Electronic Supplementary Information for

"Immobilization of papain on nanoporous silica"

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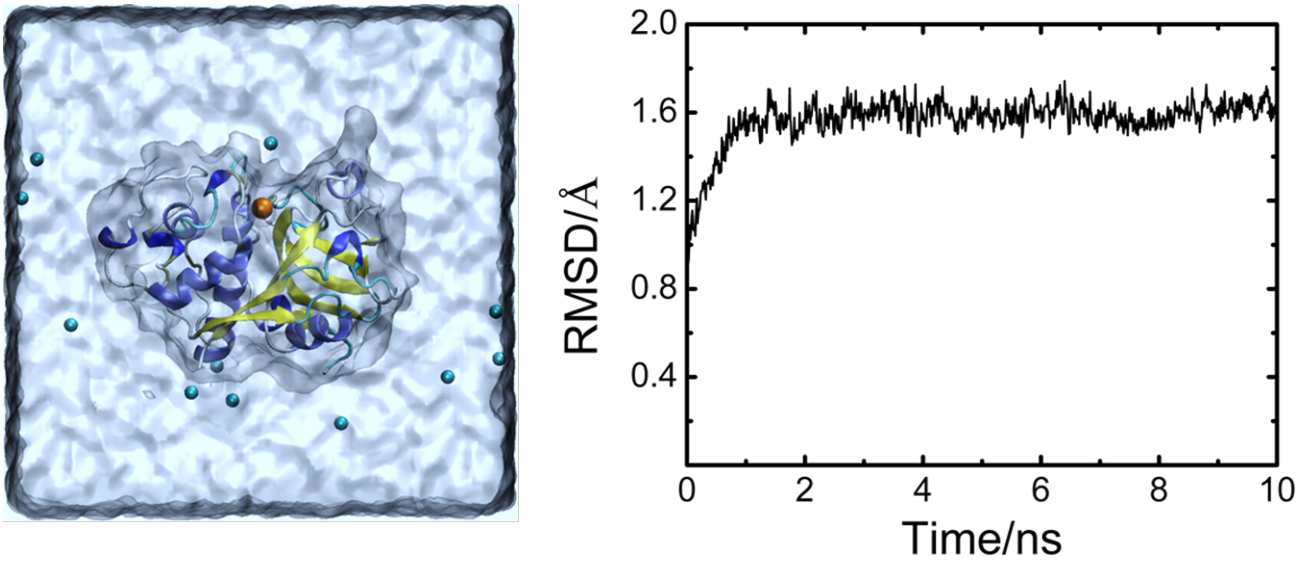

Figure S1. Time evolution of the aligned RMSD over the papain with respect to its initial structure.

Table S1. Parameters and atomic partial charges of silica used in the simulations.

Atom Type	σ (Å)	ε (kJ mol^{-1})	q (e)
Si	4.4	0.6	1.08
O	3.54	0.1521	-0.54
Oh[a]	3.54	0.1521	-0.59[b]
H	0.449	0.046	0.32

[a] Silanol O atom.

[b] q_{Oh} value from -0.54 to -0.59 e to ensure neutrality

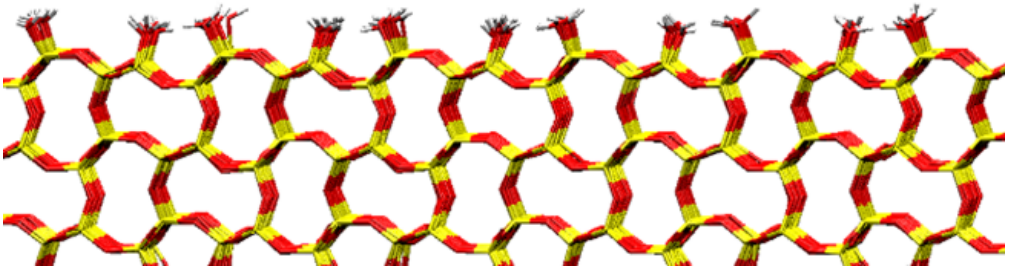

Figure S2. Structure of silica surface in the present study. The silica surface was constructed with a surface area of 103 Å × 103 Å.

