# Renxiao Wang

List of Publications by Year
in descending order



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|---|---|---|---|
| 60 papers | 10,436 citations | 101384 36 h-index | 143772 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. | 1.3 | 1,012 |
| 2 | Comparative Evaluation of 11 Scoring Functions for Molecular Docking. Journal of Medicinal Chemistry, 2003, 46, 2287-2303. | 2.9 | 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. | 2.9 | 787 |
| 4 | The PDBbind Database:Â Methodologies and Updates. Journal of Medicinal Chemistry, 2005, 48, 4111-4119. | 2.9 | 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. | 2.5 | 601 |
| 6 | Development and optimization of a binding assay for the XIAP BIR3 domain using fluorescence polarization. Analytical Biochemistry, 2004, 332, 261-273. | 1.1 | 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. | 3.3 | 460 |
| 8 | Comparative Assessment of Scoring Functions on a Diverse Test Set. Journal of Chemical Information and Modeling, 2009, 49, 1079-1093. | 2.5 | 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. | 1.8 | 375 |
| 11 | Comparative Assessment of Scoring Functions: The CASF-2016 Update. Journal of Chemical Information and Modeling, 2019, 59, 895-913. | 2.5 | 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. | 2.9 | 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. | 2.5 | 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. | 1.5 | 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. | 0.8 | 275 |
| 17 | Structure-Based Design of Potent Small-Molecule Inhibitors of Anti-Apoptotic Bcl-2 Proteins. Journal of Medicinal Chemistry, 2006, 49, 6139-6142. | 2.9 | 274 |
| 18 | Forging the Basis for Developing Proteinâ€“Ligand Interaction Scoring Functions. Accounts of Chemical Research, 2017, 50, 302-309. | 7.6 | 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. | 2.5 | 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. | 2.5 | 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. | 2.5 | 156 |
| 24 | Structure-based method for analyzing protein?protein interfaces. Journal of Molecular Modeling, 2004, 10, 44-54. | 0.8 | 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. | 0.4 | 85 |
| 26 | Assessing proteinâ€“ligand interaction scoring functions with the CASF-2013 benchmark. Nature Protocols, 2018, 13, 666-680. | 5.5 | 79 |
| 27 | AlloFinder: a strategy for allosteric modulator discovery and allosterome analyses. Nucleic Acids Research, 2018, 46, W451-W458. | 6.5 | 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. | 1.5 | 71 |
| 29 | M-Score:Â A Knowledge-Based Potential Scoring Function Accounting for Protein Atom Mobility. Journal of Medicinal Chemistry, 2006, 49, 5903-5911. | 2.9 | 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. | 2.5 | 56 |
| 31 | Hemolytic mechanism of dioscin proposed by molecular dynamics simulations. Journal of Molecular Modeling, 2010, 16, 107-118. | 0.8 | 52 |
| 32 | Pyrogallol-Based Molecules as Potent Inhibitors of the Antiapoptotic Bcl-2 Proteins. Journal of Medicinal Chemistry, 2007, 50, 1723-1726. | 2.9 | 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. | 1.6 | 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. | 2.9 | 39 |
| 35 | Calculating Partition Coefficients of Peptides by the Addition Method. Journal of Molecular Modeling, 1999, 5, 189-195. | 0.8 | 38 |
| 36 | Automatic Perception of Organic Molecules Based on Essential Structural Information. Journal of Chemical Information and Modeling, 2007, 47, 1379-1385. | 2.5 | 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. | 2.5 | 31 |
| 38 | Test MM-PB/SA on True Conformational Ensembles of Proteinâ^'Ligand Complexes. Journal of Chemical Information and Modeling, 2010, 50, 1682-1692. | 2.5 | 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. | 2.3 | 27 |
| 40 | Screening of Small-Molecule Inhibitors of Proteinâ€"Protein Interaction with Capillary Electrophoresis Frontal Analysis. Analytical Chemistry, 2016, 88, 8050-8057. | 3.2 | 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. | 2.5 | 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. | 1.3 | 19 |
| 43 | De Novo Design, Synthesis and Evaluation of Benzylpiperazine Derivatives as Highly Selective Binders of Mclâ€1. ChemMedChem, 2013, 8, 1986-2014. | 1.6 | 19 |
| 44 | A knowledge-guided strategy for improving the accuracy of scoring functions in binding affinity prediction. BMC Bioinformatics, 2010, 11, 193. | 1.2 | 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. | 2.9 | 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. | 2.5 | 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. | 1.6 | 14 |
| 48 | Enhance the performance of current scoring functions with the aid of 3D protein-ligand interaction fingerprints. BMC Bioinformatics, 2017, 18, 343. | 1.2 | 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. | 1.6 | 11 |
| 50 | Revisiting the Relationship Between Correlation Coefficient, Confidence Level, and Sample Size. Journal of Chemical Information and Modeling, 2019, 59, 4602-4612. | 2.5 | 11 |
| 51 | Crossâ€Mapping of Protein â€" Ligand Binding Data Between ChEMBL and PDBbind. Molecular Informatics, 2015, 34, 568-576. | 1.4 | 9 |
| 52 | Development of a new benchmark for assessing the scoring functions applicable to proteinâ€"protein interactions. Future Medicinal Chemistry, 2018, 10, 1555-1574. | 1.1 | 9 |
| 53 | Public Data Set of Proteinâ€"Ligand Dissociation Kinetic Constants for Quantitative Structureâ€"Kinetics Relationship Studies. ACS Omega, 2022, 7, 18985-18996. | 1.6 | 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. | 2.9 | 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. | 1.4 | 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. | 1.3 | 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. | 2.6 | 1 |
| 59 | An Extensive Test for 14 Scoring Functions Using the PDBbind Refined Set of 800 Protein?Ligand Complexes.. ChemInform, 2005, 36, no. | 0.1 | 0 |
| 60 | Computational Methods Applicable to the Discovery of Small-Molecule Inhibitors of Protein-Protein Interactions. , 2018, , 73-94. | | 0 |