

Arieh Warshel

List of Publications by Year in descending order

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158
papers

21,502
citations

14655

66
h-index

9103

144
g-index

159
all docs

159
docs citations

159
times ranked

13025
citing authors

#	ARTICLE	IF	CITATIONS
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	1.7	2,561
2	Electrostatic Basis for Enzyme Catalysis. <i>Chemical Reviews</i> , 2006, 106, 3210-3235.	47.7	1,117
3	Calculations of electrostatic interactions in biological systems and in solutions. <i>Quarterly Reviews of Biophysics</i> , 1984, 17, 283-422.	5.7	950
4	What are the dielectric constants of proteins and how to validate electrostatic models?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 44, 400-417.	2.6	865
5	An empirical valence bond approach for comparing reactions in solutions and in enzymes. <i>Journal of the American Chemical Society</i> , 1980, 102, 6218-6226.	13.7	853
6	Simulation of enzyme reactions using valence bond force fields and other hybrid quantum/classical approaches. <i>Chemical Reviews</i> , 1993, 93, 2523-2544.	47.7	797
7	Q-Chem 2.0: a high-performance ab initio electronic structure program package. <i>Journal of Computational Chemistry</i> , 2000, 21, 1532-1548.	3.3	617
8	Modeling electrostatic effects in proteins. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2006, 1764, 1647-1676.	2.3	472
9	Computer Simulations of Enzyme Catalysis: Methods, Progress, and Insights. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 2003, 32, 425-443.	18.3	467
10	Microscopic and semimicroscopic calculations of electrostatic energies in proteins by the POLARIS and ENZYMIK programs. <i>Journal of Computational Chemistry</i> , 1993, 14, 161-185.	3.3	445
11	A surface constrained all-atom solvent model for effective simulations of polar solutions. <i>Journal of Chemical Physics</i> , 1989, 91, 3647-3661.	3.0	442
12	A local reaction field method for fast evaluation of long-range electrostatic interactions in molecular simulations. <i>Journal of Chemical Physics</i> , 1992, 97, 3100-3107.	3.0	414
13	At the dawn of the 21st century: Is dynamics the missing link for understanding enzyme catalysis?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1339-1375.	2.6	399
14	Investigation of the free energy functions for electron transfer reactions. <i>Journal of Chemical Physics</i> , 1990, 93, 8682-8692.	3.0	393
15	Consistent Calculations of pKa's of Ionizable Residues in Proteins: Semi-microscopic and Microscopic Approaches. <i>Journal of Physical Chemistry B</i> , 1997, 101, 4458-4472.	2.6	357
16	Calculations of chemical processes in solutions. <i>The Journal of Physical Chemistry</i> , 1979, 83, 1640-1652.	2.9	328
17	Energetics and Dynamics of Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7887-7907.	2.6	326
18	Simulation of free energy relationships and dynamics of SN2 reactions in aqueous solution. <i>Journal of the American Chemical Society</i> , 1988, 110, 5297-5311.	13.7	287

