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Citation Report

#	Article	IF	Citations
11	Molecular simulations and visualization: introduction and overview. Faraday Discussions, 2014, 169, 9-22.	1.6	38
12	Conformational plasticity surrounding the active site of NADH oxidase from Thermus thermophilus. Protein Science, 2015, 24, 1114-1128.	3.1	4
13	The Nitrileâ€Forming Enzyme 7â€Cyanoâ€7â€Deazaguanine Synthase from Geobacillus kaustophilus: A Reverse Nitrilase?. ChemBioChem, 2015, 16, 2373-2378.	1.3	7
14	GeneStoryTeller: a mobile app for quick and comprehensive information retrieval of human genes. Database: the Journal of Biological Databases and Curation, 2015, 2015, bav048.	1.4	0
15	Light-induced structural changes in a short light, oxygen, voltage (LOV) protein revealed by molecular dynamics simulationsâ€"implications for the understanding of LOV photoactivation. Frontiers in Molecular Biosciences, 2015, 2, 55.	1.6	21
16	Functional properties of LptA and LptD in Anabaena sp. PCC 7120. Biological Chemistry, 2015, 396, 1151-1162.	1.2	5
17	Structure and Mechanism of Dimerâ€"Monomer Transition of a Plant Poly(A)-Binding Protein upon RNA Interaction: Insights into Its Poly(A) Tail Assembly. Journal of Molecular Biology, 2015, 427, 2491-2506.	2.0	5
18	A series of PDB-related databanks for everyday needs. Nucleic Acids Research, 2015, 43, D364-D368.	6.5	757
19	Comparative study of the mechanism of action of the antimicrobial peptide gomesin and its linear analogue: The role of the Î²-hairpin structure. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2414-2421.	1.4	24
20	A novel mutation in the TMC1 gene causes non-syndromic hearing loss in a Moroccan family.. Gene, 2015, 574, 28-33.	1.0	21
21	Anisotropic Crystal Growth in Flat and Nonflat Systems: The Important Influence of van der Waals Contact Molecular Stacking on Crystal Growth and Dissolution. Crystal Growth and Design, 2015, 15, 3235-3248.	1.4	23
22	Mutations in a TGF-Î² Ligand, TGFB3, CauseÂSyndromic Aortic Aneurysms andÂDissections. Journal of the American College of Cardiology, 2015, 65, 1324-1336.	1.2	238
23	New ways to boost molecular dynamics simulations. Journal of Computational Chemistry, 2015, 36, 996-1007.	1.5	711
24	Activity prediction of substrates in NADH-dependent carbonyl reductase by docking requires catalytic constraints and charge parameterization of catalytic zinc environment. Journal of Computer-Aided Molecular Design, 2015, 29, 1057-1069.	1.3	17
25	Directed evolution of the substrate specificity of dialkylglycine decarboxylase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 146-155.	1.1	14
26	Functional Analysis of the Fusarielin Biosynthetic Gene Cluster. Molecules, 2016, 21, 1710.	1.7	15
27	The Effect of Geometrical Isomerism of 3,5-Dicaffeoylquinic Acid on Its Binding Affinity to HIV-Integrase Enzyme: A Molecular Docking Study. Evidence-based Complementary and Alternative Medicine, 2016, 2016, 1-9.	0.5	17
28	Structural Elucidation and Molecular Docking of a Novel Antibiotic Compound from Cyanobacterium Nostoc sp. MGL001. Frontiers in Microbiology, 2016, 7, 1899.	1.5	25

#	Article	IF	Citations
29	An Interplay of S-Nitrosylation and Metal Ion Binding for Astrocytic S100B Protein. PLoS ONE, 2016, 11, e0154822.	1.1	15
30	MSX1 mutations and associated disease phenotypes: genotype-phenotype relations. European Journal of Human Genetics, 2016, 24, 1663-1670.	1.4	27
31	Bifunctional CYP81AA proteins catalyse identical hydroxylations but alternative regioselective phenol couplings in plant xanthone biosynthesis. Nature Communications, 2016, 7, 11472.	5.8	46
32	Intermolecular Interactions in the TMEM16A Dimer Controlling Channel Activity. Scientific Reports, 2016, 6, 38788.	1.6	11
33	Intron retention resulting from a silent mutation in the VWF gene that structurally influences the 5â€² splice site. Blood, 2016, 128, 2144-2152.	0.6	32
34	Molmil: a molecular viewer for the PDB and beyond. Journal of Cheminformatics, 2016, 8, 42.	2.8	56
35	Revisiting the mechanism of coagulation factor XIII activation and regulation from a structure/functional perspective. Scientific Reports, 2016, 6, 30105.	1.6	28
36	Semiempirical QM/MM calculations reveal a step-wise proton transfer and an unusual thiolate pocket in the mechanism of the unique arylpropionate racemase AMDase G74C. Catalysis Science and Technology, 2016, 6, 4937-4944.	2.1	4
37	Relative Orientation of POTRA Domains from Cyanobacterial Omp85 Studied by Pulsed EPR Spectroscopy. Biophysical Journal, 2016, 110, 2195-2206.	0.2	21
38	Real-time imaging of the growth-inhibitory effect of JS399-19 on Fusarium. Pesticide Biochemistry and Physiology, 2016, 134, 24-30.	1.6	14
39	Edge chlorination of hexa-peri-hexabenzocoronene investigated by density functional theory and vibrational spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 11869-11878.	1.3	17
40	A New Flexible Protocol for Docking Studies. Communications in Computer and Information Science, 2016, , 117-126.	0.4	2
41	HIV-1 adaptation to low levels of CCR5 results in V3 and V2 loop changes that increase envelope pathogenicity, CCR5 affinity and decrease susceptibility to Maraviroc. Virology, 2016, 493, 86-99.	1.1	15
42	A homology model of Xyloglucan Xylosyltransferase 2 reveals critical amino acids involved in substrate binding. Glycobiology, 2016, 26, 961-972.	1.3	7
43	Advances in Artificial Life, Evolutionary Computation and Systems Chemistry. Communications in Computer and Information Science, 2016, , .	0.4	2
44	Elucidation, functional clustering and structural characterization of Î²TrCP1 substrates through a molecular dynamics study. Molecular BioSystems, 2016, 12, 2233-2246.	2.9	10
45	Dynamic Convergent Evolution Drives the Passage Adaptation across 48 Yearsâ€™ History of H3N2 Influenza Evolution. Molecular Biology and Evolution, 2016, 33, 3133-3143.	3.5	16
46	Characterization of DprE1-Mediated Benzothiazinone Resistance in Mycobacterium tuberculosis. Antimicrobial Agents and Chemotherapy, 2016, 60, 6451-6459.	1.4	36

#	Article	IF	Citations
47	Coagulation Factor XIIIA Subunit Missense Mutations Affect Structure and Function at the Various Steps of Factor XIII Action. Human Mutation, 2016, 37, 1030-1041.	1.1	17
48	Novel mutations in Vicugna pacos (alpaca) Tyrp1 are not correlated with brown fibre colour phenotypes. Small Ruminant Research, 2016, 143, 29-34.	0.6	4
49	Revisiting sulfur H-bonds in proteins: The example of peroxiredoxin AhpE. Scientific Reports, 2016, 6, 30369.	1.6	52
50	Visual Analysis of Biomolecular Cavities: State of the Art. Computer Graphics Forum, 2016, 35, 527-551.	1.8	46
51	An engineered outer membrane pore enables an efficient oxygenation of aromatics and terpenes. Journal of Molecular Catalysis B: Enzymatic, 2016, 134, 285-294.	1.8	16
52	Structural basis of reversine selectivity in inhibiting Mps1 more potently than aurora B kinase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1761-1766.	1.5	23
53	The CebE/MsiK Transporter is a Doorway to the Cello-oligosaccharide-mediated Induction of Streptomyces scabies Pathogenicity. Scientific Reports, 2016, 6, 27144.	1.6	42
54	Enantioselective Benzylic Hydroxylation Catalysed by P450 Monooxygenases: Characterisation of a P450cam Mutant Library and Molecular Modelling. ChemBioChem, 2016, 17, 426-432.	1.3	29
55	DNA2App: Mobile sequence analyser. Scientific Phone Apps and Mobile Devices, 2016, 2, .	0.5	4
56	Building a virtual ligand screening pipeline using free software: a survey. Briefings in Bioinformatics, 2016, 17, 352-366.	3.2	74
57	MMB-GUI: a fast morphing method demonstrates a possible ribosomal tRNA translocation trajectory. Nucleic Acids Research, 2016, 44, 95-105.	6.5	11
58	Four Amino Acid Changes in HIV-2 Protease Confer Class-Wide Sensitivity to Protease Inhibitors. Journal of Virology, 2016, 90, 1062-1069.	1.5	22
59	Substrate thiophosphorylation by Arabidopsis mitogen-activated protein kinases. BMC Plant Biology, 2016, 16, 48.	1.6	14
60	Structure of a TCR-Mimic Antibody with Target Predicts Pharmacogenetics. Journal of Molecular Biology, 2016, 428, 194-205.	2.0	48
61	A hypothetical hierarchical mechanism of the self-assembly of the Escherichia coli RNA polymerase Ïƒ⁷⁰subunit. Soft Matter, 2016, 12, 1974-1982.	1.2	4
62	The Vps27/Hrs/STAM (VHS) Domain of the Signal-transducing Adaptor Molecule (STAM) Directs Associated Molecule with the SH3 Domain of STAM (AMSH) Specificity to Longer Ubiquitin Chains and Dictates the Position of Cleavage. Journal of Biological Chemistry, 2016, 291, 2033-2042.	1.6	9
63	Enzyme efficiency but not thermostability drives cefotaxime resistance evolution in TEM-1 Î²-lactamase. Molecular Biology and Evolution, 2017, 34, msx053.	3.5	48
64	Assessing the stereoselectivity of Serratia marcescens CECT 977 2,3-butanediol dehydrogenase. Catalysis Science and Technology, 2017, 7, 1831-1837.	2.1	12

#	Article	IF	Citations
65	Myosin B of Plasmodium falciparum (PfMyoB): in silico prediction of its three-dimensional structure and its possible interaction with MTIP. Parasitology Research, 2017, 116, 1373-1382.	0.6	5
66	A simple approach for preparation of affinity matrices: Simultaneous purification and reversible immobilization of a streptavidin mutein to agarose matrix. Scientific Reports, 2017, 7, 42849.	1.6	10
67	Separating Thermodynamics from Kineticsâ€"A New Understanding of the Transketolase Reaction. ChemCatChem, 2017, 9, 1808-1814.	1.8	16
68	Structural properties of amyloid Î²(1â€40) dimer explored by replica exchange molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1024-1045.	1.5	18
69	Computational study on human sphingomyelin synthase 1 (hSMS1). Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1517-1525.	1.4	17
70	Prediction of Protein Aggregation and Amyloid Formation. , 2017, , 205-263.		4
71	Immobilisation on mesoporous silica and solvent rinsing improve the transesterification abilities of feruloyl esterases from Myceliophthora thermophila. Bioresource Technology, 2017, 239, 57-65.	4.8	21
72	NewProt â€" a protein engineering portal. Protein Engineering, Design and Selection, 2017, 30, 441-447.	1.0	11
73	Missense mutations in the WD40 domain ofAHI1cause non-syndromic retinitis pigmentosa. Journal of Medical Genetics, 2017, 54, 624-632.	1.5	21
74	Identification, expression and characterization of an R-Ï‰-transaminase from Capronia semiimmersa. Applied Microbiology and Biotechnology, 2017, 101, 5677-5687.	1.7	28
75	Structural characterization of interactions between transactivation domain 1 of the p65 subunit of NF-ÎºB and transcription regulatory factors. Nucleic Acids Research, 2017, 45, 5564-5576.	6.5	51
76	Structural Stability Among Hybrid Antimicrobial Peptide Cecropin A(1â€"8)â€"Magainin 2(1â€"12) and Its Analogues: A Computational Approach. Journal of Cluster Science, 2017, 28, 2549-2563.	1.7	4
77	Architecture of the paracellular channels formed by claudins of the bloodâ€"brain barrier tight junctions. Annals of the New York Academy of Sciences, 2017, 1405, 131-146.	1.8	56
78	Deregulated Ca ²⁺ cycling underlies the development of arrhythmia and heart disease due to mutant obscurin. Science Advances, 2017, 3, e1603081.	4.7	33
79	N-(4-Hydroxyphenyl)acetamide against diiodine towards polyiodide dianion. New Journal of Chemistry, 2017, 41, 5555-5564.	1.4	0
80	Deciphering the influence of column chemistry and mass spectrometry settings for the analyses of geometrical isomers of L-chicoric acid. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2017, 1052, 73-81.	1.2	8
81	Characterization of surface binding sites in glycoside hydrolases: A computational study. Journal of Molecular Recognition, 2017, 30, e2624.	1.1	10
82	Synthesis characterization and biological activity of mixed ligand silver(I) complex of 2-benzimidazolylurea and triphenylphosphine. Polyhedron, 2017, 128, 95-103.	1.0	12

#	Article	IF	Citations
83	Histo-Blood Group Antigen Presentation Is Critical for Binding of Norovirus VLP to Glycosphingolipids in Model Membranes. ACS Chemical Biology, 2017, 12, 1288-1296.	1.6	22
84	Determination of Structure and Micellar Interactions of Small Antimicrobial Peptides by Solution-State NMR. Methods in Molecular Biology, 2017, 1548, 73-88.	0.4	3
85	Theoretical and experimental study of the antifreeze protein AFP752, trehalose and dimethyl sulfoxide cryoprotection mechanism: correlation with cryopreserved cell viability. RSC Advances, 2017, 7, 352-360.	1.7	50
86	Collapsin response mediator protein 2: high-resolution crystal structure sheds light on small-molecule binding, post-translational modifications, and conformational flexibility. Amino Acids, 2017, 49, 747-759.	1.2	22
87	Warfarin and vitamin K compete for binding to Phe55 in human VKOR. Nature Structural and Molecular Biology, 2017, 24, 77-85.	3.6	42
88	High quality rendering of protein dynamics in space filling mode. Journal of Molecular Graphics and Modelling, 2017, 78, 158-167.	1.3	4
89	Insights into the roles of non-catalytic residues in the active site of a GH10 xylanase with activity on cellulose. Journal of Biological Chemistry, 2017, 292, 19315-19327.	1.6	35
90	Streptavidin as a Scaffold for Lightâ€Induced Longâ€Lived Charge Separation. Chemistry - A European Journal, 2017, 23, 18019-18024.	1.7	3
91	Novel compound heterozygous mutations in the GPR98 (USH2C) gene identified by whole exome sequencing in a Moroccan deaf family. Molecular Biology Reports, 2017, 44, 429-434.	1.0	10
92	HIV-1 subtype CRF01_AE and B differ in utilization of low levels of CCR5, Maraviroc susceptibility and potential N-glycosylation sites. Virology, 2017, 512, 222-233.	1.1	4
93	Increase of Bacillus badius Phenylalanine dehydrogenase specificity towards phenylalanine substrate by site-directed mutagenesis. Archives of Biochemistry and Biophysics, 2017, 635, 44-51.	1.4	11
94	Glycosidase Inhibition by Multivalent Presentation of Heparan Sulfate Saccharides on Bottlebrush Polymers. Biomacromolecules, 2017, 18, 3387-3399.	2.6	25
95	A novel fluorescent solvatochromic probe for lipid bilayers. Supramolecular Chemistry, 2017, 29, 887-895.	1.5	30
96	Inversion of cpADH5 Enantiopreference and Altered Chain Length Specificity for Methyl 3â€Hydroxyalkanoates. Chemistry - A European Journal, 2017, 23, 12636-12645.	1.7	6
97	High-Throughput Automated Preparation and Simulation of Membrane Proteins with HTMD. Journal of Chemical Theory and Computation, 2017, 13, 4003-4011.	2.3	27
98	Inhibitors of nicotinamide N-methyltransferase designed to mimic the methylation reaction transition state. Organic and Biomolecular Chemistry, 2017, 15, 6656-6667.	1.5	42
99	Impact of phenylalanines outside the dimer interface on phosphotriesterase stability and function. Molecular BioSystems, 2017, 13, 2092-2106.	2.9	4
100	Molecular Dynamics Study to Investigate the Dimeric Structure of the Full-Length Î±-Synuclein in Aqueous Solution. Journal of Chemical Information and Modeling, 2017, 57, 2281-2293.	2.5	14

#	Article	IF	Citations
101	Crystal Structure and Regulation of the Citrus Pol III Repressor MAF1 by Auxin and Phosphorylation. Structure, 2017, 25, 1360-1370.e4.	1.6	22
102	A half-site multimeric enzyme achieves its cooperativity without conformational changes. Scientific Reports, 2017, 7, 16529.	1.6	14
103	Evolution of Cytochrome c Oxidase in Hypoxia Tolerant Sculpins (Cottidae, Actinopterygii). Molecular Biology and Evolution, 2017, 34, 2153-2162.	3.5	27
104	Outward-Open Model of Thyroid Hormone Transporter Monocarboxylate Transporter 8 Provides Novel Structural and Functional Insights. Endocrinology, 2017, 158, 3292-3306.	1.4	16
105	Metagenome-derived haloalkane dehalogenases with novel catalytic properties. Applied Microbiology and Biotechnology, 2017, 101, 6385-6397.	1.7	8
106	Phosphorylation regulates the secondary structure and function of dentin phosphoprotein peptides. Bone, 2017, 95, 65-75.	1.4	18
107	<scp>DNA</scp>â€binding and repressor function are prerequisites for the turnover of the tomato heat stress transcription factor HsfB1. Plant Journal, 2017, 89, 31-44.	2.8	12
108	Visualization of Biomolecular Structures: State of the Art Revisited. Computer Graphics Forum, 2017, 36, 178-204.	1.8	69
109	Humanization of Murine Monoclonal anti-hTNF Antibody: The F10 Story. Molecular Biology, 2017, 51, 921-926.	0.4	1
110	The Combined Use of in Silico, in Vitro, and in Vivo Analyses to Assess Anti-cancerous Potential of a Bioactive Compound from Cyanobacterium Nostoc sp. MGL001. Frontiers in Pharmacology, 2017, 8, 873.	1.6	12
111	2-Methyl-2,4-pentanediol (MPD) boosts as detergent-substitute the performance of ÃŸ-barrel hybrid catalyst for phenylacetylene polymerization. Beilstein Journal of Organic Chemistry, 2017, 13, 1498-1506.	1.3	12
112	Fluorinated Adenosine A2A Receptor Antagonists Inspired by Preladenant as Potential Cancer Immunotherapeutics. International Journal of Medicinal Chemistry, 2017, 2017, 1-8.	2.2	5
113	Structural aspects of nucleotide ligand binding by a bacterial 2H phosphoesterase. PLoS ONE, 2017, 12, e0170355.	1.1	6
114	An in silico and in vitro approach to elucidate the impact of residues flanking the cleavage scissile bonds of FVIII. PLoS ONE, 2017, 12, e0180456.	1.1	3
115	Molecular docking studies of 3-bromopyruvate and its derivatives to metabolic regulatory enzymes: Implication in designing of novel anticancer therapeutic strategies. PLoS ONE, 2017, 12, e0176403.	1.1	64
116	Homozygous GRID2 missense mutation predicts a shift in the D-serine binding domain of GluD2 in a case with generalized brain atrophy and unusual clinical features. BMC Medical Genetics, 2017, 18, 144.	2.1	21
117	Active phytochemicals of Pueraria tuberosa for DPP-IV inhibition: in silico and experimental approach. Journal of Diabetes and Metabolic Disorders, 2017, 16, 46.	0.8	27
118	PI(4,5)P2 controls plasma membrane PI4P and PS levels via ORP5/8 recruitment to ERâ€“PM contact sites. Journal of Cell Biology, 2018, 217, 1797-1813.	2.3	153

