Xiaoqin Zou

List of Publications by Year
in descending order

73 papers	4,552 citations	117625 34 h-index	106344 65 g-index
76 all docs	76 docs citations	76 times ranked	4438 citing authors

#	Article	IF	Citations
1	Predicting Proteinâ€“Peptide Complex Structures by Accounting for Peptide Flexibility and the Physicochemical Environment. Journal of Chemical Information and Modeling, 2022, 62, 27-39.	5.4	13
2	Carbohydrate-protein interactions: advances and challenges. Communications in Information and Systems, 2021, 21, 147-163.	0.5	9
3	Rapid Identification of Inhibitors and Prediction of Ligand Selectivity for Multiple Proteins: Application to Protein Kinases. Journal of Physical Chemistry B, 2021, 125, 2288-2298.	2.6	3
4	The three-way junction structure of the HIV-1 PBS-segment binds host enzyme important for viral infectivity. Nucleic Acids Research, 2021, 49, 5925-5942.	14.5	9
5	Modulating the voltage sensor of a cardiac potassium channel shows antiarrhythmic effects. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	6
6	INI1/SMARCB1 Rpt1 domain mimics TAR RNA in binding to integrase to facilitate HIV-1 replication. Nature Communications, 2021, 12, 2743.	12.8	9
7	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	2.6	73
8	MDock: A Suite for Molecular Inverse Docking and Target Prediction. Methods in Molecular Biology, 2021, 2266, 313-322.	0.9	7
9	A Selective Tether Recruits Activated Response Regulator CheB to Its Chemoreceptor Substrate. MBio, 2021, 12, e0310621.	4.1	4
10	Dissimilar Ligands Bind in a Similar Fashion: A Guide to Ligand Binding-Mode Prediction with Application to CELPP Studies. International Journal of Molecular Sciences, 2021, 22, 12320.	4.1	6
11	TRIC-A Channel Maintains Store Calcium Handling by Interacting With Type 2 Ryanodine Receptor in Cardiac Muscle. Circulation Research, 2020, 126, 417-435.	4.5	19
12	PepPro: A Nonredundant Structure Data Set for Benchmarking Peptideâ€“Protein Computational Docking. Journal of Computational Chemistry, 2020, 41, 362-369.	3.3	13
13	A PIP2 substitute mediates voltage sensor-pore coupling in KCNQ activation. Communications Biology, 2020, 3, 385.	4.4	22
14	Structural basis of prostate-specific membrane antigen recognition by the A9g RNA aptamer. Nucleic Acids Research, 2020, 48, 11130-11145.	14.5	15
15	Performance of human and server prediction in <scp>CAPRI</scp> rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1110-1120.	2.6	6
16	Two-stage electroâ€“mechanical coupling of a KV channel in voltage-dependent activation. Nature Communications, 2020, 11, 676.	12.8	46
17	Binding interface and impact on protease cleavage for an RNA aptamer to HIV-1 reverse transcriptase. Nucleic Acids Research, 2020, 48, 2709-2722.	14.5	22
18	Scoring functions for protein-RNA complex structure prediction: advances, applications, and future directions. Communications in Information and Systems, 2020, 20, 1-22.	0.5	3

