Philip E Bourne

List of Publications by Year in descending order

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253 papers	57,733 citations	16451 64 h-index	1158 229 g-index
279 all docs	279 docs citations	279 times ranked	69329 citing authors

#	Article	IF	Citations
1	The Protein Data Bank. Nucleic Acids Research, 2000, 28, 235-242.	14.5	31,087
2	The FAIR Guiding Principles for scientific data management and stewardship. Scientific Data, 2016, 3, 160018.	5.3	8,670
3	The Protein Data Bank. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 899-907.	2.5	2,023
4	ElliPro: a new structure-based tool for the prediction of antibody epitopes. BMC Bioinformatics, 2008, 9, 514.	2.6	1,076
5	The RCSB Protein Data Bank: redesigned web site and web services. Nucleic Acids Research, 2011, 39, D392-D401.	14.5	549
6	SuperTarget and Matador: resources for exploring drug-target relationships. Nucleic Acids Research, 2007, 36, D919-D922.	14.5	518
7	The Protein Data Bank and the challenge of structural genomics. Nature Structural Biology, 2000, 7, 957-959.	9.7	511
8	The RCSB Protein Data Bank: views of structural biology for basic and applied research and education. Nucleic Acids Research, 2015, 43, D345-D356.	14.5	461
9	How open science helps researchers succeed. ELife, 2016, 5, .	6.0	449
10	Immune epitope database analysis resource. Nucleic Acids Research, 2012, 40, W525-W530.	14.5	446
11	The RCSB Protein Data Bank: new resources for research and education. Nucleic Acids Research, 2012, 41, D475-D482.	14.5	418
12	The RCSB PDB information portal for structural genomics. Nucleic Acids Research, 2006, 34, D302-D305.	14.5	334
13	Immune epitope database analysis resource (IEDB-AR). Nucleic Acids Research, 2008, 36, W513-W518.	14.5	304
14	The RCSB Protein Data Bank: a redesigned query system and relational database based on the mmCIF schema. Nucleic Acids Research, 2004, 33, D233-D237.	14.5	303
15	Drug Discovery Using Chemical Systems Biology: Repositioning the Safe Medicine Comtan to Treat Multi-Drug and Extensively Drug Resistant Tuberculosis. PLoS Computational Biology, 2009, 5, e1000423.	3.2	283
16	History of biological metal utilization inferred through phylogenomic analysis of protein structures. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 10567-10572.	7.1	264
17	The Protein Data Bank: unifying the archive. Nucleic Acids Research, 2002, 30, 245-248.	14.5	261
18	The Molecular Biology Toolkit (MBT): a modular platform for developing molecular visualization applications. BMC Bioinformatics, 2005, 6, 21.	2.6	257

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19	Natural language processing of symptoms documented in free-text narratives of electronic health records: a systematic review. Journal of the American Medical Informatics Association: JAMIA, 2019, 26, 364-379.	4.4	253
20	Detecting evolutionary relationships across existing fold space, using sequence order-independent profileâ€“profile alignments. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5441-5446.	7.1	241
21	Structural Evolution of the Protein Kinaseâ€“Like Superfamily. PLoS Computational Biology, 2005, 1, e49.	3.2	234
22	Drug Discovery Using Chemical Systems Biology: Identification of the Protein-Ligand Binding Network To Explain the Side Effects of CETP Inhibitors. PLoS Computational Biology, 2009, 5, e1000387.	3.2	232
23	Modern proteomes contain putative imprints of ancient shifts in trace metal geochemistry. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 17822-17827.	7.1	215
24	Phylogeny determined by protein domain content. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 373-378.	7.1	205
25	PROMISCUOUS: a database for network-based drug-repositioning. Nucleic Acids Research, 2011, 39, D1060-D1066.	14.5	203
26	Antibody-protein interactions: benchmark datasets and prediction tools evaluation. BMC Structural Biology, 2007, 7, 64.	2.3	195
27	Novel Computational Approaches to Polypharmacology as a Means to Define Responses to Individual Drugs. Annual Review of Pharmacology and Toxicology, 2012, 52, 361-379.	9.4	194
28	Biodiversity data should be published, cited, and peer reviewed. Trends in Ecology and Evolution, 2013, 28, 454-461.	8.7	193
29	Drug Off-Target Effects Predicted Using Structural Analysis in the Context of a Metabolic Network Model. PLoS Computational Biology, 2010, 6, e1000938.	3.2	183
30	Pre-calculated protein structure alignments at the RCSB PDB website. Bioinformatics, 2010, 26, 2983-2985.	4.1	183
31	A Machine Learning-Based Method To Improve Docking Scoring Functions and Its Application to Drug Repurposing. Journal of Chemical Information and Modeling, 2011, 51, 408-419.	5.4	175
32	SuperTarget goes quantitative: update on drug-target interactions. Nucleic Acids Research, 2012, 40, D1113-D1117.	14.5	174
33	BioJava: an open-source framework for bioinformatics in 2012. Bioinformatics, 2012, 28, 2693-2695.	4.1	160
34	Progress with covalent small-molecule kinase inhibitors. Drug Discovery Today, 2018, 23, 727-735.	6.4	154
35	A systematic review of natural language processing and text mining of symptoms from electronic patient-authored text data. International Journal of Medical Informatics, 2019, 125, 37-46.	3.3	154
36	Drug Discovery Using Chemical Systems Biology: Weak Inhibition of Multiple Kinases May Contribute to the Anti-Cancer Effect of Nelfinavir. PLoS Computational Biology, 2011, 7, e1002037.	3.2	151