#	Article	IF	Citations
119	The single berberine bridge enzyme homolog of PhyscomitrellaÂpatens is a cellobiose oxidase. FEBS Journal, 2018, 285, 1923-1943.	2.2	17
120	Frequent novel mutations are causative for maple syrup urine disease from Southwest Iran. Meta Gene, 2018, 16, 96-104.	0.3	2
121	Study on oligomerization of glutamate decarboxylase from Lactobacillus brevis using asymmetrical flow field-flow fractionation (AF4) with light scattering techniques. Analytical and Bioanalytical Chemistry, 2018, 410, 451-458.	1.9	6
122	Insights from ion mobility-mass spectrometry, infrared spectroscopy, and molecular dynamics simulations on nicotinamide adenine dinucleotide structural dynamics: NAD⁺vs.NADH. Physical Chemistry Chemical Physics, 2018, 20, 7043-7052.	1.3	14
123	Potholing of the hydrophobic heme oxygenase-1 western region for the search of potent and selective imidazole-based inhibitors. European Journal of Medicinal Chemistry, 2018, 148, 54-62.	2.6	38
124	Xylo- and arabinoxylooligosaccharides from wheat bran by endoxylanases, utilisation by probiotic bacteria, and structural studies of the enzymes. Applied Microbiology and Biotechnology, 2018, 102, 3105-3120.	1.7	36
125	The structural and functional reliability of Circulins of Chassalia parvifolia for peptide therapeutic scaffolding. Journal of Cellular Biochemistry, 2018, 119, 3999-4008.	1.2	2
126	A computational examination of the binding interactions of amyloidÎ² and human cystatin C. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850001.	1.8	1
127	Translation initiation by capâ€dependent ribosome recruitment: Recent insights and open questions. Wiley Interdisciplinary Reviews RNA, 2018, 9, e1473.	3.2	113
128	Distinct domains in the matricellular protein Lonely heart are crucial for cardiac extracellular matrix formation and heart function in Drosophila. Journal of Biological Chemistry, 2018, 293, 7864-7879.	1.6	14
129	The Structural Basis of Calcium-Dependent Inactivation of the Transient Receptor Potential Vanilloid 5 Channel. Biochemistry, 2018, 57, 2623-2635.	1.2	18
130	Metabolites of n-Butylparaben and iso-Butylparaben Exhibit Estrogenic Properties in MCF-7 and T47D Human Breast Cancer Cell Lines. Toxicological Sciences, 2018, 164, 50-59.	1.4	17
131	Nudt19 is a renal CoA diphosphohydrolase with biochemical and regulatory properties that are distinct from the hepatic Nudt7 isoform. Journal of Biological Chemistry, 2018, 293, 4134-4148.	1.6	49
132	Transâ€species synthetic gene design allows resistance pyramiding and broadâ€spectrum engineering of virus resistance in plants. Plant Biotechnology Journal, 2018, 16, 1569-1581.	4.1	64
133	Identification of endocrine disrupting chemicals acting on human aromatase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 88-96.	1.1	27
134	Relative binding affinity prediction of farnesoid X receptor in the D3R Grand Challenge 2 using FEP+. Journal of Computer-Aided Molecular Design, 2018, 32, 265-272.	1.3	10
135	YASARA: A Tool to Obtain Structural Guidance in Biocatalytic Investigations. Methods in Molecular Biology, 2018, 1685, 43-67.	0.4	306
136	The V279F polymorphism might change protein character and immunogenicity in Lp-PLA2 protein. Egyptian Journal of Medical Human Genetics, 2018, 19, 107-112.	0.5	3

#	Article	IF	Citations
137	Missense variants in the X-linked genePRPS1cause retinal degeneration in females. Human Mutation, 2018, 39, 80-91.	1.1	23
138	Arabinoxylanase from glycoside hydrolase family 5 is a selective enzyme for production of specific arabinoxylooligosaccharides. Food Chemistry, 2018, 242, 579-584.	4.2	28
139	DNA intercalators based on (1,10-phenanthrolin-2-yl)isoxazolidin-5-yl core with better growth inhibition and selectivity than cisplatin upon head and neck squamous cells carcinoma. European Journal of Medicinal Chemistry, 2018, 143, 583-590.	2.6	19
140	Dominant-negative SMARCA4 mutants alter the accessibility landscape of tissue-unrestricted enhancers. Nature Structural and Molecular Biology, 2018, 25, 61-72.	3.6	140
141	Structural insights of Rm Xyn10A â€“ A prebiotic-producing GH10 xylanase with a non-conserved aglycone binding region. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 292-306.	1.1	14
142	Substrate specificity and transfucosylation activity of GH29 Î±-l-fucosidases for enzymatic production of human milk oligosaccharides. New Biotechnology, 2018, 41, 34-45.	2.4	58
143	Incretin hormones receptor signaling plays the key role in antidiabetic potential of PTY-2 against STZ-induced pancreatitis. Biomedicine and Pharmacotherapy, 2018, 97, 330-338.	2.5	16
144	Improved Enantioselectivity of Subtilisin Carlsberg towards Secondary Alcohols by Protein Engineering. ChemBioChem, 2018, 19, 338-346.	1.3	5
145	Molecular Dynamics and Morphing Protocols for High Accuracy Molecular Docking. Lecture Notes in Bioengineering, 2018, , 85-96.	0.3	3
146	The cereal pathogen Fusarium pseudograminearum produces a new class of active cytokinins during infection. Molecular Plant Pathology, 2018, 19, 1140-1154.	2.0	37
147	Covalently immobilized catalase on functionalized graphene: effect on the activity, immobilization efficiency, and tetramer stability. Biomaterials Science, 2018, 6, 3231-3240.	2.6	27
148	Exploring the binding pattern between pepsin and deferasirox using detailed experimental and computer simulation methods. RSC Advances, 2018, 8, 37208-37218.	1.7	8
149	Efficient discrimination of natural stereoisomers of chicoric acid, an HIV-1 integrase inhibitor. Journal of Photochemistry and Photobiology B: Biology, 2018, 189, 258-266.	1.7	13
150	Mechanism of Tetramer Dissociation, Unfolding, and Oligomer Assembly of Pneumovirus M2-1 Transcription Antiterminators. ACS Omega, 2018, 3, 14732-14745.	1.6	4
151	The 9H-Fluoren Vinyl Ether Derivative SAM461 Inhibits Bacterial Luciferase Activity and Protects Artemia franciscana From Luminescent Vibriosis. Frontiers in Cellular and Infection Microbiology, 2018, 8, 368.	1.8	1
152	Iron is a centrally bound cofactor of specifier proteins involved in glucosinolate breakdown. PLoS ONE, 2018, 13, e0205755.	1.1	34
153	In Silico Studies on Compounds Derived from Calceolaria: Phenylethanoid Glycosides as Potential Multitarget Inhibitors for the Development of Pesticides. Biomolecules, 2018, 8, 121.	1.8	26
154	A Pseudouridine Isoxazolidinyl Nucleoside Analogue Structural Analysis: A Morphological Approach. Molecules, 2018, 23, 3381.	1.7	1

#	Article	IF	Citations
155	The proton and metal binding sites responsible for the pH-dependent green-red bioluminescence color tuning in firefly luciferases. Scientific Reports, 2018, 8, 17594.	1.6	13
156	Structure and dynamics of Helicobacter pylori nickel-chaperone HypA: an integrated approach using NMR spectroscopy, functional assays and computational tools. Journal of Biological Inorganic Chemistry, 2018, 23, 1309-1330.	1.1	20
157	Novel pathogenic variants in filamin C identified in pediatric restrictive cardiomyopathy. Human Mutation, 2018, 39, 2083-2096.	1.1	21
158	Development of photoswitchable inhibitors for Î²-galactosidase. Organic and Biomolecular Chemistry, 2018, 16, 7430-7437.	1.5	16
159	Proteinase 3; a potential target in chronic obstructive pulmonary disease and other chronic inflammatory diseases. Respiratory Research, 2018, 19, 180.	1.4	36
160	Structural Basis for the Acceleration of Procollagen Processing by Procollagen C-Proteinase Enhancer-1. Structure, 2018, 26, 1384-1392.e3.	1.6	30
161	Mutated Thyroid Hormone Transporter OATP1C1 Associates with Severe Brain Hypometabolism and Juvenile Neurodegeneration. Thyroid, 2018, 28, 1406-1415.	2.4	57
162	In silico Prediction, Characterization, Molecular Docking, and Dynamic Studies on Fungal SDRs as Novel Targets for Searching Potential Fungicides Against Fusarium Wilt in Tomato. Frontiers in Pharmacology, 2018, 9, 1038.	1.6	79
163	Role of Leucine 341 in Thyroid Hormone Receptor Beta Revealed by a Novel Mutation Causing Thyroid Hormone Resistance. Thyroid, 2018, 28, 1723-1726.	2.4	4
164	Quaternary Structure, Salt Sensitivity, and Allosteric Regulation of Î²-AMYLASE2 From Arabidopsis thaliana. Frontiers in Plant Science, 2018, 9, 1176.	1.7	12
165	Oleanolic acid enhances neural stem cell migration, proliferation, and differentiation in vitro by inhibiting GSK3Î² activity. Cell Death Discovery, 2018, 4, 48.	2.0	15
166	Systematic variation of the benzoylhydrazine moiety of the GluN2A selective NMDA receptor antagonist TCN-201. European Journal of Medicinal Chemistry, 2018, 158, 259-269.	2.6	9
167	Structural insights into antigen recognition of an anti-Î²-(1,6)-Î²-(1,3)-D-glucan antibody. Scientific Reports, 2018, 8, 13652.	1.6	7
168	Two Tau binding sites on tubulin revealed by thiol-disulfide exchanges. Scientific Reports, 2018, 8, 13846.	1.6	15
169	Hsp90 Mediates Membrane Deformation and Exosome Release. Molecular Cell, 2018, 71, 689-702.e9.	4.5	103
170	Targeting heme Oxygenase-1 with hybrid compounds to overcome Imatinib resistance in chronic myeloid leukemia cell lines. European Journal of Medicinal Chemistry, 2018, 158, 937-950.	2.6	36
171	Oxidative cyclization of N-methyl-dopa by a fungal flavoenzyme of the amine oxidase family. Journal of Biological Chemistry, 2018, 293, 17021-17032.	1.6	4
172	A hydroquinone-specific screening system for directed P450 evolution. Applied Microbiology and Biotechnology, 2018, 102, 9657-9667.	1.7	16

#	Article	IF	Citations
173	In silico stressâ€“strain measurements on self-assembled protein lattices. Soft Matter, 2018, 14, 8095-8104.	1.2	2
174	VKORC1 and VKORC1L1 have distinctly different oral anticoagulant dose-response characteristics and binding sites. Blood Advances, 2018, 2, 691-702.	2.5	17
175	Priming Time: How Cellular Proteases Arm Coronavirus Spike Proteins. , 2018, , 71-98.		69
176	Loop engineering of an Î±-1,3/4-l-fucosidase for improved synthesis of human milk oligosaccharides. Enzyme and Microbial Technology, 2018, 115, 37-44.	1.6	35
177	Fragment Based Molecular Dynamics for Drug Design. Communications in Computer and Information Science, 2018, , 49-58.	0.4	1
178	Protein phenotype diagnosis of autosomal dominant calmodulin mutations causing irregular heart rhythms. Journal of Cellular Biochemistry, 2018, 119, 8233-8248.	1.2	14
179	QM/MM Studies of Dph5 â€“ A Promiscuous Methyltransferase in the Eukaryotic Biosynthetic Pathway of Diphthamide. Journal of Chemical Information and Modeling, 2018, 58, 1406-1414.	2.5	8
180	Two Strategies of Pseudomonas syringae to Avoid Recognition of the HopQ1 Effector in Nicotiana Species. Frontiers in Plant Science, 2018, 9, 978.	1.7	14
181	The Synthetic Potential of Fungal Feruloyl Esterases: A Correlation with Current Classification Systems and Predicted Structural Properties. Catalysts, 2018, 8, 242.	1.6	15
182	Protein Engineering of the Progesterone Hydroxylating P450â€Monooxygenase CYP17A1 Alters Its Regioselectivity. ChemBioChem, 2018, 19, 1954-1958.	1.3	8
183	Casesidin-like anti-bacterial peptides in peptic hydrolysate of camel milk Î²-casein. International Dairy Journal, 2018, 86, 49-56.	1.5	14
184	Comparison of Candida antarctica Lipase B Variants for Conversion of Îµ-Caprolactone in Aqueous Mediumâ€”Part 2. Polymers, 2018, 10, 524.	2.0	10
185	A Critical Note on Symmetry Contact Artifacts and the Evaluation of the Quality of Homology Models. Symmetry, 2018, 10, 25.	1.1	1
186	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. Journal of Physical Chemistry B, 2018, 122, 7668-7681.	1.2	8
187	Structural basis of exo-Î²-mannanase activity in the GH2 family. Journal of Biological Chemistry, 2018, 293, 13636-13649.	1.6	16
188	Vasodilator effects and putative guanylyl cyclase stimulation by 2-nitro-1-phenylethanone and 2-nitro-2-phenyl-propane-1,3-diol on rat aorta. European Journal of Pharmacology, 2018, 830, 105-114.	1.7	3
189	Structure of the essential peptidoglycan amidotransferase MurT/GatD complex from Streptococcus pneumoniae. Nature Communications, 2018, 9, 3180.	5.8	34
190	Efficient ionic liquid-based platform for multi-enzymatic conversion of carbon dioxide to methanol. Green Chemistry, 2018, 20, 4339-4348.	4.6	68

#	Article	IF	Citations
191	Phage display-derived antibody fragments against conserved regions of VacA toxin of Helicobacter pylori. Applied Microbiology and Biotechnology, 2018, 102, 6899-6913.	1.7	20
192	Self-Assembly Simulations of Classic Claudinsâ€"Insights into the Pore Structure, Selectivity, and Higher Order Complexes. Journal of Physical Chemistry B, 2018, 122, 7463-7474.	1.2	37
193	Deciphering Specificity Determinants for FR900359â€Derived G_qÎ± Inhibitors Based on Computational and Structureâ€"Activity Studies. ChemMedChem, 2018, 13, 1634-1643.	1.6	29
194	Genotypeâ€phenotype correlations of lowâ€frequency variants in the complement system in renal disease and ageâ€related macular degeneration. Clinical Genetics, 2018, 94, 330-338.	1.0	17
195	Insights into mechanism and functional consequences of heme binding to hemolysin-activating lysine acyltransferase HlyC from Escherichia coli. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1964-1972.	1.1	18
196	A selective Fluorescence Chemosensor: Pyrene motif Schiff base derivative for detection of Cu2+ ions in living cells. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 364, 424-432.	2.0	25
197	Evaluation of in vitro refolding vs cold shock expression: Production of a low yielding single chain variable fragment. Protein Expression and Purification, 2018, 151, 62-71.	0.6	7
198	Insights into the interaction of ulipristal acetate and human serum albumin using multi-spectroscopic methods, molecular docking, and dynamic simulation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2989-2998.	2.0	21
199	Determination of interactions between human serum albumin and niraparib through multi-spectroscopic and computational methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 126-134.	2.0	36
200	Molecular designing, virtual screening and docking study of novel curcumin analogue as mutation (S769L and K846R) selective inhibitor for EGFR. Saudi Journal of Biological Sciences, 2019, 26, 439-448.	1.8	20
201	Computational simulations assessment of mutations impact on streptokinase (SK) from a group G streptococci with enhanced activity â€" insights into the functional roles of structural dynamics flexibility of SK and stabilization of SKâ€"¼plasmin catalytic complex. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1944-1955.	2.0	6
202	Protein Structure Visualization. , 2019, , 520-538.		1
203	Bi-allelic c.181_183delTGT in BTB domain of KLHL7 is associated with overlapping phenotypes of Crisponi/CISS1-like and Bohring-Opitz like syndrome. European Journal of Medical Genetics, 2019, 62, 103528.	0.7	7
204	Discovery and development of substituted thiadiazoles as inhibitors of Staphylococcus aureus Sortase A. Bioorganic and Medicinal Chemistry, 2019, 27, 115043.	1.4	13
205	Structure functional insights into calcium binding during the activation of coagulation factor XIII A. Scientific Reports, 2019, 9, 11324.	1.6	52
206	Structural Comparison of a Promiscuous and a Highly Specific Sucrose 6F-Phosphate Phosphorylase. International Journal of Molecular Sciences, 2019, 20, 3906.	1.8	10
207	In Vitro Characterization of Human, Mouse, and Zebrafish MCT8 Orthologues. Thyroid, 2019, 29, 1499-1510.	2.4	9
208	A cytochrome P450 from the mustard leaf beetles hydroxylates geraniol, a key step in iridoid biosynthesis. Insect Biochemistry and Molecular Biology, 2019, 113, 103212.	1.2	11

#	Article	IF	Citations
209	The Sialic Acid-Dependent Nematocyst Discharge Process in Relation to Its Physical-Chemical Properties Is a Role Model for Nanomedical Diagnostic and Therapeutic Tools. Marine Drugs, 2019, 17, 469.	2.2	11
210	Effect of Conformational Diversity on the Bioactivity of Âµ-Conotoxin PIIIA Disulfide Isomers. Marine Drugs, 2019, 17, 390.	2.2	10
211	Analysis of Long Molecular Dynamics Simulations Using Interactive Focus+Context Visualization. Computer Graphics Forum, 2019, 38, 441-453.	1.8	11
212	Directed Evolution of P450 BM3 towards Functionalization of Aromatic O-Heterocycles. International Journal of Molecular Sciences, 2019, 20, 3353.	1.8	14
213	Sulfation pathways from red to green. Journal of Biological Chemistry, 2019, 294, 12293-12312.	1.6	76
214	Exploring the mechanism of PPARÎ³ phosphorylation mediated by CDK5. Journal of Structural Biology, 2019, 207, 317-326.	1.3	16
215	A novel epitope-presenting thermostable scaffold for the development of highly specific insulin-like growth factor-1/2 antibodies. Journal of Biological Chemistry, 2019, 294, 13434-13444.	1.6	3
216	The anti-parasitic drug suramin potently inhibits formation of seminal amyloid fibrils and their interaction with HIV-1. Journal of Biological Chemistry, 2019, 294, 13740-13754.	1.6	9
217	A novel potent autophagy inhibitor ECDD-S27 targets vacuolar ATPase and inhibits cancer cell survival. Scientific Reports, 2019, 9, 9177.	1.6	11
218	Revisiting silibinin as a novobiocin-like Hsp90â€¯C-terminal inhibitor: Computational modeling and experimental validation. Food and Chemical Toxicology, 2019, 132, 110645.	1.8	16
219	Insight Into Molecular Determinants of T3 vs T4 Recognition From Mutations in Thyroid Hormone Receptor Î± and Î². Journal of Clinical Endocrinology and Metabolism, 2019, 104, 3491-3500.	1.8	17
220	Binding site plasticity in viral PPxY Late domain recognition by the third WW domain of human NEDD4. Scientific Reports, 2019, 9, 15076.	1.6	12
221	Oleanolic Acid Derivatives as Potential Inhibitors of HIV-1 Protease. Journal of Natural Products, 2019, 82, 2886-2896.	1.5	29
222	Computational protein design of bacteriocins based on structural scaffold of aureocin A53. International Journal of Bioinformatics Research and Applications, 2019, 15, 129.	0.1	7
223	Effect of Single Amino Acid Substitutions by Asn and Gln on Aggregation Properties of Bence-Jones Protein BIF. International Journal of Molecular Sciences, 2019, 20, 5197.	1.8	1
224	Structure of the Human ACP-ISD11 Heterodimer. Biochemistry, 2019, 58, 4596-4609.	1.2	13
225	Presence of carbohydrate binding modules in extracellular region of class C G-protein coupled receptors (C GPCR): An in silico investigation on sweet taste receptor. Journal of Biosciences, 2019, 44, 1.	0.5	2
226	Computational Nanoscopy of Tight Junctions at the Bloodâ€“Brain Barrier Interface. International Journal of Molecular Sciences, 2019, 20, 5583.	1.8	18

#	Article	IF	Citations
227	[1]Benzothieno[3,2-d]pyrimidine derivatives as ligands for the serotonergic 5-HT7 receptor. European Journal of Medicinal Chemistry, 2019, 183, 111690.	2.6	4
228	Characterization of the mutation spectrum in a Pakistani cohort of type 3 von Willebrand disease. Haemophilia, 2019, 25, 1035-1044.	1.0	5
229	Phylodynamics of Influenza A/H1N1pdm09 in India Reveals Circulation Patterns and Increased Selection for Clade 6b Residues and Other High Mortality Mutants. Viruses, 2019, 11, 791.	1.5	9
230	Functional characterization of a SNP (F51S) found in human alpha 1â€antitrypsin. Molecular Genetics & Genomic Medicine, 2019, 7, e819.	0.6	2
231	Molecular Basis of BioJ, a Unique Gatekeeper in Bacterial Biotin Synthesis. IScience, 2019, 19, 796-808.	1.9	5
232	Volumetric Representation of Biomolecules Using Cell Decomposition and Robotics. , 2019, , .		1
233	G protein-coupled receptors of class A harness the energy of membrane potential to increase their sensitivity and selectivity. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 183051.	1.4	10
234	The In Vitro Functional Impairment of Thyroid Hormone Receptor Alpha 1 Isoform Mutants Is Mainly Dictated by Reduced Ligand Sensitivity. Thyroid, 2019, 29, 1834-1842.	2.4	2
235	Adaption of human antibody Î» and Îº light chain architectures to CDR repertoires. Protein Engineering, Design and Selection, 2019, 32, 109-127.	1.0	12
236	Structural and Dynamical Basis of G Protein Inhibition by YM-254890 and FR900359: An Inhibitor in Action. Journal of Chemical Information and Modeling, 2019, 59, 4361-4373.	2.5	22
237	Immunoinformatics approaches to explore Helicobacter Pylori proteome (Virulence Factors) to design B and T cell multi-epitope subunit vaccine. Scientific Reports, 2019, 9, 13321.	1.6	102
238	Physicochemical Characterization and Antioxidant Activity Evaluation of Idebenone/Hydroxypropyl-Î²-Cyclodextrin Inclusion Complex â€. Biomolecules, 2019, 9, 531.	1.8	51
239	Conformation and Domain Movement Analysis of Human Matrix Metalloproteinase-2: Role of Associated Zn2+ and Ca2+ Ions. International Journal of Molecular Sciences, 2019, 20, 4194.	1.8	5
240	Consensus model of a cyanobacterial light-dependent protochlorophyllide oxidoreductase in its pigment-free apo-form and photoactive ternary complex. Communications Biology, 2019, 2, 351.	2.0	9
241	Room-Temperature Phosphorescence from Encapsulated Pyrene Induced by Xenon. Journal of Physical Chemistry A, 2019, 123, 9123-9131.	1.1	12
242	Bis-anthracene derived bis-pyridine: selective fluorescence sensing of Al³⁺ ions. New Journal of Chemistry, 2019, 43, 2519-2528.	1.4	23
243	Differences between the binding modes of enantiomers S/R-nicotine to acetylcholinesterase. RSC Advances, 2019, 9, 1428-1440.	1.7	13
244	AllerCatProâ€"prediction of protein allergenicity potential from the protein sequence. Bioinformatics, 2019, 35, 3020-3027.	1.8	115

