Shina Caroline Lynn Kamerlin

List of Publications by Year
in descending order

143 papers	6,299 citations	61857 43 h-index	85405 71 g-index
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.	3.7	15
2	Adventures on the Routes of Protein Evolutionâ€"In Memoriam Dan Salah Tawfik (1955â€“2021). Journal of Molecular Biology, 2022, 434, 167462.	2.0	6
3	Essential Functional Interplay of the Catalytic Groups in Acid Phosphatase. ACS Catalysis, 2022, 12, 3357-3370.	5.5	5
4	5 suggestions to increase grant application success rates. EMBO Reports, 2022, 23, e54893.	2.0	1
5	Computational Advances in Protein Engineering and Enzyme Design. Journal of Physical Chemistry B, 2022, 126, 2449-2451.	1.2	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.	3.6	10
7	Journal Open Access and Plan S: Solving Problems or Shifting Burdens?. Development and Change, 2021, 52, 627-650.	2.0	7
8	Heme-binding enables allosteric modulation in an ancient TIM-barrel glycosidase. Nature Communications, 2021, 12, 380.	5.8	20
9	Loop Dynamics and Enzyme Catalysis in Protein Tyrosine Phosphatases. Journal of the American Chemical Society, 2021, 143, 3830-3845.	6.6	42
10	Single Residue on the WPD-Loop Affects the pH Dependency of Catalysis in Protein Tyrosine Phosphatases. Jacs Au, 2021, 1, 646-659.	3.6	14
11	Academic motherhood â€“ what happens when you can't make it happen?. EMBO Reports, 2021, 22, e52875.	2.0	4
12	Dan Salah Tawfik (1955â€2021)â€"A giant of protein evolution. EMBO Reports, 2021, 22, .	2.0	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.	1.2	6
14	Prenatal genetic screening and the evolving quest for â€œperfect babiesâ€• at what cost for genetic diversity?. EMBO Reports, 2021, 22, e53620.	2.0	1
15	How to write a successful postdoc application â€“ the PI perspective. EMBO Reports, 2021, 22, e54203.	2.0	1
16	Errors in DFT integration grids and their potential impact on chemical shift calculations. Magnetic Resonance in Chemistry, 2020, 58, 116-117.	1.1	3
17	Enzyme Evolution: An Epistatic Ratchet versus a Smooth Reversible Transition. Molecular Biology and Evolution, 2020, 37, 1133-1147.	3.5	26
18	G-Protein coupled receptors: structure and function in drug discovery. RSC Advances, 2020, 10, 36337-36348.	1.7	29

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19	The Role of Substrate-Coenzyme Crosstalk in Determining Turnover Rates in Rhodococcus ruber Alcohol Dehydrogenase. ACS Catalysis, 2020, 10, 9115-9128.	5.5	7
20	Ground-State Destabilization by Active-Site Hydrophobicity Controls the Selectivity of a Cofactor-Free Decarboxylase. Journal of the American Chemical Society, 2020, 142, 20216-20231.	6.6	6
21	Modeling the Role of a Flexible Loop and Active Site Side Chains in Hydride Transfer Catalyzed by Glycerol-3-phosphate Dehydrogenase. ACS Catalysis, 2020, 10, 11253-11267.	5.5	14
22	Enhancing ade novoenzyme activity by computationally-focused ultra-low-throughput screening. Chemical Science, 2020, 11, 6134-6148.	3.7	24
23	Harnessing Conformational Plasticity to Generate Designer Enzymes. Journal of the American Chemical Society, 2020, 142, 11324-11342.	6.6	70
24	Manipulating Conformational Dynamics To Repurpose Ancient Proteins for Modern Catalytic Functions. ACS Catalysis, 2020, 10, 4863-4870.	5.5	42
25	Managing Coronavirus Disease 2019 Spread With Voluntary Public Health Measures: Sweden as a Case Study for Pandemic Control. Clinical Infectious Diseases, 2020, 71, 3174-3181.	2.9	73
26	Female Faculty: Why So Few and Why Care?. Chemistry - A European Journal, 2020, 26, 8319-8323.	1.7	18
27	Short and simple sequences favored the emergence of N-helix phospho-ligand binding sites in the first enzymes. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5310-5318.	3.3	32
28	Recent Advances in Understanding Biological GTP Hydrolysis through Molecular Simulation. ACS Omega, 2020, 5, 4380-4385.	1.6	7
29	Modeling the Alkaline Hydrolysis of Diaryl Sulfate Diesters: A Mechanistic Study. Journal of Organic Chemistry, 2020, 85, 6489-6497.	1.7	8
30	When we increase diversity in academia, we all win. EMBO Reports, 2020, 21, e51994.	2.0	7
31	Open Access, Plan S, and researchers' needs. EMBO Reports, 2020, 21, e51568.	2.0	2
32	Open Access, Plan S, and researchersâ€™ needs. EMBO Reports, 2020, 21, e51568.	2.0	4
33	Computational physical organic chemistry using the empirical valence bond approach. Advances in Physical Organic Chemistry, 2019, 53, 69-104.	0.5	2
34	Bifunctional Substrate Activation via an Arginine Residue Drives Catalysis in Chalcone Isomerases. ACS Catalysis, 2019, 9, 8388-8396.	5.5	11
35	Uncovering the Role of Key Active-Site Side Chains in Catalysis: An Extended BrÃ¸nsted Relationship for Substrate Deprotonation Catalyzed by Wild-Type and Variants of Triosephosphate Isomerase. Journal of the American Chemical Society, 2019, 141, 16139-16150.	6.6	15
36	Structural consequence of the most frequently recurring cancer-associated substitution in DNA polymerase Îµ. Nature Communications, 2019, 10, 373.	5.8	40

