Ren-Xiao Wang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7412899/publications.pdf

Version: 2024-02-01

89 papers	7,705 citations	117625 34 h-index	53230 85 g-index
93 all docs	93 docs citations	93 times ranked	9115 citing authors

#	Article	IF	Citations
1	Analysis of the Binding Sites on BAX and the Mechanism of BAX Activators through Extensive Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2022, 62, 5208-5222.	5.4	7
2	Public Data Set of Proteinâ€“Ligand Dissociation Kinetic Constants for Quantitative Structureâ€“Kinetics Relationship Studies. ACS Omega, 2022, 7, 18985-18996.	3.5	7
3	Computational Chemistry in Asia. Journal of Chemical Information and Modeling, 2021, 61, 547-547.	5.4	2
4	The Role of Chronic Inflammation in Various Diseases and Antiâ€inflammatory Therapies Containing Natural Products. ChemMedChem, 2021, 16, 1576-1592.	3.2	25
5	The phytochemical hyperforin triggers thermogenesis in adipose tissue via a Dlat-AMPK signaling axis to curb obesity. Cell Metabolism, 2021, 33, 565-580.e7.	16.2	79
6	Mechanistic basis for receptor-mediated pathological Î±-synuclein fibril cell-to-cell transmission in Parkinson's disease. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	59
7	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
8	Optimization of Beclin 1-Targeting Stapled Peptides by Staple Scanning Leads to Enhanced Antiproliferative Potency in Cancer Cells. Journal of Medicinal Chemistry, 2021, 64, 13475-13486.	6.4	13
9	Fragment-Based Computational Method for Designing GPCR Ligands. Journal of Chemical Information and Modeling, 2020, 60, 4339-4349.	5.4	11
10	New Trends in Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4109-4111.	5.4	29
11	<scp>NMR</scp> Studies on the Interaction between Oncogene <scp>RET Gâ€Quadruplex</scp> and Berberine^{â€}. Chinese Journal of Chemistry, 2020, 38, 1656-1662.	4.9	7
12	Revealing the Unbinding Kinetics and Mechanism of Type I and Type II Protein Kinase Inhibitors by Local-Scaled Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 6620-6632.	5.3	7
13	Prediction of the Favorable Hydration Sites in a Protein Binding Pocket and Its Application to Scoring Function Formulation. Journal of Chemical Information and Modeling, 2020, 60, 4359-4375.	5.4	21
14	Synthesis of (1,3,4-thiadiazol-2-yl)-acrylamide derivatives as potential antitumor agents against acute leukemia cells. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127114.	2.2	6
15	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
16	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. Journal of Chemical Information and Modeling, 2020, 60, 5868-5869.	5.4	22
17	Colchicine selective interaction with oncogene RET G-quadruplex revealed by NMR. Chemical Communications, 2020, 56, 2099-2102.	4.1	23
18	Revisiting the Relationship Between Correlation Coefficient, Confidence Level, and Sample Size. Journal of Chemical Information and Modeling, 2019, 59, 4602-4612.	5.4	11

