

M R Gunner

List of Publications by Year in descending order

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Version: 2024-02-01

52
papers

3,194
citations

236833

25
h-index

189801

50
g-index

53
all docs

53
docs citations

53
times ranked

2690
citing authors

#	ARTICLE	IF	CITATIONS
1	On the calculation of pK _a s in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 1993, 15, 252-265.	1.5	514
2	Incorporating protein conformational flexibility into the calculation of pH-dependent protein properties. <i>Biophysical Journal</i> , 1997, 72, 2075-2093.	0.2	343
3	Calculated Protein and Proton Motions Coupled to Electron Transfer: Electron Transfer from QA to QB in Bacterial Photosynthetic Reaction Centers. <i>Biochemistry</i> , 1999, 38, 8253-8270.	1.2	243
4	Calculated coupling of electron and proton transfer in the photosynthetic reaction center of <i>Rhodospseudomonas viridis</i> . <i>Biophysical Journal</i> , 1996, 70, 2469-2492.	0.2	194
5	MCCE2: Improving protein pK _a calculations with extensive side chain rotamer sampling. <i>Journal of Computational Chemistry</i> , 2009, 30, 2231-2247.	1.5	192
6	L-2-Hydroxyglutarate production arises from noncanonical enzyme function at acidic pH. <i>Nature Chemical Biology</i> , 2017, 13, 494-500.	3.9	190
7	Are Acidic and Basic Groups in Buried Proteins Predicted to be Ionized?. <i>Journal of Molecular Biology</i> , 2005, 348, 1283-1298.	2.0	106
8	The pK _a Cooperative: A collaborative effort to advance structure-based calculations of pK _a values and electrostatic effects in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3249-3259.	1.5	105
9	Factors influencing the energetics of electron and proton transfers in proteins. What can be learned from calculations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2006, 1757, 942-968.	0.5	89
10	The importance of the protein in controlling the electrochemistry of heme metalloproteins: methods of calculation and analysis. <i>Journal of Biological Inorganic Chemistry</i> , 1997, 2, 126-134.	1.1	84
11	Backbone Dipoles Generate Positive Potentials in all Proteins: Origins and Implications of the Effect. <i>Biophysical Journal</i> , 2000, 78, 1126-1144.	0.2	82
12	Analysis of the electrochemistry of hemes with E _m s spanning 800 mV. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 719-734.	1.5	81
13	High-resolution cryo-electron microscopy structure of photosystem II from the mesophilic cyanobacterium, <i>Synechocystis</i> sp. PCC 6803. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	58
14	Modification of quinone electrochemistry by the proteins in the biological electron transfer chains: examples from photosynthetic reaction centers. <i>Journal of Bioenergetics and Biomembranes</i> , 2008, 40, 509-19.	1.0	57
15	Modeling the Effects of Mutations on the Free Energy of the First Electron Transfer from QA- to QB in Photosynthetic Reaction Centers. <i>Biochemistry</i> , 2000, 39, 5940-5952.	1.2	56
16	MCCE analysis of the pK _a s of introduced buried acids and bases in staphylococcal nuclease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3306-3319.	1.5	56
17	Characterizing the proton loading site in cytochrome c oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 12414-12419.	3.3	54
18	Proton-Coupled Electron Transfer During the S-State Transitions of the Oxygen-Evolving Complex of Photosystem II. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7366-7377.	1.2	49

