

Shina Caroline Lynn Kamerlin

List of Publications by Year in descending order

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144
papers

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citations

61984
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202
all docs

202
docs citations

202
times ranked

6385
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploiting enzyme evolution for computational protein design. Trends in Biochemical Sciences, 2022, 47, 375-389.	7.5	15
2	Adventures on the Routes of Protein Evolutionâ€”In Memoriam Dan Salah Tawfik (1955â€”2021). Journal of Molecular Biology, 2022, 434, 167462.	4.2	6
3	Essential Functional Interplay of the Catalytic Groups in Acid Phosphatase. ACS Catalysis, 2022, 12, 3357-3370.	11.2	5
4	5 suggestions to increase grant application success rates. EMBO Reports, 2022, 23, e54893.	4.5	1
5	Computational Advances in Protein Engineering and Enzyme Design. Journal of Physical Chemistry B, 2022, 126, 2449-2451.	2.6	8
6	Complex Loop Dynamics Underpin Activity, Specificity, and Evolvability in the (Î²Î±) ₈ Barrel Enzymes of Histidine and Tryptophan Biosynthesis. JACS Au, 2022, 2, 943-960.	7.9	10
7	Journal Open Access and Plan S: Solving Problems or Shifting Burdens?. Development and Change, 2021, 52, 627-650.	3.3	7
8	Heme-binding enables allosteric modulation in an ancient TIM-barrel glycosidase. Nature Communications, 2021, 12, 380.	12.8	20
9	Loop Dynamics and Enzyme Catalysis in Protein Tyrosine Phosphatases. Journal of the American Chemical Society, 2021, 143, 3830-3845.	13.7	42
10	Single Residue on the WPD-Loop Affects the pH Dependency of Catalysis in Protein Tyrosine Phosphatases. JACS Au, 2021, 1, 646-659.	7.9	14
11	Academic motherhood â€” what happens when you can't make it happen?. EMBO Reports, 2021, 22, e52875.	4.5	4
12	Dan Salah Tawfik (1955â€”2021)â€”A giant of protein evolution. EMBO Reports, 2021, 22, .	4.5	2
13	The N-terminal Helix-Turn-Helix Motif of Transcription Factors MarA and Rob Drives DNA Recognition. Journal of Physical Chemistry B, 2021, 125, 6791-6806.	2.6	6
14	Prenatal genetic screening and the evolving quest for â€œperfect babiesâ€” at what cost for genetic diversity?. EMBO Reports, 2021, 22, e53620.	4.5	1
15	How to write a successful postdoc application â€” the PI perspective. EMBO Reports, 2021, 22, e54203.	4.5	1
16	Errors in DFT integration grids and their potential impact on chemical shift calculations. Magnetic Resonance in Chemistry, 2020, 58, 116-117.	1.9	3
17	Enzyme Evolution: An Epistatic Ratchet versus a Smooth Reversible Transition. Molecular Biology and Evolution, 2020, 37, 1133-1147.	8.9	26
18	G-Protein coupled receptors: structure and function in drug discovery. RSC Advances, 2020, 10, 36337-36348.	3.6	29

