

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

61 papers	746 citations	16 h-index	24 g-index
64 ext. papers	970 ext. citations	4.2 avg, IF	4.01 L-index

#	Paper	IF	Citations
61	COVID-19 Docking Server: a meta server for docking small molecules, peptides and antibodies against potential targets of COVID-19. <i>Bioinformatics</i> , <b>2020</b> , 36, 5109-5111	7.2	78
60	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2019</b> , 87, 1200-1221	4.2	58
59	Molecular dynamics simulations of wild type and mutants of human complement receptor 2 complexed with C3d. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 1241-51	3.6	44
58	Molecular dynamics simulations of DNA-free and DNA-bound TAL effectors. <i>PLoS ONE</i> , <b>2013</b> , 8, e76045	3.7	34
57	Construction and application of the weighted amino acid network based on energy. <i>Physical Review E</i> , <b>2007</b> , 75, 051903	2.4	29
56	Molecular dynamics simulation study reveals potential substrate entry path into $\beta$ -secretase/presenilin-1. <i>Journal of Structural Biology</i> , <b>2015</b> , 191, 120-9	3.4	27
55	Substrate recognition and transport behavior analyses of amino acid antiporter with coarse-grained models. <i>Molecular BioSystems</i> , <b>2010</b> , 6, 2430-8		26
54	Protein-protein docking with binding site patch prediction and network-based terms enhanced combinatorial scoring. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2010</b> , 78, 3150-5	4.2	26
53	Insight into the selective binding mechanism of DNMT1 and DNMT3A inhibitors: a molecular simulation study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 12931-12947	3.6	23
52	Molecular Dynamics Simulations of Wild Type and Mutants of SAPAP in Complexed with Shank3. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 20,	6.3	22
51	Importance of protein flexibility in molecular recognition: a case study on Type-11/2 inhibitors of ALK. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 4851-4863	3.6	21
50	Discovery of Novel Androgen Receptor Ligands by Structure-based Virtual Screening and Bioassays. <i>Genomics, Proteomics and Bioinformatics</i> , <b>2018</b> , 16, 416-427	6.5	19
49	Stability and folding behavior analysis of zinc-finger using simple models. <i>International Journal of Molecular Sciences</i> , <b>2010</b> , 11, 4014-34	6.3	18
48	Amino acid network and its scoring application in protein-protein docking. <i>Biophysical Chemistry</i> , <b>2008</b> , 134, 111-8	3.5	18
47	Reliability of Docking-Based Virtual Screening for GPCR Ligands with Homology Modeled Structures: A Case Study of the Angiotensin II Type I Receptor. <i>ACS Chemical Neuroscience</i> , <b>2019</b> , 10, 677-689	5.7	17
46	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2021</b> , 89, 1800-1823	4.2	17
45	Molecular dynamics simulations of wild type and mutants of botulinum neurotoxin A complexed with synaptic vesicle protein 2C. <i>Molecular BioSystems</i> , <b>2015</b> , 11, 223-31		16

44	CoDockPP: A Multistage Approach for Global and Site-Specific Protein-Protein Docking. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 3556-3564	6.1	15
43	Conopeptide Vt3.1 preferentially inhibits BK potassium channels containing $\beta$ subunits via electrostatic interactions. <i>Journal of Biological Chemistry</i> , <b>2014</b> , 289, 4735-42	5.4	15
42	Complex-type-dependent scoring functions in protein-protein docking. <i>Biophysical Chemistry</i> , <b>2007</b> , 129, 1-10	3.5	14
41	Exploring the molecular basis of RNA recognition by the dimeric RNA-binding protein via molecular simulation methods. <i>RNA Biology</i> , <b>2016</b> , 13, 1133-1143	4.8	14
40	Study on the interactions between diketo-acid inhibitors and prototype foamy virus integrase-DNA complex via molecular docking and comparative molecular dynamics simulation methods. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2013</b> , 31, 734-47	3.6	12
39	Molecular Simulation Studies on the Binding Selectivity of Type-I Inhibitors in the Complexes with ROS1 versus ALK. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 977-987	6.1	11
38	Molecular Dynamics Simulations of Ternary Complexes: Comparisons of LEAFY Protein Binding to Different DNA Motifs. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 784-94	6.1	11
37	Benchmark Study Based on 2P2I to Gain Insights into the Discovery of Small-Molecule PPI Inhibitors. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 2544-2555	3.4	11
36	Unraveling the conformational determinants of LARP7 and 7SK small nuclear RNA by theoretical approaches. <i>Molecular BioSystems</i> , <b>2016</b> , 12, 2613-21		11
35	Allosteric and transport behavior analyses of a fucose transporter with network models. <i>Soft Matter</i> , <b>2011</b> , 7, 4661	3.6	11
34	Substrate recognition and motion mode analyses of PFV integrase in complex with viral DNA via coarse-grained models. <i>PLoS ONE</i> , <b>2013</b> , 8, e54929	3.7	9
33	Probing the Behaviour of Cas1-Cas2 upon Protospacer Binding in CRISPR-Cas Systems using Molecular Dynamics Simulations. <i>Scientific Reports</i> , <b>2019</b> , 9, 3188	4.9	9
32	Scoring function based on weighted residue network. <i>International Journal of Molecular Sciences</i> , <b>2011</b> , 12, 8773-86	6.3	8
31	Improvement of Prediction Performance With Conjoint Molecular Fingerprint in Deep Learning. <i>Frontiers in Pharmacology</i> , <b>2020</b> , 11, 606668	5.6	8
30	Evolving model of amino acid networks. <i>Physical Review E</i> , <b>2008</b> , 77, 061920	2.4	7
29	Inhibition of programmed cell death protein ligand-1 (PD-L1) by benzyl ether derivatives: analyses of conformational change, molecular recognition and binding free energy. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2019</b> , 37, 4801-4812	3.6	7
28	A HTRF based competitive binding assay for screening specific inhibitors of HIV-1 capsid assembly targeting the C-Terminal domain of capsid. <i>Antiviral Research</i> , <b>2019</b> , 169, 104544	10.8	6
27	Understanding peptide competitive inhibition of botulinum neurotoxin A binding to SV2 protein via molecular dynamics simulations. <i>Biopolymers</i> , <b>2015</b> , 103, 597-608	2.2	6

