Supporting Information

Probing the Binding Mode and Interactions of Proteinase K and Glutathione: Molecular Simulation and Experiments

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Content

Supplementary figures

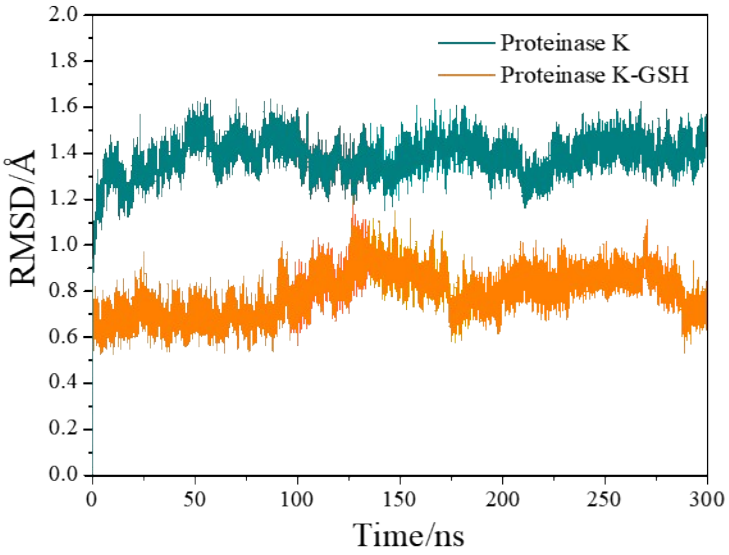

Fig. S1 RMSD fluctuations of proteinase K before and after binding to GSH.

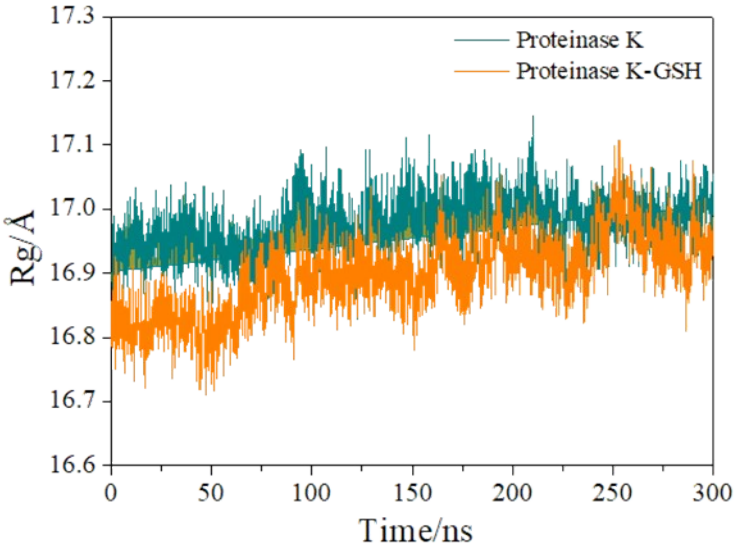

Fig. S2 Rg of proteinase K before and after binding to GSH.

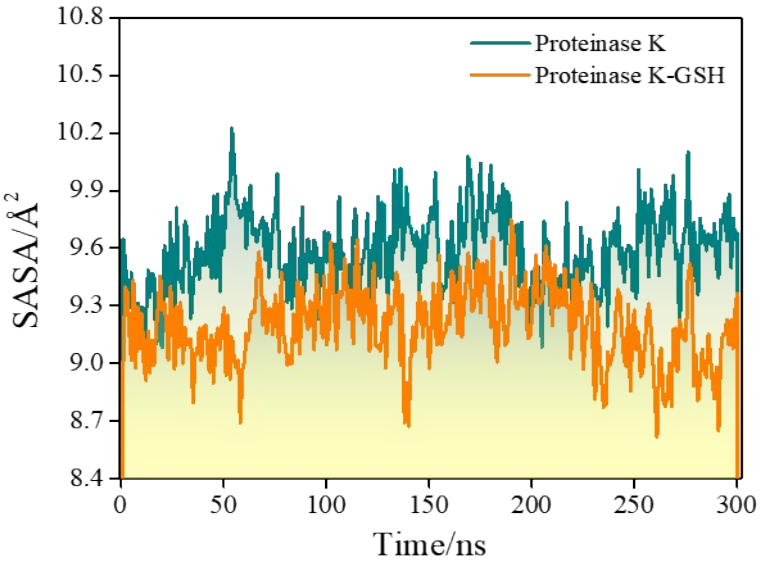

Fig. S3 SASA of proteinase K before and after binding to GSH.

