Shina Caroline Lynn Kamerlin

List of Publications by Year
in descending order

144 papers	6,299 citations	61984 43 h-index	85541 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.	2.6	399
2	Why nature really chose phosphate. Quarterly Reviews of Biophysics, 2013, 46, 1-132.	5.7	290
3	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.	2.6	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.	7.1	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.	7.1	176
6	Coarse-Grained (Multiscale) Simulations in Studies of Biophysical and Chemical Systems. Annual Review of Physical Chemistry, 2011, 62, 41-64.	10.8	176
7	Force Field Independent Metal Parameters Using a Nonbonded Dummy Model. Journal of Physical Chemistry B, 2014, 118, 4351-4362.	2.6	148
8	The empirical valence bond model: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 30-45.	14.6	141
9	Conformational dynamics and enzyme evolution. Journal of the Royal Society Interface, 2018, 15, 20180330.	3.4	140
10	Evolution of chalcone isomerase from a noncatalytic ancestor. Nature Chemical Biology, 2018, 14, 548-555.	8.0	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.	2.5	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.	2.6	101
13	The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. Faraday Discussions, 2010, 145, 71-106.	3.2	96
14	Resolving Apparent Conflicts between Theoretical and Experimental Models of Phosphate Monoester Hydrolysis. Journal of the American Chemical Society, 2015, 137, 1081-1093.	13.7	92
15	Cellular Polyamines Promote Amyloid-Beta (AÎ²) Peptide Fibrillation and Modulate the Aggregation Pathways. ACS Chemical Neuroscience, 2013, 4, 454-462.	3.5	89
16	Associative Versus Dissociative Mechanisms of Phosphate Monoester Hydrolysis: On the Interpretation of Activation Entropies. ChemPhysChem, 2008, 9, 1767-1773.	2.1	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.	2.1	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.	7.1	81

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19	Cooperativity and flexibility in enzyme evolution. Current Opinion in Structural Biology, 2018, 48, 83-92.	5.7	81
20	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.	2.8	75
21	The evolution of multiple active site configurations in a designed enzyme. Nature Communications, 2018, 9, 3900.	12.8	75
22	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.	5.8	73
23	Higher-order epistasis shapes the fitness landscape of a xenobiotic-degrading enzyme. Nature Chemical Biology, 2019, 15, 1120-1128.	8.0	71
24	Harnessing Conformational Plasticity to Generate Designer Enzymes. Journal of the American Chemical Society, 2020, 142, 11324-11342.	13.7	70
25	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.	5.3	67
26	A molecular dynamics study of WPD-loop flexibility in PTP1B. Biochemical and Biophysical Research Communications, 2007, 356, 1011-1016.	2.1	65
27	Development and Application of a Nonbonded Cu²⁺ Model That Includes the Jahnâ€“Teller Effect. Journal of Physical Chemistry Letters, 2015, 6, 2657-2662.	4.6	64
28	Cooperative Electrostatic Interactions Drive Functional Evolution in the Alkaline Phosphatase Superfamily. Journal of the American Chemical Society, 2015, 137, 9061-9076.	13.7	63
29	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.	13.7	63
30	Loop Motion in Triosephosphate Isomerase Is Not a Simple Open and Shut Case. Journal of the American Chemical Society, 2018, 140, 15889-15903.	13.7	63
31	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.	3.0	60
32	De novo active sites for resurrected Precambrian enzymes. Nature Communications, 2017, 8, 16113.	12.8	60
33	Recent advances in QM/MM free energy calculations using reference potentials. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 954-965.	2.4	56
34	Multiscale modeling of biological functions. Physical Chemistry Chemical Physics, 2011, 13, 10401.	2.8	54
35	Amyloid-Î² Peptide Interactions with Amphiphilic Surfactants: Electrostatic and Hydrophobic Effects. ACS Chemical Neuroscience, 2018, 9, 1680-1692.	3.5	51
36	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.	2.6	50