#	Article	IF	Citations
245	Morphing of Ibogaine: A Successful Attempt into the Search for Sigma-2 Receptor Ligands. International Journal of Molecular Sciences, 2019, 20, 488.	1.8	10
246	Homology models of mouse and rat estrogen receptor-Î± ligand-binding domain created by in silico mutagenesis of a human template: Molecular docking with 17Î²-estradiol, diethylstilbestrol, and paraben analogs. Computational Toxicology, 2019, 10, 1-16.	1.8	18
247	Theoretical insights into the metal chelating and antimicrobial properties of the chalcone based Schiff bases. Molecular Simulation, 2019, 45, 636-645.	0.9	19
248	Transesterification of a Tertiary Alcohol by Engineered Candida antarctica Lipaseâ€...A. ChemBioChem, 2019, 20, 1438-1443.	1.3	13
249	A new class of recombinant human albumin with multiple surface thiols exhibits stable conjugation and enhanced FcRn binding and blood circulation. Journal of Biological Chemistry, 2019, 294, 3735-3743.	1.6	15
250	Protein Disulfide Isomerase Modulates the Activation of Thyroid Hormone Receptors. Frontiers in Endocrinology, 2019, 9, 784.	1.5	6
251	Phenamacril is a reversible and noncompetitive inhibitor of Fusarium class I myosin. Journal of Biological Chemistry, 2019, 294, 1328-1337.	1.6	21
252	OligoCOOL: A mobile application for nucleotide sequence analysis. Biochemistry and Molecular Biology Education, 2019, 47, 201-206.	0.5	0
253	KnowVolution of a Fungal Laccase toward Alkaline pH. ChemBioChem, 2019, 20, 1458-1466.	1.3	40
254	Stabilization of cyclohexanone monooxygenase by computational and experimental library design. Biotechnology and Bioengineering, 2019, 116, 2167-2177.	1.7	25
255	Combined Inhibitory Effects of Citrinin, Ochratoxin-A, and T-2 Toxin on Aquaporin-2. Journal of Physical Chemistry B, 2019, 123, 5755-5768.	1.2	8
256	Ultrafast Solvation Dynamics Reveal that Octa Acid Capsuleâ€™s Interior Dryness Depends on the Guest. Journal of Physical Chemistry A, 2019, 123, 5928-5936.	1.1	13
257	Genomic analysis and lactose transporter expression in Kluyveromyces marxianus CCT 7735. Fungal Biology, 2019, 123, 687-697.	1.1	4
258	Improvement of the versatility of an arabinofuranosidase against galactofuranose for the synthesis of galactofuranoconjugates. Organic and Biomolecular Chemistry, 2019, 17, 6799-6808.	1.5	3
259	Ultrafast trans â†' cis Photoisomerization Dynamics of Alkyl-Substituted Stilbenes in a Supramolecular Capsule. Journal of Physical Chemistry A, 2019, 123, 5061-5071.	1.1	16
260	Supramolecular host-guest interactions of pseudoginsenoside F11 with Î²- and Î³-cyclodextrin: Spectroscopic/spectrometric and computational studies. Journal of Molecular Structure, 2019, 1195, 387-394.	1.8	7
261	Identification of Ezetimibe and Pranlukast as Pharmacological Chaperones for the Treatment of the Rare Disease Mucopolysaccharidosis Type IVA. Journal of Medicinal Chemistry, 2019, 62, 6175-6189.	2.9	26
262	Crystal Structure and Biophysical Analysis of Furfural-Detoxifying Aldehyde Reductase from Clostridium beijerinckii. Applied and Environmental Microbiology, 2019, 85, .	1.4	1

#	Article	IF	Citations
263	Chitin-Binding Protein of Verticillium nonalfalfae Disguises Fungus from Plant Chitinases and Suppresses Chitin-Triggered Host Immunity. Molecular Plant-Microbe Interactions, 2019, 32, 1378-1390.	1.4	72
264	Introducing a New Model of Sweet Taste Receptor, a Class C G-protein Coupled Receptor (C GPCR). Cell Biochemistry and Biophysics, 2019, 77, 227-243.	0.9	11
265	Disruption of Structural Disulfides of Coagulation FXIII-B Subunit; Functional Implications for a Rare Bleeding Disorder. International Journal of Molecular Sciences, 2019, 20, 1956.	1.8	7
266	Antiviral RNAi in Insects and Mammals: Parallels and Differences. Viruses, 2019, 11, 448.	1.5	67
267	Mapping the Allosteric Communication Network of Aminodeoxychorismate Synthase. Journal of Molecular Biology, 2019, 431, 2718-2728.	2.0	11
268	Binding assessment of methylene blue to human serum albumin and poly(acrylic acid): Experimental and computer-aided modeling studies. Journal of Molecular Liquids, 2019, 285, 811-821.	2.3	11
269	Control of anterior <scp>GR</scp> adient 2 (<scp>AGR</scp> 2) dimerization links endoplasmic reticulum proteostasis to inflammation. EMBO Molecular Medicine, 2019, 11, .	3.3	48
270	In silico and in vitro evaluation of the impact of mutations in non-severe haemophilia A patients on assay discrepancies. Annals of Hematology, 2019, 98, 1855-1865.	0.8	7
271	COL1A1 C-propeptide mutations cause ER mislocalization of procollagen and impair C-terminal procollagen processing. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2019, 1865, 2210-2223.	1.8	18
272	Examining Product Specificity in Protein Arginine Methyltransferase 7 (PRMT7) Using Quantum and Molecular Mechanical Simulations. Journal of Chemical Information and Modeling, 2019, 59, 2913-2923.	2.5	10
273	Amino Acids as Additives against Amorphous Aggregation: In Vitro and In Silico Study on Human Lysozyme. Applied Biochemistry and Biotechnology, 2019, 189, 305-317.	1.4	9
274	Stereoselectivity Switch in the Reduction of Î±-Alkyl-Î²-Arylenones by Structure-Guided Designed Variants of the Ene Reductase OYE1. Frontiers in Bioengineering and Biotechnology, 2019, 7, 89.	2.0	16
275	In Silico Approaches for TRP Channel Modulation. Methods in Molecular Biology, 2019, 1987, 187-206.	0.4	5
276	Novel mutations in MYBPC1 are associated with myogenic tremor and mild myopathy. Annals of Neurology, 2019, 86, 129-142.	2.8	27
277	Molecular screening and genetic diversity analysis of anticancer Azurin-encoding and Azurin-like genes in human gut microbiome deduced through cultivation-dependent and cultivation-independent studies. International Microbiology, 2019, 22, 437-449.	1.1	5
278	Glycosylation of the viral attachment protein of avian coronavirus is essential for host cell and receptor binding. Journal of Biological Chemistry, 2019, 294, 7797-7809.	1.6	68
279	Effects of Selective Substitution of Cysteine Residues on the Conformational Properties of Chlorotoxin Explored by Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2019, 20, 1261.	1.8	6
280	Investigating coordination flexibility of glycerophosphodiesterase (GpdQ) through interactions with mono-, di-, and triphosphoester (NPP, BNPP, GPE, and paraoxon) substrates. Physical Chemistry Chemical Physics, 2019, 21, 5499-5509.	1.3	15

#	Article	IF	Citations
281	Exploring the structural similarity yet functional distinction between coagulation factor XIII-B and complement factor H sushi domains. Journal of Thrombosis and Thrombolysis, 2019, 48, 95-102.	1.0	6
282	Chiral separation of <scp>d</scp>/<scp>l</scp>-arginine with whole cells through an engineered FhuA nanochannel. Chemical Communications, 2019, 55, 5431-5434.	2.2	17
283	Coagulation Factor XIIIa Inhibitor Tridegin: On the Role of Disulfide Bonds for Folding, Stability, and Function. Journal of Medicinal Chemistry, 2019, 62, 3513-3523.	2.9	7
284	A new Mycobacterium leprae dihydropteroate synthase variant (V39I) from Papua, Indonesia. Heliyon, 2019, 5, e01279.	1.4	7
285	Novel RU486 (mifepristone) analogues with increased activity against Venezuelan Equine Encephalitis Virus but reduced progesterone receptor antagonistic activity. Scientific Reports, 2019, 9, 2634.	1.6	13
286	Global computational mutagenesis of domain structures associated with inherited eye disease. Scientific Reports, 2019, 9, 3676.	1.6	5
287	Loss of DPP6 in neurodegenerative dementia: a genetic player in the dysfunction of neuronal excitability. Acta Neuropathologica, 2019, 137, 901-918.	3.9	37
288	Anticancer evaluation of ruthenium(III) complexes with N-donor ligands tethered to coumarin or uracil moieties. Inorganica Chimica Acta, 2019, 492, 98-107.	1.2	17
289	In Silico Analysis of the Subtype Selective Blockage of KCNA Ion Channels through the Âμ-Conotoxins PIIIA, SIIIA, and GIIIA. Marine Drugs, 2019, 17, 180.	2.2	8
290	Biological 3D Structural Databases. , 2019, , 47-73.		2
291	The extra virgin olive oil phenolic oleacein is a dual substrate-inhibitor of catechol-O-methyltransferase. Food and Chemical Toxicology, 2019, 128, 35-45.	1.8	27
292	ADS-J1 disaggregates semen-derived amyloid fibrils. Biochemical Journal, 2019, 476, 1021-1035.	1.7	14
293	Fourfold Filtered Statistical/Computational Approach for the Identification of Imidazole Compounds as HO-1 Inhibitors from Natural Products. Marine Drugs, 2019, 17, 113.	2.2	22
294	Computational and spectroscopic analysis of interaction between food colorant citrus red 2 and human serum albumin. Scientific Reports, 2019, 9, 1615.	1.6	13
295	Selection of a fully human single domain antibody specific to Helicobacter pylori urease. Applied Microbiology and Biotechnology, 2019, 103, 3407-3420.	1.7	19
296	A Glycoengineered Interferon-Î² Mutein (R27T) Generates Prolonged Signaling by an Altered Receptor-Binding Kinetics. Frontiers in Pharmacology, 2018, 9, 1568.	1.6	6
297	Synthesis of Rosmarinic Acid Amides as Antioxidative and Hypoglycemic Agents. Journal of Natural Products, 2019, 82, 573-582.	1.5	23
298	Non steroidal anti-inflammatory drug (NSAIDs) in breast cancer chemotherapy; antimony(V) salicylate a DNA binder. Inorganica Chimica Acta, 2019, 489, 39-47.	1.2	25

#	Article	IF	Citations
299	A Homozygous RAG1 Gene Mutation in a Case of Combined Immunodeficiency: Clinical, Molecular, and Computational Analysis. Human Heredity, 2019, 84, 272-278.	0.4	0
300	Molecular Modelling and Dynamics Study of nsSNP in STXBP1 Gene in Early Infantile Epileptic Encephalopathy Disease. BioMed Research International, 2019, 2019, 1-14.	0.9	8
301	Designing an improved T-cell mobilising CXCL10 mutant through enhanced GAG binding affinity. Protein Engineering, Design and Selection, 2019, 32, 367-373.	1.0	2
302	The THE ROLE OF ASTAXANTHIN COMPARED WITH METFORMIN IN PREVENTING GLYCATED HUMAN SERUM ALBUMIN FROM POSSIBLE UNFOLDING: A MOLECULAR DYNAMIC STUDY. Asian Journal of Pharmaceutical and Clinical Research, 0, , 276-282.	0.3	10
303	Measuring glycolytic flux in single yeast cells with an orthogonal synthetic biosensor. Molecular Systems Biology, 2019, 15, e9071.	3.2	34
304	Structural insights into heme binding to IL-36Î± proinflammatory cytokine. Scientific Reports, 2019, 9, 16893.	1.6	29
305	Rigorous Computational and Experimental Investigations on MDM2/MDMX-Targeted Linear and Macrocyclic Peptides. Molecules, 2019, 24, 4586.	1.7	4
306	The Plasma Factor XIII Heterotetrameric Complex Structure: Unexpected Unequal Pairing within a Symmetric Complex. Biomolecules, 2019, 9, 765.	1.8	13
307	A common mechanism allows selective targeting of GluN2B subunit-containing N-methyl-D-aspartate receptors. Communications Biology, 2019, 2, 420.	2.0	24
308	Computational Tools in the Discovery of FABP4 Ligands: A Statistical and Molecular Modeling Approach. Marine Drugs, 2019, 17, 624.	2.2	20
309	Highly thermostable carboxylic acid reductases generated by ancestral sequence reconstruction. Communications Biology, 2019, 2, 429.	2.0	34
310	Computational Analysis of nsSNPs of ADA Gene in Severe Combined Immunodeficiency Using Molecular Modeling and Dynamics Simulation. Journal of Immunology Research, 2019, 2019, 1-14.	0.9	11
311	Insight into the dimer dissociation process of the Chromobacterium violaceum (S)-selective amine transaminase. Scientific Reports, 2019, 9, 16946.	1.6	8
312	Prediction and Structural Comparison of Deleterious Coding Nonsynonymous Single Nucleotide Polymorphisms (nsSNPs) in Human LEP Gene Associated with Obesity. BioMed Research International, 2019, 2019, 1-10.	0.9	10
313	The Potential Synergistic Modulation of AMPK by Lippia citriodora Compounds as a Target in Metabolic Disorders. Nutrients, 2019, 11, 2961.	1.7	16
314	Metyrapone-Î²-cyclodextrin supramolecular interactions inferred by complementary spectroscopic/spectrometric and computational studies. Journal of Molecular Structure, 2019, 1176, 815-824.	1.8	13
315	Identification of Effective Dimeric Gramicidin-D Peptide as Antimicrobial Therapeutics over Drug Resistance: In-Silico Approach. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 575-583.	2.2	3
316	Molecular dynamics simulations of the chemokine CCL2 in complex with pull down-derived heparan sulfate hexasaccharides. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 528-533.	1.1	5

#	Article	IF	Citations
317	Biocatalytic Production of Amino Carbohydrates through Oxidoreductase and Transaminase Cascades. ChemSusChem, 2019, 12, 848-857.	3.6	32
318	Basal cell carcinomas developing independently from BAP1â€tumor predisposition syndrome in a patient with bilateral uveal melanoma. Genes Chromosomes and Cancer, 2019, 58, 357-364.	1.5	7
319	Chitosan-based magnetic adsorbent for removal of water-soluble anionic dye: Artificial neural network modeling and molecular docking insights. International Journal of Biological Macromolecules, 2019, 123, 587-599.	3.6	39
320	Gemcitabine anticancer activity enhancement by water soluble celecoxib/sulfobutyl ether-Î²-cyclodextrin inclusion complex. Carbohydrate Polymers, 2019, 206, 792-800.	5.1	37
321	Bichromophoric pyrazoline derivative with solvent-selective photoluminescence quenching. Journal of Molecular Liquids, 2019, 278, 156-163.	2.3	11
322	Structural Insights into the Dual-Substrate Recognition and Catalytic Mechanisms of a Bifunctional Acetyl Esterâ€“Xyloside Hydrolase from Caldicellulosiruptor lactoaceticus. ACS Catalysis, 2019, 9, 1739-1747.	5.5	6
323	â€˜Dusty core diseaseâ€™ (DuCD): expanding morphological spectrum of RYR1 recessive myopathies. Acta Neuropathologica Communications, 2019, 7, 3.	2.4	31
324	Molecular docking of anti-inflammatory drug diclofenac with metabolic targets: Potential applications in cancer therapeutics. Journal of Theoretical Biology, 2019, 465, 117-125.	0.8	21
325	B â€factor Guided Proline Substitutions in Chromobacterium violaceum Amine Transaminase: Evaluation of the Proline Rule as a Method for Enzyme Stabilization. ChemBioChem, 2019, 20, 1297-1304.	1.3	22
326	Specific Inhibition of Heparanase by a Glycopolymer with Well-Defined Sulfation Pattern Prevents Breast Cancer Metastasis in Mice. ACS Applied Materials & Interfaces, 2019, 11, 244-254.	4.0	46
327	Bioinformatics and enzymatics investigation of Trametes laccase for optical biosensing application. Journal of Materials Science, 2019, 54, 4970-4983.	1.7	10
328	In silico identification and evaluation of potential interaction of Azadirachta indica phytochemicals with Plasmodium falciparum heat shock protein 90. Journal of Molecular Graphics and Modelling, 2019, 87, 144-164.	1.3	14
329	Investigation of structural stability and functionality of homodimeric gramicidin towards peptideâ€based drug: a molecular simulation approach. Journal of Cellular Biochemistry, 2019, 120, 4903-4911.	1.2	13
330	Synthesis, structure, computational modeling, and biological activity of two novel bimesitylene derivatives. Research on Chemical Intermediates, 2019, 45, 453-469.	1.3	5
331	Comparative study of stability and transport of molecules through cyclic peptide nanotube and aquaporin: a molecular dynamics simulation approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 186-199.	2.0	16
332	20(S)-protopanaxadiol promotes the migration, proliferation, and differentiation of neural stem cells by targeting GSK-3Î² in the Wnt/GSK-3Î²/Î²-catenin pathway. Journal of Ginseng Research, 2020, 44, 475-482.	3.0	12
333	Halogenated derivatives of methotrexate as human dihydrofolate reductase inhibitors in cancer chemotherapy. Journal of Biomolecular Structure and Dynamics, 2020, 38, 901-917.	2.0	12
334	Molecular modelling and dynamics of CA2 missense mutations causative to carbonic anhydrase 2 deficiency syndrome. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4067-4080.	2.0	20

#	Article	IF	Citations
335	Molecular dynamics simulation exploration of the interaction between curcumin and myosin combined with the results of spectroscopy techniques. Food Hydrocolloids, 2020, 101, 105455.	5.6	103
336	Identification of deleterious missense variants of human Piwi like RNA-mediated gene silencing 1 gene and their impact on PAZ domain structure, stability, flexibility and dimension: in silico analysis. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4600-4606.	2.0	8
337	Evolutionary conservation and structural localizations suggest a physical trace of metabolismâ€™s progressive geochronological emergence. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3700-3719.	2.0	3
338	Computer-Aided Saturation Mutagenesis of Arabidopsis thaliana Ent-Copalyl Diphosphate Synthase. Interdisciplinary Sciences, Computational Life Sciences, 2020, 12, 32-43.	2.2	8
339	Baltic Fucus vesiculosus as potential bio-sorbent for Zn removal: Mechanism insight. Chemosphere, 2020, 238, 124652.	4.2	12
340	In Silico Analysis of New Potent Anti-hyperglycemic Molecule for Diabetes Type 2 Management. International Journal of Peptide Research and Therapeutics, 2020, 26, 1031-1042.	0.9	0
341	Possible dual contribution of a novel GUCY2D mutation in the development of retinal degeneration in a consanguineous population. European Journal of Medical Genetics, 2020, 63, 103750.	0.7	0
342	Designing Antiviral Substances Targeting the Ebola Virus Viral Protein 24. , 2020, , 147-177.		1
343	Thermostability enhancement of the Pseudomonas fluorescens esterase I by in vivo folding selection in Thermus thermophilus. Biotechnology and Bioengineering, 2020, 117, 30-38.	1.7	8
344	VGLUT substrates and inhibitors: A computational viewpoint. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183175.	1.4	4
345	The Protein Imager: a full-featured online molecular viewer interface with server-side HQ-rendering capabilities. Bioinformatics, 2020, 36, 2909-2911.	1.8	133
346	An Atomistic Understanding of Allosteric Inhibition of Glutamate Racemase: a Dampening of Native Activation Dynamics. ChemMedChem, 2020, 15, 376-384.	1.6	4
347	Structureâ€“Activity Relationship in Pyrazolo[4,3-c]pyridines, First Inhibitors of PEX14â€“PEX5 Proteinâ€“Protein Interaction with Trypanocidal Activity. Journal of Medicinal Chemistry, 2020, 63, 847-879.	2.9	13
348	Comparative Structural Analysis of Different Mycobacteriophage-Derived Mycolylarabinogalactan Esterases (Lysin B). Biomolecules, 2020, 10, 45.	1.8	2
349	A piperic acid CoA ligase produces a putative precursor of piperine, the pungent principle from black pepper fruits. Plant Journal, 2020, 102, 569-581.	2.8	16
350	Discovery of salicyl benzoate UDPâ€glycosyltransferase, a central enzyme in poplar salicinoid phenolic glycoside biosynthesis. Plant Journal, 2020, 102, 99-115.	2.8	31
351	Characterization of arginine preventive effect on heat-induced aggregation of insulin. International Journal of Biological Macromolecules, 2020, 145, 1039-1048.	3.6	16
352	Development of Novel Oxotriazinoindole Inhibitors of Aldose Reductase: Isosteric Sulfur/Oxygen Replacement in the Thioxotriazinoindole Cemtirestat Markedly Improved Inhibition Selectivity. Journal of Medicinal Chemistry, 2020, 63, 369-381.	2.9	20

