Dongqing Wei

List of Publications by Citations

255 papers	3,368 citations	28 h-index	43 g-index
287 ext. papers	4,815 ext. citations	4.6 avg, IF	6.2 L-index

#	Paper	IF	Citations
255	Higher infectivity of the SARS-CoV-2 new variants is associated with K417N/T, E484K, and N501Y mutants: An insight from structural data. *Journal of Cellular Physiology*, **2021**, 236, 7045-7057	7	151
254	Current updates on computer aided protein modeling and designing. *International Journal of Biological Macromolecules*, **2016**, 85, 48-62	7.9	86
253	PredT4SE-Stack: Prediction of Bacterial Type IV Secreted Effectors From Protein Sequences Using a Stacked Ensemble Method. *Frontiers in Microbiology*, **2018**, 9, 2571	5.7	77
252	Marine natural compounds as potents inhibitors against the main protease of SARS-CoV-2-a molecular dynamic study. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 3627-3637	3.6	64
251	How reliable are molecular dynamics simulations of membrane active antimicrobial peptides?. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 2280-8	3.8	64
250	DTI-CDF: a cascade deep forest model towards the prediction of drug-target interactions based on hybrid features. *Briefings in Bioinformatics*, **2021**, 22, 451-462	13.4	64
249	PDC-SGB: Prediction of effective drug combinations using a stochastic gradient boosting algorithm. *Journal of Theoretical Biology*, **2017**, 417, 1-7	2.3	63
248	Thermal decomposition of the solid phase of nitromethane: ab□nitio molecular dynamics simulations. *Physical Review Letters*, **2010**, 105, 188302	7.4	63
247	Human Intestinal Defensin 5 Inhibits SARS-CoV-2 Invasion by Cloaking ACE2. *Gastroenterology*, **2020**, 159, 1145-1147.e4	13.3	61
246	Computational identification, characterization and validation of potential antigenic peptide vaccines from hrHPVs E6 proteins using immunoinformatics and computational systems biology approaches. *PLoS ONE*, **2018**, 13, e0196484	3.7	57
245	Initial decomposition of the condensed-phase □HMX under shock waves: molecular dynamics simulations. *Journal of Physical Chemistry B*, **2012**, 116, 13696-704	3.4	56
244	Phylogenetic Analysis and Structural Perspectives of RNA-Dependent RNA-Polymerase Inhibition from SARs-CoV-2 with Natural Products. *Interdisciplinary Sciences, Computational Life Sciences*, **2020** , 12, 335-348	3.5	54
243	Immunoinformatics approaches to explore Helicobacter Pylori proteome (Virulence Factors) to design B and T cell multi-epitope subunit vaccine. *Scientific Reports*, **2019**, 9, 13321	4.9	52
242	Virtual screening-driven drug discovery of SARS-CoV2 enzyme inhibitors targeting viral attachment, replication, post-translational modification and host immunity evasion infection mechanisms. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 4316-4333	3.6	51
241	Structural insights into the mechanism of RNA recognition by the N-terminal RNA-binding domain of the SARS-CoV-2 nucleocapsid phosphoprotein. *Computational and Structural Biotechnology Journal*, **2020**, 18, 2174-2184	6.8	51
240	Destabilization of Alzheimer's A□42 Protofibrils with a Novel Drug Candidate wgx-50 by Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 11196-202	3.4	48
239	Combined drug repurposing and virtual screening strategies with molecular dynamics simulation identified potent inhibitors for SARS-CoV-2 main protease (3CLpro). *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 4659-4670	3.6	46

238	Nano-particle mediated inhibition of Parkinson's disease using computational biology approach. *Scientific Reports*, **2018**, 8, 9169	4.9	45
237	Immunoinformatics and structural vaccinology driven prediction of multi-epitope vaccine against Mayaro virus and validation through in-silico expression. *Infection, Genetics and Evolution*, **2019**, 73, 390-400	4.5	43
