Arieh Warshel

List of Publications by Citations

154 papers	18,993 citations	66 h-index	137 g-index
159 ext. papers	20,235 ext. citations	7.9 avg, IF	6.96 L-index

#	Paper	IF	Citations
154	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
153	Electrostatic basis for enzyme catalysis. *Chemical Reviews*, **2006**, 106, 3210-35	68.1	923
152	Calculations of electrostatic interactions in biological systems and in solutions. *Quarterly Reviews of Biophysics*, **1984**, 17, 283-422	7	864
151	What are the dielectric "constants" of proteins and how to validate electrostatic models?. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 400-17	4.2	785
150	An empirical valence bond approach for comparing reactions in solutions and in enzymes. *Journal of the American Chemical Society*, **1980**, 102, 6218-6226	16.4	761
149	Simulation of enzyme reactions using valence bond force fields and other hybrid quantum/classical approaches. *Chemical Reviews*, **1993**, 93, 2523-2544	68.1	720
148	Q-Chem 2.0: a high-performance ab initio electronic structure program package. *Journal of Computational Chemistry*, **2000**, 21, 1532-1548	3.5	588
147	Computer simulations of enzyme catalysis: methods, progress, and insights. *Annual Review of Biophysics and Biomolecular Structure*, **2003**, 32, 425-43		438
146	Modeling electrostatic effects in proteins. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2006**, 1764, 1647-76	4	433
145	Microscopic and semimicroscopic calculations of electrostatic energies in proteins by the POLARIS and ENZYMIX programs. *Journal of Computational Chemistry*, **1993**, 14, 161-185	3.5	422
144	A surface constrained all-atom solvent model for effective simulations of polar solutions. *Journal of Chemical Physics*, **1989**, 91, 3647-3661	3.9	410
143	A local reaction field method for fast evaluation of long-range electrostatic interactions in molecular simulations. *Journal of Chemical Physics*, **1992**, 97, 3100-3107	3.9	380
142	Investigation of the free energy functions for electron transfer reactions. *Journal of Chemical Physics*, **1990**, 93, 8682-8692	3.9	363
141	At the dawn of the 21st century: Is dynamics the missing link for understanding enzyme catalysis?. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1339-75	4.2	346
140	Consistent Calculations of pKa's of Ionizable Residues in Proteins: Semi-microscopic and Microscopic Approaches. *Journal of Physical Chemistry B*, **1997**, 101, 4458-4472	3.4	325
139	Calculations of chemical processes in solutions. *The Journal of Physical Chemistry*, **1979**, 83, 1640-1652		313
138	Energetics and Dynamics of Enzymatic Reactions. *Journal of Physical Chemistry B*, **2001**, 105, 7887-7907	3.4	299

