

# Qianqian Wang

## List of Publications by Year in descending order

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32  
papers

579  
citations

567144

15  
h-index

642610

23  
g-index

32  
all docs

32  
docs citations

32  
times ranked

990  
citing authors

#	ARTICLE	IF	CITATIONS
1	The Molecular Mechanism of Bisphenol A (BPA) as an Endocrine Disruptor by Interacting with Nuclear Receptors: Insights from Molecular Dynamics (MD) Simulations. <i>PLoS ONE</i> , 2015, 10, e0120330.	1.1	73
2	The adsorption mechanism and induced conformational changes of three typical proteins with different secondary structural features on graphene. <i>RSC Advances</i> , 2014, 4, 9953.	1.7	54
3	Molecular Mechanism of the Inhibition and Remodeling of Human Islet Amyloid Polypeptide (hIAPP <sub>1-37</sub> ) Oligomer by Resveratrol from Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15-24.	1.2	51
4	Exploring the Influence of EGCG on the $\beta$ -Sheet-Rich Oligomers of Human Islet Amyloid Polypeptide (hIAPP <sub>1-37</sub> ) and Identifying Its Possible Binding Sites from Molecular Dynamics Simulation. <i>PLoS ONE</i> , 2014, 9, e94796.	1.1	40
5	Targeting protein arginine methyltransferase 5 in cancers: Roles, inhibitors and mechanisms. <i>Biomedicine and Pharmacotherapy</i> , 2021, 144, 112252.	2.5	31
6	Selective inhibition mechanism of RVX-208 to the second bromodomain of bromo and extraterminal proteins: insight from microsecond molecular dynamics simulations. <i>Scientific Reports</i> , 2017, 7, 8857.	1.6	26
7	Identification of a Novel Protein Arginine Methyltransferase 5 Inhibitor in Non-small Cell Lung Cancer by Structure-Based Virtual Screening. <i>Frontiers in Pharmacology</i> , 2018, 9, 173.	1.6	23
8	Gasotransmitters: Potential Therapeutic Molecules of Fibrotic Diseases. <i>Oxidative Medicine and Cellular Longevity</i> , 2021, 2021, 1-18.	1.9	22
9	Computational insights into the inhibition and destabilization of morin on the oligomer of full-length human islet amyloid polypeptide. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29103-29112.	1.3	20
10	Gossypol Inhibits Non-small Cell Lung Cancer Cells Proliferation by Targeting EGFR L858R/T790M. <i>Frontiers in Pharmacology</i> , 2018, 9, 728.	1.6	20
11	Compound C620-0696, a new potent inhibitor targeting BPTF, the chromatin-remodeling factor in non-small-cell lung cancer. <i>Frontiers of Medicine</i> , 2020, 14, 60-67.	1.5	19
12	Classical molecular dynamics and metadynamics simulations decipher the mechanism of CBP30 selectively inhibiting CBP/p300 bromodomains. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 6521-6530.	1.5	17
13	Synthesis, Biological Evaluation and Molecular Docking Studies of Piperidinylpiperidines and Spirochromanones Possessing Quinoline Moieties as Acetyl-CoA Carboxylase Inhibitors. <i>Molecules</i> , 2015, 20, 16221-16234.	1.7	16
14	The folding mechanism and key metastable state identification of the PrP <sup>127-147</sup> monomer studied by molecular dynamics simulations and Markov state model analysis. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11249-11259.	1.3	16
15	Computational study on the selective inhibition mechanism of MS402 to the first and second bromodomains of BRD4. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 3-11.	1.5	16
16	Selectively targeting individual bromodomain: Drug discovery and molecular mechanisms. <i>Pharmacological Research</i> , 2021, 172, 105804.	3.1	16
17	Citronellal ameliorates doxorubicin-induced hepatotoxicity via antioxidative stress, antiapoptosis, and proangiogenesis in rats. <i>Journal of Biochemical and Molecular Toxicology</i> , 2021, 35, e22639.	1.4	15
18	TQFL12, a novel synthetic derivative of TQ, inhibits triple-negative breast cancer metastasis and invasion through activating AMPK/ACC pathway. <i>Journal of Cellular and Molecular Medicine</i> , 2021, 25, 10101-10110.	1.6	15

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19	A Natural Interruption Displays Higher Global Stability and Local Conformational Flexibility than a Similar Gly Mutation Sequence in Collagen Mimic Peptides. <i>Biochemistry</i> , 2015, 54, 6106-6113.	1.2	13
20	Hesperidin derivative-11 inhibits fibroblast-like synoviocytes proliferation by activating Secreted frizzled-related protein 2 in adjuvant arthritis rats. <i>European Journal of Pharmacology</i> , 2017, 794, 173-183.	1.7	13
21	Effects of the A117V mutation on the folding and aggregation of palindromic sequences (PrP113â€“120) in prion: insights from replica exchange molecular dynamics simulations. <i>Molecular BioSystems</i> , 2015, 11, 647-655.	2.9	11
22	Molecular dynamics simulation on the inhibition mechanism of peptideâ€“based inhibitor of islet amyloid polypeptide (<scp>IAPP</scp>) to islet amyloid polypeptide (<scp>IAPP</scp><sub>22â€“28</sub>) oligomers. <i>Chemical Biology and Drug Design</i> , 2017, 90, 31-39.	1.5	10
23	Discovery of a novel protein kinase C activator from <i>Croton tiglium</i> for inhibition of non-small cell lung cancer. <i>Phytomedicine</i> , 2019, 65, 153100.	2.3	10
24	Understanding the recognition mechanisms of ZÎ± domain of human editing enzyme ADAR1 (hZÎ±ADAR1) and various Z-DNAs from molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2014, 20, 2500.	0.8	7
25	Deciphering the Active Compounds and Mechanisms of HSBDF for Treating ALI via Integrating Chemical Bioinformatics Analysis. <i>Frontiers in Pharmacology</i> , 0, 13, .	1.6	7
26	Systematic analyses identify the anti-fibrotic role of lncRNA TP53TG1 in IPF. <i>Cell Death and Disease</i> , 2022, 13, .	2.7	6
27	Discovery and Optimization of a Novel 2<i>H</i>-Pyrazolo[3,4-d]pyrimidine Derivative as a Potent Irreversible Pan-Fibroblast Growth Factor Receptor Inhibitor. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 9078-9099.	2.9	4
28	Exploring the thermodynamic, kinetic and inhibitory mechanisms of 5-iTU targeting mitotic kinase haspin by integrated molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18404-18413.	1.3	3
29	Amorphous Selenium Nanoparticles Improve Vascular Function in Rats With Chronic Isocarbophos Poisoning via Inhibiting the Apoptosis of Vascular Endothelial Cells. <i>Frontiers in Bioengineering and Biotechnology</i> , 2021, 9, 673327.	2.0	2
30	Gasotransmitter CO Attenuates Bleomycin-Induced Fibroblast Senescence via Induction of Stress Granule Formation. <i>Oxidative Medicine and Cellular Longevity</i> , 2021, 2021, 1-21.	1.9	2
31	5Î±-Epoxyalantolactone Inhibits Metastasis of Triple-Negative Breast Cancer Cells by Covalently Binding a Conserved Cysteine of Annexin A2. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 12537-12547.	2.9	1
32	Fluorometric determination of ssDNA based on functionalized magnetic microparticles and DNA supersandwich self-assemblies. <i>Mikrochimica Acta</i> , 2019, 186, 707.	2.5	0