Dongqing Wei

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5635936/publications.pdf

Version: 2024-02-01

274	6,117	76196	138251
papers	citations	40 h-index	58 g-index

287	287	287	6043
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Higher infectivity of the SARSâ€CoVâ€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.	2.0	283
2	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.	3.2	142
3	Current updates on computer aided protein modeling and designing. International Journal of Biological Macromolecules, 2016, 85, 48-62.	3.6	123
4	PredT4SE-Stack: Prediction of Bacterial Type IV Secreted Effectors From Protein Sequences Using a Stacked Ensemble Method. Frontiers in Microbiology, 2018, 9, 2571.	1.5	107
5	Human Intestinal Defensin 5 Inhibits SARS-CoV-2 Invasion by Cloaking ACE2. Gastroenterology, 2020, 159, 1145-1147.e4.	0.6	106
6	Immunoinformatics approaches to explore Helicobacter Pylori proteome (Virulence Factors) to design B and T cell multi-epitope subunit vaccine. Scientific Reports, 2019, 9, 13321.	1.6	102
7	Marine natural compounds as potents inhibitors against the main protease of SARS-CoV-2â€"a molecular dynamic study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3627-3637.	2.0	98
8	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.	2.0	92
9	PDC-SGB: Prediction of effective drug combinations using a stochastic gradient boosting algorithm. Journal of Theoretical Biology, 2017, 417, 1-7.	0.8	85
10	How reliable are molecular dynamics simulations of membrane active antimicrobial peptides?. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2280-2288.	1.4	83
11	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.	2.2	81
12	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.	1.9	81
13	In silico and in vitro evaluation of kaempferol as a potential inhibitor of the <scp>SARSâ€CoV</scp>â€2 main protease (<scp>3CLpro</scp>). Phytotherapy Research, 2021, 35, 2841-2845.	2.8	80
14	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.	1.0	77
15	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.	1.1	75
16	Thermal Decomposition of the Solid Phase of Nitromethane:AbÂInitioMolecular Dynamics Simulations. Physical Review Letters, 2010, 105, 188302.	2.9	74
17	Bioinformatics Approaches for Anti-cancer Drug Discovery. Current Drug Targets, 2019, 21, 3-17.	1.0	73
18	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.	2.0	73

#	Article	IF	Citations
19	Destabilization of Alzheimerâ€™s AÎ²42 Protofibrils with a Novel Drug Candidate wgx-50 by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 11196-11202.	1.2	69
20	Initial Decomposition of the Condensed-Phase Î²-HMX under Shock Waves: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 13696-13704.	1.2	66
21	Human Cathelicidin Inhibits SARS-CoV-2 Infection: Killing Two Birds with One Stone. ACS Infectious Diseases, 2021, 7, 1545-1554.	1.8	64
22	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.	3.6	64
23	Conformational Preferences of Ï€â€“Ï€ Stacking Between Ligand and Protein, Analysis Derived from Crystal Structure Data Geometric Preference of Ï€â€“Ï€ Interaction. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 211-220.	2.2	63
24	Integrated PPI- and WGCNA-Retrieval of Hub Gene Signatures Shared Between Barrett's Esophagus and Esophageal Adenocarcinoma. Frontiers in Pharmacology, 2020, 11, 881.	1.6	63
25	Nano-particle mediated inhibition of Parkinsonâ€™s disease using computational biology approach. Scientific Reports, 2018, 8, 9169.	1.6	60
26	MDF-SA-DDI: predicting drugâ€“drug interaction events based on multi-source drug fusion, multi-source feature fusion and transformer self-attention mechanism. Briefings in Bioinformatics, 2022, 23, .	3.2	59
27	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.	3.9	59
28	The SARS-CoV-2 B.1.618 variant slightly alters the spike RBDâ€“ACE2 binding affinity and is an antibody escaping variant: a computational structural perspective. RSC Advances, 2021, 11, 30132-30147.	1.7	57
29	Prediction of CYP450 Enzymeâ€“Substrate Selectivity Based on the Network-Based Label Space Division Method. Journal of Chemical Information and Modeling, 2019, 59, 4577-4586.	2.5	55
30	A transformer-based model to predict peptideâ€“HLA class I binding and optimize mutated peptides for vaccine design. Nature Machine Intelligence, 2022, 4, 300-311.	8.3	55
31	A Novel Drug Candidate for Alzheimer's Disease Treatment: gx-50 Derived from Zanthoxylum Bungeanum. Journal of Alzheimer's Disease, 2013, 34, 203-213.	1.2	52
32	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.	2.0	52
33	SPVec: A Word2vec-Inspired Feature Representation Method for Drug-Target Interaction Prediction. Frontiers in Chemistry, 2019, 7, 895.	1.8	52
34	DTI-MLCD: predicting drug-target interactions using multi-label learning with community detection method. Briefings in Bioinformatics, 2021, 22, .	3.2	52
35	SARS-CoV-2 new variants: Characteristic features and impact on the efficacy of different vaccines. Biomedicine and Pharmacotherapy, 2021, 143, 112176.	2.5	51
36	Network Pharmacology: Exploring the Resources and Methodologies. Current Topics in Medicinal Chemistry, 2018, 18, 949-964.	1.0	51