137	Simulation of free energy relationships and dynamics of SN2 reactions in aqueous solution. *Journal of the American Chemical Society*, **1988**, 110, 5297-5311	16.4	267
136	Langevin Dipoles Model for ab Initio Calculations of Chemical Processes in Solution: Parametrization and Application to Hydration Free Energies of Neutral and Ionic Solutes and Conformational Analysis in Aqueous Solution. *Journal of Physical Chemistry B*, **1997**, 101, 5583-5595	3.4	259
135	Dynamics of biochemical and biophysical reactions: insight from computer simulations. *Quarterly Reviews of Biophysics*, **2001**, 34, 563-679	7	240
134	Microscopic simulations of macroscopic dielectric constants of solvated proteins. *Journal of Chemical Physics*, **1991**, 95, 4366-4377	3.9	240
133	Substrate-assisted catalysis as a mechanism for GTP hydrolysis of p21ras and other GTP-binding proteins. *Nature Structural Biology*, **1995**, 2, 36-44		234
132	Phosphate Ester Hydrolysis in Aqueous Solution: Associative versus Dissociative Mechanisms. *Journal of Physical Chemistry B*, **1998**, 102, 719-734	3.4	222
131	Simulation of the dynamics of electron transfer reactions in polar solvents: Semiclassical trajectories and dispersed polaron approaches. *Journal of Chemical Physics*, **1986**, 84, 4938-4957	3.9	210
130	Calculations of resonance Raman spectra of conjugated molecules. *Journal of Chemical Physics*, **1977**, 66, 5477-5488	3.9	207
129	The effect of protein relaxation on charge-charge interactions and dielectric constants of proteins. *Biophysical Journal*, **1998**, 74, 1744-53	2.9	200
128	Examining methods for calculations of binding free energies: LRA, LIE, PDLD-LRA, and PDLD/S-LRA calculations of ligands binding to an HIV protease. *Proteins: Structure, Function and Bioinformatics*, **2000**, 39, 393-407	4.2	186
127	Enzyme millisecond conformational dynamics do not catalyze the chemical step. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 17359-64	11.5	181
126	On the mechanism of hydrolysis of phosphate monoesters dianions in solutions and proteins. *Journal of the American Chemical Society*, **2006**, 128, 15310-23	16.4	179
125	How Important Are Quantum Mechanical Nuclear Motions in Enzyme Catalysis?. *Journal of the American Chemical Society*, **1996**, 118, 11745-11751	16.4	177
124	Evaluation of catalytic free energies in genetically modified proteins. *Journal of Molecular Biology*, **1988**, 201, 139-59	6.5	170
123	Coarse-grained (multiscale) simulations in studies of biophysical and chemical systems. *Annual Review of Physical Chemistry*, **2011**, 62, 41-64	15.7	165
122	Molecular dynamics simulations of biological reactions. *Accounts of Chemical Research*, **2002**, 35, 385-95	24.3	163
121	Multiscale modeling of biological functions: from enzymes to molecular machines (Nobel Lecture). *Angewandte Chemie - International Edition*, **2014**, 53, 10020-31	16.4	159
120	Calculations of Activation Entropies of Chemical Reactions in Solution. *Journal of Physical Chemistry B*, **2000**, 104, 4578-4584	3.4	159

119	Theoretical correlation of structure and energetics in the catalytic reaction of trypsin. *Journal of the American Chemical Society*, **1986**, 108, 6569-6579	16.4	151
118	Ab Initio QM/MM Simulation with Proper Sampling: First Principle Calculations of the Free Energy of the Autodissociation of Water in Aqueous Solution. *Journal of Physical Chemistry B*, **2002**, 106, 13333-13343	3.4	147
117	How does GAP catalyze the GTPase reaction of Ras? A computer simulation study. *Biochemistry*, **2000**, 39, 9641-51	3.2	137
116	Free energy relationships in metalloenzyme-catalyzed reactions. Calculations of the effects of metal ion substitutions in staphylococcal nuclease. *Journal of the American Chemical Society*, **1990**, 112, 2860-2868	16.4	136
115	The low barrier hydrogen bond (LBHB) proposal revisited: the case of the Asp... His pair in serine proteases. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 711-23	4.2	134
114	Computer simulation of the chemical catalysis of DNA polymerases: discriminating between alternative nucleotide insertion mechanisms for T7 DNA polymerase. *Journal of the American Chemical Society*, **2003**, 125, 8163-77	16.4	134
113	Absolute binding free energy calculations: on the accuracy of computational scoring of protein-ligand interactions. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1705-23	4.2	132
112	The empirical valence bond model: theory and applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 30-45	7.9	130
111	Remarkable rate enhancement of orotidine 5'-monophosphate decarboxylase is due to transition-state stabilization rather than to ground-state destabilization. *Biochemistry*, **2000**, 39, 14728-38	3.2	128
110	Perspective: Defining and quantifying the role of dynamics in enzyme catalysis. *Journal of Chemical Physics*, **2016**, 144, 180901	3.9	128
109	Conversion of light energy to electrostatic energy in the proton pump of Halobacterium halobium. *Photochemistry and Photobiology*, **1979**, 30, 285-90	3.6	123
108	Calculations of Hydration Entropies of Hydrophobic, Polar, and Ionic Solutes in the Framework of the Langevin Dipoles Solvation Model. *Journal of Physical Chemistry B*, **1999**, 103, 10282-10288	3.4	120
107	Role of arginine-38 in regulation of the cytochrome c oxidation-reduction equilibrium. *Biochemistry*, **1989**, 28, 3188-97	3.2	117
106	Ab Initio Frozen Density Functional Calculations of Proton Transfer Reactions in Solution. *The Journal of Physical Chemistry*, **1996**, 100, 15444-15449		107
105	Ab Initio Evaluation of the Potential Surface for General Base- Catalyzed Methanolysis of Formamide: A Reference Solution Reaction for Studies of Serine Proteases. *Journal of the American Chemical Society*, **2000**, 122, 5354-5366	16.4	107
104	Origin of the Catalytic Power of Acetylcholinesterase: Computer Simulation Studies. *Journal of the American Chemical Society*, **1998**, 120, 183-194	16.4	106
103	A Fundamental Assumption about OH- Attack in Phosphate Ester Hydrolysis Is Not Fully Justified. *Journal of the American Chemical Society*, **1997**, 119, 5473-5474	16.4	103
102	Computer simulations of protein functions: searching for the molecular origin of the replication fidelity of DNA polymerases. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6819-24	11.5	101

