Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Molecular dynamics investigation on the interaction of human angiotensin-converting enzyme with tetra-peptide inhibitors

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Table S1 Mutation Energy of Single Mutation Based on Tetra-peptide YIHP (Tyr3-Ile4-His5-Pro6) (kcal/mol).

	Tyr3	Ile4	His5	Pro6
Gly	4.04	0.71	1.37	3.38
Ala	3.36	-0.05	0.77	2.11
Val	2.15	-0.05	1.99	2.49
Leu	1.77	0.24	2.18	0.18
Ile	3.20	----	1.21	1.20
Ser	3.68	0.06	1.14	2.45
Thr	2.93	-0.51	1.14	2.41
Cys	3.16	-0.04	0.53	2.07
Met	2.50	0.41	1.92	1.20
Asp	5.11	3.28	5.47	6.64
Glu	7.27	4.26	7.83	7.16
Asn	1.45	-0.69	0.65	3.62
Gln	5.98	-0.32	2.48	1.80
Lys	1.19	-2.70	-0.82	-1.63
Arg	-0.01	-2.15	1.42	0.02
His	0.47	0.14	----	0.58
Pro	-0.76	0.27	9.09	----
Phe	-0.29	-0.48	-0.10	1.26
Tyr	----	-0.58	-0.17	1.43
Trp	1.43	5.05	2.98	2.72

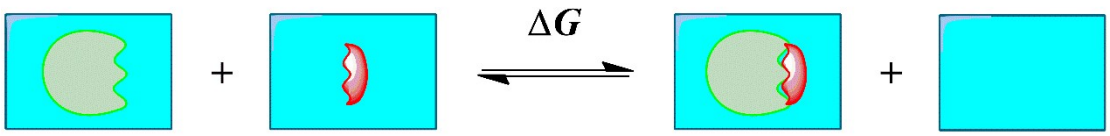
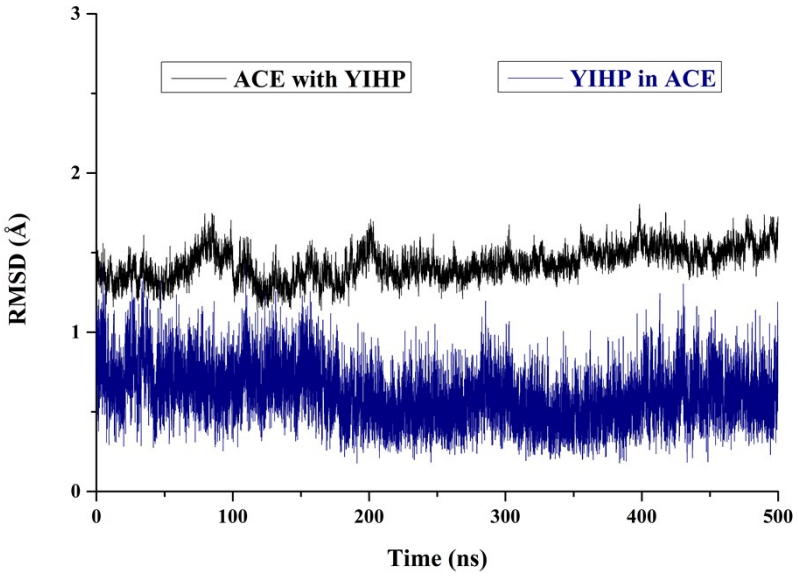
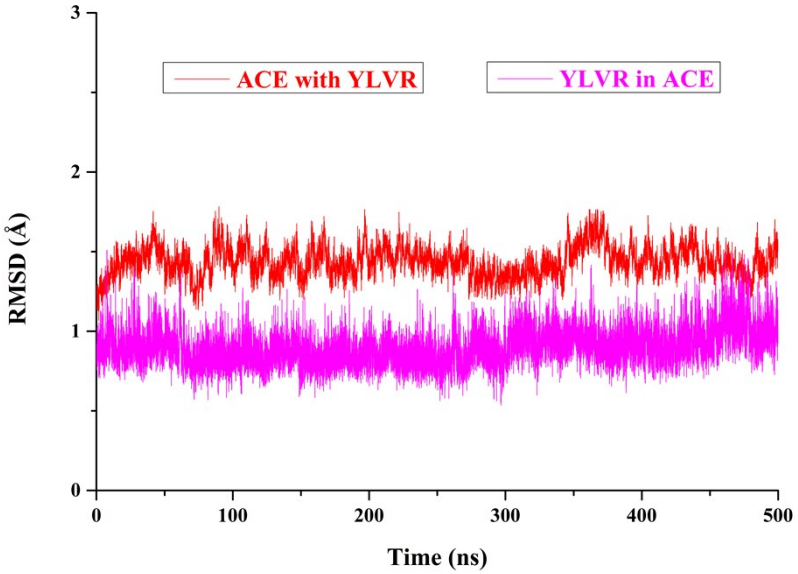