#	Article	IF	Citations
37	Artificial Neural Networks for Prediction of Tuberculosis Disease. Frontiers in Microbiology, 2019, 10, 395.	1.5	49
38	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.	2.5	48
39	Structural and free energy landscape of novel mutations in ribosomal protein S1 (rpsA) associated with pyrazinamide resistance. Scientific Reports, 2019, 9, 7482.	1.6	48
40	Preliminary Structural Data Revealed That the SARSâ€CoVâ€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.	1.3	46
41	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, .	3.2	43
42	Nanotheranostic Applications for Detection and Targeting Neurodegenerative Diseases. Frontiers in Neuroscience, 2020, 14, 305.	1.4	41
43	Gene expression profiles and protein-protein interaction networks in amyotrophic lateral sclerosis patients with C9orf72 mutation. Orphanet Journal of Rare Diseases, 2016, 11, 148.	1.2	38
44	Free Energy Calculations on the Two Drug Binding Sites in the M2 Proton Channel. Journal of the American Chemical Society, 2011, 133, 10817-10825.	6.6	37
45	Immunoinformatic and systems biology approaches to predict and validate peptide vaccines against Epsteinâ€“Barr virus (EBV). Scientific Reports, 2019, 9, 720.	1.6	37
46	Predicting protein-ligand interactions based on bow-pharmacological space and Bayesian additive regression trees. Scientific Reports, 2019, 9, 7703.	1.6	37
47	Evolutionary and structural analysis of SARS-CoV-2 specific evasion of host immunity. Genes and Immunity, 2020, 21, 409-419.	2.2	37
48	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.	1.6	37
49	Structures of SARS-CoV-2 RNA-Binding Proteins and Therapeutic Targets. Intervirology, 2021, 64, 55-68.	1.2	36
50	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.	2.2	35
51	A Negative Cooperativity Mechanism of Human CYP2E1 Inferred from Molecular Dynamics Simulations and Free Energy Calculations. Journal of Chemical Information and Modeling, 2011, 51, 3217-3225.	2.5	34
52	Structure prediction and functional analyses of a thermostable lipase obtained from Shewanella putrefaciens. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2123-2135.	2.0	34
53	SARS-CoV-2 nucleocapsid and Nsp3 binding: an in silico study. Archives of Microbiology, 2021, 203, 59-66.	1.0	34
54	Sustainable production of biomass and industrially important secondary metabolites in cell cultures of selfheal (Prunella vulgaris L.) elicited by silver and gold nanoparticles. Artificial Cells, Nanomedicine and Biotechnology, 2019, 47, 2553-2561.	1.9	33

#	Article	IF	Citations
55	Computational Screening and Analysis of Lung Cancer Related Non-Synonymous Single Nucleotide Polymorphisms on the Human Kirsten Rat Sarcoma Gene. Molecules, 2019, 24, 1951.	1.7	32
56	Cancer Immunoinformatics: A Promising Era in the Development of Peptide Vaccines for Human Papillomavirus-induced Cervical Cancer. Current Pharmaceutical Design, 2019, 24, 3791-3817.	0.9	32
57	Pressure effects on elastic and thermodynamic properties of Zr3Al intermetallic compound. Computational Materials Science, 2012, 58, 125-130.	1.4	31
58	Inhibition of Î²-Amyloid Channels with a Drug Candidate wgx-50 Revealed by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2017, 57, 2811-2821.	2.5	31
59	The first principle studies of the structural and vibrational properties of solid Î²-HMX under compression. Molecular Physics, 2008, 106, 2569-2580.	0.8	30
60	dbAMEPNI: a database of alanine mutagenic effects for proteinâ€“nucleic acid interactions. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	1.4	30
61	Prediction of Effective Drug Combinations by an Improved NaÃ¯ve Bayesian Algorithm. International Journal of Molecular Sciences, 2018, 19, 467.	1.8	30
62	ATC-NLSP: Prediction of the Classes of Anatomical Therapeutic Chemicals Using a Network-Based Label Space Partition Method. Frontiers in Pharmacology, 2019, 10, 971.	1.6	30
63	Exploring the Papillomaviral Proteome to Identify Potential Candidates for a Chimeric Vaccine against Cervix Papilloma Using Immunomics and Computational Structural Vaccinology. Viruses, 2019, 11, 63.	1.5	30
64	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.	3.6	30
65	Transmembrane Permeation Mechanism of Charged Methyl Guanidine. Journal of Chemical Theory and Computation, 2014, 10, 1717-1726.	2.3	29
66	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.	1.7	29
67	Insight into novel clinical mutants of RpsA-S324F, E325K, and G341R of Mycobacterium tuberculosis associated with pyrazinamide resistance. Computational and Structural Biotechnology Journal, 2018, 16, 379-387.	1.9	28
68	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.	2.0	28
69	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.	2.0	28
70	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, 6042-6051.	1.2	27
71	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.	1.5	26
72	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.	2.2	26

