Luhua Lai

List of Publications by Year
in descending order

165 papers	9,413 citations	50276 46 h-index	45317 90 g-index
172 all docs	172 docs citations	172 times ranked	11754 citing authors

#	Article	IF	Citations
1	PharmMapper 2017 update: a web server for potential drug target identification with a comprehensive target pharmacophore database. Nucleic Acids Research, 2017, 45, W356-W360.	14.5	802
2	A New Atom-Additive Method for Calculating Partition Coefficients. Journal of Chemical Information and Computer Sciences, 1997, 37, 615-621.	2.8	399
3	Arabidopsis pollen tube integrity and sperm release are regulated by RALF-mediated signaling. Science, 2017, 358, 1596-1600.	12.6	324
4	Biosynthesis, Purification, and Substrate Specificity of Severe Acute Respiratory Syndrome Coronavirus 3C-like Proteinase. Journal of Biological Chemistry, 2004, 279, 1637-1642.	3.4	280
5	Sequence-based prediction of protein protein interaction using a deep-learning algorithm. BMC Bioinformatics, 2017, 18, 277.	2.6	278
6	SCORE: A New Empirical Method for Estimating the Binding Affinity of a Protein-Ligand Complex. Journal of Molecular Modeling, 1998, 4, 379-394.	1.8	275
7	Deep Learning for Drug-Induced Liver Injury. Journal of Chemical Information and Modeling, 2015, 55, 2085-2093.	5.4	264
8	A protein engineered to bind uranyl selectively and with femtomolar affinity. Nature Chemistry, 2014, 6, 236-241.	13.6	262
9	LigBuilder: A Multi-Purpose Program for Structure-Based Drug Design. Journal of Molecular Modeling, 2000, 6, 498-516.	1.8	249
10	CavityPlus: a web server for protein cavity detection with pharmacophore modelling, allosteric site identification and covalent ligand binding ability prediction. Nucleic Acids Research, 2018, 46, W374-W379.	14.5	226
11	Scutellaria baicalensis extract and baicalein inhibit replication of SARS-CoV-2 and its 3C-like protease inÂvitro. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 497-503.	5.2	206
12	3C-like Proteinase from SARS Coronavirus Catalyzes Substrate Hydrolysis by a General Base Mechanism. Biochemistry, 2004, 43, 4568-4574.	2.5	189
13	Deep Learning Based Regression and Multiclass Models for Acute Oral Toxicity Prediction with Automatic Chemical Feature Extraction. Journal of Chemical Information and Modeling, 2017, 57, 2672-2685.	5.4	179
14	Transfer Learning for Drug Discovery. Journal of Medicinal Chemistry, 2020, 63, 8683-8694.	6.4	178
15	Calculating partition coefficient by atom-additive method. Journal of Computer - Aided Molecular Design, 2000, 19, 47-66.	1.0	172
16	LigBuilder 2: A Practical de Novo Drug Design Approach. Journal of Chemical Information and Modeling, 2011, 51, 1083-1091.	5.4	170
17	Binding Site Detection and Druggability Prediction of Protein Targets for Structure- Based Drug Design. Current Pharmaceutical Design, 2013, 19, 2326-2333.	1.9	167
18	Finding multiple target optimal intervention in diseaseâ€related molecular network. Molecular Systems Biology, 2008, 4, 228.	7.2	165

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19	Computational Multitarget Drug Design. Journal of Chemical Information and Modeling, 2017, 57, 403-412.	5.4	149
20	Serine synthesis through PHGDH coordinates nucleotide levels by maintaining central carbon metabolism. Nature Communications, 2018, 9, 5442.	12.8	143
21	Discovery of Multitarget Inhibitors by Combining Molecular Docking with Common Pharmacophore Matching. Journal of Medicinal Chemistry, 2008, 51, 7882-7888.	6.4	128
22	Pocket v.2:â€‰ Further Developments on Receptor-Based Pharmacophore Modeling. Journal of Chemical Information and Modeling, 2006, 46, 2684-2691.	5.4	117
