

Protein Data Bank (PDB): The Single Global Macromolecular

Methods in Molecular Biology

1607, 627-641

DOI: 10.1007/978-1-4939-7000-1_26

Citation Report

#	ARTICLE	IF	CITATIONS
1	Interleukins and their signaling pathways in the Reactome biological pathway database. Journal of Allergy and Clinical Immunology, 2018, 141, 1411-1416.	2.9	11
2	Bringing diffuse X-ray scattering into focus. Current Opinion in Structural Biology, 2018, 50, 109-116.	5.7	29
3	Searching and Extracting Data from the EMBL-EBI Complex Portal. Methods in Molecular Biology, 2018, 1764, 377-390.	0.9	7
4	Mechanism and Catalytic Site Atlas (M-CSA): a database of enzyme reaction mechanisms and active sites. Nucleic Acids Research, 2018, 46, D618-D623.	14.5	151
5	Simulating biological processes: stochastic physics from whole cells to colonies. Reports on Progress in Physics, 2018, 81, 052601.	20.1	32
6	Evaluation of variability in high-resolution protein structures by global distance scoring. Heliyon, 2018, 4, e00510.	3.2	5
7	MolProbity: More and better reference data for improved all-atom structure validation. Protein Science, 2018, 27, 293-315.	7.6	2,776
8	Ligand-biased ensemble receptor docking (LigBEnD): a hybrid ligand/receptor structure-based approach. Journal of Computer-Aided Molecular Design, 2018, 32, 187-198.	2.9	39
9	Anaerobic crystallization of proteins. Biophysical Reviews, 2018, 10, 183-189.	3.2	9
10	Target-specific toxicity knowledgebase (TsTKb): a novel toolkit for in silico predictive toxicology. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2018, 36, 219-236.	2.9	6
11	Art v 4 Protein Structure as a Representative Template for Allergen Profilins: Homology Modeling and Molecular Dynamics. ACS Omega, 2018, 3, 17254-17260.	3.5	11
12	Compositionally Biased Dark Matter in the Protein Universe. Proteomics, 2018, 18, e1800069.	2.2	11
13	Glykoinformatik: Brücken zwischen isolierten Inseln im Datenmeer. Angewandte Chemie, 2018, 130, 15202-15207.	2.0	0
14	Synchrotron Big Data Science. Small, 2018, 14, e1802291.	10.0	41
15	An Algorithm for Describing the Convex and Concave Shape of Protein Surface. Communications in Computer and Information Science, 2018, , 17-26.	0.5	0
16	Taxonomic Landscape of the Dark Proteomes: Whole-Proteome Scale Interplay Between Structural Darkness, Intrinsic Disorder, and Crystallization Propensity. Proteomics, 2018, 18, 1800243.	2.2	27
17	What's happened over the last five years with high-throughput protein crystallization screening?. Expert Opinion on Drug Discovery, 2018, 13, 691-695.	5.0	19
18	RNAfitme: a webserver for modeling nucleobase and nucleoside residue conformation in fixed-backbone RNA structures. BMC Bioinformatics, 2018, 19, 304.	2.6	12

#	ARTICLE	IF	CITATIONS
19	Glycoinformatics: Bridging Isolated Islands in the Sea of Data. Angewandte Chemie - International Edition, 2018, 57, 14986-14990.	13.8	29
20	AbDb: antibody structure database—a database of PDB-derived antibody structures. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	3.0	51
21	Improving Docking Performance Using Negative Image-Based Rescoring. Frontiers in Pharmacology, 2018, 9, 260.	3.5	20
22	TBC2target: A Resource of Predicted Target Genes of Tea Bioactive Compounds. Frontiers in Plant Science, 2018, 9, 211.	3.6	3
23	Systematic Analysis of the Binding Surfaces between tRNAs and Their Respective Aminoacyl tRNA Synthetase Based on Structural and Evolutionary Data. Frontiers in Genetics, 2017, 8, 227.	2.3	12
24	Protein engineering of enzymes involved in lipid modification. , 2018, , 11-43.		2
25	Structure-guided engineering of TGF-Î²s for the development of novel inhibitors and probing mechanism. Bioorganic and Medicinal Chemistry, 2018, 26, 5239-5246.	3.0	6
26	Control of mitotic chromosome condensation by the fission yeast transcription factor Zas1. Journal of Cell Biology, 2018, 217, 2383-2401.	5.2	3
27	RepeatsDB-lite: a web server for unit annotation of tandem repeat proteins. Nucleic Acids Research, 2018, 46, W402-W407.	14.5	18
28	Overview of the structure-based non-genomic effects of the nuclear receptor RXRÎ±. Cellular and Molecular Biology Letters, 2018, 23, 36.	7.0	9
29	Glycomics@ExPASy: Bridging the Gap. Molecular and Cellular Proteomics, 2018, 17, 2164-2176.	3.8	48
30	OpuF, a New Bacillus Compatible Solute ABC Transporter with a Substrate-Binding Protein Fused to the Transmembrane Domain. Applied and Environmental Microbiology, 2018, 84, .	3.1	35
31	Homozygous Calcium-Sensing Receptor Polymorphism R544Q Presents as Hypocalcemic Hypoparathyroidism. Journal of Clinical Endocrinology and Metabolism, 2018, 103, 2879-2888.	3.6	18
32	MobiDB 3.0: more annotations for intrinsic disorder, conformational diversity and interactions in proteins. Nucleic Acids Research, 2018, 46, D471-D476.	14.5	190
33	Protein Structure Databases. , 2019, , 460-471.		0
34	Comprehensive search for accessory proteins encoded with archaeal and bacterial type III CRISPR- <i>cas</i> gene cassettes reveals 39 new <i>cas</i> gene families. RNA Biology, 2019, 16, 530-542.	3.1	97
35	Biological Databases. , 2019, , 96-117.		1
36	Protein Structural Bioinformatics: An Overview. , 2019, , 445-459.		23

#	ARTICLE	IF	CITATIONS
37	Getting Docking into Shape Using Negative Image-Based Rescoring. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3584-3599.	5.4	22
38	Computer-aided re-engineering of nonribosomal peptide and polyketide biosynthetic assembly lines. <i>Natural Product Reports</i> , 2019, 36, 1249-1261.	10.3	35
39	Physics-Based Method for Modeling Passive Membrane Permeability and Translocation Pathways of Bioactive Molecules. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3198-3213.	5.4	41
40	RareLSD: a manually curated database of lysosomal enzymes associated with rare diseases. <i>Database: the Journal of Biological Databases and Curation</i> , 2019, 2019, .	3.0	4
41	Protein Engineering of Multi-Modular Transcription Factor Alcohol Dehydrogenase Repressor 1 (Adr1p), a Tool for Dissecting In Vitro Transcription Activation. <i>Biomolecules</i> , 2019, 9, 497.	4.0	0
42	A protein interaction free energy model based on amino acid residue contributions: Assessment of point mutation stability of T4 lysozyme. <i>Technology</i> , 2019, 07, 12-39.	1.4	2
43	AllerCatPro"prediction of protein allergenicity potential from the protein sequence. <i>Bioinformatics</i> , 2019, 35, 3020-3027.	4.1	115
44	Structural analysis of proteins using X-ray diffraction technique. , 2019, , 69-84.		3
45	Analysis of the TP53 Deleterious Single Nucleotide Polymorphisms Impact on Estrogen Receptor Alpha-p53 Interaction: A Machine Learning Approach. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2962.	4.1	8
46	A Practical Perspective: The Effect of Ligand Conformers on the Negative Image-Based Screening. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2779.	4.1	9
47	Mode-of-Action-Guided, Molecular Modeling-Based Toxicity Prediction: A Novel Approach for In Silico Predictive Toxicology. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 99-118.	0.6	2
48	The IgA Isotype of Anti- β 2 Glycoprotein I Antibodies Recognizes Epitopes in Domains 3, 4, and 5 That Are Located in a Lateral Zone of the Molecule (L-Shaped). <i>Frontiers in Immunology</i> , 2019, 10, 1031.	4.8	12
49	Molecular mechanisms involved in drug-induced liver injury caused by urate-lowering Chinese herbs: A network pharmacology study and biology experiments. <i>PLoS ONE</i> , 2019, 14, e0216948.	2.5	20
50	Structural Basis of Response Regulator Function. <i>Annual Review of Microbiology</i> , 2019, 73, 175-197.	7.3	118
51	Computational prediction of functions of intrinsically disordered regions. <i>Progress in Molecular Biology and Translational Science</i> , 2019, 166, 341-369.	1.7	27
52	Computational approach identifies protein off-targets for Isoniazid-NAD adduct: hypothesizing a possible drug resistance mechanism in <i>Mycobacterium tuberculosis</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 1-14.	3.5	5
53	Biomolecular Data Resources: Bioinformatics Infrastructure for Biomedical Data Science. <i>Annual Review of Biomedical Data Science</i> , 2019, 2, 199-222.	6.5	8
54	Computational Prediction of MoRFs, Short Disorder-to-order Transitioning Protein Binding Regions. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 454-462.	4.1	50

#	ARTICLE	IF	CITATIONS
55	Shared Signature Dynamics Tempered by Local Fluctuations Enables Fold Adaptability and Specificity. Molecular Biology and Evolution, 2019, 36, 2053-2068.	8.9	45
56	Application of In Silico Drug Repurposing in Infectious Diseases. , 2019, , 427-462.		0
57	Omics-Driven Knowledge-Based Discovery of Anthelmintic Targets and Drugs. , 2019, , 329-358.		2
58	Identification of compounds that inhibit the binding of Keap1a/Keap1b Kelch DGR domain with Nrf2 ETGE/DLG motifs in zebrafish. Basic and Clinical Pharmacology and Toxicology, 2019, 125, 259-270.	2.5	20
59	Mapping the Azolog Space Enables the Optical Control of New Biological Targets. ACS Central Science, 2019, 5, 607-618.	11.3	65
60	Computational Prediction of Secondary and Supersecondary Structures from Protein Sequences. Methods in Molecular Biology, 2019, 1958, 73-100.	0.9	11
61	Analyzing Change in Protein Stability Associated with Single Point Deletions in a Newly Defined Protein Structure Database. Journal of Proteome Research, 2019, 18, 1402-1410.	3.7	11
62	Molecular Cavity Topological Representation for Pattern Analysis: A NLP Analogy-Based Word2Vec Method. International Journal of Molecular Sciences, 2019, 20, 6019.	4.1	6
63	Targeted isolation and cultivation of uncultivated bacteria by reverse genomics. Nature Biotechnology, 2019, 37, 1314-1321.	17.5	231
64	Structural Features of Tight-Junction Proteins. International Journal of Molecular Sciences, 2019, 20, 6020.	4.1	98
65	Biosynthesis of the Stress-Protectant and Chemical Chaperon Ectoine: Biochemistry of the Transaminase EctB. Frontiers in Microbiology, 2019, 10, 2811.	3.5	39
66	A Computational Bipartite Graph-Based Drug Repurposing Method. Methods in Molecular Biology, 2019, 1903, 115-127.	0.9	7
67	RCSB Protein Data Bank: biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. Nucleic Acids Research, 2019, 47, D464-D474.	14.5	918
68	Enhancing thermostability of a psychrophilic alpha-amylase by the structural energy optimization in the trajectories of molecular dynamics simulations. International Journal of Biological Macromolecules, 2020, 142, 624-633.	7.5	27
69	Structural and functional analysis of "non-smelly" proteins. Cellular and Molecular Life Sciences, 2020, 77, 2423-2440.	5.4	16
70	The Evolutionary History of Ephs and Ephrins: Toward Multicellular Organisms. Molecular Biology and Evolution, 2020, 37, 379-394.	8.9	13
71	TMPfold: A Web Tool for Predicting Stability of Transmembrane α -Helix Association. Journal of Molecular Biology, 2020, 432, 3388-3394.	4.2	4
72	Recent advances in the improvement of enzyme thermostability by structure modification. Critical Reviews in Biotechnology, 2020, 40, 83-98.	9.0	145