#	Article	IF	Citations
73	Survey of Machine Learning Techniques for Prediction of the Isoform Specificity of Cytochrome P450 Substrates. Current Drug Metabolism, 2019, 20, 229-235.	0.7	26
74	The pressure-induced phase transition of the solid Î²â€“HMX. Molecular Physics, 2009, 107, 2373-2385.	0.8	25
75	A Hadoop-Based Method to Predict Potential Effective Drug Combination. BioMed Research International, 2014, 2014, 1-5.	0.9	25
76	Evaluation and validation of synergistic effects of amyloid-beta inhibitorâ€“gold nanoparticles complex on Alzheimerâ€™s disease using deep neural network approach. Journal of Materials Research, 2019, 34, 1845-1853.	1.2	25
77	Prognostic Impact of Tissue Inhibitor of Metalloproteinase-1 in Non- Small Cell Lung Cancer: Systematic Review and Meta-Analysis. Current Medicinal Chemistry, 2020, 26, 7694-7713.	1.2	25
78	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.	1.3	24
79	LMI-DForest: A deep forest model towards the prediction of lncRNA-miRNA interactions. Computational Biology and Chemistry, 2020, 89, 107406.	1.1	24
80	Potential Cancer- and Alzheimerâ€™s Disease-Targeting Phosphodiesterase Inhibitors from Uvaria alba: Insights from In Vitro and Consensus Virtual Screening. ACS Omega, 2021, 6, 8403-8417.	1.6	24
81	Remdesivir MD Simulations Suggest a More Favourable Binding to SARS-CoV-2 RNA Dependent RNA Polymerase Mutant P323L Than Wild-Type. Biomolecules, 2021, 11, 919.	1.8	24
82	Passive Transmembrane Permeation Mechanisms of Monovalent Ions Explored by Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 4959-4969.	2.3	23
83	T4SE-XGB: Interpretable Sequence-Based Prediction of Type IV Secreted Effectors Using eXtreme Gradient Boosting Algorithm. Frontiers in Microbiology, 2020, 11, 580382.	1.5	23
84	Exosomal ncRNAs profiling of mycobacterial infection identified miRNA-185-5p as a novel biomarker for tuberculosis. Briefings in Bioinformatics, 2021, 22, .	3.2	23
85	NeuroPpred-Fuse: an interpretable stacking model for prediction of neuropeptides by fusing sequence information and feature selection methods. Briefings in Bioinformatics, 2021, 22, .	3.2	23
86	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.	3.9	23
87	Prediction of Type II Toxin-Antitoxin Loci in Klebsiella pneumoniae Genome Sequences. Interdisciplinary Sciences, Computational Life Sciences, 2016, 8, 143-149.	2.2	22
88	Designing of CD8⁺ and CD8⁺-overlapped CD4⁺ epitope vaccine by targeting late and early proteins of human papillomavirus. Biologics: Targets and Therapy, 2018, Volume 12, 107-125.	3.0	22
89	Structural-dynamic insights into the H. pylori 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.	2.0	22
90	iEnhancer-DHF: Identification of Enhancers and Their Strengths Using Optimize Deep Neural Network With Multiple Features Extraction Methods. IEEE Access, 2021, 9, 40783-40796.	2.6	22

#	Article	IF	Citations
91	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. International Journal of Molecular Sciences, 2021, 22, 7071.	1.8	22
92	Hantavirus: The Next Pandemic We Are Waiting For?. Interdisciplinary Sciences, Computational Life Sciences, 2021, 13, 147-152.	2.2	22
93	Rare Diseases: Drug Discovery and Informatics Resource. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 195-204.	2.2	21
94	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.	2.5	21
95	Emerging mutations in envelope protein of SARS-CoV-2 and their effect on thermodynamic properties. Informatics in Medicine Unlocked, 2021, 25, 100675.	1.9	21
96	MDA-CF: Predicting MiRNA-Disease associations based on a cascade forest model by fusing multi-source information. Computers in Biology and Medicine, 2021, 136, 104706.	3.9	21
97	Initial Decomposition of the Co-crystal of CL-20/TNT: Sensitivity Decrease under Shock Loading. Journal of Physical Chemistry C, 2018, 122, 24270-24278.	1.5	20
98	Proteome-wide mapping and reverse vaccinology-based B and T cell multi-epitope subunit vaccine designing for immune response reinforcement againstPorphyromonas gingivalis. Journal of Biomolecular Structure and Dynamics, 2022, 40, 833-847.	2.0	20
99	Formation and superconducting properties of predicted ternary hydride <scp>ScYH₆</scp> under pressures. International Journal of Quantum Chemistry, 2021, 121, e26459.	1.0	20
100	Blocking key mutated hotspot residues in the RBD of the omicron variant (B.1.1.529) with medicinal compounds to disrupt the RBD-hACE2 complex using molecular screening and simulation approaches. RSC Advances, 2022, 12, 7318-7327.	1.7	20
101	Deep6mAPred: A CNN and Bi-LSTM-based deep learning method for predicting DNA N6-methyladenosine sites across plant species. Methods, 2022, 204, 142-150.	1.9	20
102	Irinotecan and vandetanib create synergies for treatment of pancreatic cancer patients with concomitant TP53 and KRAS mutations. Briefings in Bioinformatics, 2021, 22, .	3.2	19
103	Bringing Structural Implications and Deep Learning-Based Drug Identification for KRAS Mutants. Journal of Chemical Information and Modeling, 2021, 61, 571-586.	2.5	19
104	Classification Models for Predicting Cytochrome P450 Enzymeâ€Substrate Selectivity. Molecular Informatics, 2012, 31, 53-62.	1.4	18
105	Pressure-Induced Crystallization and Phase Transformation of Para-xylene. Scientific Reports, 2017, 7, 5321.	1.6	18
106	Emerging Mutations in Nsp1 of SARS-CoV-2 and Their Effect on the Structural Stability. Pathogens, 2021, 10, 1285.	1.2	18
107	Pressure induced superconductivity and electronic structure properties of scandium hydrides using first principles calculations. RSC Advances, 2016, 6, 81534-81541.	1.7	17
108	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.	2.0	17