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37	Challenges in computational studies of enzyme structure, function and dynamics. Journal of Molecular Graphics and Modelling, 2014, 54, 62-79.	2.4	50
38	How valence bond theory can help you understand your (bio)chemical reaction. Chemical Society Reviews, 2015, 44, 1037-1052.	38.1	49
39	Modeling the mechanisms of biological GTP hydrolysis. Archives of Biochemistry and Biophysics, 2015, 582, 80-90.	3.0	48
40	The role of metal ions in phosphate ester hydrolysis. Organic and Biomolecular Chemistry, 2007, 5, 2098.	2.8	47
41	Dineopentyl Phosphate Hydrolysis: Evidence for Stepwise Water Attack. Journal of Organic Chemistry, 2008, 73, 6960-6969.	3.2	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. Journal of Organic Chemistry, 2010, 75, 6391-6401.	3.2	47
43	Energetics of activation of GTP hydrolysis on the ribosome. Nature Communications, 2013, 4, 1733.	12.8	47
44	Understanding the structural and dynamic consequences of DNA epigenetic modifications: Computational insights into cytosine methylation and hydroxymethylation. Epigenetics, 2014, 9, 1604-1612.	2.7	47
45	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. SoftwareX, 2018, 7, 388-395.	2.6	47
46	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. Physical Chemistry Chemical Physics, 2013, 15, 11160.	2.8	46
47	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. Journal of the American Chemical Society, 2016, 138, 10664-10673.	13.7	46
48	CADEE: Computer-Aided Directed Evolution of Enzymes. IUCrJ, 2017, 4, 50-64.	2.2	46
49	Shuffling Active Site Substate Populations Affects Catalytic Activity: The Case of Glucose Oxidase. ACS Catalysis, 2017, 7, 6188-6197.	11.2	46
50	A targeted molecular dynamics study of WPD loop movement in PTP1B. Biochemical and Biophysical Research Communications, 2006, 345, 1161-1166.	2.1	45
51	Promiscuity and electrostatic flexibility in the alkaline phosphatase superfamily. Current Opinion in Structural Biology, 2016, 37, 14-21.	5.7	44
52	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.	13.7	44
53	Expanding the Catalytic Triad in Epoxide Hydrolases and Related Enzymes. ACS Catalysis, 2015, 5, 5702-5713.	11.2	42
54	Capturing the Role of Explicit Solvent in the Dimerization of Ru^V(bda) Water Oxidation Catalysts. Angewandte Chemie - International Edition, 2017, 56, 6962-6965.	13.8	42

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55	Manipulating Conformational Dynamics To Repurpose Ancient Proteins for Modern Catalytic Functions. ACS Catalysis, 2020, 10, 4863-4870.	11.2	42
56	Loop Dynamics and Enzyme Catalysis in Protein Tyrosine Phosphatases. Journal of the American Chemical Society, 2021, 143, 3830-3845.	13.7	42
57	Structural consequence of the most frequently recurring cancer-associated substitution in DNA polymerase Îµ. Nature Communications, 2019, 10, 373.	12.8	40
58	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.	3.2	39
59	On the Energetics of ATP Hydrolysis in Solution. Journal of Physical Chemistry B, 2009, 113, 15692-15698.	2.6	38
60	Enzyme Architecture: Modeling the Operation of a Hydrophobic Clamp in Catalysis by Triosephosphate Isomerase. Journal of the American Chemical Society, 2017, 139, 10514-10525.	13.7	38
61	Computational Protein Engineering: Bridging the Gap between Rational Design and Laboratory Evolution. International Journal of Molecular Sciences, 2012, 13, 12428-12460.	4.1	37
62	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.	4.2	37
63	Cryptic genetic variation shapes the adaptive evolutionary potential of enzymes. ELife, 2019, 8, .	6.0	35
64	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.	7.1	34
65	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.	1.9	33
66	Extending the Nonbonded Cationic Dummy Model to Account for Ion-Induced Dipole Interactions. Journal of Physical Chemistry Letters, 2017, 8, 5408-5414.	4.6	33
67	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. Biochemistry, 2016, 55, 3061-3081.	2.5	32
68	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.	7.1	32
69	On Unjustifiably Misrepresenting the EVB Approach While Simultaneously Adopting It. Journal of Physical Chemistry B, 2009, 113, 10905-10915.	2.6	31
70	Exceptionally large entropy contributions enable the high rates of GTP hydrolysis on the ribosome. Scientific Reports, 2015, 5, 15817.	3.3	31
71	The Conformation of a Catalytic Loop Is Central to GTPase Activity on the Ribosome. Biochemistry, 2015, 54, 546-556.	2.5	30
72	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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73	Catalytic promiscuity in Pseudomonas aeruginosa arylsulfatase as an example of chemistryâ€driven protein evolution. FEBS Letters, 2012, 586, 1622-1630.	2.8	29
74	G-Protein coupled receptors: structure and function in drug discovery. RSC Advances, 2020, 10, 36337-36348.	3.6	29
75	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.	13.7	28
76	Examining the promiscuous phosphatase activity of Pseudomonas aeruginosa arylsulfatase: A comparison to analogous phosphatases. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1211-1226.	2.6	27
77	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.	13.7	27
78	The Alkaline Hydrolysis of Sulfonate Esters: Challenges in Interpreting Experimental and Theoretical Data. Journal of Organic Chemistry, 2014, 79, 2816-2828.	3.2	26
79	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.	13.7	26
80	Enzyme Evolution: An Epistatic Ratchet versus a Smooth Reversible Transition. Molecular Biology and Evolution, 2020, 37, 1133-1147.	8.9	26
81	Conserved Motifs in Different Classes of GTPases Dictate their Specific Modes of Catalysis. ACS Catalysis, 2016, 6, 1737-1743.	11.2	24
82	Enhancing ade novoenzyme activity by computationally-focused ultra-low-throughput screening. Chemical Science, 2020, 11, 6134-6148.	7.4	24
83	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.	7.1	23
84	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.	3.2	23
85	Conformational diversity and enantioconvergence in potato epoxide hydrolase 1. Organic and Biomolecular Chemistry, 2016, 14, 5639-5651.	2.8	23
86	Probing the mechanisms for the selectivity and promiscuity of methyl parathion hydrolase. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160150.	3.4	23
87	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.	2.6	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. Biochemistry, 2009, 48, 5963-5971.	2.5	22
89	Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer. Faraday Discussions, 2010, 145, 281-299.	3.2	21
90	Long Time-Scale Atomistic Simulations of the Structure and Dynamics of Transcription Factor-DNA Recognition. Journal of Physical Chemistry B, 2019, 123, 3576-3590.	2.6	21