236	Molecular mechanism of Ras-related protein Rab-5A and effect of mutations in the catalytically active phosphate-binding loop. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 105-118	3.6	41
235	Prediction of CYP450 Enzyme-Substrate Selectivity Based on the Network-Based Label Space Division Method. *Journal of Chemical Information and Modeling*, **2019**, 59, 4577-4586	6.1	41
234	Identification of target gene and prognostic evaluation for lung adenocarcinoma using gene expression meta-analysis, network analysis and neural network algorithms. *Journal of Biomedical Informatics*, **2018**, 86, 120-134	10.2	38
233	A novel drug candidate for Alzheimer's disease treatment: gx-50 derived from Zanthoxylum bungeanum. *Journal of Alzheimer's Disease*, **2013**, 34, 203-13	4.3	35
232	Free energy calculations on the two drug binding sites in the M2 proton channel. *Journal of the American Chemical Society*, **2011**, 133, 10817-25	16.4	35
231	In silico and in vitro evaluation of kaempferol as a potential inhibitor of the SARS-CoV-2 main protease (3CLpro). *Phytotherapy Research*, **2021**, 35, 2841-2845	6.7	34
230	A negative cooperativity mechanism of human CYP2E1 inferred from molecular dynamics simulations and free energy calculations. *Journal of Chemical Information and Modeling*, **2011**, 51, 3217-25	6.1	31
229	Network Pharmacology: Exploring the Resources and Methodologies. *Current Topics in Medicinal Chemistry*, **2018**, 18, 949-964	3	31
228	Structure prediction and functional analyses of a thermostable lipase obtained from Shewanella putrefaciens. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2123-2135	3.6	30
227	Gene expression profiles and protein-protein interaction networks in amyotrophic lateral sclerosis patients with C9orf72 mutation. *Orphanet Journal of Rare Diseases*, **2016**, 11, 148	4.2	28
226	The first principle studies of the structural and vibrational properties of solid β-HMX under compression. *Molecular Physics*, **2008**, 106, 2569-2580	1.7	27
225	Integrated PPI- and WGCNA-Retrieval of Hub Gene Signatures Shared Between Barrett's Esophagus and Esophageal Adenocarcinoma. *Frontiers in Pharmacology*, **2020**, 11, 881	5.6	27
224	Bioinformatics Approaches for Anti-cancer Drug Discovery. *Current Drug Targets*, **2020**, 21, 3-17	3	27
223	Pressure effects on elastic and thermodynamic properties of Zr3Al intermetallic compound. *Computational Materials Science*, **2012**, 58, 125-130	3.2	26
222	Preliminary Structural Data Revealed That the SARS-CoV-2 B.1.617 Variant's RBD Binds to ACE2 Receptor Stronger Than the Wild Type to Enhance the Infectivity. *ChemBioChem*, **2021**, 22, 2641-2649	3.8	26
221	SARS-CoV-2 new variants: Characteristic features and impact on the efficacy of different vaccines. *Biomedicine and Pharmacotherapy*, **2021**, 143, 112176	7.5	26

220	Dynamics Insights Into the Gain of Flexibility by Helix-12 in ESR1 as a Mechanism of Resistance to Drugs in Breast Cancer Cell Lines. *Frontiers in Molecular Biosciences*, **2019**, 6, 159	5.6	25
219	Transmembrane Permeation Mechanism of Charged Methyl Guanidine. *Journal of Chemical Theory and Computation*, **2014**, 10, 1717-26	6.4	25
218	Immunogenomics guided design of immunomodulatory multi-epitope subunit vaccine against the SARS-CoV-2 new variants, and its validation through in silico cloning and immune simulation. *Computers in Biology and Medicine*, **2021**, 133, 104420	7	25
217	Conformational Preferences of Stacking Between Ligand and Protein, Analysis Derived from Crystal Structure Data Geometric Preference of Interaction. *Interdisciplinary Sciences, Computational Life Sciences*, **2015**, 7, 211-20	3.5	24
216	Structural comparison of the wild-type and drug-resistant mutants of the influenza A M2 proton channel by molecular dynamics simulations. *Journal of Physical Chemistry B*, **2013**, 117, 6042-51	3.4	24