#	Article	IF	Citations
109	Computational Perspective on the Current State of the Methods and New Challenges in Cancer Drug Discovery. Current Pharmaceutical Design, 2019, 24, 3725-3726.	0.9	17
110	Comprehensive epigenetic analyses reveal master regulators driving lung metastasis of breast cancer. Journal of Cellular and Molecular Medicine, 2019, 23, 5415-5431.	1.6	17
111	Structural Dynamics Behind Clinical Mutants of PncA-Asp12Ala, Pro54Leu, and His57Pro of Mycobacterium tuberculosis Associated With Pyrazinamide Resistance. Frontiers in Bioengineering and Biotechnology, 2019, 7, 404.	2.0	17
112	Pyrazinamide resistance and mutations L19R, R140H, and E144K in Pyrazinamidase of Mycobacterium tuberculosis. Journal of Cellular Biochemistry, 2019, 120, 7154-7166.	1.2	17
113	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.	1.0	17
114	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.	2.2	17
115	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.	0.9	17
116	Structural probing of HapR to identify potent phytochemicals to control Vibrio cholera through integrated computational approaches. Computers in Biology and Medicine, 2021, 138, 104929.	3.9	17
117	Computational modelling of potentially emerging SARS-CoV-2 spike protein RBDs mutations with higher binding affinity towards ACE2: A structural modelling study. Computers in Biology and Medicine, 2022, 141, 105163.	3.9	17
118	Computational prediction of the effect of mutations in the receptor-binding domain on the interaction between SARS-CoV-2 and human ACE2. Molecular Diversity, 2022, 26, 3309-3324.	2.1	17
119	Identification of Human Disease Genes from Interactome Network Using Graphlet Interaction. PLoS ONE, 2014, 9, e86142.	1.1	16
120	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.	1.3	16
121	Deciphering G-Protein-Coupled Receptor 119 Agonists as Promising Strategy against Type 2 Diabetes Using Systems Biology Approach. ACS Omega, 2018, 3, 18214-18226.	1.6	16
122	Polyvinylidene Fluoride-Added Ceramic Powder Composite Near-Field Electrospinned Piezoelectric Fiber-Based Low-Frequency Dynamic Sensors. ACS Omega, 2020, 5, 17090-17101.	1.6	16
123	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.	3.0	15
124	An Integrated Pan-Cancer Analysis and Structure-Based Virtual Screening of GPR15. International Journal of Molecular Sciences, 2019, 20, 6226.	1.8	15
125	Prediction of Recombination Spots Using Novel Hybrid Feature Extraction Method via Deep Learning Approach. Frontiers in Genetics, 2020, 11, 539227.	1.1	15
126	Lemairamin, isolated from the Zanthoxylum plants, alleviates pain hypersensitivity via spinal Î±7 nicotinic acetylcholine receptors. Biochemical and Biophysical Research Communications, 2020, 525, 1087-1094.	1.0	15

#	Article	IF	Citations
127	Gibbs Free Energy Calculation of Mutation in PncA and RpsA Associated With Pyrazinamide Resistance. Frontiers in Molecular Biosciences, 2020, 7, 52.	1.6	15
128	Comparative mutational analysis of SARS-CoV-2 isolates from Pakistan and structural-functional implications using computational modelling and simulation approaches. Computers in Biology and Medicine, 2022, 141, 105170.	3.9	15
129	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.	1.3	14
130	Recent Studies of Mitochondrial SLC25: Integration of Experimental and Computational Approaches. Current Protein and Peptide Science, 2018, 19, 507-522.	0.7	14
131	Dipeptide Frequency of Word Frequency and Graph Convolutional Networks for DTA Prediction. Frontiers in Bioengineering and Biotechnology, 2020, 8, 267.	2.0	14
132	An in-silico 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.	2.0	14
133	Antibacterial and COX-2 Inhibitory Tetrahydrobisbenzylisoquinoline Alkaloids from the Philippine Medicinal Plant Phaeanthus ophthalmicus. Plants, 2021, 10, 462.	1.6	14
134	Genome-wide screening of vaccine targets prioritization and reverse vaccinology aided design of peptides vaccine to enforce humoral immune response against Campylobacter jejuni. Computers in Biology and Medicine, 2021, 133, 104412.	3.9	14
135	Abrogation of SARS-CoV-2 interaction with host (NRP1) neuropilin-1 receptor through high-affinity marine natural compounds to curtail the infectivity: A structural-dynamics data. Computers in Biology and Medicine, 2022, 141, 104714.	3.9	14
136	Docking and molecular dynamics studies on CYP2D6. Science Bulletin, 2010, 55, 1877-1880.	1.7	13
137	Elastic, superconducting, and thermodynamic properties of the cubic metallic phase of AlH3 via first-principles calculations. Journal of Applied Physics, 2013, 114, .	1.1	13
138	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, .	1.1	13
139	Marine Natural Products and Drug Resistance in Latent Tuberculosis. Marine Drugs, 2019, 17, 549.	2.2	13
140	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.	2.2	13
141	New strategy for identifying potential natural HIV-1 non-nucleoside reverse transcriptase inhibitors against drug-resistance: an in silico study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3327-3341.	2.0	13
142	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, 162.	1.1	13
143	Development of multi-epitope subunit vaccine for protection against the norovirusâ€™ infections based on computational vaccinology. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3098-3109.	2.0	13
144	Chemomics and drug innovation. Science China Chemistry, 2013, 56, 71-85.	4.2	12