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19	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. <i>Journal of Physical Chemistry B</i> , 1997, 101, 5583-5595.	2.6	275
20	Substrate-assisted catalysis as a mechanism for GTP hydrolysis of p21ras and other GTP-binding proteins. <i>Nature Structural Biology</i> , 1995, 2, 36-44.	9.7	259
21	Dynamics of biochemical and biophysical reactions: insight from computer simulations. <i>Quarterly Reviews of Biophysics</i> , 2001, 34, 563-679.	5.7	257
22	Microscopic simulations of macroscopic dielectric constants of solvated proteins. <i>Journal of Chemical Physics</i> , 1991, 95, 4366-4377.	3.0	252
23	Phosphate Ester Hydrolysis in Aqueous Solution: Associative versus Dissociative Mechanisms. <i>Journal of Physical Chemistry B</i> , 1998, 102, 719-734.	2.6	234
24	Calculations of resonance Raman spectra of conjugated molecules. <i>Journal of Chemical Physics</i> , 1977, 66, 5477-5488.	3.0	219
25	Simulation of the dynamics of electron transfer reactions in polar solvents: Semiclassical trajectories and dispersed polaron approaches. <i>Journal of Chemical Physics</i> , 1986, 84, 4938-4957.	3.0	219
26	The Effect of Protein Relaxation on Charge-Charge Interactions and Dielectric Constants of Proteins. <i>Biophysical Journal</i> , 1998, 74, 1744-1753.	0.5	207
27	Examining methods for calculations of binding free energies: LRA, LIE, PDL-LRA, and PDL/S-LRA calculations of ligands binding to an HIV protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 39, 393-407.	2.6	202
28	Multiscale Modeling of Biological Functions: From Enzymes to Molecular Machines (Nobel Lecture). <i>Angewandte Chemie - International Edition</i> , 2014, 53, 10020-10031.	13.8	201
29	Enzyme millisecond conformational dynamics do not catalyze the chemical step. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 17359-17364.	7.1	195
30	On the Mechanism of Hydrolysis of Phosphate Monoesters Dianions in Solutions and Proteins. <i>Journal of the American Chemical Society</i> , 2006, 128, 15310-15323.	13.7	191
31	Evaluation of catalytic free energies in genetically modified proteins. <i>Journal of Molecular Biology</i> , 1988, 201, 139-159.	4.2	190
32	Molecular Dynamics Simulations of Biological Reactions. <i>Accounts of Chemical Research</i> , 2002, 35, 385-395.	15.6	186
33	How Important Are Quantum Mechanical Nuclear Motions in Enzyme Catalysis?. <i>Journal of the American Chemical Society</i> , 1996, 118, 11745-11751.	13.7	185
34	Absolute binding free energy calculations: On the accuracy of computational scoring of protein-ligand interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1705-1723.	2.6	180
35	Coarse-Grained (Multiscale) Simulations in Studies of Biophysical and Chemical Systems. <i>Annual Review of Physical Chemistry</i> , 2011, 62, 41-64.	10.8	176
36	Theoretical correlation of structure and energetics in the catalytic reaction of trypsin. <i>Journal of the American Chemical Society</i> , 1986, 108, 6569-6579.	13.7	169