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19	The Role of Substrate-Coenzyme Crosstalk in Determining Turnover Rates in <i>Rhodococcus ruber</i> Alcohol Dehydrogenase. <i>ACS Catalysis</i> , 2020, 10, 9115-9128.	11.2	7
20	Ground-State Destabilization by Active-Site Hydrophobicity Controls the Selectivity of a Cofactor-Free Decarboxylase. <i>Journal of the American Chemical Society</i> , 2020, 142, 20216-20231.	13.7	6
21	Modeling the Role of a Flexible Loop and Active Site Side Chains in Hydride Transfer Catalyzed by Glycerol-3-phosphate Dehydrogenase. <i>ACS Catalysis</i> , 2020, 10, 11253-11267.	11.2	14
22	Enhancing a <i>de novo</i> enzyme activity by computationally-focused ultra-low-throughput screening. <i>Chemical Science</i> , 2020, 11, 6134-6148.	7.4	24
23	Harnessing Conformational Plasticity to Generate Designer Enzymes. <i>Journal of the American Chemical Society</i> , 2020, 142, 11324-11342.	13.7	70
24	Manipulating Conformational Dynamics To Repurpose Ancient Proteins for Modern Catalytic Functions. <i>ACS Catalysis</i> , 2020, 10, 4863-4870.	11.2	42
25	Managing Coronavirus Disease 2019 Spread With Voluntary Public Health Measures: Sweden as a Case Study for Pandemic Control. <i>Clinical Infectious Diseases</i> , 2020, 71, 3174-3181.	5.8	73
26	Female Faculty: Why So Few and Why Care?. <i>Chemistry - A European Journal</i> , 2020, 26, 8319-8323.	3.3	18
27	Short and simple sequences favored the emergence of N-helix phospho-ligand binding sites in the first enzymes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 5310-5318.	7.1	32
28	Recent Advances in Understanding Biological GTP Hydrolysis through Molecular Simulation. <i>ACS Omega</i> , 2020, 5, 4380-4385.	3.5	7
29	Modeling the Alkaline Hydrolysis of Diaryl Sulfate Diesters: A Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2020, 85, 6489-6497.	3.2	8
30	When we increase diversity in academia, we all win. <i>EMBO Reports</i> , 2020, 21, e51994.	4.5	7
31	Open Access, Plan S, and researchers' needs. <i>EMBO Reports</i> , 2020, 21, e51568.	4.5	2
32	Open Access, Plan S, and researchers'™ needs. <i>EMBO Reports</i> , 2020, 21, e51568.	4.5	4
33	Computational physical organic chemistry using the empirical valence bond approach. <i>Advances in Physical Organic Chemistry</i> , 2019, 53, 69-104.	0.5	2
34	Bifunctional Substrate Activation via an Arginine Residue Drives Catalysis in Chalcone Isomerases. <i>ACS Catalysis</i> , 2019, 9, 8388-8396.	11.2	11
35	Uncovering the Role of Key Active-Site Side Chains in Catalysis: An Extended Brønsted Relationship for Substrate Deprotonation Catalyzed by Wild-Type and Variants of Triosephosphate Isomerase. <i>Journal of the American Chemical Society</i> , 2019, 141, 16139-16150.	13.7	15
36	Structural consequence of the most frequently recurring cancer-associated substitution in DNA polymerase β . <i>Nature Communications</i> , 2019, 10, 373.	12.8	40

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37	GTP Hydrolysis Without an Active Site Base: A Unifying Mechanism for Ras and Related GTPases. <i>Journal of the American Chemical Society</i> , 2019, 141, 10684-10701.	13.7	44
38	Chemical and Biochemical Approaches for the Synthesis of Substituted Dihydroxybutanones and Di- and Tri-Hydroxypentanones. <i>Journal of Organic Chemistry</i> , 2019, 84, 6982-6991.	3.2	2
39	Long Time-Scale Atomistic Simulations of the Structure and Dynamics of Transcription Factor-DNA Recognition. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3576-3590.	2.6	21
40	Relative Binding Energies Predict Crystallographic Binding Modes of Ethionamide Booster Lead Compounds. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2244-2249.	4.6	5
41	Higher-order epistasis shapes the fitness landscape of a xenobiotic-degrading enzyme. <i>Nature Chemical Biology</i> , 2019, 15, 1120-1128.	8.0	71
42	Human Glycerol 3-Phosphate Dehydrogenase: X-ray Crystal Structures That Guide the Interpretation of Mutagenesis Studies. <i>Biochemistry</i> , 2019, 58, 1061-1073.	2.5	15
43	In Silico-Directed Evolution Using CADEE. <i>Methods in Molecular Biology</i> , 2019, 1851, 381-415.	0.9	8
44	The role of ligand-gated conformational changes in enzyme catalysis. <i>Biochemical Society Transactions</i> , 2019, 47, 1449-1460.	3.4	12
45	Cryptic genetic variation shapes the adaptive evolutionary potential of enzymes. <i>ELife</i> , 2019, 8, .	6.0	35
46	Role of Ligand-Driven Conformational Changes in Enzyme Catalysis: Modeling the Reactivity of the Catalytic Cage of Triosephosphate Isomerase. <i>Journal of the American Chemical Society</i> , 2018, 140, 3854-3857.	13.7	27
47	Computer simulations of the catalytic mechanism of wild-type and mutant \hat{I}^2 -phosphoglucomutase. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 2060-2073.	2.8	11
48	Evolution of chalcone isomerase from a noncatalytic ancestor. <i>Nature Chemical Biology</i> , 2018, 14, 548-555.	8.0	113
49	Amyloid- \hat{I}^2 Peptide Interactions with Amphiphilic Surfactants: Electrostatic and Hydrophobic Effects. <i>ACS Chemical Neuroscience</i> , 2018, 9, 1680-1692.	3.5	51
50	Challenges and advances in the computational modeling of biological phosphate hydrolysis. <i>Chemical Communications</i> , 2018, 54, 3077-3089.	4.1	20
51	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. <i>SoftwareX</i> , 2018, 7, 388-395.	2.6	47
52	Empirical Valence Bond Simulations Suggest a Direct Hydride Transfer Mechanism for Human Diamine Oxidase. <i>ACS Omega</i> , 2018, 3, 3665-3674.	3.5	7
53	Cooperativity and flexibility in enzyme evolution. <i>Current Opinion in Structural Biology</i> , 2018, 48, 83-92.	5.7	81
54	The evolution of multiple active site configurations in a designed enzyme. <i>Nature Communications</i> , 2018, 9, 3900.	12.8	75