#	Article	IF	Citations
353	Virtual Screening to Identify Novel Inhibitors of Pan ERBB Family of Proteins from Natural Products with Known Anti-tumorigenic Properties. International Journal of Peptide Research and Therapeutics, 2020, 26, 1923-1938.	0.9	6
354	Ligand-based virtual screening, consensus molecular docking, multi-target analysis and comprehensive ADMET profiling and MD stimulation to find out noteworthy tyrosine kinase inhibitor with better efficacy and accuracy. Advances in Traditional Medicine, 2020, 20, 645-661.	1.0	5
355	Identification of the phospholipid binding regions of the envelope E protein of flaviviruses by molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5136-5147.	2.0	6
356	PEGylation of a glycosaminoglycan-binding, dominant-negative CXCL8 mutant retains bioactivity in vitro and in vivo. Cytokine, 2020, 127, 154942.	1.4	3
357	Repurposing of FDAâ€Approved Drugs for Treating Iatrogenic Botulism: A Paired 3Dâ€QSAR/Docking Approach^{â€}. ChemMedChem, 2020, 15, 256-262.	1.6	20
358	Fluorescent aptasensor based on G-quadruplex-assisted structural transformation for the detection of biomarker lipocalin 1. Biosensors and Bioelectronics, 2020, 169, 112607.	5.3	15
359	Forming nanoconjugates or inducing macroaggregates, curcumin dose effect on myosin assembling revealed by molecular dynamics simulation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2020, 607, 125415.	2.3	16
360	Targeting the aryl hydrocarbon receptor with a novel set of triarylmethanes. European Journal of Medicinal Chemistry, 2020, 207, 112777.	2.6	9
361	Herbicides That Target Acetohydroxyacid Synthase Are Potent Inhibitors of the Growth of Drug-Resistant Candida auris. ACS Infectious Diseases, 2020, 6, 2901-2912.	1.8	13
362	Sequence analysis and spatiotemporal developmental distribution of the Cat-1-type transporter slc7a1a in zebrafish (Danio rerio). Fish Physiology and Biochemistry, 2020, 46, 2281-2298.	0.9	1
363	Raw nuclear magnetic resonance data of human linker histone H1x, lacking the C-terminal domain (NGH1x), and trajectory data of nanosecond molecular dynamics simulations of GH1x- and NGH1x-chromatosomes. Data in Brief, 2020, 31, 105865.	0.5	0
364	Current advances on the development of BET inhibitors: insights from computational methods. Advances in Protein Chemistry and Structural Biology, 2020, 122, 127-180.	1.0	5
365	Natural bioactive compounds as a new source of promising G protein-coupled estrogen receptor (GPER) modulators: comprehensive in silico approach. Journal of Biomolecular Structure and Dynamics, 2020, , 1-12.	2.0	6
366	The Influence of Calcium toward Order/Disorder Conformation of Repeat-in-Toxin (RTX) Structure of Family I.3 Lipase from Pseudomonas fluorescens AMS8. Toxins, 2020, 12, 579.	1.5	3
367	10-N-heterocylic aryl-isoxazole-amides (AIMs) have robust anti-tumor activity against breast and brain cancer cell lines and useful fluorescence properties. Bioorganic and Medicinal Chemistry, 2020, 28, 115781.	1.4	7
368	Genetic polymorphism of Plasmodium falciparum circumsporozoite protein on Bioko Island, Equatorial Guinea and global comparative analysis. Malaria Journal, 2020, 19, 245.	0.8	6
369	Expanding the clinical and neuroimaging features of NKX6-2-related hereditary spastic ataxia type 8. European Journal of Medical Genetics, 2020, 63, 103868.	0.7	5
370	Top-Down Characterization of Denatured Proteins and Native Protein Complexes Using Electron Capture Dissociation Implemented within a Modified Ion Mobility-Mass Spectrometer. Analytical Chemistry, 2020, 92, 3674-3681.	3.2	35

#	Article	IF	Citations
371	Insights Into the Mechanism of MCT8 Oligomerization. Journal of the Endocrine Society, 2020, 4, bvaa080.	0.1	2
372	Probing Vulnerability of the gp41 C-Terminal Heptad Repeat as Target for Miniprotein HIV Inhibitors. Journal of Molecular Biology, 2020, 432, 5577-5592.	2.0	7
373	Study on the Influence of Chirality in the Threading of Calix[6]arene Hosts with Dialkylammonium Axles. Molecules, 2020, 25, 5323.	1.7	2
374	Assessing the Thiamine Diphosphate Dependent Pyruvate Dehydrogenase E1 Subunit for Carboligation Reactions with Aliphatic Ketoacids. International Journal of Molecular Sciences, 2020, 21, 8641.	1.8	6
375	Asymmetric Synthesis of Optically Pure Aliphatic Amines with an Engineered Robust Ï‰-Transaminase. Catalysts, 2020, 10, 1310.	1.6	10
376	Roles, Characteristics, and Analysis of Intrinsically Disordered Proteins: A Minireview. Life, 2020, 10, 320.	1.1	11
377	Synthesis and Glycosidase Inhibition Properties of Calix[8]arene-Based Iminosugar Click Clusters. Pharmaceuticals, 2020, 13, 366.	1.7	8
378	Effect of Mutations on mRNA and Globin Stability: The Cases of Hb Bernalda/Groene Hart and Hb Southern Italy. Genes, 2020, 11, 870.	1.0	4
379	A Flavone-Based Solvatochromic Probe with A Low Expected Perturbation Impact on the Membrane Physical State. Molecules, 2020, 25, 3458.	1.7	5
380	Molecular Basis for Ser/Thr Specificity in PKA Signaling. Cells, 2020, 9, 1548.	1.8	3
381	The maturase HydF enables [FeFe] hydrogenase assembly via transient, cofactor-dependent interactions. Journal of Biological Chemistry, 2020, 295, 11891-11901.	1.6	10
382	First Evidence of Acyl-Hydrolase/Lipase Activity From Human Probiotic Bacteria: Lactobacillus rhamnosus GG and Bifidobacterium longum NCC 2705. Frontiers in Microbiology, 2020, 11, 1534.	1.5	13
383	Squalamine and Aminosterol Mimics Inhibit the Peptidoglycan Glycosyltransferase Activity of PBP1b. Antibiotics, 2020, 9, 373.	1.5	8
384	RORÎ³ Structural Plasticity and Druggability. International Journal of Molecular Sciences, 2020, 21, 5329.	1.8	17
385	Quercetin metabolites from Hibiscus sabdariffa contribute to alleviate glucolipotoxicity-induced metabolic stress in vitro. Food and Chemical Toxicology, 2020, 144, 111606.	1.8	11
386	Relationship between activity and stability: Design and characterization of stable variants of human frataxin. Archives of Biochemistry and Biophysics, 2020, 691, 108491.	1.4	9
387	Ecdysteroid Derivatives that Reverse P-Glycoprotein-Mediated Drug Resistance. Journal of Natural Products, 2020, 83, 2434-2446.	1.5	14
388	Computational screening of natural and natural-like compounds to identify novel ligands for sigma-2 receptor. SAR and QSAR in Environmental Research, 2020, 31, 837-856.	1.0	5

#	Article	IF	Citations
389	(4-Oxo-2-thioxothiazolidin-3-yl)acetic acids as potent and selective aldose reductase inhibitors. Chemico-Biological Interactions, 2020, 332, 109286.	1.7	12
390	Molecular dynamics simulation of carbonyl reductase 1 clarifies the structural switch in drug metabolism. Journal of Taibah University for Science, 2020, 14, 1326-1334.	1.1	0
391	GDP-altrose as novel product of GDP-mannose 3,5-epimerase: Revisiting its reaction mechanism. International Journal of Biological Macromolecules, 2020, 165, 1862-1868.	3.6	5
392	The use of C1 symmetry imidazole-carboxylate building block and auxiliary acetate co-ligand for assembly of a 2D wave-like zinc(II) coordination polymer: experimental and theoretical study. Journal of Coordination Chemistry, 2020, 73, 2250-2264.	0.8	5
393	Inhibition of Acetylcholinesterases by Stereoisomeric Organophosphorus Compounds Containing Both Thioester andp-Nitrophenyl Leaving Groups. Chemical Research in Toxicology, 2020, 33, 2455-2466.	1.7	2
394	Targeting COVID-19 (SARS-CoV-2) main protease through active phytochemicals of ayurvedic medicinal plants â€“ Withania somnifera (Ashwagandha), Tinospora cordifolia (Giloy) and Ocimum sanctum (Tulsi) â€“ a molecular docking study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 190-203.	2.0	181
395	Similar but Not Identicalâ€”Binding Properties of LSU (Response to Low Sulfur) Proteins From Arabidopsis thaliana. Frontiers in Plant Science, 2020, 11, 1246.	1.7	15
396	Prediction of the Impact of Deleterious Nonsynonymous Single Nucleotide Polymorphisms on the Human RRM2B Gene: A Molecular Modeling Study. BioMed Research International, 2020, 2020, 1-10.	0.9	7
397	New Anti SARS-Cov-2 Targets for Quinoline Derivatives Chloroquine and Hydroxychloroquine. International Journal of Molecular Sciences, 2020, 21, 5856.	1.8	25
398	Differential Effects of IGF-1R Small Molecule Tyrosine Kinase Inhibitors BMS-754807 and OSI-906 on Human Cancer Cell Lines. Cancers, 2020, 12, 3717.	1.7	21
399	An Integrated Pharmacophore/Docking/3D-QSAR Approach to Screening a Large Library of Products in Search of Future Botulinum Neurotoxin A Inhibitors. International Journal of Molecular Sciences, 2020, 21, 9470.	1.8	20
400	Synthesis of two new lipid mediators from docosahexaenoic acid by combinatorial catalysis involving enzymatic and chemical reaction. Scientific Reports, 2020, 10, 18849.	1.6	7
401	Repurposing FDA Approved Drugs as JNK3 Inhibitor for Prevention of Neuroinflammation Induced by MCAO in Rats. Journal of Inflammation Research, 2020, Volume 13, 1185-1205.	1.6	24
402	Epidemiology, evolutionary origin, and malariaâ€induced positive selection effects of G6PDâ€deficient alleles in Chinese populations. Molecular Genetics & Genomic Medicine, 2020, 8, e1540.	0.6	9
403	The physicochemical properties role of a functionalized alkyl-peptide in nanofibre formation and neural progenitor cells viability and survival. Polymer Testing, 2020, 91, 106829.	2.3	0
404	Detailed epitope mapping of neutralizing anti-drug antibodies against recombinant Î±-galactosidase A in patients with Fabry disease. Molecular Genetics and Metabolism, 2020, 131, 229-234.	0.5	6
405	New Multifunctional Agents Based on Conjugates of 4-Amino-2,3-polymethylenequinoline and Butylated Hydroxytoluene for Alzheimerâ€™s Disease Treatment. Molecules, 2020, 25, 5891.	1.7	28
406	When a foreign gene meets its native counterpart: computational biophysics analysis of two PgiC loci in the grass Festuca ovina. Scientific Reports, 2020, 10, 18752.	1.6	0

#	Article	IF	Citations
407	Study of the Interaction of a Novel Semi-Synthetic Peptide with Model Lipid Membranes. Membranes, 2020, 10, 294.	1.4	9
408	Naturally-Occurring Rare Mutations Cause Mild to Catastrophic Effects in the Multifunctional and Cancer-Associated NQO1 Protein. Journal of Personalized Medicine, 2020, 10, 207.	1.1	8
409	A Highly Conserved Iron-Sulfur Cluster Assembly Machinery between Humans and Amoeba Dictyostelium discoideum: The Characterization of Frataxin. International Journal of Molecular Sciences, 2020, 21, 6821.	1.8	3
410	The TRIOBP Isoforms and Their Distinct Roles in Actin Stabilization, Deafness, Mental Illness, and Cancer. Molecules, 2020, 25, 4967.	1.7	13
411	A Multibasic Cleavage Site in the Spike Protein of SARS-CoV-2 Is Essential for Infection of Human Lung Cells. Molecular Cell, 2020, 78, 779-784.e5.	4.5	1,527
412	The ancillary N-terminal region of the yeast AP-1 transcription factor Yap8 contributes to its DNA binding specificity. Nucleic Acids Research, 2020, 48, 5426-5441.	6.5	7
413	Improvement of enzymatic performance of Asclepias curassavica L. proteases by immobilization. Application to the synthesis of an antihypertensive peptide. Process Biochemistry, 2020, 95, 36-46.	1.8	2
414	Investigating the role of endogenous opioid system in chloroquineâ€induced phospholipidosis in rat liver by morphological, biochemical and molecular modelling studies. Clinical and Experimental Pharmacology and Physiology, 2020, 47, 1575-1583.	0.9	1
415	Novel Indole-Based Hydrazones as Potent Inhibitors of the Î±-class Carbonic Anhydrase from Pathogenic Bacterium Vibrio cholerae. International Journal of Molecular Sciences, 2020, 21, 3131.	1.8	3
416	Potential Drugs Targeting Early Innate Immune Evasion of SARS-Coronavirus 2 via 2â€™-O-Methylation of Viral RNA. Viruses, 2020, 12, 525.	1.5	75
417	Î²-N-Acetylhexosaminidases for Carbohydrate Synthesis via Trans-Glycosylation. Catalysts, 2020, 10, 365.	1.6	19
418	Selective Enzymatic Release and Gel Formation by Cross-Linking of Feruloylated Glucurono-Arabinoxylan from Corn Bran. ACS Sustainable Chemistry and Engineering, 2020, 8, 8164-8174.	3.2	17
419	Crystal Structure and Active Site Engineering of a Halophilic Î³-Carbonic Anhydrase. Frontiers in Microbiology, 2020, 11, 742.	1.5	16
420	Reversal of Regioselectivity in Zincâ€Dependent Mediumâ€Chain Alcohol Dehydrogenase fromRhodococcus erythropolistoward Octanone Derivatives. ChemBioChem, 2020, 21, 2957-2965.	1.3	6
421	Discovery of 2-aryl and 2-pyridinylbenzothiazoles endowed with antimicrobial and aryl hydrocarbon receptor agonistic activities. European Journal of Pharmaceutical Sciences, 2020, 151, 105386.	1.9	6
422	Amantadine copper(II) chloride conjugate with possible implementation in influenza virus inhibition. Polyhedron, 2020, 185, 114590.	1.0	20
423	Mutational Effects on Carbapenem Hydrolysis of YEM-1, a New Subclass B2 Metallo-Î²-Lactamase from Yersinia mollaretii. Antimicrobial Agents and Chemotherapy, 2020, 64, .	1.4	5
424	Solubility of 5-aminosalicylic acid in N-methyl-2-pyrrolidone + water mixtures at various temperatures. Journal of Molecular Liquids, 2020, 310, 113143.	2.3	32

#	Article	IF	Citations
425	A Sequence Homology and Bioinformatic Approach Can Predict Candidate Targets for Immune Responses to SARS-CoV-2. Cell Host and Microbe, 2020, 27, 671-680.e2.	5.1	893
426	Deletion and Randomization of Structurally Variable Regions in B. subtilis Lipase A (BSLA) Alter Its Stability and Hydrolytic Performance Against Long Chain Fatty Acid Esters. International Journal of Molecular Sciences, 2020, 21, 1990.	1.8	6
427	Polymer assisted ultrafiltration of AO7 anionic dye from aqueous solutions: Experimental design, multivariate optimization, and molecular docking insights. Journal of Membrane Science, 2020, 604, 118054.	4.1	12
428	Solubility of ketoconazole in 1,4-dioxaneÂ+Âwater mixtures at TÂ=Â(293.2 to 313.2) K. Journal of Molecular Liquids, 2020, 306, 112830.	2.3	7
429	Characterization of the inhibition mechanism of a tissuefactor inhibiting single-chain variable fragment: a combined computational approach. Journal of Molecular Modeling, 2020, 26, 87.	0.8	0
430	Rare genetic variants in interleukin-37 link this anti-inflammatory cytokine to the pathogenesis and treatment of gout. Annals of the Rheumatic Diseases, 2020, 79, 536-544.	0.5	44
431	Molecular Dynamics Analysis of a Rationally Designed Aldehyde Dehydrogenase Gives Insights into Improved Activity for the Non-Native Cofactor NAD⁺. ACS Synthetic Biology, 2020, 9, 920-929.	1.9	13
432	Modulating Heparanase Activity: Tuning Sulfation Pattern and Glycosidic Linkage of Oligosaccharides. Journal of Medicinal Chemistry, 2020, 63, 4227-4255.	2.9	10
433	Phenolic Compounds from Morus nigra Regulate Viability and Apoptosis of Pancreatic Î²-Cells Possibly via SERCA Activity. ACS Medicinal Chemistry Letters, 2020, 11, 1006-1013.	1.3	5
434	Boron Effect on Sugarâ€Based Organogelators. Chemistry - A European Journal, 2020, 26, 13927-13934.	1.7	8
435	In Vivo Performance of Innovative Polyelectrolyte Matrices for Hot Melt Extrusion of Amorphous Drug Systems. Molecular Pharmaceutics, 2020, 17, 3053-3061.	2.3	4
436	In silico tools to study molecular targets of neglected diseases: inhibition of TcSir2rp3, an epigenetic enzyme of Trypanosoma cruzi. Advances in Protein Chemistry and Structural Biology, 2020, 122, 203-229.	1.0	10
437	Undefeatedâ€"Changing the phenamacril scaffold is not enough to beat resistant Fusarium. PLoS ONE, 2020, 15, e0235568.	1.1	1
438	Structure-based machine-guided mapping of amyloid sequence space reveals uncharted sequence clusters with higher solubilities. Nature Communications, 2020, 11, 3314.	5.8	54
440	Catalytically-active inclusion bodies for biotechnologyâ€"general concepts, optimization, and application. Applied Microbiology and Biotechnology, 2020, 104, 7313-7329.	1.7	46
441	Molecular basis of the beta-lactamase protein using comparative modelling, drug screening and molecular dynamics studies to understand the resistance of Î²-lactam antibiotics. Journal of Molecular Modeling, 2020, 26, 200.	0.8	1
442	Application of real sample analysis and biosensing: Synthesis of new naphthyl derived chemosensor for detection of Al3+ ions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 241, 118684.	2.0	37
443	Production of rebaudioside D from stevioside using a UGTSL2 Asn358Phe mutant in a multiâ€enzyme system. Microbial Biotechnology, 2020, 13, 974-983.	2.0	28

#	Article	IF	Citations
444	Probing remote residues important for catalysis in Escherichia coli ornithine transcarbamoylase. PLoS ONE, 2020, 15, e0228487.	1.1	4
445	Identification and characterization of a novel variant in C-terminal region of Antithrombin (Ala427Thr) associated with type II AT deficiency leading to polymer formation. Journal of Thrombosis and Thrombolysis, 2020, 50, 678-685.	1.0	3
446	A specific amino acid context in EGFR and HER2 phosphorylation sites enables selective binding to the active site of Src homology phosphatase 2 (SHP2). Journal of Biological Chemistry, 2020, 295, 3563-3575.	1.6	16
447	Directed evolution of VanR biosensor specificity in yeast. Biotechnology Notes, 2020, 1, 9-15.	0.7	17
448	Metronidazole and Secnidazole Carbamates: Synthesis, Antiprotozoal Activity, and Molecular Dynamics Studies. Molecules, 2020, 25, 793.	1.7	12
449	Effects of the deglycosylation on the structure and activity of chloroperoxidase: Molecular dynamics simulation approach. Journal of Molecular Graphics and Modelling, 2020, 97, 107570.	1.3	3
450	Solubility of 5-aminosalicylic acid in {N-methyl-2-pyrrolidoneÂ+Âethanol} mixtures at TÂ=Â(293.2 to 313.2) K. Journal of Molecular Liquids, 2020, 306, 112774.	2.3	8
451	Molecular Simulation Elaborating the Mechanism of 1Î²-Hydroxy Alantolactone Inhibiting Ubiquitin-Conjugating Enzyme UbcH5s. Scientific Reports, 2020, 10, 141.	1.6	11
452	Engineering of Laccase CueO for Improved Electron Transfer in Bioelectrocatalysis by Semiâ€Rational Design. Chemistry - A European Journal, 2020, 26, 4974-4979.	1.7	11
453	Robust Ï‰-Transaminases by Computational Stabilization of the Subunit Interface. ACS Catalysis, 2020, 10, 2915-2928.	5.5	52
454	Characterization and diversity of the complete set of GH family 3 enzymes from Rhodothermus marinus DSM 4253. Scientific Reports, 2020, 10, 1329.	1.6	9
455	Structural Changes of Sarco/Endoplasmic Reticulum Ca2+-ATPase Induced by Rutin Arachidonate: A Molecular Dynamics Study. Biomolecules, 2020, 10, 214.	1.8	3
456	Putative Inhibitors of SARS-CoV-2 Main Protease from A Library of Marine Natural Products: A Virtual Screening and Molecular Modeling Study. Marine Drugs, 2020, 18, 225.	2.2	237
457	Engineered P450 BM3 and cpADH5 coupled cascade reaction for Î²-oxo fatty acid methyl ester production in whole cells. Enzyme and Microbial Technology, 2020, 138, 109555.	1.6	8
458	Ranking Plasticizers for Polymers with Atomistic Simulations: PVT, Mechanical Properties, and the Role of Hydrogen Bonding in Thermoplastic Starch. ACS Applied Polymer Materials, 2020, 2, 2016-2026.	2.0	29
459	A Potent Host Defense Peptide Triggers DNA Damage and Is Active against Multidrug-Resistant Gram-Negative Pathogens. ACS Infectious Diseases, 2020, 6, 1250-1263.	1.8	13
460	Loop engineering of aryl sulfotransferase B for improving catalytic performance in regioselective sulfation. Catalysis Science and Technology, 2020, 10, 2369-2377.	2.1	6
461	Multifunctional Acidocin 4356 Combats Pseudomonas aeruginosa through Membrane Perturbation and Virulence Attenuation: Experimental Results Confirm Molecular Dynamics Simulation. Applied and Environmental Microbiology, 2020, 86, .	1.4	5