215	The SARS-CoV-2 B.1.618 variant slightly alters the spike RBD-ACE2 binding affinity and is an antibody escaping variant: a computational structural perspective.. *RSC Advances*, **2021**, 11, 30132-30147	3.7	24
214	Cancer Immunoinformatics: A Promising Era in the Development of Peptide Vaccines for Human Papillomavirus-induced Cervical Cancer. *Current Pharmaceutical Design*, **2018**, 24, 3791-3817	3.3	23
213	Exploring the Papillomaviral Proteome to Identify Potential Candidates for a Chimeric Vaccine against Cervix Papilloma Using Immunomics and Computational Structural Vaccinology. *Viruses*, **2019**, 11,	6.2	23
212	DTI-MLCD: predicting drug-target interactions using multi-label learning with community detection method. *Briefings in Bioinformatics*, **2021**, 22,	13.4	23
211	Artificial Neural Networks for Prediction of Tuberculosis Disease. *Frontiers in Microbiology*, **2019**, 10, 395	5.7	22
210	Inhibition of Amyloid Channels with a Drug Candidate wgx-50 Revealed by Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2017**, 57, 2811-2821	6.1	22
209	Evolutionary and structural analysis of SARS-CoV-2 specific evasion of host immunity. *Genes and Immunity*, **2020**, 21, 409-419	4.4	21
208	Human Cathelicidin Inhibits SARS-CoV-2 Infection: Killing Two Birds with One Stone. *ACS Infectious Diseases*, **2021**, 7, 1545-1554	5.5	21
207	Immunoinformatic and systems biology approaches to predict and validate peptide vaccines against Epstein-Barr virus (EBV). *Scientific Reports*, **2019**, 9, 720	4.9	20
206	Sustainable production of biomass and industrially important secondary metabolites in cell cultures of selfheal (L.) elicited by silver and gold nanoparticles. *Artificial Cells, Nanomedicine and Biotechnology*, **2019**, 47, 2553-2561	6.1	20
205	Structural and free energy landscape of novel mutations in ribosomal protein S1 (rpsA) associated with pyrazinamide resistance. *Scientific Reports*, **2019**, 9, 7482	4.9	20
204	Deep-learning-based target screening and similarity search for the predicted inhibitors of the pathways in Parkinson's disease.. *RSC Advances*, **2019**, 9, 10326-10339	3.7	20
203	A hadoop-based method to predict potential effective drug combination. *BioMed Research International*, **2014**, 2014, 196858	3	20

202	The pressure-induced phase transition of the solid HMX. *Molecular Physics*, **2009**, 107, 2373-2385	1.7	20
201	dbAMEPNI: a database of alanine mutagenic effects for protein-nucleic acid interactions. *Database: the Journal of Biological Databases and Curation*, **2018**, 2018,	5	20
200	Nanotheranostic Applications for Detection and Targeting Neurodegenerative Diseases. *Frontiers in Neuroscience*, **2020**, 14, 305	5.1	19
199	SPVec: A Word2vec-Inspired Feature Representation Method for Drug-Target Interaction Prediction. *Frontiers in Chemistry*, **2019**, 7, 895	5	19
198	Prediction of Type II Toxin-Antitoxin Loci in Klebsiella pneumoniae Genome Sequences. *Interdisciplinary Sciences, Computational Life Sciences*, **2016**, 8, 143-149	3.5	19
197	The systematic modeling studies and free energy calculations of the phenazine compounds as anti-tuberculosis agents. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 4051-4069	3.6	19
196	Towards the low-sensitive and high-energetic co-crystal explosive CL-20/TNT: from intermolecular interactions to structures and properties. *Physical Chemistry Chemical Physics*, **2018**, 20, 17253-17261	3.6	19
195	Prognostic Impact of Tissue Inhibitor of Metalloproteinase-1 in Non- Small Cell Lung Cancer: Systematic Review and Meta-Analysis. *Current Medicinal Chemistry*, **2019**, 26, 7694-7713	4.3	18
194	Survey of Machine Learning Techniques for Prediction of the Isoform Specificity of Cytochrome P450 Substrates. *Current Drug Metabolism*, **2019**, 20, 229-235	3.5	18
193	Combining in silico and in vitro approaches to identification of potent inhibitor against phospholipase A2 (PLA2). *International Journal of Biological Macromolecules*, **2020**, 144, 53-66	7.9	18
