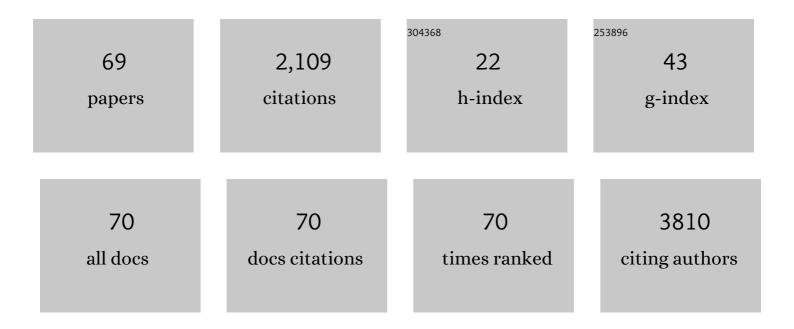
## Zhiwei Yang

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Mechanism of Glycans Modulating Cholesteryl Ester Transfer Protein: Unveiled by Molecular Dynamics Simulation. Journal of Chemical Information and Modeling, 2022, 62, 5246-5257.	2.5	7
2	Facilely prepared aggregation-induced emission (AIE) nanocrystals with deep-red emission for super-resolution imaging. Chemical Science, 2022, 13, 1270-1280.	3.7	24
3	TAB1 binding induced p38α conformation change: an accelerated molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2022, 24, 10506-10513.	1.3	2
4	Sequence Matching between Hemagglutinin and Neuraminidase through Sequence Analysis Using Machine Learning. Viruses, 2022, 14, 469.	1.5	1
5	Aggregation-Induced Emission (AIE) in Super-resolution Imaging: Cationic AIE Luminogens (AIEgens) for Tunable Organelle-Specific Imaging and Dynamic Tracking in Nanometer Scale. ACS Nano, 2022, 16, 5932-5942.	7.3	26
6	Gold Nanorods/Metal–Organic Framework Hybrids: Photo-Enhanced Peroxidase-Like Activity and SERS Performance for Organic Dyestuff Degradation and Detection. Analytical Chemistry, 2022, 94, 4484-4494.	3.2	45
7	Accounting Conformational Dynamics into Structural Modeling Reflected by Cryo-EM with Deep Learning. Combinatorial Chemistry and High Throughput Screening, 2022, 25, .	0.6	0
8	Molecular insights into the binding variance of the SARS-CoV-2 spike with human, cat and dog ACE2 proteins. Physical Chemistry Chemical Physics, 2021, 23, 13752-13759.	1.3	5
9	Bimetallic Metal–Organic Frameworks: Enhanced Peroxidase-like Activities for the Self-Activated Cascade Reaction. ACS Applied Materials & Interfaces, 2021, 13, 36106-36116.	4.0	41
10	Molecular Insights into the Recruiting Between UCP2 and DDX5/UBAP2L in the Metabolic Plasticity of Non-Small-Cell Lung Cancer. Journal of Chemical Information and Modeling, 2021, 61, 3978-3987.	2.5	8
11	Donor-Acceptor Typed AIE Luminogens with Near-infrared Emission for Super-resolution Imaging. Chemical Research in Chinese Universities, 2021, 37, 143-149.	1.3	9
12	Computational identification of potential chemoprophylactic agents according to dynamic behavior of peroxisome proliferator-activated receptor gamma. RSC Advances, 2021, 11, 147-159.	1.7	5
13	Thermal Decomposition of Photocurable Energetic APNIMMO Polymer. Propellants, Explosives, Pyrotechnics, 2021, 46, 1767.	1.0	4
14	Computational Simulation of HIV Protease Inhibitors to the Main Protease (Mpro) of SARS-CoV-2: Implications for COVID-19 Drugs Design. Molecules, 2021, 26, 7385.	1.7	6
15	Bindings of PPARÎ <sup>3</sup> ligand-binding domain with 5-cholesten-3β, 25-diol, 3-sulfate: accurate prediction by molecular simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1918-1926.	2.0	3
16	Assessing the performance of the g_mmpbsa tools to simulate the inhibition of oseltamivir to influenza virus neuraminidase by molecular mechanics Poisson–Boltzmann surface area methods. Journal of the Chinese Chemical Society, 2020, 67, 46-53.	0.8	43
17	Structure-based methoxyflavone derivatives with potent inhibitory activity against various influenza neuraminidases. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4617-4624.	2.0	4
18	Tuning molecular aggregation to achieve highly bright AIE dots for NIR-II fluorescence imaging and NIR-I photoacoustic imaging. Chemical Science, 2020, 11, 8157-8166.	3.7	70

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19	CD147-spike protein is a novel route for SARS-CoV-2 infection to host cells. Signal Transduction and Targeted Therapy, 2020, 5, 283.	7.1	806
20	Crosstalk between the Akt/mTORC1 and NF-κB signaling pathways promotes hypoxia-induced pulmonary hypertension by increasing DPP4 expression in PASMCs. Acta Pharmacologica Sinica, 2019, 40, 1322-1333.	2.8	43
21	One-step synthesis of cross-linked and hollow microporous organic–inorganic hybrid nanoreactors for selective redox reactions. Nanoscale, 2019, 11, 15017-15022.	2.8	5
22	Chemically Controlled Helical Polymorphism in Protein Tubes by Selective Modulation of Supramolecular Interactions. Journal of the American Chemical Society, 2019, 141, 19448-19457.	6.6	34