Fig. S1 Schematic diagram of a ligand binding with a receptor in aqueous solution. On the left side, a ligand is so far away from its receptor that the interaction between them can be ignored. Correspondingly, on the right side, a ligand and a receptor form a complex, and the solution area occupied by the ligand returns to an isotropic and homogeneous state.





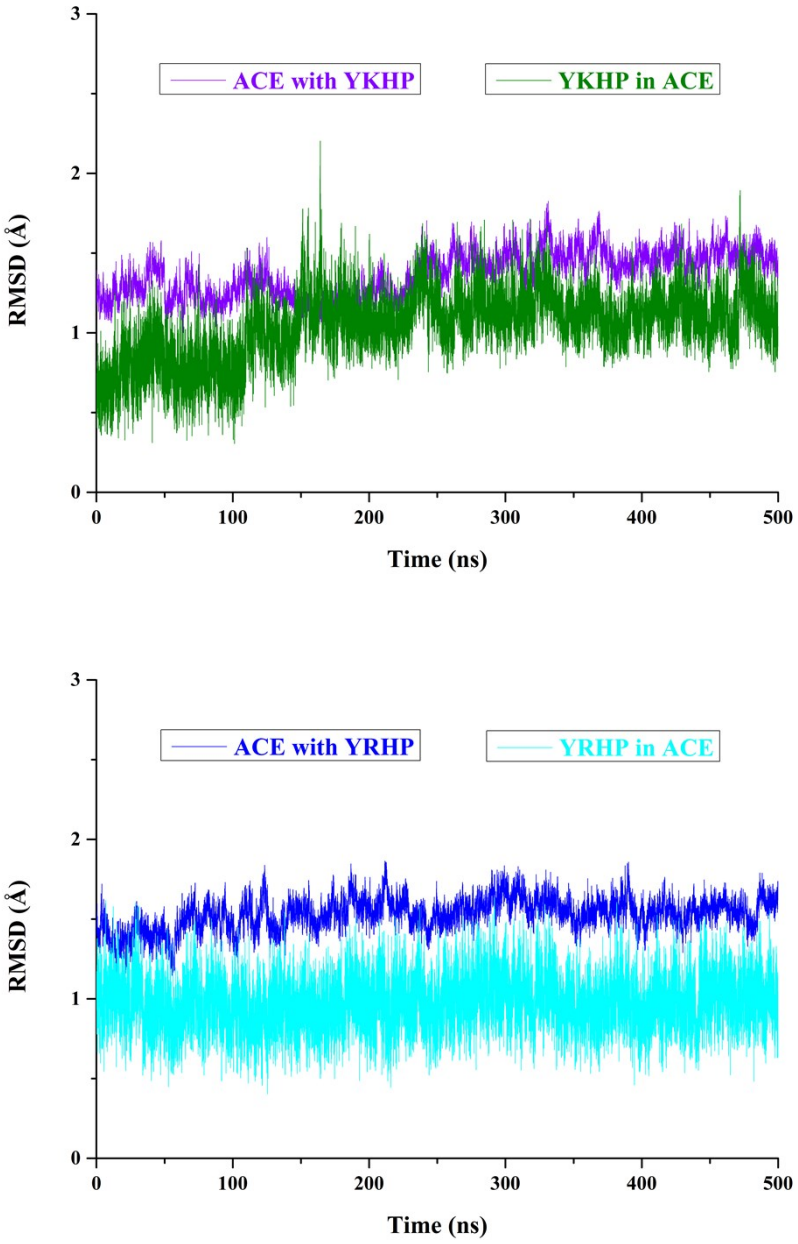
