

Shina Caroline Lynn Kamerlin

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3923095/publications.pdf>

Version: 2024-02-01

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	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
2	Why nature really chose phosphate. Quarterly Reviews of Biophysics, 2013, 46, 1-132.	2.4	290
3	Progress in <i>Ab Initio</i> 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
4	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
5	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
6	Coarse-Grained (Multiscale) Simulations in Studies of Biophysical and Chemical Systems. Annual Review of Physical Chemistry, 2011, 62, 41-64.	4.8	176
7	Force Field Independent Metal Parameters Using a Nonbonded Dummy Model. Journal of Physical Chemistry B, 2014, 118, 4351-4362.	1.2	148
8	The empirical valence bond model: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 30-45.	6.2	141
9	Conformational dynamics and enzyme evolution. Journal of the Royal Society Interface, 2018, 15, 20180330.	1.5	140
10	Evolution of chalcone isomerase from a noncatalytic ancestor. Nature Chemical Biology, 2018, 14, 548-555.	3.9	113
11	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
12	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
13	The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. Faraday Discussions, 2010, 145, 71-106.	1.6	96
14	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
15	Cellular Polyamines Promote Amyloid-Beta (A β) Peptide Fibrillation and Modulate the Aggregation Pathways. ACS Chemical Neuroscience, 2013, 4, 454-462.	1.7	89
16	Associative Versus Dissociative Mechanisms of Phosphate Monoester Hydrolysis: On the Interpretation of Activation Entropies. ChemPhysChem, 2008, 9, 1767-1773.	1.0	85
17	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
18	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

#	ARTICLE	IF	CITATIONS
19	Cooperativity and flexibility in enzyme evolution. <i>Current Opinion in Structural Biology</i> , 2018, 48, 83-92.	2.6	81
20	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.	1.3	75
21	The evolution of multiple active site configurations in a designed enzyme. <i>Nature Communications</i> , 2018, 9, 3900.	5.8	75
22	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.	2.9	73
23	Higher-order epistasis shapes the fitness landscape of a xenobiotic-degrading enzyme. <i>Nature Chemical Biology</i> , 2019, 15, 1120-1128.	3.9	71
24	Harnessing Conformational Plasticity to Generate Designer Enzymes. <i>Journal of the American Chemical Society</i> , 2020, 142, 11324-11342.	6.6	70
25	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.	2.3	67
26	A molecular dynamics study of WPD-loop flexibility in PTP1B. <i>Biochemical and Biophysical Research Communications</i> , 2007, 356, 1011-1016.	1.0	65
27	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.	2.1	64
28	Cooperative Electrostatic Interactions Drive Functional Evolution in the Alkaline Phosphatase Superfamily. <i>Journal of the American Chemical Society</i> , 2015, 137, 9061-9076.	6.6	63
29	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.	6.6	63
30	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.	6.6	63
31	Characterization of Mn(II) ion binding to the amyloid- β^2 peptide in Alzheimer's disease. <i>Journal of Trace Elements in Medicine and Biology</i> , 2016, 38, 183-193.	1.5	60
32	De novo active sites for resurrected Precambrian enzymes. <i>Nature Communications</i> , 2017, 8, 16113.	5.8	60
33	Recent advances in QM/MM free energy calculations using reference potentials. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 954-965.	1.1	56
34	Multiscale modeling of biological functions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10401.	1.3	54
35	Amyloid- β^2 Peptide Interactions with Amphiphilic Surfactants: Electrostatic and Hydrophobic Effects. <i>ACS Chemical Neuroscience</i> , 2018, 9, 1680-1692.	1.7	51
36	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.	1.5	50

