M R Gunner

List of Publications by Year
in descending order

52 papers	3,194 citations	236925 25 h-index	189892 50 g-index
53 all docs	53 docs citations	53 times ranked	2690 citing authors

#	ARTICLE	IF	CITATIONS
1	On the calculation of pKas in proteins. Proteins: Structure, Function and Bioinformatics, 1993, 15, 252-265.	2.6	514
2	Incorporating protein conformational flexibility into the calculation of pH-dependent protein properties. Biophysical Journal, 1997, 72, 2075-2093.	0.5	343
3	Calculated Protein and Proton Motions Coupled to Electron Transfer:Â Electron Transfer from QA-to QBin Bacterial Photosynthetic Reaction Centersâ€. Biochemistry, 1999, 38, 8253-8270.	2.5	243
4	Calculated coupling of electron and proton transfer in the photosynthetic reaction center of Rhodopseudomonas viridis. Biophysical Journal, 1996, 70, 2469-2492.	0.5	194
5	MCCE2: Improving protein p<i>K</i>_a calculations with extensive side chain rotamer sampling. Journal of Computational Chemistry, 2009, 30, 2231-2247.	3.3	192
6	L-2-Hydroxyglutarate production arises from noncanonical enzyme function at acidic pH. Nature Chemical Biology, 2017, 13, 494-500.	8.0	190
7	Are Acidic and Basic Groups in Buried Proteins Predicted to be Ionized?. Journal of Molecular Biology, 2005, 348, 1283-1298.	4.2	106
8	The p<i>K</i>_a Cooperative: A collaborative effort to advance structureâ€based calculations of p<i>K</i>_a values and electrostatic effects in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3249-3259.	2.6	105
9	Factors influencing the energetics of electron and proton transfers in proteins. What can be learned from calculations. Biochimica Et Biophysica Acta - Bioenergetics, 2006, 1757, 942-968.	1.0	89
10	The importance of the protein in controlling the electrochemistry of heme metalloproteins: methods of calculation and analysis. Journal of Biological Inorganic Chemistry, 1997, 2, 126-134.	2.6	84
11	Backbone Dipoles Generate Positive Potentials in all Proteins: Origins and Implications of the Effect. Biophysical Journal, 2000, 78, 1126-1144.	0.5	82
12	Analysis of the electrochemistry of hemes with <i>E</i>_ms spanning 800 mV. Proteins: Structure, Function and Bioinformatics, 2009, 75, 719-734.	2.6	81
13	High-resolution cryo-electron microscopy structure of photosystem II from the mesophilic cyanobacterium, <i>Synechocystis</i> sp. PCC 6803. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	58
14	Modification of quinone electrochemistry by the proteins in the biological electron transfer chains: examples from photosynthetic reaction centers. Journal of Bioenergetics and Biomembranes, 2008, 40, 509-19.	2.3	57
15	Modeling the Effects of Mutations on the Free Energy of the First Electron Transfer from QA- to QB in Photosynthetic Reaction Centers. Biochemistry, 2000, 39, 5940-5952.	2.5	56
16	MCCE analysis of the p<i>K</i>_as of introduced buried acids and bases in staphylococcal nuclease. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3306-3319.	2.6	56
17	Characterizing the proton loading site in cytochrome <i>c</i> oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 12414-12419.	7.1	54
18	Proton-Coupled Electron Transfer During the S-State Transitions of the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2015, 119, 7366-7377.	2.6	49