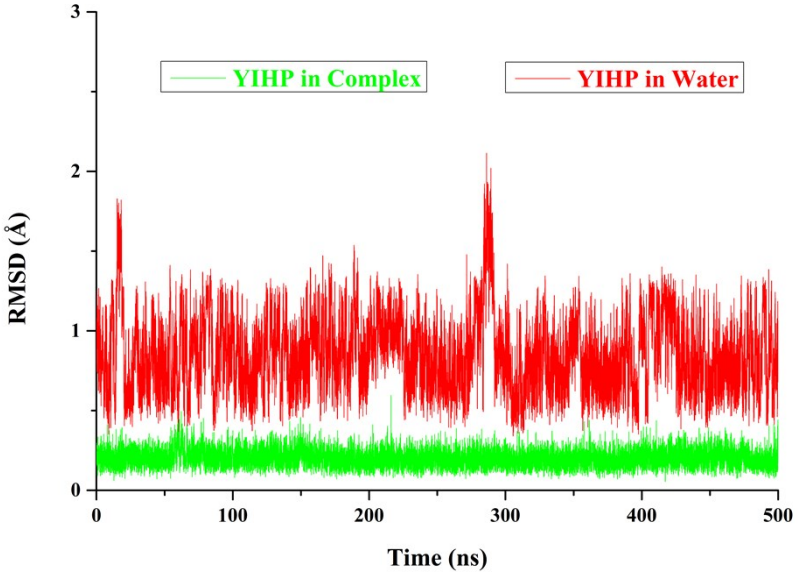
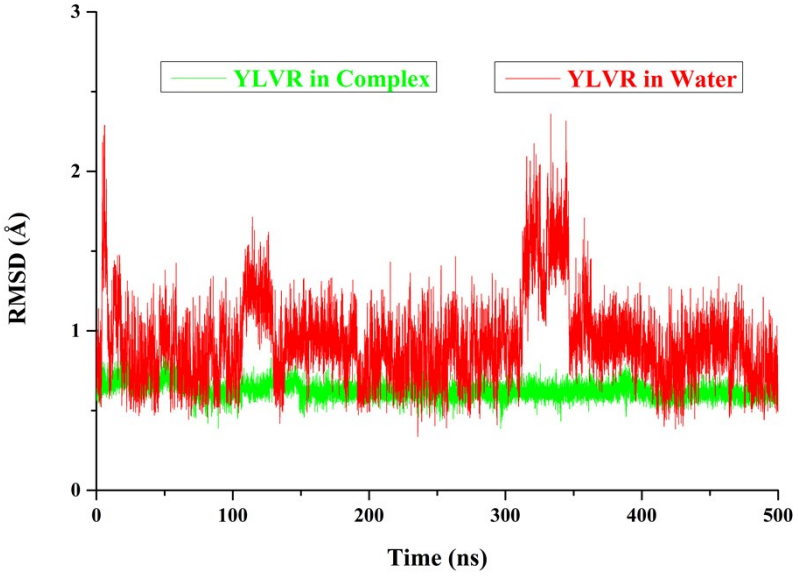


Fig. S2 RMSD curves of the backbone atoms of hACEs and tetrapeptides in the four complex systems during the production simulation phase. Taking the initially constructed model as the reference, the structural superimpositions were performed on the basis of the hACE backbone atoms prior to the RMSD calculation.