23	Isatin Compounds as Noncovalent SARS Coronavirus 3C-like Protease Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 3440-3443.	6.4	110
24	Automatic retrosynthetic route planning using template-free models. Chemical Science, 2020, 11, 3355-3364.	7.4	105
25	Rational Design of Selective Allosteric Inhibitors of PHGDH and Serine Synthesis with Anti-tumor Activity. Cell Chemical Biology, 2017, 24, 55-65.	5.2	102
26	Synergistic and Antagonistic Drug Combinations Depend on Network Topology. PLoS ONE, 2014, 9, e93960.	2.5	99
27	Activation of Glutathione Peroxidase 4 as a Novel Anti-inflammatory Strategy. Frontiers in Pharmacology, 2018, 9, 1120.	3.5	98
28	Targeting intrinsically disordered proteins at the edge of chaos. Drug Discovery Today, 2019, 24, 217-227.	6.4	98
29	Discovering Potent Small Molecule Inhibitors of Cyclophilin A Using de Novo Drug Design Approach. Journal of Medicinal Chemistry, 2009, 52, 5295-5298.	6.4	92
30	Novel Allosteric Activators for Ferroptosis Regulator Glutathione Peroxidase 4. Journal of Medicinal Chemistry, 2019, 62, 266-275.	6.4	91
31	Dynamic Simulations on the Arachidonic Acid Metabolic Network. PLoS Computational Biology, 2007, 3, e55.	3.2	90
32	Deep learning for molecular generation. Future Medicinal Chemistry, 2019, 11, 567-597.	2.3	88
33	Prediction of Human Cytochrome P450 Inhibition Using a Multitask Deep Autoencoder Neural Network. Molecular Pharmaceutics, 2018, 15, 4336-4345.	4.6	85
34	Structure-based de novo drug design using 3D deep generative models. Chemical Science, 2021, 12, 13664-13675.	7.4	82
35	Ligand Clouds around Protein Clouds: A Scenario of Ligand Binding with Intrinsically Disordered Proteins. PLoS Computational Biology, 2013, 9, e1003249.	3.2	79
36	Structure-based Inhibitor Design for the Intrinsically Disordered Protein c-Myc. Scientific Reports, 2016, 6, 22298.	3.3	79

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37	Systems Biology Brings New Dimensions for Structure-Based Drug Design. Journal of the American Chemical Society, 2014, 136, 11556-11565.	13.7	75
38	Prediction of liquidâ€“liquid phase separating proteins using machine learning. BMC Bioinformatics, 2022, 23, 72.	2.6	74
39	Self-Learning Perfect Optical Chirality via a Deep Neural Network. Physical Review Letters, 2019, 123, 213902.	7.8	72
40	Motions of Allosteric and Orthosteric Ligand-Binding Sites in Proteins are Highly Correlated. Journal of Chemical Information and Modeling, 2016, 56, 1725-1733.	5.4	70
41	Mechanism of DNAâ€Induced Phase Separation for Transcriptional Repressor VRN1. Angewandte Chemie - International Edition, 2019, 58, 4858-4862.	13.8	69
42	All-Orientation Search and All-Placement Search in Comparative Molecular Field Analysis. Journal of Molecular Modeling, 1998, 4, 276-283.	1.8	67
43	RALF peptide signaling controls the polytubey block in Arabidopsis. Science, 2022, 375, 290-296.	12.6	65
44	Diverse Ways of Perturbing the Human Arachidonic Acid Metabolic Network To Control Inflammation. Accounts of Chemical Research, 2015, 48, 2242-2250.	15.6	59
45	Dynamic Modeling of Human 5-Lipoxygenaseâ€“Inhibitor Interactions Helps To Discover Novel Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 2597-2605.	6.4	56
46	De Novo Design of Multitarget Ligands with an Iterative Fragment-Growing Strategy. Journal of Chemical Information and Modeling, 2014, 54, 1235-1241.	5.4	54
47	Maturation Mechanism of Severe Acute Respiratory Syndrome (SARS) Coronavirus 3C-like Proteinase. Journal of Biological Chemistry, 2010, 285, 28134-28140.	3.4	50
48	Identifying Allosteric Binding Sites in Proteins with a Two-State Goì... Model for Novel Allosteric Effector Discovery. Journal of Chemical Theory and Computation, 2012, 8, 2962-2971.	5.3	46