23	Sp1â€mediated epigenetic dysregulation dictates HDAC inhibitor susceptibility of HER2â€overexpressing breast cancer. International Journal of Cancer, 2019, 145, 3285-3298.	2.3	20
24	Caspase cleavage of Mcl-1 impairs its anti-apoptotic activity and proteasomal degradation in non-small lung cancer cells. Apoptosis: an International Journal on Programmed Cell Death, 2018, 23, 54-64.	2.2	12
25	Fluorescent Organic Nanoparticles Constructed by a Facile "Self-Isolation Enhanced Emission― Strategy for Cell Imaging. ACS Applied Nano Materials, 2018, 1, 2324-2331.	2.4	23
26	Binding profiles of cholesterol ester transfer protein with current inhibitors: a look at mechanism and drawback. Journal of Biomolecular Structure and Dynamics, 2018, 36, 2567-2580.	2.0	7
27	Cefminox, a Dual Agonist of Prostacyclin Receptor and Peroxisome Proliferator-Activated Receptor-Gamma Identified by Virtual Screening, Has Therapeutic Efficacy against Hypoxia-Induced Pulmonary Hypertension in Rats. Frontiers in Pharmacology, 2018, 9, 134.	1.6	16
28	Role of glycans in cholesteryl ester transfer protein revealed by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2018, 86, 882-891.	1.5	4
29	Cover Image, Volume 86, Issue 8. Proteins: Structure, Function and Bioinformatics, 2018, 86, C4-C4.	1.5	0
30	Screening allergic components of Yejuhua injection using LAD2 cell membrane chromatography model online with high performance liquid chromatography-ion trap-time of flight-mass spectrum system. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2017, 1055-1056, 119-124.	1.2	10
31	Lightweight, interconnected VO <sub>2</sub> nanoflowers hydrothermally grown on 3D graphene networks for wide-voltage-window supercapacitors. RSC Advances, 2017, 7, 35558-35564.	1.7	42
32	Membrane Fusion Involved in Neurotransmission: Glimpse from Electron Microscope and Molecular Simulation. Frontiers in Molecular Neuroscience, 2017, 10, 168.	1.4	18
33	Uncoupling protein 2 downregulation by hypoxia through repression of peroxisome proliferator-activated receptor 1 <sup>3</sup> promotes chemoresistance of non-small cell lung cancer. Oncotarget, 2017, 8, 8083-8094.	0.8	29
34	Zwitterionic structures: from physicochemical properties toward computer-aided drug designs. Future Medicinal Chemistry, 2016, 8, 2245-2262.	1.1	22
35	Novel binding patterns between ganoderic acids and neuraminidase: Insights from docking, molecular dynamics and MM/PBSA studies. Journal of Molecular Graphics and Modelling, 2016, 65, 27-34.	1.3	24
36	TOPK promotes lung cancer resistance to EGFR tyrosine kinase inhibitors by phosphorylating and activating c-Jun. Oncotarget, 2016, 7, 6748-6764.	0.8	40

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37	miR-26a desensitizes non-small cell lung cancer cells to tyrosine kinase inhibitors by targeting PTPN13. Oncotarget, 2016, 7, 45687-45701.	0.8	25
38	Metabolomics studies of prostate cancer using gas chromatography-mass spectrometery. Translational Cancer Research, 2016, 5, 302-314.	0.4	2
39	Bacterial cellulose-templated synthesis of free-standing silica nanotubes with a three-dimensional network structure. RSC Advances, 2015, 5, 48875-48880.	1.7	15
40	Construction of nanoparticles based on amphiphilic PEI–PA polymers for bortezomib and paclitaxel co-delivery. RSC Advances, 2015, 5, 15453-15460.	1.7	8
41	A general strategy of decorating 3D carbon nanofiber aerogels derived from bacterial cellulose with nano-Fe <sub>3</sub> O <sub>4</sub> for high-performance flexible and binder-free lithium-ion battery anodes. Journal of Materials Chemistry A, 2015, 3, 15386-15393.	5.2	91
42	Construction of nanoparticles based on amphiphilic copolymers of poly(γ-glutamic acid) Tj ETQq0 0 0 rgBT /Over Journal of Colloid and Interface Science, 2014, 413, 54-64.	lock 10 Tf 5.0	50 547 Td (0 14
43	Transferrin conjugated poly (γ-glutamic acid-maleimide-co- l) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 507 T drug delivery. Colloids and Surfaces B: Biointerfaces, 2014, 123, 787-796.	d (-lactide 2.5	)-1,2-dipalm 18
44	Mutation effects of neuraminidases and their docking with ligands: a molecular dynamics and free energy calculation study. Journal of Computer-Aided Molecular Design, 2013, 27, 935-950.	1.3	28
45	The Direct Hydroxylation of Benzene to Phenol Catalyzed by Fe-ZSM-5 Zeolite: A DFT and Hybrid MP2:DFT Calculation. Catalysis Letters, 2013, 143, 260-266.	1.4	16