101	Why ion pair reversal by protein engineering is unlikely to succeed. *Nature*, **1988**, 334, 270-2	50.4	95
100	Paradynamics: an effective and reliable model for ab initio QM/MM free-energy calculations and related tasks. *Journal of Physical Chemistry B*, **2011**, 115, 7950-62	3.4	94
99	The Physics and Physical Chemistry of Molecular Machines. *ChemPhysChem*, **2016**, 17, 1719-41	3.2	85
98	Orientation of the OH Dipole of Tyrosine (M)210 and Its Effect on Electrostatic Energies in Photosynthetic Bacterial Reaction Centers. *The Journal of Physical Chemistry*, **1996**, 100, 16761-16770		84
97	The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. *Faraday Discussions*, **2010**, 145, 71-106	3.6	77
96	Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center. *Proteins: Structure, Function and Bioinformatics*, **1999**, 36, 484-500	4.2	77
95	Ketosteroid isomerase provides further support for the idea that enzymes work by electrostatic preorganization. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 4075-80	11.5	74
94	Converting conformational changes to electrostatic energy in molecular motors: The energetics of ATP synthase. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 14834-9	11.5	74
93	Electrostatic origin of the mechanochemical rotary mechanism and the catalytic dwell of F1-ATPase. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 20550-5	11.5	73
92	Electrostatic contributions to protein-protein binding affinities: application to Rap/Raf interaction. *Proteins: Structure, Function and Bioinformatics*, **1998**, 30, 407-23	4.2	73
91	Computer aided enzyme design and catalytic concepts. *Current Opinion in Chemical Biology*, **2014**, 21, 56-62	9.7	70
90	Calculations of free energy profiles for the staphylococcal nuclease catalyzed reaction. *Biochemistry*, **1989**, 28, 4680-9	3.2	70
89	Exploring the Dependence of QM/MM Calculations of Enzyme Catalysis on the Size of the QM Region. *Journal of Physical Chemistry B*, **2016**, 120, 9913-21	3.4	68
88	Electrostatic contributions to binding of transition state analogues can be very different from the corresponding contributions to catalysis: phenolates binding to the oxyanion hole of ketosteroid isomerase. *Biochemistry*, **2007**, 46, 1466-76	3.2	65
87	Quantum-mechanical calculations of solvation free energies. A combined ab initio pseudopotential free-energy perturbation approach. *Journal of Chemical Physics*, **1992**, 97, 4264-4271	3.9	65
86	Ab Initio Evaluation of the Free Energy Surfaces for the General Base/Acid Catalyzed Thiolysis of Formamide and the Hydrolysis of Methyl Thiolformate:□A Reference Solution Reaction for Studies of Cysteine Proteases. *Journal of Physical Chemistry B*, **2001**, 105, 4471-4484	3.4	62
85	On the Reactivity of Phosphate Monoester Dianions in Aqueous Solution: Brønsted Linear Free-Energy Relationships Do Not Have an Unique Mechanistic Interpretation. *Journal of the American Chemical Society*, **1998**, 120, 11524-11525	16.4	60
84	The surface constraint all atom model provides size independent results in calculations of hydration free energies. *Journal of Chemical Physics*, **1998**, 109, 7940-7944	3.9	57