#	ARTICLE	IF	CITATIONS
37	Challenges in computational studies of enzyme structure, function and dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 54, 62-79.	1.3	50
38	How valence bond theory can help you understand your (bio)chemical reaction. <i>Chemical Society Reviews</i> , 2015, 44, 1037-1052.	18.7	49
39	Modeling the mechanisms of biological GTP hydrolysis. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 80-90.	1.4	48
40	The role of metal ions in phosphate ester hydrolysis. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 2098.	1.5	47
41	Dineopentyl Phosphate Hydrolysis: Evidence for Stepwise Water Attack. <i>Journal of Organic Chemistry</i> , 2008, 73, 6960-6969.	1.7	47
42	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. <i>Journal of Organic Chemistry</i> , 2010, 75, 6391-6401.	1.7	47
43	Energetics of activation of GTP hydrolysis on the ribosome. <i>Nature Communications</i> , 2013, 4, 1733.	5.8	47
44	Understanding the structural and dynamic consequences of DNA epigenetic modifications: Computational insights into cytosine methylation and hydroxymethylation. <i>Epigenetics</i> , 2014, 9, 1604-1612.	1.3	47
45	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. <i>SoftwareX</i> , 2018, 7, 388-395.	1.2	47
46	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11160.	1.3	46
47	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. <i>Journal of the American Chemical Society</i> , 2016, 138, 10664-10673.	6.6	46
48	<i>CADEE</i> : Computer-Aided Directed Evolution of Enzymes. <i>IUCr</i> , 2017, 4, 50-64.	1.0	46
49	Shuffling Active Site Substate Populations Affects Catalytic Activity: The Case of Glucose Oxidase. <i>ACS Catalysis</i> , 2017, 7, 6188-6197.	5.5	46
50	A targeted molecular dynamics study of WPD loop movement in PTP1B. <i>Biochemical and Biophysical Research Communications</i> , 2006, 345, 1161-1166.	1.0	45
51	Promiscuity and electrostatic flexibility in the alkaline phosphatase superfamily. <i>Current Opinion in Structural Biology</i> , 2016, 37, 14-21.	2.6	44
52	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.	6.6	44
53	Expanding the Catalytic Triad in Epoxide Hydrolases and Related Enzymes. <i>ACS Catalysis</i> , 2015, 5, 5702-5713.	5.5	42
54	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.	7.2	42

#	ARTICLE	IF	CITATIONS
55	Manipulating Conformational Dynamics To Repurpose Ancient Proteins for Modern Catalytic Functions. <i>ACS Catalysis</i> , 2020, 10, 4863-4870.	5.5	42
56	Loop Dynamics and Enzyme Catalysis in Protein Tyrosine Phosphatases. <i>Journal of the American Chemical Society</i> , 2021, 143, 3830-3845.	6.6	42
57	Structural consequence of the most frequently recurring cancer-associated substitution in DNA polymerase β . <i>Nature Communications</i> , 2019, 10, 373.	5.8	40
58	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.	1.7	39
59	On the Energetics of ATP Hydrolysis in Solution. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15692-15698.	1.2	38
60	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.	6.6	38
61	Computational Protein Engineering: Bridging the Gap between Rational Design and Laboratory Evolution. <i>International Journal of Molecular Sciences</i> , 2012, 13, 12428-12460.	1.8	37
62	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.	2.0	37
63	Cryptic genetic variation shapes the adaptive evolutionary potential of enzymes. <i>ELife</i> , 2019, 8, .	2.8	35
64	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.	3.3	34
65	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.	0.9	33
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.	2.1	33
67	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. <i>Biochemistry</i> , 2016, 55, 3061-3081.	1.2	32
68	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.	3.3	32
69	On Unjustifiably Misrepresenting the EVB Approach While Simultaneously Adopting It. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10905-10915.	1.2	31
70	Exceptionally large entropy contributions enable the high rates of GTP hydrolysis on the ribosome. <i>Scientific Reports</i> , 2015, 5, 15817.	1.6	31
71	The Conformation of a Catalytic Loop Is Central to GTPase Activity on the Ribosome. <i>Biochemistry</i> , 2015, 54, 546-556.	1.2	30
72	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.	0.5	29

