Wenbo Yu

List of Publications by Year in Descending Order

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	Application of Site-Identification by Ligand Competitive Saturation in Computer-Aided Drug Design.. *New Journal of Chemistry*, **2022**, 46, 919-932	3.6	1
51	Cholecalciferol complexation with hydroxypropyl-β-cyclodextrin (HPBCD) and its molecular dynamics simulation.. *Pharmaceutical Development and Technology*, **2022**, 1-10	3.4	0
50	Development of CHARMM Additive Potential Energy Parameters for β-Methyl Amino Acids. *Journal of Physical Chemistry B*, **2021**, 125, 11687-11696	3.4	
49	Profiling the Tox21 Chemical Collection for Acetylcholinesterase Inhibition. *Environmental Health Perspectives*, **2021**, 129, 47008	8.4	6
48	Small molecules inhibitors of the heterogeneous ribonuclear protein A18 (hnRNP A18): a regulator of protein translation and an immune checkpoint. *Nucleic Acids Research*, **2021**, 49, 1235-1246	20.1	2
47	Specificity of Molecular Fragments Binding to S100B versus S100A1 as Identified by NMR and Site Identification by Ligand Competitive Saturation (SILCS). *Molecules*, **2021**, 26,	4.8	2
46	Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae. *PLoS ONE*, **2021**, 16, e0244967	3.7	7
45	Rapid and accurate estimation of protein-ligand relative binding affinities using site-identification by ligand competitive saturation. *Chemical Science*, **2021**, 12, 8844-8858	9.4	5
44	Impact of electronic polarizability on protein-functional group interactions. *Physical Chemistry Chemical Physics*, **2020**, 22, 6848-6860	3.6	7
43	Optimization of a Benzothiazole Indolene Scaffold Targeting Bacterial Cell Wall Assembly. *Drug Design, Development and Therapy*, **2020**, 14, 567-574	4.4	4
42	Structure of the cell-binding component of the binary toxin reveals a di-heptamer macromolecular assembly. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 1049-1058	11.5	12
41	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches **2020**, 81-108		
40	Identification and characterization of fragment binding sites for allosteric ligand design using the site identification by ligand competitive saturation hotspots approach (SILCS-Hotspots). *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129519	4	15
39	The SKI complex is a broad-spectrum, host-directed antiviral drug target for coronaviruses, influenza, and filoviruses. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 30687-30698	11.5	7
38	Optimization and Evaluation of Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target-Based Ligand Optimization. *Journal of Chemical Information and Modeling*, **2019**, 59, 3018-3035	6.1	27
37	Second harmonic generation detection of Ras conformational changes and discovery of a small molecule binder. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 17290-17297	11.5	11
36	An activating mutation of the NSD2 histone methyltransferase drives oncogenic reprogramming in acute lymphocytic leukemia. *Oncogene*, **2019**, 38, 671-686	9.2	23

35	Exploring protein-protein interactions using the site-identification by ligand competitive saturation methodology. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 289-301	4.2	10
34	Structure-based design and biological evaluation of inhibitors of the pseudomonas aeruginosa heme oxygenase (pa-HemO). *Bioorganic and Medicinal Chemistry Letters*, **2018**, 28, 1024-1029	2.9	9
33	Identification of Thiourea-Based Inhibitors of the B-Cell Lymphoma 6 BTB Domain via NMR-Based Fragment Screening and Computer-Aided Drug Design. *Journal of Medicinal Chemistry*, **2018**, 61, 7573-7588	8.3	22
32	Iodobenzene-Catalyzed Synthesis of Phenanthridinones via Oxidative C-H Amidation. *Journal of Organic Chemistry*, **2017**, 82, 3589-3596	4.2	36
31	Computer-Aided Drug Design Methods. *Methods in Molecular Biology*, **2017**, 1520, 85-106	1.4	160
30	The Expanding Role of the BCL6 Oncoprotein as a Cancer Therapeutic Target. *Clinical Cancer Research*, **2017**, 23, 885-893	12.9	85
29	Novel protein-inhibitor interactions in site 3 of Ca(2+)-bound S100B as discovered by X-ray crystallography. *Acta Crystallographica Section D: Structural Biology*, **2016**, 72, 753-60	5.5	10
28	Structure-based design of N-substituted 1-hydroxy-4-sulfamoyl-2-naphthoates as selective inhibitors of the Mcl-1 oncoprotein. *European Journal of Medicinal Chemistry*, **2016**, 113, 273-92	6.8	34
27	Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma. *Journal of Clinical Investigation*, **2016**, 126, 3351-62	15.9	92
26	Iminoguanidines as Allosteric Inhibitors of the Iron-Regulated Heme Oxygenase (HemO) of Pseudomonas aeruginosa. *Journal of Medicinal Chemistry*, **2016**, 59, 6929-42	8.3	26
25	Estimating glycosaminoglycan-protein interaction affinity: water dominates the specific antithrombin-heparin interaction. *Glycobiology*, **2016**, 26, 1041-1047	5.8	17
24	Mapping functional group free energy patterns at protein occluded sites: nuclear receptors and G-protein coupled receptors. *Journal of Chemical Information and Modeling*, **2015**, 55, 700-8	6.1	40
23	Structure-activity exploration of a small-molecule Lipid II inhibitor. *Drug Design, Development and Therapy*, **2015**, 9, 2383-94	4.4	6
22	Facile Synthesis of Spirocyclic Lactams from Keto Carboxylic Acids. *Organic Letters*, **2015**, 17, 3070-3	6.2	17
21	Pharmacophore modeling using site-identification by ligand competitive saturation (SILCS) with multiple probe molecules. *Journal of Chemical Information and Modeling*, **2015**, 55, 407-20	6.1	48
20	Sampling of Organic Solutes in Aqueous and Heterogeneous Environments Using Oscillating Excess Chemical Potentials in Grand Canonical-like Monte Carlo-Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 2281-2290	6.4	48
19	Site-Identification by Ligand Competitive Saturation (SILCS) assisted pharmacophore modeling. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 491-507	4.2	46
18	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. *Molecular Cancer*, **2013**, 12, 42	42.1	69

