Luhua Lai

List of Publications by Year
in descending order

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165 papers	9,413 citations	50170 46 h-index	46693 89 g-index
172 all docs	172 docs citations	172 times ranked	11754 citing authors

#	Article	IF	Citations
1	RALF peptide signaling controls the polytubey block in Arabidopsis. Science, 2022, 375, 290-296.	6.0	65
2	Tailoring Escherichia coli Chemotactic Sensing towards Cadmium by Computational Redesign of Ribose-Binding Protein. MSystems, 2022, , e0108421.	1.7	2
3	Uncovering the Dominant Motion Modes of Allosteric Regulation Improves Allosteric Site Prediction. Journal of Chemical Information and Modeling, 2022, 62, 187-195.	2.5	14
4	Prediction of liquidâ€“liquid phase separating proteins using machine learning. BMC Bioinformatics, 2022, 23, 72.	1.2	74
5	Pinpointing Cancer Sub-Type Specific Metabolic Tasks Facilitates Identification of Anti-cancer Targets. Frontiers in Medicine, 2022, 9, 872024.	1.2	1
6	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.	1.7	4
7	The Regulatory Roles of Intrinsically Disordered Linker in VRN1-DNA Phase Separation. International Journal of Molecular Sciences, 2022, 23, 4594.	1.8	2
8	Advances and Challenges in De Novo Drug Design Using Three-Dimensional Deep Generative Models. Journal of Chemical Information and Modeling, 2022, 62, 2269-2279.	2.5	25
9	Quantitative Analysis of Dynamic Allostery. Journal of Chemical Information and Modeling, 2022, 62, 2538-2549.	2.5	2
10	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.	2.6	8
11	CavitySpace: A Database of Potential Ligand Binding Sites in the Human Proteome. Biomolecules, 2022, 12, 967.	1.8	16
12	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.	1.0	8
13	Dimerization of PHGDH via the catalytic unit is essential for its enzymatic function. Journal of Biological Chemistry, 2021, 296, 100572.	1.6	7
14	Multiple Target Drug Design Using LigBuilder 3. Methods in Molecular Biology, 2021, 2266, 279-298.	0.4	0
15	Structure-based de novo drug design using 3D deep generative models. Chemical Science, 2021, 12, 13664-13675.	3.7	82
16	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.	7.1	25
17	Allosteric Type and Pathways Are Governed by the Forces of Proteinâ€“Ligand Binding. Journal of Physical Chemistry Letters, 2021, 12, 5404-5412.	2.1	20
18	A transferable deep learning approach to fast screen potential antiviral drugs against SARS-CoV-2. Briefings in Bioinformatics, 2021, 22, .	3.2	29