#	Article	IF	Citations
462	In silico molecular docking analysis of cancer biomarkers with GC/MS identified compounds of Scytonema sp.. Network Modeling Analysis in Health Informatics and Bioinformatics, 2020, 9, 1.	1.2	1
463	Defective Sec61Î±1 underlies a novel cause of autosomal dominant severe congenital neutropenia. Journal of Allergy and Clinical Immunology, 2020, 146, 1180-1193.	1.5	32
464	Development of Thiazolidinones as Fungal Carbonic Anhydrase Inhibitors. International Journal of Molecular Sciences, 2020, 21, 2960.	1.8	15
465	Characterization of a novel pathogenic variation c.1237T>G in the FZD4 gene presenting new inheritance from an Iranian individual suffering vitreoretinopathy. Intractable and Rare Diseases Research, 2020, 9, 48-53.	0.3	1
466	Noncompetitive tightâ€binding inhibition of Anticarsia gemmatalis trypsins by Adenanthera pavonina protease inhibitor affects larvae survival. Archives of Insect Biochemistry and Physiology, 2020, 104, e21687.	0.6	10
467	High-affinity binding and catalytic activity of His/Tyr-based sequences: Extending heme-regulatory motifs beyond CP. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129603.	1.1	20
468	Interaction of cobalt and iron hydroperoxo bleomycin with deoxyribonucleic acid (DNA): Dynamic vs. electronic structure considerations. Inorganica Chimica Acta, 2020, 509, 119682.	1.2	4
469	Structure and Molecular Recognition Mechanism of IMP-13 Metallo-Î²-Lactamase. Antimicrobial Agents and Chemotherapy, 2020, 64, .	1.4	8
470	A molecular dynamics investigation on transporting mechanism of glucose through a cyclic peptide nanotube. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2230-2241.	2.0	3
471	Structural and functional characterization of chitin binding lectin from Datura stramonium: insights from phylogenetic analysis, protein structure prediction, molecular docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1698-1716.	2.0	4
472	Molecular Insights and Functional Consequences of the Interaction of Heme with Activated Protein C. Antioxidants and Redox Signaling, 2021, 34, 32-48.	2.5	14
473	Complex Evolution of Light-Dependent Protochlorophyllide Oxidoreductases in Aerobic Anoxygenic Phototrophs: Origin, Phylogeny, and Function. Molecular Biology and Evolution, 2021, 38, 819-837.	3.5	6
474	Towards Photochromic Azobenzeneâ€Based Inhibitors for Tryptophan Synthase. Chemistry - A European Journal, 2021, 27, 2439-2451.	1.7	11
475	MPM motifs of the yeast SKT protein Trk1 can assemble to form a functional K+-translocation system. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183513.	1.4	5
476	Engineering DNA-Templated Nonribosomal Peptide Synthesis. Cell Chemical Biology, 2021, 28, 221-227.e7.	2.5	23
477	Synergistic Computational Modeling Approaches as Team Players in the Game of Solubility Predictions. Journal of Pharmaceutical Sciences, 2021, 110, 22-34.	1.6	13
478	Reprogramming the Specificity of a Protein Interface by Computational and Data-Driven Design. Structure, 2021, 29, 292-304.e3.	1.6	2
479	The virus that shook the world: questions and answers about SARS-CoV-2 and COVID-19. Biotechnology and Biotechnological Equipment, 2021, 35, 74-102.	0.5	13

#	Article	IF	Citations
480	Dehydroquinate dehydratase/shikimate dehydrogenases involved in gallate biosynthesis of the aluminum-tolerant tree species Eucalyptus camaldulensis. Planta, 2021, 253, 3.	1.6	17
481	Stabilizing AqdC, a Pseudomonas Quinolone Signalâ€Cleaving Dioxygenase from Mycobacteria, by FRESCOâ€Based Protein Engineering. ChemBioChem, 2021, 22, 733-742.	1.3	7
482	Structural Insights into the Interaction of Heme with Protein Tyrosine Kinase JAK2**. ChemBioChem, 2021, 22, 861-864.	1.3	5
483	Interhelical interactions within the STIM1 CC1 domain modulate CRAC channel activation. Nature Chemical Biology, 2021, 17, 196-204.	3.9	22
484	ChemVA: Interactive Visual Analysis of Chemical Compound Similarity in Virtual Screening. IEEE Transactions on Visualization and Computer Graphics, 2021, 27, 891-901.	2.9	6
485	Unravelling the molecular effect of ocellatin-1, F1, K1 and S1, the frog-skin antimicrobial peptides to enhance its therapeuticsâ€"quantum and molecular mechanical approaches. Journal of Molecular Modeling, 2021, 27, 10.	0.8	3
486	A capsaicinoid-based soft drug, AG1529, for attenuating TRPV1-mediated histaminergic and inflammatory sensory neuron excitability. Scientific Reports, 2021, 11, 246.	1.6	16
487	Modeling and simulation in medical sciences: an overview of specific applications based on research experience in EMRI (Endocrinology and Metabolism Research Institute of Tehran University of Medical) Tj ETQq1 1 0.784314 rgBT /Ov	0.8	0
488	Monte-Carlo method-based QSAR model to discover phytochemical urease inhibitors using SMILES and GRAPH descriptors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5090-5099.	2.0	11
489	LAHMA: structure analysis through local annotation of homology-matched amino acids. Acta Crystallographica Section D: Structural Biology, 2021, 77, 28-40.	1.1	5
490	Improving the binding affinity and interaction of 5-Pentyl-2-Phenoxyphenol against Mycobacterium Enoyl ACP reductase by computational approach. Informatics in Medicine Unlocked, 2021, 23, 100528.	1.9	8
491	Molecular Dynamics Simulations and in silico Analysis of Supramolecular Self-assembled Structures. , 2021, , 357-371.		0
492	Identification of Amino Acid Residues in Human IgM Fc Receptor (FcÂµR) Critical for IgM Binding. Frontiers in Immunology, 2020, 11, 618327.	2.2	11
493	Engineering of Biological Pathways: Complex Formation and Signal Transduction. Methods in Molecular Biology, 2021, 2315, 59-70.	0.4	2
494	In Silico Study of Polyunsaturated Fatty Acids as Potential SARS-CoV-2 Spike Protein Closed Conformation Stabilizers: Epidemiological and Computational Approaches. Molecules, 2021, 26, 711.	1.7	37
495	Enyzmes | Lipoprotein Lipase. , 2021, , 307-320.		0
496	Understanding substrate binding and the role of gatekeeping residues in PigC access tunnels. Chemical Communications, 2021, 57, 2681-2684.	2.2	10
497	Structure-guided evolution of a ketoreductase for efficient and stereoselective bioreduction of bulky Î±-amino Î²-keto esters. Catalysis Science and Technology, 2021, 11, 6755-6769.	2.1	8

#	Article	IF	Citations
498	Teaching Multidimensional Heteronuclear NMR Analysis to Undergraduate Students. ACS Symposium Series, 2021, , 239-251.	0.5	0
499	Possible host-adaptation of SARS-CoV-2 due to improved ACE2 receptor binding in mink. Virus Evolution, 2021, 7, veaa094.	2.2	50
500	KnowVolution of prodigiosin ligase PigC towards condensation of short-chain prodiginines. Catalysis Science and Technology, 2021, 11, 2805-2815.	2.1	9
501	Microwave-assisted xylanase reaction: impact in the production of prebiotic xylooligosaccharides. RSC Advances, 2021, 11, 11882-11888.	1.7	6
502	Dynamics of Anthracene Excimer Formation within a Water-Soluble Nanocavity at Room Temperature. Journal of the American Chemical Society, 2021, 143, 2025-2036.	6.6	33
503	From thiol-subtilisin to omniligase: Design and structure of a broadly applicable peptide ligase. Computational and Structural Biotechnology Journal, 2021, 19, 1277-1287.	1.9	11
504	High affinity promoter binding of STOP1 is essential for early expression of novel aluminum-induced resistance genes GDH1 and GDH2 in Arabidopsis. Journal of Experimental Botany, 2021, 72, 2769-2789.	2.4	28
505	Reaction mechanism of the farnesyl pyrophosphate C-methyltransferase towards the biosynthesis of pre-sodorifen pyrophosphate byÂSerratia plymuthicaÂ4Rx13. Scientific Reports, 2021, 11, 3182.	1.6	9
506	d-Amino acid substituted peptides as potential alternatives of homochiral l-configurations. Amino Acids, 2021, 53, 265-280.	1.2	5
508	CA10 regulates neurexin heparan sulfate addition via a direct binding in the secretory pathway. EMBO Reports, 2021, 22, e51349.	2.0	7
510	Bis (Diamines) Cu and Zn Complexes of Flurbiprofen as Potential Cholinesterase Inhibitors: In Vitro Studies and Docking Simulations. Crystals, 2021, 11, 208.	1.0	2
511	Proteolytic enzymes in the salivary glands of the Neotropical brown stink bugEuschistus heros: Reduced activities in imidaclopridâ€resistant strains. Annals of Applied Biology, 2021, 179, 85-95.	1.3	4
512	Biocatalytic Aromaticity-Breaking Epoxidation of Naphthalene and Nucleophilic Ring-Opening Reactions. ACS Catalysis, 2021, 11, 2644-2649.	5.5	14
513	Heterologous Expression and Characterization of Plant Lipase LIP2 from Elaeis guineensis Jacq. Oil Palm Mesocarp in Escherichia coli. Catalysts, 2021, 11, 244.	1.6	2
514	Revisiting the interaction of heme with hemopexin. Biological Chemistry, 2021, 402, 675-691.	1.2	13
515	Site-Specific O-Glycosylation Analysis of SARS-CoV-2 Spike Protein Produced in Insect and Human Cells. Viruses, 2021, 13, 551.	1.5	57
516	Homology modeling and global computational mutagenesis of human myosin VIIa. Journal of Analytical & Pharmaceutical Research, 2021, 10, 41-48.	0.3	2
517	Genetic diversity and natural selection on the thrombospondin-related adhesive protein (TRAP) gene of Plasmodium falciparum on Bioko Island, Equatorial Guinea and global comparative analysis. Malaria Journal, 2021, 20, 124.	0.8	1

#	Article	IF	Citations
518	Dual inhibition of SARS-CoV-2 and human rhinovirus with protease inhibitors in clinical development. Antiviral Research, 2021, 187, 105020.	1.9	37
519	ADP-dependent glucose/glucosamine kinase from Thermococcus kodakarensis: cloning and characterization. International Journal of Biological Macromolecules, 2021, 173, 168-179.	3.6	6
520	ERRÎ³ ligand HPB2 upregulates BDNF-TrkB and enhances dopaminergic neuronal phenotype. Pharmacological Research, 2021, 165, 105423.	3.1	12
521	Steroid disulfates - Sulfation double trouble. Molecular and Cellular Endocrinology, 2021, 524, 111161.	1.6	9
522	Synthesis of benzaldehyde-grafted polysilane: A highly stable and selective â€œturn-onâ€•fluorescent sensor for cytosine. Journal of Molecular Liquids, 2021, 326, 115300.	2.3	3
523	DFT and molecular dynamics studies of astaxanthin-metal ions (Cu2+ and Zn2+) complex to prevent glycated human serum albumin from possible unfolding. Heliyon, 2021, 7, e06548.	1.4	7
524	Combined docking methods and molecular dynamics to identify effective antiviral 2, 5-diaminobenzophenonederivatives against SARS-CoV-2. Journal of King Saud University - Science, 2021, 33, 101352.	1.6	30
525	The Dose-Dependent Pleiotropic Effects of the UBB+1 Ubiquitin Mutant. Frontiers in Molecular Biosciences, 2021, 8, 650730.	1.6	2
526	MAPRE2 mutations result in altered human cranial neural crest migration, underlying craniofacial malformations in CSC-KT syndrome. Scientific Reports, 2021, 11, 4976.	1.6	10
527	Molecular docking and density functional theory studies of potent 1,3-disubstituted-9H-pyrido[3,4-b]indoles antifilarial compounds. Structural Chemistry, 2021, 32, 1925-1947.	1.0	4
528	Efficacy of Phytochemicals Derived from Avicennia officinalis for the Management of COVID-19: A Combined In Silico and Biochemical Study. Molecules, 2021, 26, 2210.	1.7	68
529	Synthesis, Enzymatic Degradation, and Polymer-Miscibility Evaluation of Nonionic Antimicrobial Hyperbranched Polyesters with Indole or Isatin Functionalities. Biomacromolecules, 2021, 22, 2256-2271.	2.6	8
530	Secondary <scp>CoQ₁₀</scp> deficiency, bioenergetics unbalance in disease and aging. BioFactors, 2021, 47, 551-569.	2.6	19
531	Discovery of a Novel Acetylcholinesterase Inhibitor by Fragment-Based Design and Virtual Screening. Molecules, 2021, 26, 2058.	1.7	9
532	Non-canonical substrates for terpene synthases in bacteria are synthesized by a new family of methyltransferases. FEMS Microbiology Reviews, 2021, 45, .	3.9	3
533	Poly(Ethylene Glycol)/Î²-Cyclodextrin Pseudorotaxane Complexes as Sustainable Dispersing and Retarding Materials in a Cement-Based Mortar. ACS Omega, 2021, 6, 12250-12260.	1.6	5
534	High Throughput Virtual Screening and Molecular Dynamics Simulation for Identifying a Putative Inhibitor of Bacterial CTX-M-15. Antibiotics, 2021, 10, 474.	1.5	10
535	Modeled 3D-Structures of Proteobacterial Transglycosylases from Glycoside Hydrolase Family 17 Give Insight in Ligand Interactions Explaining Differences in Transglycosylation Products. Applied Sciences (Switzerland), 2021, 11, 4048.	1.3	3

#	Article	IF	Citations
536	Drug Development for Target Ribosomal Protein rpL35/uL29 for Repair of LAMB3R635X in Rare Skin Disease Epidermolysis Bullosa. Skin Pharmacology and Physiology, 2021, 34, 167-182.	1.1	8
537	Computationally-guided exchange of substrate selectivity motifs in a modular polyketide synthase acyltransferase. Nature Communications, 2021, 12, 2193.	5.8	20
538	Two Novel, Flavin-Dependent Halogenases from the Bacterial Consortia of Botryococcus braunii Catalyze Mono- and Dibromination. Catalysts, 2021, 11, 485.	1.6	5
539	Tailor-made recombinant prokaryotic lectins for characterisation of glycoproteins. Analytica Chimica Acta, 2021, 1155, 338352.	2.6	12
540	Molecular Docking and Dynamics Simulation of a Screening Library from Life Chemicals Database for Potential Protein-Protein Interactions (PPIs) Inhibitors against SARS-CoV-2 Spike Protein. Journal of Pharmaceutical Research International, 0, , 74-84.	1.0	3
541	Identification of Kaurane-Type Diterpenes as Inhibitors of Leishmania Pteridine Reductase I. Molecules, 2021, 26, 3076.	1.7	11
542	Addition of hydrophobic side chains improve the apoptosis inducibility of the human glyoxalase I inhibitor, TLSC702. Bioorganic and Medicinal Chemistry Letters, 2021, 40, 127918.	1.0	3
543	Laboratory Variants GES G170L , GES G170K , and GES G170H Increase Carbapenem Hydrolysis and Confer Resistance to Clavulanic Acid. Antimicrobial Agents and Chemotherapy, 2021, 65, .	1.4	1
544	CACNA1A Mutations Causing Early Onset Ataxia: Profiling Clinical, Dysmorphic and Structural-Functional Findings. International Journal of Molecular Sciences, 2021, 22, 5180.	1.8	5
546	Analysis of natural compounds against the activity of SARS-CoV-2 NSP15 protein towards an effective treatment against COVID-19: a theoretical and computational biology approach. Journal of Molecular Modeling, 2021, 27, 160.	0.8	10
547	Cryo-EM structure of the mature and infective Mayaro virus at 4.4â€‰Ã… resolution reveals features of arthritogenic alphaviruses. Nature Communications, 2021, 12, 3038.	5.8	28
548	In silico virtual screening of lead compounds for major antigenic sites in respiratory syncytial virus fusion protein. Emergent Materials, 2022, 5, 295-305.	3.2	4
549	Analysis of electrostatic coupling throughout the laboratory evolution of a designed retroaldolase. Protein Science, 2021, 30, 1617-1627.	3.1	5
550	PAD4 takes charge during neutrophil activation: Impact of PAD4 mediated NET formation on immuneâ€mediated disease. Journal of Thrombosis and Haemostasis, 2021, 19, 1607-1617.	1.9	63
551	Synthesis of novel oligomeric anionic alkyl glycosides using laccase/TEMPO oxidation and cyclodextrin glucanotransferase (CGTase)â€catalyzed transglycosylation. Biotechnology and Bioengineering, 2021, 118, 2548-2558.	1.7	6
552	Discovery of Novel eEF2K Inhibitors Using HTS Fingerprint Generated from Predicted Profiling of Compound-Protein Interactions. Medicines (Basel, Switzerland), 2021, 8, 23.	0.7	1
553	Effects of Curcumin and Ferulic Acid on the Folding of Amyloid-Î² Peptide. Molecules, 2021, 26, 2815.	1.7	10
554	Quinoline-sulfamoyl carbamates/sulfamide derivatives: Synthesis, cytotoxicity, carbonic anhydrase activity, and molecular modelling studies. Bioorganic Chemistry, 2021, 110, 104778.	2.0	6

#	Article	IF	Citations
556	Factors Controlling Persistent Needle Crystal Growth: The Importance of Dominant One-Dimensional Secondary Bonding, Stacked Structures, and van der Waals Contact. Crystal Growth and Design, 2021, 21, 3449-3460.	1.4	21
557	Autocitrullination of PAD4 does not alter its enzymatic activity: In vitro and in silico studies. International Journal of Biochemistry and Cell Biology, 2021, 134, 105938.	1.2	8
558	Global spectrum of populationâ€specific common missense variation in cytochrome P450 pharmacogenes. Human Mutation, 2021, 42, 1107-1123.	1.1	1
559	An insect acetylcholinesterase biosensor utilizing WO3/g-C3N4 nanocomposite modified pencil graphite electrode for phosmet detection in stored grains. Food Chemistry, 2021, 346, 128894.	4.2	56
560	The importance of hydrophobic interactions in the structure of transcription systems. European Biophysics Journal, 2021, 50, 951-961.	1.2	5
561	Arginine methylation of METTL14 promotes RNA N6-methyladenosine modification and endoderm differentiation of mouse embryonic stem cells. Nature Communications, 2021, 12, 3780.	5.8	34
562	Simulations of the Upper Critical Solution Temperature Behavior of Poly(ornithine-co-citrulline)s Using MARTINI-Based Coarse-Grained Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 4499-4511.	2.3	2
564	Structural and functional analyses of a novel manganese-catalase from Bacillus subtilis R5. International Journal of Biological Macromolecules, 2021, 180, 222-233.	3.6	8
565	Novel xylan degrading enzymes from polysaccharide utilizing loci of Prevotella copri DSM18205. Glycobiology, 2021, 31, 1330-1349.	1.3	9
567	ptFVa (Pseudonaja Textilis Venom-Derived Factor Va) Retains Structural Integrity Following Proteolysis by Activated Protein C. Arteriosclerosis, Thrombosis, and Vascular Biology, 2021, 41, 2263-2276.	1.1	0
568	Characterization of Temperature-Dependent Kinetics of Oculocutaneous Albinism-Causing Mutants of Tyrosinase. International Journal of Molecular Sciences, 2021, 22, 7771.	1.8	4
569	Mechanistic insights into the three steps of poly(ADP-ribosylation) reversal. Nature Communications, 2021, 12, 4581.	5.8	34
570	How hydrophilic group affects drugâ€"protein binding modes: Differences in interaction between sirtuins inhibitors Tenovin-1/Tenovin-6 and human serum albumin. Journal of Pharmaceutical and Biomedical Analysis, 2021, 201, 114121.	1.4	4
571	Reconstruction of the Fas-Based Death-Inducing Signaling Complex (DISC) Using a Proteinâ€"Protein Docking Meta-Approach. Journal of Chemical Information and Modeling, 2021, 61, 3543-3558.	2.5	8
572	Inherited Variants in SCARB1 Cause Severe Early-Onset Coronary Artery Disease. Circulation Research, 2021, 129, 296-307.	2.0	12
573	In silico Study of Potential Non-oxime Reactivator for Sarin-inhibited Human Acetylcholinesterase. Pertanika Journal of Science and Technology, 2021, 29, .	0.3	0
574	Computational Insights into the Deleterious Impacts of Missense Variants on N-Acetyl-d-glucosamine Kinase Structure and Function. International Journal of Molecular Sciences, 2021, 22, 8048.	1.8	6
575	An Integrated Clinical-Biological Approach to Identify Interindividual Variability and Atypical Phenotype-Genotype Correlations in Myopathies: Experience on A Cohort of 156 Families. Genes, 2021, 12, 1199.	1.0	8