#	Article	IF	Citations
145	CEBPE expression is an independent prognostic factor for acute myeloid leukemia. Journal of Translational Medicine, 2019, 17, 188.	1.8	12
146	CytoMegaloVirus Infection Database: A Public Omics Database for Systematic and Comparable Information of CMV. Interdisciplinary Sciences, Computational Life Sciences, 2020, 12, 169-177.	2.2	12
147	A comparative chemogenic analysis for predicting Drug-Target Pair via Machine Learning Approaches. Scientific Reports, 2020, 10, 6870.	1.6	12
148	Identifying potential drug targets and candidate drugs for COVID-19: biological networks and structural modeling approaches. F1000Research, 2021, 10, 127.	0.8	12
149	Immunoinformatics and Immunogenetics-Based Design of Immunogenic Peptides Vaccine against the Emerging Tick-Borne Encephalitis Virus (TBEV) and Its Validation through In Silico Cloning and Immune Simulation. Vaccines, 2021, 9, 1210.	2.1	12
150	Ab initioand molecular dynamics studies of solid Î²-HMX: effects of hydrostatic pressure and high temperature. Molecular Simulation, 2010, 36, 670-681.	0.9	11
151	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.	2.2	11
152	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.	1.6	11
153	Prediction of Blood-Brain Barrier Permeability of Compounds by Fusing Resampling Strategies and eXtreme Gradient Boosting. IEEE Access, 2021, 9, 9557-9566.	2.6	11
154	Discovering potent inhibitors against the Mpro of the SARS-CoV-2. A medicinal chemistry approach. Computers in Biology and Medicine, 2022, 143, 105235.	3.9	11
155	Molecular dynamics simulations exploring drug resistance in HIV-1 proteases. Science Bulletin, 2010, 55, 2677-2683.	1.7	10
156	Mechanical instability and ideal strengths of layered M2SC (Mâ€‰=â€‰Ti, Zr, and Hf) compounds. Journal of Applied Physics, 2013, 113, .	1.1	10
157	Detoxification of aflatoxins on prospective approach: effect on structural, mechanical, and optical properties under pressures. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 311-319.	2.2	10
158	Survey of Computational Approaches for Prediction of DNA-Binding Residues on Protein Surfaces. Methods in Molecular Biology, 2018, 1754, 223-234.	0.4	10
159	A-CaMP: a tool for anti-cancer and antimicrobial peptide generation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 285-293.	2.0	10
160	Identifying potential drug targets and candidate drugs for COVID-19: biological networks and structural modeling approaches. F1000Research, 0, 10, 127.	0.8	10
161	Potential Immunogenic Activity of Computationally Designed mRNA- and Peptide-Based Prophylactic Vaccines against MERS, SARS-CoV, and SARS-CoV-2: A Reverse Vaccinology Approach. Molecules, 2022, 27, 2375.	1.7	10
162	Subtractive proteomics assisted therapeutic targets mining and designing ensemble vaccine against Candida auris for immune response induction. Computers in Biology and Medicine, 2022, 145, 105462.	3.9	10

#	Article	IF	Citations
163	Mesoscopic simulation of aggregate behaviour of fluoropolymers in the TATB-based PBX. Molecular Simulation, 2011, 37, 237-242.	0.9	9
164	Catalytic mechanism and origin of high activity of cellulase TmCel12A at high temperature: a quantum mechanical/molecular mechanical study. Cellulose, 2014, 21, 937-949.	2.4	9
165	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.	1.7	9
166	Free Energy Calculation of Transmembrane Ion Permeation: Sample with a Single Reaction Coordinate and Analysis along Transition Path. Journal of Chemical Theory and Computation, 2019, 15, 1216-1225.	2.3	9
167	Proteome wide vaccine targets prioritization and designing of antigenic vaccine candidate to trigger the host immune response against the Mycoplasma genitalium infection. Microbial Pathogenesis, 2021, 152, 104771.	1.3	9
168	Towards an Ensemble Vaccine against the Pegivirus Using Computational Modelling Approaches and Its Validation through In Silico Cloning and Immune Simulation. Vaccines, 2021, 9, 818.	2.1	9
169	CytomegaloVirusDb: Multi-omics knowledge database for cytomegaloviruses. Computers in Biology and Medicine, 2021, 135, 104563.	3.9	9
170	A novel formulation of theranostic nanomedicine for targeting drug delivery to gastrointestinal tract cancer. Cancer Nanotechnology, 2021, 12, .	1.9	9
171	New coupling mechanism of the silane coupling agents in the TATB-based PBX. Molecular Simulation, 2013, 39, 423-427.	0.9	8
172	Molecular dynamics simulation of chitinase I from Thermomyces lanuginosus SSBP to ensure optimal activity. Molecular Simulation, 2017, 43, 480-490.	0.9	8
173	Two-Dimensional Infrared Spectra of Cationic Dopamine under Different Electric Fields: Theoretical Studies from the Density Function Theory Anharmonic Potential. Journal of Physical Chemistry C, 2018, 122, 17994-18004.	1.5	8
174	Extraction of molecular features for the drug discovery targeting proteinâ€protein interaction ofHelicobacter pyloriCagA and tumor suppressor protein ASSP2. Proteins: Structure, Function and Bioinformatics, 2019, 87, 837-849.	1.5	8
175	Helix-Switch Enables C99 Dimer Transition between the Multiple Conformations. Journal of Chemical Information and Modeling, 2019, 59, 339-350.	2.5	8
176	Pyrazinamide resistance of novel mutations inpncAand their dynamic behavior. RSC Advances, 2020, 10, 35565-35573.	1.7	8
177	LUNAR :Drug Screening for Novel Coronavirus Based on Representation Learning Graph Convolutional Network. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 1290-1298.	1.9	8
178	Insight into the drug resistance whole genome of Mycobacterium tuberculosis isolates from Khyber Pakhtunkhwa, Pakistan. Infection, Genetics and Evolution, 2021, 92, 104861.	1.0	8
179	A computational perspective on the dynamic behaviour of recurrent drug resistance mutations in the pncA gene from Mycobacterium tuberculosis. RSC Advances, 2021, 11, 2476-2486.	1.7	8
180	Improved Prediction of Michaelis Constants in CYP450-Mediated Reactions by Resilient Back Propagation Algorithm. Current Drug Metabolism, 2016, 17, 673-680.	0.7	8