192	Passive Transmembrane Permeation Mechanisms of Monovalent Ions Explored by Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2016**, 12, 4959-4969	6.4	18
191	Prediction of Effective Drug Combinations by an Improved Naïve Bayesian Algorithm. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	18
190	Predicting protein-ligand interactions based on bow-pharmacological space and Bayesian additive regression trees. *Scientific Reports*, **2019**, 9, 7703	4.9	17
189	Molecular docking and molecular dynamics simulation studies to identify potent AURKA inhibitors: assessing the performance of density functional theory, MM-GBSA and mass action kinetics calculations. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 4325-4335	3.6	17
188	Designing of CD8 and CD8-overlapped CD4 epitope vaccine by targeting late and early proteins of human papillomavirus. *Biologics: Targets and Therapy*, **2018**, 12, 107-125	4.4	17
187	Computational Screening and Analysis of Lung Cancer Related Non-Synonymous Single Nucleotide Polymorphisms on the Human Kirsten Rat Sarcoma Gene. *Molecules*, **2019**, 24,	4.8	16
186	An Integrated Systems Biology and Network-Based Approaches to Identify Novel Biomarkers in Breast Cancer Cell Lines Using Gene Expression Data. *Interdisciplinary Sciences, Computational Life Sciences*, **2020**, 12, 155-168	3.5	16
185	Rare Diseases: Drug Discovery and Informatics Resource. *Interdisciplinary Sciences, Computational Life Sciences*, **2018**, 10, 195-204	3.5	16

184	Classification Models for Predicting Cytochrome P450 Enzyme-Substrate Selectivity. *Molecular Informatics*, **2012**, 31, 53-62	3.8	16
183	Evaluation and validation of synergistic effects of amyloid-beta inhibitor–gold nanoparticles complex on Alzheimer's disease using deep neural network approach. *Journal of Materials Research*, **2019**, 34, 1845-1853	2.5	15
182	The Omicron (B.1.1.529) variant of SARS-CoV-2 binds to the hACE2 receptor more strongly and escapes the antibody response: Insights from structural and simulation data.. *International Journal of Biological Macromolecules*, **2022**, 200, 438-448	7.9	15
181	Insight into novel clinical mutants of RpsA-S324F, E325K, and G341R of associated with pyrazinamide resistance. *Computational and Structural Biotechnology Journal*, **2018**, 16, 379-387	6.8	15
180	Pressure induced superconductivity and electronic structure properties of scandium hydrides using first principles calculations. *RSC Advances*, **2016**, 6, 81534-81541	3.7	14
179	Prediction and validation of potent peptides against herpes simplex virus type 1 via immunoinformatic and systems biology approach. *Chemical Biology and Drug Design*, **2019**, 94, 1868-1883	2.9	14
178	Deciphering G-Protein-Coupled Receptor 119 Agonists as Promising Strategy against Type 2 Diabetes Using Systems Biology Approach. *ACS Omega*, **2018**, 3, 18214-18226	3.9	14
177	ATC-NLSP: Prediction of the Classes of Anatomical Therapeutic Chemicals Using a Network-Based Label Space Partition Method. *Frontiers in Pharmacology*, **2019**, 10, 971	5.6	13
176	Allosteric ligands for the pharmacologically important Flavivirus target (NS5) from ZINC database based on pharmacophoric points, free energy calculations and dynamics correlation. *Journal of Molecular Graphics and Modelling*, **2018**, 82, 37-47	2.8	13
175	Identification of novel drug targets for diamond-blackfan anemia based on RPS19 gene mutation using protein-protein interaction network. *BMC Systems Biology*, **2018**, 12, 39	3.5	13
174	Structural-dynamic insights into the cytotoxin-associated gene A (CagA) and its abrogation to interact with the tumor suppressor protein ASPP2 using decoy peptides. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 4035-4050	3.6	13
