# Alexey Aleksandrov

List of Publications by Year
in descending order



| 27 | 652 | 706676 14 | 651938 25 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 27 | 27 | 27 | 1008 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | 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 Î±-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<sup>+</sup> Oxidoreductase. Journal of the American Chemical Society, 2021, 143, 2757-2768. | 6.6 | 12 |
| 7 | pKa Calculations with the Polarizable Drude Force Field and Poissonâ€“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 Poissonâ€“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 |

| # | 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 temperamentalâ€‰â€¦. 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 |