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37	[30] Macromolecular crystallographic information file. Methods in Enzymology, 1997, 277, 571-590.	1.0	148
38	Homology Modeling. Methods of Biochemical Analysis, 2005, 44, 509-523.	0.2	142
39	Big Data Science: Opportunities and Challenges to Address Minority Health and Health Disparities in the 21st Century. Ethnicity and Disease, 2017, 27, 95.	2.3	141
40	Structure-based systems biology for analyzing off-target binding. Current Opinion in Structural Biology, 2011, 21, 189-199.	5.7	131
41	A robust and efficient algorithm for the shape description of protein structures and its application in predicting ligand binding sites. BMC Bioinformatics, 2007, 8, S9.	2.6	123
42	Preprints for the life sciences. Science, 2016, 352, 899-901.	12.6	119
43	The distribution and query systems of the RCSB Protein Data Bank. Nucleic Acids Research, 2004, 32, 223D-225.	14.5	108
44	Evidence for treatment with estradiol for women with SARS-CoV-2 infection. BMC Medicine, 2020, 18, 369.	5.5	106
45	Perspective: Sustaining the big-data ecosystem. Nature, 2015, 527, S16-S17.	27.8	104
46	Determining Cysteines Available for Covalent Inhibition Across the Human Kinome. Journal of Medicinal Chemistry, 2017, 60, 2879-2889.	6.4	104
47	Partitioning Protein Structures into Domains: Why Is it so Difficult?. Journal of Molecular Biology, 2006, 361, 562-590.	4.2	100
48	CE-MC: a multiple protein structure alignment server. Nucleic Acids Research, 2004, 32, W100-W103.	14.5	98
49	The Mycobacterium tuberculosis Drugome and Its Polypharmacological Implications. PLoS Computational Biology, 2010, 6, e1000976.	3.2	98
50	The protein kinase resource. Trends in Biochemical Sciences, 1997, 22, 444-446.	7.5	96
51	Quantifying Reproducibility in Computational Biology: The Case of the Tuberculosis Drugome. PLoS ONE, 2013, 8, e80278.	2.5	91
52	Ten Simple Rules for Better Figures. PLoS Computational Biology, 2014, 10, e1003833.	3.2	90
53	A unified statistical model to support local sequence order independent similarity searching for ligand-binding sites and its application to genome-based drug discovery. Bioinformatics, 2009, 25, i305-i312.	4.1	89
54	An alternative view of protein fold space. Proteins: Structure, Function and Bioinformatics, 2000, 38, 247-260.	2.6	88