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91	Challenges and advances in the computational modeling of biological phosphate hydrolysis. Chemical Communications, 2018, 54, 3077-3089.	4.1	20
92	Heme-binding enables allosteric modulation in an ancient TIM-barrel glycosidase. Nature Communications, 2021, 12, 380.	12.8	20
93	The effect of magnesium ions on triphosphate hydrolysis. Pure and Applied Chemistry, 2017, 89, 715-727.	1.9	18
94	Micelle Maker: An Online Tool for Generating Equilibrated Micelles as Direct Input for Molecular Dynamics Simulations. ACS Omega, 2017, 2, 4524-4530.	3.5	18
95	Female Faculty: Why So Few and Why Care?. Chemistry - A European Journal, 2020, 26, 8319-8323.	3.3	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. ACS Catalysis, 2018, 8, 7526-7538.	11.2	17
97	Linking coupled motions and entropic effects to the catalytic activity of 2-deoxyribose-5-phosphate aldolase (DERA). Chemical Science, 2016, 7, 1415-1421.	7.4	15
98	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.	13.7	15
99	Human Glycerol 3-Phosphate Dehydrogenase: X-ray Crystal Structures That Guide the Interpretation of Mutagenesis Studies. Biochemistry, 2019, 58, 1061-1073.	2.5	15
100	Exploiting enzyme evolution for computational protein design. Trends in Biochemical Sciences, 2022, 47, 375-389.	7.5	15
101	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.	11.2	14
102	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
103	The effect of leaving group on mechanistic preference in phosphate monoester hydrolysis. Organic and Biomolecular Chemistry, 2011, 9, 5394.	2.8	12
104	The role of ligand-gated conformational changes in enzyme catalysis. Biochemical Society Transactions, 2019, 47, 1449-1460.	3.4	12
105	Computer simulations of the catalytic mechanism of wild-type and mutant Î²-phosphoglucomutase. Organic and Biomolecular Chemistry, 2018, 16, 2060-2073.	2.8	11
106	Bifunctional Substrate Activation via an Arginine Residue Drives Catalysis in Chalcone Isomerases. ACS Catalysis, 2019, 9, 8388-8396.	11.2	11
107	Capturing the Role of Explicit Solvent in the Dimerization of Ru^V(bda) Water Oxidation Catalysts. Angewandte Chemie, 2017, 129, 7066-7069.	2.0	10
108	Enhancing the Steroid Sulfatase Activity of the Arylsulfatase from Pseudomonas aeruginosa. ACS Catalysis, 2018, 8, 8902-8914.	11.2	10