#	ARTICLE	IF	CITATIONS
19	Ligand preference and orientation in <i>bâ€‹</i> and <i>câ€‹</i>type hemeâ€binding proteins. Proteins: Structure, Function and Bioinformatics, 2008, 73, 690-704.	2.6	46
20	Evaluation of logÂP, pKa, and logÂD predictions from the SAMPL7 blind challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 771-802.	2.9	42
21	Using Multiconformation Continuum Electrostatics to Compare Chloride Binding Motifs in Î±-Amylase, Human Serum Albumin, and Omp32. Journal of Molecular Biology, 2009, 387, 840-856.	4.2	41
22	Photosystem II oxygen-evolving complex photoassembly displays an inverse H/D solvent isotope effect under chloride-limiting conditions. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18917-18922.	7.1	41
23	Temperature Dependence of the Free Energy, Enthalpy, and Entropy of P+QA-Charge Recombination inRhodobacter sphaeroidesR-26 Reaction Centers. Journal of Physical Chemistry B, 2000, 104, 8035-8043.	2.6	38
24	Molecular mechanisms for generating transmembrane proton gradients. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 892-913.	1.0	37
25	Network analysis of a proposed exit pathway for protons to the P-side of cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 997-1005.	1.0	35
26	Proton exit pathways surrounding the oxygen evolving complex of photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148446.	1.0	30
27	Continuum Electrostatics Approaches to Calculating pKas and Ems in Proteins. Methods in Enzymology, 2016, 578, 1-20.	1.0	27
28	Halorhodopsin pumps Cl ^{â€“} and bacteriorhodopsin pumps protons by a common mechanism that uses conserved electrostatic interactions. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 16377-16382.	7.1	24
29	Overview of the SAMPL6 pKa challenge: evaluating small molecule microscopic and macroscopic pKa predictions. Journal of Computer-Aided Molecular Design, 2021, 35, 131-166.	2.9	23
30	Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 9220-9230.	13.7	22
31	Thermodynamics of the S₂-to-S₃ state transition of the oxygen-evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2019, 21, 20840-20848.	2.8	21
32	Hydrogen bond network analysis reveals the pathway for the proton transfer in the E-channel of T. thermophilus Complex I. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148240.	1.0	20
33	Standard state free energies, not pKas, are ideal for describing small molecule protonation and tautomeric states. Journal of Computer-Aided Molecular Design, 2020, 34, 561-573.	2.9	20
34	Relative stability of the S2 isomers of the oxygen evolving complex of photosystem II. Photosynthesis Research, 2019, 141, 331-341.	2.9	18
35	Unraveling the mechanism of proton translocation in the extracellular halfâ€channel of bacteriorhodopsin. Proteins: Structure, Function and Bioinformatics, 2016, 84, 639-654.	2.6	17
36	Two Cl Ions and a Glu Compete for a Helix Cage inÂthe CLC Proton/Clâˆ' Antiporter. Biophysical Journal, 2017, 113, 1025-1036.	0.5	16

#	Article	IF	Citations
37	Protein Motifs for Proton Transfers That Build the Transmembrane Proton Gradient. Frontiers in Chemistry, 2021, 9, 660954.	3.6	15
38	X-ray Free Electron Laser Radiation Damage through the S-State Cycle of the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2017, 121, 9382-9388.	2.6	14
39	Mesoscopic to Macroscopic Electron Transfer by Hopping in a Crystal Network of Cytochromes. Journal of the American Chemical Society, 2020, 142, 10459-10467.	13.7	13
40	Identifying the proton loading site cluster in the ba cytochrome c oxidase that loads and traps protons. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148239.	1.0	13
41	The measured and calculated affinity of methylâ€•and methoxyâ€substituted benzoquinones for the Q_Asite of bacterial reaction centers. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2638-2654.	2.6	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. Journal of Computational Biophysics and Chemistry, 2021, 20, 111-130.	1.7	11
43	Comparison of proton transfer paths to the QA and QB sites of the Rb. sphaeroides photosynthetic reaction centers. Photosynthesis Research, 2022, 152, 153-165.	2.9	10
44	Characterizing Protein Protonation Microstates Using Monte Carlo Sampling. Journal of Physical Chemistry B, 2022, 126, 2476-2485.	2.6	9
45	Affinity and activity of non-native quinones at the QB site of bacterial photosynthetic reaction centers. Photosynthesis Research, 2014, 120, 181-196.	2.9	6
46	Characterization of a symmetrized mutant RC with 42 residues from the QA site replacing residues in the Q(B) site. Photosynthesis Research, 2000, 64, 41-52.	2.9	5
47	Identification of a Na⁺-Binding Site near the Oxygen-Evolving Complex of Spinach Photosystem II. Biochemistry, 2020, 59, 2823-2831.	2.5	5
48	The design features cells use to build their transmembrane proton gradient. Physical Biology, 2017, 14, 013001.	1.8	4
49	Computational analysis of photosynthetic systems. Photosynthesis Research, 2008, 97, 1-3.	2.9	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. Journal of Theoretical and Computational Chemistry, 0, , 2042001.	1.8	2
51	Poor Personâ€™s pH Simulation of Membrane Proteins. Methods in Molecular Biology, 2021, 2315, 197-217.	0.9	1
52	Modeling the First Electron Transfer from QA to QB in Reaction Center Proteins from Rb. sphaeroid. ACS Symposium Series, 2004, , 93-106.	0.5	0