#	Article	IF	Citations
19	Simplifying Submission Requirements for the Journal of Medicinal Chemistry. Journal of Medicinal Chemistry, 2021, 64, 7877-7878.	2.9	0
20	ePharmer : An integrated and graphical software for pharmacophoreâ€based virtual screening. Journal of Computational Chemistry, 2021, 42, 2181-2195.	1.5	0
21	Charge Segregation in the Intrinsically Disordered Region Governs VRN1 and DNA Liquid-like Phase Separation Robustness. Journal of Molecular Biology, 2021, 433, 167269.	2.0	14
22	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.	3.7	19
23	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.	2.5	206
24	Transfer Learning for Drug Discovery. Journal of Medicinal Chemistry, 2020, 63, 8683-8694.	2.9	178
25	Potent inhibitors of SARS-CoV-2 3C-like protease derived from N-substituted isatin compounds. European Journal of Medicinal Chemistry, 2020, 206, 112702.	2.6	45
26	Glycopeptide Self-Assembly Modulated by Glycan Stereochemistry through Glycanâ€“Aromatic Interactions. Journal of the American Chemical Society, 2020, 142, 17015-17023.	6.6	21
27	Novel mutations in the PLCZ1 gene associated with human low or failed fertilization. Molecular Genetics & Genomic Medicine, 2020, 8, e1470.	0.6	15
28	Discovery of Targeted Covalent Natural Products against PLK1 by Herb-Based Screening. Journal of Chemical Information and Modeling, 2020, 60, 4350-4358.	2.5	12
29	Protein Fibrils Formed by Rationally Designed Î±-Helical Peptides. Langmuir, 2020, 36, 6126-6131.	1.6	3
30	Chemical perturbations reveal that RUVBL2 regulates the circadian phase in mammals. Science Translational Medicine, 2020, 12, .	5.8	25
31	Editorial overview: Allosteric assemblies. Current Opinion in Structural Biology, 2020, 62, vi-vii.	2.6	0
32	Discovery of Small Molecule Inhibitors Targeting the Sonic Hedgehog. Frontiers in Chemistry, 2020, 8, 498.	1.8	8
33	LigBuilder V3: A Multi-Target de novo Drug Design Approach. Frontiers in Chemistry, 2020, 8, 142.	1.8	46
34	Automatic retrosynthetic route planning using template-free models. Chemical Science, 2020, 11, 3355-3364.	3.7	105
35	Protein topology and allostery. Current Opinion in Structural Biology, 2020, 62, 158-165.	2.6	22
36	Allostery of multidomain proteins with disordered linkers. Current Opinion in Structural Biology, 2020, 62, 175-182.	2.6	28

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37	A combined computational and experimental strategy identifies mutations conferring resistance to drugs targeting the BCR-ABL fusion protein. Communications Biology, 2020, 3, 18.	2.0	12
38	Integrative structural modeling of a multidomain polo-like kinase. Physical Chemistry Chemical Physics, 2020, 22, 27581-27589.	1.3	5
39	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.	1.3	7
40	Identification of Cancerâ€"associated metabolic vulnerabilities by modeling multi-objective optimality in metabolism. Cell Communication and Signaling, 2019, 17, 124.	2.7	19
41	Deep learning for molecular generation. Future Medicinal Chemistry, 2019, 11, 567-597.	1.1	88
42	Efficient ligand discovery from natural herbs by integrating virtual screening, affinity mass spectrometry and targeted metabolomics. Analyst, The, 2019, 144, 2881-2890.	1.7	25
43	Computational design and optimization of novel <scp>d</scp>â€peptide <scp>TNF</scp>Î± inhibitors. FEBS Letters, 2019, 593, 1292-1302.	1.3	9
44	Investigating targets for neuropharmacological intervention by molecular dynamics simulations. Biochemical Society Transactions, 2019, 47, 909-918.	1.6	1
45	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.	0.5	27
46	Mechanism of DNAâ€Induced Phase Separation for Transcriptional Repressor VRN1. Angewandte Chemie, 2019, 131, 4912-4916.	1.6	13
47	Mechanism of DNAâ€Induced Phase Separation for Transcriptional Repressor VRN1. Angewandte Chemie - International Edition, 2019, 58, 4858-4862.	7.2	69
48	Efficient molecular encoders for virtual screening. Drug Discovery Today: Technologies, 2019, 32-33, 19-27.	4.0	1
49	Discovery of novel helix binding sites at protein-protein interfaces. Computational and Structural Biotechnology Journal, 2019, 17, 1396-1403.	1.9	4
50	Self-Learning Perfect Optical Chirality via a Deep Neural Network. Physical Review Letters, 2019, 123, 213902.	2.9	72
51	Legionella effector SetA as a general O-glucosyltransferase for eukaryotic proteins. Nature Chemical Biology, 2019, 15, 213-216.	3.9	21
52	Targeting intrinsically disordered proteins at the edge of chaos. Drug Discovery Today, 2019, 24, 217-227.	3.2	98
53	Novel Allosteric Activators for Ferroptosis Regulator Glutathione Peroxidase 4. Journal of Medicinal Chemistry, 2019, 62, 266-275.	2.9	91
54	Correlation Between Allosteric and Orthosteric Sites. Advances in Experimental Medicine and Biology, 2019, 1163, 89-105.	0.8	10