83	Continuum and Dipole-Lattice Models of Solvation. *Journal of Physical Chemistry B*, **1997**, 101, 11254-11264	3.4	49
82	Dissecting the role of the ε subunit in the rotary-chemical coupling and torque generation of F1-ATPase. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 2746-51	11.5	47
81	Realistic simulations of the coupling between the protomotive force and the mechanical rotation of the F0-ATPase. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 14876-81	11.5	46
80	Constraining the electron densities in DFT method as an effective way for ab initio studies of metal-catalyzed reactions. *Journal of Computational Chemistry*, **2000**, 21, 1554-1561	3.5	42
79	The extended Ewald method: A general treatment of long-range electrostatic interactions in microscopic simulations. *Journal of Chemical Physics*, **1988**, 89, 3751-3759	3.9	42
78	Dineopentyl phosphate hydrolysis: evidence for stepwise water attack. *Journal of Organic Chemistry*, **2008**, 73, 6960-9	4.2	39
77	Computer simulation studies of the fidelity of DNA polymerases. *Biopolymers*, **2003**, 68, 286-99	2.2	37
76	Simulating electrostatic energies in proteins: perspectives and some recent studies of pKas, redox, and other crucial functional properties. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3469-84	4.2	36
75	An effective coarse-grained model for biological simulations: recent refinements and validations. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1168-85	4.2	35
74	Prechemistry versus preorganization in DNA replication fidelity. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2900-19	4.2	35
73	A stringent test of the cavity concept in continuum dielectrics. *Journal of Chemical Physics*, **1997**, 107, 7975-7978	3.9	35
72	Exploring the free-energy landscape of GPCR activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 10327-10332	11.5	27
71	Exploring the Development of Ground-State Destabilization and Transition-State Stabilization in Two Directed Evolution Paths of Kemp Eliminases. *ACS Catalysis*, **2017**, 7, 3301-3305	13.1	25
70	Prechemistry barriers and checkpoints do not contribute to fidelity and catalysis as long as they are not rate limiting. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	25
69	DNA polymerase β catalytic efficiency mirrors the Asn279–dCTP H-bonding strength. *FEBS Letters*, **2007**, 581, 775-780	3.8	25
68	Effect of Solvent Discreteness on Solvation. *Journal of Physical Chemistry B*, **1998**, 102, 5348-5357	3.4	25
67	Refining the treatment of membrane proteins by coarse-grained models. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 92-117	4.2	25
66	Renormalizing SMD: the renormalization approach and its use in long time simulations and accelerated PMF calculations of macromolecules. *Journal of Physical Chemistry B*, **2010**, 114, 12720-8	3.4	24

65	Simulating the dynamics of the mechanochemical cycle of myosin-V. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2259-2264	11.5	23
64	Critical Differences between the Binding Features of the Spike Proteins of SARS-CoV-2 and SARS-CoV. *Journal of Physical Chemistry B*, **2020**, 124, 5907-5912	3.4	23
63	The FF ATP synthase: from atomistic three-dimensional structure to the rotary-chemical function. *Photosynthesis Research*, **2017**, 134, 1-15	3.7	23
62	Exploring the Mechanism of Covalent Inhibition: Simulating the Binding Free Energy of Ketoamide Inhibitors of the Main Protease of SARS-CoV-2. *Biochemistry*, **2020**, 59, 4601-4608	3.2	23
61	Revisiting the protomotive vectorial motion of F-ATPase. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 19484-19489	11.5	22
60	The entropic contributions in vitamin B12 enzymes still reflect the electrostatic paradigm. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 4328-33	11.5	22
59	Simulating the fidelity and the three Mg mechanism of pol and clarifying the validity of transition state theory in enzyme catalysis. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 1446-1453	4.2	21
58	Reply to Karplus: Conformational dynamics have no role in the chemical step. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, E72-E72	11.5	21
57	Quantum Mechanical-Molecular Mechanical Approaches for Studying Chemical Reactions in Proteins and Solution. *ACS Symposium Series*, **1998**, 16-34	0.4	21
56	Torque, chemistry and efficiency in molecular motors: a study of the rotary-chemical coupling in F1-ATPase. *Quarterly Reviews of Biophysics*, **2015**, 48, 395-403	7	20
55	Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase. *Structural Chemistry*, **1996**, 7, 131-138	1.8	20
54	Enhancing Paradynamics for QM/MM Sampling of Enzymatic Reactions. *Journal of Physical Chemistry B*, **2016**, 120, 2155-64	3.4	20
53	Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer. *Faraday Discussions*, **2010**, 145, 281-299	3.6	19
52	Exploring the challenges of computational enzyme design by rebuilding the active site of a dehalogenase. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 389-394	11.5	19
51	ZnT2 is an electroneutral proton-coupled vesicular antiporter displaying an apparent stoichiometry of two protons per zinc ion. *PLoS Computational Biology*, **2019**, 15, e1006882	5	18
50	Simulating the function of sodium/proton antiporters. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 12378-83	11.5	18
49	Quantized semiclassical trajectory approach for evaluation of vibronic transitions in anharmonic molecules. *Journal of Chemical Physics*, **1985**, 82, 1756-1771	3.9	18
48	Exploring the mechanism of DNA polymerases by analyzing the effect of mutations of active site acidic groups in Polymerase *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 1644-1657	4.2	17