17	Six-site polarizable model of water based on the classical Drude oscillator. *Journal of Chemical Physics*, **2013**, 138, 034508	3.9	92
16	Computational approaches for the design of protein–protein interaction inhibitors **2013**, 90-102		3
15	Inclusion of multiple fragment types in the site identification by ligand competitive saturation (SILCS) approach. *Journal of Chemical Information and Modeling*, **2013**, 53, 3384-98	6.1	79
14	Turning defense into offense: defensin mimetics as novel antibiotics targeting lipid II. *PLoS Pathogens*, **2013**, 9, e1003732	7.6	41
13	Comprehensive conformational studies of five tripeptides and a deduced method for efficient determinations of peptide structures. *Journal of Physical Chemistry B*, **2012**, 116, 2269-83	3.4	15
12	Prospects of Modulating Protein–Protein Interactions **2012**, 295-329		3
11	Extension of the CHARMM General Force Field to sulfonyl-containing compounds and its utility in biomolecular simulations. *Journal of Computational Chemistry*, **2012**, 33, 2451-68	3.5	447
10	Reproducing crystal binding modes of ligand functional groups using Site-Identification by Ligand Competitive Saturation (SILCS) simulations. *Journal of Chemical Information and Modeling*, **2011**, 51, 877-96	6.1	85
9	Targeting zymogen activation to control the matriptase-prostasin proteolytic cascade. *Journal of Medicinal Chemistry*, **2011**, 54, 7567-78	8.3	13
8	Comprehensive density functional theory study on the mechanism of activation of the nonapeptide hormone oxytocin by metal ions. *Journal of Physical Chemistry B*, **2010**, 114, 1417-23	3.4	13
7	Comparison of some representative density functional theory and wave function theory methods for the studies of amino acids. *Journal of Computational Chemistry*, **2009**, 30, 589-600	3.5	53
6	Extensive conformational searches of 13 representative dipeptides and an efficient method for dipeptide structure determinations based on amino acid conformers. *Journal of Computational Chemistry*, **2009**, 30, 2105-21	3.5	28
5	Electronic structures and electron detachment energies of halogen substituted acetate anions, XCH2COO- (X=F,Cl,Br). *Journal of Chemical Physics*, **2007**, 126, 114301	3.9	1
4	Coexistence of dihydrogen, blue- and red-shifting hydrogen bonds in an ultrasmall system: valine. *ChemPhysChem*, **2006**, 7, 828-30	3.2	37
3	Gaseous arginine conformers and their unique intramolecular interactions. *Journal of Physical Chemistry A*, **2006**, 110, 12282-91	2.8	96
2	Exploration of the full conformational landscapes of gaseous aromatic amino acid phenylalanine: An ab initio study. *Computational and Theoretical Chemistry*, **2006**, 758, 195-202		67
1	First-principle studies of gaseous aromatic amino acid histidine. *Computational and Theoretical Chemistry*, **2006**, 801, 7-20		35