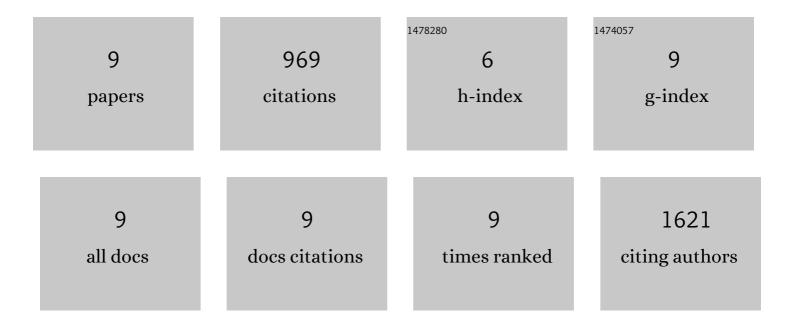


## List of Publications by Year in descending order

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Yi Li

#	Article	IF	CITATIONS
1	Insights into Protein–Ligand Interactions: Mechanisms, Models, and Methods. International Journal of Molecular Sciences, 2016, 17, 144.	1.8	885
2	Insights into the role of electrostatics in temperature adaptation: a comparative study of psychrophilic, mesophilic, and thermophilic subtilisin-like serine proteases. RSC Advances, 2018, 8, 29698-29713.	1.7	20
3	Comparative thermal unfolding study of psychrophilic and mesophilic subtilisin-like serine proteases by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1500-1517.	2.0	19
4	Molecular dynamics simulations reveal distinct differences in conformational dynamics and thermodynamics between the unliganded and CD4-bound states of HIV-1 gp120. Physical Chemistry Chemical Physics, 2020, 22, 5548-5560.	1.3	12
5	Effects of CD4 Binding on Conformational Dynamics, Molecular Motions, and Thermodynamics of HIV-1 gp120. International Journal of Molecular Sciences, 2019, 20, 260.	1.8	10
6	Insights into the molecular mechanism underlying CD4-dependency and neutralization sensitivity of HIV-1: a comparative molecular dynamics study on gp120s from isolates with different phenotypes. RSC Advances, 2018, 8, 14355-14368.	1.7	9
7	CD4-binding obstacles in conformational transitions and allosteric communications of HIV gp120. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183217.	1.4	6
8	Deciphering gp120 sequence variation and structural dynamics in <scp>HIV</scp> neutralization phenotype by molecular dynamics simulations and graph machine learning. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1413-1424.	1.5	5
9	Probing intrinsic dynamics and conformational transition of HIV gp120 by molecular dynamics simulation. RSC Advances, 2020, 10, 30499-30507.	1.7	3