26	Network analysis of protein-protein interaction. <i>Science Bulletin</i> , <b>2010</b> , 55, 814-822		6
25	Disruption of the EGFR-SQSTM1 interaction by a stapled peptide suppresses lung cancer via activating autophagy and inhibiting EGFR signaling. <i>Cancer Letters</i> , <b>2020</b> , 474, 23-35	9.9	6
24	A holistic molecular docking approach for predicting protein-protein complex structure. <i>Science China Life Sciences</i> , <b>2010</b> , 53, 1152-61	8.5	5
23	Study on the drug resistance and the binding mode of HIV-1 integrase with LCA inhibitor. <i>Science in China Series B: Chemistry</i> , <b>2007</b> , 50, 665-674		5
22	Applications of Molecular Simulation in the Discovery of Antituberculosis Drugs: A Review. <i>Protein and Peptide Letters</i> , <b>2019</b> , 26, 648-663	1.9	5
21	Two- and three-dimensional QSAR studies on hURAT1 inhibitors with flexible linkers: topomer CoMFA and HQSAR. <i>Molecular Diversity</i> , <b>2020</b> , 24, 141-154	3.1	5
20	Exploring the RNA-bound and RNA-free human Argonaute-2 by molecular dynamics simulation method. <i>Chemical Biology and Drug Design</i> , <b>2017</b> , 90, 753-763	2.9	4
19	Understanding the folding and stability of a designed WW domain protein with replica exchange molecular dynamics simulations. <i>Molecular Simulation</i> , <b>2013</b> , 39, 828-836	2	4
18	A filter enhanced sampling and combinatorial scoring study for protein docking in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2007</b> , 69, 859-65	4.2	4
17	Multitask deep networks with grid featurization achieve improved scoring performance for protein-ligand binding. <i>Chemical Biology and Drug Design</i> , <b>2020</b> , 96, 973-983	2.9	4
16	Study on The Binding Mode and Mobility of HIV-1 Integrase With L708, 906 Inhibitor*. <i>Progress in Biochemistry and Biophysics</i> , <b>2011</b> , 38, 338-346		3
15	Clinical recommendations for perioperative immunotherapy-induced adverse events in patients with non-small cell lung cancer. <i>Thoracic Cancer</i> , <b>2021</b> , 12, 1469-1488	3.2	3
14	Template-based modeling and ab-initio docking using CoDock in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2020</b> , 88, 1100-1109	4.2	2
13	Computational model for protein unfolding simulation. <i>Physical Review E</i> , <b>2011</b> , 83, 061910	2.4	2
12	Network models reveal stability and structural rearrangement of signal recognition particle. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2012</b> , 30, 150-9	3.6	2
11	Scoring Function for the Other-type Protein Complexes. <i>Acta Physico-chimica Sinica</i> , <b>2006</b> , 22, 622-626		2
10	Molecular dynamics simulations of wild type and mutant of Pin1 peptidyl-prolyl isomerase. <i>Molecular Simulation</i> , <b>2016</b> , 42, 1281-1291	2	2
9	Helix-Based RNA Landscape Partition and Alternative Secondary Structure Determination. <i>ACS Omega</i> , <b>2019</b> , 4, 15407-15413	3.9	1

8	Novel natural scaffold as hURAT1 inhibitor identified by 3D-shape-based, docking-based virtual screening approach and biological evaluation. <i>Bioorganic Chemistry</i> , <b>2021</b> , 117, 105444	5.1	1
7	Recent Progress of Deep Learning in Drug Discovery. <i>Current Pharmaceutical Design</i> , <b>2021</b> , 27, 2088-2096	5.3	1
6	Potential Role of the Last Half Repeat in TAL Effectors Revealed by a Molecular Simulation Study. <i>BioMed Research International</i> , <b>2016</b> , 2016, 8036450	3	1
5	Study on Molecular Recognition between Euphorbia Factor L713283 and $\alpha$ -Tubulin via Molecular Simulation Methods. <i>Journal of Chemistry</i> , <b>2015</b> , 2015, 1-13	2.3	0
4	An Overview of Computational Tools of Nucleic Acid Binding Site Prediction for Site-specific Proteins and Nucleases. <i>Protein and Peptide Letters</i> , <b>2020</b> , 27, 370-384	1.9	0
3	Log odds of positive lymph nodes is a better prognostic factor for oesophageal signet ring cell carcinoma than N stage. <i>World Journal of Clinical Cases</i> , <b>2021</b> , 9, 24-35	1.6	0
2	Exploiting Surroundedness and Superpixel cues for salient region detection. <i>Multimedia Tools and Applications</i> , <b>2020</b> , 79, 10935-10951	2.5	
1	Nomogram for predicting the overall survival of the patients with oesophageal signet ring cell carcinoma. <i>Journal of Thoracic Disease</i> , <b>2021</b> , 13, 1315-1326	2.6	