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55	Loop Motion in Triosephosphate Isomerase Is Not a Simple Open and Shut Case. <i>Journal of the American Chemical Society</i> , 2018, 140, 15889-15903.	13.7	63
56	Stereo- and Regioselectivity in Catalyzed Transformation of a 1,2-Disubstituted Vicinal Diol and the Corresponding Diketone by Wild Type and Laboratory Evolved Alcohol Dehydrogenases. <i>ACS Catalysis</i> , 2018, 8, 7526-7538.	11.2	17
57	Evolutionary repurposing of a sulfatase: A new Michaelis complex leads to efficient transition state charge offset. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E7293-E7302.	7.1	34
58	Conformational dynamics and enzyme evolution. <i>Journal of the Royal Society Interface</i> , 2018, 15, 20180330.	3.4	140
59	Enhancing the Steroid Sulfatase Activity of the Arylsulfatase from <i>Pseudomonas aeruginosa</i> . <i>ACS Catalysis</i> , 2018, 8, 8902-8914.	11.2	10
60	Empirical Valence Bond Simulations of Organophosphate Hydrolysis: Theory and Practice. <i>Methods in Enzymology</i> , 2018, 607, 3-51.	1.0	0
61	Epoxide hydrolysis as a model system for understanding flux through a branched reaction scheme. <i>IUCr</i> , 2018, 5, 269-282.	2.2	5
62	The effect of magnesium ions on triphosphate hydrolysis. <i>Pure and Applied Chemistry</i> , 2017, 89, 715-727.	1.9	18
63	Capturing the Role of Explicit Solvent in the Dimerization of Ru ^V (bda) Water Oxidation Catalysts. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6962-6965.	13.8	42
64	CADEE: Computer-Aided Directed Evolution of Enzymes. <i>IUCr</i> , 2017, 4, 50-64.	2.2	46
65	Active Site Hydrophobicity and the Convergent Evolution of Paraoxonase Activity in Structurally Divergent Enzymes: The Case of Serum Paraoxonase 1. <i>Journal of the American Chemical Society</i> , 2017, 139, 1155-1167.	13.7	63
66	Extending the Nonbonded Cationic Dummy Model to Account for Ion-Induced Dipole Interactions. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5408-5414.	4.6	33
67	De novo active sites for resurrected Precambrian enzymes. <i>Nature Communications</i> , 2017, 8, 16113.	12.8	60
68	DNA Polymerase β Active Site Favors a Mutagenic Mismatch between the Enol Form of Deoxyguanosine Triphosphate Substrate and the Keto Form of Thymidine Template: A Free Energy Perturbation Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 7813-7822.	2.6	23
69	Capturing the Role of Explicit Solvent in the Dimerization of Ru ^V (bda) Water Oxidation Catalysts. <i>Angewandte Chemie</i> , 2017, 129, 7066-7069.	2.0	10
70	Shuffling Active Site Substate Populations Affects Catalytic Activity: The Case of Glucose Oxidase. <i>ACS Catalysis</i> , 2017, 7, 6188-6197.	11.2	46
71	Micelle Maker: An Online Tool for Generating Equilibrated Micelles as Direct Input for Molecular Dynamics Simulations. <i>ACS Omega</i> , 2017, 2, 4524-4530.	3.5	18
72	Simulating the reactions of substituted pyridinio-N-phosphonates with pyridine as a model for biological phosphoryl transfer. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7308-7316.	2.8	5

