Hai-Bo Yu

List of Publications by Year
in descending order

108 papers	4,948 citations	134610 34 h-index	107981 68 g-index
123 all docs	123 docs citations	123 times ranked	6459 citing authors

#	Article	IF	Citations
1	Discovery of 7-alkyloxy- [1,2,4] triazolo[1,5-a] pyrimidine derivatives as selective positive modulators of GABAA1 and GABAA4 receptors with potent antiepileptic activity. Bioorganic Chemistry, 2022, 119, 105565.	2.0	4
2	Urokinase plasminogen activator as an anti-metastasis target: inhibitor design principles, recent amiloride derivatives, and issues with human/mouse species selectivity. Biophysical Reviews, 2022, 14, 277-301.	1.5	6
3	Direct S_N2 or S_N2X Manifoldâ”€Mechanistic Study of Ion-Pair-Catalyzed Carbon(sp³)â€“Carbon(sp³) Bond Formation. Journal of Organic Chemistry, 2022, 87, 4029-4039.	1.7	1
4	Disruption of Water Networks is the Cause of Human/Mouse Species Selectivity in Urokinase Plasminogen Activator (uPA) Inhibitors Derived from Hexamethylene Amiloride (HMA). Journal of Medicinal Chemistry, 2022, 65, 1933-1945.	2.9	5
5	1,6;2,3-Bis-BN Cyclohexane: Synthesis, Structure, and Hydrogen Release. Journal of the American Chemical Society, 2022, 144, 8434-8438.	6.6	5
6	Hydrogen bonding penalty used for virtual screening to discover potent inhibitors for Papainâ€Like cysteine proteases of SARSâ€CoVâ€². Chemical Biology and Drug Design, 2022, 100, 502-514.	1.5	4
7	Synthesis and biological evaluation of selective phosphonate-bearing 1,2,3-triazole-linked sialyltransferase inhibitors. RSC Medicinal Chemistry, 2021, 12, 1680-1689.	1.7	3
8	A First-Principles Study of Impurity-Enhanced Adhesion and Lubricity of Graphene on Iron Oxide Surface. Journal of Physical Chemistry C, 2021, 125, 4310-4321.	1.5	6
9	Postsynthetic Modification of Half-Sandwich Ruthenium Complexes by Mechanochemical Synthesis. Inorganic Chemistry, 2021, 60, 4313-4321.	1.9	8
10	An Amineâ€“Borane System Featuring Roomâ€Temperature Dehydrogenation and Regeneration. Angewandte Chemie - International Edition, 2021, 60, 11725-11729.	7.2	11
11	An Amineâ€“Borane System Featuring Roomâ€Temperature Dehydrogenation and Regeneration. Angewandte Chemie, 2021, 133, 11831-11835.	1.6	3
12	Identification of WP1066, an inhibitor of JAK2 and STAT3, as a K_V1.3 potassium channel blocker. British Journal of Pharmacology, 2021, 178, 2617-2631.	2.7	4
13	The Detosylation of Chiral 1,2-Bis(tosylamides). Journal of Organic Chemistry, 2021, 86, 9163-9180.	1.7	5
14	Computational Tribochemistry: A Review from Classical and Quantum Mechanics Studies. Journal of Physical Chemistry C, 2021, 125, 16875-16891.	1.5	12
15	Comparative studies of IR spectra of deprotonated serine with classical and thermostated ring polymer molecular dynamics simulations. Structural Dynamics, 2021, 8, 054101.	0.9	0
16	Sialyltransferase Inhibitors as Potential Anti-Cancer Agents. Australian Journal of Chemistry, 2021, 74, 758-766.	0.5	4
17	Indole alkaloid glycosides with a 1â€²-(phenyl)ethyl unit from Isatis indigotica leaves. Acta Pharmaceutica Sinica B, 2020, 10, 895-902.	5.7	16
18	Discovery of [1,2,4]-triazolo [1,5-a]pyrimidine-7(4H)-one derivatives as positive modulators of GABAA1 receptor with potent anticonvulsant activity and low toxicity. European Journal of Medicinal Chemistry, 2020, 185, 111824.	2.6	31

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19	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	1.5	31
20	Structural basis of the potency and selectivity of Urotoxin, a potent Kv1 blocker from scorpion venom. Biochemical Pharmacology, 2020, 174, 113782.	2.0	12
