

Ren-Xiao Wang

List of Publications by Year in descending order

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89
papers

7,705
citations

117625

34
h-index

53230

85
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93
all docs

93
docs citations

93
times ranked

9115
citing authors

#	ARTICLE	IF	CITATIONS
1	Further development and validation of empirical scoring functions for structure-based binding affinity prediction. <i>Journal of Computer-Aided Molecular Design</i> , 2002, 16, 11-26.	2.9	1,012
2	Computation of Octanol-Water Partition Coefficients by Guiding an Additive Model with Knowledge. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2140-2148.	5.4	601
3	Development and optimization of a binding assay for the XIAP BIR3 domain using fluorescence polarization. <i>Analytical Biochemistry</i> , 2004, 332, 261-273.	2.4	479
4	Comparative Assessment of Scoring Functions on a Diverse Test Set. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1079-1093.	5.4	444
5	A New Atom-Additive Method for Calculating Partition Coefficients. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 615-621.	2.8	399
6	PDB-wide collection of binding data: current status of the PDBbind database. <i>Bioinformatics</i> , 2015, 31, 405-412.	4.1	375
7	Comparative Assessment of Scoring Functions: The CASF-2016 Update. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 895-913.	5.4	367
8	Comparative Assessment of Scoring Functions on an Updated Benchmark: 2. Evaluation Methods and General Results. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1717-1736.	5.4	294
9	Evaluation of the performance of four molecular docking programs on a diverse set of protein-ligand complexes. <i>Journal of Computational Chemistry</i> , 2010, 31, 2109-2125.	3.3	277
10	CRISPR-Cpf1 assisted genome editing of <i>Corynebacterium glutamicum</i> . <i>Nature Communications</i> , 2017, 8, 15179.	12.8	276
11	SCORE: A New Empirical Method for Estimating the Binding Affinity of a Protein-Ligand Complex. <i>Journal of Molecular Modeling</i> , 1998, 4, 379-394.	1.8	275
12	Forging the Basis for Developing Protein-Ligand Interaction Scoring Functions. <i>Accounts of Chemical Research</i> , 2017, 50, 302-309.	15.6	257
13	LigBuilder: A Multi-Purpose Program for Structure-Based Drug Design. <i>Journal of Molecular Modeling</i> , 2000, 6, 498-516.	1.8	249
14	Classification of Current Scoring Functions. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 475-482.	5.4	218
15	Comparative Assessment of Scoring Functions on an Updated Benchmark: 1. Compilation of the Test Set. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1700-1716.	5.4	175
16	Calculating partition coefficient by atom-additive method. <i>Journal of Computer - Aided Molecular Design</i> , 2000, 19, 47-66.	1.0	172
17	Systematic Derivation of AMBER Force Field Parameters Applicable to Zinc-Containing Systems. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1852-1870.	5.3	100
18	Current Experimental Methods for Characterizing Protein-Protein Interactions. <i>ChemMedChem</i> , 2016, 11, 738-756.	3.2	82