YIHP in Complex
YIHP in Water
RMSD (Å)
Time (ns)
0
1
2
3
0
100
200
300
400
500


YLVR in Complex
YLVR in Water
RMSD (Å)
Time (ns)
0
1
2
3
0
100
200
300
400
500

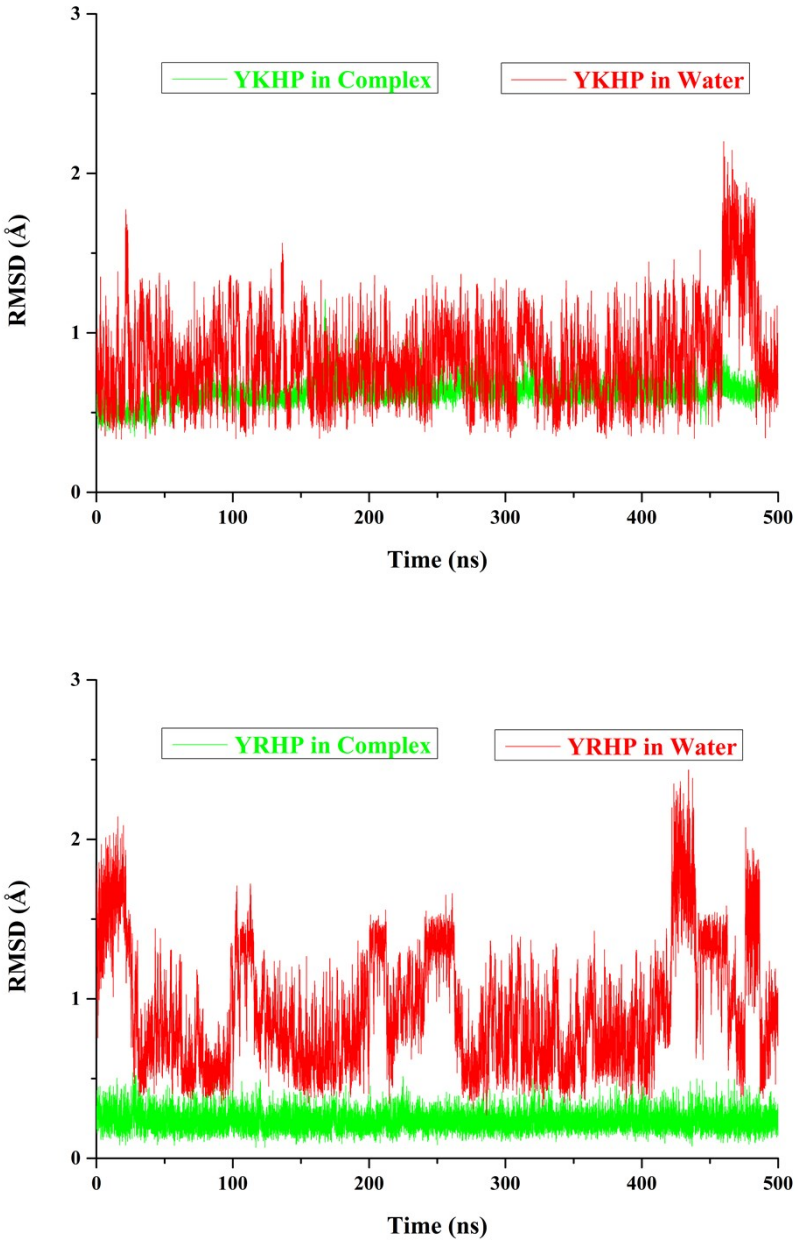
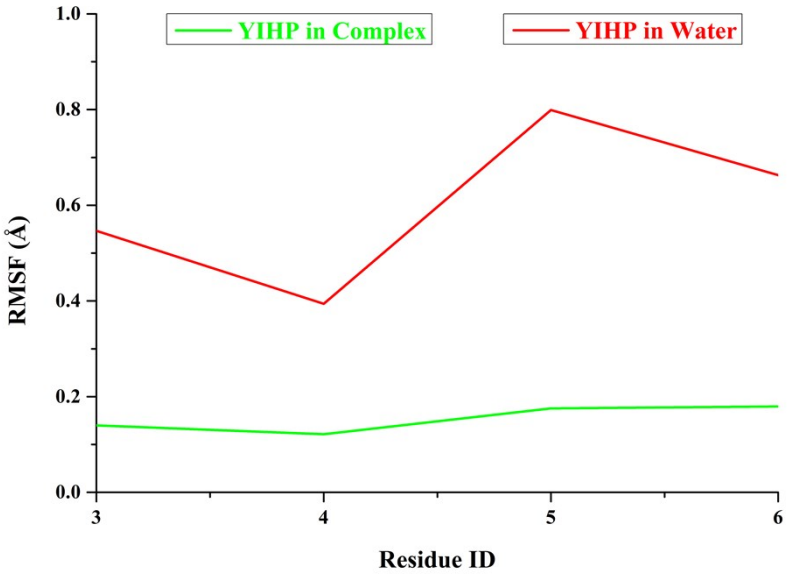
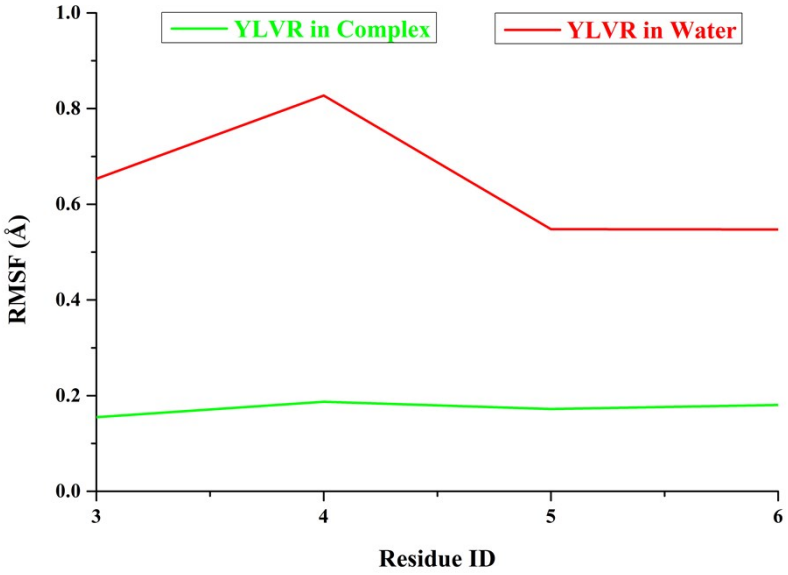