#	ARTICLE	IF	CITATIONS
73	Breaking the Glass Ceiling in Simulation and Modeling: Women in Pharmaceutical Discovery. Journal of Medicinal Chemistry, 2020, 63, 1929-1936.	6.4	3
74	Modeling beta-sheet peptide-protein interactions: Rosetta FlexPepDock in CAPRI rounds 38-45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1037-1049.	2.6	10
75	New Features of Carbohydrate Structure Database Notation (CSDB Linear), As Compared to Other Carbohydrate Notations. Journal of Chemical Information and Modeling, 2020, 60, 1276-1289.	5.4	11
76	A tiered high-throughput screening approach for evaluation of estrogen and androgen receptor modulation by environmentally relevant bisphenol A substitutes. Science of the Total Environment, 2020, 717, 134743.	8.0	30
77	Enhancing Protein Crystallization under a Magnetic Field. Crystals, 2020, 10, 821.	2.2	9
78	Nature of the copper-nitrosyl intermediates of copper nitrite reductases during catalysis. Chemical Science, 2020, 11, 12485-12492.	7.4	6
79	Identification of novel vaccine candidates against carbapenem resistant Klebsiella pneumoniae: A systematic reverse proteomic approach. Computational Biology and Chemistry, 2020, 89, 107380.	2.3	9
80	ConoMode, a database for conopeptide binding modes. Database: the Journal of Biological Databases and Curation, 2020, 2020, .	3.0	2
81	Data-driven rational biosynthesis design: from molecules to cell factories. Briefings in Bioinformatics, 2020, 21, 1238-1248.	6.5	9
82	Characterisation of plasmodial transketolases and identification of potential inhibitors: an in silico study. Malaria Journal, 2020, 19, 442.	2.3	5
83	An Educational Bioinformatics Project to Improve Genome Annotation. Frontiers in Microbiology, 2020, 11, 577497.	3.5	6
84	Identification of A Putative T6SS Immunity Islet in Salmonella Typhi. Pathogens, 2020, 9, 559.	2.8	7
85	Identification of continuous immunoglobulin G epitopes of Dermatophagoides farinae allergens by peptide microarray immunoassay. IUBMB Life, 2020, 72, 1976-1985.	3.4	2
86	Three-Dimensional Structures of Carbohydrates and Where to Find Them. International Journal of Molecular Sciences, 2020, 21, 7702.	4.1	22
87	Exploration and identification of novel inhibitors against Knowpain-4 of P. knowlesi using a combinatorial 3D pharmacophore modeling approach. Network Modeling Analysis in Health Informatics and Bioinformatics, 2020, 9, 1.	2.1	0
88	Identification of New Rofecoxib-Based Cyclooxygenase-2 Inhibitors: A Bioinformatics Approach. Pharmaceuticals, 2020, 13, 209.	3.8	52
89	Molecular Dynamics Simulations of Mite Aquaporin DerfAQP1 from the Dust Mite Dermatophagoides farinae (Acariformes: Pyroglyphidae). BioMed Research International, 2020, 2020, 1-7.	1.9	1
90	Multifunctional Proteins. Biophysics (Russian Federation), 2020, 65, 390-403.	0.7	3

#	ARTICLE	IF	CITATIONS
91	A SNP-mediated lncRNA (LOC146880) and microRNA (miR-539-5p) interaction and its potential impact on the NSCLC risk. <i>Journal of Experimental and Clinical Cancer Research</i> , 2020, 39, 157.	8.6	21
92	Identification of Potential Inhibitors of 3CL Protease of SARS-CoV-2 From ZINC Database by Molecular Docking-Based Virtual Screening. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 603037.	3.5	29
93	Identification of potential inhibitors of Zika virus NS5 RNA-dependent RNA polymerase through virtual screening and molecular dynamic simulations. <i>Saudi Pharmaceutical Journal</i> , 2020, 28, 1580-1591.	2.7	12
94	Molecular docking analyses of CYP450 monooxygenases of <i>Tribolium castaneum</i> (Herbst) reveal synergism of quercetin with paraoxon and tetraethyl pyrophosphate: in vivo and in silico studies. <i>Toxicology Research</i> , 2020, 9, 212-221.	2.1	4
95	Teaching and Learning Computational Drug Design: Student Investigations of 3D Quantitative Structure–Activity Relationships through Web Applications. <i>Journal of Chemical Education</i> , 2020, 97, 1922-1930.	2.3	27
96	Prediction of protein-binding residues: dichotomy of sequence-based methods developed using structured complexes versus disordered proteins. <i>Bioinformatics</i> , 2020, 36, 4729-4738.	4.1	16
97	Functional Heterologous Expression of Mature Lipase LipA from <i>Pseudomonas aeruginosa</i> PSA01 in <i>Escherichia coli</i> SHuffle and BL21 (DE3): Effect of the Expression Host on Thermal Stability and Solvent Tolerance of the Enzyme Produced. <i>International Journal of Molecular Sciences</i> , 2020, 21, 3925.	4.1	7
98	LigBuilder V3: A Multi-Target de novo Drug Design Approach. <i>Frontiers in Chemistry</i> , 2020, 8, 142.	3.6	46
99	Pseudo-Symmetric Assembly of Protodomains as a Common Denominator in the Evolution of Polytropic Helical Membrane Proteins. <i>Journal of Molecular Evolution</i> , 2020, 88, 319-344.	1.8	5
100	In silico Analysis of the tryptophan hydroxylase 2 (TPH2) protein variants related to psychiatric disorders. <i>PLoS ONE</i> , 2020, 15, e0229730.	2.5	14
101	Tools to Ease the Choice and Design of Protein Crystallisation Experiments. <i>Crystals</i> , 2020, 10, 95.	2.2	7
102	Identifying Synergistic Mechanisms of Multiple Ingredients in Shuangbai Tablets against Proteinuria by Virtual Screening and a Network Pharmacology Approach. <i>Evidence-based Complementary and Alternative Medicine</i> , 2020, 2020, 1-15.	1.2	4
103	User guide for the discovery of potential drugs via protein structure prediction and ligand docking simulation. <i>Journal of Microbiology</i> , 2020, 58, 235-244.	2.8	25
104	Computational approaches for identifying potential inhibitors on targeting protein interactions in drug discovery. <i>Advances in Protein Chemistry and Structural Biology</i> , 2020, 121, 25-47.	2.3	9
105	In silico identification and structure function analysis of a putative coclaurine N-methyltransferase from <i>Aristolochia fimbriata</i> . <i>Computational Biology and Chemistry</i> , 2020, 85, 107201.	2.3	1
106	Genomic variance of the 2019-nCoV coronavirus. <i>Journal of Medical Virology</i> , 2020, 92, 522-528.	5.0	353
107	Master Regulator Analysis of the SARS-CoV-2/Human Interactome. <i>Journal of Clinical Medicine</i> , 2020, 9, 982.	2.4	160
108	Big data and artificial intelligence discover novel drugs targeting proteins without 3D structure and overcome the undruggable targets. <i>Stroke and Vascular Neurology</i> , 2020, 5, 381-387.	3.3	10

#	ARTICLE	IF	CITATIONS
109	MPTherm: database for membrane protein thermodynamics for understanding folding and stability. Briefings in Bioinformatics, 2021, 22, 2119-2125.	6.5	18
110	MDeePred: novel multi-channel protein featurization for deep learning-based binding affinity prediction in drug discovery. Bioinformatics, 2021, 37, 693-704.	4.1	61
111	The <scp>BioGRID</scp> database: A comprehensive biomedical resource of curated protein, genetic, and chemical interactions. Protein Science, 2021, 30, 187-200.	7.6	769
112	Classification of the glyphosate target enzyme (5-enolpyruvylshikimate-3-phosphate synthase) for assessing sensitivity of organisms to the herbicide. Journal of Hazardous Materials, 2021, 408, 124556.	12.4	55
113	Analyses of structural dynamics revealed flexible binding mechanism for the <scp><i>Agrilus mali</i></scp> odorant binding protein 8 towards plant volatiles. Pest Management Science, 2021, 77, 1642-1653.	3.4	15
114	Network Pharmacology and bioinformatics analyses identify intersection genes of niacin and COVID-19 as potential therapeutic targets. Briefings in Bioinformatics, 2021, 22, 1279-1290.	6.5	100
115	Identification of Dominant Transcripts in Oxidative Stress Response by a Full-Length Transcriptome Analysis. Molecular and Cellular Biology, 2021, 41, .	2.3	7
116	ProThermDB: thermodynamic database for proteins and mutants revisited after 15 years. Nucleic Acids Research, 2021, 49, D420-D424.	14.5	102
117	How to use the <scp><i>MEROPS</i></scp> database and website to help understand peptidase specificity. Protein Science, 2021, 30, 83-92.	7.6	44
118	Negative Image-Based Screening: Rigid Docking Using Cavity Information. Methods in Molecular Biology, 2021, 2266, 125-140.	0.9	1
119	Structural binding site comparisons reveal Crizotinib as a novel LRRK2 inhibitor. Computational and Structural Biotechnology Journal, 2021, 19, 3674-3681.	4.1	9
120	Negative Image-Based Rescoring: Using Cavity Information to Improve Docking Screening. Methods in Molecular Biology, 2021, 2266, 141-154.	0.9	0
121	Resources for Docking-Based Virtual Screening. , 2021, , 179-203.		1
122	Cold-Shock Domainsâ€™ Abundance, Structure, Properties, and Nucleic-Acid Binding. Cancers, 2021, 13, 190.	3.7	35
123	Structural Bioinformatics to Unveil Weaknesses of Coronavirus Spike Glycoprotein Stability. Methods in Pharmacology and Toxicology, 2021, , 203.	0.2	0
125	MINERVA, A Platform for the Exploration of Disease Maps. , 2021, , 480-489.		0
126	Online Resource and Tools for the Development of Drugs Against Novel Coronavirus. Methods in Pharmacology and Toxicology, 2021, , 735-759.	0.2	7
127	TMPSS: A Deep Learning-Based Predictor for Secondary Structure and Topology Structure Prediction of Alpha-Helical Transmembrane Proteins. Frontiers in Bioengineering and Biotechnology, 2020, 8, 629937.	4.1	14

#	ARTICLE	IF	CITATIONS
128	Drug Design and Discovery: Theory, Applications, Open Issues and Challenges. Studies in Computational Intelligence, 2021, , 337-358.	0.9	0
129	Getting to know each other: PPIMem, a novel approach for predicting transmembrane protein-protein complexes. Computational and Structural Biotechnology Journal, 2021, 19, 5184-5197.	4.1	5
130	Retrieval and Investigation of Data on SARS-CoV-2 and COVID-19 Using Bioinformatics Approach. Advances in Experimental Medicine and Biology, 2021, 1318, 839-857.	1.6	23
131	Applications of Protein Secondary Structure Algorithms in SARS-CoV-2 Research. Journal of Proteome Research, 2021, 20, 1457-1463.	3.7	3
132	Chemical composition and pharmacological mechanism of ephedra-glycyrrhiza drug pair against coronavirus disease 2019 (COVID-19). Aging, 2021, 13, 4811-4830.	3.1	29
133	Bioinformatics in Microbial Biotechnology: A Genomics and Proteomics Perspective. , 2021, , 54-69.		0
134	Exploring the Oxidative Stress Mechanism of Buyang Huanwu Decoction in Intervention of Vascular Dementia Based on Systems Biology Strategy. Oxidative Medicine and Cellular Longevity, 2021, 2021, 1-29.	4.0	10
135	Molecular storytelling for online structural biology outreach and education. Structural Dynamics, 2021, 8, 020401.	2.3	7
136	MCPdb: The bacterial microcompartment database. PLoS ONE, 2021, 16, e0248269.	2.5	11
137	Exploring the new potential antiviral constituents of Moringa oliefera for SARS-COV-2 pathogenesis: An in silico molecular docking and dynamic studies. Chemical Physics Letters, 2021, 767, 138379.	2.6	58
138	Comprehensive Identification of Bridge Genes to Explain the Progression from Chronic Hepatitis B Virus Infection to Hepatocellular Carcinoma. Journal of Inflammation Research, 2021, Volume 14, 1613-1624.	3.5	4
139	Pharmacological Mechanisms Underlying the Anti-asthmatic Effects of Modified Guomin Decoction Determined by Network Pharmacology and Molecular Docking. Frontiers in Molecular Biosciences, 2021, 8, 644561.	3.5	6
140	Performance improvement for a 2D convolutional neural network by using SSC encoding on proteinâ€protein interaction tasks. BMC Bioinformatics, 2021, 22, 184.	2.6	10
141	Assessing the functional relevance of splice isoforms. NAR Genomics and Bioinformatics, 2021, 3, lqab044.	3.2	13
142	Contribution of structural accessibility to the cooperative relationship of TF-lncRNA in myopia. Briefings in Bioinformatics, 2021, 22, .	6.5	3
143	Computational Identification of Potential Anti-Inflammatory Natural Compounds Targeting the p38 Mitogen-Activated Protein Kinase (MAPK): Implications for COVID-19-Induced Cytokine Storm. Biomolecules, 2021, 11, 653.	4.0	25
144	Based on Network Pharmacology and Molecular Docking to Explore the Underlying Mechanism of Huangqi Gegen Decoction for Treating Diabetic Nephropathy. Evidence-based Complementary and Alternative Medicine, 2021, 2021, 1-14.	1.2	9
145	Molecular Docking and Virtual Screening Based Prediction of Drugs for COVID-19. Combinatorial Chemistry and High Throughput Screening, 2021, 24, 716-728.	1.1	39