21	Ab initio study on physical and chemical interactions at borates and iron oxide interface at high temperature. Chemical Physics, 2020, 529, 110548.	0.9	8
22	Mechanisms of Pressure-Induced Structural Transformation in Confined Sodium Borate Glasses. Journal of Physical Chemistry B, 2020, 124, 277-287.	1.2	5
23	Atomistic Insights into Photoprotein Formation: Computational Prediction of the Properties of Coelenterazine and Oxygen Binding in Obelin. Journal of Computational Chemistry, 2020, 41, 587-603.	1.5	5
24	Predicting phosphirane air stability using density functional theory. Journal of Physical Organic Chemistry, 2020, 33, e4110.	0.9	0
25	Exploration of the Dehydrogenation Pathways of Ammonia Diborane and Diammoniate of Diborane by Molecular Dynamics Simulations Using Reactive Force Fields. Journal of Physical Chemistry A, 2020, 124, 1698-1704.	1.1	19
26	Surface transformation and interactions of iron oxide in glassy lubricant: An ab initio study. Chemical Physics, 2020, 538, 110919.	0.9	4
27	Structural response of alkali metal borates at Fe2O3 sliding interface: The effect of alkali cations. Computational Materials Science, 2020, 184, 109930.	1.4	4
28	Design, synthesis and evaluation of carbamate-linked uridyl-based inhibitors of human ST6Gal I. Bioorganic and Medicinal Chemistry, 2020, 28, 115561.	1.4	15
29	A new class of quadruplex DNA-binding nickel Schiff base complexes. Dalton Transactions, 2020, 49, 4843-4860.	1.6	12
30	Polarisable force fields: what do they add in biomolecular simulations?. Current Opinion in Structural Biology, 2020, 61, 182-190.	2.6	63
31	Enhanced Potassium Ion Battery by Inducing Interlayer Anionic Ligands in MoS_{1.5}Se_{0.5} Nanosheets with Exploration of the Mechanism. Advanced Energy Materials, 2020, 10, 1904162.	10.2	48
32	Divergent Pd-catalyzed cross-coupling of allenyloxazolidinones to give chiral 1,3-dienes and vinyloxazolidinones. Chemical Science, 2019, 10, 9051-9056.	3.7	16
33	Electrocatalytically inactive SnS2 promotes water adsorption/dissociation on molybdenum dichalcogenides for accelerated alkaline hydrogen evolution. Nano Energy, 2019, 64, 103918.	8.2	58
34	11B NMR Chemical Shift Predictions via Density Functional Theory and Gauge-Including Atomic Orbital Approach: Applications to Structural Elucidations of Boron-Containing Molecules. ACS Omega, 2019, 4, 12385-12392.	1.6	20
35	Theoretical Investigation on the Single Transition-Metal Atom-Decorated Defective MoS₂ for Electrocatalytic Ammonia Synthesis. ACS Applied Materials & Interfaces, 2019, 11, 36506-36514.	4.0	88
36	Theoretical Screening of Single Transition Metal Atoms Embedded in MXene Defects as Superior Electrocatalyst of Nitrogen Reduction Reaction. Small Methods, 2019, 3, 1900337.	4.6	213

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37	Comparative studies of catalytic pathways for Streptococcus pneumoniae sialidases NanA, NanB and NanC. Scientific Reports, 2019, 9, 2157.	1.6	12
38	Three new phenylspirodrimane derivatives with inhibitory effect towards potassium channel Kv1.3 from the fungus Stachybotrys chartarum. Journal of Asian Natural Products Research, 2019, 21, 887-894.	0.7	10
39	Towards an Accurate Prediction of Nitrogen Chemical Shifts by Density Functional Theory and Gaugeâ€Including Atomic Orbital. Advanced Theory and Simulations, 2019, 2, 1800148.	1.3	12
40	Heteroatomâ€doped MoSe₂ Nanosheets with Enhanced Hydrogen Evolution Kinetics for Alkaline Water Splitting. Chemistry - an Asian Journal, 2019, 14, 301-306.	1.7	41
41	Depolymerization of sodium polyphosphates on an iron oxide surface at high temperature. Physical Chemistry Chemical Physics, 2018, 20, 7819-7835.	1.3	15