173	Pyrazinamide resistance and mutations L19R, R140H, and E144K in Pyrazinamidase of Mycobacterium tuberculosis. *Journal of Cellular Biochemistry*, **2018**, 120, 7154	4.7	13
172	Recent Studies of Mitochondrial SLC25: Integration of Experimental and Computational Approaches. *Current Protein and Peptide Science*, **2018**, 19, 507-522	2.8	12
171	Elastic, superconducting, and thermodynamic properties of the cubic metallic phase of AlH3 via first-principles calculations. *Journal of Applied Physics*, **2013**, 114, 114905	2.5	12
170	Insights into the Mechanisms of the Pyrazinamide Resistance of Three Pyrazinamidase Mutants N11K, P69T, and D126N. *Journal of Chemical Information and Modeling*, **2019**, 59, 498-508	6.1	12
169	Comprehensive epigenetic analyses reveal master regulators driving lung metastasis of breast cancer. *Journal of Cellular and Molecular Medicine*, **2019**, 23, 5415-5431	5.6	11
168	Chemomics and drug innovation. *Science China Chemistry*, **2013**, 56, 71-85	7.9	11
167	Ab initio and molecular dynamics studies of solid β-HMX: effects of hydrostatic pressure and high temperature. *Molecular Simulation*, **2010**, 36, 670-681	2	11

166	SARS-CoV-2 nucleocapsid and Nsp3 binding: an in silico study. *Archives of Microbiology*, **2021**, 203, 59-66	3	11
165	Structures of SARS-CoV-2 RNA-Binding Proteins and Therapeutic Targets. *Intervirology*, **2021**, 64, 55-68	2.5	11
164	Protection of Primary Dopaminergic Midbrain Neurons Through Impact of Small Molecules Using Virtual Screening of GPR139 Supported by Molecular Dynamic Simulation and Systems Biology. *Interdisciplinary Sciences, Computational Life Sciences*, **2019**, 11, 247-257	3.5	10
163	Pressure-Induced Crystallization and Phase Transformation of Para-xylene. *Scientific Reports*, **2017**, 7, 5321	4.9	10
162	Identification of human disease genes from interactome network using graphlet interaction. *PLoS ONE*, **2014**, 9, e86142	3.7	10
161	Viewing the Emphasis on State-of-the-Art Magnetic Nanoparticles: Synthesis, Physical Properties, and Applications in Cancer Theranostics. *Current Pharmaceutical Design*, **2019**, 25, 1505-1523	3.3	10
160	Subtractive proteomics and immunoinformatics approaches to explore Bartonella bacilliformis proteome (virulence factors) to design B and T cell multi-epitope subunit vaccine. *Infection, Genetics and Evolution*, **2020**, 85, 104551	4.5	10
159	Structural Dynamics Behind Clinical Mutants of PncA-Asp12Ala, Pro54Leu, and His57Pro of Associated With Pyrazinamide Resistance. *Frontiers in Bioengineering and Biotechnology*, **2019**, 7, 404	5.8	10
158	The dynamic binding of cholesterol to the multiple sites of C99: as revealed by coarse-grained and all-atom simulations. *Physical Chemistry Chemical Physics*, **2017**, 19, 3845-3856	3.6	9
157	Shock response of 1,3,5-trinitroperhydro-1,3,5-triazine (RDX): The C-N bond scission studied by molecular dynamics simulations. *Journal of Applied Physics*, **2017**, 122, 135901	2.5	9
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155	Survey of Computational Approaches for Prediction of DNA-Binding Residues on Protein Surfaces. *Methods in Molecular Biology*, **2018**, 1754, 223-234	1.4	9
154	Docking and molecular dynamics studies on CYP2D6. *Science Bulletin*, **2010**, 55, 1877-1880		9
153	T4SE-XGB: Interpretable Sequence-Based Prediction of Type IV Secreted Effectors Using eXtreme Gradient Boosting Algorithm. *Frontiers in Microbiology*, **2020**, 11, 580382	5.7	9
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151	Are the Allergic Reactions of COVID-19 Vaccines Caused by mRNA Constructs or Nanocarriers? Immunological Insights. *Interdisciplinary Sciences, Computational Life Sciences*, **2021**, 13, 344-347	3.5	9
150	Irinotecan and vandetanib create synergies for treatment of pancreatic cancer patients with concomitant TP53 and KRAS mutations. *Briefings in Bioinformatics*, **2021**, 22,	13.4	9