#	ARTICLE	IF	CITATIONS
147	Computational Biology and Machine Learning Approaches to Understand Mechanistic Microbiome-Host Interactions. <i>Frontiers in Microbiology</i> , 2021, 12, 618856.	3.5	19
148	Functional and Material Properties in Nanocatalyst Design: A Data Handling and Sharing Problem. <i>International Journal of Molecular Sciences</i> , 2021, 22, 5176.	4.1	6
149	Thermodynamics-Based Molecular Modeling of Î±-Helices in Membranes and Micelles. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2884-2896.	5.4	6
150	Evaluation of potency of the selected bioactive molecules from Indian medicinal plants with MPro of SARS-CoV-2 through in silico analysis. <i>Journal of Ayurveda and Integrative Medicine</i> , 2022, 13, 100449.	1.7	21
151	A trimethoprim derivative impedes antibiotic resistance evolution. <i>Nature Communications</i> , 2021, 12, 2949.	12.8	41
152	Uncovering the Mechanism of Curcuma in the Treatment of Ulcerative Colitis Based on Network Pharmacology, Molecular Docking Technology, and Experiment Verification. <i>Evidence-based Complementary and Alternative Medicine</i> , 2021, 2021, 1-14.	1.2	13
153	Integrated Core Proteomics, Subtractive Proteomics, and Immunoinformatics Investigation to Unveil a Potential Multi-Epitope Vaccine against Schistosomiasis. <i>Vaccines</i> , 2021, 9, 658.	4.4	30
154	Elucidation of ligand binding and dimerization of NADPH :protochlorophyllide (Pchl _{id}) oxidoreductase from pea (<i>Pisum sativum</i> L.) by structural analysis and simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1300-1314.	2.6	1
155	Study of the Active Components and Molecular Mechanism of <i>Tripterygium wilfordii</i> in the Treatment of Diabetic Nephropathy. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 664416.	3.5	9
156	Dissecting the novel mechanism of reduning injection in treating Coronavirus Disease 2019 (COVID-19) based on network pharmacology and experimental verification. <i>Journal of Ethnopharmacology</i> , 2021, 273, 113871.	4.1	23
158	Cyclic Peptides as T-Type Calcium Channel Blockers: Characterization and Molecular Mapping of the Binding Site. <i>ACS Pharmacology and Translational Science</i> , 2021, 4, 1379-1389.	4.9	3
160	The clinical importance of tandem exon duplication-derived substitutions. <i>Nucleic Acids Research</i> , 2021, 49, 8232-8246.	14.5	11
161	Computational Analysis of the Crystal and Cryo-EM Structures of P-Loop Channels with Drugs. <i>International Journal of Molecular Sciences</i> , 2021, 22, 8143.	4.1	3
162	Computational drug repurposing study of antiviral drugs against main protease, RNA polymerase, and spike proteins of SARS-CoV-2 using molecular docking method. <i>Journal of Basic and Clinical Physiology and Pharmacology</i> , 2022, 33, 85-95.	1.3	6
163	Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021, 43, 128079.	2.2	29
164	Network Pharmacology-Based Investigation on the Anti-Osteoporosis Mechanism of Astragaloside IV. <i>Natural Product Communications</i> , 2021, 16, 1934578X2110295.	0.5	2
165	Predicting Proteinâ€“Protein Interactions Between Rice and Blast Fungus Using Structure-Based Approaches. <i>Frontiers in Plant Science</i> , 2021, 12, 690124.	3.6	9
166	The Potential Effect of <i>Rhizoma coptidis</i> on Polycystic Ovary Syndrome Based on Network Pharmacology and Molecular Docking. <i>Evidence-based Complementary and Alternative Medicine</i> , 2021, 2021, 1-12.	1.2	5

#	ARTICLE	IF	CITATIONS
167	Identification of Potential Bioactive Ingredients and Mechanisms of the Guanxin Suhe Pill on Angina Pectoris by Integrating Network Pharmacology and Molecular Docking. Evidence-based Complementary and Alternative Medicine, 2021, 2021, 1-13.	1.2	2
168	Recent structural insights into bacterial microcompartment shells. Current Opinion in Microbiology, 2021, 62, 51-60.	5.1	18
170	Comparison and Analysis on the Existing Single-Herbal Strategies against Viral Myocarditis. Genetical Research, 2021, 2021, 1-12.	0.9	4
171	Integrated Phytochemical Analysis Based on UPLC-MS/MS and Network Pharmacology Approaches to Explore the Effect of <i>Odontites vulgaris</i> Moench on Rheumatoid Arthritis. Frontiers in Pharmacology, 2021, 12, 707687.	3.5	6
172	Topological and Structural Plasticity of the Single Ig Fold and the Double Ig Fold Present in CD19. Biomolecules, 2021, 11, 1290.	4.0	5
173	Rational Design of Constrained Peptides as Protein Interface Inhibitors. Antibodies, 2021, 10, 32.	2.5	0
174	Features and Functions of the A-Minor Motif, the Most Common Motif in RNA Structure. Biochemistry (Moscow), 2021, 86, 952-961.	1.5	2
175	Exploration of the molecular targets and mechanisms of suxiao xintong dropping pills for myocardial infarction by network pharmacology method. Bioscience Reports, 2021, 41, .	2.4	5
176	Prediction of antischistosomal small molecules using machine learning in the era of big data. Molecular Diversity, 2021, , 1.	3.9	1
178	Modeling SARS-CoV-2 proteins in the CASP-commons experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1987-1996.	2.6	24
179	Discovery of novel anti-inflammatory and analgesic compounds from the traditional Chinese medicine <i>Salvia miltiorrhiza</i> using network pharmacology and molecular docking. Frontiers in Pharmacology, 2021, 12, 707687.	3.5	6
180	Uncovering the mechanism of the Shenzhi Jiannao formula against vascular dementia using a combined network pharmacology approach and molecular biology. Phytomedicine, 2021, 90, 153637.	5.3	20
181	Microglia Mediate the Occurrence and Development of Alzheimer's Disease Through Ligand-Receptor Axis Communication. Frontiers in Aging Neuroscience, 2021, 13, 731180.	3.4	15
183	Exploring the mechanism of Danggui Buxue Decoction in regulating atherosclerotic disease network based on integrated pharmacological methods. Bioscience Reports, 2021, 41, .	2.4	1
184	virusMED: an atlas of hotspots of viral proteins. IUCr, 2021, 8, 931-942.	2.2	5
185	Multitarget mechanism of Yiqi Jiedu Huayu decoction on diabetic cardiomyopathy based on network pharmacology. European Journal of Integrative Medicine, 2021, 47, 101388.	1.7	1
186	Amyloid β fibrils disruption by kolaviron: Molecular docking and extended molecular dynamics simulation studies. Computational Biology and Chemistry, 2021, 94, 107557.	2.3	14
187	Cheminformatics-Based Identification of Potential Novel Anti-SARS-CoV-2 Natural Compounds of African Origin. Molecules, 2021, 26, 406.	3.8	35

#	ARTICLE	IF	CITATIONS
188	Computational Study of the Interactions between Antimalarial Chemotherapies with Folate Pathway Receptors and Telomerase Reverse Transcriptase. Computational Chemistry, 2021, 09, 197-214.	0.7	0
189	Structural genomics and the Protein Data Bank. Journal of Biological Chemistry, 2021, 296, 100747.	3.4	11
190	Genomics Reveals the Origins of Historical Specimens. Molecular Biology and Evolution, 2021, 38, 2166-2176.	8.9	24
197	Homology-based loop modeling yields more complete crystallographic protein structures. IUCr, 2018, 5, 585-594.	2.2	27
198	A comprehensive overview of sequence-based protein-binding residue predictions for structured and disordered regions. , 2020, , 33-58.		4
199	Best practice data life cycle approaches for the life sciences. F1000Research, 2017, 6, 1618.	1.6	21
200	Best practice data life cycle approaches for the life sciences. F1000Research, 2017, 6, 1618.	1.6	23
201	FilterDCA: Interpretable supervised contact prediction using inter-domain coevolution. PLoS Computational Biology, 2020, 16, e1007621.	3.2	8
202	Mapping the landscape of Artificial Intelligence applications against COVID-19. Journal of Artificial Intelligence Research, 0, 69, 807-845.	7.0	275
204	Therapeutic Targets and Computational Approaches on Drug Development for COVID-19. Current Topics in Medicinal Chemistry, 2020, 20, 2210-2220.	2.1	16
206	Discovery of several thousand highly diverse circular DNA viruses. ELife, 2020, 9, .	6.0	131
207	Identification of Aloperine as an anti-apoptotic Bcl2 protein inhibitor in glioma cells. PeerJ, 2019, 7, e7652.	2.0	13
208	Investigation of anti-osteoporosis mechanisms of Rehmanniae Radix Preparata based on network pharmacology and experimental verification. Journal of Orthopaedic Surgery and Research, 2021, 16, 599.	2.3	11
209	The GH19 Engineering Database: Sequence diversity, substrate scope, and evolution in glycoside hydrolase family 19. PLoS ONE, 2021, 16, e0256817.	2.5	14
210	Screening Potential Drugs for COVID-19 Based on Bound Nuclear Norm Regularization. Frontiers in Genetics, 2021, 12, 749256.	2.3	5
211	Study on the mechanism of treating COVID-19 with Shenqi Wan based on network pharmacology. Drug Development and Industrial Pharmacy, 2021, , 1-11.	2.0	8
215	Application of Bioinformatics to Asthma. Translational Bioinformatics, 2018, , 349-359.	0.0	0
218	Elaboration of Simplest Folding Structures in 2-Dimensional Lattice with Delta-Hemolysin and Its Variants in HP Model. Journal of Biomedical Science and Engineering, 2019, 12, 293-309.	0.4	0