42	Molecular Quantum Dot Cellular Automata Based on Diboryl Monoradical Anions. Journal of Physical Chemistry C, 2018, 122, 2454-2460.	1.5	30
43	Differential-Mobility Spectrometry of 1-Deoxysphingosine Isomers: New Insights into the Gas Phase Structures of Ionized Lipids. Analytical Chemistry, 2018, 90, 5343-5351.	3.2	31
44	Molecular Docking Studies to Explore Potential Binding Pockets and Inhibitors for Chikungunya Virus Envelope Glycoproteins. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 515-524.	2.2	14
45	Chemical Origin of Sodium Phosphate Interactions on Iron and Iron Oxide Surfaces by First Principle Calculations. Journal of Physical Chemistry C, 2018, 122, 635-647.	1.5	29
46	Computerâ€aided design of human sialyltransferase inhibitors of hST8Sia III. Journal of Molecular Recognition, 2018, 31, e2684.	1.1	8
47	A systematic benchmarking of computational vibrational spectroscopy with DFTB3: Normal mode analysis and fast Fourier transform dipole autocorrelation function. Journal of Computational Chemistry, 2018, 39, 2067-2078.	1.5	7
48	Remodeling the endoplasmic reticulum proteostasis network restores proteostasis of pathogenic GABAA receptors. PLoS ONE, 2018, 13, e0207948.	1.1	26
49	The effect of DNA backbone on the triplet mechanism of UV-induced thymine-thymine (6â€“4) dimer formation. Journal of Molecular Modeling, 2018, 24, 319.	0.8	2
50	Loperamide inhibits sodium channels to alleviate inflammatory hyperalgesia. Neuropharmacology, 2017, 117, 282-291.	2.0	15
51	Computational Glycobiology: Mechanistic Studies of Carbohydrate-Active Enzymes and Implication for Inhibitor Design. Advances in Protein Chemistry and Structural Biology, 2017, 109, 25-76.	1.0	28
52	Theoretical pK prediction of the Î±-phosphate moiety of uridine 5â€²-diphosphate-GlcNAc. Chemical Physics Letters, 2017, 667, 220-225.	1.2	7
53	Transition state-based ST6Gal I inhibitors: Mimicking the phosphodiester linkage with a triazole or carbamate through an enthalpy-entropy compensation. Scientific Reports, 2017, 7, 14428.	1.6	20
54	P2123The timing for elective percutaneous coronary intervention and in-hospital outcomes in patients with ST-segment elevation myocardial infarction. European Heart Journal, 2017, 38, .	1.0	0

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55	Computational characterisation of the interactions between human ST6Gal I and transition-state analogue inhibitors: insights for inhibitor design. Journal of Molecular Recognition, 2016, 29, 210-222.	1.1	17
56	Ammonium Aminodiboranate: A Longâ€Sought Isomer of Diammoniate of Diborane and Ammonia Borane Dimer. Chemistry - A European Journal, 2016, 22, 7727-7729.	1.7	15
57	Rationalising pK_a shifts in Bacillus circulans xylanase with computational studies. Physical Chemistry Chemical Physics, 2016, 18, 30305-30312.	1.3	11
58	Selective binding modes and allosteric inhibitory effects of lupane triterpenes on protein tyrosine phosphatase 1B. Scientific Reports, 2016, 6, 20766.	1.6	57
59	High throughput screening technologies for ion channels. Acta Pharmacologica Sinica, 2016, 37, 34-43.	2.8	102
60	Investigation of miscellaneous hERG inhibition in large diverse compound collection using automated patch-clamp assay. Acta Pharmacologica Sinica, 2016, 37, 111-123.	2.8	44
61	Effect of <scp>t</scp>yrphostin <scp>AG</scp>879 on <scp>K</scp>_v4.2 and <scp>K</scp>_v4.3 potassium channels. British Journal of Pharmacology, 2015, 172, 3370-3382.	2.7	2
62	Identification of chikungunya virus nsP2 protease inhibitors using structure-base approaches. Journal of Molecular Graphics and Modelling, 2015, 57, 1-8.	1.3	41