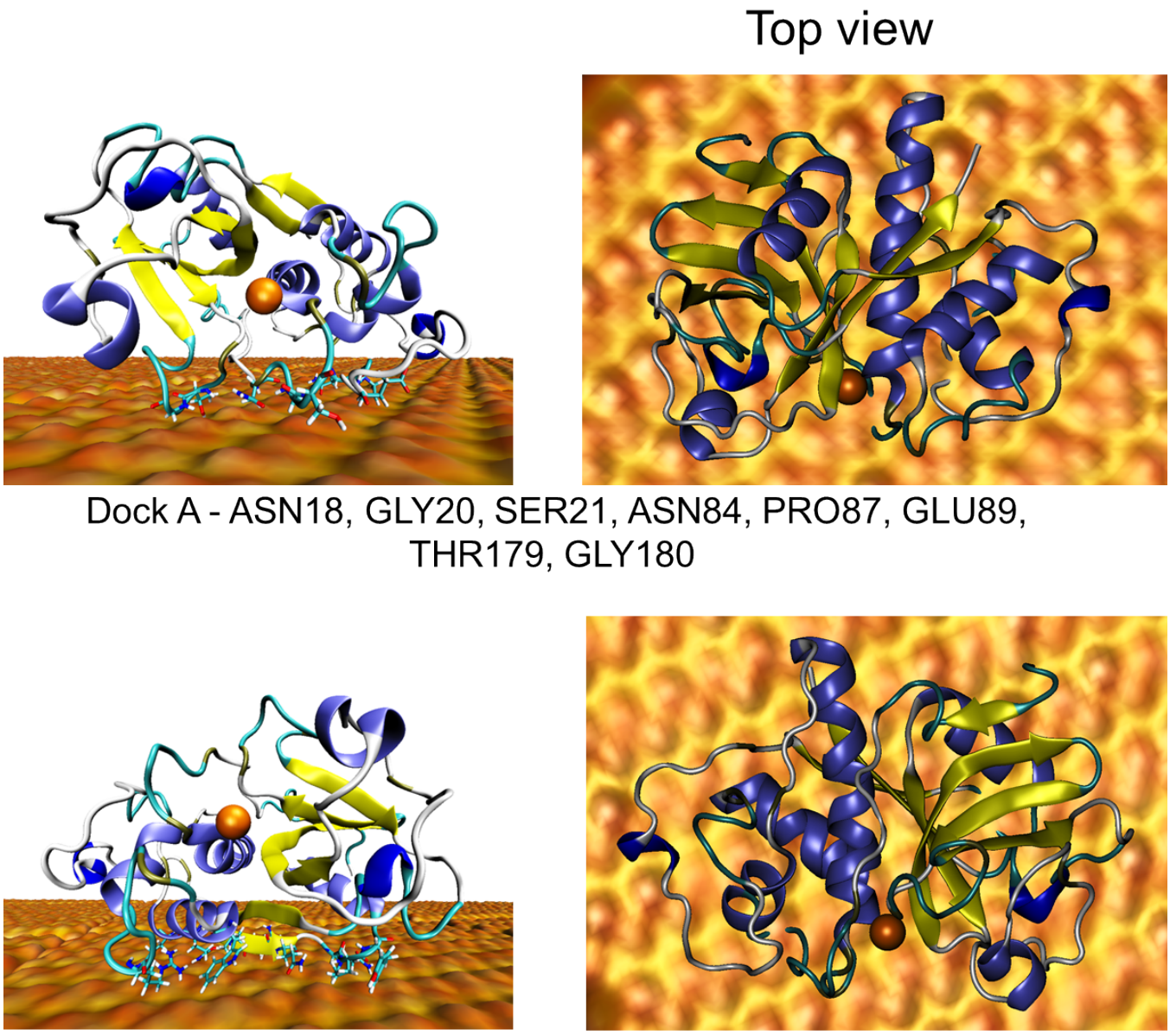

Figure S3. Conformations of the top two docked complexes obtained by the PatchDock and FireDock package. The two orientations in Dock A and B were used as representative orientations in adsorption simulations, denoted as Orientation I and II, respectively. The atom S of residue CYS25 in active center is highlighted by orange sphere.

Table S2. Detail of systems for MD simulation. The simulations of each orientation were repeated five times.

Orientation	Number of Atoms			
	Papain	Silica	Water	Ion
Orientation I	3253	10227	73842	11
Orientation II	3253	10227	73854	11