49	Discovery of novel chemoeffectors and rational design of Escherichia coli chemoreceptor specificity. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 16814-16819.	7.1	46
50	LigBuilder V3: A Multi-Target de novo Drug Design Approach. Frontiers in Chemistry, 2020, 8, 142.	3.6	46
51	Potent inhibitors of SARS-CoV-2 3C-like protease derived from N-substituted isatin compounds. European Journal of Medicinal Chemistry, 2020, 206, 112702.	5.5	45
52	Discovery of Dual Target Inhibitors against Cyclooxygenases and Leukotriene A₄ Hydrolyase. Journal of Medicinal Chemistry, 2011, 54, 3650-3660.	6.4	44
53	Discovery of Novel 15-Lipoxygenase Activators To Shift the Human Arachidonic Acid Metabolic Network toward Inflammation Resolution. Journal of Medicinal Chemistry, 2016, 59, 4202-4209.	6.4	43
54	Prediction of Drug-Likeness Using Deep Autoencoder Neural Networks. Frontiers in Genetics, 2018, 9, 585.	2.3	43

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55	A Flux Balance of Glucose Metabolism Clarifies the Requirements of the Warburg Effect. Biophysical Journal, 2016, 111, 1088-1100.	0.5	42
56	Computational Chemical Synthesis Analysis and Pathway Design. Frontiers in Chemistry, 2018, 6, 199.	3.6	41
57	RASSE:â€‰ A New Method for Structure-Based Drug Design. Journal of Chemical Information and Computer Sciences, 1996, 36, 1187-1194.	2.8	39
58	Dynamic eicosanoid responses upon different inhibitor and combination treatments on the arachidonic acid metabolic network. Molecular BioSystems, 2012, 8, 1585.	2.9	39
59	Both piston-like and rotational motions are present in bacterial chemoreceptor signaling. Scientific Reports, 2015, 5, 8640.	3.3	39
60	Origin of the Reflectin Gene and Hierarchical Assembly of Its Protein. Current Biology, 2017, 27, 2833-2842.e6.	3.9	39
61	Calculating Partition Coefficients of Peptides by the Addition Method. Journal of Molecular Modeling, 1999, 5, 189-195.	1.8	38
62	A fast and efficient program for modeling protein loops. Biopolymers, 1997, 41, 61-72.	2.4	35
63	A comprehensive analysis of the influence of drug binding kinetics on drug action at molecular and systems levels. Molecular BioSystems, 2013, 9, 1381.	2.9	35
64	A novel mutation in the TUBB8 gene is associated with complete cleavage failure in fertilized eggs. Journal of Assisted Reproduction and Genetics, 2018, 35, 1349-1356.	2.5	35
65	Computational design of ligand-binding proteins. Current Opinion in Structural Biology, 2017, 45, 67-73.	5.7	33
66	Protein loops on structurally similar scaffolds: Database and conformational analysis. , 1999, 49, 481-495.		32
67	Benzo[d]isothiazole 1,1-dioxide derivatives as dual functional inhibitors of 5-lipoxygenase and microsomal prostaglandin E2 synthase-1. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2764-2767.	2.2	31
68	Tuning SpyTagâ€“SpyCatcher mutant pairs toward orthogonal reactivity encryption. Chemical Science, 2017, 8, 6577-6582.	7.4	31
69	Discovery of Highly Potent Microsomal Prostaglandin E₂ Synthase 1 Inhibitors Using the Active Conformation Structural Model and Virtual Screen. Journal of Medicinal Chemistry, 2013, 56, 3296-3309.	6.4	30
70	iDrug: a web-accessible and interactive drug discovery and design platform. Journal of Cheminformatics, 2014, 6, 28.	6.1	30
71	Activation and inhibition of leukotriene A4 hydrolase aminopeptidase activity by diphenyl ether and derivatives. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 6549-6552.	2.2	29
72	A transferable deep learning approach to fast screen potential antiviral drugs against SARS-CoV-2. Briefings in Bioinformatics, 2021, 22, .	6.5	29

