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List of Publications by Year in descending order

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51 papers	1,443 citations	394421 19 h-index	345221 36 g-index
52 all docs	52 docs citations	52 times ranked	2102 citing authors

#	Article	IF	Citations
1	Protein Allostery and Conformational Dynamics. Chemical Reviews, 2016, 116, 6503-6515.	47.7	306
2	A Safe Polyzwitterionic Hydrogel Electrolyte for Longâ€Life Quasiâ€Solid State Zinc Metal Batteries. Advanced Functional Materials, 2020, 30, 2001317.	14.9	188
3	Divergent Total Syntheses of (â^')â€Daphnilongeraninâ€...B and (â^')â€Daphenylline. Angewandte Chemie - International Edition, 2018, 57, 947-951.	13.8	84
4	Two Pathways Mediate Interdomain Allosteric Regulation in Pin1. Structure, 2015, 23, 237-247.	3.3	70
5	Artificial K⁺ Channels Formed by Pillarareneâ€Cyclodextrin Hybrid Molecules: Tuning Cation Selectivity and Generating Membrane Potential. Angewandte Chemie - International Edition, 2019, 58, 2779-2784.	13.8	58
6	The adsorption mechanism and induced conformational changes of three typical proteins with different secondary structural features on graphene. RSC Advances, 2014, 4, 9953.	3.6	54
7	Exploring the Influence of Carbon Nanoparticles on the Formation of Î²-Sheet-Rich Oligomers of IAPP22â€“28 Peptide by Molecular Dynamics Simulation. PLoS ONE, 2013, 8, e65579.	2.5	48
8	Potential of esterase DmtH in transforming plastic additive dimethyl terephthalate to less toxic mono-methyl terephthalate. Ecotoxicology and Environmental Safety, 2020, 187, 109848.	6.0	41
9	Exploring the Influence of EGCG on the Î²-Sheet-Rich Oligomers of Human Islet Amyloid Polypeptide (hIAPP1â€“37) and Identifying Its Possible Binding Sites from Molecular Dynamics Simulation. PLoS ONE, 2014, 9, e94796.	2.5	40
10	A Short Peptide Hydrogel with High Stiffness Induced by 3₁₀â€Helices to Î²â€Sheet Transition in Water. Advanced Science, 2019, 6, 1901173.	11.2	36
11	Brazilin inhibits fibrillogenesis of human islet amyloid polypeptide, disassembles mature fibrils, and alleviates cytotoxicity. RSC Advances, 2017, 7, 43491-43501.	3.6	33
12	Influence of the pathogenic mutations T188K/R/A on the structural stability and misfolding of human prion protein: Insight from molecular dynamics simulations. Biochimica Et Biophysica Acta - General Subjects, 2012, 1820, 116-123.	2.4	32
13	Hinge-Shift Mechanism Modulates Allosteric Regulations in Human Pin1. Journal of Physical Chemistry B, 2018, 122, 5623-5629.	2.6	30
14	Brazilin inhibits the Zn2+-mediated aggregation of amyloid Î²-protein and alleviates cytotoxicity. Journal of Inorganic Biochemistry, 2017, 177, 183-189.	3.5	26
15	Dynamically Driven Protein Allostery Exhibits Disparate Responses for Fast and Slow Motions. Biophysical Journal, 2015, 108, 2771-2774.	0.5	25
16	Exploring structural and thermodynamic stabilities of human prion protein pathogenic mutants D202N, E211Q and Q217R. Journal of Structural Biology, 2012, 178, 225-232.	2.8	24
17	Stabilities and structures of islet amyloid polypeptide (IAPP22â€“28) oligomers: From dimer to 16-mer. Biochimica Et Biophysica Acta - General Subjects, 2014, 1840, 357-366.	2.4	24
18	The molecular basis of IGF-II/IGF2R recognition: a combined molecular dynamics simulation, free-energy calculation and computational alanine scanning study. Journal of Molecular Modeling, 2012, 18, 1421-1430.	1.8	21