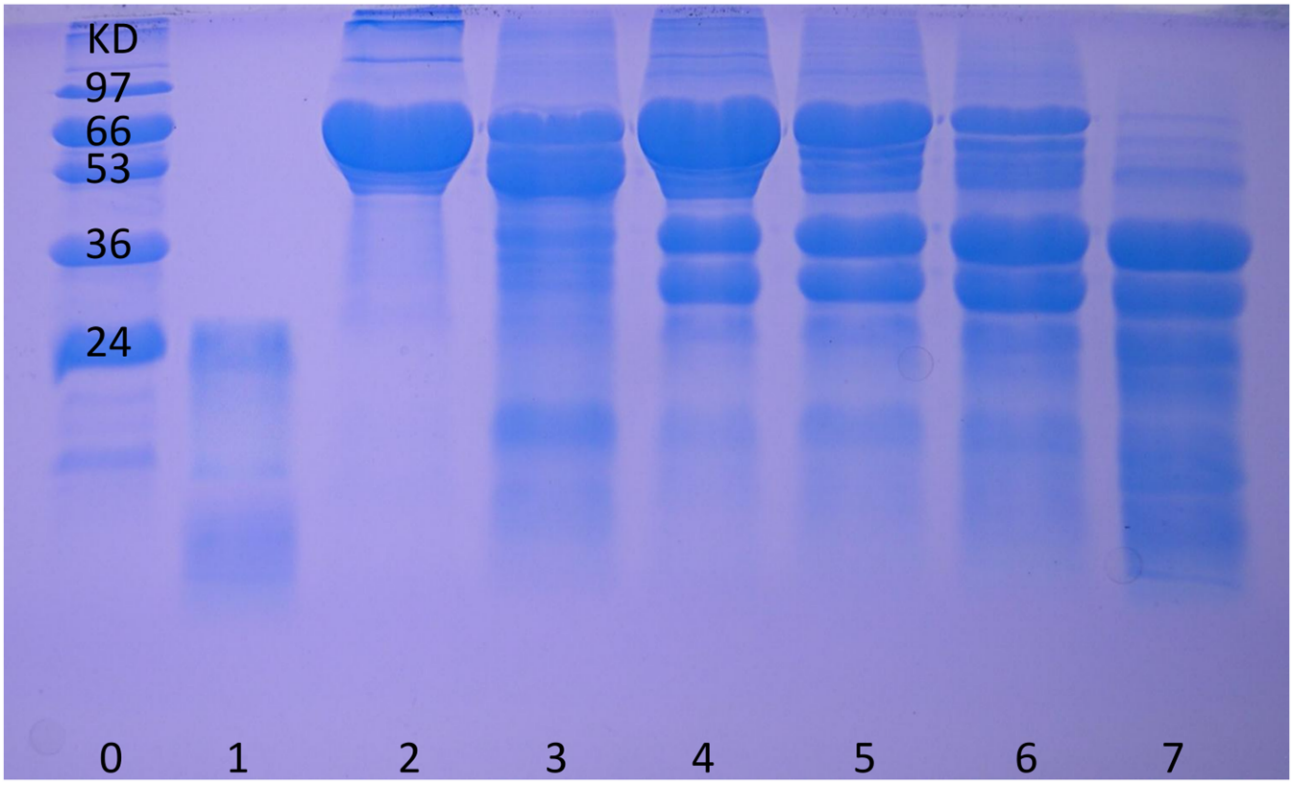

Figure S4. The digestive pattern of different concentrations of bovine serum albumin (BSA) digested by papain. The amounts in each wells are as follows: lane 0, protein molecular weight maker; lane 1, 5 mg ml^{-1} papain; lane 2, 4 mg ml^{-1} BSA; lane 3-7, papain:BSA (w/w) is 1:100, 1:20, 1:10, 1:4, respectively.

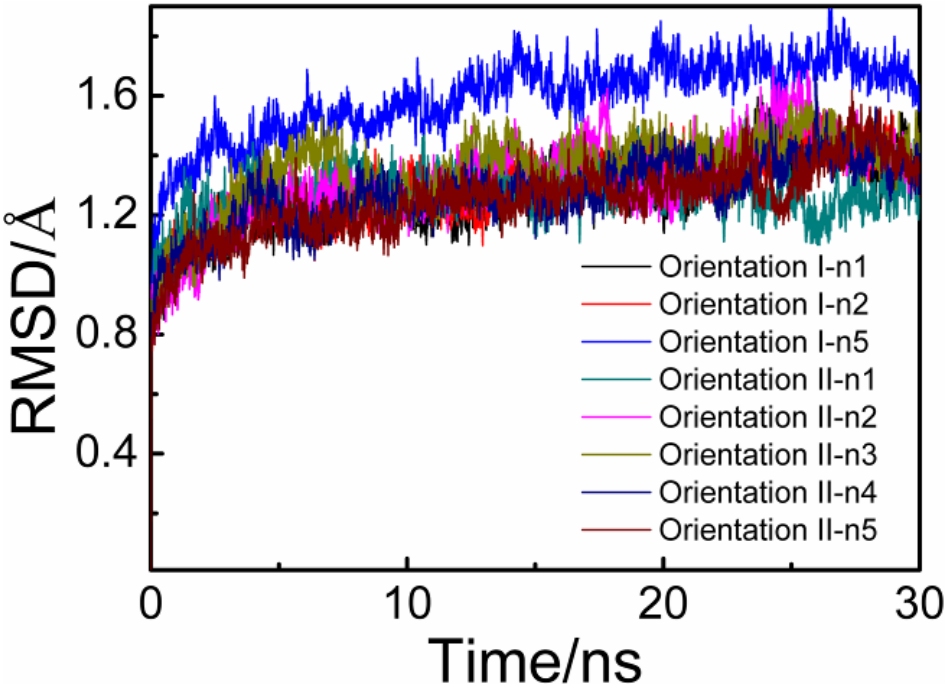

Figure S5. Time evolution of the aligned RMSD over the papain with respect to its initial structure for each adsorption system.