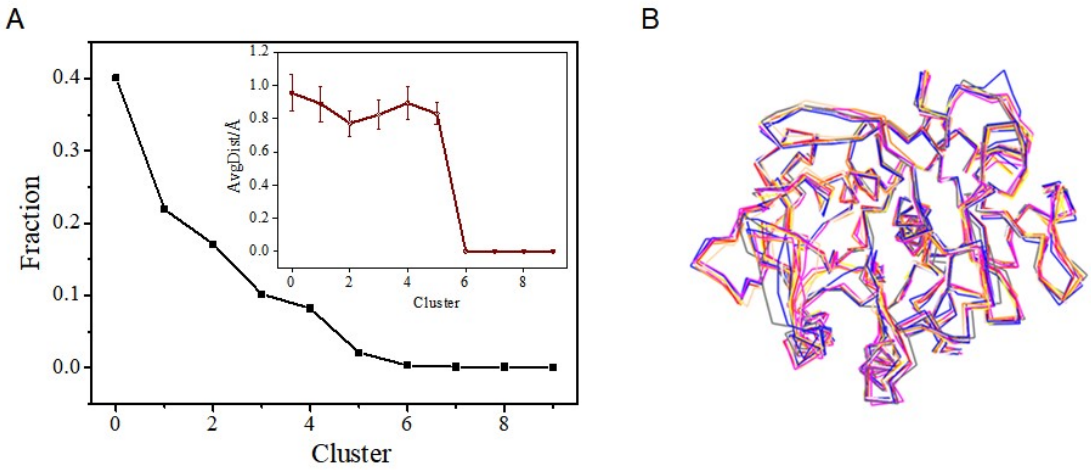

Fig. S4 (A) The clusters of proteinase K-GSH complex. (B) The spatial conformation of clusters.

Supplementary tables

Table S1 Energetic contributions of significant residues of proteinase K bindings with GSH

Residue	B_{vdw} [a)]	S_{vdw} [a)]	B_{ele} [a)]	S_{ele} [a)]	Polar solv. [a)]	Total [a)]
Asp39	-0.122	1.142	-0.024	-24.455	16.349	-7.154
His69	-0.178	-0.528	0.421	-0.746	0.797	-0.362
Leu96	-0.039	-0.961	-0.047	0.282	-0.056	-1.049
Leu133	-0.596	-1.569	-1.373	0.240	0.961	-2.476
Glu135	-0.575	-0.322	-1.419	0.239	1.176	-1.044
Asn161	-0.180	-0.405	-0.265	-0.277	0.975	-0.244
Asn162	-0.067	-0.191	-0.054	-1.971	1.721	-0.713
Ser224	-0.076	-0.328	-0.462	0.229	0.324	-0.351

[a)] All energy units are kJ mol^{-1}. B_{vdw} represents the van der Waals forces of the backbone of amino acid residues; S_{vdw} represents the van der Waals forces of the side chain of amino acid residues; B_{ele} represents the electrostatic interactions of the backbone of amino acid residues; S_{ele} represents the electrostatic interactions of the side chain of amino acid residues; Polar solv. represents the free energy of polar solvation.

Table S2 Hydrogen bonding interactions of GSH with proteinase K

Acceptor	DonorH	Donor	Frac/%	AvgDist/Å	AvgAng/deg
Asp39@OD1	GSH@HO4	GSH@O4	29.47	2.6572	162.2084
Asp39@OD2	GSH@HO4	GSH@O4	22.22	2.6493	161.5201
Gly100@O	GSH@HO4	GSH@O4	8.99	2.7413	156.8901
Ser132@O	GSH@H7	GSH@N1	7.61	2.8690	153.0704
GSH@O1	Ser224@H	Ser224@N	23.23	2.8852	164.3316
GSH@O6	Asn161@HD21	Asn161@ND2	21.85	2.8355	151.5626
GSH@O6	Asn161@H	Asn161@N	15.05	2.8764	158.3816
GSH@O2	Gly134@H	Gly134@N	12.34	2.8713	159.2309
GSH@O6	Asn162@HD21	Asn162@ND2	9.31	2.8654	156.0028

Table S3 The quenching constants of the interaction of proteinase K with GSH.

T/K	K_{sv}/(L·mol^{-1})	K_q/(L·mol^{-1}·s^{-1})	R^2
298	4821.1	4.82×10^{11}	0.994
303	4727.6	4.73×10^{11}	0.995
308	4305.1	4.31×10^{11}	0.989

Table S4 The content of secondary structures of proteinase K with GSH.

Sample	Alpha helix (%)	Beta sheet (%)	Turn (%)	Unordered (%)
proteinase K	7.9	27.7	10.9	53.5
proteinase K + 34 μM GSH	7.9	29.5	11.4	51.2
proteinase K + 170 μM GSH	7.1	34	7.5	51.4
proteinase K + 340 μM GSH	6.6	33.9	6.7	52.8
proteinase K + 680 μM GSH	6.8	34.2	6.9	52.1