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19	Ligand preference and orientation in α - and γ -type heme-binding proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 690-704.	1.5	46
20	Evaluation of log $\hat{A}P$, pKa, and log $\hat{A}D$ predictions from the SAMPL7 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 771-802.	1.3	42
21	Using Multiconformation Continuum Electrostatics to Compare Chloride Binding Motifs in α -Amylase, Human Serum Albumin, and Omp32. <i>Journal of Molecular Biology</i> , 2009, 387, 840-856.	2.0	41
22	Photosystem II oxygen-evolving complex photoassembly displays an inverse H/D solvent isotope effect under chloride-limiting conditions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 18917-18922.	3.3	41
23	Temperature Dependence of the Free Energy, Enthalpy, and Entropy of P+QA-Charge Recombination in <i>Rhodobacter sphaeroides</i> R-26 Reaction Centers. <i>Journal of Physical Chemistry B</i> , 2000, 104, 8035-8043.	1.2	38
24	Molecular mechanisms for generating transmembrane proton gradients. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2013, 1827, 892-913.	0.5	37
25	Network analysis of a proposed exit pathway for protons to the P-side of cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2018, 1859, 997-1005.	0.5	35
26	Proton exit pathways surrounding the oxygen evolving complex of photosystem II. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2021, 1862, 148446.	0.5	30
27	Continuum Electrostatics Approaches to Calculating pKas and Ems in Proteins. <i>Methods in Enzymology</i> , 2016, 578, 1-20.	0.4	27
28	Halorhodopsin pumps Cl ⁻ and bacteriorhodopsin pumps protons by a common mechanism that uses conserved electrostatic interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 16377-16382.	3.3	24
29	Overview of the SAMPL6 pKa challenge: evaluating small molecule microscopic and macroscopic pKa predictions. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 131-166.	1.3	23
30	Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. <i>Journal of the American Chemical Society</i> , 2020, 142, 9220-9230.	6.6	22
31	Thermodynamics of the S ₂ -to-S ₃ state transition of the oxygen-evolving complex of photosystem II. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20840-20848.	1.3	21
32	Hydrogen bond network analysis reveals the pathway for the proton transfer in the E-channel of T. thermophilus Complex I. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2020, 1861, 148240.	0.5	20
33	Standard state free energies, not pKas, are ideal for describing small molecule protonation and tautomeric states. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 561-573.	1.3	20
34	Relative stability of the S2 isomers of the oxygen evolving complex of photosystem II. <i>Photosynthesis Research</i> , 2019, 141, 331-341.	1.6	18
35	Unraveling the mechanism of proton translocation in the extracellular half-channel of bacteriorhodopsin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 639-654.	1.5	17
36	Two Cl Ions and a Glu Compete for a Helix Cage in the CLC Proton/Cl ⁻ Antiporter. <i>Biophysical Journal</i> , 2017, 113, 1025-1036.	0.2	16

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37	Protein Motifs for Proton Transfers That Build the Transmembrane Proton Gradient. <i>Frontiers in Chemistry</i> , 2021, 9, 660954.	1.8	15
38	X-ray Free Electron Laser Radiation Damage through the S-State Cycle of the Oxygen-Evolving Complex of Photosystem II. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9382-9388.	1.2	14
39	Mesoscopic to Macroscopic Electron Transfer by Hopping in a Crystal Network of Cytochromes. <i>Journal of the American Chemical Society</i> , 2020, 142, 10459-10467.	6.6	13
40	Identifying the proton loading site cluster in the ba cytochrome c oxidase that loads and traps protons. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2020, 1861, 148239.	0.5	13
41	The measured and calculated affinity of methyl- and methoxy-substituted benzoquinones for the Q _A site of bacterial reaction centers. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2638-2654.	1.5	11
42	Characterizing the Water Wire in the Gramicidin Channel Found by Monte Carlo Sampling Using Continuum Electrostatics and in Molecular Dynamics Trajectories with Conventional or Polarizable Force Fields. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 111-130.	1.0	11
43	Comparison of proton transfer paths to the QA and QB sites of the Rb. sphaeroides photosynthetic reaction centers. <i>Photosynthesis Research</i> , 2022, 152, 153-165.	1.6	10
44	Characterizing Protein Protonation Microstates Using Monte Carlo Sampling. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2476-2485.	1.2	9
45	Affinity and activity of non-native quinones at the QB site of bacterial photosynthetic reaction centers. <i>Photosynthesis Research</i> , 2014, 120, 181-196.	1.6	6
46	Characterization of a symmetrized mutant RC with 42 residues from the QA site replacing residues in the Q(B) site. <i>Photosynthesis Research</i> , 2000, 64, 41-52.	1.6	5
47	Identification of a Na ⁺ -Binding Site near the Oxygen-Evolving Complex of Spinach Photosystem II. <i>Biochemistry</i> , 2020, 59, 2823-2831.	1.2	5
48	The design features cells use to build their transmembrane proton gradient. <i>Physical Biology</i> , 2017, 14, 013001.	0.8	4
49	Computational analysis of photosynthetic systems. <i>Photosynthesis Research</i> , 2008, 97, 1-3.	1.6	3
50	Characterizing the water wire in the Gramicidin channel found by Monte Carlo sampling using continuum electrostatics and in molecular dynamics trajectories with conventional or polarizable force fields. <i>Journal of Theoretical and Computational Chemistry</i> , 0, , 2042001.	1.8	2
51	Poor Person's pH Simulation of Membrane Proteins. <i>Methods in Molecular Biology</i> , 2021, 2315, 197-217.	0.4	1
52	Modeling the First Electron Transfer from QA to QB in Reaction Center Proteins from Rb. sphaeroid. <i>ACS Symposium Series</i> , 2004, , 93-106.	0.5	0