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37	Calculations of Activation Entropies of Chemical Reactions in Solution. <i>Journal of Physical Chemistry B</i> , 2000, 104, 4578-4584.	2.6	166
38	Perspective: Defining and quantifying the role of dynamics in enzyme catalysis. <i>Journal of Chemical Physics</i> , 2016, 144, 180901.	3.0	163
39	The low barrier hydrogen bond (LBHB) proposal revisited: The case of the Asp ⁺ His pair in serine proteases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 711-723.	2.6	155
40	How Does GAP Catalyze the GTPase Reaction of Ras? A Computer Simulation Study. <i>Biochemistry</i> , 2000, 39, 9641-9651.	2.5	153
41	Free energy relationships in metalloenzyme-catalyzed reactions. Calculations of the effects of metal ion substitutions in staphylococcal nuclease. <i>Journal of the American Chemical Society</i> , 1990, 112, 2860-2868.	13.7	151
42	Ab Initio QM/MM Simulation with Proper Sampling: First Principle Calculations of the Free Energy of the Autodissociation of Water in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2002, 106, 13333-13343.	2.6	150
43	Computer Simulation of the Chemical Catalysis of DNA Polymerases: Discriminating between Alternative Nucleotide Insertion Mechanisms for T7 DNA Polymerase. <i>Journal of the American Chemical Society</i> , 2003, 125, 8163-8177.	13.7	145
44	The empirical valence bond model: theory and applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 30-45.	14.6	141
45	Remarkable Rate Enhancement of Orotidine 5'-Monophosphate Decarboxylase Is Due to Transition-State Stabilization Rather Than to Ground-State Destabilization. <i>Biochemistry</i> , 2000, 39, 14728-14738.	2.5	135
46	Calculations of Hydration Entropies of Hydrophobic, Polar, and Ionic Solutes in the Framework of the Langevin Dipoles Solvation Model. <i>Journal of Physical Chemistry B</i> , 1999, 103, 10282-10288.	2.6	131
47	CONVERSION OF LIGHT ENERGY TO ELECTROSTATIC ENERGY IN THE PROTON PUMP OF <i>HALOBACTERIUM HALOBIIUM</i> . <i>Photochemistry and Photobiology</i> , 1979, 30, 285-290.	2.5	130
48	Role of arginine-38 in regulation of the cytochrome c oxidation-reduction equilibrium. <i>Biochemistry</i> , 1989, 28, 3188-3197.	2.5	126
49	The Physics and Physical Chemistry of Molecular Machines. <i>ChemPhysChem</i> , 2016, 17, 1719-1741.	2.1	120
50	Origin of the Catalytic Power of Acetylcholinesterase: A Computer Simulation Studies. <i>Journal of the American Chemical Society</i> , 1998, 120, 183-194.	13.7	116
51	Ab Initio Evaluation of the Potential Surface for General Base-Catalyzed Methanolysis of Formamide: A Reference Solution Reaction for Studies of Serine Proteases. <i>Journal of the American Chemical Society</i> , 2000, 122, 5354-5366.	13.7	115
52	Ab Initio Frozen Density Functional Calculations of Proton Transfer Reactions in Solution. <i>The Journal of Physical Chemistry</i> , 1996, 100, 15444-15449.	2.9	112
53	A Fundamental Assumption about OH-Attack in Phosphate Ester Hydrolysis Is Not Fully Justified. <i>Journal of the American Chemical Society</i> , 1997, 119, 5473-5474.	13.7	107
54	Why ion pair reversal by protein engineering is unlikely to succeed. <i>Nature</i> , 1988, 334, 270-272.	27.8	104

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55	Computer simulations of protein functions: Searching for the molecular origin of the replication fidelity of DNA polymerases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6819-6824.	7.1	103
56	Paradynamics: An Effective and Reliable Model for Ab Initio QM/MM Free-Energy Calculations and Related Tasks. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7950-7962.	2.6	101
57	The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. <i>Faraday Discussions</i> , 2010, 145, 71-106.	3.2	96
58	Exploring the Dependence of QM/MM Calculations of Enzyme Catalysis on the Size of the QM Region. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9913-9921.	2.6	94
59	Electrostatic origin of the mechanochemical rotary mechanism and the catalytic dwell of F1-ATPase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 20550-20555.	7.1	93
60	Orientation of the OH Dipole of Tyrosine (M)210 and Its Effect on Electrostatic Energies in Photosynthetic Bacterial Reaction Centers. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16761-16770.	2.9	90
61	Calculations of free energy profiles for the staphylococcal nuclease catalyzed reaction. <i>Biochemistry</i> , 1989, 28, 4680-4689.	2.5	81
62	Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodospirillum rubrum reaction center. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 36, 484-500.	2.6	81
63	Ketosteroid isomerase provides further support for the idea that enzymes work by electrostatic preorganization. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 4075-4080.	7.1	81
64	Computer aided enzyme design and catalytic concepts. <i>Current Opinion in Chemical Biology</i> , 2014, 21, 56-62.	6.1	78
65	Electrostatic contributions to protein-protein binding affinities: Application to Rap/Raf interaction. <i>Journal of Molecular Biology</i> , 1998, 30, 407-423.		77
66	Converting conformational changes to electrostatic energy in molecular motors: The energetics of ATP synthase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 14834-14839.	7.1	75
67	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. <i>Biochemistry</i> , 2007, 46, 1466-1476.	2.5	71
68	Quantum-mechanical calculations of solvation free energies. A combined ab initio pseudopotential free energy perturbation approach. <i>Journal of Chemical Physics</i> , 1992, 97, 4264-4271.	3.0	68
69	Ab Initio Evaluation of the Free Energy Surfaces for the General Base/Acid Catalyzed Thiolysis of Formamide and the Hydrolysis of Methyl Thiolfornate: A Reference Solution Reaction for Studies of Cysteine Proteases. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4471-4484.	2.6	66
70	On the Reactivity of Phosphate Monoester Dianions in Aqueous Solution: Brønsted Linear Free-Energy Relationships Do Not Have a Unique Mechanistic Interpretation. <i>Journal of the American Chemical Society</i> , 1998, 120, 11524-11525.	13.7	62
71	The surface constraint all atom model provides size independent results in calculations of hydration free energies. <i>Journal of Chemical Physics</i> , 1998, 109, 7940-7944.	3.0	60
72	Continuum and Dipole-Lattice Models of Solvation. <i>Journal of Physical Chemistry B</i> , 1997, 101, 11254-11264.	2.6	54