#	Article	IF	Citations
181	Structural-Dynamics and Binding Analysis of RBD from SARS-CoV-2 Variants of Concern (VOCs) and GRP78 Receptor Revealed Basis for Higher Infectivity. Microorganisms, 2021, 9, 2331.	1.6	8
182	Characterization of rifampicin-resistant Mycobacterium tuberculosis in Khyber Pakhtunkhwa, Pakistan. Scientific Reports, 2021, 11, 14194.	1.6	7
183	Identification of novel acetylcholinesterase inhibitors through 3D-QSAR, molecular docking, and molecular dynamics simulation targeting Alzheimerâ€™s disease. Journal of Molecular Modeling, 2021, 27, 302.	0.8	7
184	Discovery of a Natural Product with Potent Efficacy Against SARS-CoV-2 by Drug Screening. Interdisciplinary Sciences, Computational Life Sciences, 2022, 14, 55-63.	2.2	7
185	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. Current Drug Targets, 2020, 21, 132-147.	1.0	7
186	MMV-db: vaccinomics and RNA-based therapeutics database for infectious hemorrhagic fever-causing mammarenaviruses. Database: the Journal of Biological Databases and Curation, 2021, 2021, .	1.4	7
187	Evaluation of the Whole Proteome of Achromobacter xylosoxidans to Identify Vaccine Targets for mRNA and Peptides-Based Vaccine Designing Against the Emerging Respiratory and Lung Cancer-Causing Bacteria. Frontiers in Medicine, 2021, 8, 825876.	1.2	7
188	Progress in the applications of flux analysis of metabolic networks. Science Bulletin, 2010, 55, 2315-2322.	1.7	6
189	The PPI network analysis of mRNA expression profile of uterus from primary dysmenorrheal rats. Scientific Reports, 2018, 8, 351.	1.6	6
190	High-pressure transformations of ortho-xylene probed by combined infrared and Raman spectroscopies. Solid State Communications, 2018, 269, 96-101.	0.9	6
191	Estimation of Probability Distribution and Its Application in Bayesian Classification and Maximum Likelihood Regression. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 559-574.	2.2	6
192	The Disulfide Bond between Cys22 and Cys27 in the Protease Domain Modulate Clotting Activity of Coagulation Factor X. Thrombosis and Haemostasis, 2019, 119, 871-881.	1.8	6
193	Computational Advances in Chronic Diseases Diagnostics and Therapy - I. Current Drug Targets, 2019, 21, 1-2.	1.0	6
194	SARS-CoV-2 Genome from the Khyber Pakhtunkhwa Province of Pakistan. ACS Omega, 2021, 6, 6588-6599.	1.6	6
195	Diketopiperazine Modulates Arabidopsis thaliana Root System Architecture by Promoting Interactions of Auxin Receptor TIR1 and IAA7/17 Proteins. Plant and Cell Physiology, 2022, 63, 57-69.	1.5	6
196	A protein coupling and molecular simulation analysis of the clinical mutants of androgen receptor revealed a higher binding for Leupaxin, to increase the prostate cancer invasion and motility. Computers in Biology and Medicine, 2022, 146, 105537.	3.9	6
197	Role of dipole elongation in orientationally ordered liquids. Physical Review E, 2011, 83, 061703.	0.8	5
198	Applications of rare event dynamics on the free energy calculations for membrane protein systems. Canadian Journal of Chemistry, 2013, 91, 769-774.	0.6	5

#	Article	IF	Citations
199	Theoretical Studies of Intracellular Concentration of Micro-organismsâ€™ Metabolites. Scientific Reports, 2017, 7, 9048.	1.6	5
200	Free Energy Calculations on the Water-Chain-Assisted and the Dehydration Mechanisms of Transmembrane Ion Permeation. Journal of Chemical Theory and Computation, 2020, 16, 700-710.	2.3	5
201	Characterization and synthetic biology of lipase from Bacillus amyloliquefaciens strain. Archives of Microbiology, 2020, 202, 1497-1506.	1.0	5
202	Structural insights of catalytic mechanism in mutant pyrazinamidase ofMycobacterium tuberculosis. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1-14.	2.0	5
203	Molecular dynamics simulation and binding free energy calculations of microcin J25 binding to the FhuA receptor. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2585-2594.	2.0	5
204	ACPS: An accurate bioinformatics tool for precisionâ€based antiâ€cancer peptide generation via omics data. Chemical Biology and Drug Design, 2021, 97, 372-382.	1.5	5
205	Identifying potential drug targets and candidate drugs for COVID-19: biological networks and structural modeling approaches. F1000Research, 2021, 10, 127.	0.8	5
206	Insights Into Mutations Induced Conformational Changes and Rearrangement of Fe2+ Ion in pncA Gene of Mycobacterium tuberculosis to Decipher the Mechanism of Resistance to Pyrazinamide. Frontiers in Molecular Biosciences, 2021, 8, 633365.	1.6	5
207	Interrogation of Bacillus anthracis SrtA active site loop forming open/close lid conformations through extensive MD simulations for understanding binding selectivity of SrtA inhibitors. Saudi Journal of Biological Sciences, 2021, 28, 3650-3659.	1.8	5
208	CoronaPep: An Anti-Coronavirus Peptide Generation Tool. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 1299-1304.	1.9	5
209	Globally ncRNAs Expression Profiling of TNBC and Screening of Functional lncRNA. Frontiers in Bioengineering and Biotechnology, 2020, 8, 523127.	2.0	5
210	A novel method of affinity purification and characterization of polygalacturonase of Aspergillus flavus by galacturonic acid engineered magnetic nanoparticle. Food Chemistry, 2022, 372, 131317.	4.2	5
211	OUP accepted manuscript. Briefings in Bioinformatics, 2022, 23, .	3.2	5
212	Inhibitory effect of thymoquinone from Nigella sativa against SARS-CoV-2 main protease. An in-silico study. Brazilian Journal of Biology, 2022, 84, e250667.	0.4	5
213	Enhancer-LSTMAtt: A Bi-LSTM and Attention-Based Deep Learning Method for Enhancer Recognition. Biomolecules, 2022, 12, 995.	1.8	5
214	A THEORETICAL STUDY ON THE MECHANISM OF 2:1 1, 3 DIPOLAR CYCLOADDITION REACTIONS. Journal of Theoretical and Computational Chemistry, 2007, 06, 861-867.	1.8	4
215	Molecular dynamics simulations of dipolar fluids in orientationally ordered phases. Physical Review E, 2007, 75, 061702.	0.8	4
216	PCLâ€“DOX microdroplets: an evaluation of the enhanced intracellular delivery of doxorubicin in metastatic cancer cells via in silico and in vitro approaches. New Journal of Chemistry, 2019, 43, 12241-12256.	1.4	4