#	ARTICLE	IF	CITATIONS
221	High-Performance Hybrid Computing for Bioinformatic Analysis of Protein Superfamilies. Communications in Computer and Information Science, 2019, , 249-264.	0.5	0
222	Binding of metal ions and water molecules to nucleic acid bases: the influence of water molecule coordination to a metal ion on water's nucleic acid base hydrogen bonds. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 301-309.	1.1	1
224	In Silico Laboratory: Tools for Similarity-Based Drug Discovery. Methods in Molecular Biology, 2020, 2089, 1-28.	0.9	2
229	Recent Advancement in Predicting Subcellular Localization of Mycobacterial Protein with Machine Learning Methods. Medicinal Chemistry, 2020, 16, 605-619.	1.5	2
230	Heterogeneous Composition of Oxygen-Evolving Complexes in Crystal Structures of Dark-Adapted Photosystem II. Biochemistry, 2021, 60, 3374-3384.	2.5	8
231	Data- and diversity-driven development of a Shotgun crystallization screen using the Protein Data Bank. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1437-1450.	2.3	3
232	Crosstalk between Circulatory Microenvironment and Vascular Endothelial Cells in Acute Myocardial Infarction. Journal of Inflammation Research, 2021, Volume 14, 5597-5610.	3.5	2
233	Spatial arrangement of proteins in planar and curved membranes by <scp>PPM</scp> 3.0. Protein Science, 2022, 31, 209-220.	7.6	89
234	Characterization of Schistosoma mansoni Dihydrofolate Reductase (DHFR). Methods in Molecular Biology, 2020, 2151, 159-172.	0.9	1
237	RBM8A Promotes Glioblastoma Growth and Invasion Through the Notch/STAT3 Pathway. Frontiers in Oncology, 2021, 11, 736941.	2.8	12
238	The inhibitory effect of KN-93 and KN-62 as a result of CaM-directed blocking animal CaMK2 and plant CDPK activation. Faktori Eksperimental Noi Evolucii Organizmiv, 0, 26, 298-304.	0.0	0
239	Potential Therapeutic Approaches to Alzheimer's Disease By Bioinformatics, Cheminformatics And Predicted Adme-Tox Tools. Current Neuropharmacology, 2020, 18, 696-719.	2.9	10
240	Tyrophagus putrescentiae group 4 allergen allergenicity and epitope prediction. Allergologia Et Immunopathologia, 2020, 48, 619-625.	1.7	3
241	EMPAS: Electron Microscopy Screening for Endogenous Protein Architectures. Molecules and Cells, 2020, 43, 804-812.	2.6	0
242	Annotating Putative Proteins Using I-TASSER. MicroPublication Biology, 2021, 2021, .	0.1	0
243	Novel dynamic residue network analysis approaches to study allosteric modulation: SARS-CoV-2 Mpro and its evolutionary mutations as a case study. Computational and Structural Biotechnology Journal, 2021, 19, 6431-6455.	4.1	14
244	Instructional Design for an Undergraduate Laboratory Course in Molecular Biophysics. The Biophysicist, 2021, 2, 41-54.	0.3	0
246	Configurational Differences and Binding Mechanisms of Interleukin-1 Receptor-Associated Kinase 1. , 2020, , .		0

#	ARTICLE	IF	CITATIONS
247	Probing In Silico the Benzimidazole Privileged Scaffold for the Development of Drug-like Anti-RSV Agents. <i>Pharmaceuticals</i> , 2021, 14, 1307.	3.8	17
248	The intrinsically disordered TSSC4 protein acts as a helicase inhibitor, placeholder and multi-interaction coordinator during snRNP assembly and recycling. <i>Nucleic Acids Research</i> , 2022, 50, 2938-2958.	14.5	11
249	Noise-Transfer2Clean: denoising cryo-EM images based on noise modeling and transfer. <i>Bioinformatics</i> , 2022, 38, 2022-2029.	4.1	13
250	Prediction and Modeling of Protein-Protein Interactions Using Spotted Peptides with a Template-Based Approach. <i>Biomolecules</i> , 2022, 12, 201.	4.0	1
251	Computational design of a cutinase for plastic biodegradation by mining molecular dynamics simulations trajectories. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 459-470.	4.1	27
252	Merging NMR Data and Computation Facilitates Data-Centered Research. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 817175.	3.5	2
253	In silico study to identify new monoamine oxidase type a (MAO-A) selective inhibitors from natural source by virtual screening and molecular dynamics simulation. <i>Journal of Molecular Structure</i> , 2022, 1254, 132244.	3.6	6
254	Classification Model for the Second Extracellular Loop of Class A GPCRs. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 511-522.	5.4	25
255	A novel sequence-based predictor for identifying and characterizing thermophilic proteins using estimated propensity scores of dipeptides. <i>Scientific Reports</i> , 2021, 11, 23782.	3.3	24
256	Elucidating the role of N440K mutation in SARS-CoV-2 spike ACE-2 binding affinity and COVID-19 severity by virtual screening, molecular docking and dynamics approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-18.	3.5	11
258	Structural Prediction of Peptide-MHC Binding Modes. <i>Methods in Molecular Biology</i> , 2022, 2405, 245-282.	0.9	7
259	Network pharmacology analysis and molecular docking to unveil the potential mechanisms of San-Huang-Chai-Zhu formula treating cholestasis. <i>PLoS ONE</i> , 2022, 17, e0264398.	2.5	5
260	Hepatoprotective mechanism of <i>Silybum marianum</i> on nonalcoholic fatty liver disease based on network pharmacology and experimental verification. <i>Bioengineered</i> , 2022, 13, 5216-5235.	3.2	24
261	In Silico Screening of Bioactive Compounds of Representative Seaweeds to Inhibit SARS-CoV-2 ACE2-Bound Omicron B.1.1.529 Spike Protein Trimer. <i>Marine Drugs</i> , 2022, 20, 148.	4.6	19
262	Molecular Mechanism Investigation on Monomer Kaempferol of the Traditional Medicine Dingqing Tablet in Promoting Apoptosis of Acute Myeloid Leukemia HL-60 Cells. <i>Evidence-based Complementary and Alternative Medicine</i> , 2022, 2022, 1-11.	1.2	4
263	Discovery and Characterization of the Naturally Occurring Inhibitors Against Human Pancreatic Lipase in <i>Ampelopsis grossedentata</i> . <i>Frontiers in Nutrition</i> , 2022, 9, 844195.	3.7	6
264	A Decomposition and Dominance-Based Multiobjective Artificial Bee Colony Algorithm for Multiple Sequence Alignment. <i>Mobile Information Systems</i> , 2022, 2022, 1-13.	0.6	1
265	Network Pharmacological Study on Mechanism of the Therapeutic Effect of Modified Duhuo Jisheng Decoction in Osteoporosis. <i>Frontiers in Endocrinology</i> , 2022, 13, 860649.	3.5	2

#	ARTICLE	IF	CITATIONS
266	Identification of the potential mechanism of Radix pueraria in colon cancer based on network pharmacology. Scientific Reports, 2022, 12, 3765.	3.3	4
267	The Mechanism of Ginseng and Astragalus Decoction in the Treatment of Malignant Pleural Effusion Based on Network Pharmacology and Molecular Docking Technology. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-11.	1.2	0
268	A Network Pharmacology Approach to Reveal the Underlying Mechanisms of Rhizoma Dioscoreae Nipponicae in the Treatment of Asthma. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-17.	1.2	1
269	Adipose-derived mesenchymal stem cells may reduce intestinal epithelial damage in ulcerative colitis by communicating with macrophages and blocking inflammatory pathways: an analysis in silico. Aging, 2022, 14, 2665-2677.	3.1	6
270	Natural alkaloids targeting EGFR in non-small cell lung cancer: Molecular docking and ADMET predictions. Chemico-Biological Interactions, 2022, 358, 109901.	4.0	11
271	The mechanism of dioscin preventing lung cancer based on network pharmacology and experimental validation. Journal of Ethnopharmacology, 2022, 292, 115138.	4.1	13
272	GCRNN: graph convolutional recurrent neural network for compound-protein interaction prediction. BMC Bioinformatics, 2021, 22, 616.	2.6	6
273	Structure-Based Virtual Screening of Benzaldehyde Thiosemicarbazone Derivatives against DNA Gyrase B of Mycobacterium tuberculosis. Evidence-based Complementary and Alternative Medicine, 2021, 2021, 1-11.	1.2	1
274	A computational biology approach for the identification of potential SARS-CoV-2 main protease inhibitors from natural essential oil compounds.. F1000Research, 0, 10, 1313.	1.6	1
275	Identification of novel potential anti-diabetic candidates targeting human pancreatic α -amylase and human α -glucosidase: an exhaustive structure-based screening. Canadian Journal of Chemistry, 2022, 100, 338-352.	1.1	7
276	HDContact: a novel predictor of residue-residue contacts on hetero-dimer interfaces via sequential information and transfer learning strategy. Briefings in Bioinformatics, 2022, 23, .	6.5	5
277	Novel adamantyl clubbed iminothiazolidinones as promising elastase inhibitors: design, synthesis, molecular docking, ADMET and DFT studies. RSC Advances, 2022, 12, 11974-11991.	3.6	28
291	HORDB a comprehensive database of peptide hormones. Scientific Data, 2022, 9, 187.	5.3	5
294	Effects of Koumiss on Intestinal Immune Modulation in Immunosuppressed Rats. Frontiers in Nutrition, 2022, 9, 765499.	3.7	10
295	SCAMPER: Accurate Type-Specific Prediction of Calcium-Binding Residues Using Sequence-Derived Features. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2023, 20, 1406-1416.	3.0	0
296	Membranome 3.0: Database of single-pass membrane proteins with α -Fold models. Protein Science, 2022, 31, e4318.	7.6	20
297	Network Pharmacology and Molecular Docking-Based Strategy to Investigate the Multitarget Mechanisms of Shenqi Yizhi Granule on Alzheimer's Disease. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-14.	1.2	2
298	Wangzaozin A, a potent novel microtubule stabilizer, targets both the taxane and laulimalide sites on β -tubulin through molecular dynamics simulations. Life Sciences, 2022, 301, 120583.	4.3	1

#	ARTICLE	IF	CITATIONS
299	Exploring the Mechanism of Ling-Gui-Zhu-Gan Decoction in Ventricular Remodeling after Acute Myocardial Infarction Based on UPLC and In Vivo Experiments. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-14.	1.2	4
300	Optimal learning of Markov $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e86" altimg="si603.svg"} \rangle \langle \text{mml:mi} \rangle k \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -tree topology. Journal of Computational Mathematics and Data Science, 2022, 4, 100046.	2.3	24
301	Protein language-model embeddings for fast, accurate, and alignment-free protein structure prediction. Structure, 2022, 30, 1169-1177.e4.	3.3	52
302	Exploring the Effect and Mechanism of Si-Miao-Yong-An Decoction on Abdominal Aortic Aneurysm Based on Mice Experiment and Bioinformatics Analysis. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-15.	1.2	0
304	Identifying Candidate Flavonoids for Non-Alcoholic Fatty Liver Disease by Network-Based Strategy. Frontiers in Pharmacology, 0, 13, .	3.5	4
305	Dual transcriptome based reconstruction of Salmonella-human integrated metabolic network to screen potential drug targets. PLoS ONE, 2022, 17, e0268889.	2.5	7
306	Amentoflavone derivatives significantly act towards the main protease (3CLPRO/M ^{PRO}) of SARS-CoV-2: in silico admet profiling, molecular docking, molecular dynamics simulation, network pharmacology. Molecular Diversity, 2023, 27, 857-871.	3.9	26
307	Homology Modeling, de Novo Design of Ligands, and Molecular Docking Identify Potential Inhibitors of Leishmania donovani 24-Sterol Methyltransferase. Frontiers in Cellular and Infection Microbiology, 2022, 12, .	3.9	8
308	Immunoinformatics guided design of a next generation epitope-based vaccine against Kaposi Sarcoma. Informatics in Medicine Unlocked, 2022, , 100986.	3.4	0
309	Identifying molecular structural features by pattern recognition methods. RSC Advances, 2022, 12, 17559-17569.	3.6	0
310	The Anti-Tumor Efficacy of Verbascoside on Ovarian Cancer via Facilitating CCN1-AKT/NF- κ B Pathway-Mediated M1 Macrophage Polarization. Frontiers in Oncology, 0, 12, .	2.8	3
311	Study the Mechanism of Gualou Niubang Decoction in Treating Plasma Cell Mastitis Based on Network Pharmacology and Molecular Docking. BioMed Research International, 2022, 2022, 1-21.	1.9	6
312	Integrative illustration of a JCVI-syn3A minimal cell. Journal of Integrative Bioinformatics, 2022, 19, .	1.5	6
313	Characterizing the Antitumor Effect of Coptis chinensis and Mume Fructus against Colorectal Cancer Based on Pharmacological Analysis. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-14.	1.2	3
314	Exploring the potential mechanism of emetine against coronavirus disease 2019 combined with lung adenocarcinoma: bioinformatics and molecular simulation analyses. BMC Cancer, 2022, 22, .	2.6	3
315	A computational biology approach for the identification of potential SARS-CoV-2 main protease inhibitors from natural essential oil compounds.. F1000Research, 0, 10, 1313.	1.6	2
316	In Vitro and In Silico Antistaphylococcal Activity of Indole Alkaloids Isolated from Tabernaemontana cymosa Jacq (Apocynaceae). Scientia Pharmaceutica, 2022, 90, 38.	2.0	3
317	Comprehensive Bioinformatics Analysis to Reveal Key RNA Targets and Hub Competitive Endogenous RNA Network of Keratoconus. Frontiers in Genetics, 0, 13, .	2.3	2