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73	Quaternary Structure, Substrate Selectivity and Inhibitor Design for SARS 3C-Like Proteinase. Current Pharmaceutical Design, 2006, 12, 4555-4564.	1.9	28
74	An autoimmune disease variant of IgG1 modulates B cell activation and differentiation. Science, 2018, 362, 700-705.	12.6	28
75	Allostery of multidomain proteins with disordered linkers. Current Opinion in Structural Biology, 2020, 62, 175-182.	5.7	28
76	Protein ligand docking based on empirical method for binding affinity estimation. , 2001, 15, 429-446.		27
77	Understanding molecular mechanisms of traditional Chinese medicine for the treatment of influenza viruses infection by computational approaches. Molecular BioSystems, 2013, 9, 2696.	2.9	27
78	Sequencing of the MHC region defines HLA-DQA1 as the major genetic risk for seropositive rheumatoid arthritis in Han Chinese population. Annals of the Rheumatic Diseases, 2019, 78, 773-780.	0.9	27
79	Herb-target interaction network analysis helps to disclose molecular mechanism of traditional Chinese medicine. Scientific Reports, 2016, 6, 36767.	3.3	26
80	Discovery of Novel Allosteric Effectors Based on the Predicted Allosteric Sites for Escherichia coli D-3-Phosphoglycerate Dehydrogenase. PLoS ONE, 2014, 9, e94829.	2.5	26
81	Disordered linkers in multidomain allosteric proteins: Entropic effect to favor the open state or enhanced local concentration to favor the closed state?. Protein Science, 2018, 27, 1600-1610.	7.6	25
82	Efficient ligand discovery from natural herbs by integrating virtual screening, affinity mass spectrometry and targeted metabolomics. Analyst, The, 2019, 144, 2881-2890.	3.5	25
83	Chemical perturbations reveal that RUVBL2 regulates the circadian phase in mammals. Science Translational Medicine, 2020, 12, .	12.4	25
84	Bardoxolone and bardoxolone methyl, two Nrf2 activators in clinical trials, inhibit SARS-CoV-2 replication and its 3C-like protease. Signal Transduction and Targeted Therapy, 2021, 6, 212.	17.1	25
85	Advances and Challenges in De Novo Drug Design Using Three-Dimensional Deep Generative Models. Journal of Chemical Information and Modeling, 2022, 62, 2269-2279.	5.4	25
86	Novel Inhibitors of Toxin HipA Reduce Multidrug Tolerant Persisters. ACS Medicinal Chemistry Letters, 2016, 7, 449-453.	2.8	23
87	Statistical Analysis and Prediction of Covalent Ligand Targeted Cysteine Residues. Journal of Chemical Information and Modeling, 2017, 57, 1453-1460.	5.4	23
88	Protein-Protein Interface Analysis and Hot Spots Identification for Chemical Ligand Design. Current Pharmaceutical Design, 2014, 20, 1192-1200.	1.9	23
89	Protein topology and allostery. Current Opinion in Structural Biology, 2020, 62, 158-165.	5.7	22
90	Structural Features of Toxic Chemicals for Specific Toxicity. Journal of Chemical Information and Computer Sciences, 1999, 39, 1173-1189.	2.8	21

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91	Molecular mechanism of 15-lipoxygenase allosteric activation and inhibition. Physical Chemistry Chemical Physics, 2018, 20, 14785-14795.	2.8	21
92	Legionella effector SetA as a general O-glucosyltransferase for eukaryotic proteins. Nature Chemical Biology, 2019, 15, 213-216.	8.0	21
93	Glycopeptide Self-Assembly Modulated by Glycan Stereochemistry through Glycanâ€“Aromatic Interactions. Journal of the American Chemical Society, 2020, 142, 17015-17023.	13.7	21
94	Discovery of highly potent TNFÎ± inhibitors using virtual screen. European Journal of Medicinal Chemistry, 2014, 85, 119-126.	5.5	20