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73	Realistic simulations of the coupling between the protomotive force and the mechanical rotation of the FO-ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14876-14881.	7.1	54
74	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.	2.6	52
75	Dissecting the role of the \hat{F}_1 -subunit in the rotary chemical coupling and torque generation of F_1F_0 -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2746-2751.	7.1	51
76	Dineopentyl Phosphate Hydrolysis: Evidence for Stepwise Water Attack. Journal of Organic Chemistry, 2008, 73, 6960-6969.	3.2	47
77	The extended Ewald method: A general treatment of long-range electrostatic interactions in microscopic simulations. Journal of Chemical Physics, 1988, 89, 3751-3759.	3.0	45
78	An effective Coarse-grained model for biological simulations: Recent refinements and validations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1168-1185.	2.6	45
79	Exploring the Mechanism of Covalent Inhibition: Simulating the Binding Free Energy of \hat{I} -Ketoamide Inhibitors of the Main Protease of SARS-CoV-2. Biochemistry, 2020, 59, 4601-4608.	2.5	45
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.	3.3	44
81	Simulating electrostatic energies in proteins: Perspectives and some recent studies of pKa's, redox, and other crucial functional properties. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3469-3484.	2.6	44
82	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.	7.1	43
83	Computer simulation studies of the fidelity of DNA polymerases. Biopolymers, 2003, 68, 286-299.	2.4	39
84	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.	13.7	39
85	A stringent test of the cavity concept in continuum dielectrics. Journal of Chemical Physics, 1997, 107, 7975-7978.	3.0	37
86	Prechemistry versus preorganization in DNA replication fidelity. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2900-2919.	2.6	37
87	Refining the treatment of membrane proteins by coarse-grained models. Proteins: Structure, Function and Bioinformatics, 2016, 84, 92-117.	2.6	37
88	Revisiting the protomotive vectorial motion of F_0F_1 -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19484-19489.	7.1	36
89	Zn ²⁺ is an electroneutral proton-coupled vesicular antiporter displaying an apparent stoichiometry of two protons per zinc ion. PLoS Computational Biology, 2019, 15, e1006882.	3.2	31
90	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.	1.4	29