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73	Similar Active Sites and Mechanisms Do Not Lead to Cross-Promiscuity in Organophosphate Hydrolysis: Implications for Biotherapeutic Engineering. <i>Journal of the American Chemical Society</i> , 2017, 139, 17533-17546.	13.7	26
74	Enzyme Architecture: Modeling the Operation of a Hydrophobic Clamp in Catalysis by Triosephosphate Isomerase. <i>Journal of the American Chemical Society</i> , 2017, 139, 10514-10525.	13.7	38
75	Promiscuity and electrostatic flexibility in the alkaline phosphatase superfamily. <i>Current Opinion in Structural Biology</i> , 2016, 37, 14-21.	5.7	44
76	Conformational diversity and enantioconvergence in potato epoxide hydrolase 1. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 5639-5651.	2.8	23
77	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. <i>Biochemistry</i> , 2016, 55, 3061-3081.	2.5	32
78	Characterization of Mn(II) ion binding to the amyloid- β peptide in Alzheimer's disease. <i>Journal of Trace Elements in Medicine and Biology</i> , 2016, 38, 183-193.	3.0	60
79	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. <i>Journal of the American Chemical Society</i> , 2016, 138, 10664-10673.	13.7	46
80	Probing the mechanisms for the selectivity and promiscuity of methyl parathion hydrolase. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2016, 374, 20160150.	3.4	23
81	Linking coupled motions and entropic effects to the catalytic activity of 2-deoxyribose-5-phosphate aldolase (DERA). <i>Chemical Science</i> , 2016, 7, 1415-1421.	7.4	15
82	Conserved Motifs in Different Classes of GTPases Dictate their Specific Modes of Catalysis. <i>ACS Catalysis</i> , 2016, 6, 1737-1743.	11.2	24
83	Where are the female science professors? A personal perspective. <i>F1000Research</i> , 2016, 5, 1224.	1.6	6
84	Where are the female science professors? A personal perspective. <i>F1000Research</i> , 2016, 5, 1224.	1.6	4
85	Exceptionally large entropy contributions enable the high rates of GTP hydrolysis on the ribosome. <i>Scientific Reports</i> , 2015, 5, 15817.	3.3	31
86	Resolving Apparent Conflicts between Theoretical and Experimental Models of Phosphate Monoester Hydrolysis. <i>Journal of the American Chemical Society</i> , 2015, 137, 1081-1093.	13.7	92
87	Recent advances in QM/MM free energy calculations using reference potentials. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 954-965.	2.4	56
88	Catalytic Stimulation by Restrained Active-Site Floppiness—The Case of High Density Lipoprotein-Bound Serum Paraoxonase-1. <i>Journal of Molecular Biology</i> , 2015, 427, 1359-1374.	4.2	37
89	Cooperative Electrostatic Interactions Drive Functional Evolution in the Alkaline Phosphatase Superfamily. <i>Journal of the American Chemical Society</i> , 2015, 137, 9061-9076.	13.7	63
90	Development and Application of a Nonbonded Cu ²⁺ Model That Includes the Jahn–Teller Effect. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2657-2662.	4.6	64

