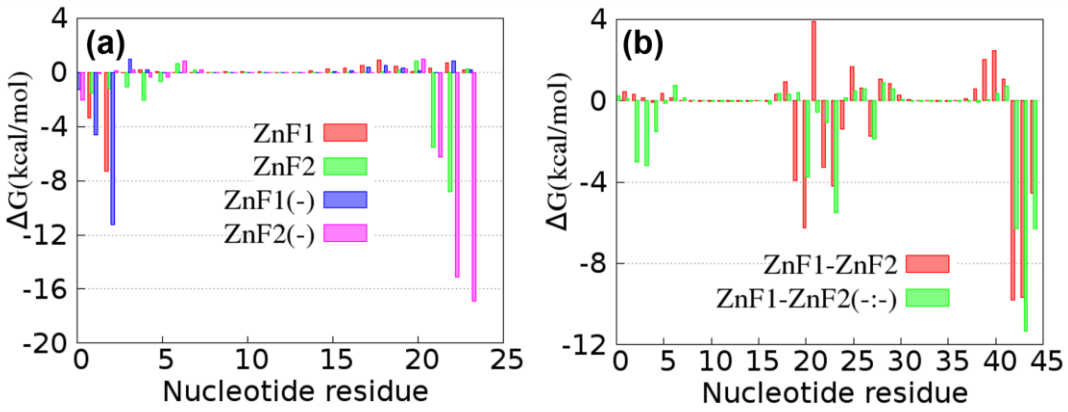

Fig S4. The per-nucleotide-residue energy contribution spectrum of DSB and SSB. (a) The comparison of per residue energy contribution spectrum of DSB binding with ZnF1/ZnF2/ZnF1(-)/ZnF2(-). (b) The comparison of per residue energy contribution spectrum of SSB binding with ZnF1-ZnF2 and ZnF1-ZnF2(-:-).

Table S1. The calculated (MM/GBSA) binding free energies of ZnF1/ZnF3/DSB and ZnF1(-)/ZnF3(-)/DSB complex

Terms	**ZnF1/DSB**	**ZnF3/DSB**	**ZnF1(-)/DSB**	**ZnF3(-)/DSB**
ΔE_{vdw} [a]	-51.01	-10.26	-51.11	-10.43
ΔE_{ele} [b]	-774.63	-420.70	-856.52	-642.66
ΔE_{polar} [c]	778.03	435.07	854.76	656.91
$\Delta E_{nonpolar}$ [d]	-6.14	-1.43	-6.37	-1.59
ΔG [e]	-53.75	2.68	-59.24	2.23

[a] Van der Waals energy.

[b] Electrostatic energy.

[c] Polar solvation free energy.

[d] Non-polar solvation free energy.

[e] Calculated Gibbs free energy. All the energy terms are in Kcal/mol.