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55	Will a Biological Database Be Different from a Biological Journal?. PLoS Computational Biology, 2005, 1, e34.	3.2	87
56	IL-13 is a driver of COVID-19 severity. JCI Insight, 2021, 6, .	5.0	80
57	Exploiting sequence and structure homologs to identify protein-protein binding sites. Proteins: Structure, Function and Bioinformatics, 2005, 62, 630-640.	2.6	79
58	Raloxifene attenuates Pseudomonas aeruginosa pyocyanin production and virulence. International Journal of Antimicrobial Agents, 2012, 40, 246-251.	2.5	79
59	The Evolutionary History of Protein Domains Viewed by Species Phylogeny. PLoS ONE, 2009, 4, e8378.	2.5	79
60	STAR/mmCIF: An ontology for macromolecular structure. Bioinformatics, 2000, 16, 159-168.	4.1	78
61	Fold Recognition Methods. Methods of Biochemical Analysis, 2005, 44, 525-546.	0.2	78
62	In Silico Elucidation of the Molecular Mechanism Defining the Adverse Effect of Selective Estrogen Receptor Modulators. PLoS Computational Biology, 2007, 3, e217.	3.2	78
63	Ten Simple Rules for a Successful Collaboration. PLoS Computational Biology, 2007, 3, e44.	3.2	77
64	Ten simple rules to consider regarding preprint submission. PLoS Computational Biology, 2017, 13, e1005473.	3.2	77
65	A Multidimensional Strategy to Detect Polypharmacological Targets in the Absence of Structural and Sequence Homology. PLoS Computational Biology, 2010, 6, e1000648.	3.2	72
66	The NIH Big Data to Knowledge (BD2K) initiative. Journal of the American Medical Informatics Association: JAMIA, 2015, 22, 1114-1114.	4.4	68
67	Cloud computing applications for biomedical science: A perspective. PLoS Computational Biology, 2018, 14, e1006144.	3.2	67
68	Functional Coverage of the Human Genome by Existing Structures, Structural Genomics Targets, and Homology Models. PLoS Computational Biology, 2005, 1, e31.	3.2	63
69	Ten Simple Rules for a Good Poster Presentation. PLoS Computational Biology, 2007, 3, e102.	3.2	62
70	Towards Structural Systems Pharmacology to Study Complex Diseases and Personalized Medicine. PLoS Computational Biology, 2014, 10, e1003554.	3.2	61
71	Outcome of a Workshop on Archiving Structural Models of Biological Macromolecules. Structure, 2006, 14, 1211-1217.	3.3	60
72	SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison. Nucleic Acids Research, 2010, 38, W441-W444.	14.5	59

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73	IEDB-3D: structural data within the immune epitope database. Nucleic Acids Research, 2011, 39, D1164-D1170.	14.5	59
74	Ten Simple Rules for Getting Published. PLoS Computational Biology, 2005, 1, e57.	3.2	54
75	The Small Î²-Barrel Domain: A Survey-Based Structural Analysis. Structure, 2019, 27, 6-26.	3.3	51
76	The Cath Domain Structure Database. Methods of Biochemical Analysis, 2005, 44, 249-271.	0.2	50
77	Harnessing Big Data for Systems Pharmacology. Annual Review of Pharmacology and Toxicology, 2017, 57, 245-262.	9.4	50
78	Erabutoxin b. Initial protein refinement and sequence analysis at 0.140-nm resolution. FEBS Journal, 1985, 153, 521-527.	0.2	49
79	Developing multi-target therapeutics to fine-tune the evolutionary dynamics of the cancer ecosystem. Frontiers in Pharmacology, 2015, 6, 209.	3.5	47
80	Ten Simple Rules for Making Good Oral Presentations. PLoS Computational Biology, 2007, 3, e77.	3.2	46
81	Toward effective software solutions for big biology. Nature Biotechnology, 2015, 33, 686-687.	17.5	46
82	Systems biology of the structural proteome. BMC Systems Biology, 2016, 10, 26.	3.0	46
83	Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology. BMC Bioinformatics, 2016, 17, 90.	2.6	45
84	Limitations of Ab Initio Predictions of Peptide Binding to MHC Class II Molecules. PLoS ONE, 2010, 5, e9272.	2.5	45
85	EpitopeViewer: a Java application for the visualization and analysis of immune epitopes in the Immune Epitope Database and Analysis Resource (IEDB). Immunome Research, 2007, 3, 3.	0.1	44
86	Systematic Detection of Internal Symmetry in Proteins Using CE-Symm. Journal of Molecular Biology, 2014, 426, 2255-2268.	4.2	44
87	Delineation of Polypharmacology across the Human Structural Kinome Using a Functional Site Interaction Fingerprint Approach. Journal of Medicinal Chemistry, 2016, 59, 4326-4341.	6.4	39
88	An ontology for immune epitopes: application to the design of a broad scope database of immune reactivities. Immunome Research, 2005, 1, 2.	0.1	37
89	Conserved key amino acid positions (CKAAPs) derived from the analysis of common substructures in proteins. Proteins: Structure, Function and Bioinformatics, 2001, 42, 148-163.	2.6	36
90	Insights into the binding mode of MEK type-III inhibitors. A step towards discovering and designing allosteric kinase inhibitors across the human kinome. PLoS ONE, 2017, 12, e0179936.	2.5	34