#	ARTICLE	IF	CITATIONS
318	A Mechanistic Exploratory Study on the Therapeutic Efficacy of Astragaloside IV Against Diabetic Retinopathy Revealed by Network Pharmacology. <i>Frontiers in Pharmacology</i> , 0, 13, .	3.5	3
319	Scopolin obtained from <i>Smilax china</i> L. against hepatocellular carcinoma by inhibiting glycolysis: A network pharmacology and experimental study. <i>Journal of Ethnopharmacology</i> , 2022, 296, 115469.	4.1	6
320	Systems Pharmacology and Molecular Docking Reveals the Mechanisms of Nux Vomica for the Prevention of Myasthenia Gravis. <i>Evidence-based Complementary and Alternative Medicine</i> , 2022, 2022, 1-19.	1.2	2
321	Identification of Potential Natural Bioactive Compounds from <i>Glycyrrhiza glabra</i> as Sars-CoV-2 Main Protease (MPRO) Inhibitors: In-Silico Approach. <i>Magl̂allat̂ Al-Muá²-tar Li-l-ÊžulÅ«m</i> , 2022, 37, 150-161.	0.1	0
322	Docking cyclic peptides formed by a disulfide bond through a hierarchical strategy. <i>Bioinformatics</i> , 2022, 38, 4109-4116.	4.1	5
323	Artificial intelligence and machine-learning approaches in structure and ligand-based discovery of drugs affecting central nervous system. <i>Molecular Diversity</i> , 2023, 27, 959-985.	3.9	11
324	Proteinâ€“Ligand Docking in the Machine-Learning Era. <i>Molecules</i> , 2022, 27, 4568.	3.8	37
325	The Pharmacological Mechanism of Xianping Injection for the Treatment of Novel Coronavirus Pneumonia (COVID-19): Based on Network Pharmacology Strategy. <i>Evidence-based Complementary and Alternative Medicine</i> , 2022, 2022, 1-18.	1.2	0
326	Identification of molecular mechanisms underlying the therapeutic effects of Xintong granule in coronary artery disease by a network pharmacology and molecular docking approach. <i>Medicine (United States)</i> , 2022, 101, e29829.	1.0	2
327	Charge-based interactions through peptide position 4 drive diversity of antigen presentation by human leukocyte antigen class I molecules. , 2022, 1, .		3
328	IDPsBind: a repository of binding sites for intrinsically disordered proteins complexes with known 3D structures. <i>BMC Molecular and Cell Biology</i> , 2022, 23, .	2.0	2
329	Mechanism of action of Bu Zhong Yi Qi Decoction in the treatment of chronic fatigue syndrome based on network pharmacology and molecular docking. <i>Pharmacological Research Modern Chinese Medicine</i> , 2022, 4, 100139.	1.2	0
330	Assessment of pulmonary infectious disease treatment with Mongolian medicine formulae based on data mining, network pharmacology and molecular docking. <i>Chinese Herbal Medicines</i> , 2022, 14, 432-448.	3.0	8
331	Study on the Action Mechanism of the Yifei Jianpi Tongfu Formula in Treatment of Colorectal Cancer Lung Metastasis Based on Network Analysis, Molecular Docking, and Experimental Validation. <i>Evidence-based Complementary and Alternative Medicine</i> , 2022, 2022, 1-14.	1.2	2
333	Integrating Network Pharmacology, Molecular Docking, and Experimental Validation to Investigate the Mechanism of (-)-Guaio Against Lung Adenocarcinoma. <i>Medical Science Monitor</i> , 0, 28, .	1.1	0
334	Mechanism of Zhinao Capsule in Treating Alzheimerâ€™s Disease Based on Network Pharmacology Analysis and Molecular Docking Validation. <i>Journal of Healthcare Engineering</i> , 2022, 2022, 1-12.	1.9	0
335	cpxDeepMSA: A Deep Cascade Algorithm for Constructing Multiple Sequence Alignments of Proteinâ€“Protein Interactions. <i>International Journal of Molecular Sciences</i> , 2022, 23, 8459.	4.1	2
336	Network Pharmacology, Molecular Docking and Molecular Dynamics Simulation Studies of the Molecular Targets and Mechanisms of ChuanKeZhi in the Treatment of COVID-19. <i>Natural Product Communications</i> , 2022, 17, 1934578X2211169.	0.5	3

#	ARTICLE	IF	CITATIONS
338	Viral informatics: bioinformatics-based solution for managing viral infections. Briefings in Bioinformatics, 2022, 23, .	6.5	10
339	Phytoncides could potentially inhibit the spike protein of <scp>SARSâ€CoV</scp>â€2 variants. Phytotherapy Research, 2022, 36, 4020-4023.	5.8	0
340	Network pharmacology and molecular docking technology-based predictive study of the active ingredients and potential targets of rhubarb for the treatment of diabetic nephropathy. BMC Complementary Medicine and Therapies, 2022, 22, .	2.7	13
341	An in silico reverse vaccinology study of Brachyspira pilosicoli, the causative organism of intestinal spirochaetosis, to identify putative vaccine candidates. Process Biochemistry, 2022, 122, 128-148.	3.7	0
342	Immunoinformatics-Based Proteome Mining to Develop a Next-Generation Vaccine Design against Borrelia burgdorferi: The Cause of Lyme Borreliosis. Vaccines, 2022, 10, 1239.	4.4	2
344	Identifying potential pharmacological targets and mechanisms of vitamin D for hepatocellular carcinoma and COVID-19. Frontiers in Immunology, 0, 13, .	4.8	1
345	Ellagic Acid as a Potential Inhibitor against the Nonstructural Protein NS3 Helicase of Zika Virus: A Molecular Modelling Study. BioMed Research International, 2022, 2022, 1-15.	1.9	3
347	Exploring the mechanism of action of licorice in the treatment of COVID-19 through bioinformatics analysis and molecular dynamics simulation. Frontiers in Pharmacology, 0, 13, .	3.5	7
348	Synthesis, biological evaluation and computational investigations of S-benzyl dithiocarbamates as the cholinesterase and monoamine oxidase inhibitors. Journal of Molecular Structure, 2023, 1271, 134138.	3.6	5
349	Quantum machine learning for chemistry and physics. Chemical Society Reviews, 2022, 51, 6475-6573.	38.1	40
350	Data Fusion Analysis for Determining Localization of Proteins Associated to Escherichia coli. , 2022, , .		0
351	Mechanisms and network pharmacological analysis of Yangyin Fuzheng Jiedu prescription in the treatment of hepatocellular carcinoma. Cancer Medicine, 2023, 12, 3237-3259.	2.8	3
352	Exploring the mechanism of action of dapansutril in the treatment of gouty arthritis based on molecular docking and molecular dynamics. Frontiers in Physiology, 0, 13, .	2.8	7
353	<i>CCP</i>4 Cloud for structure determination and project management in macromolecular crystallography. Acta Crystallographica Section D: Structural Biology, 2022, 78, 1079-1089.	2.3	21
355	APPRIS principal isoforms and MANE Select transcripts define reference splice variants. Bioinformatics, 2022, 38, ii89-ii94.	4.1	6
357	Network pharmacological investigation into the mechanism of Kaixinsan powder for the treatment of depression. Metabolic Brain Disease, 2022, 37, 2903-2914.	2.9	3
358	Computer-Aided Drug Design Boosts RAS Inhibitor Discovery. Molecules, 2022, 27, 5710.	3.8	6
359	Research on the Mechanism of Liuwei Dihuang Decoction for Osteoporosis Based on Systematic Biological Strategies. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-22.	1.2	2

#	ARTICLE	IF	CITATIONS
360	Exploring the mechanism of Shexiang Tongxin dropping pill in the treatment of microvascular angina through network pharmacology and molecular docking. <i>Annals of Translational Medicine</i> , 2022, 10, 983-983.	1.7	2
361	Molecular mechanism of Sishen pills in the treatment of diarrheal diabetic enteropathy based on network pharmacology. <i>Medicine (United States)</i> , 2022, 101, e30096.	1.0	1
362	Weipiling decoction alleviates N-methyl-N-nitro-N ² -nitrosoguanidine-induced gastric precancerous lesions via NF- κ B signalling pathway inhibition. <i>Chinese Medicine</i> , 2022, 17, .	4.0	4
363	Expression pattern and clinical value of Key RNA methylation modification regulators in ischemic stroke. <i>Frontiers in Genetics</i> , 0, 13, .	2.3	0
364	Snakebite Envenoming: A Comprehensive Review on Epidemiology, Diagnosis, Potential Treatments Role of Proteomics and Bioinformatics. <i>International Journal of Pharmaceutical Research and Allied Sciences</i> , 2022, 11, 108-122.	0.9	0
365	Implications of Microorganisms in Alzheimer's Disease. <i>Current Issues in Molecular Biology</i> , 2022, 44, 4584-4615.	2.4	11
366	Effect of Curcumin on Attenuation of Liver Cirrhosis via Genes/Proteins and Pathways: A System Pharmacology Study. <i>Nutrients</i> , 2022, 14, 4344.	4.1	9
367	Network pharmacology and molecular docking analysis on the mechanism of Baihe Zhimu decoction in the treatment of postpartum depression. <i>Medicine (United States)</i> , 2022, 101, e29323.	1.0	3
369	<sc>RCSB</sc> Protein Data bank: Tools for visualizing and understanding biological macromolecules in <sc>3D</sc>. <i>Protein Science</i> , 2022, 31, .	7.6	25
370	Clinical variant interpretation and biologically relevant reference transcripts. <i>Npj Genomic Medicine</i> , 2022, 7, .	3.8	2
371	Small NRPS-like enzymes in <i>Aspergillus</i> sections Flavi and Circumdati selectively form substituted pyrazinone metabolites. <i>Frontiers in Fungal Biology</i> , 0, 3, .	2.0	0
372	Proteins from Thermophilic <i>Thermus thermophilus</i> Often Do Not Fold Correctly in a Mesophilic Expression System Such as <i>Escherichia coli</i> . <i>ACS Omega</i> , 2022, 7, 37797-37806.	3.5	2
373	Comparison of Intermolecular Interactions of Irreversible and Reversible Inhibitors with Bruton's Tyrosine Kinase via Molecular Dynamics Simulations. <i>Molecules</i> , 2022, 27, 7451.	3.8	1
374	Protein encoder: An autoencoder-based ensemble feature selection scheme to predict protein secondary structure. <i>Expert Systems With Applications</i> , 2023, 213, 119081.	7.6	5
375	AI in Translational Bioinformatics and Precision Medicine. , 2022, , 391-429.		0
376	Improved inter-residue contact prediction via a hybrid generative model and dynamic loss function. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 6138-6148.	4.1	3
377	Origins and Evolution of Human Tandem Duplicated Exon Substitution Events. <i>Genome Biology and Evolution</i> , 2022, 14, .	2.5	1
378	Nearest neighbor search on embeddings rapidly identifies distant protein relations. <i>Frontiers in Bioinformatics</i> , 0, 2, .	2.1	13