149	Initial Decomposition of the Co-crystal of CL-20/TNT: Sensitivity Decrease under Shock Loading. *Journal of Physical Chemistry C*, **2018**, 122, 24270-24278	3.8	9

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147	Lemairamin, isolated from the Zanthoxylum plants, alleviates pain hypersensitivity via spinal α7 nicotinic acetylcholine receptors. *Biochemical and Biophysical Research Communications*, **2020**, 525, 1087-1094	3.1	8
146	Systems Biology Integration and Screening of Reliable Prognostic Markers to Create Synergies in the Control of Lung Cancer Patients. *Frontiers in Molecular Biosciences*, **2020**, 7, 47	5.6	8
145	STS-NLSP: A Network-Based Label Space Partition Method for Predicting the Specificity of Membrane Transporter Substrates Using a Hybrid Feature of Structural and Semantic Similarity. *Frontiers in Bioengineering and Biotechnology*, **2019**, 7, 306	5.8	8
144	Mesoscopic simulation of aggregate behaviour of fluoropolymers in the TATB-based PBX. *Molecular Simulation*, **2011**, 37, 237-242	2	8
143	Improved Prediction of Michaelis Constants in CYP450-Mediated Reactions by Resilient Back Propagation Algorithm. *Current Drug Metabolism*, **2016**, 17, 673-80	3.5	8
142	Structural probing of HapR to identify potent phytochemicals to control Vibrio cholera through integrated computational approaches. *Computers in Biology and Medicine*, **2021**, 138, 104929	7	8
141	CytoMegaloVirus Infection Database: A Public Omics Database for Systematic and Comparable Information of CMV. *Interdisciplinary Sciences, Computational Life Sciences*, **2020**, 12, 169-177	3.5	8
140	LMI-DForest: A deep forest model towards the prediction of lncRNA-miRNA interactions. *Computational Biology and Chemistry*, **2020**, 89, 107406	3.6	8
139	An approach to identify the potential hot spots in SARS-CoV-2 spike RBD to block the interaction with ACE2 receptor. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-16	3.6	8
138	Potential Cancer- and Alzheimer's Disease-Targeting Phosphodiesterase Inhibitors from : Insights from and Consensus Virtual Screening. *ACS Omega*, **2021**, 6, 8403-8417	3.9	8
137	An Integrated Pan-Cancer Analysis and Structure-Based Virtual Screening of GPR15. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	8
136	New strategy for identifying potential natural HIV-1 non-nucleoside reverse transcriptase inhibitors against drug-resistance: an study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3327-3341	3.6	8
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134	Catalytic mechanism and origin of high activity of cellulase TmCel12A at high temperature: a quantum mechanical/molecular mechanical study. *Cellulose*, **2014**, 21, 937-949	5.5	7
133	Mechanical instability and ideal strengths of layered M2SC (M = Ti, Zr, and Hf) compounds. *Journal of Applied Physics*, **2013**, 113, 083516	2.5	7
132	MDA-GCNFTG: identifying miRNA-disease associations based on graph convolutional networks via graph sampling through the feature and topology graph. *Briefings in Bioinformatics*, **2021**, 22,	13.4	7
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129	In Silico Mutagenesis-Based Remodelling of SARS-CoV-1 Peptide (ATLQAIAS) to Inhibit SARS-CoV-2: Structural-Dynamics and Free Energy Calculations. *Interdisciplinary Sciences, Computational Life Sciences*, **2021**, 13, 521-534	3.5	7
128	Progress in the applications of flux analysis of metabolic networks. *Science Bulletin*, **2010**, 55, 2315-2322		6
127	Molecular dynamics simulations exploring drug resistance in HIV-1 proteases. *Science Bulletin*, **2010** , 55, 2677-2683		6
126	Proteome-wide mapping and reverse vaccinology-based B and T cell multi-epitope subunit vaccine designing for immune response reinforcement against. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-15	3.6	6
