Dongqing Wei

List of Publications by Year in Descending Order

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	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	3.9	0
254	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
253	Discovering potent inhibitors against the Mpro of the SARS-CoV-2. A medicinal chemistry approach.. *Computers in Biology and Medicine*, **2022**, 143, 105235	7	4
252	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**, 1	3.1	2
251	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	7	0
250	A novel method of affinity purification and characterization of polygalacturonase of Aspergillus flavus by galacturonic acid engineered magnetic nanoparticle. *Food Chemistry*, **2022**, 372, 131317	8.5	2
249	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	3.7	2
248	A transformer-based model to predict peptide–HLA class I binding and optimize mutated peptides for vaccine design. *Nature Machine Intelligence*, **2022**, 4, 300-311	22.5	1
247	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	7	1
246	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	7	
245	Computational Methods for Structure-Based Drug Design Through System Biology. *Methods in Molecular Biology*, **2022**, 2385, 161-174	1.4	
244	Deep6mAPred: A CNN and Bi-LSTM-based deep learning method for predicting DNA N6-methyladenosine sites across plant species.. *Methods*, **2022**,	4.6	3
243	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	7	1
242	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	7	0
241	Ion permeation across the membrane: A comprehensive comparison analysis on passive permeations of differently charged ions. *Journal of Molecular Liquids*, **2022**, 359, 119339	6	
240	Inhibitory effect of thymoquinone from Nigella sativa against SARS-CoV-2 main protease. An in-silico study.. *Brazilian Journal of Biology*, **2022**, 84, e250667	1.5	2
239	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

238	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
237	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
236	Structural insights of catalytic mechanism in mutant pyrazinamidase of. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 3172-3185	3.6	4
235	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*, **2021**, 140, 105122	7	0
234	Evaluation of the Whole Proteome of 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	4.9	2
233	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,	4.9	3
232	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*, **2021**, 141, 105163	7	3
231	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*, **2021**, 141, 105170	7	0
230	Exploring the Molecular Basis of Substrate and Product Selectivities of Nocardicin Bifunctional Thioesterase. *Interdisciplinary Sciences, Computational Life Sciences*, **2021**, 1	3.5	0
229	A novel formulation of theranostic nanomedicine for targeting drug delivery to gastrointestinal tract cancer. *Cancer Nanotechnology*, **2021**, 12,	7.9	4
228	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,	4.8	1
227	MMV-db: vaccinomics and RNA-based therapeutics database for infectious hemorrhagic fever-causing mammarenaviruses. *Database: the Journal of Biological Databases and Curation*, **2021**, 2021,	5	2
226	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,	5.3	1
225	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
224	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
223	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	3.8	5
222	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
221	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

220	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
219	Antibacterial and COX-2 Inhibitory Tetrahydrobisbenzylisoquinoline Alkaloids from the Philippine Medicinal Plant. *Plants*, **2021**, 10,	4.5	3
218	Human Cathelicidin Inhibits SARS-CoV-2 Infection: Killing Two Birds with One Stone. *ACS Infectious Diseases*, **2021**, 7, 1545-1554	5.5	21
217	Insights Into Mutations Induced Conformational Changes and Rearrangement of Fe Ion in Gene of to Decipher the Mechanism of Resistance to Pyrazinamide. *Frontiers in Molecular Biosciences*, **2021**, 8, 633365	5.6	2
216	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
215	Identifying potential drug targets and candidate drugs for COVID-19: biological networks and structural modeling approaches. *F1000Research*, **2021**, 10, 127	3.6	5
214	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
213	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	7
212	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
211	Exosomal ncRNAs profiling of mycobacterial infection identified miRNA-185-5p as a novel biomarker for tuberculosis. *Briefings in Bioinformatics*, **2021**, 22,	13.4	2
210	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
209	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	7	7
208	Prediction of Protein Solubility Based on Sequence Feature Fusion and DDcCNN. *Interdisciplinary Sciences, Computational Life Sciences*, **2021**, 13, 703-716	3.5	0
207	Characterization of rifampicin-resistant Mycobacterium tuberculosis in Khyber Pakhtunkhwa, Pakistan. *Scientific Reports*, **2021**, 11, 14194	4.9	2
206	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*, **2021**, 141, 104714	7	6
205	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
204	Application of Artificial Intelligence in Drug Repurposing: A mini-review. *Current Chinese Science*, **2021**, 1, 333-345	0.2	1
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	3.6	4