#	ARTICLE	IF	CITATIONS
379	The impact of AlphaFold Protein Structure Database on the fields of life sciences. <i>Proteomics</i> , 2023, 23, .	2.2	29
380	Structure based Drug Designing Approaches in SARS-CoV-2 Spike Inhibitor Design. <i>Current Topics in Medicinal Chemistry</i> , 2022, 22, 2396-2409.	2.1	2
381	Network Pharmacology and Molecular Docking Analysis on Molecular Targets and Mechanisms of Bushen Hugu Decoction in the Treatment of Malignant Tumor Bone Metastases. <i>BioMed Research International</i> , 2022, 2022, 1-16.	1.9	0
382	Introducing the Bacterial and Viral Bioinformatics Resource Center (BV-BRC): a resource combining PATRIC, IRD and ViPR. <i>Nucleic Acids Research</i> , 2023, 51, D678-D689.	14.5	229
384	AutoDock Koto: A Gradient Boosting Differential Evolution for Molecular Docking. <i>IEEE Transactions on Evolutionary Computation</i> , 2023, 27, 1648-1662.	10.0	1
385	The alkaloids of <i>Isatis indigotica</i> as promising candidates against COVID-19: A molecular docking simulation for drug development. <i>Journal of Reports in Pharmaceutical Sciences</i> , 2022, 11, 165.	0.8	0
386	Mr.Vc v2: An updated version of database with increased data of transcriptome and experimental validated interactions. <i>Frontiers in Microbiology</i> , 0, 13, .	3.5	1
390	A systematic review of state-of-the-art strategies for machine learning-based protein function prediction. <i>Computers in Biology and Medicine</i> , 2023, 154, 106446.	7.0	1
391	Pesticide informatics expands the opportunity for structure-based molecular design and optimization. , 2022, 1, 139-147.		11
392	Exploring the potential anti-Alzheimer disease mechanisms of <i>Alpiniae Oxyphyllae Fructus</i> by network pharmacology study and molecular docking. <i>Metabolic Brain Disease</i> , 2023, 38, 933-944.	2.9	1
393	Identification and screening of potential inhibitors obtained from <i>Plumeria rubra</i> L. compounds against type 2 diabetes mellitus. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 10081-10095.	3.5	3
394	SDEGen: learning to evolve molecular conformations from thermodynamic noise for conformation generation. <i>Chemical Science</i> , 2023, 14, 1557-1568.	7.4	6
395	IDENTIFICATION OF PHYTOCOMPOUNDS FROM ARGEMONE MEXICANA AS INHIBITORS OF EPSTEIN-BARR NUCLEAR ANTIGEN TO COMBAT INFECTIOUS MONONUCLEOSIS. <i>Innovare Journal of Medical Sciences</i> , 0, , 9-14.	0.2	0
396	Miracle fruit seed as a potential supplement for the treatment of learning and memory disorders in Alzheimer's disease. <i>Frontiers in Pharmacology</i> , 0, 13, .	3.5	1
397	Yupingfeng San exhibits anticancer effect in hepatocellular carcinoma cells via the MAPK pathway revealed by HTS2 technology. <i>Journal of Ethnopharmacology</i> , 2023, 306, 116134.	4.1	4
398	Transcriptomics Based Network Analyses and Molecular Docking Highlighted Potentially Therapeutic Biomarkers for Colon Cancer. <i>Biochemical Genetics</i> , 0, , .	1.7	0
399	Obacunone targets macrophage migration inhibitory factor (MIF) to impede osteoclastogenesis and alleviate ovariectomy-induced bone loss. <i>Journal of Advanced Research</i> , 2023, 53, 235-248.	9.5	6
400	Identification of therapeutic targets for osteosarcoma by integrating single-cell RNA sequencing and network pharmacology. <i>Frontiers in Pharmacology</i> , 0, 13, .	3.5	0

#	ARTICLE	IF	CITATIONS
401	Marmesin and Marmelosin Interact with the Heparan Sulfatase-2 Active Site: Potential Mechanism for Phytochemicals from Bael Fruit Extract as Antitumor Therapeutics. <i>Oxidative Medicine and Cellular Longevity</i> , 2023, 2023, 1-19.	4.0	0
402	Scavenger receptor B1 facilitates the endocytosis of <i>Escherichia coli</i> via TLR4 signaling in mammary gland infection. <i>Cell Communication and Signaling</i> , 2023, 21, .	6.5	2
403	S-PDB: Analysis and Classification of SARS-CoV-2 Spike Protein Structures. , 2022, , .		4
404	Free energy and kinetic rate calculation via non-equilibrium molecular simulation: application to biomolecules. <i>Biophysical Reviews</i> , 2022, 14, 1303-1314.	3.2	3
405	Computational biophysics and structural biology of proteinsâ€™a Special Issue in honor of Prof. Haruki Nakamuraâ€™s 70th birthday. <i>Biophysical Reviews</i> , 2022, 14, 1211-1222.	3.2	3
406	Network Pharmacology and Molecular Docking Analysis of Shufeiya Recipe in the Treatment of Pulmonary Hypertension. <i>BioMed Research International</i> , 2022, 2022, 1-12.	1.9	7
407	Repurposed benzydamine targeting CDK2 suppresses the growth of esophageal squamous cell carcinoma. <i>Frontiers of Medicine</i> , 2023, 17, 290-303.	3.4	3
409	How AlphaFold2 Predicts Conditionally Folding Regions Annotated in an Intrinsically Disordered Protein Database, IDEAL. <i>Biology</i> , 2023, 12, 182.	2.8	3
410	Structure of <i>Helicobacter pylori</i> dihydroneopterin aldolase suggests a fragment-based strategy for isozyme-specific inhibitor design. <i>Current Research in Structural Biology</i> , 2023, 5, 100095.	2.2	0
411	Systematic Analysis of the Mechanism of Polygoni Multiflori Caulis in Improving Depressive Disorder in Mice via Network Pharmacology Combined with Ultra-High Performance Liquid Chromatography Coupled with Quadrupole Exactive Orbitrap Mass Spectrometer. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2023, 26, .	1.1	0
412	In Silico Structural and Functional Analyses of NLRP3 Inflammasomes to Provide Insights for Treating Neurodegenerative Diseases. <i>BioMed Research International</i> , 2023, 2023, 1-16.	1.9	1
413	Bioinformatics and computational chemistry approaches to explore the mechanism of the anti-depressive effect of ligustilide. <i>Scientific Reports</i> , 2023, 13, .	3.3	1
414	PSAC-PDB: Analysis and classification of protein structures. <i>Computers in Biology and Medicine</i> , 2023, 158, 106814.	7.0	2
415	Pharmacokinetic analysis and structural optimization of inophyllamine-I to forecast as a possible drug candidate. <i>Phytomedicine Plus</i> , 2023, 3, 100422.	2.0	1
416	Identification of Potent Small-Molecule PCSK9 Inhibitors Based on Quantitative Structure-Activity Relationship, Pharmacophore Modeling, and Molecular Docking Procedure. <i>Current Problems in Cardiology</i> , 2023, 48, 101660.	2.4	2
417	Network pharmacology study of the mechanism underlying the therapeutic effect of Zhujing pill and its main component oleanolic acid against diabetic retinopathy. <i>Bioscience Reports</i> , 2023, 43, .	2.4	1
418	Computational Approaches to Enzyme Inhibition by Marine Natural Products in the Search for New Drugs. <i>Marine Drugs</i> , 2023, 21, 100.	4.6	4
419	Computational Prediction of Protein Intrinsically Disordered Region Related Interactions and Functions. <i>Genes</i> , 2023, 14, 432.	2.4	2

#	ARTICLE	IF	CITATIONS
420	The opportunities and challenges posed by the new generation of deep learning-based protein structure predictors. <i>Current Opinion in Structural Biology</i> , 2023, 79, 102543.	5.7	11
421	Exploring Myocardial Ischemia-Reperfusion Injury Mechanism of Cinnamon by Network Pharmacology, Molecular Docking, and Experiment Validation. <i>Computational and Mathematical Methods in Medicine</i> , 2023, 2023, 1-14.	1.3	1
422	4'-methyhbavachalcone inhibits succinate induced cardiomyocyte hypertrophy via the NFATc4 pathway. <i>Experimental and Therapeutic Medicine</i> , 2023, 25, .	1.8	0
423	Threat of respiratory syncytial virus infection knocking the door: a proposed potential drug candidate through molecular dynamics simulations, a future alternative. <i>Journal of Molecular Modeling</i> , 2023, 29, .	1.8	7
424	The mechanism of action of paeoniae radix rubra“angelicae sinensis radix drug pair in the treatment of rheumatoid arthritis through PI3K/AKT/NF- κ B signaling pathway. <i>Frontiers in Pharmacology</i> , 0, 14, .	3.5	2
426	Identification of Potential Inhibitors for the Treatment of Alkaptonuria Using an Integrated In Silico Computational Strategy. <i>Molecules</i> , 2023, 28, 2623.	3.8	4
427	Structural and Phylogenetic Analysis of CXCR4 Protein Reveals New Insights into Its Role in Emerging and Re-Emerging Diseases in Mammals. <i>Vaccines</i> , 2023, 11, 671.	4.4	0
428	Functional metagenomics uncovers nitrile-hydrolysing enzymes in a coal metagenome. <i>Frontiers in Molecular Biosciences</i> , 0, 10, .	3.5	3
429	DRAVP: A Comprehensive Database of Antiviral Peptides and Proteins. <i>Viruses</i> , 2023, 15, 820.	3.3	5
430	DRUG REPURPOSING OF COMMERCIALY AVAILABLE AZOLES AGAINST ASPERGILLOSIS PEROXIREDOXIN ASP F3 ALLERGEN DRUGS. <i>Innovare Journal of Medical Sciences</i> , 0, , 15-19.	0.2	0
431	Docking and Molecular Dynamics Identify Leads against 5 Alpha Reductase 2 for Benign Prostate Hyperplasia Treatment. <i>Journal of Chemistry</i> , 2023, 2023, 1-20.	1.9	2
432	Cheminformatics-Based Study Identifies Potential Ebola VP40 Inhibitors. <i>International Journal of Molecular Sciences</i> , 2023, 24, 6298.	4.1	8
433	Escherichia coli: Analysis of Features for Protein Localization Classification Employing Fusion Data. <i>Communications in Computer and Information Science</i> , 2023, , 31-43.	0.5	0
434	Introduction of the Korea BioData Station (K-BDS) for sharing biological data. <i>Genomics and Informatics</i> , 2023, 21, e12.	0.8	4
437	<sc>CDK6</sc> is activated by the atypical cyclin I to promote <sc>E2F</sc>-mediated gene expression and cancer cell proliferation. <i>Molecular Oncology</i> , 2023, 17, 1228-1245.	4.6	0
438	Using a Graph Transformer Network to Predict 3D Coordinates of Proteins via Geometric Algebra Modelling. <i>Lecture Notes in Computer Science</i> , 2023, , 83-95.	1.3	0
439	Exploring the inhibitory potential of novel piperidine-derivatives against main protease (Mpro) of SARS-CoV-2: A hybrid approach consisting of molecular docking, MD simulations and MMPBSA analysis. <i>Journal of Molecular Liquids</i> , 2023, 382, 121904.	4.9	2
440	Identification of key upregulated genes involved in foam cell formation and the modulatory role of statin therapy. <i>International Immunopharmacology</i> , 2023, 119, 110209.	3.8	1