46	Computational investigation of interaction mechanisms between juglone and influenza virus surface glycoproteins. Molecular Simulation, 2013, 39, 788-795.	0.9	5
47	SUSCEPTIBILITY OF COMMERCIAL NEURAMINIDASE INHIBITORS AGAINST 2013 A/H7N9 INFLUENZA VIRUS: A DOCKING AND MOLECULAR DYNAMICS STUDY. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350069.	1.8	2
48	Editorial (Applications of Docking and Molecular Dynamics in Drug Design). Current Computer-Aided Drug Design, 2013, 9, 506-506.	0.8	2
49	Genome-Wide Identification and in Silico Analysis of Poplar Peptide Deformylases. International Journal of Molecular Sciences, 2012, 13, 5112-5124.	1.8	4
50	EXPLORING THE MOLECULAR BASIS OF H5N1 HEMAGGLUTININ BINDING WITH CATECHINS IN GREEN TEA: A FLEXIBLE DOCKING AND MOLECULAR DYNAMICS STUDY. Journal of Theoretical and Computational Chemistry, 2012, 11, 111-125.	1.8	9
51	Understanding the chiral recognitions between neuraminidases and inhibitors: Studies with DFT, docking, and MD methods. International Journal of Quantum Chemistry, 2012, 112, 909-921.	1.0	13
52	<i>In Vitro</i> Antioxidant Properties, DNA Damage Protective Activity, and Xanthine Oxidase Inhibitory Effect of Cajaninstilbene Acid, a Stilbene Compound Derived from Pigeon Pea [ <i>Cajanus cajan</i> (L.) Millsp.] Leaves. Journal of Agricultural and Food Chemistry, 2011, 59, 437-443.	2.4	58
53	Comparative Anti-Infectious Bronchitis Virus (IBV) Activity of (-)-Pinene: Effect on Nucleocapsid (N) Protein. Molecules, 2011, 16, 1044-1054.	1.7	40
54	Antioxidant and antibacterial activities of Camptotheca acuminate D. seed oil. African Journal of Microbiology Research, 2011, 5, .	0.4	3

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55	The systematic characterization of poplar CK2α and its theoretical studies on phosphorylation of P-protein C-terminal domain. African Journal of Microbiology Research, 2011, 5, .	0.4	Ο
56	Synergistic effects in the designs of neuraminidase ligands: Analysis from docking and molecular dynamics studies. Journal of Theoretical Biology, 2010, 267, 363-374.	0.8	23
57	A revisit to proline-catalyzed aldol reaction: Interactions with acetone and catalytic mechanisms. Journal of Molecular Catalysis A, 2010, 316, 112-117.	4.8	29
58	Computer-Based De Novo Designs of Tripeptides as Novel Neuraminidase Inhibitors. International Journal of Molecular Sciences, 2010, 11, 4932-4951.	1.8	12
59	Anti-Infectious Bronchitis Virus (IBV) Activity of 1,8-cineole: Effect on Nucleocapsid (N) Protein. Journal of Biomolecular Structure and Dynamics, 2010, 28, 323-330.	2.0	53
60	The conformational analysis and proton transfer of neuraminidase inhibitors: a theoretical study. Physical Chemistry Chemical Physics, 2009, 11, 10035.	1.3	21
61	MOLECULAR DYNAMIC SIMULATIONS ON THE FOLDING AND CONFORMATIONAL INSIGHTS OF THE TRUNCATED PEPTIDES. Journal of Theoretical and Computational Chemistry, 2009, 08, 317-331.	1.8	5
62	Medicinal Chemistry of Paclitaxel and its Analogues. Current Medicinal Chemistry, 2009, 16, 3966-3985.	1.2	103
63	A Proline-Based Neuraminidase Inhibitor: DFT Studies on the Zwitterion Conformation, Stability and Formation. International Journal of Molecular Sciences, 2009, 10, 3918-3930.	1.8	11
64	Conformational Dynamics and Thermal Stabilities of the αβ-Tubulin Dimer: A Molecular Dynamics Simulation Study. In Silico Biology, 2009, 9, 271-284.	0.4	2
65	Temperature-Controlled Molecular Dynamics Studies on the Folding Mechanism of the Tubulin Active Peptides. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2009, 25, 773-782.	2.2	4
66	Synthesis and antitumor activity of novel 10-substituted camptothecin analogues. Bioorganic and Medicinal Chemistry, 2006, 14, 7175-7182.	1.4	21
67	Novel Potent Neutralizing Antibodies Revealed the Domain I of HCMV Glycoprotein B for Vaccine Design. SSRN Electronic Journal, 0, , .	0.4	0
68	Boosting the AIEgen-based photo-theranostic platform by balancing radiative decay and non-radiative decay. Materials Chemistry Frontiers, 0, , .	3.2	11
69	Organelle Interaction and Drug Discovery: Towards Correlative Nanoscopy and Molecular Dynamics Simulation. Frontiers in Pharmacology, 0, 13, .	1.6	1