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91	Understanding thio-effects in simple phosphoryl systems: role of solvent effects and nucleophile charge. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 5391-5398.	2.8	7
92	Expanding the Catalytic Triad in Epoxide Hydrolases and Related Enzymes. <i>ACS Catalysis</i> , 2015, 5, 5702-5713.	11.2	42
93	Modeling the mechanisms of biological GTP hydrolysis. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 80-90.	3.0	48
94	The Conformation of a Catalytic Loop Is Central to GTPase Activity on the Ribosome. <i>Biochemistry</i> , 2015, 54, 546-556.	2.5	30
95	How valence bond theory can help you understand your (bio)chemical reaction. <i>Chemical Society Reviews</i> , 2015, 44, 1037-1052.	38.1	49
96	Theoretical modelling of epigenetically modified DNA sequences. <i>F1000Research</i> , 2015, 4, 52.	1.6	10
97	Hypercompetition in biomedical research evaluation and its impact on young scientist careers. <i>International Microbiology</i> , 2015, 18, 253-61.	2.4	2
98	Understanding the structural and dynamic consequences of DNA epigenetic modifications: Computational insights into cytosine methylation and hydroxymethylation. <i>Epigenetics</i> , 2014, 9, 1604-1612.	2.7	47
99	Concerted or Stepwise: How Much Do Free-Energy Landscapes Tell Us about the Mechanisms of Elimination Reactions?. <i>Journal of Organic Chemistry</i> , 2014, 79, 1280-1288.	3.2	23
100	The Alkaline Hydrolysis of Sulfonate Esters: Challenges in Interpreting Experimental and Theoretical Data. <i>Journal of Organic Chemistry</i> , 2014, 79, 2816-2828.	3.2	26
101	Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B catalyzed metabolism of dopamine. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 3347-3355.	2.6	50
102	Challenges in computational studies of enzyme structure, function and dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 54, 62-79.	2.4	50
103	Editorial overview: Mechanisms: Chemical and computational probes of biological mechanism. <i>Current Opinion in Chemical Biology</i> , 2014, 21, viii-x.	6.1	2
104	Force Field Independent Metal Parameters Using a Nonbonded Dummy Model. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4351-4362.	2.6	148
105	Energetics of activation of GTP hydrolysis on the ribosome. <i>Nature Communications</i> , 2013, 4, 1733.	12.8	47
106	Cellular Polyamines Promote Amyloid-Beta (A β) Peptide Fibrillation and Modulate the Aggregation Pathways. <i>ACS Chemical Neuroscience</i> , 2013, 4, 454-462.	3.5	89
107	Why nature really chose phosphate. <i>Quarterly Reviews of Biophysics</i> , 2013, 46, 1-132.	5.7	290
108	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11160.	2.8	46

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109	Computational Protein Engineering: Bridging the Gap between Rational Design and Laboratory Evolution. <i>International Journal of Molecular Sciences</i> , 2012, 13, 12428-12460.	4.1	37
110	Base-Catalyzed Dehydration of 3-Substituted Benzene cis-1,2-Dihydrodiols: Stabilization of a Cyclohexadienide Anion Intermediate by Negative Aromatic Hyperconjugation. <i>Journal of the American Chemical Society</i> , 2012, 134, 14056-14069.	13.7	28
111	Computational Study of the pKa Values of Potential Catalytic Residues in the Active Site of Monoamine Oxidase B. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3864-3870.	5.3	67
112	Prechemistry barriers and checkpoints do not contribute to fidelity and catalysis as long as they are not rate limiting. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	29
113	Examining the promiscuous phosphatase activity of <i>Pseudomonas aeruginosa</i> arylsulfatase: A comparison to analogous phosphatases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1211-1226.	2.6	27
114	Catalytic promiscuity in <i>Pseudomonas aeruginosa</i> arylsulfatase as an example of chemistry-driven protein evolution. <i>FEBS Letters</i> , 2012, 586, 1622-1630.	2.8	29
115	Multiscale modeling of biological functions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10401.	2.8	54
116	Theoretical Comparison of <i>p</i> -Nitrophenyl Phosphate and Sulfate Hydrolysis in Aqueous Solution: Implications for Enzyme-Catalyzed Sulfuryl Transfer. <i>Journal of Organic Chemistry</i> , 2011, 76, 9228-9238.	3.2	39
117	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
118	Catalysis by dihydrofolate reductase and other enzymes arises from electrostatic preorganization, not conformational motions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 14115-14120.	7.1	176
119	The effect of leaving group on mechanistic preference in phosphate monoester hydrolysis. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5394.	2.8	12
120	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
121	The empirical valence bond model: theory and applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 30-45.	14.6	141
122	Examining the case for the effect of barrier compression on tunneling, vibrationally enhanced catalysis, catalytic entropy and related issues. <i>FEBS Letters</i> , 2010, 584, 2759-2766.	2.8	75
123	An analysis of all the relevant facts and arguments indicates that enzyme catalysis does <i>not</i> involve large contributions from nuclear tunneling. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 677-684.	1.9	33
124	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
125	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
126	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