#	ARTICLE	IF	CITATIONS
441	Comparative Analysis and Classification of SARS-CoV-2 Spike Protein Structures in PDB. Covid, 2023, 3, 452-471.	1.5	1
442	A Systematic Study of Traditional Chinese Medicine for the Treatment of Lung Adenocarcinoma Using a Reverse Network of Key Targets Based on Bioinformatics and Molecular Docking: Curcumin and Trans-Resveratrol as Potential Drug Candidates for Lung Adenocarcinoma. Natural Product Communications. 2023, 18, 1934578X2311693.	0.5	0
443	Mechanism of action of Asparagus officinalis extract against multiple myeloma using bioinformatics tools, in silico and in vitro study. Frontiers in Pharmacology, 0, 14, .	3.5	1
444	Revealing the structural and molecular interaction landscape of the favipiravir-RTP and SARS-CoV-2 RdRp complex through integrative bioinformatics: Insights for developing potent drugs targeting SARS-CoV-2 and other viruses. Journal of Infection and Public Health, 2023, 16, 1048-1056.	4.1	3
447	Molecular evolution of the pathogen recognition peptidoglycan proteins regulates the immune response against infectious diseases in Drosophila melanogaster. Journal of King Saud University - Science, 2023, 35, 102710.	3.5	0
448	RBM38 Reverses Sorafenib Resistance in Hepatocellular Carcinoma Cells by Combining and Promoting lncRNA-GAS5. Cancers, 2023, 15, 2897.	3.7	2
452	Recent advancement of HDAC inhibitors against breast cancer. , 2023, 40, .		6
453	Comprehensive computational study in the identification of novel potential cholesterol lowering agents targeting proprotein convertase subtilisin/kexin type 9. Journal of Biomolecular Structure and Dynamics, 0, , 1-12.	3.5	2
454	Mechanism of ligusticum cycloprolactam against neuroinflammation based on network pharmacology and experimental verification. Clinical and Experimental Pharmacology and Physiology, 2023, 50, 647-663.	1.9	0
455	Systems-wide analysis of <i>A. fumigatus</i> using kinetic modeling of metabolic pathways to identify putative drug targets. Journal of Biomolecular Structure and Dynamics, 0, , 1-16.	3.5	0
456	Allosteric inhibition of dengue virus RNA-dependent RNA polymerase by <i>Litsea cubeba</i> phytochemicals: a computational study. Journal of Biomolecular Structure and Dynamics, 0, , 1-13.	3.5	2
457	PASSer: fast and accurate prediction of protein allosteric sites. Nucleic Acids Research, 2023, 51, W427-W431.	14.5	13
458	Facing Antitubercular Resistance: Identification of Potential Direct Inhibitors Targeting InhA Enzyme and Generation of 3D-pharmacophore Model by in silico Approach. Advances and Applications in Bioinformatics and Chemistry, 0, Volume 16, 49-59.	2.6	0
459	Development of Potential Inhibitors for Human T-lymphotropic Virus Type I Integrase Enzyme: A Molecular Modeling Approach. Current Computer-Aided Drug Design, 2024, 20, 72-86.	1.2	1
460	Pancreatic lipase related protein 1 as a potential target in triglyceride breakdown: A molecular docking studies with in vitro appraisal. Results in Chemistry, 2023, 5, 100960.	2.0	1
461	Guiqi Baizhu prescription ameliorates cytarabine-induced intestinal mucositis by targeting JAK2 to inhibit M1 macrophage polarization. Biomedicine and Pharmacotherapy, 2023, 164, 114902.	5.6	2
462	Identification of a covert evolutionary pathway between two protein folds. Nature Communications, 2023, 14, .	12.8	7
463	In-silico study of protein-protein interactions in wheat blast using docking and molecular dynamics simulation approach. Journal of Biomolecular Structure and Dynamics, 0, , 1-11.	3.5	0

#	ARTICLE	IF	CITATIONS
464	The potential effects and mechanism of echinacoside powder in the treatment of Hirschsprung's Disease. Mathematical Biosciences and Engineering, 2023, 20, 14222-14240.	1.9	0
465	Exploring Machine Learning Algorithms and Protein Language Models Strategies to Develop Enzyme Classification Systems. Lecture Notes in Computer Science, 2023, , 307-319.	1.3	2
466	Target specific inhibition of West Nile virus envelope glycoprotein and methyltransferase using phytocompounds: an in silico strategy leveraging molecular docking and dynamics simulation. Frontiers in Microbiology, 0, 14, .	3.5	1
468	Generating interacting protein sequences using domain-to-domain translation. Bioinformatics, 2023, 39, .	4.1	1
469	Evaluation of mechanical features and antibacterial potential of fluoroquinolone against β -ketoacyl-ACP synthases (FabB, FabF & FabH) via computational approaches. Archives of Biochemistry and Biophysics, 2023, 744, 109674.	3.0	0
471	MOLECULAR DOCKING AND INVESTIGATION OF BOSWELLIA SERRATA PHYTOCOMPOUNDS AS CANCER THERAPEUTICS TO TARGET GROWTH FACTOR RECEPTORS: AN IN SILICO APPROACH. International Journal of Applied Pharmaceutics, 0, , 173-183.	0.3	3
472	Optimization and theoretical analysis of lipase-catalyzed enzymatic esterification of glycerol for efficient glycerides synthesis. Biochemical Engineering Journal, 2023, 198, 109033.	3.6	4
474	Fluid protein fold space and its implications. BioEssays, 2023, 45, .	2.5	2
475	RDKG-115: Assisting drug repurposing and discovery for rare diseases by trimodal knowledge graph embedding. Computers in Biology and Medicine, 2023, 164, 107262.	7.0	1
476	Exploring the Molecular Targets for the Antidepressant and Antisuicidal Effects of Ketamine Enantiomers by Using Network Pharmacology and Molecular Docking. Pharmaceuticals, 2023, 16, 1013.	3.8	2
477	A soft-computation hybrid method for search of the antibiotic-resistant gene in <i>Mycobacterium tuberculosis</i> for promising drug target identification and antimycobacterial lead discovery. Bioinformatics Advances, 0, , .	2.4	1
478	Adopting Autodock Koto for Virtual Screening of COVID-19. Lecture Notes in Computer Science, 2023, , 752-763.	1.3	0
479	Prognostic significance and mechanisms of CXCL genes in clear cell renal cell carcinoma. Aging, 0, , .	3.1	0
480	Exploring the pharmacological mechanism of Qufeng Tongluo Formula in the treatment of rheumatoid arthritis using network pharmacology methods and in vitro experimental validation. Pharmacological Research Modern Chinese Medicine, 2023, 8, 100298.	1.2	0
481	Synthesis, DFT and molecular docking of novel (Z)-4-bromo-N-(4-butyl-3-oxo-1-phenyl-1H-pyrazol-5-yl)thiophene-2-carboxamide. Journal of Molecular Structure, 2023, 1282, 132883.	3.8	0
482	Exploration of human pancreatic alpha-amylase inhibitors from Physalis peruviana for the treatment of type 2 diabetes. Journal of Biomolecular Structure and Dynamics, 0, , 1-16.	3.5	0
483	Fabrication and Evaluation of Anticancer Potential of Eugenol Incorporated Chitosan-Silver Nanocomposites: In Vitro, In Vivo, and In Silico Studies. AAPS PharmSciTech, 2023, 24, .	3.3	1
484	PASSerRank: Prediction of allosteric sites with learning to rank. Journal of Computational Chemistry, 2023, 44, 2223-2229.	3.3	8

#	ARTICLE	IF	CITATIONS
485	Antibacterial, Antibiofilm, Antiswarming, and Antioxidant Activities of Flavonoids Isolated from <i>Allium colchicifolium</i> Leaves. <i>Journal of Food Biochemistry</i> , 2023, 2023, 1-14.	2.9	0
486	Perspectives of Proteomics in Respiratory Allergic Diseases. <i>International Journal of Molecular Sciences</i> , 2023, 24, 12924.	4.1	0
489	In Silico Structural Analysis Exploring Conformational Folding of Protein Variants in Alzheimer's Disease. <i>International Journal of Molecular Sciences</i> , 2023, 24, 13543.	4.1	2
491	<i>Klebsiella</i> phage KP34gp57 capsular depolymerase structure and function: from a serendipitous finding to the design of active mini-enzymes against <i>K. pneumoniae</i> . <i>MBio</i> , 2023, 14, .	4.1	2
492	Novel computational and drug design strategies for inhibition of monkeypox virus and <i>Babesia microti</i> : molecular docking, molecular dynamic simulation and drug design approach by natural compounds. <i>Frontiers in Microbiology</i> , 0, 14, .	3.5	1
493	Systems pharmacology dissection of pharmacological mechanisms of Xiaochaihu decoction against human coronavirus. <i>BMC Complementary Medicine and Therapies</i> , 2023, 23, .	2.7	0
494	Interaction of Vanadium Complexes with Proteins: Revisiting the Reported Structures in the Protein Data Bank (PDB) since 2015. <i>Molecules</i> , 2023, 28, 6538.	3.8	1
495	Exploring the role and mechanism of <i>Astragalus membranaceus</i> and <i>radix paeoniae rubra</i> in idiopathic pulmonary fibrosis through network pharmacology and experimental validation. <i>Scientific Reports</i> , 2023, 13, .	3.3	0
496	A pharmacophore-guided deep learning approach for bioactive molecular generation. <i>Nature Communications</i> , 2023, 14, .	12.8	2
497	SARS-CoV-2 external structures interacting with nanospheres using docking and molecular dynamics. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-16.	3.5	0
498	Evaluation of the pH effect on complex formation between bovine β -lactoglobulin and aflatoxin M1: a molecular dynamic simulation and molecular docking study. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-11.	3.5	0
499	Homologous Pairs of Low and High Temperature Originating Proteins Spanning the Known Prokaryotic Universe. <i>Scientific Data</i> , 2023, 10, .	5.3	1
500	Network Pharmacology, Molecular Docking, Molecular Dynamics Simulation, and in vitro Experiments to Explore the Mechanism of Asiatic Acid Inhibiting Acetaldehyde-Induced Activation of Hepatic Stellate Cells. <i>Natural Product Communications</i> , 2023, 18, .	0.5	0
503	Accelerating Molecular Dynamics Simulations for Drug Discovery. <i>Methods in Molecular Biology</i> , 2024, , 187-202.	0.9	0
504	Gene LY96 is an M2 macrophage-related biomarker and is associated with immunosuppression in renal cell carcinoma. , 2023, 2, .		1
505	Bioinformatics, Molecular Docking Simulation and <i>in Vitro</i> Experiments Reveal the Bioactive Compounds and Mechanism of <i>Coptis Chinensis</i> Franch. Against Colorectal Adenocarcinoma. <i>Pharmacognosy Magazine</i> , 0, , .	0.6	0
506	Reverse Docking Approach Reveals the Negative Effect of Caffeine Toxicity on Glutamate GluR2 Receptor. <i>Toxicology International</i> , 0, , 317-323.	0.1	0
507	E2EDA: Protein Domain Assembly Based on End-to-End Deep Learning. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 6451-6461.	5.4	2

#	ARTICLE	IF	CITATIONS
508	Medicinal Chemistry Assignment Requiring Undergraduate Pharmacy Students To Utilize Free Web-Based Resources. Journal of Chemical Education, 0, , .	2.3	0
509	Study on tumour cell-derived hybrid exosomes as dasatinib nanocarriers for pancreatic cancer therapy. Artificial Cells, Nanomedicine and Biotechnology, 2023, 51, 532-546.	2.8	0
510	Learning on topological surface and geometric structure for 3D molecular generation. Nature Computational Science, 2023, 3, 849-859.	8.0	4
511	Discovery of druggable potent inhibitors of serine proteases and farnesoid X receptor by ligand-based virtual screening to obstruct SARS-CoV-2. International Journal of Biological Macromolecules, 2023, 253, 127379.	7.5	1
512	<i>In silico</i> screening applied in drug discovery: T001-10026247 as a novel fourth-generation EGFR inhibitor. New Journal of Chemistry, 2023, 47, 20405-20416.	2.8	1
513	Revolutionizing antiretroviral therapy for human immunodeficiency virus/AIDS: A computational approach using molecular docking, virtual screening, and 3D pharmacophore building to address therapeutic failure and propose highly effective candidates. International Journal of Immunopathology and Pharmacology, 2023, 37, .	2.1	0
514	Lead phytochemicals and marine compounds against ceruloplasmin in cancer targeting. Journal of Biomolecular Structure and Dynamics, 0, , 1-17.	3.5	0
515	The neuroprotective mechanisms of naringenin: Inhibition of apoptosis through the PI3K/AKT pathway after hypoxic-ischemic brain damage. Journal of Ethnopharmacology, 2024, 318, 116941.	4.1	3
516	Glucose restriction in <i>Saccharomyces cerevisiae</i> modulates the phosphorylation pattern of the 20S proteasome and increases its activity. Scientific Reports, 2023, 13, .	3.3	0
517	Development of AKR1B10 inhibitors from <i>Ajuga nipponensis</i> based on diseases and targets. <i>FÄ-toterapÄ-Ä</i> , 2024, 172, 105742.	2.2	1
518	CLOOME: contrastive learning unlocks bioimaging databases for queries with chemical structures. Nature Communications, 2023, 14, .	12.8	2
519	Impact of N221S missense mutation in human ribonucleotide reductase small subunit b on mitochondrial DNA depletion syndrome. Scientific Reports, 2023, 13, .	3.3	0
520	High-throughput virtual screening of potential inhibitors of GPR52 using docking and biased sampling method for Huntingtonâ€™s disease therapy. Molecular Diversity, 0, , .	3.9	0
521	Comprehensive analysis reveals key genes and environmental toxin exposures underlying treatment response in ulcerative colitis based on in-silico analysis and mendelian randomization. Aging, 0, , .	3.1	0
522	Network pharmacology analysis of a patented Chinese herbal medicine for alleviating anxiety disorder in in vitro fertilization-embryo transfer. Journal of Traditional and Complementary Medicine, 2024, 14, 191-202.	2.7	0
523	Molecular dynamic simulation reveals spider antimicrobial peptide Latarcin-1 and human eosinophil cationic protein as peptide inhibitors of SARS-CoV-2 variants. Journal of Biomolecular Structure and Dynamics, 0, , 1-11.	3.5	0
525	MOLECULAR DOCKING AND DYNAMIC SIMULATION-BASED SCREENING IDENTIFIES INHIBITORS OF TARGETED SARS-COV-2 3CLPRO AND HUMAN ACE2. International Journal of Applied Pharmaceutics, 0, , 297-308.	0.3	2
526	<i>SSDraw</i> : <i>Software</i> for generating comparative protein secondary structure diagrams. Protein Science, 2023, 32, .	7.6	1