47	Exploring the Catalytic Mechanism of Cas9 Using Information Inferred from Endonuclease VII. *ACS Catalysis*, **2019**, 9, 1329-1336	13.1	17
46	Misunderstanding the preorganization concept can lead to confusions about the origin of enzyme catalysis. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 2157-2161	4.2	16
45	Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions. *Journal of Computational Chemistry*, **2000**, 21, 607-625	3.5	16
44	On the control of the proton current in the voltage-gated proton channel Hv1. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 10321-10326	11.5	16
43	Multiskalenmodellierung biologischer Funktionen: Von Enzymen zu molekularen Maschinen (Nobel-Aufsatz). *Angewandte Chemie*, **2014**, 126, 10182-10194	3.6	15
42	Oscillations of the energy gap for the initial electron-transfer step in bacterial reaction centers. *Photosynthesis Research*, **1998**, 55, 147-152	3.7	15
41	Comment on Effect of Active Site Mutation Phe93 -nTrp in the Horse Liver Alcohol Dehydrogenase Enzyme on Catalysis: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2003**, 107, 12370-12371	3.4	15
40	Energetics of Light-Induced Charge Separation Across Membranes. *Israel Journal of Chemistry*, **1981**, 21, 341-347	3.4	14
39	Modeling gating charge and voltage changes in response to charge separation in membrane proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 11353-8	11.5	13
38	Reexamining the origin of the directionality of myosin V. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 10426-10431	11.5	13
37	Microscopic simulation of quantum dynamics and nuclear tunneling in bacterial reaction centers. *Photosynthesis Research*, **1989**, 22, 39-46	3.7	13
36	EF-Tu and EF-G are activated by allosteric effects. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 3386-3391	11.5	12
35	Origin of the Non-Arrhenius Behavior of the Rates of Enzymatic Reactions. *Journal of Physical Chemistry B*, **2017**, 121, 6520-6526	3.4	11
34	Validating the Water Flooding Approach by Comparing It to Grand Canonical Monte Carlo Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 9358-9365	3.4	11
33	Inverting the selectivity of aquaporin 6: gating versus direct electrostatic interaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 1813-4	11.5	9
32	Ab initio/LD studies of chemical reactions in solution: Reference free-energy surfaces for acylation reactions occurring in serine and cysteine proteases. *International Journal of Quantum Chemistry*, **2000**, 77, 44-53	2.1	9
31	Energetics and Dynamics of Transition States of Reactions in Enzymes and Solutions. *ACS Symposium Series*, **1999**, 489-499	0.4	9
30	Exploring the Effectiveness of Binding Free Energy Calculations. *Journal of Physical Chemistry B*, **2019**, 123, 8910-8915	3.4	8