95	Novel mutations and polymorphisms in the CFTR gene associated withÂthree subtypes of congenital absence of vas deferens. Fertility and Sterility, 2015, 104, 1268-1275.e2.	1.0	20
96	Conformational Flexibility of a Short Loop near the Active Site of the SARS-3CLpro is Essential to Maintain Catalytic Activity. Scientific Reports, 2016, 6, 20918.	3.3	20
97	Allosteric Type and Pathways Are Governed by the Forces of Proteinâ€“Ligand Binding. Journal of Physical Chemistry Letters, 2021, 12, 5404-5412.	4.6	20
98	Computational Design of Helical Peptides Targeting TNFÎ±. Angewandte Chemie - International Edition, 2013, 52, 11059-11062.	13.8	19
99	Identification of Cancerâ€“associated metabolic vulnerabilities by modeling multi-objective optimality in metabolism. Cell Communication and Signaling, 2019, 17, 124.	6.5	19
100	Computational strategy for intrinsically disordered protein ligand design leads to the discovery of p53 transactivation domain I binding compounds that activate the p53 pathway. Chemical Science, 2021, 12, 3004-3016.	7.4	19
101	A continuous fluorescence assay for phospholipase A2 with nontagged lipid. Analytical Biochemistry, 2006, 351, 11-17.	2.4	17
102	Allosteric sites can be identified based on the residue-residue interaction energy difference. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1375-1384.	2.6	17
103	Identification of acylthiourea derivatives as potent Plk1 PBD inhibitors. European Journal of Medicinal Chemistry, 2016, 124, 229-236.	5.5	17
104	CavitySpace: A Database of Potential Ligand Binding Sites in the Human Proteome. Biomolecules, 2022, 12, 967.	4.0	16
105	Construction of protein binding sites in scaffold structures. Biopolymers, 2000, 54, 515-523.	2.4	15
106	Discovery of Novel Polo-Like Kinase 1 Polo-Box Domain Inhibitors to Induce Mitotic Arrest in Tumor Cells. Journal of Medicinal Chemistry, 2016, 59, 7089-7096.	6.4	15
107	Novel mutations in the PLCZ1 gene associated with human low or failed fertilization. Molecular Genetics & Genomic Medicine, 2020, 8, e1470.	1.2	15
108	Quinoline-4-acetamides as sPLA2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 1639-1641.	2.2	14

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109	Charge Segregation in the Intrinsically Disordered Region Governs VRN1 and DNA Liquid-like Phase Separation Robustness. Journal of Molecular Biology, 2021, 433, 167269.	4.2	14
110	Uncovering the Dominant Motion Modes of Allosteric Regulation Improves Allosteric Site Prediction. Journal of Chemical Information and Modeling, 2022, 62, 187-195.	5.4	14
111	Data Mining of Toxic Chemicals: Structure Patterns and QSAR. Journal of Molecular Modeling, 1999, 5, 252-262.	1.8	13
112	Mechanism of DNAâ€Induced Phase Separation for Transcriptional Repressor VRN1. Angewandte Chemie, 2019, 131, 4912-4916.	2.0	13
113	Discovery of Targeted Covalent Natural Products against PLK1 by Herb-Based Screening. Journal of Chemical Information and Modeling, 2020, 60, 4350-4358.	5.4	12
114	A combined computational and experimental strategy identifies mutations conferring resistance to drugs targeting the BCR-ABL fusion protein. Communications Biology, 2020, 3, 18.	4.4	12
115	Optimization of 5-hydroxytryptamines as dual function inhibitors targeting phospholipase A2 and leukotriene A4 hydrolase. European Journal of Medicinal Chemistry, 2013, 59, 160-167.	5.5	11
116	Differential simulated annealing: a robust and efficient global optimization algorithm for parameter estimation of biological networks. Molecular BioSystems, 2014, 10, 1385-1392.	2.9	11
117	A novel allosteric inhibitor that prevents IKKÎ² activation. MedChemComm, 2018, 9, 239-243.	3.4	11