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37	GTP Hydrolysis Without an Active Site Base: A Unifying Mechanism for Ras and Related GTPases. Journal of the American Chemical Society, 2019, 141, 10684-10701.	6.6	44
38	Chemical and Biochemical Approaches for the Synthesis of Substituted Dihydroxybutanones and Di- and Tri-Hydroxypentanones. Journal of Organic Chemistry, 2019, 84, 6982-6991.	1.7	2
39	Long Time-Scale Atomistic Simulations of the Structure and Dynamics of Transcription Factor-DNA Recognition. Journal of Physical Chemistry B, 2019, 123, 3576-3590.	1.2	21
40	Relative Binding Energies Predict Crystallographic Binding Modes of Ethionamide Booster Lead Compounds. Journal of Physical Chemistry Letters, 2019, 10, 2244-2249.	2.1	5
41	Higher-order epistasis shapes the fitness landscape of a xenobiotic-degrading enzyme. Nature Chemical Biology, 2019, 15, 1120-1128.	3.9	71
42	Human Glycerol 3-Phosphate Dehydrogenase: X-ray Crystal Structures That Guide the Interpretation of Mutagenesis Studies. Biochemistry, 2019, 58, 1061-1073.	1.2	15
43	In Silico-Directed Evolution Using CADEE. Methods in Molecular Biology, 2019, 1851, 381-415.	0.4	8
44	The role of ligand-gated conformational changes in enzyme catalysis. Biochemical Society Transactions, 2019, 47, 1449-1460.	1.6	12
45	Cryptic genetic variation shapes the adaptive evolutionary potential of enzymes. ELife, 2019, 8, .	2.8	35
46	Role of Ligand-Driven Conformational Changes in Enzyme Catalysis: Modeling the Reactivity of the Catalytic Cage of Triosephosphate Isomerase. Journal of the American Chemical Society, 2018, 140, 3854-3857.	6.6	27
47	Computer simulations of the catalytic mechanism of wild-type and mutant Î²-phosphoglucomutase. Organic and Biomolecular Chemistry, 2018, 16, 2060-2073.	1.5	11
48	Evolution of chalcone isomerase from a noncatalytic ancestor. Nature Chemical Biology, 2018, 14, 548-555.	3.9	113
49	Amyloid-Î² Peptide Interactions with Amphiphilic Surfactants: Electrostatic and Hydrophobic Effects. ACS Chemical Neuroscience, 2018, 9, 1680-1692.	1.7	51
50	Challenges and advances in the computational modeling of biological phosphate hydrolysis. Chemical Communications, 2018, 54, 3077-3089.	2.2	20
51	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. SoftwareX, 2018, 7, 388-395.	1.2	47
52	Empirical Valence Bond Simulations Suggest a Direct Hydride Transfer Mechanism for Human Diamine Oxidase. ACS Omega, 2018, 3, 3665-3674.	1.6	7
53	Cooperativity and flexibility in enzyme evolution. Current Opinion in Structural Biology, 2018, 48, 83-92.	2.6	81
54	The evolution of multiple active site configurations in a designed enzyme. Nature Communications, 2018, 9, 3900.	5.8	75

