

Alexey Aleksandrov

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

26

papers

426

citations

13

h-index

20

g-index

27

ext. papers

535

ext. citations

6.6

avg, IF

3.86

L-index

#	Paper	IF	Citations
26	Molecular dynamics simulations show that conformational selection governs the binding preferences of imatinib for several tyrosine kinases. <i>Journal of Biological Chemistry</i> , 2010 , 285, 13807-15	5.4	65
25	Alchemical free energy simulations for biological complexes: powerful but temperamental. <i>Journal of Molecular Recognition</i> , 2010 , 23, 117-27	2.6	46
24	Additive CHARMM force field for naturally occurring modified ribonucleotides. <i>Journal of Computational Chemistry</i> , 2016 , 37, 896-912	3.5	36
23	Protonation patterns in tetracycline:tet repressor recognition: simulations and experiments. <i>ChemBioChem</i> , 2007 , 8, 675-85	3.8	32
22	Tet repressor induction by tetracycline: a molecular dynamics, continuum electrostatics, and crystallographic study. <i>Journal of Molecular Biology</i> , 2008 , 378, 898-912	6.5	29
21	Predicting the acid/base behavior of proteins: a constant-pH Monte Carlo approach with generalized born solvent. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 10634-48	3.4	28
20	Mechanism and dynamics of fatty acid photodecarboxylase. <i>Science</i> , 2021 , 372,	33.3	28
19	Molecular dynamics simulations of the 30S ribosomal subunit reveal a preferred tetracycline binding site. <i>Journal of the American Chemical Society</i> , 2008 , 130, 1114-5	16.4	24
18	Mechanism of activation of elongation factor Tu by ribosome: catalytic histidine activates GTP by protonation. <i>Rna</i> , 2013 , 19, 1218-25	5.8	18
17	Identification of a second GTP-bound magnesium ion in archaeal initiation factor 2. <i>Nucleic Acids Research</i> , 2015 , 43, 2946-57	20.1	18
16	A hybrid elastic band string algorithm for studies of enzymatic reactions. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12544-53	3.6	18
15	Combining the polarizable Drude force field with a continuum electrostatic Poisson-Boltzmann implicit solvation model. <i>Journal of Computational Chemistry</i> , 2018 , 39, 1707-1719	3.5	13
14	Tetracycline-tet repressor binding specificity: insights from experiments and simulations. <i>Biophysical Journal</i> , 2009 , 97, 2829-38	2.9	13
13	The mechanism of citryl-coenzyme A formation catalyzed by citrate synthase. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 4505-13	3.4	11
12	A Molecular Mechanics Model for Flavins. <i>Journal of Computational Chemistry</i> , 2019 , 40, 2834-2842	3.5	9
11	p Calculations with the Polarizable Drude Force Field and Poisson-Boltzmann Solvation Model. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4655-4668	6.4	7
10	Cyclization Reaction Catalyzed by Cyclodipeptide Synthases Relies on a Conserved Tyrosine Residue. <i>Scientific Reports</i> , 2018 , 8, 7031	4.9	6

9	Advances and challenges in drug design against tuberculosis: application of in silico approaches. <i>Expert Opinion on Drug Discovery</i> , 2019 , 14, 35-46	6.2	6
8	Additive CHARMM36 Force Field for Nonstandard Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3554-3570	6.4	5
7	Aminoacylation Reaction Catalyzed by Leucyl-tRNA Synthetase Operates via a Self-Assisted Mechanism Using a Conserved Residue and the Aminoacyl Substrate. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 4388-98	3.4	5
6	Electrostatic free energies in translational GTPases: Classic allostery and the rest. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015 , 1850, 1006-1016	4	4
5	Characterization of Light-Induced, Short-Lived Interacting Radicals in the Active Site of Flavoprotein Ferredoxin-NADP Oxidoreductase. <i>Journal of the American Chemical Society</i> , 2021 , 143, 2757-2768	16.4	2
4	An atomistic model for simulations of nilotinib and nilotinib/kinase binding. <i>Theoretical Chemistry Accounts</i> , 2011 , 129, 747-756	1.9	1
3	Mechanism of Naphthoquinone Selectivity of Thymidylate Synthase ThyX. <i>Biophysical Journal</i> , 2020 , 119, 2508-2516	2.9	1
2	Photochemical processes in flavo-enzymes as a probe for active site dynamics: TrmFO of <i>Thermus thermophilus</i> . <i>Photochemical and Photobiological Sciences</i> , 2021 , 20, 663-670	4.2	0
1	Cyclodipeptide Synthases of the NYH Subfamily Recognize tRNA Using an β -Helix Enriched with Positive Residues. <i>Biochemistry</i> , 2021 , 60, 64-76	3.2	