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55	A novel allosteric inhibitor that prevents IKKÎ² activation. MedChemComm, 2018, 9, 239-243.	3.5	11
56	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.	1.2	35
57	Prediction of Drug-Likeness Using Deep Autoencoder Neural Networks. Frontiers in Genetics, 2018, 9, 585.	1.1	43
58	Serine synthesis through PHGDH coordinates nucleotide levels by maintaining central carbon metabolism. Nature Communications, 2018, 9, 5442.	5.8	143
59	Activation of Glutathione Peroxidase 4 as a Novel Anti-inflammatory Strategy. Frontiers in Pharmacology, 2018, 9, 1120.	1.6	98
60	An autoimmune disease variant of IgG1 modulates B cell activation and differentiation. Science, 2018, 362, 700-705.	6.0	28
61	Prediction of Human Cytochrome P450 Inhibition Using a Multitask Deep Autoencoder Neural Network. Molecular Pharmaceutics, 2018, 15, 4336-4345.	2.3	85
62	Synthetic lethality in drug development: the dawn is coming. Future Medicinal Chemistry, 2018, 10, 2129-2132.	1.1	8
63	Singular value decomposition for the correlation of atomic fluctuations with arbitrary angle. Proteins: Structure, Function and Bioinformatics, 2018, 86, 1075-1087.	1.5	5
64	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.	3.1	25
65	Design, Synthesis, and Evaluation of Dihydrobenzo[cd]indole-6-sulfonamide as TNF-Î± Inhibitors. Frontiers in Chemistry, 2018, 6, 98.	1.8	10
66	Computational Chemical Synthesis Analysis and Pathway Design. Frontiers in Chemistry, 2018, 6, 199.	1.8	41
67	Molecular mechanism of 15-lipoxygenase allosteric activation and inhibition. Physical Chemistry Chemical Physics, 2018, 20, 14785-14795.	1.3	21
68	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.	6.5	226
69	Computational Multitarget Drug Design. Journal of Chemical Information and Modeling, 2017, 57, 403-412.	2.5	149
70	PharmMapper 2017 update: a web server for potential drug target identification with a comprehensive target pharmacophore database. Nucleic Acids Research, 2017, 45, W356-W360.	6.5	802
71	Statistical Analysis and Prediction of Covalent Ligand Targeted Cysteine Residues. Journal of Chemical Information and Modeling, 2017, 57, 1453-1460.	2.5	23
72	Sequence-based prediction of protein protein interaction using a deep-learning algorithm. BMC Bioinformatics, 2017, 18, 277.	1.2	278

