Wenbo Yu

List of Publications by Year
in descending order

54 papers	2,858 citations	218662 26 h-index	189881 50 g-index
57 all docs	57 docs citations	57 times ranked	4120 citing authors

#	Article	IF	Citations
1	Extension of the CHARMM general force field to sulfonylâ€containing compounds and its utility in biomolecular simulations. Journal of Computational Chemistry, 2012, 33, 2451-2468.	3.3	659
2	Computer-Aided Drug Design Methods. Methods in Molecular Biology, 2017, 1520, 85-106.	0.9	317
3	The Expanding Role of the BCL6 Oncoprotein as a Cancer Therapeutic Target. Clinical Cancer Research, 2017, 23, 885-893.	7.0	133
4	Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma. Journal of Clinical Investigation, 2016, 126, 3351-3362.	8.2	133
5	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, 877-896.	5.4	105
6	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	3.0	103
7	Inclusion of Multiple Fragment Types in the Site Identification by Ligand Competitive Saturation (SILCS) Approach. Journal of Chemical Information and Modeling, 2013, 53, 3384-3398.	5.4	101
8	Gaseous Arginine Conformers and Their Unique Intramolecular Interactions. Journal of Physical Chemistry A, 2006, 110, 12282-12291.	2.5	100
9	The novel BH3 Î±-helix mimetic JY-1-106 induces apoptosis in a subset of cancer cells (lung cancer, colon) Tj ETQq1 1 0.784314 rgBT / Molecular Cancer, 2013, 12, 42.	19.2	78
10	Exploration of the full conformational landscapes of gaseous aromatic amino acid phenylalanine: An ab initio study. Computational and Theoretical Chemistry, 2006, 758, 195-202.	1.5	70
11	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.	5.3	69
12	Pharmacophore Modeling Using Site-Identification by Ligand Competitive Saturation (SILCS) with Multiple Probe Molecules. Journal of Chemical Information and Modeling, 2015, 55, 407-420.	5.4	62
13	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.	3.3	61
14	Site-Identification by Ligand Competitive Saturation (SILCS) assisted pharmacophore modeling. Journal of Computer-Aided Molecular Design, 2014, 28, 491-507.	2.9	56
15	Iodobenzene-Catalyzed Synthesis of Phenanthridinones via Oxidative Câ€“H Amidation. Journal of Organic Chemistry, 2017, 82, 3589-3596.	3.2	52
16	Turning Defense into Offense: Defensin Mimetics as Novel Antibiotics Targeting Lipid II. PLoS Pathogens, 2013, 9, e1003732.	4.7	50
17	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, 700-708.	5.4	48
18	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.	5.4	47

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19	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, 273-292.	5.5	42
20	Coexistence of Dihydrogen, Blue- and Red-Shifting Hydrogen Bonds in an Ultrasmall System: Valine. ChemPhysChem, 2006, 7, 828-830.	2.1	40
21	An activating mutation of the NSD2 histone methyltransferase drives oncogenic reprogramming in acute lymphocytic leukemia. Oncogene, 2019, 38, 671-686.	5.9	39
22	First-principle studies of gaseous aromatic amino acid histidine. Computational and Theoretical Chemistry, 2006, 801, 7-20.	1.5	35
23	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.	6.4	35
24	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.	2.4	34
25	Iminoguanidines as Allosteric Inhibitors of the Iron-Regulated Heme Oxygenase (HemO) of Pseudomonas aeruginosa. Journal of Medicinal Chemistry, 2016, 59, 6929-6942.	6.4	33
26	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, 2105-2121.	3.3	32
27	Structure of the cell-binding component of the Clostridium difficile 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.	7.1	23
28	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.	7.1	22
29	Facile Synthesis of Spirocyclic Lactams from Î²-Keto Carboxylic Acids. Organic Letters, 2015, 17, 3070-3073.	4.6	21
30	Exploring proteinâ€protein interactions using the siteâ€identification by ligand competitive saturation methodology. Proteins: Structure, Function and Bioinformatics, 2019, 87, 289-301.	2.6	21
31	Profiling the Tox21 Chemical Collection for Acetylcholinesterase Inhibition. Environmental Health Perspectives, 2021, 129, 47008.	6.0	21
32	Estimating glycosaminoglycanâ€“protein interaction affinity: water dominates the specific antithrombinâ€“heparin interaction. Glycobiology, 2016, 26, 1041-1047.	2.5	19
33	Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae. PLoS ONE, 2021, 16, e0244967.	2.5	19
34	Rapid and accurate estimation of proteinâ€“ligand relative binding affinities using site-identification by ligand competitive saturation. Chemical Science, 2021, 12, 8844-8858.	7.4	18
35	Comprehensive Conformational Studies of Five Tripeptides and a Deduced Method for Efficient Determinations of Peptide Structures. Journal of Physical Chemistry B, 2012, 116, 2269-2283.	2.6	17
36	Targeting Zymogen Activation To Control the Matriptase-Prostasin Proteolytic Cascade. Journal of Medicinal Chemistry, 2011, 54, 7567-7578.	6.4	16

