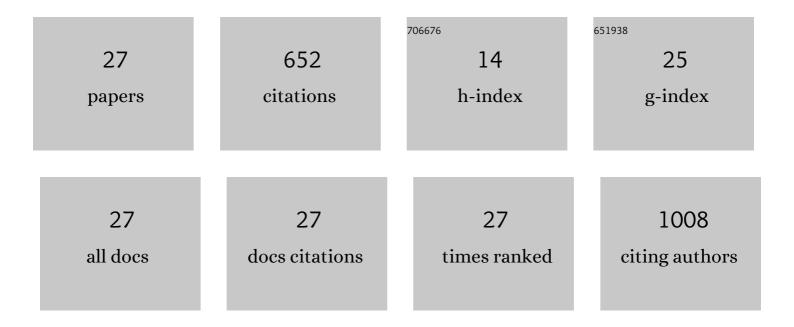
Alexey Aleksandrov

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Ultrafast photooxidation of protein-bound anionic flavin radicals. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	9
2	Cyclodipeptide Synthases of the NYH Subfamily Recognize tRNA Using an α-Helix Enriched with Positive Residues. Biochemistry, 2021, 60, 64-76.	1.2	0
3	Mechanism and dynamics of fatty acid photodecarboxylase. Science, 2021, 372, .	6.0	93
4	Additive CHARMM36 Force Field for Nonstandard Amino Acids. Journal of Chemical Theory and Computation, 2021, 17, 3554-3570.	2.3	39
5	Photochemical processes in flavo-enzymes as a probe for active site dynamics: TrmFO of Thermus thermophilus. Photochemical and Photobiological Sciences, 2021, 20, 663-670.	1.6	3
6	Characterization of Light-Induced, Short-Lived Interacting Radicals in the Active Site of Flavoprotein Ferredoxin-NADP ⁺ Oxidoreductase. Journal of the American Chemical Society, 2021, 143, 2757-2768.	6.6	12
7	pKa Calculations with the Polarizable Drude Force Field and Poisson–Boltzmann Solvation Model. Journal of Chemical Theory and Computation, 2020, 16, 4655-4668.	2.3	14
8	Mechanism of Naphthoquinone Selectivity of Thymidylate Synthase ThyX. Biophysical Journal, 2020, 119, 2508-2516.	0.2	2
9	A Molecular Mechanics Model for Flavins. Journal of Computational Chemistry, 2019, 40, 2834-2842.	1.5	18
10	Advances and challenges in drug design against tuberculosis: application of in silico approaches. Expert Opinion on Drug Discovery, 2019, 14, 35-46.	2.5	10
11	Combining the polarizable Drude force field with a continuum electrostatic Poisson–Boltzmann implicit solvation model. Journal of Computational Chemistry, 2018, 39, 1707-1719.	1.5	15
12	Cyclization Reaction Catalyzed by Cyclodipeptide Synthases Relies on a Conserved Tyrosine Residue. Scientific Reports, 2018, 8, 7031.	1.6	8
13	Aminoacetylation Reaction Catalyzed by Leucyl-tRNA Synthetase Operates via a Self-Assisted Mechanism Using a Conserved Residue and the Aminoacyl Substrate. Journal of Physical Chemistry B, 2016, 120, 4388-4398.	1.2	6
14	Additive <scp>CHARMM</scp> force field for naturally occurring modified ribonucleotides. Journal of Computational Chemistry, 2016, 37, 896-912.	1.5	63
15	Identification of a second GTP-bound magnesium ion in archaeal initiation factor 2. Nucleic Acids Research, 2015, 43, 2946-2957.	6.5	28
16	Electrostatic free energies in translational GTPases: Classic allostery and the rest. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1006-1016.	1.1	5
17	The Mechanism of Citryl-Coenzyme A Formation Catalyzed by Citrate Synthase. Journal of Physical Chemistry B, 2014, 118, 4505-4513.	1.2	12
18	Mechanism of activation of elongation factor Tu by ribosome: Catalytic histidine activates GTP by protonation. Rna. 2013. 19. 1218-1225.	1.6	20

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#	Article	IF	CITATIONS
19	A hybrid elastic band string algorithm for studies of enzymatic reactions. Physical Chemistry Chemical Physics, 2012, 14, 12544.	1.3	21
20	An atomistic model for simulations of nilotinib and nilotinib/kinase binding. Theoretical Chemistry Accounts, 2011, 129, 747-756.	0.5	1
21	Alchemical free energy simulations for biological complexes: powerful but temperamental …. Journal of Molecular Recognition, 2010, 23, 117-127.	1.1	54
22	Molecular Dynamics Simulations Show That Conformational Selection Governs the Binding Preferences of Imatinib for Several Tyrosine Kinases. Journal of Biological Chemistry, 2010, 285, 13807-13815.	1.6	70
23	Predicting the Acid/Base Behavior of Proteins: A Constant-pH Monte Carlo Approach with Generalized Born Solvent. Journal of Physical Chemistry B, 2010, 114, 10634-10648.	1.2	29
24	Tetracycline-Tet Repressor Binding Specificity: Insights from Experiments and Simulations. Biophysical Journal, 2009, 97, 2829-2838.	0.2	16
25	Tet Repressor Induction by Tetracycline: A Molecular Dynamics, Continuum Electrostatics, and Crystallographic Study. Journal of Molecular Biology, 2008, 378, 898-912.	2.0	34
26	Molecular Dynamics Simulations of the 30S Ribosomal Subunit Reveal a Preferred Tetracycline Binding Site. Journal of the American Chemical Society, 2008, 130, 1114-1115.	6.6	30
27	Protonation Patterns in Tetracycline:Tet Repressor Recognition: Simulations and Experiments. ChemBioChem, 2007, 8, 675-685.	1.3	40