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91	Ten Simple Rules for Getting Grants. PLoS Computational Biology, 2006, 2, e12.	3.2	33
92	Ten Simple Rules for Building and Maintaining a Scientific Reputation. PLoS Computational Biology, 2011, 7, e1002108.	3.2	33
93	Zeta Inhibitory Peptide Disrupts Electrostatic Interactions That Maintain Atypical Protein Kinase C in Its Active Conformation on the Scaffold p62. Journal of Biological Chemistry, 2015, 290, 21845-21856.	3.4	33
94	Nothing about protein structure classification makes sense except in the light of evolution. Current Opinion in Structural Biology, 2009, 19, 329-334.	5.7	32
95	Superimpose: a 3D structural superposition server. Nucleic Acids Research, 2008, 36, W47-W54.	14.5	31
96	Ten Simple Rules for Reviewers. PLoS Computational Biology, 2006, 2, e110.	3.2	30
97	Rethinking Proteasome Evolution: Two Novel Bacterial Proteasomes. Journal of Molecular Evolution, 2008, 66, 494-504.	1.8	30
98	BioLit: integrating biological literature with databases. Nucleic Acids Research, 2008, 36, W385-W389.	14.5	30
99	Structural Insights into Characterizing Binding Sites in Epidermal Growth Factor Receptor Kinase Mutants. Journal of Chemical Information and Modeling, 2019, 59, 453-462.	5.4	30
100	The Protein Data Bank. , 2003, , 389-405.		29
101	Translational Health Disparities Research in a Data-Rich World. Health Equity, 2019, 3, 588-600.	1.9	29
102	Institutional Profile: University of California San Diego Pharmacogenomics Education Program (PharmGenEdâ„¢): bridging the gap between science and practice. Pharmacogenomics, 2011, 12, 149-153.	1.3	28
103	The origin of a derived superkingdom: how a gram-positive bacterium crossed the desert to become an archaeon. Biology Direct, 2011, 6, 16.	4.6	28
104	Realâ€world evidence from over one million <scp>COVID</scp>â€19 vaccinations is consistent with reactivation of the varicellaâ€zoster virus. Journal of the European Academy of Dermatology and Venereology, 2022, 36, 1342-1348.	2.4	28
105	Structural analysis of polarizing indels: an emerging consensus on the root of the tree of life. Biology Direct, 2009, 4, 30.	4.6	27
106	A New Scoring Function and Associated Statistical Significance for Structure Alignment by CE. Journal of Computational Biology, 2004, 11, 787-799.	1.6	26
107	Wiggleâ€”Predicting Functionally Flexible Regions from Primary Sequence. PLoS Computational Biology, 2006, 2, e90.	3.2	26
108	Computational Biology Resources Lack Persistence and Usability. PLoS Computational Biology, 2008, 4, e1000136.	3.2	26

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109	Ten Simple Rules for Cultivating Open Science and Collaborative R&D. PLoS Computational Biology, 2013, 9, e1003244.	3.2	26
110	Analyzing the symmetrical arrangement of structural repeats in proteins with CE-Symm. PLoS Computational Biology, 2019, 15, e1006842.	3.2	26
111	A comparative proteomics resource: proteins of Arabidopsis thaliana. Genome Biology, 2003, 4, R51.	9.6	25
112	Prediction in 1D: Secondary Structure, Membrane Helices, and Accessibility. Methods of Biochemical Analysis, 2005, , 559-587.	0.2	25
113	Peptide Identification by Database Search of Mixture Tandem Mass Spectra. Molecular and Cellular Proteomics, 2011, 10, M111.010017.	3.8	25
114	Building the biomedical data science workforce. PLoS Biology, 2017, 15, e2003082.	5.6	25
115	Achievements and challenges in structural bioinformatics and computational biophysics. Bioinformatics, 2015, 31, 146-150.	4.1	24
116	Computational Prediction of Potential Inhibitors of the Main Protease of SARS-CoV-2. Frontiers in Chemistry, 2020, 8, 590263.	3.6	24
117	Structural Quality Assurance. Methods of Biochemical Analysis, 2005, , 273-303.	0.2	23
118	Topic Pages: PLoS Computational Biology Meets Wikipedia. PLoS Computational Biology, 2012, 8, e1002446.	3.2	23
119	Antibacterial mechanisms identified through structural systems pharmacology. BMC Systems Biology, 2013, 7, 102.	3.0	23
120	WhatBig Datameans to me. Journal of the American Medical Informatics Association: JAMIA, 2014, 21, 194-194.	4.4	23
121	The encyclopedia of life project: Grid software and deployment. New Generation Computing, 2004, 22, 127-136.	3.3	21
122	Intrinsic evaluation of text mining tools may not predict performance on realistic tasks. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2008, , 640-51.	0.7	21
123	The Protein Data Bank and lessons in data management. Briefings in Bioinformatics, 2004, 5, 23-30.	6.5	20
124	Prediction of Protein-Protein Interactions from Evolutionary Information. Methods of Biochemical Analysis, 2005, , 409-426.	0.2	20
125	Assigning new GO annotations to protein data bank sequences by combining structure and sequence homology. Proteins: Structure, Function and Bioinformatics, 2005, 58, 855-865.	2.6	20
126	The PDB Format, mmCIF Formats, and Other Data Formats. Methods of Biochemical Analysis, 2005, , 159-179.	0.2	20