Fig. S3 RMSD curves of the backbone atoms of four tetrapeptides in the complex (green) and aqueous (red) systems during the production simulation phase. Taking the initial conformation of each tetrapeptide in the complex system as the reference, the structural superimpositions were performed on the basis of the backbone atoms prior to the RMSD calculation.


YIHP in Complex
YIHP in Water
RMSF (Å)
1.0
0.8
0.6
0.4
0.2
0.0
3
4
5
6
Residue ID


YLVR in Complex
YLVR in Water
RMSF (Å)
1.0
0.8
0.6
0.4
0.2
0.0
3
4
5
6
Residue ID

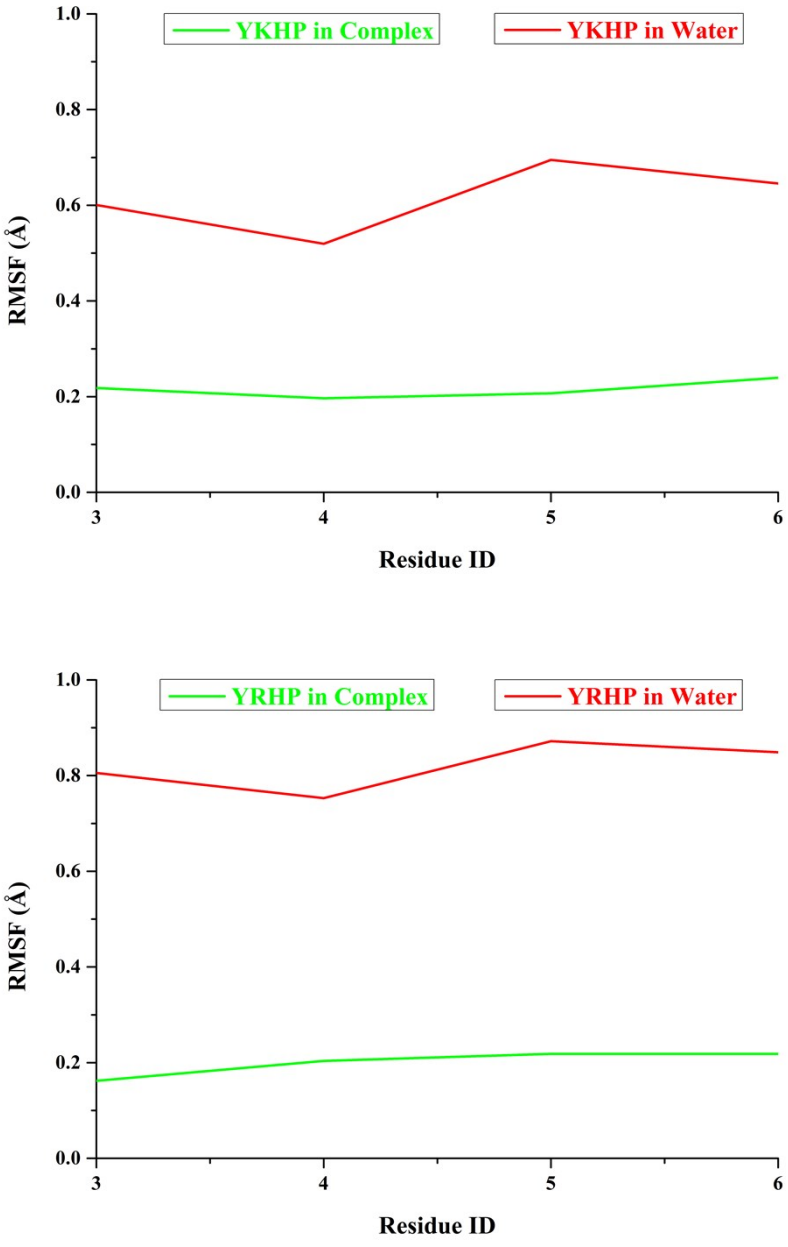


Fig. S4 RMSF curves of the Cα atoms of four tetrapeptides in the complex (green) and aqueous (red) systems during the production simulation phase. The structural superimpositions were performed on the basis of the Cα atoms prior to the RMSF calculation.