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124	Formation and superconducting properties of predicted ternary hydride ScYH6 under pressures. *International Journal of Quantum Chemistry*, **2021**, 121, e26459	2.1	6
123	A-CaMP: a tool for anti-cancer and antimicrobial peptide generation. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 285-293	3.6	6
122	MDF-SA-DDI: predicting drug-drug interaction events based on multi-source drug fusion, multi-source feature fusion and transformer self-attention mechanism. *Briefings in Bioinformatics*, **2021**,	13.4	6
121	Emerging mutations in envelope protein of SARS-CoV-2 and their effect on thermodynamic properties. *Informatics in Medicine Unlocked*, **2021**, 25, 100675	5.3	6
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119	Identification of novel acetylcholinesterase inhibitors through 3D-QSAR, molecular docking, and molecular dynamics simulation targeting Alzheimer's disease. *Journal of Molecular Modeling*, **2021**, 27, 302	2	6
118	Bringing Structural Implications and Deep Learning-Based Drug Identification for Mutants. *Journal of Chemical Information and Modeling*, **2021**, 61, 571-586	6.1	6
117	Extraction of molecular features for the drug discovery targeting protein-protein interaction of Helicobacter pylori CagA and tumor suppressor protein ASSP2. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 837-849	4.2	5
116	Dipeptide Frequency of Word Frequency and Graph Convolutional Networks for DTA Prediction. *Frontiers in Bioengineering and Biotechnology*, **2020**, 8, 267	5.8	5
115	The PPI network analysis of mRNA expression profile of uterus from primary dysmenorrheal rats. *Scientific Reports*, **2018**, 8, 351	4.9	5
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112	Evaluation of anti-EGFR-iRGD recombinant protein with GOLD nanoparticles: synergistic effect on antitumor efficiency using optimized deep neural networks.. *RSC Advances*, **2019**, 9, 19261-19270	3.7	5
111	Molecular dynamics simulation of chitinase I from Thermomyces lanuginosus SSBP to ensure optimal activity. *Molecular Simulation*, **2017**, 43, 480-490	2	5
110	New coupling mechanism of the silane coupling agents in the TATB-based PBX. *Molecular Simulation*, **2013**, 39, 423-427	2	5
109	Bioinformatics analysis of the differences in the binding profile of the wild-type and mutants of the SARS-CoV-2 spike protein variants with the ACE2 receptor. *Computers in Biology and Medicine*, **2021** , 138, 104936	7	5
108	Circulating miR-1246 Targeting UBE2C, TNNI3, TRAIP, UCHL1 Genes and Key Pathways as a Potential Biomarker for Lung Adenocarcinoma: Integrated Biological Network Analysis. *Journal of Personalized Medicine*, **2020**, 10,	3.6	5
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105	Identifying potential drug targets and candidate drugs for COVID-19: biological networks and structural modeling approaches. *F1000Research*, **2021**, 10, 127	3.6	5
104	Remdesivir MD Simulations Suggest a More Favourable Binding to SARS-CoV-2 RNA Dependent RNA Polymerase Mutant P323L Than Wild-Type. *Biomolecules*, **2021**, 11,	5.9	5
103	Identification of chlorprothixene as a potential drug that induces apoptosis and autophagic cell death in acute myeloid leukemia cells. *FEBS Journal*, **2020**, 287, 1645-1665	5.7	5
102	Identifying potential drug targets and candidate drugs for COVID-19: biological networks and structural modeling approaches. *F1000Research*, **2021**, 10, 127	3.6	5
101	CytomegaloVirusDb: Multi-omics knowledge database for cytomegaloviruses. *Computers in Biology and Medicine*, **2021**, 135, 104563	7	5
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99	Marine Natural Products and Drug Resistance in Latent Tuberculosis. *Marine Drugs*, **2019**, 17,	6	4
98	Structural insights of catalytic mechanism in mutant pyrazinamidase of. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 3172-3185	3.6	4
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