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19	MDockPeP: A Web Server for Blind Prediction of Proteinâ€“Peptide Complex Structures. Methods in Molecular Biology, 2020, 2165, 259-272.	0.9	4
20	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
21	Predicting proteinâ€“ligand binding modes for CELPP and GC3: workflows and insight. Journal of Computer-Aided Molecular Design, 2019, 33, 367-374.	2.9	11
22	Identifying the molecular target sites for CFTR potentiators GLPG1837 and VX-770. Journal of General Physiology, 2019, 151, 912-928.	1.9	57
23	Docking-based inverse virtual screening: methods, applications, and challenges. Biophysics Reports, 2018, 4, 1-16.	0.8	99
24	MDockServer: An Efficient Docking Platform for Inverse Virtual Screening. Biophysical Journal, 2018, 114, 56a.	0.5	1
25	Lessons learned from participating in D3R 2016 Grand Challenge 2: compounds targeting the farnesoid X receptor. Journal of Computer-Aided Molecular Design, 2018, 32, 103-111.	2.9	12
26	MDockPeP: An abâ€initio proteinâ€“peptide docking server. Journal of Computational Chemistry, 2018, 39, 2409-2413.	3.3	59
27	The Usage of ACCLUSTER for Peptide Binding Site Prediction. Methods in Molecular Biology, 2017, 1561, 3-9.	0.9	2
28	Modeling of flux, binding and substitution of urea molecules in the urea transporter dvUT. Journal of Molecular Graphics and Modelling, 2017, 76, 504-511.	2.4	3
29	Performance of MDockPP in CAPRI rounds 28â€29 and 31â€35 including the prediction of waterâ€mediated interactions. Proteins: Structure, Function and Bioinformatics, 2017, 85, 424-434.	2.6	11
30	Improving binding mode and binding affinity predictions of docking by ligand-based search of protein conformations: evaluation in D3R grand challenge 2015. Journal of Computer-Aided Molecular Design, 2017, 31, 689-699.	2.9	15
31	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	2.6	148
32	SM-TF: A structural database of small molecule-transcription factor complexes. Journal of Computational Chemistry, 2016, 37, 1559-1564.	3.3	4
33	Fully Blind Docking at the Atomic Level for Protein-Peptide Complex Structure Prediction. Structure, 2016, 24, 1842-1853.	3.3	86
34	Iterative Knowledge-Based Scoring Functions Derived from Rigid and Flexible Decoy Structures: Evaluation with the 2013 and 2014 CSAR Benchmarks. Journal of Chemical Information and Modeling, 2016, 56, 1013-1021.	5.4	21
35	MDock: An Ensemble Docking Suite for Molecular Docking, Scoring and In Silico Screening. Methods in Pharmacology and Toxicology, 2015, , 153-166.	0.2	8
36	Computation and Simulation of the Structural Characteristics of the Kidney Urea Transporter and Behaviors of Urea Transport. Journal of Physical Chemistry B, 2015, 119, 5124-5131.	2.6	13

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37	Predicting peptide binding sites on protein surfaces by clustering chemical interactions. Journal of Computational Chemistry, 2015, 36, 49-61.	3.3	41
38	A knowledge-based scoring function for protein-RNA interactions derived from a statistical mechanics-based iterative method. Nucleic Acids Research, 2014, 42, e55-e55.	14.5	110
39	A Bayesian statistical approach of improving knowledgeâ€based scoring functions for proteinâ€“ligand interactions. Journal of Computational Chemistry, 2014, 35, 932-943.	3.3	10
40	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	2.6	50
41	Challenges, Applications, and Recent Advances of Protein-Ligand Docking in Structure-Based Drug Design. Molecules, 2014, 19, 10150-10176.	3.8	163
42	ITScorePro: An Efficient Scoring Program for Evaluating the Energy Scores of Protein Structures for Structure Prediction. Methods in Molecular Biology, 2014, 1137, 71-81.	0.9	5
43	Inclusion of the orientational entropic effect and lowâ€resolution experimental information for proteinâ€“protein docking in Critical Assessment of PRedicted Interactions (CAPRI). Proteins: Structure, Function and Bioinformatics, 2013, 81, 2183-2191.	2.6	18
44	A nonredundant structure dataset for benchmarking proteinâ€RNA computational docking. Journal of Computational Chemistry, 2013, 34, 311-318.	3.3	46
45	Automated Large-Scale File Preparation, Docking, and Scoring: Evaluation of ITScore and STScore Using the 2012 Community Structureâ€“Activity Resource Benchmark. Journal of Chemical Information and Modeling, 2013, 53, 1905-1914.	5.4	18
46	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	2.6	87
47	Rational Truncation of an RNA Aptamer to Prostate-Specific Membrane Antigen Using Computational Structural Modeling. Nucleic Acid Therapeutics, 2011, 21, 299-314.	3.6	106
48	Construction and Test of Ligand Decoy Sets Using MDock: Community Structureâ€“Activity Resource Benchmarks for Binding Mode Prediction. Journal of Chemical Information and Modeling, 2011, 51, 2107-2114.	5.4	21
49	Scoring and Lessons Learned with the CSAR Benchmark Using an Improved Iterative Knowledge-Based Scoring Function. Journal of Chemical Information and Modeling, 2011, 51, 2097-2106.	5.4	31
50	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	4.2	131
51	Statistical mechanicsâ€based method to extract atomic distanceâ€dependent potentials from protein structures. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2648-2661.	2.6	60
52	An inverse docking approach for identifying new potential anti-cancer targets. Journal of Molecular Graphics and Modelling, 2011, 29, 795-799.	2.4	60
53	MDockPP: A hierarchical approach for proteinâ€protein docking and its application to CAPRI rounds 15â€“19. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3096-3103.	2.6	65
54	Ion sensing in the RCK1 domain of BK channels. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 18700-18705.	7.1	78