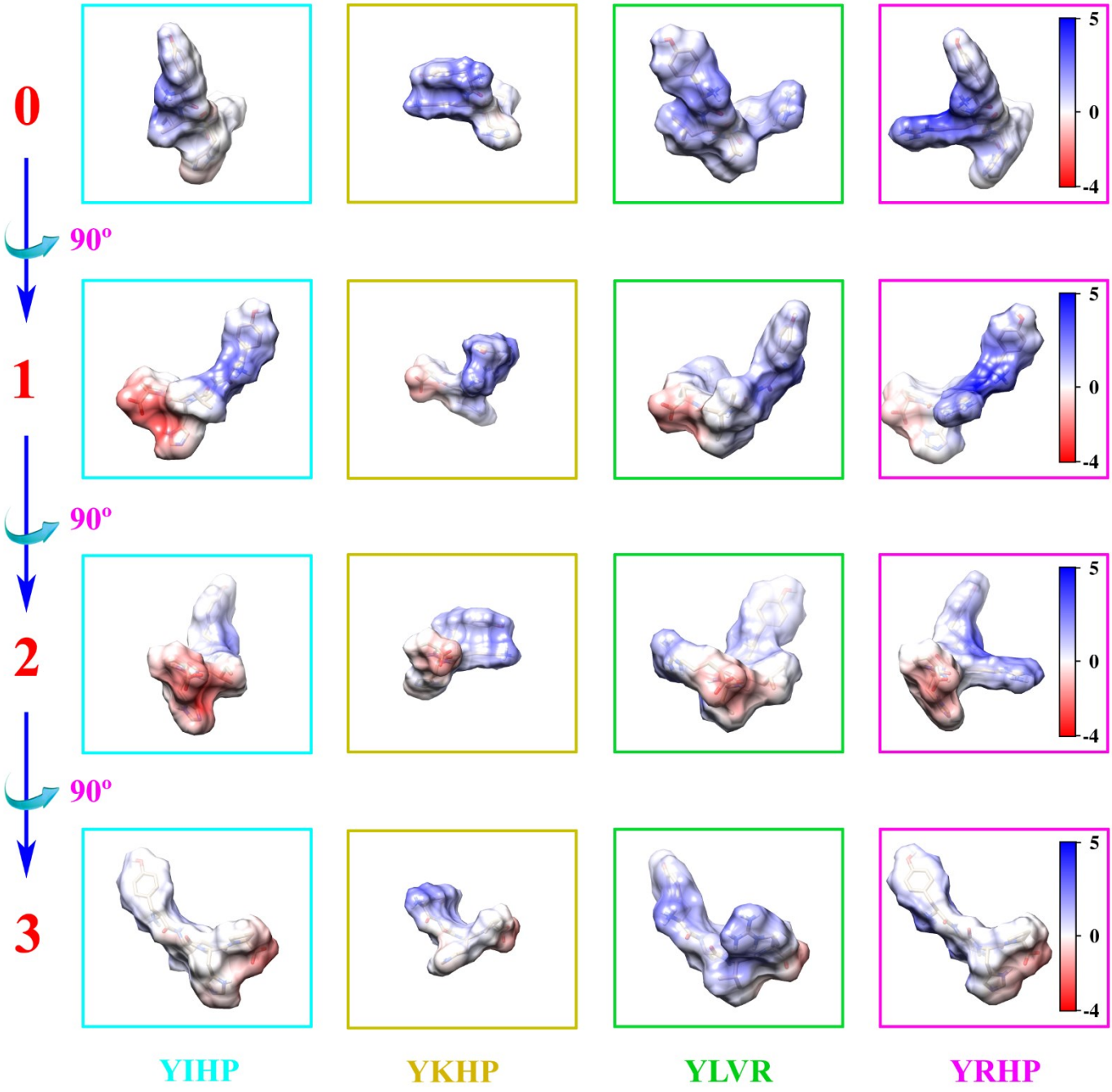


Fig. S5 The electrostatic potential surface for the representative conformations of four ligands. All the ligands were first superimposed and then calculated the electrostatic potential surface.

