Renxiao Wang

List of Publications by Year
in descending order

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60 papers	10,436 citations	101543 36 h-index	144013 57 g-index
60 all docs	60 docs citations	60 times ranked	10004 citing authors

#	Article	IF	Citations
1	Further development and validation of empirical scoring functions for structure-based binding affinity prediction. Journal of Computer-Aided Molecular Design, 2002, 16, 11-26.	2.9	1,012
2	Comparative Evaluation of 11 Scoring Functions for Molecular Docking. Journal of Medicinal Chemistry, 2003, 46, 2287-2303.	6.4	834
3	The PDBbind Database:Â Collection of Binding Affinities for Proteinâ^'Ligand Complexes with Known Three-Dimensional Structures. Journal of Medicinal Chemistry, 2004, 47, 2977-2980.	6.4	787
4	The PDBbind Database:Â Methodologies and Updates. Journal of Medicinal Chemistry, 2005, 48, 4111-4119.	6.4	632
5	Computation of Octanolâ^'Water Partition Coefficients by Guiding an Additive Model with Knowledge. Journal of Chemical Information and Modeling, 2007, 47, 2140-2148.	5.4	601
6	Development and optimization of a binding assay for the XIAP BIR3 domain using fluorescence polarization. Analytical Biochemistry, 2004, 332, 261-273.	2.4	479
7	A low-molecular-weight compound discovered through virtual database screening inhibits Stat3 function in breast cancer cells. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 4700-4705.	7.1	460
8	Comparative Assessment of Scoring Functions on a Diverse Test Set. Journal of Chemical Information and Modeling, 2009, 49, 1079-1093.	5.4	444
9	A New Atom-Additive Method for Calculating Partition Coefficients. Journal of Chemical Information and Computer Sciences, 1997, 37, 615-621.	2.8	399
10	PDB-wide collection of binding data: current status of the PDBbind database. Bioinformatics, 2015, 31, 405-412.	4.1	375
11	Comparative Assessment of Scoring Functions: The CASF-2016 Update. Journal of Chemical Information and Modeling, 2019, 59, 895-913.	5.4	367
12	Discovery of Embelin as a Cell-Permeable, Small-Molecular Weight Inhibitor of XIAP through Structure-Based Computational Screening of a Traditional Herbal Medicine Three-Dimensional Structure Database. Journal of Medicinal Chemistry, 2004, 47, 2430-2440.	6.4	335
13	Comparative Assessment of Scoring Functions on an Updated Benchmark: 2. Evaluation Methods and General Results. Journal of Chemical Information and Modeling, 2014, 54, 1717-1736.	5.4	294
14	How Does Consensus Scoring Work for Virtual Library Screening? An Idealized Computer Experiment. Journal of Chemical Information and Computer Sciences, 2001, 41, 1422-1426.	2.8	279
15	Evaluation of the performance of four molecular docking programs on a diverse set of proteinâ€ligand complexes. Journal of Computational Chemistry, 2010, 31, 2109-2125.	3.3	277
16	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
17	Structure-Based Design of Potent Small-Molecule Inhibitors of Anti-Apoptotic Bcl-2 Proteins. Journal of Medicinal Chemistry, 2006, 49, 6139-6142.	6.4	274
18	Forging the Basis for Developing Proteinâ€"Ligand Interaction Scoring Functions. Accounts of Chemical Research, 2017, 50, 302-309.	15.6	257