63	Four basic residues critical for the ion selectivity and pore blocker sensitivity of TMEM16A calcium-activated chloride channels. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3547-3552.	3.3	65
64	Discovery of in silico hits targeting the nsP3 macro domain of chikungunya virus. Journal of Molecular Modeling, 2014, 20, 2216.	0.8	34
65	pKa cycling of the general acid/base in glycoside hydrolase families 33 and 34. Physical Chemistry Chemical Physics, 2014, 16, 5785.	1.3	10
66	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. Faraday Discussions, 2013, 160, 135-149.	1.6	102
67	Allosteric Activation Transitions in Enzymes and Biomolecular Motors: Insights from Atomistic and Coarse-Grained Simulations. Topics in Current Chemistry, 2013, 337, 139-164.	4.0	12
68	Molecular Mechanisms of K+ Selectivity in Na/K Pump. Australian Journal of Chemistry, 2012, 65, 448.	0.5	6
69	Engineering the hERG1 Selectivity Filter into the NaK Pore Domain. Biophysical Journal, 2011, 100, 584a.	0.2	0
70	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	0.9	142
71	Protonation of key acidic residues is critical for the K+-selectivity of the Na/K pump. Nature Structural and Molecular Biology, 2011, 18, 1159-1163.	3.6	54
72	Two mechanisms of ion selectivity in protein binding sites. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20329-20334.	3.3	83

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73	Selectivity of externally facing ion-binding sites in the Na/K pump to alkali metals and organic cations. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 18718-18723.	3.3	31
74	Assessing the accuracy of approximate treatments of ion hydration based on primitive quasichemical theory. Journal of Chemical Physics, 2010, 132, 234101.	1.2	24
75	Microscopic Mechanism of Ion Selectivity in the Nak Pump. Biophysical Journal, 2010, 98, 330a.	0.2	0
76	A Combined Experimental and Theoretical Study of Ion Solvation in Liquid N-Methylacetamide. Journal of the American Chemical Society, 2010, 132, 10847-10856.	6.6	35
77	Ion-Selectivity of Externally Facing Na+-Exclusive and Na+/K+-Shared Sites in the Na/K-Pump. Biophysical Journal, 2010, 98, 168a.	0.2	0
78	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	2.3	401
79	The Role of Architectural and Structural Forces in Ion Selectivity. Biophysical Journal, 2010, 98, 330a.	0.2	0
80	Hydration Number, Topological Control, and Ion Selectivity. Journal of Physical Chemistry B, 2009, 113, 8725-8730.	1.2	34
81	On the Utilization of Energy Minimization to the Study of Ion Selectivity. Biophysical Journal, 2009, 97, L15-L17.	0.2	17
82	Development of a Drude Polarizable Force Field for Ion-water and Ion-NMA Interactions and Application to Selectivity in Ion Channels. Biophysical Journal, 2009, 96, 660a.	0.2	0
83	Geometry and excitation energy fluctuations of NMA in aqueous solution with CHARMM, AMBER, OPLS, and GROMOS force fields: Implications for protein ultraviolet spectra simulation. Chemical Physics Letters, 2008, 452, 78-83.	1.2	20
84	Extensive Conformational Transitions Are Required to Turn On ATP Hydrolysis in Myosin. Journal of Molecular Biology, 2008, 381, 1407-1420.	2.0	71
85	Description of Phosphate Hydrolysis Reactions with the Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB) Theory. 1. Parameterization. Journal of Chemical Theory and Computation, 2008, 4, 2067-2084.	2.3	87
86	Amino acids with an intermolecular proton bond as proton storage site in bacteriorhodopsin. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19672-19677.	3.3	87