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91	Effect of Solvent Discreteness on Solvation. <i>Journal of Physical Chemistry B</i> , 1998, 102, 5348-5357.	2.6	28
92	The FOF1 ATP synthase: from atomistic three-dimensional structure to the rotary-chemical function. <i>Photosynthesis Research</i> , 2017, 134, 1-15.	2.9	28
93	On the control of the proton current in the voltage-gated proton channel Hv1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 10321-10326.	7.1	28
94	Exploring the challenges of computational enzyme design by rebuilding the active site of a dehalogenase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 389-394.	7.1	28
95	Simulating the fidelity and the three Mg mechanism of pol $\hat{\nu}$ and clarifying the validity of transition state theory in enzyme catalysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1446-1453.	2.6	27
96	Exploring the Development of Ground-State Destabilization and Transition-State Stabilization in Two Directed Evolution Paths of Kemp Eliminases. <i>ACS Catalysis</i> , 2017, 7, 3301-3305.	11.2	27
97	Renormalizing SMD: The Renormalization Approach and Its Use in Long Time Simulations and Accelerated PMF Calculations of Macromolecules. <i>Journal of Physical Chemistry B</i> , 2010, 114, 12720-12728.	2.6	26
98	The entropic contributions in vitamin B ₁₂ enzymes still reflect the electrostatic paradigm. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 4328-4333.	7.1	26
99	Exploring the Catalytic Mechanism of Cas9 Using Information Inferred from Endonuclease VII. <i>ACS Catalysis</i> , 2019, 9, 1329-1336.	11.2	26
100	DNA polymerase $\hat{\nu}^2$ catalytic efficiency mirrors the Asn279-dCTP H-bonding strength. <i>FEBS Letters</i> , 2007, 581, 775-780.	2.8	25
101	Simulating the dynamics of the mechanochemical cycle of myosin-V. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2259-2264.	7.1	25
102	Torque, chemistry and efficiency in molecular motors: a study of the rotary chemical coupling in F ₁ -ATPase. <i>Quarterly Reviews of Biophysics</i> , 2015, 48, 395-403.	5.7	24
103	Reply to Karplus: Conformational dynamics have no role in the chemical step. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, E72-E72.	7.1	23
104	Simulating the function of sodium/proton antiporters. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 12378-12383.	7.1	23
105	Misunderstanding the preorganization concept can lead to confusions about the origin of enzyme catalysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 2157-2161.	2.6	23
106	Quantum Mechanical-Molecular Mechanical Approaches for Studying Chemical Reactions in Proteins and Solution. <i>ACS Symposium Series</i> , 1998, , 16-34.	0.5	22
107	Enhancing Paradynamics for QM/MM Sampling of Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2155-2164.	2.6	22
108	Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase. <i>Structural Chemistry</i> , 1996, 7, 131-138.	2.0	21

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109	Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer. <i>Faraday Discussions</i> , 2010, 145, 281-299.	3.2	21
110	Oscillations of the energy gap for the initial electron-transfer step in bacterial reaction centers. <i>Photosynthesis Research</i> , 1998, 55, 147-152.	2.9	20
111	Quantized semiclassical trajectory approach for evaluation of vibronic transitions in anharmonic molecules. <i>Journal of Chemical Physics</i> , 1985, 82, 1756-1771.	3.0	18
112	Exploring the mechanism of DNA polymerases by analyzing the effect of mutations of active site acidic groups in Polymerase β . <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 1644-1657.	2.6	18
113	EF-Tu and EF-G are activated by allosteric effects. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 3386-3391.	7.1	18
114	Exploring the Catalytic Reaction of Cysteine Proteases. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11349-11356.	2.6	18
115	Enhancing computational enzyme design by a maximum entropy strategy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	7.1	18
116	Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions. <i>Journal of Computational Chemistry</i> , 2000, 21, 607-625.	3.3	17
117	Exploring alternative catalytic mechanisms of the Cas9 HNH domain. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 260-264.	2.6	17
118	Reexamining the origin of the directionality of myosin V. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 10426-10431.	7.1	16
119	Exploring the Effectiveness of Binding Free Energy Calculations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8910-8915.	2.6	16
120	Combinatorial Approach for Exploring Conformational Space and Activation Barriers in Computer-Aided Enzyme Design. <i>ACS Catalysis</i> , 2020, 10, 6002-6012.	11.2	16
121	Energetics of Light-Induced Charge Separation Across Membranes. <i>Israel Journal of Chemistry</i> , 1981, 21, 341-347.	2.3	15
122	Comment on 'Effect of Active Site Mutation Phe93 \rightarrow Trp in the Horse Liver Alcohol Dehydrogenase Enzyme on Catalysis: A Molecular Dynamics Study'. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12370-12371.	2.6	15
123	Multiskalenmodellierung biologischer Funktionen: Von Enzymen zu molekularen Maschinen (Nobel-Aufsatz). <i>Angewandte Chemie</i> , 2014, 126, 10182-10194.	2.0	15
124	Exploring the activation pathway and G _i -coupling specificity of the μ -opioid receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 26218-26225.	7.1	15
125	Microscopic simulation of quantum dynamics and nuclear tunneling in bacterial reaction centers. <i>Photosynthesis Research</i> , 1989, 22, 39-46.	2.9	14
126	Origin of the Non-Arrhenius Behavior of the Rates of Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6520-6526.	2.6	14