#	Article	IF	Citations
19	An Extensive Test of 14 Scoring Functions Using the PDBbind Refined Set of 800 Proteinâ^'Ligand Complexes. Journal of Chemical Information and Computer Sciences, 2004, 44, 2114-2125.	2.8	234
20	Classification of Current Scoring Functions. Journal of Chemical Information and Modeling, 2015, 55, 475-482.	5.4	218
21	Comparative Assessment of Scoring Functions on an Updated Benchmark: 1. Compilation of the Test Set. Journal of Chemical Information and Modeling, 2014, 54, 1700-1716.	5.4	175
22	Calculating partition coefficient by atom-additive method. Journal of Computer - Aided Molecular Design, 2000, 19, 47-66.	1.0	172
23	Analysis of Ligand-Bound Water Molecules in High-Resolution Crystal Structures of Proteinâ^'Ligand Complexes. Journal of Chemical Information and Modeling, 2007, 47, 668-675.	5.4	156
24	Structure-based method for analyzing protein?protein interfaces. Journal of Molecular Modeling, 2004, 10, 44-54.	1.8	96
25	Breast Cancer Cells Can Evade Apoptosis-Mediated Selective Killing by a Novel Small Molecule Inhibitor of Bcl-2. Cancer Research, 2004, 64, 7947-7953.	0.9	85
26	Assessing proteinâ€“ligand interaction scoring functions with the CASF-2013 benchmark. Nature Protocols, 2018, 13, 666-680.	12.0	79
27	AlloFinder: a strategy for allosteric modulator discovery and allosterome analyses. Nucleic Acids Research, 2018, 46, W451-W458.	14.5	79
28	TopPâ€“S: Persistent homologyâ€based multiâ€task deep neural networks for simultaneous predictions of partition coefficient and aqueous solubility. Journal of Computational Chemistry, 2018, 39, 1444-1454.	3.3	71
29	M-Score:Â A Knowledge-Based Potential Scoring Function Accounting for Protein Atom Mobility. Journal of Medicinal Chemistry, 2006, 49, 5903-5911.	6.4	63
30	Tapping on the Black Box: How Is the Scoring Power of a Machine-Learning Scoring Function Dependent on the Training Set?. Journal of Chemical Information and Modeling, 2020, 60, 1122-1136.	5.4	56
31	Hemolytic mechanism of dioscin proposed by molecular dynamics simulations. Journal of Molecular Modeling, 2010, 16, 107-118.	1.8	52
32	Pyrogallol-Based Molecules as Potent Inhibitors of the Antiapoptotic Bcl-2 Proteins. Journal of Medicinal Chemistry, 2007, 50, 1723-1726.	6.4	44
33	Discovery and Development of Thiazolo[3,2â€a]pyrimidinone Derivatives as General Inhibitors of Bclâ€2 Family Proteins. ChemMedChem, 2011, 6, 904-921.	3.2	44
34	Structure-Based Design of Flavonoid Compounds As a New Class of Small-Molecule Inhibitors of the Anti-apoptotic Bcl-2 Proteins. Journal of Medicinal Chemistry, 2007, 50, 3163-3166.	6.4	39
35	Calculating Partition Coefficients of Peptides by the Addition Method. Journal of Molecular Modeling, 1999, 5, 189-195.	1.8	38
36	Automatic Perception of Organic Molecules Based on Essential Structural Information. Journal of Chemical Information and Modeling, 2007, 47, 1379-1385.	5.4	37