87	Mechanochemical Coupling in the Myosin Motor Domain. I. Insights from Equilibrium Active-Site Simulations. PLoS Computational Biology, 2007, 3, e21.	1.5	44
88	Mechanochemical Coupling in the Myosin Motor Domain. II. Analysis of Critical Residues. PLoS Computational Biology, 2007, 3, e23.	1.5	63
89	The vibrational spectra of protonated water clusters: A benchmark for self-consistent-charge density-functional tight binding. Journal of Chemical Physics, 2007, 127, 234504.	1.2	53
90	Molecular dynamics simulation of human interleukin-4: comparison with NMR data and effect of pH, counterions and force field on tertiary structure stability. Molecular Simulation, 2007, 33, 1143-1154.	0.9	2

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91	Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method:â€‰ Third-Order Expansion of the Density Functional Theory Total Energy and Introduction of a Modified Effective Coulomb Interaction. Journal of Physical Chemistry A, 2007, 111, 10861-10873.	1.1	265
92	Development of Effective Quantum Mechanical/Molecular Mechanical (QM/MM) Methods for Complex Biological Processes. Journal of Physical Chemistry B, 2006, 110, 6458-6469.	1.2	290
93	â€œProton Holesâ€•in Long-Range Proton Transfer Reactions in Solution and Enzymes:Â A Theoretical Analysis. Journal of the American Chemical Society, 2006, 128, 16302-16311.	6.6	125
94	Molecular dynamics study of the stabilities of consensus designed ankyrin repeat proteins. Proteins: Structure, Function and Bioinformatics, 2006, 65, 285-295.	1.5	13
95	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	7.2	503
96	Molecular dynamics simulations of liquid methanol and methanolâ€“water mixtures with polarizable models. Journal of Computational Chemistry, 2006, 27, 1494-1504.	1.5	103
97	Role of potassium channels in AÎ²1â€“40-activated apoptotic pathway in cultured cortical neurons. Journal of Neuroscience Research, 2006, 84, 1475-1484.	1.3	35
98	Accounting for polarization in molecular simulation. Computer Physics Communications, 2005, 172, 69-85.	3.0	209
99	On the transferability of the SPC/L water model to biomolecular simulation. Brazilian Journal of Physics, 2004, 34, 116-125.	0.7	5
100	Charge-on-spring polarizable water models revisited: From water clusters to liquid water to ice. Journal of Chemical Physics, 2004, 121, 9549-9564.	1.2	191
101	Effect of methylation on the stability and solvation free energy of amylose and cellulose fragments: a molecular dynamics study. Carbohydrate Research, 2004, 339, 1697-1709.	1.1	43
102	Comparison of Properties of Aib-Rich Peptides in Crystal and Solution: A Molecular Dynamics Study. ChemPhysChem, 2004, 5, 633-641.	1.0	15
103	Molecular dynamics simulations of peptides containing an unnatural amino acid: Dimerization, folding, and protein binding. Proteins: Structure, Function and Bioinformatics, 2003, 54, 116-127.	1.5	17
104	Development of a simple, self-consistent polarizable model for liquid water. Journal of Chemical Physics, 2003, 118, 221-234.	1.2	209
105	Novel Magnetic Resonance Signal Enhancing Coating Material. Advanced Materials, 2001, 13, 490-493.	11.1	9
106	Design of new selective inhibitors of cyclooxygenase-2 by dynamic assembly of molecular building blocks. Journal of Computer-Aided Molecular Design, 2001, 15, 447-463.	1.3	15
107	capillary wave study of linear and branched polysiloxanes at the air/water interface. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 1046-1055.	0.9	3
108	Technique of surfaceâ€wave scattering and calibration with simple liquids. Review of Scientific Instruments, 1986, 57, 1158-1162.	0.6	71