

# Wenbo Yu

## List of Publications by Citations

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52  
papers

2,013  
citations

23  
h-index

44  
g-index

57  
ext. papers

2,419  
ext. citations

6.4  
avg, IF

5.05  
L-index

#	Paper	IF	Citations
52	Extension of the CHARMM General Force Field to sulfonyl-containing compounds and its utility in biomolecular simulations. <i>Journal of Computational Chemistry</i> , <b>2012</b> , 33, 2451-68	3.5	447
51	Computer-Aided Drug Design Methods. <i>Methods in Molecular Biology</i> , <b>2017</b> , 1520, 85-106	1.4	160
50	Gaseous arginine conformers and their unique intramolecular interactions. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 12282-91	2.8	96
49	Six-site polarizable model of water based on the classical Drude oscillator. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 034508	3.9	92
48	Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma. <i>Journal of Clinical Investigation</i> , <b>2016</b> , 126, 3351-62	15.9	92
47	The Expanding Role of the BCL6 Oncoprotein as a Cancer Therapeutic Target. <i>Clinical Cancer Research</i> , <b>2017</b> , 23, 885-893	12.9	85
46	Reproducing crystal binding modes of ligand functional groups using Site-Identification by Ligand Competitive Saturation (SILCS) simulations. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 877-96	6.1	85
45	Inclusion of multiple fragment types in the site identification by ligand competitive saturation (SILCS) approach. <i>Journal of Chemical Information and Modeling</i> , <b>2013</b> , 53, 3384-98	6.1	79
44	The novel BH3 helix mimetic JY-1-106 induces apoptosis in a subset of cancer cells (lung cancer, colon cancer and mesothelioma) by disrupting Bcl-xL and Mcl-1 protein-protein interactions with Bak. <i>Molecular Cancer</i> , <b>2013</b> , 12, 42	42.1	69
43	Exploration of the full conformational landscapes of gaseous aromatic amino acid phenylalanine: An ab initio study. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 758, 195-202		67
42	Comparison of some representative density functional theory and wave function theory methods for the studies of amino acids. <i>Journal of Computational Chemistry</i> , <b>2009</b> , 30, 589-600	3.5	53
41	Sampling of Organic Solutes in Aqueous and Heterogeneous Environments Using Oscillating Excess Chemical Potentials in Grand Canonical-like Monte Carlo-Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2281-2290	6.4	48
40	Pharmacophore modeling using site-identification by ligand competitive saturation (SILCS) with multiple probe molecules. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 407-20	6.1	48
39	Site-Identification by Ligand Competitive Saturation (SILCS) assisted pharmacophore modeling. <i>Journal of Computer-Aided Molecular Design</i> , <b>2014</b> , 28, 491-507	4.2	46
38	Turning defense into offense: defensin mimetics as novel antibiotics targeting lipid II. <i>PLoS Pathogens</i> , <b>2013</b> , 9, e1003732	7.6	41
37	Mapping functional group free energy patterns at protein occluded sites: nuclear receptors and G-protein coupled receptors. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 700-8	6.1	40
36	Coexistence of dihydrogen, blue- and red-shifting hydrogen bonds in an ultrasmall system: valine. <i>ChemPhysChem</i> , <b>2006</b> , 7, 828-30	3.2	37