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19	Assessing protein-ligand interaction scoring functions with the CASF-2013 benchmark. <i>Nature Protocols</i> , 2018, 13, 666-680.	12.0	79
20	AlloFinder: a strategy for allosteric modulator discovery and allosterome analyses. <i>Nucleic Acids Research</i> , 2018, 46, W451-W458.	14.5	79
21	The phytochemical hyperforin triggers thermogenesis in adipose tissue via a Dlat-AMPK signaling axis to curb obesity. <i>Cell Metabolism</i> , 2021, 33, 565-580.e7.	16.2	79
22	A computational analysis of the binding affinities of FKBP12 inhibitors using the MM-PB/SA method. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 64, 1058-1068.	2.6	71
23	TopoP&S: Persistent homology-based multi-task deep neural networks for simultaneous predictions of partition coefficient and aqueous solubility. <i>Journal of Computational Chemistry</i> , 2018, 39, 1444-1454.	3.3	71
24	All-Orientation Search and All-Placement Search in Comparative Molecular Field Analysis. <i>Journal of Molecular Modeling</i> , 1998, 4, 276-283.	1.8	67
25	Mechanistic basis for receptor-mediated pathological α -synuclein fibril cell-to-cell transmission in Parkinson's disease. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	59
26	Tapping on the Black Box: How Is the Scoring Power of a Machine-Learning Scoring Function Dependent on the Training Set?. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1122-1136.	5.4	56
27	The domain responsible for sphingomyelin synthase (SMS) activity. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2008, 1781, 610-617.	2.4	53
28	Hemolytic mechanism of dioscin proposed by molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2010, 16, 107-118.	1.8	52
29	Targeting the potent Beclin 1-UVRAG coiled-coil interaction with designed peptides enhances autophagy and endolysosomal trafficking. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E5669-E5678.	7.1	45
30	Molecular modeling of the three-dimensional structure of GLP-1R and its interactions with several agonists. <i>Journal of Molecular Modeling</i> , 2009, 15, 53-65.	1.8	44
31	Discovery and Development of Thiazolo[3,2-a]pyrimidinone Derivatives as General Inhibitors of Bcl-2 Family Proteins. <i>ChemMedChem</i> , 2011, 6, 904-921.	3.2	44
32	RASSE: A New Method for Structure-Based Drug Design. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 1187-1194.	2.8	39
33	Calculating Partition Coefficients of Peptides by the Addition Method. <i>Journal of Molecular Modeling</i> , 1999, 5, 189-195.	1.8	38
34	Automatic Perception of Organic Molecules Based on Essential Structural Information. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1379-1385.	5.4	37
35	Target-oriented design and biosynthesis of thiostrepton-derived thiopeptide antibiotics with improved pharmaceutical properties. <i>Organic Chemistry Frontiers</i> , 2015, 2, 106-109.	4.5	32
36	Interpretation of the Binding Affinities of PTP1B Inhibitors with the MM-GB/SA Method and the X-Score Scoring Function. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1033-1048.	5.4	31

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37	Test MM-PB/SA on True Conformational Ensembles of Protein-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1682-1692.	5.4	31
38	Alloscore: a method for predicting allosteric ligand-protein interactions. <i>Bioinformatics</i> , 2016, 32, 1574-1576.	4.1	31
39	New Trends in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4109-4111.	5.4	29
40	Geometrical Preferences of the Hydrogen Bonds on Protein-Ligand Binding Interface Derived from Statistical Surveys and Quantum Mechanics Calculations. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1959-1973.	5.3	27
41	Enantioselective Synthesis of (α)-Stemoamide. <i>Synthesis</i> , 2012, 44, 3432-3440.	2.3	26
42	Screening of Small-Molecule Inhibitors of Protein-Protein Interaction with Capillary Electrophoresis Frontal Analysis. <i>Analytical Chemistry</i> , 2016, 88, 8050-8057.	6.5	25
43	The Role of Chronic Inflammation in Various Diseases and Anti-inflammatory Therapies Containing Natural Products. <i>ChemMedChem</i> , 2021, 16, 1576-1592.	3.2	25
44	AutoT&T v.2: An Efficient and Versatile Tool for Lead Structure Generation and Optimization. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 435-453.	5.4	24
45	Identification of small molecule sphingomyelin synthase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2014, 73, 1-7.	5.5	23
46	Colchicine selective interaction with oncogene <i>RET</i> G-quadruplex revealed by NMR. <i>Chemical Communications</i> , 2020, 56, 2099-2102.	4.1	23
47	Small-Molecule Regulators of Autophagy and Their Potential Therapeutic Applications. <i>ChemMedChem</i> , 2013, 8, 694-707.	3.2	22
48	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5868-5869.	5.4	22
49	Prediction of the Favorable Hydration Sites in a Protein Binding Pocket and Its Application to Scoring Function Formulation. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4359-4375.	5.4	21
50	Rational design of Tamiflu derivatives targeting at the open conformation of neuraminidase subtype 1. <i>Journal of Molecular Graphics and Modelling</i> , 2009, 28, 203-219.	2.4	19
51	De Novo Design, Synthesis and Evaluation of Benzylpiperazine Derivatives as Highly Selective Binders of Mcl-1. <i>ChemMedChem</i> , 2013, 8, 1986-2014.	3.2	19
52	Synthesis and anti-tumor activities of N ² -benzylidene-2-(4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)acetohydrazone derivatives. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 6662-6666.	2.2	17
53	Mutagenesis of Key Residues in the Binding Center of <i>Aspartate Semialdehyde Dehydrogenase</i> from <i>Escherichia coli</i> Enhances Utilization of the Cofactor NAD(H). <i>ChemBioChem</i> , 2016, 17, 56-64.	2.6	17
54	2-Aminoethoxydiphenylborane sensitizes anti-tumor effect of bortezomib via suppression of calcium-mediated autophagy. <i>Cell Death and Disease</i> , 2018, 9, 361.	6.3	16