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55	Loop Motion in Triosephosphate Isomerase Is Not a Simple Open and Shut Case. Journal of the American Chemical Society, 2018, 140, 15889-15903.	6.6	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. ACS Catalysis, 2018, 8, 7526-7538.	5.5	17
57	Evolutionary repurposing of a sulfatase: A new Michaelis complex leads to efficient transition state charge offset. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7293-E7302.	3.3	34
58	Conformational dynamics and enzyme evolution. Journal of the Royal Society Interface, 2018, 15, 20180330.	1.5	140
59	Enhancing the Steroid Sulfatase Activity of the Arylsulfatase from Pseudomonas aeruginosa. ACS Catalysis, 2018, 8, 8902-8914.	5.5	10
60	Empirical Valence Bond Simulations of Organophosphate Hydrolysis: Theory and Practice. Methods in Enzymology, 2018, 607, 3-51.	0.4	0
61	Epoxide hydrolysis as a model system for understanding flux through a branched reaction scheme. IUCrJ, 2018, 5, 269-282.	1.0	5
62	The effect of magnesium ions on triphosphate hydrolysis. Pure and Applied Chemistry, 2017, 89, 715-727.	0.9	18
63	Capturing the Role of Explicit Solvent in the Dimerization of Ru^V(bda) Water Oxidation Catalysts. Angewandte Chemie - International Edition, 2017, 56, 6962-6965.	7.2	42
64	CADEE: Computer-Aided Directed Evolution of Enzymes. IUCrJ, 2017, 4, 50-64.	1.0	46
65	Active Site Hydrophobicity and the Convergent Evolution of Paraoxonase Activity in Structurally Divergent Enzymes: The Case of Serum Paraoxonase 1. Journal of the American Chemical Society, 2017, 139, 1155-1167.	6.6	63
66	Extending the Nonbonded Cationic Dummy Model to Account for Ion-Induced Dipole Interactions. Journal of Physical Chemistry Letters, 2017, 8, 5408-5414.	2.1	33
67	De novo active sites for resurrected Precambrian enzymes. Nature Communications, 2017, 8, 16113.	5.8	60
68	DNA Polymerase Î» Active Site Favors a Mutagenic Mispair between the Enol Form of Deoxyguanosine Triphosphate Substrate and the Keto Form of Thymidine Template: A Free Energy Perturbation Study. Journal of Physical Chemistry B, 2017, 121, 7813-7822.	1.2	23
69	Capturing the Role of Explicit Solvent in the Dimerization of Ru^V(bda) Water Oxidation Catalysts. Angewandte Chemie, 2017, 129, 7066-7069.	1.6	10
70	Shuffling Active Site Substate Populations Affects Catalytic Activity: The Case of Glucose Oxidase. ACS Catalysis, 2017, 7, 6188-6197.	5.5	46
71	Micelle Maker: An Online Tool for Generating Equilibrated Micelles as Direct Input for Molecular Dynamics Simulations. ACS Omega, 2017, 2, 4524-4530.	1.6	18
72	Simulating the reactions of substituted pyridinio-N-phosphonates with pyridine as a model for biological phosphoryl transfer. Organic and Biomolecular Chemistry, 2017, 15, 7308-7316.	1.5	5

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73	Similar Active Sites and Mechanisms Do Not Lead to Cross-Promiscuity in Organophosphate Hydrolysis: Implications for Biotherapeutic Engineering. Journal of the American Chemical Society, 2017, 139, 17533-17546.	6.6	26
74	Enzyme Architecture: Modeling the Operation of a Hydrophobic Clamp in Catalysis by Triosephosphate Isomerase. Journal of the American Chemical Society, 2017, 139, 10514-10525.	6.6	38
75	Promiscuity and electrostatic flexibility in the alkaline phosphatase superfamily. Current Opinion in Structural Biology, 2016, 37, 14-21.	2.6	44
76	Conformational diversity and enantioconvergence in potato epoxide hydrolase 1. Organic and Biomolecular Chemistry, 2016, 14, 5639-5651.	1.5	23
77	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. Biochemistry, 2016, 55, 3061-3081.	1.2	32
78	Characterization of Mn(II) ion binding to the amyloid-Î² peptide in Alzheimerâ¿¿s disease. Journal of Trace Elements in Medicine and Biology, 2016, 38, 183-193.	1.5	60
79	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. Journal of the American Chemical Society, 2016, 138, 10664-10673.	6.6	46
80	Probing the mechanisms for the selectivity and promiscuity of methyl parathion hydrolase. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160150.	1.6	23
81	Linking coupled motions and entropic effects to the catalytic activity of 2-deoxyribose-5-phosphate aldolase (DERA). Chemical Science, 2016, 7, 1415-1421.	3.7	15
82	Conserved Motifs in Different Classes of GTPases Dictate their Specific Modes of Catalysis. ACS Catalysis, 2016, 6, 1737-1743.	5.5	24
83	Where are the female science professors? A personal perspective. F1000Research, 2016, 5, 1224.	0.8	6
84	Where are the female science professors? A personal perspective. F1000Research, 2016, 5, 1224.	0.8	4
85	Exceptionally large entropy contributions enable the high rates of GTP hydrolysis on the ribosome. Scientific Reports, 2015, 5, 15817.	1.6	31
86	Resolving Apparent Conflicts between Theoretical and Experimental Models of Phosphate Monoester Hydrolysis. Journal of the American Chemical Society, 2015, 137, 1081-1093.	6.6	92
87	Recent advances in QM/MM free energy calculations using reference potentials. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 954-965.	1.1	56
88	Catalytic Stimulation by Restrained Active-Site Floppinessâ€"The Case of High Density Lipoprotein-Bound Serum Paraoxonase-1. Journal of Molecular Biology, 2015, 427, 1359-1374.	2.0	37
89	Cooperative Electrostatic Interactions Drive Functional Evolution in the Alkaline Phosphatase Superfamily. Journal of the American Chemical Society, 2015, 137, 9061-9076.	6.6	63
90	Development and Application of a Nonbonded Cu²⁺ Model That Includes the Jahnâ€"Teller Effect. Journal of Physical Chemistry Letters, 2015, 6, 2657-2662.	2.1	64