#	ARTICLE	IF	CITATIONS
528	Structural similarities between SAM and ATP recognition motifs and detection of ATP binding in a SAM binding DNA methyltransferase. <i>Current Research in Structural Biology</i> , 2023, 6, 100108.	2.2	0
529	Spatially Resolved Transcriptomics Reveals Local Invasion-Related Genes in Liver Hepatocellular Carcinoma: Exploring the Therapeutic Potential of a Chimeric Protein Targeting Glypican-3. <i>Journal of Computational Biophysics and Chemistry</i> , 2024, 23, 321-332.	1.7	0
530	Exploring the Potential of Plant Bioactive Compounds against Male Infertility: An In Silico and In Vivo Study. <i>Molecules</i> , 2023, 28, 7693.	3.8	0
531	Protective effect of <i>Amauroderma rugosum</i> ethanol extract and its primary bioactive compound, ergosterol, against acute gastric ulcers based on LXR-mediated gastric mucus secretions. <i>Phytomedicine</i> , 2024, 123, 155236.	5.3	0
532	Qi Fu Yin ameliorates neuroinflammation through inhibiting RAGE and TLR4/NF- κ B pathway in AD model rats. <i>Aging</i> , 2023, 15, 13239-13264.	3.1	0
534	Effects of D128N Mutation on OsSERK2 in Xa21-Mediated Immune Complex: An In Silico Study. <i>Advances in Agriculture</i> , 2023, 2023, 1-9.	0.9	0
535	Ribosomal stalk-captured CARF-RelE ribonuclease inhibits translation following CRISPR signaling. <i>Science</i> , 2023, 382, 1036-1041.	12.6	3
537	Network pharmacology identifies the inhibitory effect of Yiqi yangyin quyu prescription on salivary gland inflammation in Sjögren's syndrome. <i>Medicine (United States)</i> , 2023, 102, e36144.	1.0	1
538	Structural organization of the retriever-CCC endosomal recycling complex. <i>Nature Structural and Molecular Biology</i> , 0, , .	8.2	2
539	Exploration and validation of key genes associated with early lymph node metastasis in thyroid carcinoma using weighted gene co-expression network analysis and machine learning. <i>Frontiers in Endocrinology</i> , 0, 14, .	3.5	0
540	QiDiTangShen granules alleviates diabetic nephropathy podocyte injury: A network pharmacology study and experimental validation in vivo and vitro. <i>Heliyon</i> , 2024, 10, e23535.	3.2	0
541	Exploring the mechanism of tenghuang jianggu wan in osteoporosis treatment based on network pharmacology, molecular docking and experimental pharmacology. <i>Chinese Journal of Analytical Chemistry</i> , 2024, 52, 100351.	1.7	0
542	Molecular Dynamics and Machine Learning reveal distinguishing mechanisms of Competitive Ligands to perturb β -Tubulin. <i>Computational Biology and Chemistry</i> , 2024, 108, 108004.	2.3	0
543	Licochalcone A alleviates ferroptosis in doxorubicin-induced cardiotoxicity via the PI3K/AKT/MDM2/p53 pathway. <i>Naunyn-Schmiedeberg's Archives of Pharmacology</i> , 0, , .	3.0	0
544	Advances in Artificial Intelligence (AI)-assisted approaches in drug screening. , 2024, 2, 100039.		0
545	N ⁺ -Ferrocenylmethyl-N-phenylbenzohydrazide as a potential DNA binding compound: a combined experimental and computational study. <i>Journal of Coordination Chemistry</i> , 2023, 76, 1984-1998.	2.2	1
546	Potential Hepatoprotective Effects of <i>Chamaecyparis lawsoniana</i> against Methotrexate-Induced Liver Injury: Integrated Phytochemical Profiling, Target Network Analysis, and Experimental Validation. <i>Antioxidants</i> , 2023, 12, 2118.	5.1	0
547	Modulation of Kr ^{1/4} ppel-like factors (KLFs) interaction with their binding partners in cancers through acetylation and phosphorylation. <i>Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms</i> , 2024, 1867, 195003.	1.9	0

#	ARTICLE	IF	CITATIONS
551	Principal Component Analysis (PCA) of Molecular Descriptors for Improving Permeation through the Blood–Brain Barrier of Quercetin Analogues. <i>International Journal of Molecular Sciences</i> , 2024, 25, 192.	4.1	0
552	Integrated Network Pharmacology Approach to Evaluate Bioactive Phytochemicals of <i>Acalypha indica</i> and Their Mechanistic Actions to Suppress Target Genes of Tuberculosis. <i>ACS Omega</i> , 0, , .	3.5	0
554	CRD: A de novo design algorithm for the prediction of cognate protein receptors for small molecule ligands. <i>Structure</i> , 2024, 32, 362-375.e4.	3.3	0
556	Limitations of Protein Structure Prediction Algorithms in Therapeutic Protein Development. <i>BioMedInformatics</i> , 2024, 4, 98-112.	2.0	0
557	LAMP3 is a potent uterine corpus endometrial carcinoma prognostic biomarker associated with immune behavior. <i>Aging</i> , 0, , .	3.1	0
558	Mechanism of Ligand Binding to Theophylline RNA Aptamer. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 1017-1029.	5.4	0
559	AlphaFold for a medicinal chemist: tool or toy?. <i>Russian Chemical Reviews</i> , 2024, 93, RCR5107.	6.5	0
560	ROS scavenging, DNA binding and NADPH oxidase inhibition potential of Ni^{TM} -Ferrocenylmethyl- Ni^{TM} -phenylpropionohydrazide using cyclic voltammetry and molecular docking. <i>Journal of Organometallic Chemistry</i> , 2024, 1007, 123026.	1.8	0
561	PandoraRLO: Unveiling Protein-Ligand Interactions with Reinforcement Learning for Optimized Pose Prediction. , 2023, , .		0
562	Probing Transmembrane Proteins Binding Domain via Multi-level Molecule Learning. , 2023, , .		0
563	Oligomeric Symmetry of Purine Nucleoside Phosphorylases. <i>Symmetry</i> , 2024, 16, 124.	2.2	0
564	New thiazolyl-isoxazole derivatives as potential anti-infective agents: design, synthesis, <i>in vitro</i> and <i>in silico</i> antimicrobial efficacy. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-15.	3.5	0
565	Investigation on the antipyretic mechanism of Chaiqin Qingning capsule for the treatment of fever based on network pharmacology, molecular docking, and <i>in vitro</i> experimental validation. <i>Chemical Biology and Drug Design</i> , 2024, 103, .	3.2	0
566	TM-search: An Efficient and Effective Tool for Protein Structure Database Search. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 1043-1049.	5.4	0
567	Investigation of natural compounds as methyltransferase inhibitors against dengue virus: an <i>in silico</i> approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-16.	3.5	2
568	Proposal of pharmacophore model for HIV reverse transcriptase inhibitors: Combined mutational effect analysis, molecular dynamics, molecular docking and pharmacophore modeling study. <i>International Journal of Immunopathology and Pharmacology</i> , 2024, 38, .	2.1	0
570	Geometric Algebra Models of Proteins for Three-Dimensional Structure Prediction. <i>Lecture Notes in Computer Science</i> , 2024, , 63-74.	1.3	0
571	Identification of hub genes significantly linked to temporal lobe epilepsy and apoptosis via bioinformatics analysis. <i>Frontiers in Molecular Neuroscience</i> , 0, 17, .	2.9	0

#	ARTICLE	IF	CITATIONS
572	Mutational analysis of consanguineous families and their targeted therapy against dwarfism. Journal of Biomolecular Structure and Dynamics, 0, , 1-18.	3.5	0
573	Use of hybrid molecular simulation techniques for systematic analysis of polyphenols as promising therapeutic agent against SARS-CoV-2. Journal of Molecular Structure, 2024, 1305, 137744.	3.6	0
574	Phytocompounds as potential inhibitors of mycobacterial multidrug efflux pump Rv1258c: an in silico approach. AMB Express, 2024, 14, .	3.0	0
575	A comprehensive computational benchmark for evaluating deep learning-based protein function prediction approaches. Briefings in Bioinformatics, 2024, 25, .	6.5	0
576	Genome Sequence Analysis of Native Xenorhabdus Strains Isolated from Entomopathogenic Nematodes in Argentina. Toxins, 2024, 16, 108.	3.4	0
578	Dynamic Docking-Assisted Engineering of Hydrolases for Efficient PET Depolymerization. ACS Catalysis, 2024, 14, 3627-3639.	11.2	0
579	Exploring the mechanism of Erteng-Sanjie capsule in treating gastric and colorectal cancers via network pharmacology and in-vivo validation. Journal of Ethnopharmacology, 2024, 327, 117945.	4.1	0
580	Network pharmacology and experimental validation to investigate the mechanism of Nao-Ling-Su capsule in the treatment of ischemia/reperfusion-induced acute kidney injury. Journal of Ethnopharmacology, 2024, 326, 117958.	4.1	0
581	Design, synthesis, and biochemical and computational screening of novel oxindole derivatives as inhibitors of Aurora A kinase and SARS-CoV-2 spike/host ACE2 interaction. Medicinal Chemistry Research, 2024, 33, 620-634.	2.4	0
582	DVA: predicting the functional impact of single nucleotide missense variants. BMC Bioinformatics, 2024, 25, .	2.6	0
583	Elucidating the role of <i>Rhodiola rosea</i> L. in sepsis-induced acute lung injury via network pharmacology: emphasis on inflammatory response, oxidative stress, and the PI3K-AKT pathway. Pharmaceutical Biology, 2024, 62, 272-284.	2.9	0
584	GSTP alleviates acute lung injury by S-glutathionylation of KEAP1 and subsequent activation of NRF2 pathway. Redox Biology, 2024, 71, 103116.	9.0	0
585	5-chloro-3-(2-(2,4-dinitrophenyl) hydrazono)indolin-2-one: synthesis, characterization, biochemical and computational screening against SARS-CoV-2. Chemical Papers, 2024, 78, 3431-3441.	2.2	0
589	<sc>Xplor–NIH</sc>: Better parameters and protocols for <sc>NMR</sc> protein structure determination. Protein Science, 2024, 33, .	7.6	0
590	Investigation of some plant stilbenoids and their fragments for the identification of inhibitors of SARS-CoV-2 viral spike/ACE2 protein binding. , 2024, 3, 100059.		0
591	Molecular mechanisms of quetiapine bidirectional regulation of bipolar depression and mania based on network pharmacology and molecular docking: Evidence from computational biology. Journal of Affective Disorders, 2024, 355, 528-539.	4.1	0
592	Diverse models of cavity engineering in enzyme modification: Creation, filling, and reshaping. Biotechnology Advances, 2024, 72, 108346.	11.7	0