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37	Interpretation of the Binding Affinities of PTP1B Inhibitors with the MM-GB/SA Method and the X-Score Scoring Function. Journal of Chemical Information and Modeling, 2009, 49, 1033-1048.	5.4	31
38	Test MM-PB/SA on True Conformational Ensembles of Proteinâ^'Ligand Complexes. Journal of Chemical Information and Modeling, 2010, 50, 1682-1692.	5.4	31
39	Geometrical Preferences of the Hydrogen Bonds on Proteinâ^'Ligand Binding Interface Derived from Statistical Surveys and Quantum Mechanics Calculations. Journal of Chemical Theory and Computation, 2008, 4, 1959-1973.	5.3	27
40	Screening of Small-Molecule Inhibitors of Proteinâ€"Protein Interaction with Capillary Electrophoresis Frontal Analysis. Analytical Chemistry, 2016, 88, 8050-8057.	6.5	25
41	AutoT&T v.2: An Efficient and Versatile Tool for Lead Structure Generation and Optimization. Journal of Chemical Information and Modeling, 2016, 56, 435-453.	5.4	24
42	Rational design of Tamiflu derivatives targeting at the open conformation of neuraminidase subtype 1. Journal of Molecular Graphics and Modelling, 2009, 28, 203-219.	2.4	19
43	De Novo Design, Synthesis and Evaluation of Benzylpiperazine Derivatives as Highly Selective Binders of Mclâ€1. ChemMedChem, 2013, 8, 1986-2014.	3.2	19
44	A knowledge-guided strategy for improving the accuracy of scoring functions in binding affinity prediction. BMC Bioinformatics, 2010, 11, 193.	2.6	18
45	A Systematic Analysis of the Effect of Small-Molecule Binding on Protein Flexibility of the Ligand-Binding Sites. Journal of Medicinal Chemistry, 2005, 48, 5648-5650.	6.4	17
46	Automatic Tailoring and Transplanting: A Practical Method that Makes Virtual Screening More Useful. Journal of Chemical Information and Modeling, 2011, 51, 1474-1491.	5.4	15
47	Characterization of the Stereochemical Structures of 2Hâ€Thiazolo[3,2â€a]pyrimidine Compounds and Their Binding Affinities for Antiâ€apoptotic Bclâ€2 Family Proteins. ChemMedChem, 2013, 8, 1345-1352.	3.2	14
48	Enhance the performance of current scoring functions with the aid of 3D protein-ligand interaction fingerprints. BMC Bioinformatics, 2017, 18, 343.	2.6	14
49	Development of 3â€Phenylâ€Nâ€(2â€(3â€phenylureido)ethyl)â€thiopheneâ€2â€sulfonamide Compounds as Inhibitors of Antiapoptotic Bclâ€2 Family Proteins. ChemMedChem, 2014, 9, 1436-1452.	3.2	11
50	Revisiting the Relationship Between Correlation Coefficient, Confidence Level, and Sample Size. Journal of Chemical Information and Modeling, 2019, 59, 4602-4612.	5.4	11
51	Crossâ€Mapping of Protein â€" Ligand Binding Data Between ChEMBL and PDBbind. Molecular Informatics, 2015, 34, 568-576.	2.5	9
52	Development of a new benchmark for assessing the scoring functions applicable to proteinâ€"protein interactions. Future Medicinal Chemistry, 2018, 10, 1555-1574.	2.3	9
53	Public Data Set of Proteinâ€"Ligand Dissociation Kinetic Constants for Quantitative Structureâ€"Kinetics Relationship Studies. ACS Omega, 2022, 7, 18985-18996.	3.5	7
54	Structure-Based Optimization of 3-Phenyl-N-(2-(3-phenylureido)ethyl)thiophene-2-sulfonamide Derivatives as Selective Mcl-1 Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 10260-10285.	6.4	6

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55	A Statistical Survey on the Binding Constants of Covalently Bound Proteinâ€“Ligand Complexes. Molecular Informatics, 2010, 29, 87-96.	2.5	4
56	I-SOLV: A new surface-based empirical model for computing solvation free energies. Journal of Molecular Graphics and Modelling, 2007, 26, 368-377.	2.4	3
57	Experimental Methods Used for Identifying Small-Molecule Inhibitors of Protein-Protein Interaction. , 2018, , 95-133.		2
58	Synthesis of 4â€(2â€Phenylhydrazono)â€1â€(4â€phenylthiazolâ€2â€yl)â€1Hâ€pyrazolâ€5(4H)â€one Compounds and Characterization of Their Affinities to Antiâ€apoptotic Bclâ€2 Family Proteins. Chinese Journal of Chemistry, 2013, 31, 1133-1138.	4.9	1
59	An Extensive Test for 14 Scoring Functions Using the PDBbind Refined Set of 800 Protein?Ligand Complexes.. ChemInform, 2005, 36, no.	0.0	0
60	Computational Methods Applicable to the Discovery of Small-Molecule Inhibitors of Protein-Protein Interactions. , 2018, , 73-94.		0