118	SYNTHESIS OF NOVEL DERIVATIVES OF 2-CYANO-3-METHYLTHIO-3â€²-BENZYLAMINO ACRYLATES(ACRYLAMIDES) AND THEIR BIOLOGICAL ACTIVITY. Phosphorus, Sulfur and Silicon and the Related Elements, 1999, 148, 235-241.	1.6	10
119	Design, Synthesis, and Evaluation of Dihydrobenzo[cd]indole-6-sulfonamide as TNF-Î± Inhibitors. Frontiers in Chemistry, 2018, 6, 98.	3.6	10
120	Correlation Between Allosteric and Orthosteric Sites. Advances in Experimental Medicine and Biology, 2019, 1163, 89-105.	1.6	10
121	Calculation of Protein Surface Loops Using Monte-Carlo Simulated Annealing Simulation. Journal of Molecular Modeling, 2000, 6, 1-8.	1.8	9
122	Quinoline-4-methyl esters as human nonpancreatic secretory phospholipase A2 inhibitors. Bioorganic and Medicinal Chemistry, 2011, 19, 3361-3366.	3.0	9
123	Development of 3,5-dinitrobenzoate-based 5-lipoxygenase inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 2396-2402.	3.0	9
124	Rational design of TNFÎ± binding proteins based on the de novo designed protein DS119. Protein Science, 2016, 25, 2066-2075.	7.6	9
125	Computational design and optimization of novel <scp>d</scp>â€peptide <scp>TNF</scp>Î± inhibitors. FEBS Letters, 2019, 593, 1292-1302.	2.8	9
126	Discovery of Nonâ€ATPâ€Competitive Inhibitors of Poloâ€like Kinaseâ€...1. ChemMedChem, 2016, 11, 713-717.	3.2	8

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127	Synthetic lethality in drug development: the dawn is coming. Future Medicinal Chemistry, 2018, 10, 2129-2132.	2.3	8
128	Discovery of Small Molecule Inhibitors Targeting the Sonic Hedgehog. Frontiers in Chemistry, 2020, 8, 498.	3.6	8
129	Ligand-based optimization and biological evaluation of N-(2,2,2-trichloro-1-(3-phenylthioureido)ethyl)acetamide derivatives as potent intrinsically disordered protein c-Myc inhibitors. Bioorganic and Medicinal Chemistry Letters, 2021, 31, 127711.	2.2	8
130	Discovery of 2-(furan-2-ylmethylene)hydrazine-1-carbothioamide derivatives as novel inhibitors of SARS-CoV-2 main protease. European Journal of Medicinal Chemistry, 2022, 238, 114508.	5.5	8
131	A new protein folding recognition potential function. Proteins: Structure, Function and Bioinformatics, 1995, 21, 127-129.	2.6	7
132	Grafting of Protein-Protein Interaction Epitope. Journal of Biomolecular Structure and Dynamics, 2000, 17, 821-828.	3.5	7
133	NF-ÎºB signaling and cell-fate decision induced by a fast-dissociating tumor necrosis factor mutant. Biochemical and Biophysical Research Communications, 2017, 489, 287-292.	2.1	7
134	How calcium ion binding induces the conformational transition of the calmodulin N-terminal domainâ€”an atomic level characterization. Physical Chemistry Chemical Physics, 2019, 21, 19795-19804.	2.8	7
135	Dimerization of PHGDH via the catalytic unit is essential for its enzymatic function. Journal of Biological Chemistry, 2021, 296, 100572.	3.4	7
136	Designed inhibitor for nuclear localization signal of poloâ€like kinase 1 induces mitotic arrest. Chemical Biology and Drug Design, 2017, 89, 732-740.	3.2	5
137	Singular value decomposition for the correlation of atomic fluctuations with arbitrary angle. Proteins: Structure, Function and Bioinformatics, 2018, 86, 1075-1087.	2.6	5
138	Integrative structural modeling of a multidomain polo-like kinase. Physical Chemistry Chemical Physics, 2020, 22, 27581-27589.	2.8	5
139	Modeling the third loop of short-chain snake venom neurotoxins: Roles of the short-range and long-range interactions. Proteins: Structure, Function and Bioinformatics, 2001, 42, 6-16.	2.6	4
140	Antibacterial properties of recombinant human non-pancreatic secretory phospholipase A2. Biochemical and Biophysical Research Communications, 2013, 441, 453-456.	2.1	4