202	SARS-CoV-2 nucleocapsid and Nsp3 binding: an in silico study. *Archives of Microbiology*, **2021**, 203, 59-66	3	11
201	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
200	ACPS: An accurate bioinformatics tool for precision-based anti-cancer peptide generation via omics data. *Chemical Biology and Drug Design*, **2021**, 97, 372-382	2.9	2
199	DTI-MLCD: predicting drug-target interactions using multi-label learning with community detection method. *Briefings in Bioinformatics*, **2021**, 22,	13.4	23
198	Formation and superconducting properties of predicted ternary hydride ScYH6 under pressures. *International Journal of Quantum Chemistry*, **2021**, 121, e26459	2.1	6
197	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
196	A-CaMP: a tool for anti-cancer and antimicrobial peptide generation. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 285-293	3.6	6
195	iEnhancer-DHF: Identification of Enhancers and Their Strengths Using Optimize Deep Neural Network With Multiple Features Extraction Methods. *IEEE Access*, **2021**, 9, 40783-40796	3.5	4
194	BC-TFdb: a database of transcription factor drivers in breast cancer. *Database: the Journal of Biological Databases and Curation*, **2021**, 2021,	5	1
193	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
192	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
191	Computational Method for Classification of Avian Influenza A Virus Using DNA Sequence Information and Physicochemical Properties. *Frontiers in Genetics*, **2021**, 12, 599321	4.5	2
190	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
189	Structures of SARS-CoV-2 RNA-Binding Proteins and Therapeutic Targets. *Intervirology*, **2021**, 64, 55-68	2.5	11
188	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
187	Identifying potential drug targets and candidate drugs for COVID-19: biological networks and structural modeling approaches. *F1000Research*, **2021**, 10, 127	3.6	5
186	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	3.6	2
185	SARS-CoV-2 Genome from the Khyber Pakhtunkhwa Province of Pakistan. *ACS Omega*, **2021**, 6, 6588-6599	3.9	2

184	Interrogation of 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	4	3
183	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	3	2
182	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
181	CoronaPep: An Anti-Coronavirus Peptide Generation Tool. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2021**, 18, 1299-1304	3	2
180	Towards an Ensemble Vaccine against the Pegivirus Using Computational Modelling Approaches and Its Validation through In Silico Cloning and Immune Simulation. *Vaccines*, **2021**, 9,	5.3	2
179	CytomegaloVirusDb: Multi-omics knowledge database for cytomegaloviruses. *Computers in Biology and Medicine*, **2021**, 135, 104563	7	5
178	NeuroPpred-Fuse: an interpretable stacking model for prediction of neuropeptides by fusing sequence information and feature selection methods. *Briefings in Bioinformatics*, **2021**, 22,	13.4	4
177	Insight into the drug resistance whole genome of Mycobacterium tuberculosis isolates from Khyber Pakhtunkhwa, Pakistan. *Infection, Genetics and Evolution*, **2021**, 92, 104861	4.5	2
176	Diketopiperazine Modulates Arabidopsis Thaliana Root System Architecture by Promoting Interactions of Auxin Receptor TIR1 and IAA7/17 Proteins. *Plant and Cell Physiology*, **2021**,	4.9	1
175	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	7	4
174	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
173	Discovery of a Natural Product with Potent Efficacy Against SARS-CoV-2 by Drug Screening. *Interdisciplinary Sciences, Computational Life Sciences*, **2021**, 1	3.5	1
172	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	1.7	0
171	SARS-CoV-2 new variants: Characteristic features and impact on the efficacy of different vaccines. *Biomedicine and Pharmacotherapy*, **2021**, 143, 112176	7.5	26
170	HantavirusesDB: Vaccinomics and RNA-based therapeutics database for the potentially emerging human respiratory pandemic agents. *Microbial Pathogenesis*, **2021**, 160, 105161	3.8	0
169	Hantavirus: The Next Pandemic We Are Waiting For?. *Interdisciplinary Sciences, Computational Life Sciences*, **2021**, 13, 147-152	3.5	2
168	Bringing Structural Implications and Deep Learning-Based Drug Identification for Mutants. *Journal of Chemical Information and Modeling*, **2021**, 61, 571-586	6.1	6
167	A Static Analysis of Wnt/Catenin and Wnt/Ca2+ Biological Regulatory Networks for ARVC Using Automata Network Model. *IEEE Access*, **2021**, 9, 107611-107624	3.5	