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55	Advances and Challenges in Protein-Ligand Docking. International Journal of Molecular Sciences, 2010, 11, 3016-3034.	4.1	418
56	Scoring functions and their evaluation methods for proteinâ€“ligand docking: recent advances and future directions. Physical Chemistry Chemical Physics, 2010, 12, 12899.	2.8	380
57	Mean-Force Scoring Functions for Proteinâ€“Ligand Binding. Annual Reports in Computational Chemistry, 2010, , 280-296.	1.7	11
58	Inclusion of Solvation and Entropy in the Knowledge-Based Scoring Function for Proteinâ^'Ligand Interactions. Journal of Chemical Information and Modeling, 2010, 50, 262-273.	5.4	118
59	Molecular modeling of the heterodimer of human CFTRâ€™s nucleotide-binding domains using a proteinâ€“protein docking approach. Journal of Molecular Graphics and Modelling, 2009, 27, 822-828.	2.4	31
60	Multiscale Generalized Born Modeling of Ligand Binding Energies for Virtual Database Screening. Journal of Physical Chemistry B, 2009, 113, 11793-11799.	2.6	11
61	An iterative knowledgeâ€based scoring function for proteinâ€“protein recognition. Proteins: Structure, Function and Bioinformatics, 2008, 72, 557-579.	2.6	242
62	Electrostatics of Ligand Binding:Â Parametrization of the Generalized Born Model and Comparison with the Poissonâ^'Boltzmann Approach. Journal of Physical Chemistry B, 2006, 110, 9304-9313.	2.6	48
63	Ensemble docking of multiple protein structures: Considering protein structural variations in molecular docking. Proteins: Structure, Function and Bioinformatics, 2006, 66, 399-421.	2.6	314
64	Efficient molecular docking of NMR structures: Application to HIV-1 protease. Protein Science, 2006, 16, 43-51.	7.6	93
65	An iterative knowledge-based scoring function to predict proteinâ€“ligand interactions: I. Derivation of interaction potentials. Journal of Computational Chemistry, 2006, 27, 1866-1875.	3.3	167
66	An iterative knowledge-based scoring function to predict proteinâ€“ligand interactions: II. Validation of the scoring function. Journal of Computational Chemistry, 2006, 27, 1876-1882.	3.3	141
67	The Two ATP Binding Sites of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) Play Distinct Roles in Gating Kinetics and Energetics. Journal of General Physiology, 2006, 128, 413-422.	1.9	71
68	High affinity ATP/ADP analogues as new tools for studying CFTR gating. Journal of Physiology, 2005, 569, 447-457.	2.9	45
69	CFTR Gating II. Journal of General Physiology, 2005, 125, 377-394.	1.9	52
70	Pairwise GB/SA Scoring Function for Structure-based Drug Design. Journal of Physical Chemistry B, 2004, 108, 5453-5462.	2.6	56
71	ATP Hydrolysis-Coupled Gating of CFTR Chloride Channels:â€‰ Structure and Function. Biochemistry, 2001, 40, 5579-5586.	2.5	22
72	Design, docking, and evaluation of multiple libraries against multiple targets. Proteins: Structure, Function and Bioinformatics, 2001, 42, 296-318.	2.6	66

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73	Inclusion of Solvation in Ligand Binding Free Energy Calculations Using the Generalized-Born Model. Journal of the American Chemical Society, 1999, 121, 8033-8043.	13.7	228