29	Brønsted slopes based on single-molecule imaging data help to unveil the chemically coupled rotation in F1-ATPase. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 14121-2	11.5	8
28	Exploring the Proteolysis Mechanism of the Proteasomes. *Journal of Physical Chemistry B*, **2020**, 124, 5626-5635	3.4	8
27	Microscopic Based Density Matrix Treatments of Electron-Transfer Reactions in Condensed Phases. *Journal of Physical Chemistry A*, **1999**, 103, 11378-11386	2.8	8
26	Exploring the Catalytic Reaction of Cysteine Proteases. *Journal of Physical Chemistry B*, **2020**, 124, 11349-11356	3.4	8
25	A free-energy landscape for the glucagon-like peptide 1 receptor GLP1R. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 127-134	4.2	8
24	Demonstrating aspects of multiscale modeling by studying the permeation pathway of the human ZnT2 zinc transporter. *PLoS Computational Biology*, **2018**, 14, e1006503	5	8
23	Exploring the Drug Resistance of HCV Protease. *Journal of Physical Chemistry B*, **2017**, 121, 6831-6840	3.4	7
22	Quantum Catalysis: The Modeling of Catalytic Transition States. *ACS Symposium Series*, **1999**, 2-17	0.4	7
21	Predicting Mutational Effects on Receptor Binding of the Spike Protein of SARS-CoV-2 Variants. *Journal of the American Chemical Society*, **2021**, 143, 17646-17654	16.4	7
20	The control of the discrimination between dNTP and rNTP in DNA and RNA polymerase. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 1616-1624	4.2	7
19	Combinatorial Approach for Exploring Conformational Space and Activation Barriers in Computer-Aided Enzyme Design. *ACS Catalysis*, **2020**, 10, 6002-6012	13.1	6
18	Perspective on "The energetics of enzymatic reactions". *Theoretical Chemistry Accounts*, **2000**, 103, 337-339	2.9	6
17	Exploring alternative catalytic mechanisms of the Cas9 HNH domain. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 260-264	4.2	6
16	Analyzing the electrogenicity of cytochrome c oxidase. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 7810-5	11.5	5
15	A Microscopic Capacitor Model of Voltage Coupling in Membrane Proteins: Gating Charge Fluctuations in Ci-VSD. *Journal of Physical Chemistry B*, **2016**, 120, 418-32	3.4	5
14	Validating a Coarse-Grained Voltage Activation Model by Comparing Its Performance to the Results of Monte Carlo Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 11284-11291	3.4	5
13	Chapter 15:Challenges and Progresses in Calculations of Binding Free Energies "What Does it Take to Quantify Electrostatic Contributions to Protein–ligand Interactions?. *RSC Biomolecular Sciences*, **2007**, 268-290		5
12	Equilibrium fluctuation relations for voltage coupling in membrane proteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 2985-97	3.8	4

11	Exploring the activation pathway and G-coupling specificity of the δ-opioid receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 26218-26225	11.5	4
10	The catalytic dwell in ATPases is not crucial for movement against applied torque. *Nature Chemistry* , **2020**, 12, 1187-1192	17.6	4
9	A new class of α-ketoamide derivatives with potent anticancer and anti-SARS-CoV-2 activities. *European Journal of Medicinal Chemistry*, **2021**, 215, 113267	6.8	4
8	Simulating the Function of the MjNhaP1 Transporter. *Journal of Physical Chemistry B*, **2016**, 120, 10951-10958	3.4	4
7	Exploring the Activation Process of the β2AR-G Complex. *Journal of the American Chemical Society*, **2021**, 143, 11044-11051	16.4	4
6	Examining methods for calculations of binding free energies: LRA, LIE, PDLD-LRA, and PDLD/S-LRA calculations of ligands binding to an HIV protease **2000**, 39, 393		4
5	Simulating the directional translocation of a substrate by the AAA+ motor in the 26S proteasome. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	3
4	Q-Chem 2.0: a high-performance ab initio electronic structure program package **2000**, 21, 1532		2
3	Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center **1999**, 36, 484		1
2	Cover Image, Volume 84, Issue 11. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, C4-C4	4.2	
1	Computer Simulations of Proton Transfer in Proteins and Solutions1171-1205		