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127	Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer. Faraday Discussions, 2010, 145, 281-299.	3.2	21
128	On Catalytic Preorganization in Oxyanion Holes: Highlighting the Problems with the Gas-Phase Modeling of Oxyanion Holes and Illustrating the Need for Complete Enzyme Models. Journal of Organic Chemistry, 2010, 75, 6391-6401.	3.2	47
129	The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. Faraday Discussions, 2010, 145, 71-106.	3.2	96
130	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, 17359-17364.	7.1	195
131	Are Mixed Explicit/Implicit Solvation Models Reliable for Studying Phosphate Hydrolysis? A Comparative Study of Continuum, Explicit and Mixed Solvation Models. ChemPhysChem, 2009, 10, 1125-1134.	2.1	81
132	On Unjustifiably Misrepresenting the EVB Approach While Simultaneously Adopting It. Journal of Physical Chemistry B, 2009, 113, 10905-10915.	2.6	31
133	A Computational Study of the Hydrolysis of dGTP Analogues with Halomethylene-Modified Leaving Groups in Solution: Implications for the Mechanism of DNA Polymerases. Biochemistry, 2009, 48, 5963-5971.	2.5	22
134	Progress in <i>Ab Initio</i> QM/MM Free-Energy Simulations of Electrostatic Energies in Proteins: Accelerated QM/MM Studies of p <i>K_a</i> , Redox Reactions and Solvation Free Energies. Journal of Physical Chemistry B, 2009, 113, 1253-1272.	2.6	267
135	On the Energetics of ATP Hydrolysis in Solution. Journal of Physical Chemistry B, 2009, 113, 15692-15698.	2.6	38
136	Associative Versus Dissociative Mechanisms of Phosphate Monoester Hydrolysis: On the Interpretation of Activation Entropies. ChemPhysChem, 2008, 9, 1767-1773.	2.1	85
137	On the Interpretation of the Observed Linear Free Energy Relationship in Phosphate Hydrolysis: A Thorough Computational Study of Phosphate Diester Hydrolysis in Solution. Biochemistry, 2008, 47, 3725-3735.	2.5	103
138	Dineopentyl Phosphate Hydrolysis: Evidence for Stepwise Water Attack. Journal of Organic Chemistry, 2008, 73, 6960-6969.	3.2	47
139	A molecular dynamics study of WPD-loop flexibility in PTP1B. Biochemical and Biophysical Research Communications, 2007, 356, 1011-1016.	2.1	65
140	The role of metal ions in phosphate ester hydrolysis. Organic and Biomolecular Chemistry, 2007, 5, 2098.	2.8	47
141	A targeted molecular dynamics study of WPD loop movement in PTP1B. Biochemical and Biophysical Research Communications, 2006, 345, 1161-1166.	2.1	45
142	A Structural View into the Complexity of Carbon Dioxide Fixation. ACS Central Science, 0, , .	11.3	0
143	Theoretical modelling of epigenetically modified DNA sequences. F1000Research, 0, , .	1.6	0
144	Late-term termination of pregnancy for medical reasons: when abortion isn't really by choice. EMBO Reports, 0, , .	4.5	1