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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.	7.1	16
38	Impact of electronic polarizability on protein-functional group interactions. Physical Chemistry Chemical Physics, 2020, 22, 6848-6860.	2.8	16
39	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, 1417-1423.	2.6	14
40	Novel proteinâ€“inhibitor interactions in site 3 of Ca²⁺-bound S100B as discovered by X-ray crystallography. Acta Crystallographica Section D: Structural Biology, 2016, 72, 753-760.	2.3	10
41	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.	14.5	10
42	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.	2.2	9
43	Application of site-identification by ligand competitive saturation in computer-aided drug design. New Journal of Chemistry, 2022, 46, 919-932.	2.8	8
44	Structure–activity exploration of a small-molecule Lipid II inhibitor. Drug Design, Development and Therapy, 2015, 9, 2383.	4.3	7
45	Specificity of Molecular Fragments Binding to S100B versus S100A1 as Identified by NMR and Site Identification by Ligand Competitive Saturation (SILCS). Molecules, 2021, 26, 381.	3.8	6
46	Optimization of a Benzothiazole Indolene Scaffold Targeting Bacterial Cell Wall Assembly . Drug Design, Development and Therapy, 2020, Volume 14, 567-574.	4.3	5
47	Cholecalciferol complexation with hydroxypropyl-Î²-cyclodextrin (HPBCD) and its molecular dynamics simulation. Pharmaceutical Development and Technology, 2022, 27, 389-398.	2.4	5
48	Scale-Up Preparation of Crocins I and II from Gardeniajasminoides by a Two-Step Chromatographic Approach and Their Inhibitory Activity Against ATP Citrate Lyase. Molecules, 2021, 26, 3137.	3.8	4
49	Scaffold hopping from indoles to indazoles yields dual MCL-1/BCL-2 inhibitors from MCL-1 selective leads. RSC Medicinal Chemistry, 2022, 13, 963-969.	3.9	4
50	hERG Blockade Prediction by Combining Site Identification by Ligand Competitive Saturation and Physicochemical Properties. Chemistry, 2022, 4, 630-646.	2.2	4
51	Electronic structures and electron detachment energies of halogen substituted acetate anions, XCH2COOâ^' (X=F,Cl,Br). Journal of Chemical Physics, 2007, 126, 114301.	3.0	1
52	Optimization of a BCL6 Inhibitor using the Site-Identification by Ligand Competitive Saturation (SILCS). Biophysical Journal, 2011, 100, 394a.	0.5	0
53	Development of CHARMM Additive Potential Energy Parameters for Î±-Methyl Amino Acids. Journal of Physical Chemistry B, 2021, 125, 11687-11696.	2.6	0
54	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches. , 2020, , 81-108.		0