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127	Ten Simple Rules for Selecting a Postdoctoral Position. PLoS Computational Biology, 2006, 2, e121.	3.2	20
128	Inferring Protein Function from Structure. Methods of Biochemical Analysis, 2005, , 387-407.	0.2	19
129	Combinatorial Approach for Large-scale Identification of Linked Peptides from Tandem Mass Spectrometry Spectra. Molecular and Cellular Proteomics, 2014, 13, 1128-1136.	3.8	19
130	Structural Insights into the Binding Modes of Viral RNA-Dependent RNA Polymerases Using a Function-Site Interaction Fingerprint Method for RNA Virus Drug Discovery. Journal of Proteome Research, 2020, 19, 4698-4705.	3.7	19
131	Harnessing systematic proteinâ€“ligand interaction fingerprints for drug discovery. Drug Discovery Today, 2022, 27, 103319.	6.4	19
132	What Do I Want from the Publisher of the Future?. PLoS Computational Biology, 2010, 6, e1000787.	3.2	18
133	Protein structure resources. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 908-915.	2.5	17
134	MixGF: Spectral Probabilities for Mixture Spectra from more than One Peptide. Molecular and Cellular Proteomics, 2014, 13, 3688-3697.	3.8	17
135	Real-world evidence for improved outcomes with histamine antagonists and aspirin in 22,560 COVID-19 patients. Signal Transduction and Targeted Therapy, 2021, 6, 267.	17.1	17
136	CASP and CAFASP Experiments and Their Findings. Methods of Biochemical Analysis, 2005, , 499-507.	0.2	16
137	Open Access: Taking Full Advantage of the Content. PLoS Computational Biology, 2008, 4, e1000037.	3.2	16
138	Ten Simple Rules for Writing a PLOS Ten Simple Rules Article. PLoS Computational Biology, 2014, 10, e1003858.	3.2	16
139	Ten Simple Rules for Doing Your Best Research, According to Hamming. PLoS Computational Biology, 2007, 3, e213.	3.2	16
140	Ab Initio Methods. Methods of Biochemical Analysis, 2005, 44, 547-557.	0.2	15
141	Structure Comparison and Alignment. Methods of Biochemical Analysis, 2005, , 321-337.	0.2	15
142	dConsensus: a tool for displaying domain assignments by multiple structure-based algorithms and for construction of a consensus assignment. BMC Bioinformatics, 2010, 11, 310.	2.6	15
143	Ten Simple Rules To Commercialize Scientific Research. PLoS Computational Biology, 2012, 8, e1002712.	3.2	14
144	Structural biology meets data science: does anything change?. Current Opinion in Structural Biology, 2018, 52, 95-102.	5.7	14