141	Discovery of Novel Secretory Phospholipase A₂ Inhibitors Using Virtual Screen. Chemical Biology and Drug Design, 2014, 84, 216-222.	3.2	4
142	Germline mutations in theVHLgene associated with 3 different renal lesions in a Chinese von Hippel-Lindau disease family. Cancer Biology and Therapy, 2016, 17, 599-603.	3.4	4
143	Discovery of novel helix binding sites at protein-protein interfaces. Computational and Structural Biotechnology Journal, 2019, 17, 1396-1403.	4.1	4
144	Discovery of a New Chemoeffector for Escherichia coli Chemoreceptor Tsr and Identification of a Molecular Mechanism of Repellent Sensing. ACS Bio & Med Chem Au, 2022, 2, 386-394.	3.7	4

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145	Bio-rational design of photosystem II inhibitors (I). Science Bulletin, 1998, 43, 652-656.	1.7	3
146	Bio-rational design of photosystem II inhibitors (VIII). Science in China Series B: Chemistry, 1999, 42, 326-331.	0.8	3
147	Molecular recognition: monomer of the yeast transcriptional activator GCN4 recognizes its dimer DNA binding target sites specifically. Science in China Series B: Chemistry, 2000, 43, 466-476.	0.8	3
148	De novo design of helical peptides to inhibit tumor necrosis factor-Î± by disrupting its trimer formation. MedChemComm, 2016, 7, 725-729.	3.4	3
149	Protein Fibrils Formed by Rationally Designed Î±-Helical Peptides. Langmuir, 2020, 36, 6126-6131.	3.5	3
150	Predictive toxicology of chemicals and database mining. Science Bulletin, 2000, 45, 1093-1097.	1.7	2
151	Solidâ€phase synthesis, metal binding and folding properties of caulimovirusâ€related â€˜zinc fingerâ€™. International Journal of Peptide and Protein Research, 1996, 48, 461-464.	0.1	2
152	Tailoring Escherichia coli Chemotactic Sensing towards Cadmium by Computational Redesign of Ribose-Binding Protein. MSystems, 2022, , e0108421.	3.8	2
153	The Regulatory Roles of Intrinsically Disordered Linker in VRN1-DNA Phase Separation. International Journal of Molecular Sciences, 2022, 23, 4594.	4.1	2
154	Quantitative Analysis of Dynamic Allostery. Journal of Chemical Information and Modeling, 2022, 62, 2538-2549.	5.4	2
155	Receptor Mapping by Comparative Molecular Field Analysis of Phospholipase A₂ Inhibitors. Journal of the Chinese Chemical Society, 1995, 42, 739-744.	1.4	1
156	Grafting of protein-protein binding sites. Science Bulletin, 2000, 45, 1707-1712.	1.7	1
157	High activity of Mj HSP16.5 under acidic condition. Science in China Series B: Chemistry, 2009, 52, 325-331.	0.8	1
158	Investigating targets for neuropharmacological intervention by molecular dynamics simulations. Biochemical Society Transactions, 2019, 47, 909-918.	3.4	1
159	Efficient molecular encoders for virtual screening. Drug Discovery Today: Technologies, 2019, 32-33, 19-27.	4.0	1
160	Pinpointing Cancer Sub-Type Specific Metabolic Tasks Facilitates Identification of Anti-cancer Targets. Frontiers in Medicine, 2022, 9, 872024.	2.6	1
161	Rational screenning in combinatorial peptide libraries of protein functional loop. Science Bulletin, 1999, 44, 2150-2154.	1.7	0
162	Editorial overview: Allosteric assemblies. Current Opinion in Structural Biology, 2020, 62, vi-vii.	5.7	0

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163	Multiple Target Drug Design Using LigBuilder 3. Methods in Molecular Biology, 2021, 2266, 279-298.	0.9	0
164	Simplifying Submission Requirements for the Journal of Medicinal Chemistry. Journal of Medicinal Chemistry, 2021, 64, 7877-7878.	6.4	0
165	ePharmer : An integrated and graphical software for pharmacophoreâ€based virtual screening. Journal of Computational Chemistry, 2021, 42, 2181-2195.	3.3	0