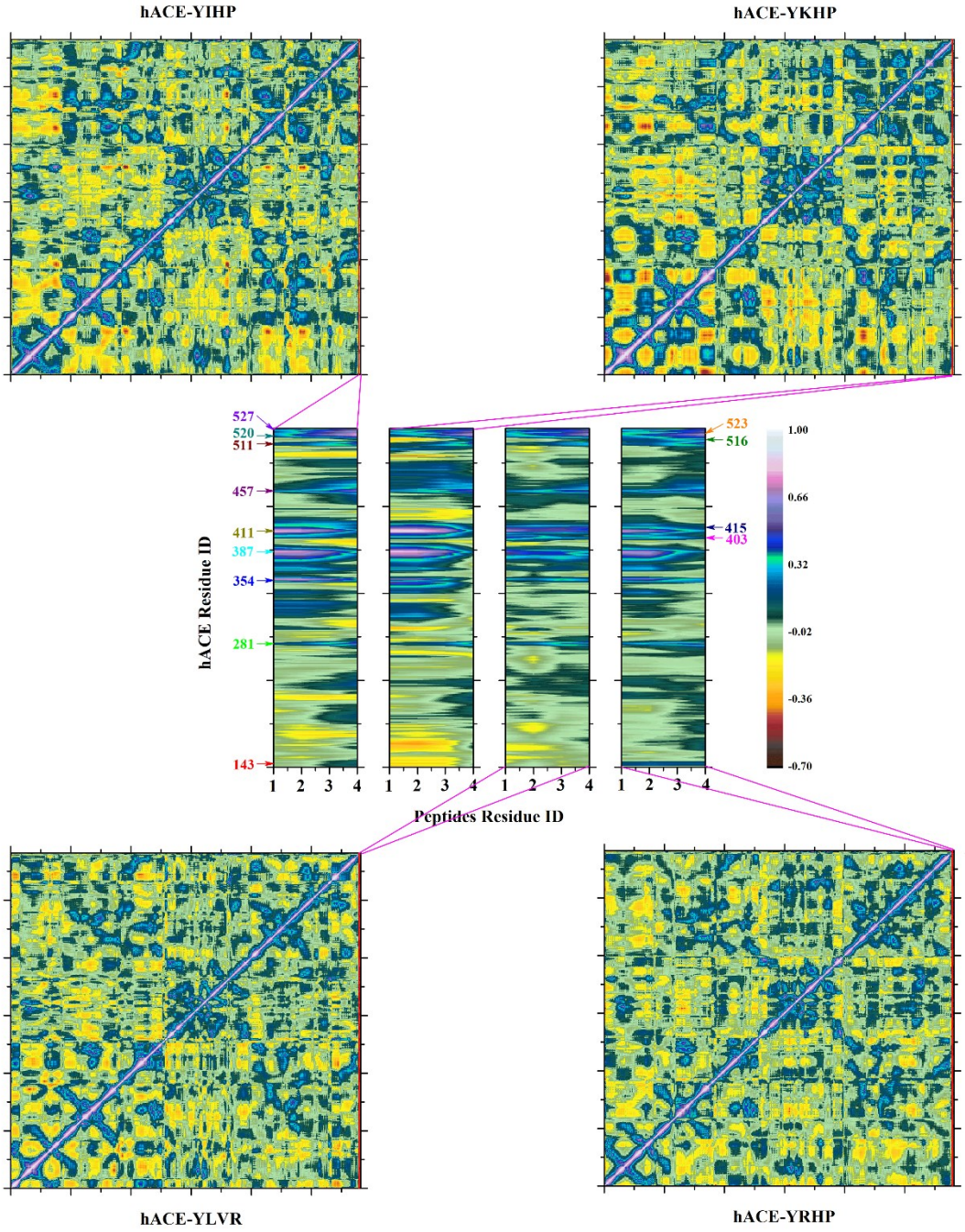


Fig. S6 Correlation analysis of the motion based on the Cα atoms during the 500 ns MD production simulation of the hACE-tetrapeptide complexes. At the center is the corresponding detail view of the correlation map for each complex.

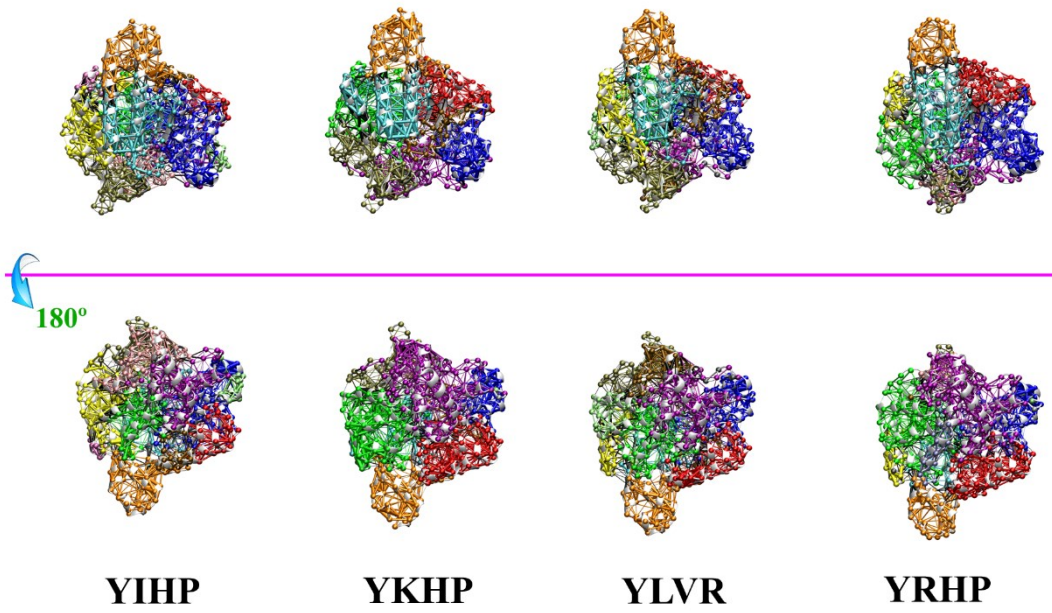


Fig. S7 Community distribution of four complex systems. The communities with the same color have the greatest similarity to each other.