#	ARTICLE	IF	CITATIONS
73	Catalytic promiscuity in <i>Pseudomonas aeruginosa</i> arylsulfatase as an example of chemistry-driven protein evolution. <i>FEBS Letters</i> , 2012, 586, 1622-1630.	1.3	29
74	G-Protein coupled receptors: structure and function in drug discovery. <i>RSC Advances</i> , 2020, 10, 36337-36348.	1.7	29
75	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.	6.6	28
76	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.	1.5	27
77	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.	6.6	27
78	The Alkaline Hydrolysis of Sulfonate Esters: Challenges in Interpreting Experimental and Theoretical Data. <i>Journal of Organic Chemistry</i> , 2014, 79, 2816-2828.	1.7	26
79	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.	6.6	26
80	Enzyme Evolution: An Epistatic Ratchet versus a Smooth Reversible Transition. <i>Molecular Biology and Evolution</i> , 2020, 37, 1133-1147.	3.5	26
81	Conserved Motifs in Different Classes of GTPases Dictate their Specific Modes of Catalysis. <i>ACS Catalysis</i> , 2016, 6, 1737-1743.	5.5	24
82	Enhancing a <i>de novo</i> enzyme activity by computationally-focused ultra-low-throughput screening. <i>Chemical Science</i> , 2020, 11, 6134-6148.	3.7	24
83	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.	3.3	23
84	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.	1.7	23
85	Conformational diversity and enantioconvergence in potato epoxide hydrolase 1. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 5639-5651.	1.5	23
86	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.	1.6	23
87	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.	1.2	23
88	A Computational Study of the Hydrolysis of dGTP Analogues with Halomethylene-Modified Leaving Groups in Solution: Implications for the Mechanism of DNA Polymerases. <i>Biochemistry</i> , 2009, 48, 5963-5971.	1.2	22
89	Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer. <i>Faraday Discussions</i> , 2010, 145, 281-299.	1.6	21
90	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.	1.2	21

#	ARTICLE	IF	CITATIONS
91	Challenges and advances in the computational modeling of biological phosphate hydrolysis. <i>Chemical Communications</i> , 2018, 54, 3077-3089.	2.2	20
92	Heme-binding enables allosteric modulation in an ancient TIM-barrel glycosidase. <i>Nature Communications</i> , 2021, 12, 380.	5.8	20
93	The effect of magnesium ions on triphosphate hydrolysis. <i>Pure and Applied Chemistry</i> , 2017, 89, 715-727.	0.9	18
94	Micelle Maker: An Online Tool for Generating Equilibrated Micelles as Direct Input for Molecular Dynamics Simulations. <i>ACS Omega</i> , 2017, 2, 4524-4530.	1.6	18
95	Female Faculty: Why So Few and Why Care?. <i>Chemistry - A European Journal</i> , 2020, 26, 8319-8323.	1.7	18
96	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.	5.5	17
97	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.	3.7	15
98	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.	6.6	15
99	Human Glycerol 3-Phosphate Dehydrogenase: X-ray Crystal Structures That Guide the Interpretation of Mutagenesis Studies. <i>Biochemistry</i> , 2019, 58, 1061-1073.	1.2	15
100	Exploiting enzyme evolution for computational protein design. <i>Trends in Biochemical Sciences</i> , 2022, 47, 375-389.	3.7	15
101	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.	5.5	14
102	Single Residue on the WPD-Loop Affects the pH Dependency of Catalysis in Protein Tyrosine Phosphatases. <i>Jacs Au</i> , 2021, 1, 646-659.	3.6	14
103	The effect of leaving group on mechanistic preference in phosphate monoester hydrolysis. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5394.	1.5	12
104	The role of ligand-gated conformational changes in enzyme catalysis. <i>Biochemical Society Transactions</i> , 2019, 47, 1449-1460.	1.6	12
105	Computer simulations of the catalytic mechanism of wild-type and mutant $\hat{1}^2$ -phosphoglucomutase. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 2060-2073.	1.5	11
106	Bifunctional Substrate Activation via an Arginine Residue Drives Catalysis in Chalcone Isomerases. <i>ACS Catalysis</i> , 2019, 9, 8388-8396.	5.5	11
107	Capturing the Role of Explicit Solvent in the Dimerization of Ru ^V (bda) Water Oxidation Catalysts. <i>Angewandte Chemie</i> , 2017, 129, 7066-7069.	1.6	10
108	Enhancing the Steroid Sulfatase Activity of the Arylsulfatase from <i>Pseudomonas aeruginosa</i> . <i>ACS Catalysis</i> , 2018, 8, 8902-8914.	5.5	10