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73	NF-Î²B signaling and cell-fate decision induced by a fast-dissociating tumor necrosis factor mutant. Biochemical and Biophysical Research Communications, 2017, 489, 287-292.	1.0	7
74	Rational Design of Selective Allosteric Inhibitors of PHGDH and Serine Synthesis with Anti-tumor Activity. Cell Chemical Biology, 2017, 24, 55-65.	2.5	102
75	Computational design of ligand-binding proteins. Current Opinion in Structural Biology, 2017, 45, 67-73.	2.6	33
76	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.	2.5	179
77	Origin of the Reflectin Gene and Hierarchical Assembly of Its Protein. Current Biology, 2017, 27, 2833-2842.e6.	1.8	39
78	Tuning SpyTagâ€“SpyCatcher mutant pairs toward orthogonal reactivity encryption. Chemical Science, 2017, 8, 6577-6582.	3.7	31
79	Arabidopsis pollen tube integrity and sperm release are regulated by RALF-mediated signaling. Science, 2017, 358, 1596-1600.	6.0	324
80	Designed inhibitor for nuclear localization signal of poloâ€like kinase 1 induces mitotic arrest. Chemical Biology and Drug Design, 2017, 89, 732-740.	1.5	5
81	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.	1.6	20
82	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.	1.5	4
83	A Flux Balance of Glucose Metabolism Clarifies the Requirements of the Warburg Effect. Biophysical Journal, 2016, 111, 1088-1100.	0.2	42
84	Rational design of TNFÎ± binding proteins based on the de novo designed protein DS119. Protein Science, 2016, 25, 2066-2075.	3.1	9
85	Motions of Allosteric and Orthosteric Ligand-Binding Sites in Proteins are Highly Correlated. Journal of Chemical Information and Modeling, 2016, 56, 1725-1733.	2.5	70
86	Identification of acylthiourea derivatives as potent Plk1 PBD inhibitors. European Journal of Medicinal Chemistry, 2016, 124, 229-236.	2.6	17
87	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.	2.9	15
88	Structure-based Inhibitor Design for the Intrinsically Disordered Protein c-Myc. Scientific Reports, 2016, 6, 22298.	1.6	79
89	Herb-target interaction network analysis helps to disclose molecular mechanism of traditional Chinese medicine. Scientific Reports, 2016, 6, 36767.	1.6	26
90	Novel Inhibitors of Toxin HipA Reduce Multidrug Tolerant Persisters. ACS Medicinal Chemistry Letters, 2016, 7, 449-453.	1.3	23

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91	Discovery of Nonâ€ATPâ€Competitive Inhibitors of Poloâ€like Kinaseâ€…1. ChemMedChem, 2016, 11, 713-717.	1.6	8
92	De novo design of helical peptides to inhibit tumor necrosis factor-Î± by disrupting its trimer formation. MedChemComm, 2016, 7, 725-729.	3.5	3
93	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.	2.9	43
94	Both piston-like and rotational motions are present in bacterial chemoreceptor signaling. Scientific Reports, 2015, 5, 8640.	1.6	39
95	Diverse Ways of Perturbing the Human Arachidonic Acid Metabolic Network To Control Inflammation. Accounts of Chemical Research, 2015, 48, 2242-2250.	7.6	59
96	Deep Learning for Drug-Induced Liver Injury. Journal of Chemical Information and Modeling, 2015, 55, 2085-2093.	2.5	264
97	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.	0.5	20
98	Allosteric sites can be identified based on the residue-residue interaction energy difference. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1375-1384.	1.5	17
99	De Novo Design of Multitarget Ligands with an Iterative Fragment-Growing Strategy. Journal of Chemical Information and Modeling, 2014, 54, 1235-1241.	2.5	54
100	Discovery of Novel Secretory Phospholipase A₂ Inhibitors Using Virtual Screen. Chemical Biology and Drug Design, 2014, 84, 216-222.	1.5	4
101	Development of 3,5-dinitrobenzoate-based 5-lipoxygenase inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 2396-2402.	1.4	9
102	A protein engineered to bind uranyl selectively and with femtomolar affinity. Nature Chemistry, 2014, 6, 236-241.	6.6	262
103	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
104	Systems Biology Brings New Dimensions for Structure-Based Drug Design. Journal of the American Chemical Society, 2014, 136, 11556-11565.	6.6	75
105	Discovery of highly potent TNFÎ± inhibitors using virtual screen. European Journal of Medicinal Chemistry, 2014, 85, 119-126.	2.6	20
106	iDrug: a web-accessible and interactive drug discovery and design platform. Journal of Cheminformatics, 2014, 6, 28.	2.8	30
107	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.	1.0	31
108	Synergistic and Antagonistic Drug Combinations Depend on Network Topology. PLoS ONE, 2014, 9, e93960.	1.1	99