#	Article	IF	Citations
217	Immunomics Datasets and Tools: To Identify Potential Epitope Segments for Designing Chimeric Vaccine Candidate to Cervix Papilloma. Data, 2019, 4, 31.	1.2	4
218	Mechanistic analysis of A46V, H57Y, and D129N in pyrazinamidase associated with pyrazinamide resistance. Saudi Journal of Biological Sciences, 2020, 27, 3150-3156.	1.8	4
219	Core amino acid substitutions in HCV-3a isolates from Pakistan and opportunities for multi-epitopic vaccines. Journal of Biomolecular Structure and Dynamics, 2020, , 1-16.	2.0	4
220	Robust Biomarker Screening Using Spares Learning Approach for Liver Cancer Prognosis. Frontiers in Bioengineering and Biotechnology, 2020, 8, 241.	2.0	4
221	Computational Method for Classification of Avian Influenza A Virus Using DNA Sequence Information and Physicochemical Properties. Frontiers in Genetics, 2021, 12, 599321.	1.1	4
222	HantavirusesDB: Vaccinomics and RNA-based therapeutics database for the potentially emerging human respiratory pandemic agents. Microbial Pathogenesis, 2021, 160, 105161.	1.3	4
223	Predicting Protein-Ligand Interactions Based on Chemical Preference Features with its Application to New D-Amino Acid Oxidase Inhibitor Discovery. Current Pharmaceutical Design, 2014, 20, 5202-5211.	0.9	4
224	Recent Progress on Computer-Aided Inhibitor Design of H5N1 Influenza A Virus. Current Computer-Aided Drug Design, 2010, 6, 139-146.	0.8	4
225	Computational Evaluation of Abrogation of HBx-Bcl-xL Complex with High-Affinity Carbon Nanotubes (Fullerene) to Halt the Hepatitis B Virus Replication. Molecules, 2021, 26, 6433.	1.7	4
226	Structure-guided design of multi-epitopes vaccine against variants of concern (VOCs) of SARS-CoV-2 and validation through In silico cloning and immune simulations. Computers in Biology and Medicine, 2022, 140, 105122.	3.9	4
227	Investigation of the binding and dynamic features of A.30 variant revealed higher binding of RBD for hACE2 and escapes the neutralizing antibody: A molecular simulation approach. Computers in Biology and Medicine, 2022, 146, 105574.	3.9	4
228	mAMBER: A CPU/MIC collaborated parallel framework for AMBER on Tianhe-2 supercomputer. , 2016, , .		3
229	A pH based molecular dynamics simulations of chitinase II isolated from Thermomyces lanuginosus SSBP. Cogent Biology, 2016, 2, 1168336.	1.7	3
230	Membrane defect and water leakage caused by passive calcium permeation. Journal of Molecular Liquids, 2018, 270, 227-233.	2.3	3
231	Blending effect between n-decane and toluene in oxidation: a ReaxFF study. Molecular Simulation, 2018, 44, 21-33.	0.9	3
232	An unexpected dynamic binding mode between coagulation factor X and Rivaroxaban reveals importance of flexibility in drug binding. Chemical Biology and Drug Design, 2019, 94, 1664-1671.	1.5	3
233	G-protein-coupled receptors function as logic gates for nanoparticle binding using systems and synthetic biology approach. Journal of Materials Research, 2019, 34, 1854-1867.	1.2	3
234	Emerging Trends on Nanoparticles and Nano-Materials in Biomedical Applications-I. Current Pharmaceutical Design, 2019, 25, 1441-1442.	0.9	3