#	Article	IF	Citations
19	New Trends in Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 3603-3604.	5.4	9
20	Comparative Assessment of Scoring Functions: The CASF-2016 Update. Journal of Chemical Information and Modeling, 2019, 59, 895-913.	5.4	367
21	Assessing proteinâ€“ligand interaction scoring functions with the CASF-2013 benchmark. Nature Protocols, 2018, 13, 666-680.	12.0	79
22	2-Aminoethoxydiphenylborane sensitizes anti-tumor effect of bortezomib via suppression of calcium-mediated autophagy. Cell Death and Disease, 2018, 9, 361.	6.3	16
23	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
24	11â€Azaâ€artemisinin Derivatives Exhibit Anticancer Activities by Targeting the Fatty Acid Binding Protein 6 (FABP6). Chinese Journal of Chemistry, 2018, 36, 1197-1201.	4.9	2
25	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
26	Experimental Methods Used for Identifying Small-Molecule Inhibitors of Protein-Protein Interaction. , 2018, , 95-133.		2
27	Experimental Characterization of the Binding Affinities between Proapoptotic BH3 Peptides and Antiapoptotic Bclâ€2 Proteins. ChemMedChem, 2018, 13, 1763-1770.	3.2	16
28	AlloFinder: a strategy for allosteric modulator discovery and allosterome analyses. Nucleic Acids Research, 2018, 46, W451-W458.	14.5	79
29	Targeting the potent Beclin 1â€“UVRAG coiled-coil interaction with designed peptides enhances autophagy and endolysosomal trafficking. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E5669-E5678.	7.1	45
30	Forging the Basis for Developing Proteinâ€“Ligand Interaction Scoring Functions. Accounts of Chemical Research, 2017, 50, 302-309.	15.6	257
31	CRISPR-Cpf1 assisted genome editing of Corynebacterium glutamicum. Nature Communications, 2017, 8, 15179.	12.8	276
32	Proposed Hydrogen-Bonding Index of Donor or Acceptor Reflecting Its Intrinsic Contribution to Hydrogen-Bonding Strength. Journal of Chemical Information and Modeling, 2017, 57, 1535-1547.	5.4	12
33	Enhance the performance of current scoring functions with the aid of 3D protein-ligand interaction fingerprints. BMC Bioinformatics, 2017, 18, 343.	2.6	14
34	Temperatureâ€Responsive Chiral (A)₆B Supramolecular Cages Based on Conformational Preferences. Chemistry - an Asian Journal, 2016, 11, 465-469.	3.3	2
35	Current Experimental Methods for Characterizing Proteinâ€“Protein Interactions. ChemMedChem, 2016, 11, 738-756.	3.2	82
36	Small-Molecule Regulators of Autophagy as Potential Anti-cancer Therapy. Current Cancer Research, 2016, , 39-57.	0.2	0

#	Article	IF	Citations
37	Mutagenesis of Key Residues in the Binding Center of <scp>lâ€</scp>Aspartateâ€²â€Semialdehyde Dehydrogenase from Escherichia coli Enhances Utilization of the Cofactor NAD(H). ChemBioChem, 2016, 17, 56-64.	2.6	17
38	Screening of Small-Molecule Inhibitors of Proteinâ€“Protein Interaction with Capillary Electrophoresis Frontal Analysis. Analytical Chemistry, 2016, 88, 8050-8057.	6.5	25
39	An unusual UMP C-5 methylase in nucleoside antibiotic polyoxin biosynthesis. Protein and Cell, 2016, 7, 673-683.	11.0	9
40	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
41	Alloscore: a method for predicting allosteric ligandâ€“protein interactions. Bioinformatics, 2016, 32, 1574-1576.	4.1	31
42	Structure-based Mechanistic Insights into Terminal Amide Synthase in Nosiheptide-Represented Thiopeptides Biosynthesis. Scientific Reports, 2015, 5, 12744.	3.3	12
43	Crossâ€Mapping of Protein â€“ Ligand Binding Data Between ChEMBL and PDBbind. Molecular Informatics, 2015, 34, 568-576.	2.5	9
44	Target-oriented design and biosynthesis of thiostrepton-derived thiopeptide antibiotics with improved pharmaceutical properties. Organic Chemistry Frontiers, 2015, 2, 106-109.	4.5	32
45	Classification of Current Scoring Functions. Journal of Chemical Information and Modeling, 2015, 55, 475-482.	5.4	218
46	Discovery, synthesis and biological evaluation of 2-(4-(N-phenethylsulfamoyl)phenoxy)acetamides (SAPAs) as novel sphingomyelin synthase 1 inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 6173-6184.	3.0	12
47	PDB-wide collection of binding data: current status of the PDBbind database. Bioinformatics, 2015, 31, 405-412.	4.1	375
48	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
49	Identification of small molecule sphingomyelin synthase inhibitors. European Journal of Medicinal Chemistry, 2014, 73, 1-7.	5.5	23
50	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
51	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
52	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
53	De Novo Design, Synthesis and Evaluation of Benzylpiperazine Derivatives as Highly Selective Binders of Mclâ€1. ChemMedChem, 2013, 8, 1986-2014.	3.2	19
54	Rise of the Selective Inhibitors of Antiâ€Apoptotic Bclâ€2 Family Proteins. ChemMedChem, 2013, 8, 1437-1440.	3.2	6