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19	Kinetic Insights into Zn²⁺-Induced Amyloid Î²-Protein Aggregation Revealed by Stopped-Flow Fluorescence Spectroscopy. Journal of Physical Chemistry B, 2017, 121, 3909-3917.	2.6	20
20	A unimolecular channel formed by dual helical peptide modified pillar[5]arene: correlating transmembrane transport properties with antimicrobial activity and haemolytic toxicity. Chemical Communications, 2017, 53, 11492-11495.	4.1	20
21	The role of Cys179â€“Cys214 disulfide bond in the stability and folding of prion protein: insights from molecular dynamics simulations. Journal of Molecular Modeling, 2014, 20, 2106.	1.8	19
22	Artificial K⁺ Channels Formed by Pillararenecyclodextrin Hybrid Molecules: Tuning Cation Selectivity and Generating Membrane Potential. Angewandte Chemie, 2019, 131, 2805-2810.	2.0	19
23	Response of microbial membranes to butanol: interdigitationvs.disorder. Physical Chemistry Chemical Physics, 2019, 21, 11903-11915.	2.8	19
24	A novel highly selective near-infrared and naked-eye fluorescence probe for imaging peroxynitrite. Analytical Methods, 2019, 11, 1522-1529.	2.7	17
25	Molecular mechanism of the enhanced virulence of 2009 pandemic Influenza A (H1N1) virus from D222G mutation in the hemagglutinin: a molecular modeling study. Journal of Molecular Modeling, 2012, 18, 4355-4366.	1.8	16
26	Divergent Total Syntheses of (â^')Daphnilongeraninâ€…B and (â^')Daphenylline. Angewandte Chemie, 2018, 130, 959-963.	2.0	16
27	Allosteric activation of SENP1 by SUMO1 Î²-grasp domain involves a dock-and-coalesce mechanism. ELife, 2016, 5, .	6.0	15
28	Molecular Mechanism of Ca²⁺ in the Allosteric Regulation of Human Parathyroid Hormone Receptor-1. Journal of Chemical Information and Modeling, 2022, 62, 5110-5119.	5.4	14
29	Structural Diversity and Initial Oligomerization of PrP106â€“126 Studied by Replica-Exchange and Conventional Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e87266.	2.5	13
30	Fluorimetric investigation of supramolecular system by modified Î²-cyclodextrin and its analytical application. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1553-1559.	3.9	11
31	Distinct Dynamic and Conformational Features of Human STING in Response to 2â€²3â€²â€cGAMP and câ€diâ€GMP. ChemBioChem, 2019, 20, 1838-1847.	2.6	10
32	Bacterial lipopolysaccharide core structures mediate effects of butanol ingress. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183150.	2.6	9
33	Investigation on a hostâ€“guest inclusion system by Î²-cyclodextrin derivative and its analytical application. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 1113-1117.	2.2	8
34	One-pot formation of hydrazide macrocycles with modified cavities: an example of pH-sensitive unimolecular cation channels. Chemical Communications, 2017, 53, 5322-5325.	4.1	8
35	How graphene affects the misfolding of human prion protein: A combined experimental and molecular dynamics simulation study. Environmental Research, 2019, 171, 1-10.	7.5	7
36	Study on the stereoselective binding of cytosine nucleoside enantiomers to human serum albumin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 224, 117452.	3.9	7

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37	Pyruvate kinase from Plasmodium falciparum: Structural and kinetic insights into the allosteric mechanism. Biochemical and Biophysical Research Communications, 2020, 532, 370-376.	2.1	7
38	Deciphering the T790M/L858R-Selective Inhibition Mechanism of an Allosteric Inhibitor of EGFR: Insights from Molecular Simulations. ACS Chemical Neuroscience, 2021, 12, 462-472.	3.5	7
39	Critical Extracellular Ca²⁺ Dependence of the Binding between PTH1R and a G-Protein Peptide Revealed by MD Simulations. ACS Chemical Neuroscience, 2022, 13, 1666-1674.	3.5	7
40	Fabrication of a fiberglass-packed channel in a microchip for flow injection analysis. Mikrochimica Acta, 2007, 159, 191-199.	5.0	6
41	Pyruvate Kinase Regulates the Pentose-Phosphate Pathway in Response to Hypoxia in Mycobacterium tuberculosis. Journal of Molecular Biology, 2019, 431, 3690-3705.	4.2	6
42	The solvent at antigen-binding site regulated C3dâ€“CR2 interactions through the C-terminal tail of C3d at different ion strengths: insights from molecular dynamics simulation. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2220-2231.	2.4	5
43	Conformational dynamics is critical for the allosteric inhibition of cGAS upon acetyl-mimic mutations. Physical Chemistry Chemical Physics, 2021, 23, 2154-2165.	2.8	4
44	Uncovering the Molecular Basis for the Better Gefitinib Sensitivity of EGFR with Complex Mutations over Single Rare Mutation: Insights from Molecular Simulations. Molecules, 2022, 27, 3844.	3.8	4
45	Insights into the negative regulation of EGFR upon the binding of an allosteric inhibitor. Chemical Biology and Drug Design, 2022, 99, 650-661.	3.2	3
46	The molecular mechanism of two coreceptor binding site antibodies X5 and 17b neutralizing <scp>HIV</scp>â€1: Insights from molecular dynamics simulation. Chemical Biology and Drug Design, 2018, 92, 1357-1365.	3.2	2
47	The Evolution of HLAâ€B*3501 Binding Affinity to Variable Immunodominant NP_{418â€426} Peptides from 1918 to 2009 Pandemic Influenza A Virus: A Molecular Dynamics Simulation and Free Energy Calculation Study. Chemical Biology and Drug Design, 2012, 79, 1025-1032.	3.2	1
48	Two Pathways Mediate Inter-Domain Allosteric Regulation in Pin1. Biophysical Journal, 2015, 108, 528a.	0.5	1
49	Probing the Binding of Bicyclol and Human Serum Albumin by Multispectral Technologies and Molecular Docking Method. Journal of Solution Chemistry, 2019, 48, 1519-1534.	1.2	1
50	Investigating the Permeation Mechanism of Typical Phthalic Acid Esters (PAEs) and Membrane Response Using Molecular Dynamics Simulations. Membranes, 2022, 12, 596.	3.0	1
51	The molecular mechanism of pHâ€regulating C3dâ€CR2 interactions: Insights from molecular dynamics simulation. Chemical Biology and Drug Design, 2019, 93, 628-637.	3.2	0