#	Article	IF	Citations
235	WeiBI (web-based platform): Enriching integrated interaction network with increased coverage and functional proteins from genome-wide experimental OMICS data. Scientific Reports, 2020, 10, 5618.	1.6	3
236	Computational insights of twoâ€dimensional infrared spectroscopy under electric fields in phosphorylcholine. International Journal of Quantum Chemistry, 2020, 120, e26169.	1.0	3
237	BC-TFdb: a database of transcription factor drivers in breast cancer. Database: the Journal of Biological Databases and Curation, 2021, 2021, .	1.4	3
238	Pan-Cancer Analysis and Drug Formulation for GPR139 and GPR142. Frontiers in Pharmacology, 2020, 11, 521245.	1.6	3
239	Targeting the N-terminal domain of the RNA-binding protein of the SARS-CoV-2 with high affinity natural compounds to abrogate the protein-RNA interaction: a molecular dynamics study. Journal of Biomolecular Structure and Dynamics, 2021, , 1-9.	2.0	3
240	Prediction of Protein Solubility Based on Sequence Feature Fusion and DDcCNN. Interdisciplinary Sciences, Computational Life Sciences, 2021, 13, 703-716.	2.2	3
241	Controlling the Substrate Specificity of an Enzyme through Structural Flexibility by Varying the Salt-Bridge Density. Molecules, 2021, 26, 5693.	1.7	3
242	Quasi-Static Two-Dimensional Infrared Spectra of the Carboxyhemoglobin Subsystem under Electric Fields: A Theoretical Study. Journal of Physical Chemistry B, 2020, 124, 9570-9578.	1.2	3
243	Evaluation and identification of essential therapeutic proteins and vaccinomics approach towards multi-epitopes vaccine designing against Legionella pneumophila for immune response instigation. Computers in Biology and Medicine, 2022, 143, 105291.	3.9	3
244	Core-Proteomics-Based Annotation of Antigenic Targets and Reverse-Vaccinology-Assisted Design of Ensemble Immunogen against the Emerging Nosocomial Infection-Causing Bacterium Elizabethkingia meningoseptica. International Journal of Environmental Research and Public Health, 2022, 19, 194.	1.2	3
245	Interactions of CYP2C9 with Different Substrates and its Implications for Metabolic Mechanism. , 2008, , .		2
246	Prediction of the functional consequences of single amino acid substitution in human cytochrome P450. Molecular Simulation, 2012, 38, 1297-1307.	0.9	2
247	Ab initio molecular metadynamics simulation for S-nitrosylation by nitric oxide: S-nitroxide as the key intermediate. Molecular Simulation, 2017, 43, 1134-1141.	0.9	2
248	A Study of the Dynamic Relation between Physiological Changes and Spontaneous Expressions. Scientific Reports, 2017, 7, 7081.	1.6	2
249	Computational Modeling of Immune Response Triggering Immunogenic Peptide Vaccine Against the Human Papillomaviruses to Induce Immunity Against Cervical Cancer. Viral Immunology, 2021, 34, 457-469.	0.6	2
250	Identification of Novel Therapeutic Targets in Myelodysplastic Syndrome Using Protein-Protein Interaction Approach and Neural Networks. Journal of Computer Science and Systems Biology, 2018, 11, .	0.0	2
251	Exploring the Molecular Basis of Substrate and Product Selectivities of Nocardicin Bifunctional Thioesterase. Interdisciplinary Sciences, Computational Life Sciences, 2022, 14, 233-244.	2.2	2
252	Annotation of Potential Vaccine Targets and Design of a Multi-Epitope Subunit Vaccine against Yersinia pestis through Reverse Vaccinology and Validation through an Agent-Based Modeling Approach. Vaccines, 2021, 9, 1327.	2.1	2

#	Article	IF	Citations
253	Intermolecular Vibration Energy Transfer Process in Two CL-20-Based Cocrystals Theoretically Revealed by Two-Dimensional Infrared Spectra. Molecules, 2022, 27, 2153.	1.7	2
254	Crystal structure of Acetyl-CoA carboxylase (AccB) from Streptomyces antibioticus and insights into the substrate-binding through in silico mutagenesis and biophysical investigations. Computers in Biology and Medicine, 2022, 145, 105439.	3.9	2
255	Ion permeation across the membrane: A comprehensive comparison analysis on passive permeations of differently charged ions. Journal of Molecular Liquids, 2022, 359, 119339.	2.3	2
256	Effect of Cholesterol on C99 Dimerization: Revealed by Molecular Dynamics Simulations. Frontiers in Molecular Biosciences, 0, 9, .	1.6	2
257	Genetic insight of the H5N1 hemagglutinin cleavage site. Science Bulletin, 2007, 52, 2374-2379.	1.7	1
258	Recent Progress on Structural Bioinformatics Research of Cytochrome P450 and Its Impact on Drug Discovery. Advances in Experimental Medicine and Biology, 2015, 827, 327-339.	0.8	1
259	Recent progresses of simulations on passive membrane permeations in China. Molecular Simulation, 2016, 42, 799-808.	0.9	1
260	Emerging Trends on Nanoparticles and Nano-materials in Biomedical Applications -II. Current Pharmaceutical Design, 2019, 25, 2607-2608.	0.9	1
261	Application of Artificial Intelligence in Drug Repurposing: A mini-review. Current Chinese Science, 2021, 1, 333-345.	0.2	1
262	Editorial: Computational Genomics and Molecular Medicine for Emerging COVID-19. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 1227-1229.	1.9	1
263	Revealing the Relationship between Electric Fields and the Conformation of Oxytocin Using Quasi-Static Amide-I Two-Dimensional Infrared Spectra. ACS Omega, 2022, 7, 3758-3767.	1.6	1
264	Computational Methods for Structure-Based Drug Design Through System Biology. Methods in Molecular Biology, 2022, 2385, 161-174.	0.4	1
265	Repositioning of experimentally validated anti-breast cancer peptides to target FAK-PAX complex to halt the breast cancer progression: a biomolecular simulation approach. Molecular Diversity, 0, , .	2.1	1
266	Discovery of Anti-Hiv Drugs Using Computer Aided Drug Designing Tools. , 2007, , .		0
267	Molecular Modeling of CYP Proteins and its Implication for Personal Drug Design. , 0, , 273-292.		0
268	Extraordinary mechanical properties of monatomic C3N2chain. Molecular Simulation, 2015, 41, 256-261.	0.9	0
269	Personalized clinical data screening: Special issue on health informatics. Computers in Biology and Medicine, 2015, 61, 161-162.	3.9	0
270	A drug information embedding method based on graph convolution neural network. , 2021, , .		0

#	Article	IF	Citations
271	A Static Analysis of Wnt/Î²-Catenin and Wnt/Ca 2+ Biological Regulatory Networks for ARVC Using Automata Network Model. IEEE Access, 2021, 9, 107611-107624.	2.6	0
272	Novel positive allosteric modulators of the human Î±7 nicotinic acetylcholine receptor. FASEB Journal, 2012, 26, .	0.2	0
273	The Reaction and Microscopic Electron Properties from Dynamic Evolutions of Condensed-Phase RDX Under Shock Loading. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2020, 75, 285-291.	0.7	0
274	Computational Chemistry in the Fight Against SARS-CoV-2.. Combinatorial Chemistry and High Throughput Screening, 2022, 25, .	0.6	0