35	Iodobenzene-Catalyzed Synthesis of Phenanthridinones via Oxidative C-H Amidation. <i>Journal of Organic Chemistry</i> , <b>2017</b> , 82, 3589-3596	4.2	36
34	First-principle studies of gaseous aromatic amino acid histidine. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 801, 7-20		35
33	Structure-based design of N-substituted 1-hydroxy-4-sulfamoyl-2-naphthoates as selective inhibitors of the Mcl-1 oncoprotein. <i>European Journal of Medicinal Chemistry</i> , <b>2016</b> , 113, 273-92	6.8	34
32	Extensive conformational searches of 13 representative dipeptides and an efficient method for dipeptide structure determinations based on amino acid conformers. <i>Journal of Computational Chemistry</i> , <b>2009</b> , 30, 2105-21	3.5	28
31	Optimization and Evaluation of Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target-Based Ligand Optimization. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 3018-3035	6.4	27
30	Iminoguanidines as Allosteric Inhibitors of the Iron-Regulated Heme Oxygenase (HemO) of <i>Pseudomonas aeruginosa</i> . <i>Journal of Medicinal Chemistry</i> , <b>2016</b> , 59, 6929-42	8.3	26
29	An activating mutation of the NSD2 histone methyltransferase drives oncogenic reprogramming in acute lymphocytic leukemia. <i>Oncogene</i> , <b>2019</b> , 38, 671-686	9.2	23
28	Identification of Thiourea-Based Inhibitors of the B-Cell Lymphoma 6 BTB Domain via NMR-Based Fragment Screening and Computer-Aided Drug Design. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 7573-7588	8.3	22
27	Facile Synthesis of Spirocyclic Lactams from $\beta$ -Keto Carboxylic Acids. <i>Organic Letters</i> , <b>2015</b> , 17, 3070-3	6.2	17
26	Estimating glycosaminoglycan-protein interaction affinity: water dominates the specific antithrombin-heparin interaction. <i>Glycobiology</i> , <b>2016</b> , 26, 1041-1047	5.8	17
25	Comprehensive conformational studies of five tripeptides and a deduced method for efficient determinations of peptide structures. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 2269-83	3.4	15
24	Identification and characterization of fragment binding sites for allosteric ligand design using the site identification by ligand competitive saturation hotspots approach (SILCS-Hotspots). <i>Biochimica Et Biophysica Acta - General Subjects</i> , <b>2020</b> , 1864, 129519	4	15
23	Targeting zymogen activation to control the matriptase-prostasin proteolytic cascade. <i>Journal of Medicinal Chemistry</i> , <b>2011</b> , 54, 7567-78	8.3	13
22	Comprehensive density functional theory study on the mechanism of activation of the nonapeptide hormone oxytocin by metal ions. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 1417-23	3.4	13
21	Structure of the cell-binding component of the binary toxin reveals a di-heptamer macromolecular assembly. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 1049-1058	11.5	12
20	Second harmonic generation detection of Ras conformational changes and discovery of a small molecule binder. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 17290-17297	11.5	11
19	Novel protein-inhibitor interactions in site 3 of Ca(2+)-bound S100B as discovered by X-ray crystallography. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2016</b> , 72, 753-60	5.5	10
18	Exploring protein-protein interactions using the site-identification by ligand competitive saturation methodology. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2019</b> , 87, 289-301	4.2	10

17	Structure-based design and biological evaluation of inhibitors of the pseudomonas aeruginosa heme oxygenase (pa-HemO). <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2018</b> , 28, 1024-1029	2.9	9
16	Impact of electronic polarizability on protein-functional group interactions. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 6848-6860	3.6	7
15	The SKI complex is a broad-spectrum, host-directed antiviral drug target for coronaviruses, influenza, and filoviruses. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 30687-30698	11.5	7
14	Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae. <i>PLoS ONE</i> , <b>2021</b> , 16, e0244967	3.7	7
13	Structure-activity exploration of a small-molecule Lipid II inhibitor. <i>Drug Design, Development and Therapy</i> , <b>2015</b> , 9, 2383-94	4.4	6
12	Profiling the Tox21 Chemical Collection for Acetylcholinesterase Inhibition. <i>Environmental Health Perspectives</i> , <b>2021</b> , 129, 47008	8.4	6
11	Rapid and accurate estimation of protein-ligand relative binding affinities using site-identification by ligand competitive saturation. <i>Chemical Science</i> , <b>2021</b> , 12, 8844-8858	9.4	5
10	Optimization of a Benzothiazole Indolene Scaffold Targeting Bacterial Cell Wall Assembly. <i>Drug Design, Development and Therapy</i> , <b>2020</b> , 14, 567-574	4.4	4
9	Computational approaches for the design of protein-protein interaction inhibitors <b>2013</b> , 90-102		3
8	Prospects of Modulating Protein-Protein Interactions <b>2012</b> , 295-329		3
7	Small molecules inhibitors of the heterogeneous ribonuclear protein A18 (hnRNP A18): a regulator of protein translation and an immune checkpoint. <i>Nucleic Acids Research</i> , <b>2021</b> , 49, 1235-1246	20.1	2
6	Specificity of Molecular Fragments Binding to S100B versus S100A1 as Identified by NMR and Site Identification by Ligand Competitive Saturation (SILCS). <i>Molecules</i> , <b>2021</b> , 26,	4.8	2
5	Electronic structures and electron detachment energies of halogen substituted acetate anions, XCH <sub>2</sub> COO <sup>-</sup> (X=F,Cl,Br). <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 114301	3.9	1
4	Application of Site-Identification by Ligand Competitive Saturation in Computer-Aided Drug Design.. <i>New Journal of Chemistry</i> , <b>2022</b> , 46, 919-932	3.6	1
3	Cholecalciferol complexation with hydroxypropyl-β-cyclodextrin (HPBCD) and its molecular dynamics simulation.. <i>Pharmaceutical Development and Technology</i> , <b>2022</b> , 1-10	3.4	0
2	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches <b>2020</b> , 81-108		
1	Development of CHARMM Additive Potential Energy Parameters for β-Methyl Amino Acids. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 11687-11696	3.4	