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91	Understanding thio-effects in simple phosphoryl systems: role of solvent effects and nucleophile charge. Organic and Biomolecular Chemistry, 2015, 13, 5391-5398.	1.5	7
92	Expanding the Catalytic Triad in Epoxide Hydrolases and Related Enzymes. ACS Catalysis, 2015, 5, 5702-5713.	5.5	42
93	Modeling the mechanisms of biological GTP hydrolysis. Archives of Biochemistry and Biophysics, 2015, 582, 80-90.	1.4	48
94	The Conformation of a Catalytic Loop Is Central to GTPase Activity on the Ribosome. Biochemistry, 2015, 54, 546-556.	1.2	30
95	How valence bond theory can help you understand your (bio)chemical reaction. Chemical Society Reviews, 2015, 44, 1037-1052.	18.7	49
96	Theoretical modelling of epigenetically modified DNA sequences. F1000Research, 2015, 4, 52.	0.8	10
97	Hypercompetition in biomedical research evaluation and its impact on young scientist careers. International Microbiology, 2015, 18, 253-61.	1.1	2
98	Understanding the structural and dynamic consequences of DNA epigenetic modifications: Computational insights into cytosine methylation and hydroxymethylation. Epigenetics, 2014, 9, 1604-1612.	1.3	47
99	Concerted or Stepwise: How Much Do Free-Energy Landscapes Tell Us about the Mechanisms of Elimination Reactions?. Journal of Organic Chemistry, 2014, 79, 1280-1288.	1.7	23
100	The Alkaline Hydrolysis of Sulfonate Esters: Challenges in Interpreting Experimental and Theoretical Data. Journal of Organic Chemistry, 2014, 79, 2816-2828.	1.7	26
101	Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B catalyzed metabolism of dopamine. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3347-3355.	1.5	50
102	Challenges in computational studies of enzyme structure, function and dynamics. Journal of Molecular Graphics and Modelling, 2014, 54, 62-79.	1.3	50
103	Editorial overview: Mechanisms: Chemical and computational probes of biological mechanism. Current Opinion in Chemical Biology, 2014, 21, viii-x.	2.8	2
104	Force Field Independent Metal Parameters Using a Nonbonded Dummy Model. Journal of Physical Chemistry B, 2014, 118, 4351-4362.	1.2	148
105	Energetics of activation of GTP hydrolysis on the ribosome. Nature Communications, 2013, 4, 1733.	5.8	47
106	Cellular Polyamines Promote Amyloid-Beta (AÎ²) Peptide Fibrillation and Modulate the Aggregation Pathways. ACS Chemical Neuroscience, 2013, 4, 454-462.	1.7	89
107	Why nature really chose phosphate. Quarterly Reviews of Biophysics, 2013, 46, 1-132.	2.4	290
108	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. Physical Chemistry Chemical Physics, 2013, 15, 11160.	1.3	46