#	ARTICLE	IF	CITATIONS
109	Theoretical modelling of epigenetically modified DNA sequences. <i>F1000Research</i> , 2015, 4, 52.	0.8	10
110	Complex Loop Dynamics Underpin Activity, Specificity, and Evolvability in the β 8 Barrel Enzymes of Histidine and Tryptophan Biosynthesis. <i>Jacs Au</i> , 2022, 2, 943-960.	3.6	10
111	In Silico-Directed Evolution Using CADEE. <i>Methods in Molecular Biology</i> , 2019, 1851, 381-415.	0.4	8
112	Modeling the Alkaline Hydrolysis of Diaryl Sulfate Diesters: A Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2020, 85, 6489-6497.	1.7	8
113	Computational Advances in Protein Engineering and Enzyme Design. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2449-2451.	1.2	8
114	Understanding thio-effects in simple phosphoryl systems: role of solvent effects and nucleophile charge. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 5391-5398.	1.5	7
115	Empirical Valence Bond Simulations Suggest a Direct Hydride Transfer Mechanism for Human Diamine Oxidase. <i>ACS Omega</i> , 2018, 3, 3665-3674.	1.6	7
116	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.	5.5	7
117	Recent Advances in Understanding Biological GTP Hydrolysis through Molecular Simulation. <i>ACS Omega</i> , 2020, 5, 4380-4385.	1.6	7
118	Journal Open Access and Plan S: Solving Problems or Shifting Burdens?. <i>Development and Change</i> , 2021, 52, 627-650.	2.0	7
119	When we increase diversity in academia, we all win. <i>EMBO Reports</i> , 2020, 21, e51994.	2.0	7
120	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.	6.6	6
121	The N-terminal Helix-Turn-Helix Motif of Transcription Factors MarA and Rob Drives DNA Recognition. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6791-6806.	1.2	6
122	Where are the female science professors? A personal perspective. <i>F1000Research</i> , 2016, 5, 1224.	0.8	6
123	Adventures on the Routes of Protein Evolution—In Memoriam Dan Salah Tawfik (1955–2021). <i>Journal of Molecular Biology</i> , 2022, 434, 167462.	2.0	6
124	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.	1.5	5
125	Relative Binding Energies Predict Crystallographic Binding Modes of Ethionamide Booster Lead Compounds. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2244-2249.	2.1	5
126	Epoxide hydrolysis as a model system for understanding flux through a branched reaction scheme. <i>IUCr</i> , 2018, 5, 269-282.	1.0	5

#	ARTICLE	IF	CITATIONS
127	Essential Functional Interplay of the Catalytic Groups in Acid Phosphatase. ACS Catalysis, 2022, 12, 3357-3370.	5.5	5
128	Academic motherhood â€“ what happens when you can't make it happen?. EMBO Reports, 2021, 22, e52875.	2.0	4
129	Where are the female science professors? A personal perspective. F1000Research, 2016, 5, 1224.	0.8	4
130	Open Access, Plan S, and researchersâ€™ needs. EMBO Reports, 2020, 21, e51568.	2.0	4
131	Errors in DFT integration grids and their potential impact on chemical shift calculations. Magnetic Resonance in Chemistry, 2020, 58, 116-117.	1.1	3
132	Editorial overview: Mechanisms: Chemical and computational probes of biological mechanism. Current Opinion in Chemical Biology, 2014, 21, viii-x.	2.8	2
133	Computational physical organic chemistry using the empirical valence bond approach. Advances in Physical Organic Chemistry, 2019, 53, 69-104.	0.5	2
134	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
135	Dan Salah Tawfik (1955â€“2021)â€™A giant of protein evolution. EMBO Reports, 2021, 22, .	2.0	2
136	Open Access, Plan S, and researchers' needs. EMBO Reports, 2020, 21, e51568.	2.0	2
137	Hypercompetition in biomedical research evaluation and its impact on young scientist careers. International Microbiology, 2015, 18, 253-61.	1.1	2
138	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
139	How to write a successful postdoc application â€“ the PI perspective. EMBO Reports, 2021, 22, e54203.	2.0	1
140	5 suggestions to increase grant application success rates. EMBO Reports, 2022, 23, e54893.	2.0	1
141	Lateâ€™termination of pregnancy for medical reasons: when abortion isnâ€™t <i>really</i> by choice. EMBO Reports, 0, , .	2.0	1
142	Empirical Valence Bond Simulations of Organophosphate Hydrolysis: Theory and Practice. Methods in Enzymology, 2018, 607, 3-51.	0.4	0
143	A Structural View into the Complexity of Carbon Dioxide Fixation. ACS Central Science, 0, , .	5.3	0