#	Article	IF	Citations
55	Smallâ€Molecule Regulators of Autophagy and Their Potential Therapeutic Applications. ChemMedChem, 2013, 8, 694-707.	3.2	22
56	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
57	Special Issue of "Medicinal Chemistry". Chinese Journal of Chemistry, 2013, 31, 1115-1115.	4.9	0
58	Probing the Key Interactions between Human Atg5 and Atg16 Proteins: A Prospective Application of Molecular Modeling. ChemMedChem, 2013, 8, 1270-1275.	3.2	8
59	Enantioselective Synthesis of (â€“)-Stemoamide. Synthesis, 2012, 44, 3432-3440.	2.3	26
60	Theoretical Analysis of Fas Ligandâ€Induced Apoptosis with an Ordinary Differential Equation Model. Molecular Informatics, 2012, 31, 793-807.	2.5	2
61	Synthesis and anti-tumor activities of Nâ€²-benzylidene-2-(4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)acetohydrazone derivatives. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 6662-6666.	2.2	17
62	Molecular Modeling of the Threeâ€Dimensional Structure of Human Sphingomyelin Synthase. Chinese Journal of Chemistry, 2011, 29, 1567-1575.	4.9	10
63	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
64	Hemolytic mechanism of dioscin proposed by molecular dynamics simulations. Journal of Molecular Modeling, 2010, 16, 107-118.	1.8	52
65	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
66	A Statistical Survey on the Binding Constants of Covalently Bound Proteinâ€“Ligand Complexes. Molecular Informatics, 2010, 29, 87-96.	2.5	4
67	Synthesis and anti-tumor activities of methyl 2-O-aryl-6-O-arylâ€²-d-glucopyranosides. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2855-2858.	2.2	7
68	Systematic Derivation of AMBER Force Field Parameters Applicable to Zinc-Containing Systems. Journal of Chemical Theory and Computation, 2010, 6, 1852-1870.	5.3	100
69	Test MM-PB/SA on True Conformational Ensembles of Proteinâˆ’Ligand Complexes. Journal of Chemical Information and Modeling, 2010, 50, 1682-1692.	5.4	31
70	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
71	Automatic Identification of Antibodies in the Protein Data Bank. Chinese Journal of Chemistry, 2009, 27, 23-28.	4.9	6
72	Molecular modeling of the three-dimensional structure of GLP-1R and its interactions with several agonists. Journal of Molecular Modeling, 2009, 15, 53-65.	1.8	44

#	Article	IF	Citations
73	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
74	Comparative Assessment of Scoring Functions on a Diverse Test Set. Journal of Chemical Information and Modeling, 2009, 49, 1079-1093.	5.4	444
75	The domain responsible for sphingomyelin synthase (SMS) activity. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2008, 1781, 610-617.	2.4	53
76	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
77	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
78	Automatic Perception of Organic Molecules Based on Essential Structural Information. Journal of Chemical Information and Modeling, 2007, 47, 1379-1385.	5.4	37
79	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
80	A computational analysis of the binding affinities of FKBP12 inhibitors using the MM-PB/SA method. Proteins: Structure, Function and Bioinformatics, 2006, 64, 1058-1068.	2.6	71
81	Development and optimization of a binding assay for the XIAP BIR3 domain using fluorescence polarization. Analytical Biochemistry, 2004, 332, 261-273.	2.4	479
82	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
83	Calculating partition coefficient by atom-additive method. Journal of Computer - Aided Molecular Design, 2000, 19, 47-66.	1.0	172
84	LigBuilder: A Multi-Purpose Program for Structure-Based Drug Design. Journal of Molecular Modeling, 2000, 6, 498-516.	1.8	249
85	Calculating Partition Coefficients of Peptides by the Addition Method. Journal of Molecular Modeling, 1999, 5, 189-195.	1.8	38
86	All-Orientation Search and All-Placement Search in Comparative Molecular Field Analysis. Journal of Molecular Modeling, 1998, 4, 276-283.	1.8	67
87	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
88	A New Atom-Additive Method for Calculating Partition Coefficients. Journal of Chemical Information and Computer Sciences, 1997, 37, 615-621.	2.8	399
89	RASSE:â€‰ A New Method for Structure-Based Drug Design. Journal of Chemical Information and Computer Sciences, 1996, 36, 1187-1194.	2.8	39