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109	Discovery of Novel Allosteric Effectors Based on the Predicted Allosteric Sites for Escherichia coli D-3-Phosphoglycerate Dehydrogenase. PLoS ONE, 2014, 9, e94829.	1.1	26
110	Protein-Protein Interface Analysis and Hot Spots Identification for Chemical Ligand Design. Current Pharmaceutical Design, 2014, 20, 1192-1200.	0.9	23
111	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
112	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.	3.3	46
113	Antibacterial properties of recombinant human non-pancreatic secretory phospholipase A2. Biochemical and Biophysical Research Communications, 2013, 441, 453-456.	1.0	4
114	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.	2.9	30
115	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
116	Optimization of 5-hydroxytryptamines as dual function inhibitors targeting phospholipase A2 and leukotriene A4 hydrolase. European Journal of Medicinal Chemistry, 2013, 59, 160-167.	2.6	11
117	Ligand Clouds around Protein Clouds: A Scenario of Ligand Binding with Intrinsically Disordered Proteins. PLoS Computational Biology, 2013, 9, e1003249.	1.5	79
118	Computational Design of Helical Peptides Targeting TNFÎ±. Angewandte Chemie - International Edition, 2013, 52, 11059-11062.	7.2	19
119	Binding Site Detection and Druggability Prediction of Protein Targets for Structure- Based Drug Design. Current Pharmaceutical Design, 2013, 19, 2326-2333.	0.9	167
120	Dynamic Modeling of Human 5-Lipoxygenaseâ€“Inhibitor Interactions Helps To Discover Novel Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 2597-2605.	2.9	56
121	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.	2.3	46
122	Dynamic eicosanoid responses upon different inhibitor and combination treatments on the arachidonic acid metabolic network. Molecular BioSystems, 2012, 8, 1585.	2.9	39
123	Discovery of Dual Target Inhibitors against Cyclooxygenases and Leukotriene A₄ Hydrolyase. Journal of Medicinal Chemistry, 2011, 54, 3650-3660.	2.9	44
124	LigBuilder 2: A Practical de Novo Drug Design Approach. Journal of Chemical Information and Modeling, 2011, 51, 1083-1091.	2.5	170
125	Quinoline-4-methyl esters as human nonpancreatic secretory phospholipase A2 inhibitors. Bioorganic and Medicinal Chemistry, 2011, 19, 3361-3366.	1.4	9
126	Maturation Mechanism of Severe Acute Respiratory Syndrome (SARS) Coronavirus 3C-like Proteinase. Journal of Biological Chemistry, 2010, 285, 28134-28140.	1.6	50

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127	High activity of Mj HSP16.5 under acidic condition. Science in China Series B: Chemistry, 2009, 52, 325-331.	0.8	1
128	Discovering Potent Small Molecule Inhibitors of Cyclophilin A Using de Novo Drug Design Approach. Journal of Medicinal Chemistry, 2009, 52, 5295-5298.	2.9	92
129	Activation and inhibition of leukotriene A4 hydrolase aminopeptidase activity by diphenyl ether and derivatives. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 6549-6552.	1.0	29
130	Finding multiple target optimal intervention in diseaseâ€related molecular network. Molecular Systems Biology, 2008, 4, 228.	3.2	165
131	Discovery of Multitarget Inhibitors by Combining Molecular Docking with Common Pharmacophore Matching. Journal of Medicinal Chemistry, 2008, 51, 7882-7888.	2.9	128
132	Dynamic Simulations on the Arachidonic Acid Metabolic Network. PLoS Computational Biology, 2007, 3, e55.	1.5	90
133	Pocket v.2:â€‰ Further Developments on Receptor-Based Pharmacophore Modeling. Journal of Chemical Information and Modeling, 2006, 46, 2684-2691.	2.5	117
134	Isatin Compounds as Noncovalent SARS Coronavirus 3C-like Protease Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 3440-3443.	2.9	110
135	A continuous fluorescence assay for phospholipase A2 with nontagged lipid. Analytical Biochemistry, 2006, 351, 11-17.	1.1	17
136	Quaternary Structure, Substrate Selectivity and Inhibitor Design for SARS 3C-Like Proteinase. Current Pharmaceutical Design, 2006, 12, 4555-4564.	0.9	28
137	Biosynthesis, Purification, and Substrate Specificity of Severe Acute Respiratory Syndrome Coronavirus 3C-like Proteinase. Journal of Biological Chemistry, 2004, 279, 1637-1642.	1.6	280
138	3C-like Proteinase from SARS Coronavirus Catalyzes Substrate Hydrolysis by a General Base Mechanism. Biochemistry, 2004, 43, 4568-4574.	1.2	189
139	Quinoline-4-acetamides as sPLA2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 1639-1641.	1.0	14
140	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.	1.5	4
141	Protein ligand docking based on empirical method for binding affinity estimation. , 2001, 15, 429-446.		27
142	Construction of protein binding sites in scaffold structures. Biopolymers, 2000, 54, 515-523.	1.2	15
143	Calculating partition coefficient by atom-additive method. Journal of Computer - Aided Molecular Design, 2000, 19, 47-66.	1.0	172
144	Calculation of Protein Surface Loops Using Monte-Carlo Simulated Annealing Simulation. Journal of Molecular Modeling, 2000, 6, 1-8.	0.8	9