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109	Computational Protein Engineering: Bridging the Gap between Rational Design and Laboratory Evolution. International Journal of Molecular Sciences, 2012, 13, 12428-12460.	1.8	37
110	Base-Catalyzed Dehydration of 3-Substituted Benzene cis-1,2-Dihydrodiols: Stabilization of a Cyclohexadienide Anion Intermediate by Negative Aromatic Hyperconjugation. Journal of the American Chemical Society, 2012, 134, 14056-14069.	6.6	28
111	Computational Study of the pKa Values of Potential Catalytic Residues in the Active Site of Monoamine Oxidase B. Journal of Chemical Theory and Computation, 2012, 8, 3864-3870.	2.3	67
112	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.	0.5	29
113	Examining the promiscuous phosphatase activity of Pseudomonas aeruginosa arylsulfatase: A comparison to analogous phosphatases. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1211-1226.	1.5	27
114	Catalytic promiscuity in Pseudomonas aeruginosa arylsulfatase as an example of chemistryâ€driven protein evolution. FEBS Letters, 2012, 586, 1622-1630.	1.3	29
115	Multiscale modeling of biological functions. Physical Chemistry Chemical Physics, 2011, 13, 10401.	1.3	54
116	Theoretical Comparison ofp-Nitrophenyl Phosphate and Sulfate Hydrolysis in Aqueous Solution: Implications for Enzyme-Catalyzed Sulfuryl Transfer. Journal of Organic Chemistry, 2011, 76, 9228-9238.	1.7	39
117	Paradynamics: An Effective and Reliable Model for Ab Initio QM/MM Free-Energy Calculations and Related Tasks. Journal of Physical Chemistry B, 2011, 115, 7950-7962.	1.2	101
118	Catalysis by dihydrofolate reductase and other enzymes arises from electrostatic preorganization, not conformational motions. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 14115-14120.	3.3	176
119	The effect of leaving group on mechanistic preference in phosphate monoester hydrolysis. Organic and Biomolecular Chemistry, 2011, 9, 5394.	1.5	12
120	Coarse-Grained (Multiscale) Simulations in Studies of Biophysical and Chemical Systems. Annual Review of Physical Chemistry, 2011, 62, 41-64.	4.8	176
121	The empirical valence bond model: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 30-45.	6.2	141
122	Examining the case for the effect of barrier compression on tunneling, vibrationally enhanced catalysis, catalytic entropy and related issues. FEBS Letters, 2010, 584, 2759-2766.	1.3	75
123	An analysis of all the relevant facts and arguments indicates that enzyme catalysis does not involve large contributions from nuclear tunneling. Journal of Physical Organic Chemistry, 2010, 23, 677-684.	0.9	33
124	At the dawn of the 21st century: Is dynamics the missing link for understanding enzyme catalysis?. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1339-1375.	1.5	399
125	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, 4075-4080.	3.3	81
126	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.	3.3	23

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127	Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer. Faraday Discussions, 2010, 145, 281-299.	1.6	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.	1.7	47
129	The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. Faraday Discussions, 2010, 145, 71-106.	1.6	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.	3.3	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.	1.0	81
132	On Unjustifiably Misrepresenting the EVB Approach While Simultaneously Adopting It. Journal of Physical Chemistry B, 2009, 113, 10905-10915.	1.2	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.	1.2	22
134	Progress in Ab Initio QM/MM Free-Energy Simulations of Electrostatic Energies in Proteins: Accelerated QM/MM Studies of pK_a, Redox Reactions and Solvation Free Energies. Journal of Physical Chemistry B, 2009, 113, 1253-1272.	1.2	267
135	On the Energetics of ATP Hydrolysis in Solution. Journal of Physical Chemistry B, 2009, 113, 15692-15698.	1.2	38
136	Associative Versus Dissociative Mechanisms of Phosphate Monoester Hydrolysis: On the Interpretation of Activation Entropies. ChemPhysChem, 2008, 9, 1767-1773.	1.0	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.	1.2	103
138	Dineopentyl Phosphate Hydrolysis: Evidence for Stepwise Water Attack. Journal of Organic Chemistry, 2008, 73, 6960-6969.	1.7	47
139	A molecular dynamics study of WPD-loop flexibility in PTP1B. Biochemical and Biophysical Research Communications, 2007, 356, 1011-1016.	1.0	65
140	The role of metal ions in phosphate ester hydrolysis. Organic and Biomolecular Chemistry, 2007, 5, 2098.	1.5	47
141	A targeted molecular dynamics study of WPD loop movement in PTP1B. Biochemical and Biophysical Research Communications, 2006, 345, 1161-1166.	1.0	45
142	A Structural View into the Complexity of Carbon Dioxide Fixation. ACS Central Science, 0, , .	5.3	0
143	Lateâ€termination of pregnancy for medical reasons: when abortion isnâ€™t really by choice. EMBO Reports, 0, , .	2.0	1