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109	Theoretical modelling of epigenetically modified DNA sequences. F1000Research, 2015, 4, 52.	1.6	10
110	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
111	In Silico-Directed Evolution Using CADEE. Methods in Molecular Biology, 2019, 1851, 381-415.	0.9	8
112	Modeling the Alkaline Hydrolysis of Diaryl Sulfate Diesters: A Mechanistic Study. Journal of Organic Chemistry, 2020, 85, 6489-6497.	3.2	8
113	Computational Advances in Protein Engineering and Enzyme Design. Journal of Physical Chemistry B, 2022, 126, 2449-2451.	2.6	8
114	Understanding thio-effects in simple phosphoryl systems: role of solvent effects and nucleophile charge. Organic and Biomolecular Chemistry, 2015, 13, 5391-5398.	2.8	7
115	Empirical Valence Bond Simulations Suggest a Direct Hydride Transfer Mechanism for Human Diamine Oxidase. ACS Omega, 2018, 3, 3665-3674.	3.5	7
116	The Role of Substrate-Coenzyme Crosstalk in Determining Turnover Rates in Rhodococcus ruber Alcohol Dehydrogenase. ACS Catalysis, 2020, 10, 9115-9128.	11.2	7
117	Recent Advances in Understanding Biological GTP Hydrolysis through Molecular Simulation. ACS Omega, 2020, 5, 4380-4385.	3.5	7
118	Journal Open Access and Plan S: Solving Problems or Shifting Burdens?. Development and Change, 2021, 52, 627-650.	3.3	7
119	When we increase diversity in academia, we all win. EMBO Reports, 2020, 21, e51994.	4.5	7
120	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.	13.7	6
121	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
122	Where are the female science professors? A personal perspective. F1000Research, 2016, 5, 1224.	1.6	6
123	Adventures on the Routes of Protein Evolutionâ€"In Memoriam Dan Salah Tawfik (1955â€“2021). Journal of Molecular Biology, 2022, 434, 167462.	4.2	6
124	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.	2.8	5
125	Relative Binding Energies Predict Crystallographic Binding Modes of Ethionamide Booster Lead Compounds. Journal of Physical Chemistry Letters, 2019, 10, 2244-2249.	4.6	5
126	Epoxide hydrolysis as a model system for understanding flux through a branched reaction scheme. IUCrJ, 2018, 5, 269-282.	2.2	5

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127	Essential Functional Interplay of the Catalytic Groups in Acid Phosphatase. ACS Catalysis, 2022, 12, 3357-3370.	11.2	5
128	Academic motherhood â€“ what happens when you can't make it happen?. EMBO Reports, 2021, 22, e52875.	4.5	4
129	Where are the female science professors? A personal perspective. F1000Research, 2016, 5, 1224.	1.6	4
130	Open Access, Plan S, and researchersâ€™ needs. EMBO Reports, 2020, 21, e51568.	4.5	4
131	Errors in DFT integration grids and their potential impact on chemical shift calculations. Magnetic Resonance in Chemistry, 2020, 58, 116-117.	1.9	3
132	Editorial overview: Mechanisms: Chemical and computational probes of biological mechanism. Current Opinion in Chemical Biology, 2014, 21, viii-x.	6.1	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.	3.2	2
135	Dan Salah Tawfik (1955â€2021)â€”A giant of protein evolution. EMBO Reports, 2021, 22, .	4.5	2
136	Open Access, Plan S, and researchers' needs. EMBO Reports, 2020, 21, e51568.	4.5	2
137	Hypercompetition in biomedical research evaluation and its impact on young scientist careers. International Microbiology, 2015, 18, 253-61.	2.4	2
138	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
139	How to write a successful postdoc application â€“ the PI perspective. EMBO Reports, 2021, 22, e54203.	4.5	1
140	5 suggestions to increase grant application success rates. EMBO Reports, 2022, 23, e54893.	4.5	1
141	Lateâ€termination of pregnancy for medical reasons: when abortion isnâ€™t really by choice. EMBO Reports, 0, , .	4.5	1
142	Empirical Valence Bond Simulations of Organophosphate Hydrolysis: Theory and Practice. Methods in Enzymology, 2018, 607, 3-51.	1.0	0
143	A Structural View into the Complexity of Carbon Dioxide Fixation. ACS Central Science, 0, , .	11.3	0
144	Theoretical modelling of epigenetically modified DNA sequences. F1000Research, 0, , .	1.6	0