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145	Predictive toxicology of chemicals and database mining. Science Bulletin, 2000, 45, 1093-1097.	1.7	2
146	Grafting of protein-protein binding sites. Science Bulletin, 2000, 45, 1707-1712.	1.7	1
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	LigBuilder: A Multi-Purpose Program for Structure-Based Drug Design. Journal of Molecular Modeling, 2000, 6, 498-516.	0.8	249
149	Grafting of Protein-Protein Interaction Epitope. Journal of Biomolecular Structure and Dynamics, 2000, 17, 821-828.	2.0	7
150	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.	0.8	10
151	Rational screenning in combinatorial peptide libraries of protein functional loop. Science Bulletin, 1999, 44, 2150-2154.	1.7	0
152	Bio-rational design of photosystem II inhibitors (VIII). Science in China Series B: Chemistry, 1999, 42, 326-331.	0.8	3
153	Calculating Partition Coefficients of Peptides by the Addition Method. Journal of Molecular Modeling, 1999, 5, 189-195.	0.8	38
154	Data Mining of Toxic Chemicals: Structure Patterns and QSAR. Journal of Molecular Modeling, 1999, 5, 252-262.	0.8	13
155	Protein loops on structurally similar scaffolds: Database and conformational analysis. , 1999, 49, 481-495.		32
156	Structural Features of Toxic Chemicals for Specific Toxicity. Journal of Chemical Information and Computer Sciences, 1999, 39, 1173-1189.	2.8	21
157	All-Orientation Search and All-Placement Search in Comparative Molecular Field Analysis. Journal of Molecular Modeling, 1998, 4, 276-283.	0.8	67
158	SCORE: A New Empirical Method for Estimating the Binding Affinity of a Protein-Ligand Complex. Journal of Molecular Modeling, 1998, 4, 379-394.	0.8	275
159	Bio-rational design of photosystem II inhibitors (I). Science Bulletin, 1998, 43, 652-656.	1.7	3
160	A New Atom-Additive Method for Calculating Partition Coefficients. Journal of Chemical Information and Computer Sciences, 1997, 37, 615-621.	2.8	399
161	A fast and efficient program for modeling protein loops. Biopolymers, 1997, 41, 61-72.	1.2	35
162	RASSE:â€‰ A New Method for Structure-Based Drug Design. Journal of Chemical Information and Computer Sciences, 1996, 36, 1187-1194.	2.8	39

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163	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
164	A new protein folding recognition potential function. Proteins: Structure, Function and Bioinformatics, 1995, 21, 127-129.	1.5	7
165	Receptor Mapping by Comparative Molecular Field Analysis of Phospholipase A₂ Inhibitors. Journal of the Chinese Chemical Society, 1995, 42, 739-744.	0.8	1