#	Article	IF	Citations
576	Motions around conserved helical weak spots facilitate <scp>GPCR</scp> activation. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1577-1586.	1.5	2
577	Hydrophobic Residues Confer the Helicity and Membrane Permeability of Ocellatin-1 Antimicrobial Peptide Scaffold Towards Therapeutics. International Journal of Peptide Research and Therapeutics, 2021, 27, 2459-2470.	0.9	4
578	Computational Screening of FDA Approved Drugs from ZINC Database for Potential Inhibitors of Zika Virus NS2B/NS3 Protease: A Molecular Docking and Dynamics Simulation Study. Journal of Pharmaceutical Research International, 0, , 308-319.	1.0	1
579	Metformin Is a Pyridoxal-5â€²-phosphate (PLP)-Competitive Inhibitor of SHMT2. Cancers, 2021, 13, 4009.	1.7	15
580	Functional Classification of Super-Large Families of Enzymes Based on Substrate Binding Pocket Residues for Biocatalysis and Enzyme Engineering Applications. Frontiers in Bioengineering and Biotechnology, 2021, 9, 701120.	2.0	5
581	Sequence-specific dynamics of DNA response elements and their flanking sites regulate the recognition by AP-1 transcription factors. Nucleic Acids Research, 2021, 49, 9280-9293.	6.5	21
582	Dolutegravir Inhibition of Matrix Metalloproteinases Affects Mouse Neurodevelopment. Molecular Neurobiology, 2021, 58, 5703-5721.	1.9	12
583	Structural determinants and distribution of phosphate specificity in ribonucleotide reductases. Journal of Biological Chemistry, 2021, 297, 101008.	1.6	4
585	Probing the Increased Virulence of Severe Acute Respiratory Syndrome Coronavirus 2 B.1.617 (Indian) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.2	3
586	Interaction between Curcumin and Î²-Casein: Multi-Spectroscopic and Molecular Dynamics Simulation Methods. Molecules, 2021, 26, 5092.	1.7	10
587	In silico screening of Pueraria tuberosa (PTY-2) for targeting COVID-19 by countering dual targets Mpro and TMPRSS2. Journal of Biomolecular Structure and Dynamics, 2021, , 1-14.	2.0	2
588	Interactome analysis of Bag-1 isoforms reveals novel interaction partners in endoplasmic reticulum-associated degradation. PLoS ONE, 2021, 16, e0256640.	1.1	3
589	Biased Coupling to Î²-Arrestin of Two Common Variants of the CB2 Cannabinoid Receptor. Frontiers in Endocrinology, 2021, 12, 714561.	1.5	10
591	Formation of the Metal-Binding Core of the ZRT/IRT-like Protein (ZIP) Family Zinc Transporter. Biochemistry, 2021, 60, 2727-2738.	1.2	8
592	Effectiveness of Natural Antioxidants against SARS-CoV-2? Insights from the In-Silico World. Antibiotics, 2021, 10, 1011.	1.5	41
593	Adamantane-derived scaffolds targeting the sigma-2 receptor; an in vitro and in silico study. Saudi Pharmaceutical Journal, 2021, 29, 1166-1172.	1.2	2
594	Synthesis, in silico, and in vivo anti-inflammatory evaluation of 3Î²-cinnamoyloxy substituted pregna-4,16-diene-6,20-diones derivatives. Journal of Biomolecular Structure and Dynamics, 2021, , 1-10.	2.0	0
595	Discovery of Novel Acetamide-Based Heme Oxygenase-1 Inhibitors with Potent In Vitro Antiproliferative Activity. Journal of Medicinal Chemistry, 2021, 64, 13373-13393.	2.9	14

#	Article	IF	Citations
598	Involvement of CYP347W1 in neurotoxin 3â€•nitropropionic acidâ€•based chemical defense in mustard leaf beetle Phaedon cochleariae. Insect Science, 2021, , .	1.5	0
599	Population genetic analysis of the Plasmodium falciparum erythrocyte binding antigen-175 (EBA-175) gene in Equatorial Guinea. Malaria Journal, 2021, 20, 374.	0.8	2
600	A supernumerary â€œB-sexâ€•chromosome drives male sex determination in the PachÃ³n cavefish, Astyanax mexicanus. Current Biology, 2021, 31, 4800-4809.e9.	1.8	34
601	Copper(II) salicylideneimine complexes revisited: From a novel derivative and extended characterization of two homologues to interaction with BSA and antiproliferative activity. Inorganica Chimica Acta, 2021, 525, 120460.	1.2	5
602	Current views on N-glycolylneuraminic acid in therapeutic recombinant proteins. Trends in Pharmacological Sciences, 2021, 42, 943-956.	4.0	5
603	Modulation of the Activity and Regioselectivity of a Glycosidase: Development of a Convenient Tool for the Synthesis of Specific Disaccharides. Molecules, 2021, 26, 5445.	1.7	0
604	Chirality Transfer in a Calixarene-Based Directional Pseudorotaxane Complex. Chemistry, 2021, 3, 1089-1100.	0.9	2
605	Assembly of Biomolecular Gigastructures and Visualization with the Vulkan Graphics API. Journal of Chemical Information and Modeling, 2021, 61, 5293-5303.	2.5	17
606	Nano-assembly and optical properties of difluoroboron dibenzoylmethane-polysilane. Polymer, 2021, 232, 124188.	1.8	5
607	Synthesis of Îł-l-Araf and Î²-d-Galf series furanobiosides using mutants of a GH51 Îł-l-arabinofuranosidase. Bioorganic Chemistry, 2021, 116, 105245.	2.0	2
608	Revisiting the CooJ family, a potential chaperone for nickel delivery to [NiFe]â€‘carbon monoxide dehydrogenase. Journal of Inorganic Biochemistry, 2021, 225, 111588.	1.5	1
609	Structure-function relationship of extremozymes. , 2022, , 9-30.		2
610	Inhibition of the Vesicular Glutamate Transporter (VGLUT) with Congo Red Analogs: New Binding Insights. Neurochemical Research, 2021, 46, 494-503.	1.6	2
611	Could Dermaseptin Analogue be a Competitive Inhibitor for ACE2 Towards Binding with Viral Spike Protein Causing COVID19?: Computational Investigation. International Journal of Peptide Research and Therapeutics, 2021, 27, 1043-1056.	0.9	8
612	5-[Aryloxypyridyl (or nitrophenyl)]-4H-1,2,4-triazoles as novel flexible benzodiazepine analogues: Synthesis, receptor binding affinity and lipophilicity-dependent anti-seizure onset of action. Bioorganic Chemistry, 2021, 106, 104504.	2.0	8
613	Pseudo-Dipeptide Bearing Îł,Îł-Difluoromethyl Ketone Moiety as Electrophilic Warhead with Activity against Coronaviruses. International Journal of Molecular Sciences, 2021, 22, 1398.	1.8	25
614	Solvatochromic and pH-Sensitive Fluorescent Membrane Probes for Imaging of Live Cells. ACS Chemical Neuroscience, 2021, 12, 719-734.	1.7	5
615	Solution X-Ray Scattering for Membrane Proteins. Methods in Molecular Biology, 2020, 2168, 177-197.	0.4	4

#	Article	IF	Citations
616	Distinct 3-disulfide-bonded isomers of tridegin differentially inhibit coagulation factor XIIIa: The influence of structural stability on bioactivity. European Journal of Medicinal Chemistry, 2020, 201, 112474.	2.6	4
617	Predicting selectivity of paracellular pores for biomimetic applications. Molecular Systems Design and Engineering, 2020, 5, 686-696.	1.7	7
618	Visualizing protein structures â€" tools and trends. Biochemical Society Transactions, 2020, 48, 499-506.	1.6	16
619	Engineering CGTase to improve synthesis of alkyl glycosides. Glycobiology, 2021, 31, 603-612.	1.3	7
620	Vaccinia virus-free rescue of fluorescent replication-defective vesicular stomatitis virus and pseudotyping with Puumala virus glycoproteins for use in neutralization tests. Journal of General Virology, 2016, 97, 1052-1059.	1.3	18
621	Mapping of human B-cell epitopes of Sindbis virus. Journal of General Virology, 2016, 97, 2243-2254.	1.3	2
628	Assessment of the interaction between the fluxâ€signaling metabolite fructoseâ€1,6â€bisphosphate and the bacterial transcription factors CggR and Cra. Molecular Microbiology, 2018, 109, 278-290.	1.2	24
629	Conservancy of mAb Epitopes in Ebolavirus Glycoproteins of Previous and 2014 Outbreaks. PLOS Currents, 2014, 6, .	1.4	14
630	Molecular Dynamics of "Fuzzy" Transcriptional Activator-Coactivator Interactions. PLoS Computational Biology, 2016, 12, e1004935.	1.5	13
631	The Effect of a Novel c.820C>T (Arg274Trp) Mutation in the Mitofusin 2 Gene on Fibroblast Metabolism and Clinical Manifestation in a Patient. PLoS ONE, 2017, 12, e0169999.	1.1	13
632	Crystal Structure and Catalytic Mechanism of CouO, a Versatile C-Methyltransferase from Streptomyces rishiriensis. PLoS ONE, 2017, 12, e0171056.	1.1	16
633	Novel compound heterozygous MYO7A mutations in Moroccan families with autosomal recessive non-syndromic hearing loss. PLoS ONE, 2017, 12, e0176516.	1.1	8
634	A novel FLNC frameshift and an OBSCN variant in a family with distal muscular dystrophy. PLoS ONE, 2017, 12, e0186642.	1.1	29
635	Autonomous aggregation suppression by acidic residues explains why chaperones favour basic residues. EMBO Journal, 2020, 39, e102864.	3.5	33
636	Resveratrol targets PD-L1 glycosylation and dimerization to enhance antitumor T-cell immunity. Aging, 2020, 12, 8-34.	1.4	99
637	The LSD1 inhibitor iadademstat (ORY-1001) targets SOX2-driven breast cancer stem cells: a potential epigenetic therapy in luminal-B and HER2-positive breast cancer subtypes. Aging, 2020, 12, 4794-4814.	1.4	38
638	Requirement of novel amino acid fragments of orphan nuclear receptor TR3/Nur77 for its functions in angiogenesis. Oncotarget, 2015, 6, 24261-24276.	0.8	6
639	In vitro and in silico Activity of Iridoids Against Leishmania amazonensis. Current Drug Discovery Technologies, 2019, 16, 173-183.	0.6	6

#	Article	IF	Citations
640	A Systematic Review on Popularity, Application and Characteristics of Protein Secondary Structure Prediction Tools. Current Drug Discovery Technologies, 2019, 16, 159-172.	0.6	9
641	Virtual Screening, Docking, Synthesis and Bioactivity Evaluation of Thiazolidinediones as Potential PPARÎ³ Partial Agonists for Preparation of Antidiabetic Agents. Letters in Drug Design and Discovery, 2019, 16, 608-617.	0.4	3
643	Early transmission patterns of coronavirus disease 2019 (COVID-19) in travellers from Wuhan to Thailand, January 2020. Eurosurveillance, 2020, 25, .	3.9	109
644	In Silico Analysis of Ethanol Binding Activity in Neuronal Nicotinic Acetylcholine Receptors. Malaysian Journal of Applied Sciences, 2020, 5, 54-61.	0.2	1
645	Molecular docking analysis of candidate compounds derived from medicinal plants with type 2 diabetes mellitus targets. Bioinformation, 2019, 15, 179-188.	0.2	17
646	Molecular docking and dynamics simulation of FDA approved drugs with the main protease from 2019 novel coronavirus. Bioinformation, 2020, 16, 236-244.	0.2	61
647	Viral factors in influenza pandemic risk assessment. ELife, 2016, 5, .	2.8	82
648	Refining the reaction mechanism of O₂towards its co-substrate in cofactor-free dioxygenases. PeerJ, 2016, 4, e2805.	0.9	18
649	Lid opening and conformational stability of T1 Lipase is mediated by increasing chain length polar solvents. PeerJ, 2017, 5, e3341.	0.9	20
650	Dynamic tracing of sugar metabolism reveals the mechanisms of action of synthetic sugar analogs. Glycobiology, 2022, 32, 239-250.	1.3	15
651	Multivalent resorcinarene clusters decorated with DAB-1 inhitopes: targeting Golgi Î±-mannosidase from Drosophila melanogaster. Organic Chemistry Frontiers, 2021, 8, 6648-6656.	2.3	3
652	Analysis of SARS-CoV-2 Genomes from West Java, Indonesia. Viruses, 2021, 13, 2097.	1.5	15
653	mRNA Analysis of Frameshift Mutations with Stop Codon in the Last Exon: The Case of Hemoglobins Campania [Î±1 cod95 (â^'C)] and Sciacca [Î±1 cod109 (â^'C)]. Biomedicines, 2021, 9, 1390.	1.4	5
654	Two fungal flavonoid-specific glucosidases/rutinosidases for rutin hydrolysis and rutinoside synthesis under homogeneous and heterogeneous reaction conditions. AMB Express, 2021, 11, 136.	1.4	5
655	Computational Prediction of Ï‰-Transaminase Specificity by a Combination of Docking and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 5569-5580.	2.5	17
656	Norfloxacin Loaded Lipid Polymer Hybrid Nanoparticles for Oral Administration: Fabrication, Characterization, In Silico Modelling and Toxicity Evaluation. Pharmaceutics, 2021, 13, 1632.	2.0	7
657	Identifying the Most Potent Dual-Targeting Compound(s) against 3CLprotease and NSP15exonuclease of SARS-CoV-2 from Nigella sativa: Virtual Screening via Physicochemical Properties, Docking and Dynamic Simulation Analysis. Processes, 2021, 9, 1814.	1.3	9
658	Molecular simulation unravels the amyloidogenic misfolding of nascent ApoA1 protein, driven by deleterious point mutations occurring in between 170â€“178 hotspot region. Journal of Biomolecular Structure and Dynamics, 2021, , 1-13.	2.0	2

#	Article	IF	Citations
659	Removal of Dyes by Polymer-Enhanced Ultrafiltration: An Overview. Polymers, 2021, 13, 3450.	2.0	16
660	Computer-Aided Design and Synthesis of a New Class of PEX14 Inhibitors: Substituted 2,3,4,5-Tetrahydrobenzo[F][1,4]oxazepines as Potential New Trypanocidal Agents. Journal of Chemical Information and Modeling, 2021, 61, 5256-5268.	2.5	1
661	ERK5 signalling pathway is a novel target of sorafenib: Implication in EGF biology. Journal of Cellular and Molecular Medicine, 2021, 25, 10591-10603.	1.6	7
662	Conformational selection of vasopressin upon V1a receptor binding. Computational and Structural Biotechnology Journal, 2021, 19, 5826-5833.	1.9	7
663	Role of aspartic acid residues D87 and D89 in APS kinase domain of human 3â€²-phosphoadenosine 5â€²-phosphosulfate synthase 1 and 2b: A commonality with phosphatases/kinases. Biochemistry and Biophysics Reports, 2021, 28, 101155.	0.7	0
664	Growing the molecular architecture of imidazole-like ligands in HO-1 complexes. Bioorganic Chemistry, 2021, 117, 105428.	2.0	7
665	Conformational flexibility of the conserved hydrophobic pocket of HIV-1 gp41. Implications for the discovery of small-molecule fusion inhibitors. International Journal of Biological Macromolecules, 2021, 192, 90-99.	3.6	4
669	Protein Docking and Drug Design. Advances in Bioinformatics and Biomedical Engineering Book Series, 2018, , 207-241.	0.2	0
673	Protein Docking and Drug Design. , 2019, , 889-922.		0
674	High-Performance Hybrid Computing for Bioinformatic Analysis of Protein Superfamilies. Communications in Computer and Information Science, 2019, , 249-264.	0.4	0
680	Deleterious amino acid substitutions with a series of putative damaging effects on egg components are revealed in the ovalbumin gene family; an in silico approach. Nova Biotechnologica Et Chimica, 2019, 18, 115-123.	0.1	0
682	Prediction of B-cell epitope by in silico analysis of Mycobacterium tuberculosis Ag85B antigen. Asia-Pacific Journal of Molecular Biology and Biotechnology, 0, , 101-109.	0.2	0
684	Synthesis and in vitro evaluation of chlorogenic acid amides as potential hypoglycemic agents and their synergistic effect with acarbose. Bioorganic Chemistry, 2021, 117, 105458.	2.0	11
685	Site-Specific Incorporation of Non-canonical Amino Acids by Amber Stop Codon Suppression in Escherichia coli. Springer Protocols, 2020, , 267-281.	0.1	0
686	Bioinformatics in Plant Pathology. , 2021, , 725-844.		0
687	Structural Studies of a Fungal Polyphenol Oxidase with Application to Bioremediation of Contaminated Water. Proceedings (mdpi), 2020, 66, .	0.2	1
690	Reconstruction and Visualization of Protein Structures by exploiting Bidirectional Neural Networks and Discrete Classes. , 2021, , .		2
692	Structural anomalies in a published NMR-derived structure of IRAK-M. Journal of Molecular Graphics and Modelling, 2022, 111, 108061.	1.3	1

#	Article	IF	Citations
693	Functional consequences of TCF4 missense substitutions associated with Pitt-Hopkins syndrome, mild intellectual disability, and schizophrenia. Journal of Biological Chemistry, 2021, 297, 101381.	1.6	10
695	Conformational stability, dynamics and function of human frataxin: Tryptophan side chain interplay. Archives of Biochemistry and Biophysics, 2022, 715, 109086.	1.4	3
696	Assessment of pesticide induced inhibition of Apis mellifera (honeybee) acetylcholinesterase by means of N-doped carbon dots/BSA nanocomposite modified electrochemical biosensor. Bioelectrochemistry, 2022, 144, 107999.	2.4	18
697	Identification of ligand binding sites in intrinsically disordered proteins with a differential binding score. Scientific Reports, 2021, 11, 22583.	1.6	4
698	Advanced Bioinformatics Tools in the Pharmacokinetic Profiles of Natural and Synthetic Compounds with Anti-Diabetic Activity. Biomolecules, 2021, 11, 1692.	1.8	11
700	In silicoscreening and covalent binding of phytochemicals ofOcimum sanctumagainst SARS-CoV-2 (COVID 19) main protease. Journal of Biomolecular Structure and Dynamics, 2023, 41, 435-444.	2.0	18
701	Identification, Characterization, and In Silico Analysis of New Imine Reductases From Native Streptomyces Genomes. Frontiers in Catalysis, 2021, 1, .	1.8	1
702	Albuminâ€“Hyaluronan Interactions: Influence of Ionic Composition Probed by Molecular Dynamics. International Journal of Molecular Sciences, 2021, 22, 12360.	1.8	12
703	Software to Visualize Proteins and Perform Structural Alignments. Current Protocols, 2021, 1, e292.	1.3	11
704	Evidence for Quantum Chemical Effects in Receptor-Ligand Binding Between Integrin and Collagen Fragments â€" A Computational Investigation With an Impact on Tissue Repair, Neurooncolgy and Glycobiology. Frontiers in Molecular Biosciences, 2021, 8, 756701.	1.6	2
705	Interactions of Urea-Based Inhibitors with Prostate-Specific Membrane Antigen for Boron Neutron Capture Therapy. ACS Omega, 2021, 6, 33354-33369.	1.6	2
706	The effects of molecular crowding and CpG hypermethylation on DNA G-quadruplexes formed by the C9orf72 nucleotide repeat expansion. Scientific Reports, 2021, 11, 23213.	1.6	5
707	Effect of Chitosan Deacetylation on Its Affinity to Type III Collagen: A Molecular Dynamics Study. Materials, 2022, 15, 463.	1.3	7
708	Decrypting a cryptic allosteric pocket in H. pylori glutamate racemase. Communications Chemistry, 2021, 4, .	2.0	4
709	Pseudomonas aeruginosa Biofilm Dispersion by the Human Atrial Natriuretic Peptide. Advanced Science, 2022, 9, e2103262.	5.6	20
710	Functional Analysis of Variants in Complement Factor I Identified in Age-Related Macular Degeneration and Atypical Hemolytic Uremic Syndrome. Frontiers in Immunology, 2021, 12, 789897.	2.2	9
711	Hydroxypropyl Cellulose for Drug Precipitation Inhibition: From the Potential of Molecular Interactions to Performance Considering Microrheology. Molecular Pharmaceutics, 2022, 19, 690-703.	2.3	6
712	Synthesis and in Silico Docking Studies of Ethyl 2â€(2â€Arylideneâ€1â€alkylhydrazinyl)thiazoleâ€4â€carboxylates as Antiglycating Agents. Chemistry and Biodiversity, 2022, 19, .	1.0	7

