

Yingjie Wang

List of Publications by Year in descending order

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papers

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1441
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#	ARTICLE	IF	CITATIONS
1	Alternatingly Amphiphilic Antimicrobial Oligoguanidines: Structure–Property Relationship and Usage as the Coating Material with Unprecedented Hemocompatibility. <i>Chemistry of Materials</i> , 2022, 34, 3670-3682.	3.2	6
2	Solvation Induction of Free Energy Barriers of Decarboxylation Reactions in Aqueous Solution from Dual-Level QM/MM Simulations. <i>Jacs Au</i> , 2021, 1, 233-244.	3.6	8
3	SARS-CoV-2 spike protein N501Y mutation causes differential species transmissibility and antibody sensitivity: a molecular dynamics and alchemical free energy study. <i>Molecular Systems Design and Engineering</i> , 2021, 6, 964-974.	1.7	8
4	Defective internal allosteric network imparts dysfunctional ATP/substrate-binding cooperativity in oncogenic chimera of protein kinase A. <i>Communications Biology</i> , 2021, 4, 321.	2.0	21
5	Activation mechanism of <i>Drosophila</i> cryptochrome through an allosteric switch. <i>Science Advances</i> , 2021, 7, .	4.7	14
6	An alternatingly amphiphilic, resistance-resistant antimicrobial oligoguanidine with dual mechanisms of action. <i>Biomaterials</i> , 2021, 275, 120858.	5.7	28
7	Is Disrupted Nucleotide-Substrate Cooperativity a Common Trait for Cushing's Syndrome Driving Mutations of Protein Kinase A?. <i>Journal of Molecular Biology</i> , 2021, 433, 167123.	2.0	8
8	Identification of the New Covalent Allosteric Binding Site of Fructose-1,6-bisphosphatase with Disulfiram Derivatives toward Glucose Reduction. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 6238-6247.	2.9	17
9	Enhanced receptor binding of SARS-CoV-2 through networks of hydrogen-bonding and hydrophobic interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 13967-13974.	3.3	291
10	Dynamical and allosteric regulation of photoprotection in light harvesting complex II. <i>Science China Chemistry</i> , 2020, 63, 1121-1133.	4.2	29
11	Multi-state recognition pathway of the intrinsically disordered protein kinase inhibitor by protein kinase A. <i>ELife</i> , 2020, 9, .	2.8	16
12	Cushing's syndrome driver mutation disrupts protein kinase A allosteric network, altering both regulation and substrate specificity. <i>Science Advances</i> , 2019, 5, eaaw9298.	4.7	43
13	Globally correlated conformational entropy underlies positive and negative cooperativity in a kinase's enzymatic cycle. <i>Nature Communications</i> , 2019, 10, 799.	5.8	40
14	A Cushing Syndrome Mutation of Protein Kinase A γ -subunit Disrupts the Internal Allosteric Network Affecting Regulation and Substrate Specificity. <i>FASEB Journal</i> , 2019, 33, 478.11.	0.2	1
15	Conformational Landscape of the PRKACA-DNAJB1 Chimeric Kinase, the Driver for Fibrolamellar Hepatocellular Carcinoma. <i>Scientific Reports</i> , 2018, 8, 720.	1.6	23
16	A Semiautomated Assignment Protocol for Methyl Group Side Chains in Large Proteins. <i>Methods in Enzymology</i> , 2016, 566, 35-57.	0.4	2
17	Probing Residue-Specific Water–Protein Interactions in Oriented Lipid Membranes via Solid-State NMR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10959-10968.	1.2	6
18	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. <i>Israel Journal of Chemistry</i> , 2014, 54, 1250-1263.	1.0	45

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19	Explicit Polarization: A Quantum Mechanical Framework for Developing Next Generation Force Fields. <i>Accounts of Chemical Research</i> , 2014, 47, 2837-2845.	7.6	82
20	Multilevel X-Pol: A Fragment-Based Method with Mixed Quantum Mechanical Representations of Different Fragments. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6781-6788.	1.2	32