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55	Experimental Characterization of the Binding Affinities between Proapoptotic BH3 Peptides and Antiapoptotic Bcl-2 Proteins. <i>ChemMedChem</i> , 2018, 13, 1763-1770.	3.2	16
56	Characterization of the Stereochemical Structures of 2-Hydroxythiazolo[3,2-a]pyrimidine Compounds and Their Binding Affinities for Antiapoptotic Bcl-2 Family Proteins. <i>ChemMedChem</i> , 2013, 8, 1345-1352.	3.2	14
57	Enhance the performance of current scoring functions with the aid of 3D protein-ligand interaction fingerprints. <i>BMC Bioinformatics</i> , 2017, 18, 343.	2.6	14
58	Optimization of Beclin 1-Targeting Stapled Peptides by Staple Scanning Leads to Enhanced Antiproliferative Potency in Cancer Cells. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 13475-13486.	6.4	13
59	Structure-based Mechanistic Insights into Terminal Amide Synthase in Nosiheptide-Represented Thiopeptides Biosynthesis. <i>Scientific Reports</i> , 2015, 5, 12744.	3.3	12
60	Discovery, synthesis and biological evaluation of 2-(4-(N-phenethylsulfamoyl)phenoxy)acetamides (SAPAs) as novel sphingomyelin synthase 1 inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 6173-6184.	3.0	12
61	Proposed Hydrogen-Bonding Index of Donor or Acceptor Reflecting Its Intrinsic Contribution to Hydrogen-Bonding Strength. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1535-1547.	5.4	12
62	Development of 3-Phenyl-N-(2-(3-phenylureido)ethyl)thiophene-2-sulfonamide Compounds as Inhibitors of Antiapoptotic Bcl-2 Family Proteins. <i>ChemMedChem</i> , 2014, 9, 1436-1452.	3.2	11
63	Revisiting the Relationship Between Correlation Coefficient, Confidence Level, and Sample Size. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4602-4612.	5.4	11
64	Fragment-Based Computational Method for Designing GPCR Ligands. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4339-4349.	5.4	11
65	Molecular Modeling of the Three-Dimensional Structure of Human Sphingomyelin Synthase. <i>Chinese Journal of Chemistry</i> , 2011, 29, 1567-1575.	4.9	10
66	Cross-Mapping of Protein-Ligand Binding Data Between ChEMBL and PDBbind. <i>Molecular Informatics</i> , 2015, 34, 568-576.	2.5	9
67	An unusual UMP C-5 methylase in nucleoside antibiotic polyoxin biosynthesis. <i>Protein and Cell</i> , 2016, 7, 673-683.	11.0	9
68	Development of a new benchmark for assessing the scoring functions applicable to protein-protein interactions. <i>Future Medicinal Chemistry</i> , 2018, 10, 1555-1574.	2.3	9
69	New Trends in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3603-3604.	5.4	9
70	Probing the Key Interactions between Human Atg5 and Atg16 Proteins: A Prospective Application of Molecular Modeling. <i>ChemMedChem</i> , 2013, 8, 1270-1275.	3.2	8
71	Synthesis and anti-tumor activities of methyl 2-O-aryl-6-O-aryl- β -d-glucopyranosides. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 2855-2858.	2.2	7
72	¹ H NMR Studies on the Interaction between Oncogene RET-G-Quadruplex and Berberine. <i>Chinese Journal of Chemistry</i> , 2020, 38, 1656-1662.	4.9	7