#	Article	IF	Citations
713	Symmetry of Post-Translational Modifications in a Human Enzyme. Symmetry, 2022, 14, 212.	1.1	0
714	p21-Activated Kinase 1 Promotes Breast Tumorigenesis via Phosphorylation and Activation of the Calcium/Calmodulin-Dependent Protein Kinase II. Frontiers in Cell and Developmental Biology, 2021, 9, 759259.	1.8	5
716	Hot Flows: Evolving an Archaeal Glucose Dehydrogenase for Ultrastable Carba-NADP⁺ Using Microfluidics at Elevated Temperatures. ACS Catalysis, 2022, 12, 1841-1846.	5.5	9
717	Humanâ€“Device Interaction in the Life Science Laboratory. Advances in Biochemical Engineering/Biotechnology, 2022, , 83-113.	0.6	3
718	In Silico and Experimental ADAM17 Kinetic Modeling as Basis for Future Screening System for Modulators. International Journal of Molecular Sciences, 2022, 23, 1368.	1.8	4
720	The Endo-Î±(1,4) Specific Fucoidanase Fhf2 From Formosa haliotis Releases Highly Sulfated Fucoidan Oligosaccharides. Frontiers in Plant Science, 2022, 13, 823668.	1.7	11
721	Versatility of subtilisin: A review on structure, characteristics, and applications. Biotechnology and Applied Biochemistry, 2022, 69, 2599-2616.	1.4	19
722	Study on the interactions between nicotine Î³-rezocine formic acid salt and pepsin: Multispectroscopy, molecular docking, and molecular dynamics simulation. Journal of Molecular Structure, 2022, 1254, 132414.	1.8	4
723	Envelope E protein of dengue virus and phospholipid binding to the late endosomal membrane. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183889.	1.4	9
724	Strigolactone Analogs: Two New Potential Bioactiphores for Glioblastoma. ACS Chemical Neuroscience, 2022, 13, 572-580.	1.7	4
725	Bis-Amiridines as Acetylcholinesterase and Butyrylcholinesterase Inhibitors: N-Functionalization Determines the Multitarget Anti-Alzheimerâ€™s Activity Profile. Molecules, 2022, 27, 1060.	1.7	10
727	An Engineered Cholesterol Oxidase Catalyses Enantioselective Oxidation of Nonâ€steroidal Secondary Alcohols. ChemBioChem, 2022, 23, .	1.3	5
728	Estrogenic Activity of Tetrazole Derivatives Bearing Bisphenol Structures: Computational Studies, Synthesis, and In Vitro Assessment. Journal of Chemical Information and Modeling, 2022, , .	2.5	1
729	Adaptive Recombinant Nanoworms from Genetically Encodable Star Amphiphiles. Biomacromolecules, 2022, 23, 863-876.	2.6	4
730	Computational Chemistry and Molecular Modelling Basics. Chemical Biology, 2017, , 1-38.	0.1	9
732	Presence of carbohydrate binding modules in extracellular region of class C G-protein coupled receptors (C GPCR): An investigation on sweet taste receptor. Journal of Biosciences, 2019, 44, .	0.5	2
733	Phage-Displayed Mimotopes of SARS-CoV-2 Spike Protein Targeted to Authentic and Alternative Cellular Receptors. Viruses, 2022, 14, 384.	1.5	10
735	Molecular modelling studies and identification of novel phytochemical inhibitor of DLL3. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3089-3109.	2.0	0

#	Article	IF	Citations
736	Stress-induced tyrosine phosphorylation of RtcB modulates IRE1 activity and signaling outputs. Life Science Alliance, 2022, 5, e202201379.	1.3	8
737	Synthesis, antiâ€TB activities, and molecular docking studies of 4â€(1,2,3â€triazoyl)arylmethanone derivatives. Journal of Biochemical and Molecular Toxicology, 2022, 36, e22998.	1.4	2
738	Unravelling the Biology of EhActo as the First Cofilin From Entamoeba histolytica. Frontiers in Cell and Developmental Biology, 2022, 10, 785680.	1.8	1
739	Targeting the HIV-1 Tat and Human Tat Protein Complex through Natural Products: An In Silico Docking and Molecular Dynamics Simulation Approach. Letters in Drug Design and Discovery, 2022, 19, 982-995.	0.4	3
740	Broad-spectrum in vitro activity of macrophage infectivity potentiator inhibitors against Gram-negative bacteria and Leishmania major. Journal of Antimicrobial Chemotherapy, 2022, 77, 1625-1634.	1.3	5
741	Functional Characterization of the Novel and Specific Thyroid Hormone Transporter SLC17A4. Thyroid, 2022, 32, 326-335.	2.4	5
742	Evolution of E. coli Phytase Toward Improved Hydrolysis of Inositol Tetraphosphate. Frontiers in Chemical Engineering, 2022, 4, .	1.3	5
743	Drug Discovery of Plausible Lead Natural Compounds That Target the Insulin Signaling Pathway: Bioinformatics Approaches. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-42.	0.5	6
744	Conformational Stabilization of Gp41-Mimetic Miniproteins Opens Up New Ways of Inhibiting HIV-1 Fusion. International Journal of Molecular Sciences, 2022, 23, 2794.	1.8	3
745	A Water Soluble 2-Phenyl-5-(pyridin-3-yl)-1,3,4-oxadiazole Based Probe: Antimicrobial Activity and Colorimetric/Fluorescence pH Response. Molecules, 2022, 27, 1824.	1.7	5
746	Structural modeling of human AKAP3 protein and in silico analysis of single nucleotide polymorphisms associated with sperm motility. Scientific Reports, 2022, 12, 3656.	1.6	3
747	Detection of a new deleterious SGCE gene variant in Moroccan family with inherited myoclonusâ€“dystonia. Clinical Case Reports (discontinued), 2022, 10, e05568.	0.2	1
748	NKX2-5 Variant in Two Siblings with Thyroid Hemiagenesis. International Journal of Molecular Sciences, 2022, 23, 3414.	1.8	0
749	Genetic heterogeneity in GJB2, COL4A3, ATP6V1B1 and EDNRB variants detected among hearing impaired families in Morocco. Molecular Biology Reports, 2022, 49, 3949-3954.	1.0	2
750	In Silico and In Vitro Evaluations of Fluorophoric Thiazolo-[2,3-b]quinazolinones as Anti-cancer Agents Targeting EGFR-TKD. Applied Biochemistry and Biotechnology, 2022, 194, 4292-4318.	1.4	13
752	CPR-C4 is a highly conserved novel protease from the Candidate Phyla Radiation with remote structural homology to human vasohibins. Journal of Biological Chemistry, 2022, 298, 101919.	1.6	2
753	Encapsulation of phenolics in Î²-lactoglobulin: Stability, antioxidant activity, and inhibition of advanced glycation end products. LWT - Food Science and Technology, 2022, 162, 113437.	2.5	9
754	Discovery of a new generation of angiotensin receptor blocking drugs: Receptor mechanisms and in silico binding to enzymes relevant to SARS-CoV-2. Computational and Structural Biotechnology Journal, 2022, 20, 2091-2111.	1.9	18

#	Article	IF	Citations
755	Molecular modeling, mutational analysis and steroid specificity of the ligand binding pocket of mPRÎ± (PAQR7): Shared ligand binding with AdipoR1 and its structural basis. Journal of Steroid Biochemistry and Molecular Biology, 2022, 219, 106082.	1.2	14
756	Machine learning assessment of the binding region as a tool for more efficient computational receptor-ligand docking. Journal of Molecular Liquids, 2022, 353, 118759.	2.3	4
757	Salt-dependent intermolecular interactions of hyaluronan molecules mediate the formation of temporary duplex structures. Carbohydrate Polymers, 2022, 286, 119288.	5.1	4
758	pyKVFinder: an efficient and integrable Python package for biomolecular cavity detection and characterization in data science. BMC Bioinformatics, 2021, 22, 607.	1.2	11
759	From Far West to East: Joining the Molecular Architecture of Imidazole-like Ligands in HO-1 Complexes. Pharmaceuticals, 2021, 14, 1289.	1.7	2
760	Screening and Functional Analysis of TEK Mutations in Chinese Children With Primary Congenital Glaucoma. Frontiers in Genetics, 2021, 12, 764509.	1.1	7
761	Identification of a glucose-insensitive variant of Gal2 from Saccharomyces cerevisiae exhibiting a high pentose transport capacity. Scientific Reports, 2021, 11, 24404.	1.6	6
762	Structure-Sweetness Relationship of Sweet Proteins: A Systematic Review on â€œSweet Proteinâ€•Studies as a Sub-Group of â€œSweetenerâ€•Investigations. Moscow University Biological Sciences Bulletin, 2021, 76, 175-190.	0.1	1
763	Molecular dynamics and structural analysis of the binding of <scp>COP1 E3</scp> ubiquitin ligase to Î²â€catenin and <scp>TRIB</scp> pseudokinases. Proteins: Structure, Function and Bioinformatics, 2022, 90, 993-1004.	1.5	3
764	Enhancing the Thermostability of Engineered Laccases in Aqueous Betaine-Based Natural Deep Eutectic Solvents. ACS Sustainable Chemistry and Engineering, 2022, 10, 572-581.	3.2	14
765	SSBP1-Disease Update: Expanding the Genetic and Clinical Spectrum, Reporting Variable Penetrance and Confirming Recessive Inheritance. , 2021, 62, 12.		4
766	2,3-Dihydroquinazolin-4(1H)-one as a New Class of Anti-Leishmanial Agents: A Combined Experimental and Computational Study. Crystals, 2022, 12, 44.	1.0	2
767	Production and analysis of titin kinase: Exploiting active/inactive kinase homologs in pseudokinase validation. Methods in Enzymology, 2022, 667, 147-181.	0.4	2
784	Evolutionary changes between pre- and post-vaccine South African group A G2P[4] rotavirus strains, 2003â€“2017. Microbial Genomics, 2022, 8, .	1.0	3
785	Molecular interaction of inhibitors with human brain butyrylcholinesterase.. EXCLI Journal, 2021, 20, 1597-1607.	0.5	4
786	A novel DPH5-related diphthamide-deficiency syndrome causing embryonic lethality or profound neurodevelopmental disorder. Genetics in Medicine, 2022, 24, 1567-1582.	1.1	5
787	Dromedary camel nanobodies broadly neutralize SARS-CoV-2 variants. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2201433119.	3.3	19
788	Drug repurposing for SARS-CoV-2: a high-throughput molecular docking, molecular dynamics, machine learning, and DFT study. Journal of Materials Science, 2022, , 1-23.	1.7	8

#	Article	IF	Citations
789	Structural analysis of TrkA mutations in patients with congenital insensitivity to pain reveals PLCÎ³ as an analgesic drug target. Science Signaling, 2022, 15, eabm6046.	1.6	3
790	Computational studies on potential new anti-Covid-19 agents with a multi-target mode of action. Journal of King Saud University - Science, 2022, 34, 102086.	1.6	11
791	The Ry_{sto} immune receptor recognises a broadly conserved feature of potyviral coat proteins. New Phytologist, 2022, 235, 1179-1195.	3.5	10
792	One-Pot Synthesis of Benzopyrano-Pyrimidine Derivatives Catalyzed by P-Toluene Sulphonic Acid and Their Nematicidal and Molecular Docking Study. Catalysts, 2022, 12, 531.	1.6	4
793	Structural dynamics of SARS-CoV-2 nucleocapsid protein induced by RNA binding. PLoS Computational Biology, 2022, 18, e1010121.	1.5	19
794	In-situ thickness control of centimetre-scale 2D-Like polydopamine films with large scalability. Materials Today Chemistry, 2022, 24, 100935.	1.7	9
795	Physicochemical properties and formation mechanism of whey protein isolate-sodium alginate complexes: Experimental and computational study. Food Hydrocolloids, 2022, 131, 107786.	5.6	22
798	Modeling and Molecular Dynamics of Aquaporin from an Antarctic Pseudomonas sp. Strain AMS3. Pertanika Journal of Science and Technology, 2022, 30, 1755-1770.	0.3	1
800	Thermodynamic analysis of amyloid fibril structures reveals a common framework for stability in amyloid polymorphs. Structure, 2022, 30, 1178-1189.e3.	1.6	11
802	Syndromic Hearing Loss in Moroccan families is associated to homozygous missense variants in COL4A3 and MASP1. , 2022, 33, 201053.		0
803	Exploring the molecular interaction of pheniramine with Enterococcus faecalis homoserine kinase: Inâ€silico studies. Journal of Molecular Recognition, 2022, 35, .	1.1	0
804	Novel Tyrosine Kinase Inhibitors to Target Chronic Myeloid Leukemia. Molecules, 2022, 27, 3220.	1.7	3
805	Functionalized Mesoporous Silica as Doxorubicin Carriers and Cytotoxicity Boosters. Nanomaterials, 2022, 12, 1823.	1.9	7
807	Ab initio derivation of flavin hyperfine interactions for the protein magnetosensor cryptochrome. Physical Chemistry Chemical Physics, 2022, 24, 16784-16798.	1.3	4
808	A novel construct of an electrochemical acetylcholinesterase biosensor for the investigation of malathion sensitivity to three different insect species using a NiCr₂O₄/g-C₃N₄ composite integrated pencil graphite electrode. RSC Advances, 2022, 12, 16860-16874.	1.7	3
809	Protein structural bioinformatics: An overview. Computers in Biology and Medicine, 2022, 147, 105695.	3.9	15
810	Identification of dual active sites in Caenorhabditis elegans GANA-1 protein: an ortholog of the human Î±-GAL a and Î±-NAGA enzymes. Journal of Biomolecular Structure and Dynamics, 0, , 1-16.	2.0	1
811	Effect of Ion and Binding Site on the Conformation of Chosen Glycosaminoglycans at the Albumin Surface. Entropy, 2022, 24, 811.	1.1	7

#	Article	IF	Citations
813	Molecular Analysis and Conformational Dynamics of Human MC4R Disease-Causing Mutations. Molecules, 2022, 27, 4037.	1.7	1
814	Sizing up DNA nanostructure assembly with native mass spectrometry and ion mobility. Nature Communications, 2022, 13, .	5.8	6
815	Computer-aided directed evolution ofl-threonine aldolase for asymmetric biocatalytic synthesis of a chloramphenicol intermediate. Bioorganic and Medicinal Chemistry, 2022, 68, 116880.	1.4	5
816	Computational method for the systematic alignment of analogue series with structure-activity relationship transfer potential across different targets. European Journal of Medicinal Chemistry, 2022, 239, 114558.	2.6	3
817	Binding mechanism and antioxidant activity of piperine to hemoglobin. Food Chemistry, 2022, 394, 133558.	4.2	24
818	Oleuropein as a Potent Compound against Neurological Complications Linked with COVID-19: A Computational Biology Approach. Entropy, 2022, 24, 881.	1.1	3
819	Role of C-terminal domain in a manganese-catalase from Geobacillus thermopakistaniensis. Journal of Bioscience and Bioengineering, 2022, , .	1.1	0
820	Photoswitching of Feedback Inhibition by Tryptophan in Anthranilate Synthase. ACS Synthetic Biology, 2022, 11, 2846-2856.	1.9	2
821	Purification, Biochemical Characterization, and DPPâ€IV and Î±â€amylase inhibitory activity of Berberine from Cardiospermum halicacabum. Journal of Molecular Recognition, 0, , .	1.1	3
822	An inhibitor of interaction between the transcription factor NRF2 and the E3 ubiquitin ligase adapter Î²-TrCP delivers anti-inflammatory responses in mouse liver. Redox Biology, 2022, 55, 102396.	3.9	8
823	10-Alkoxy-anthracenyl-isoxazole analogs have sub-micromolar activity against a Glioblastoma multiforme cell line. Bioorganic and Medicinal Chemistry, 2022, 69, 116911.	1.4	2
824	Directed evolution of a carbonyl reductase LsCR for the enantioselective synthesis of (1S)-2-chloro-1-(3,4-difluorophenyl) ethanol. Bioorganic Chemistry, 2022, 127, 105991.	2.0	6
825	Best templates outperform homology models in predicting the impact of mutations on protein stability. Bioinformatics, 2022, 38, 4312-4320.	1.8	13
826	Targeting Human CD22/Siglec-2 with Dimeric Sialosides as Novel Oligosaccharide Mimetics. Journal of Medicinal Chemistry, 2022, 65, 10588-10610.	2.9	4
827	Dithymoquinone Analogues as Potential Candidate(s) for Neurological Manifestation Associated with COVID-19: A Therapeutic Strategy for Neuro-COVID. Life, 2022, 12, 1076.	1.1	2
828	A Model Peptide Reveals Insights into the Interaction of Human Hemopexin with Heme. International Journal of Peptide Research and Therapeutics, 2022, 28, .	0.9	2
829	Molecular docking and dynamics simulation analysis of nucleoprotein from the Crimea-Congo hemorrhagic fever virus strain Baghdad-12 with FDA approved drugs. Bioinformation, 2022, 18, 442-449.	0.2	0
830	Feasible Cluster Model Method for Simulating the Redox Potentials of Laccase CueO and Its Variant. Frontiers in Bioengineering and Biotechnology, 0, 10, .	2.0	1

#	Article	IF	Citations
831	The Inhibitory Potential of Ferulic Acid Derivatives against the SARS-CoV-2 Main Protease: Molecular Docking, Molecular Dynamics, and ADMET Evaluation. Biomedicines, 2022, 10, 1787.	1.4	4
832	Actions of Novel Angiotensin Receptor Blocking Drugs, Bisartans, Relevant for COVID-19 Therapy: Biased Agonism at Angiotensin Receptors and the Beneficial Effects of Neprilysin in the Renin Angiotensin System. Molecules, 2022, 27, 4854.	1.7	4
833	Toward protein NMR at physiological concentrations by hyperpolarized waterâ€"Finding and mapping uncharted conformational spaces. Science Advances, 2022, 8, .	4.7	8
835	YAMACS: a graphical interface for GROMACS. Bioinformatics, 2022, 38, 4645-4646.	1.8	7
836	Mechanical strain stimulates <scp>COPII</scp>â€dependent secretory trafficking via Rac1. EMBO Journal, 2022, 41, .	3.5	9
837	Unfolding of an alpha-helical peptide exposed to high temperature: suggesting a critical residue in the process. Structural Chemistry, 0, , .	1.0	0
838	New Materials Based on Molecular Interaction between Hyaluronic Acid and Bovine Albumin. Molecules, 2022, 27, 4956.	1.7	3
839	Enhancement of thermostability and catalytic properties of ammonia lyase through disulfide bond construction and backbone cyclization. International Journal of Biological Macromolecules, 2022, 219, 804-811.	3.6	10
841	Theoretical insight and molecular recognition of oxatub[4]arene-based organic macrocycle as a supramolecular host for antipsychotic drug risperidone. Journal of Molecular Liquids, 2022, 366, 120195.	2.3	2
842	Enhanced conversion and extraction of ginsenoside Rg1 from Panax notoginseng using Î²-xylosidase mutants and an endoxylanase. Industrial Crops and Products, 2022, 187, 115514.	2.5	3
843	Towards specie-specific ensemble vaccine candidates against mammarenaviruses using optimized structural vaccinology pipeline and molecular modelling approaches. Microbial Pathogenesis, 2022, 172, 105793.	1.3	5
844	Extracellular matrix stiffness regulates degradation of MST2 via SCF Î²TrCP. Biochimica Et Biophysica Acta - General Subjects, 2022, 1866, 130238.	1.1	5
845	The structural differences between mushroom and human tyrosinase cleared by investigating the inhibitory activities of stilbenes. Journal of Molecular Structure, 2023, 1272, 134180.	1.8	8
846	Molecular dynamic simulation with protein and detection of repurposable drugs for COVID-19. , 2022, , 273-297.		0
847	Evaluation of temperature effect on conformation of protein interaction E-cadherin..ADTC5 complex: Molecular dynamic simulation. AIP Conference Proceedings, 2022, , .	0.3	1
848	Molecular docking analysis and dynamics simulation of salbutamol with the monoamine oxidase B (MAO-B) enzyme. Bioinformation, 2022, 18, 304-309.	0.2	1
849	Structural modeling of protein ensembles between E3 RING ligases and SARS-CoV-2: The role of zinc binding domains. Journal of Trace Elements in Medicine and Biology, 2023, 75, 127089.	1.5	2
850	Novel Hits for N-Myristoyltransferase Inhibition Discovered by Docking-Based Screening. Molecules, 2022, 27, 5478.	1.7	3

#	Article	IF	Citations
851	Novel insights into heme binding to hemoglobin. Biological Chemistry, 2022, .	1.2	2
853	Simultaneously improving the specific activity and thermostability of Î±-amylase BLA by rational design. Bioprocess and Biosystems Engineering, 2022, 45, 1839-1848.	1.7	7
854	Binding of Glycans to the SARS CoVâ€2 Spike Protein, an Open Question: NMR Data on Binding Site Localization, Affinity, and Selectivity. Chemistry - A European Journal, 2022, 28, .	1.7	3
856	Cobalt Ferrite Particles Produced by Sol-Gel Autocombustion and Embedded in Polysilane: An Innovative Route to Magnetically-Induced Fluorescence Composites. Molecules, 2022, 27, 6393.	1.7	2
857	Host and viral proteins involved in <scp>SARSâ€CoV</scp>â€2 infection differentially bind heme. Protein Science, 2022, 31, .	3.1	6
858	Unique structural features of claudinâ€5 and claudinâ€15 lead to functionally distinct tight junction strand architecture. Annals of the New York Academy of Sciences, 2022, 1517, 225-233.	1.8	6
860	In Planta, In Vitro and In Silico Studies of Chiral N6-Benzyladenine Derivatives: Discovery of Receptor-Specific S-Enantiomers with Cytokinin or Anticytokinin Activities. International Journal of Molecular Sciences, 2022, 23, 11334.	1.8	5
861	Targeting the SARS-CoV-2 HR1 with Small Molecules as Inhibitors of the Fusion Process. International Journal of Molecular Sciences, 2022, 23, 10067.	1.8	11
862	Design, Synthesis, Biological Activity, and Structural Analysis of Novel Des-C-Ring and Aromatic-D-Ring Analogues of 1Î±,25-Dihydroxyvitamin D₃. Journal of Medicinal Chemistry, 2022, 65, 13112-13124.	2.9	4
863	Circulating rotavirus P[8]â€lineage IV, unlike P[8]â€lineage III, significantly related to nonsecretors status in Iranian children. Journal of Medical Virology, 2023, 95, .	2.5	0
864	Screening Active Phytochemicals of Some Ayurvedic Medicinal Plants to Identify Potential Inhibitors against SARS-CoV-2 Mpro by Computational Investigation. Letters in Drug Design and Discovery, 2023, 20, 1380-1392.	0.4	0
865	A Potential Anticancer Mechanism of Finger Root (Boesenbergia rotunda) Extracts against a Breast Cancer Cell Line. Scientifica, 2022, 2022, 1-17.	0.6	5
866	Interaction, bioaccessibility and stability of bovine serum albumin-gamma-oryzanol complex: Spectroscopic and computational approaches. Food Chemistry, 2023, 402, 134493.	4.2	5
867	Expression pattern and clinical value of Key RNA methylation modification regulators in ischemic stroke. Frontiers in Genetics, 0, 13, .	1.1	0
868	<scp>MHC2AffyPred</scp>: A machineâ€learning approach to estimate affinity of <scp>MHC</scp> class <scp>II</scp> peptides based on structural interaction fingerprints. Proteins: Structure, Function and Bioinformatics, 2023, 91, 277-289.	1.5	1
869	Convertible cellulosic platforms with manageable loads of 1-hydroxybenzotriazole: their preparation and conductive behavior. Cellulose, 2022, 29, 9847-9863.	2.4	5
870	Galactaric acid production by engineering substrate specificity in glucose oxidase from Aspergillus niger. Biochemical Engineering Journal, 2022, 187, 108646.	1.8	1
871	Multiscale modelling of claudin-based assemblies: A magnifying glass for novel structures of biological interfaces. Computational and Structural Biotechnology Journal, 2022, 20, 5984-6010.	1.9	5