166	A computational perspective on the dynamic behaviour of recurrent drug resistance mutations in the pncA gene from .. *RSC Advances*, **2021**, 11, 2476-2486	3.7	3
165	Prediction of Blood-Brain Barrier Permeability of Compounds by Fusing Resampling Strategies and eXtreme Gradient Boosting. *IEEE Access*, **2021**, 9, 9557-9566	3.5	5
164	Core-Proteomics-Based Annotation of Antigenic Targets and Reverse-Vaccinology-Assisted Design of Ensemble Immunogen against the Emerging Nosocomial Infection-Causing Bacterium .. *International Journal of Environmental Research and Public Health*, **2021**, 19,	4.6	3
163	Nanotheranostic Applications for Detection and Targeting Neurodegenerative Diseases. *Frontiers in Neuroscience*, **2020**, 14, 305	5.1	19
162	Lemairamin, isolated from the Zanthoxylum plants, alleviates pain hypersensitivity via spinal α7 nicotinic acetylcholine receptors. *Biochemical and Biophysical Research Communications*, **2020**, 525, 1087-1094	3.4	8
161	Characterization and synthetic biology of lipase from Bacillus amyloliquefaciens strain. *Archives of Microbiology*, **2020**, 202, 1497-1506	3	3
160	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
159	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
158	A comparative chemogenic analysis for predicting Drug-Target Pair via Machine Learning Approaches. *Scientific Reports*, **2020**, 10, 6870	4.9	9
157	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	4.9	1
156	Dipeptide Frequency of Word Frequency and Graph Convolutional Networks for DTA Prediction. *Frontiers in Bioengineering and Biotechnology*, **2020**, 8, 267	5.8	5
155	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
154	Robust Biomarker Screening Using Spares Learning Approach for Liver Cancer Prognosis. *Frontiers in Bioengineering and Biotechnology*, **2020**, 8, 241	5.8	2
153	Gibbs Free Energy Calculation of Mutation in PncA and RpsA Associated With Pyrazinamide Resistance. *Frontiers in Molecular Biosciences*, **2020**, 7, 52	5.6	4
152	Computational insights of two-dimensional infrared spectroscopy under electric fields in phosphorylcholine. *International Journal of Quantum Chemistry*, **2020**, 120, e26169	2.1	2
151	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	1.4	
150	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	3.4	1
149	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. *Current Drug Targets*, **2020**, 21, 132-147	3	2

148	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
147	Human Intestinal Defensin 5 Inhibits SARS-CoV-2 Invasion by Cloaking ACE2. *Gastroenterology*, **2020**, 159, 1145-1147.e4	13.3	61
146	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
145	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
144	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	6.4	3
143	Prediction of Recombination Spots Using Novel Hybrid Feature Extraction Method via Deep Learning Approach. *Frontiers in Genetics*, **2020**, 11, 539227	4.5	4
142	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
141	LMI-DForest: A deep forest model towards the prediction of lncRNA-miRNA interactions. *Computational Biology and Chemistry*, **2020**, 89, 107406	3.6	8
140	Mechanistic analysis of A46V, H57Y, and D129N in pyrazinamidase associated with pyrazinamide resistance. *Saudi Journal of Biological Sciences*, **2020**, 27, 3150-3156	4	3
139	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
138	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
137	Polyvinylidene Fluoride-Added Ceramic Powder Composite Near-Field Electrospinned Piezoelectric Fiber-Based Low-Frequency Dynamic Sensors. *ACS Omega*, **2020**, 5, 17090-17101	3.9	9
136	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	3.6	1
135	Development of multi-epitope subunit vaccine for protection against the norovirus' infections based on computational vaccinology. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-12	3.6	4
134	Evolutionary and structural analysis of SARS-CoV-2 specific evasion of host immunity. *Genes and Immunity*, **2020**, 21, 409-419	4.4	21
133	Pyrazinamide resistance of novel mutations in and their dynamic behavior.. *RSC Advances*, **2020**, 10, 35565-35573	3.7	33
132	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
131	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

130	Bioinformatics Approaches for Anti-cancer Drug Discovery. *Current Drug Targets*, **2020**, 21, 3-17	3	27
129	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
128	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
127	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
126	Pan-Cancer Analysis and Drug Formulation for GPR139 and GPR142. *Frontiers in Pharmacology*, **2020**, 11, 521245	5.6	1
125	Globally ncRNAs Expression Profiling of TNBC and Screening of Functional lncRNA. *Frontiers in Bioengineering and Biotechnology*, **2020**, 8, 523127	5.8	4
124	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
123	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
122	Marine Natural Products and Drug Resistance in Latent Tuberculosis. *Marine Drugs*, **2019**, 17,	6	4
121	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	6.4	7
120	Immunoinformatic and systems biology approaches to predict and validate peptide vaccines against Epstein-Barr virus (EBV). *Scientific Reports*, **2019**, 9, 720	4.9	20
119	Predicting protein-ligand interactions based on bow-pharmacological space and Bayesian additive regression trees. *Scientific Reports*, **2019**, 9, 7703	4.9	17
118	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
117	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
116	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
115	CEBPE expression is an independent prognostic factor for acute myeloid leukemia. *Journal of Translational Medicine*, **2019**, 17, 188	8.5	8
114	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
113	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

112	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
111	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
110	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	2.9	1
109	Artificial Neural Networks for Prediction of Tuberculosis Disease. *Frontiers in Microbiology*, **2019**, 10, 395	5.7	22
108	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
107	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	7	3
106	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	2.5	2
105	Immunomics Datasets and Tools: To Identify Potential Epitope Segments for Designing Chimeric Vaccine Candidate to Cervix Papilloma. *Data*, **2019**, 4, 31	2.3	2
104	Evaluation and validation of synergistic effects of amyloid-beta inhibitor□gold nanoparticles complex on Alzheimer□ disease using deep neural network approach. *Journal of Materials Research*, **2019**, 34, 1845-1853	2.5	15
103	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
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