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73	Revealing the Unbinding Kinetics and Mechanism of Type I and Type II Protein Kinase Inhibitors by Local-Scaled Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6620-6632.	5.3	7
74	Analysis of the Binding Sites on BAX and the Mechanism of BAX Activators through Extensive Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5208-5222.	5.4	7
75	Public Data Set of Protein-Ligand Dissociation Kinetic Constants for Quantitative Structure-Kinetics Relationship Studies. <i>ACS Omega</i> , 2022, 7, 18985-18996.	3.5	7
76	Automatic Identification of Antibodies in the Protein Data Bank. <i>Chinese Journal of Chemistry</i> , 2009, 27, 23-28.	4.9	6
77	Rise of the Selective Inhibitors of Anti-Apoptotic Bcl-2 Family Proteins. <i>ChemMedChem</i> , 2013, 8, 1437-1440.	3.2	6
78	Synthesis of (1,3,4-thiadiazol-2-yl)-acrylamide derivatives as potential antitumor agents against acute leukemia cells. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127114.	2.2	6
79	Structure-Based Optimization of 3-Phenyl-N-(2-(3-phenylureido)ethyl)thiophene-2-sulfonamide Derivatives as Selective Mcl-1 Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 10260-10285.	6.4	6
80	A Statistical Survey on the Binding Constants of Covalently Bound Protein-Ligand Complexes. <i>Molecular Informatics</i> , 2010, 29, 87-96.	2.5	4
81	I-SOLV: A new surface-based empirical model for computing solvation free energies. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 368-377.	2.4	3
82	Theoretical Analysis of Fas Ligand-Induced Apoptosis with an Ordinary Differential Equation Model. <i>Molecular Informatics</i> , 2012, 31, 793-807.	2.5	2
83	Temperature-Responsive Chiral (A) ₆ B Supramolecular Cages Based on Conformational Preferences. <i>Chemistry - an Asian Journal</i> , 2016, 11, 465-469.	3.3	2
84	11-Aza-Artemisinin Derivatives Exhibit Anticancer Activities by Targeting the Fatty Acid Binding Protein 6 (FABP6). <i>Chinese Journal of Chemistry</i> , 2018, 36, 1197-1201.	4.9	2
85	Experimental Methods Used for Identifying Small-Molecule Inhibitors of Protein-Protein Interaction. , 2018, , 95-133.		2
86	Computational Chemistry in Asia. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 547-547.	5.4	2
87	Synthesis of 4-(2-Phenylhydrazono)-1-(4-phenylthiazol-2-yl)-1H-pyrazol-5(4H)-one Compounds and Characterization of Their Affinities to Anti-Apoptotic Bcl-2 Family Proteins. <i>Chinese Journal of Chemistry</i> , 2013, 31, 1133-1138.	4.9	1
88	Special Issue of "Medicinal Chemistry". <i>Chinese Journal of Chemistry</i> , 2013, 31, 1115-1115.	4.9	0
89	Small-Molecule Regulators of Autophagy as Potential Anti-cancer Therapy. <i>Current Cancer Research</i> , 2016, , 39-57.	0.2	0