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127	Exploring the Activation Process of the β 2AR-G _s Complex. Journal of the American Chemical Society, 2021, 143, 11044-11051.	13.7	14
128	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, 11353-11358.	7.1	13
129	Validating the Water Flooding Approach by Comparing It to Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry B, 2017, 121, 9358-9365.	2.6	13
130	Demonstrating aspects of multiscale modeling by studying the permeation pathway of the human ZnT2 zinc transporter. PLoS Computational Biology, 2018, 14, e1006503.	3.2	13
131	A new class of β -ketoamide derivatives with potent anticancer and anti-SARS-CoV-2 activities. European Journal of Medicinal Chemistry, 2021, 215, 113267.	5.5	13
132	Electrostatic influence on IL-1 transport through the GSDMD pore. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	13
133	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.	2.6	12
134	Exploring the Proteolysis Mechanism of the Proteasomes. Journal of Physical Chemistry B, 2020, 124, 5626-5635.	2.6	12
135	A free-energy landscape for the glucagon-like peptide 1 receptor GLP1R. Proteins: Structure, Function and Bioinformatics, 2020, 88, 127-134.	2.6	11
136	The catalytic dwell in ATPases is not crucial for movement against applied torque. Nature Chemistry, 2020, 12, 1187-1192.	13.6	11
137	Energetics and Dynamics of Transition States of Reactions in Enzymes and Solutions. ACS Symposium Series, 1999, , 489-499.	0.5	10
138	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, 1813-1814.	7.1	10
139	Fast and Effective Prediction of the Absolute Binding Free Energies of Covalent Inhibitors of SARS-CoV-2 Main Protease and 20S Proteasome. Journal of the American Chemical Society, 2022, 144, 7568-7572.	13.7	10
140	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.	2.0	9
141	Microscopic Based Density Matrix Treatments of Electron-Transfer Reactions in Condensed Phases. Journal of Physical Chemistry A, 1999, 103, 11378-11386.	2.5	8
142	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, 14121-14122.	7.1	8
143	The control of the discrimination between dNTP and rNTP in DNA and RNA polymerase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1616-1624.	2.6	8
144	Exploring the Drug Resistance of HCV Protease. Journal of Physical Chemistry B, 2017, 121, 6831-6840.	2.6	8

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145	Quantum Catalysis: The Modeling of Catalytic Transition States. ACS Symposium Series, 1999, , 2-17.	0.5	7
146	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, .	7.1	7
147	Chapter 15. Challenges and Progresses in Calculations of Binding Free Energies â€“ What Does it Take to Quantify Electrostatic Contributions to Proteinâ€™Ligand Interactions?. RSC Biomolecular Sciences, 2007, , 268-290.	0.4	7
148	Perspective on "The energetics of enzymatic reactions". Theoretical Chemistry Accounts, 2000, 103, 337-339.	1.4	6
149	Equilibrium fluctuation relations for voltage coupling in membrane proteins. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2985-2997.	2.6	6
150	Analyzing the electrogenicity of cytochrome <i>c</i> oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 7810-7815.	7.1	6
151	A Microscopic Capacitor Model of Voltage Coupling in Membrane Proteins: Gating Charge Fluctuations in Ci-VSD. Journal of Physical Chemistry B, 2016, 120, 418-432.	2.6	6
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