#	Article	IF	Citations
872	Novel chimeric proteins mimicking SARS-CoV-2 spike epitopes with broad inhibitory activity. International Journal of Biological Macromolecules, 2022, 222, 2467-2478.	3.6	6
873	Characterization of Synovial Fluid Components: Albumin-Chondroitin Sulfate Interactions Seen through Molecular Dynamics. Materials, 2022, 15, 6935.	1.3	2
874	DNA opening during transcription initiation by RNA polymerase II in atomic detail. Biophysical Journal, 2022, , .	0.2	1
875	In depth molecular interaction analyses of the complex of a proposed CTXM-inhibitor bound to the bacterial enzyme. Journal of Biomolecular Structure and Dynamics, 0, , 1-11.	2.0	1
876	Maize <scp>CDKA2</scp>;1a and <scp>CDKB1</scp>;1 kinases have different requirements for their activation and participate in substrate recognition. FEBS Journal, 2023, 290, 2463-2488.	2.2	1
877	Aptamerâ€"Protein Structures Guide In Silico and Experimental Discovery of Aptamerâ€"Short Peptide Recognition Complexes or Aptamerâ€"Amino Acid Cluster Complexes. Journal of Physical Chemistry B, 0, , .	1.2	1
879	Recruitment of distinct <scp>UDP</scp>â€glycosyltransferase families demonstrates dynamic evolution of chemical defense within Eucalyptus L'HÃ©r. New Phytologist, 2023, 237, 999-1013.	3.5	1
880	Identification and characterization of alternative sites and molecular probes for SARS-CoV-2 target proteins. Frontiers in Chemistry, 0, 10, .	1.8	0
881	High-resolution structure of a fish aquaporin reveals a novel extracellular fold. Life Science Alliance, 2022, 5, e202201491.	1.3	0
882	Selection of synthetic proteins to modulate the human frataxin function. Biotechnology and Bioengineering, 2023, 120, 409-425.	1.7	0
883	Molecular dynamics simulation of the interaction of food proteins with small molecules. Food Chemistry, 2023, 405, 134824.	4.2	50
884	The structure and dynamics of bottlebrushes: Simulation and experimental studies combined. Polymer, 2022, 261, 125409.	1.8	4
885	Structural adaptation of thermostable carboxylic acid reductase from Mycobacterium phlei. Molecular Catalysis, 2022, 532, 112747.	1.0	0
886	Computational study of the potential impact of AURKC missense SNPs on AURKC-INCENP interaction and their correlation to macrozoospermia. Journal of Biomolecular Structure and Dynamics, 2023, 41, 9503-9522.	2.0	1
887	Collagen type IIâ€"hyaluronan interactions â€" the effect of proline hydroxylation: a molecular dynamics study. Journal of Materials Chemistry B, 2022, 10, 9713-9723.	2.9	2
888	Selecting Better Biocatalysts by Complementing Recoded Bacteria**. Angewandte Chemie - International Edition, 2023, 62, .	7.2	5
889	Selecting Better Biocatalysts by Complementing Recoded Bacteria. Angewandte Chemie, 0, , .	1.6	0
890	Chemical Characterization, Antioxidant, Antimicrobial, Cytotoxicity and in Silico Studies of Hexane Extract and Essential Oils from Citrus limon Leaves. Chemistry and Biodiversity, 2023, 20, .	1.0	3

#	Article	IF	Citations
891	In Silico Approach for the Evaluation of the Potential Antiviral Activity of Extra Virgin Olive Oil (EVOO) Bioactive Constituents Oleuropein and Oleocanthal on Spike Therapeutic Drug Target of SARS-CoV-2. Molecules, 2022, 27, 7572.	1.7	3
892	Friedelin, a novel inhibitor of CYP17A1 in prostate cancer from Cassia tora. Journal of Biomolecular Structure and Dynamics, 2023, 41, 9695-9720.	2.0	4
893	Structural remodeling of SARS-CoV-2 spike protein glycans reveals the regulatory roles in receptor-binding affinity. Glycobiology, 2023, 33, 126-137.	1.3	11
894	Computational search for potential COVID-19 drugs from ayurvedic medicinal plants to identify potential inhibitors against SARS-CoV-2 targets. Current Computer-Aided Drug Design, 2022, 19, .	0.8	1
895	In Vivo and In Silico Assessment of the Cardioprotective Effect of Thymus linearis Extract against Ischemic Myocardial Injury. ACS Omega, 2022, 7, 43635-43646.	1.6	3
896	Intermolecular interaction and molecular dynamics study of carboxymethyl Chitosanâ€¦ Vitamin C molecular complex for understanding encapsulation and kinetics-controlled released mechanism. AIP Conference Proceedings, 2022, , .	0.3	0
897	Abnormal methylation in the NDUFA13 gene promoter of breast cancer cells breaks the cooperative DNA recognition by transcription factors. QRB Discovery, 2022, 3, .	0.6	2
898	The effect of temperature on interaction and dynamical study of protease inhibitors as a SARS-CoV-2 potential drug. AIP Conference Proceedings, 2022, , .	0.3	0
902	AlphaFill: enriching AlphaFold models with ligands and cofactors. Nature Methods, 2023, 20, 205-213.	9.0	145
903	Computation-Aided Engineering of Cytochrome P450 for the Production of Pravastatin. ACS Catalysis, 2022, 12, 15028-15044.	5.5	6
904	Deciphering the anti-filarial potential of bioactive compounds from Ocimum sanctum : a combined experimental and computational study. Pharmaceutical Biology, 2022, 60, 2237-2252.	1.3	1
905	Novel Function of CtXyn5A from Acetivibrio thermocellus: Dual Arabinoxylanase and Feruloyl Esterase Activity in the Same Active Site. ChemBioChem, 0, , .	1.3	2
906	DeepPROTACs is a deep learning-based targeted degradation predictor for PROTACs. Nature Communications, 2022, 13, .	5.8	23
908	Successes and Failures of Static Aptamer-Target 3D Docking Models. International Journal of Molecular Sciences, 2022, 23, 14410.	1.8	3
909	SARS-CoV-2 Antibody Effectiveness Is Influenced by Non-Epitope Mutation/Binding-Induced Denaturation of the Epitope 3D Architecture. Pathogens, 2022, 11, 1437.	1.2	2
910	The free fatty acidâ€“binding pocket is a conserved hallmark in pathogenic Î²-coronavirus spike proteins from SARS-CoV to Omicron. Science Advances, 2022, 8, .	4.7	21
914	SARS-CoV-2 proteases Mpro and PLpro: Design of inhibitors with predicted high potency and low mammalian toxicity using artificial neural networks, ligand-protein docking, molecular dynamics simulations, and ADMET calculations. Computers in Biology and Medicine, 2023, 153, 106449.	3.9	9
915	Understanding Selfâ€Assembly of Silicaâ€Precipitating Peptides to Control Silica Particle Morphology. Advanced Materials, 2023, 35, .	11.1	4

#	Article	IF	Citations
916	Hepatoprotective Activity of Lignin-Derived Polyphenols Dereplicated Using High-Resolution Mass Spectrometry, In Vivo Experiments, and Deep Learning. International Journal of Molecular Sciences, 2022, 23, 16025.	1.8	2
917	The PROSCOOP10 Gene Encodes Two Extracellular Hydroxylated Peptides and Impacts Flowering Time in Arabidopsis. Plants, 2022, 11, 3554.	1.6	4
918	Molecular Epidemiology of the Norwegian SARS-CoV-2 Delta Lineage AY.63. Viruses, 2022, 14, 2734.	1.5	1
919	Exploring Highly Conserved Regions of SARS-CoV-2 Spike S2 Subunit as Targets for Fusion Inhibition Using Chimeric Proteins. International Journal of Molecular Sciences, 2022, 23, 15511.	1.8	3
920	A new serotonin 2A receptor antagonist with potential benefits in Non-Alcoholic Fatty Liver Disease. Life Sciences, 2023, 314, 121315.	2.0	3
921	TMPRSS6 rs855791 polymorphism is associated with iron deficiency in a cohort of Sri Lankan pregnant women. Egyptian Journal of Medical Human Genetics, 2022, 23, .	0.5	0
922	Collagen Type IIâ€"Chitosan Interactions as Dependent on Hydroxylation and Acetylation Inferred from Molecular Dynamics Simulations. Molecules, 2023, 28, 154.	1.7	2
923	Rational Strategy for Designing Peptidomimetic Small Molecules Based on Cyclic Peptides Targeting Proteinâ€"Protein Interaction between CTLA-4 and B7-1. Pharmaceuticals, 2022, 15, 1506.	1.7	1
925	Chemical Attachment of 5-Nitrosalicylaldimine Motif to Silatrane Resulting in an Organicâ€"Inorganic Structure with High Medicinal Significance. Pharmaceutics, 2022, 14, 2838.	2.0	3
926	In silico analysis decodes transthyretin (TTR) binding and thyroid disrupting effects of per- and polyfluoroalkyl substances (PFAS). Archives of Toxicology, 2023, 97, 755-768.	1.9	7
927	Synthesis, characterization, and in vitro anti-cholinesterase screening of novel indole amines. RSC Advances, 2023, 13, 1203-1215.	1.7	3
928	A role of salt bridges in mediating drug potency: A lesson from the N-myristoyltransferase inhibitors. Frontiers in Molecular Biosciences, 0, 9, .	1.6	10
929	Inâ€silico identification of Tyr232 in <scp>AMPKÎ±2</scp> as a dephosphorylation site for the protein tyrosine phosphatase <scp>PTPâ€PEST</scp>. Proteins: Structure, Function and Bioinformatics, 2023, 91, 831-846.	1.5	2
930	Synthesis of an amantadine-based novel Schiff base and its transition metal complexes as potential ALP, Î±-amylase, and Î±-glucosidase inhibitors. RSC Advances, 2023, 13, 2756-2767.	1.7	6
931	Enzymatic (2 R ,4 R)â€Pentanediol Synthesis â€" â€œPutting a Bottle on the Tableâ€• Chemie-Ingenieur-Technik, 0, , .	0.4	1
932	Comparison of In Vitro and In Silico Assessments of Human Galactose-1-Phosphate Uridylyltransferase Coding Variants. Cureus, 2023, , .	0.2	0
933	Synthesis, Spectroscopic Characterization, DFT and Molecular Dynamics of Quinoline-based Peptoids. Arabian Journal of Chemistry, 2023, , 104570.	2.3	0
934	Identification of Compounds Preventing A. fumigatus Biofilm Formation by Inhibition of the Galactosaminogalactan Deacetylase Agd3. International Journal of Molecular Sciences, 2023, 24, 1851.	1.8	2

#	Article	IF	Citations
935	Antioxidant and Anti-inflammatory Activity of Sea Cucumber (Holothuria scabra) Active Compounds against KEAP1 and iNOS Protein. Bioinformatics and Biology Insights, 2023, 17, 117793222211496.	1.0	1
936	Molecular dynamics simulation and structural analysis of aquaporin Z from an Antarctic Pseudomonas sp. strain AMS3. Journal of Biomolecular Structure and Dynamics, 0, , 1-12.	2.0	2
937	Revealing the critical role of Leucine145 of Î±-glucosidase AglA for enhancing Î±-arbutin production. Molecular Catalysis, 2023, 537, 112943.	1.0	0
938	Modelling the Transitioning of SARS-CoV-2 nsp3 and nsp4 Lumenal Regions towards a More Stable State on Complex Formation. International Journal of Molecular Sciences, 2023, 24, 720.	1.8	7
939	Curcumin Decreases Viability and Inhibits Proliferation of Imatinib-Sensitive and Imatinib-Resistant Chronic Myeloid Leukemia Cell Lines. Metabolites, 2023, 13, 58.	1.3	5
940	Switching Heavy Chain Constant Domains Denatures the Paratope 3D Architecture of Influenza Monoclonal Antibodies. Pathogens, 2023, 12, 51.	1.2	0
941	Molecular Epidemiology of SARS-CoV-2: The Dominant Role of Arginine in Mutations and Infectivity. Viruses, 2023, 15, 309.	1.5	6
943	Conjugates of Tacrine and Salicylic Acid Derivatives as New Promising Multitarget Agents for Alzheimerâ€™s Disease. International Journal of Molecular Sciences, 2023, 24, 2285.	1.8	7
944	Synthesis and Biological Evaluation of a Series of Quinolineâ€Based Quinazolinones and Carbamic Anhydride Derivatives. ChemistrySelect, 2023, 8, .	0.7	2
945	Inhibition of Neutral Sphingomyelinase 2 by Novel Small Molecule Inhibitors Results in Decreased Release of Extracellular Vesicles by Vascular Smooth Muscle Cells and Attenuated Calcification. International Journal of Molecular Sciences, 2023, 24, 2027.	1.8	3
946	The ubiquitination landscape of the influenza A virus polymerase. Nature Communications, 2023, 14, .	5.8	8
947	DNA methylation of the promoter region at the CREB1 binding site is a mechanism for the epigenetic regulation of brain-specific PKMÎ¶. Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms, 2023, 1866, 194909.	0.9	1
948	Structural modeling and analyses of genetic variations in the human XPC nucleotide excision repair protein. Journal of Biomolecular Structure and Dynamics, 2023, 41, 13535-13562.	2.0	1
949	Ultra-rare complement factor 8 coding variants in families with age-related macular degeneration. IScience, 2023, 26, 106417.	1.9	3
950	In-silico prediction of highly promising natural fungicides against the destructive blast fungus Magnaporthe oryzae. Heliyon, 2023, 9, e15113.	1.4	1
951	Neurotensin(8â€“13) analogs as dual NTS1 and NTS2 receptor ligands with enhanced effects on a mouse model of Parkinson's disease. European Journal of Medicinal Chemistry, 2023, 254, 115386.	2.6	2
954	Metalloproteaseâ€mediated cleavage of CD95 ligand. FEBS Journal, 2023, 290, 3145-3164.	2.2	1
955	The in-silico evaluation of important GLUT9 residue for uric acid transport based on renal hypouricemia type 2. Chemico-Biological Interactions, 2023, 373, 110378.	1.7	1

#	Article	IF	Citations
956	An Insight into the Metabolism of 2,5-Disubstituted Monotetrazole Bearing Bisphenol Structures: Emerging Bisphenol A Structural Congeners. Molecules, 2023, 28, 1465.	1.7	0
957	Redox sensitive human mitochondrial aconitase and its interaction with frataxin: In vitro and in silico studies confirm that it takes two to tango. Free Radical Biology and Medicine, 2023, 197, 71-84.	1.3	3
958	Molecular interaction of a putative inhibitor with bacterial SHV, an enzyme associated with antibiotic resistance. Royal Society Open Science, 2023, 10, .	1.1	1
959	Structural differences between hypoxanthine phosphoribosyltransferase family members highlight opportunities for antiparasitic drug design in neglected diseases. Archives of Biochemistry and Biophysics, 2023, 737, 109550.	1.4	0
960	Physiological and genomic insights into abiotic stress of halophilic archaeon Natrinema altunense 4.1R isolated from a saline ecosystem of Tunisian desert. Genetica, 2023, 151, 133-152.	0.5	2
961	Coevolving stability and activity of LsCR by a single point mutation and constructing neat substrate bioreaction system. Biotechnology and Bioengineering, 2023, 120, 1521-1530.	1.7	1
962	Structural Insights into Pseudomonas aeruginosa Exotoxin Aâ€“Elongation Factor 2 Interactions: A Molecular Dynamics Study. Journal of Chemical Information and Modeling, 2023, 63, 1578-1591.	2.5	2
963	Physiological Buffer Effects in Drug Supersaturation - A Mechanistic Study of Hydroxypropyl Cellulose as Precipitation Inhibitor. Journal of Pharmaceutical Sciences, 2023, , .	1.6	1
964	N-Glycan on the Non-Consensus N-X-C Glycosylation Site Impacts Activity, Stability, and Localization of the Sda Synthase B4GALNT2. International Journal of Molecular Sciences, 2023, 24, 4139.	1.8	0
965	Inhibition of matrix metalloproteinases by HIV-1 integrase strand transfer inhibitors. Frontiers in Toxicology, 0, 5, .	1.6	3
966	A novel chemical attack on Notch-mediated transcription by targeting the NACK ATPase. Molecular Therapy - Oncolytics, 2023, 28, 307-320.	2.0	1
967	Evolution of enzyme functionality in the flavin-containing monooxygenases. Nature Communications, 2023, 14, .	5.8	11
968	Heparan Sulfate and Enoxaparin Interact at the Interface of the Spike Protein of HCoV-229E but Not with HCoV-OC43. Viruses, 2023, 15, 663.	1.5	3
969	GRB2 dimerization mediated by SH2 domain-swapping is critical for T cell signaling and cytokine production. Scientific Reports, 2023, 13, .	1.6	1
970	In Vitro and Silico Studies on the N-Doped Carbon Dots Potential in ACE2 Expression Modulation. ACS Omega, 2023, 8, 10077-10085.	1.6	1
972	In Silico-Based Structural Evaluation to Categorize the Pathogenicity of Mutations Identified in the RAD Class of Proteins. ACS Omega, 2023, 8, 10266-10277.	1.6	0
973	Pharmacophore modelling-based drug repurposing approaches for monkeypox therapeutics. Journal of Biomolecular Structure and Dynamics, 0, , 1-12.	2.0	1
974	Computationally Supported Inversion of Ketoreductase Stereoselectivity. ChemBioChem, 2023, 24, .	1.3	2

#	Article	IF	Citations
975	Steered Molecular Dynamics Simulations Study on FABP4 Inhibitors. Molecules, 2023, 28, 2731.	1.7	2
976	Rapid adaptations of Legionella pneumophila to the human host. Microbial Genomics, 2023, 9, .	1.0	0
977	Crystal structure of the Fusarium oxysporum tannaseâ€like feruloyl esterase <scp>FaeC</scp> in complex with pâ€coumaric acid provides insight into ligand binding. FEBS Letters, 2023, 597, 1415-1427.	1.3	1
978	Unravelling the epidemiological diversity of Zika virus by analyzing key protein variations. Archives of Virology, 2023, 168, .	0.9	0
979	Maleimide constrained BAD BH3 domain peptides as BCL-xL Inhibitors: A versatile approach to rapidly identify sites compatible with peptide constraining. Bioorganic and Medicinal Chemistry Letters, 2023, 87, 129260.	1.0	1
980	Kaurane-Type Diterpenoids as Potential Inhibitors of Dihydrofolate Reductase-Thymidylate Synthase in New World Leishmania Species. Antibiotics, 2023, 12, 663.	1.5	3
981	Therapeutic Role of DGJ (1â€deoxygalactonojirimycin) in Fabry Disease: Theoretical Insights. ChemistrySelect, 2023, 8, .	0.7	0
982	The E2 glycoprotein holds key residues for Mayaro virus adaptation to the urban Aedes aegypti mosquito. PLoS Pathogens, 2023, 19, e1010491.	2.1	4
983	An Affordable Topography-Based Protocol for Assigning a Residueâ€™s Character on a Hydropathy (PARCH) Scale. Journal of Chemical Theory and Computation, 2024, 20, 1656-1672.	2.3	4
985	The IgG4 hinge with CD28 transmembrane domain improves VHH-based CAR T cells targeting a membrane-distal epitope of GPC1 in pancreatic cancer. Nature Communications, 2023, 14, .	5.8	8
986	Structural and Pathogenic Impacts of ABCA4 Variants in Retinal Degenerationsâ€”An In-Silico Study. International Journal of Molecular Sciences, 2023, 24, 7280.	1.8	1
987	An In silico Investigation to Identify Promising Inhibitors for SARS-CoV-2 Mpro Target. Medicinal Chemistry, 2023, 19, 925-938.	0.7	0
988	Molecular modeling of ARF6 dysregulation caused by mutations in IQSEC2. Journal of Biomolecular Structure and Dynamics, 2024, 42, 1268-1279.	2.0	0
1021	Computational Modeling of DYRK1A Inhibitors as Potential Anti-Alzheimer Agents. Neuromethods, 2023, , 295-324.	0.2	0
1119	In-Silico Analysis of the High-Risk Missense Variants in PTH1R Gene and Association with Primary Failure of Tooth Eruption (PFE). Lecture Notes in Networks and Systems, 2024, , 264-287.	0.5	0