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145	CASP and CAFASP experiments and their findings. Methods of Biochemical Analysis, 2003, 44, 501-7.	0.2	14
146	Secondary Structure Assignment. Methods of Biochemical Analysis, 2005, , 339-363.	0.2	13
147	Teaching Bioinformatics at the Secondary School Level. PLoS Computational Biology, 2011, 7, e1002242.	3.2	13
148	Ten Simple Rules for Graduate Students. PLoS Computational Biology, 2007, 3, e229.	3.2	12
149	Con-Struct Map: a comparative contact map analysis tool. Bioinformatics, 2007, 23, 2491-2492.	4.1	12
150	RCSB PDB Mobile : iOS and Android mobile apps to provide data access and visualization to the RCSB Protein Data Bank. Bioinformatics, 2015, 31, 126-127.	4.1	12
151	Detection of circular permutations within protein structures using CE-CP. Bioinformatics, 2015, 31, 1316-1318.	4.1	12
152	INTRINSIC EVALUATION OF TEXT MINING TOOLS MAY NOT PREDICT PERFORMANCE ON REALISTIC TASKS. , 2007, , .		12
153	Macromolecular Structure Determination by NMR Spectroscopy. Methods of Biochemical Analysis, 2005, , 89-113.	0.2	11
154	ANTI-INFECTIOUS DRUG REPURPOSING USING AN INTEGRATED CHEMICAL GENOMICS AND STRUCTURAL SYSTEMS BIOLOGY APPROACH. , 2013, , .		11
155	Let's Make Gender Diversity in Data Science a Priority Right from the Start. PLoS Biology, 2015, 13, e1002206.	5.6	11
156	Principles and Methods of Docking and Ligand Design. Methods of Biochemical Analysis, 2005, , 441-476.	0.2	10
157	Electrostatic Interactions. Methods of Biochemical Analysis, 2005, , 427-440.	0.2	10
158	High-throughput identification of interacting protein-protein binding sites. BMC Bioinformatics, 2007, 8, 223.	2.6	10
159	Is â€œbioinformaticsâ€•dead?. PLoS Biology, 2021, 19, e3001165.	5.6	10
160	Announcement of the BioSync web site. Nature Structural Biology, 2001, 8, 663-663.	9.7	9
161	CKAAPs DB: a conserved key amino acid positions database. Nucleic Acids Research, 2001, 29, 329-331.	14.5	9
162	Structural Bioinformatics in Drug Discovery. Methods of Biochemical Analysis, 2005, 44, 477-497.	0.2	9

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163	I Am Not a Scientist, I Am a Number. PLoS Computational Biology, 2008, 4, e1000247.	3.2	9
164	Confronting the Ethical Challenges of Big Data in Public Health. PLoS Computational Biology, 2015, 11, e1004073.	3.2	9
165	The Urfold: Structural similarity just above the superfold level?. Protein Science, 2019, 28, 2119-2126.	7.6	9
166	Ten Simple Rules for avoiding and resolving conflicts with your colleagues. PLoS Computational Biology, 2019, 15, e1006708.	3.2	9
167	Ten simple rules for starting (and sustaining) an academic data science initiative. PLoS Computational Biology, 2021, 17, e1008628.	3.2	9
168	Analysis of the Human Kinome Using Methods Including Fold Recognition Reveals Two Novel Kinases. PLoS ONE, 2008, 3, e1597.	2.5	9
169	Anti-infectious drug repurposing using an integrated chemical genomics and structural systems biology approach. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2014, , 136-47.	0.7	9
170	A Comparative Analysis of COVID-19 Vaccines Based on over 580,000 Cases from the Vaccination Adverse Event Reporting System. Vaccines, 2022, 10, 408.	4.4	9
171	Design and implementation of a collaborative molecular graphics environment. Journal of Molecular Graphics and Modelling, 2001, 19, 280-287.	2.4	8
172	Identifying Structural Domains in Proteins. Methods of Biochemical Analysis, 2005, , 365-385.	0.2	8
173	Save the tree of life or get lost in the woods. Biology Direct, 2010, 5, 44.	4.6	8
174	Cobweb: a Java applet for network exploration and visualisation. Bioinformatics, 2011, 27, 1725-1726.	4.1	8
175	Ten Simple Rules to Protect Your Intellectual Property. PLoS Computational Biology, 2012, 8, e1002766.	3.2	8
176	BioJava-ModFinder: identification of protein modifications in 3D structures from the Protein Data Bank. Bioinformatics, 2017, 33, 2047-2049.	4.1	8
177	Ten simple rules in considering a career in academia versus government. PLoS Computational Biology, 2017, 13, e1005729.	3.2	8
178	Revealing Acquired Resistance Mechanisms of Kinase-Targeted Drugs Using an on-the-Fly, Function-Site Interaction Fingerprint Approach. Journal of Chemical Theory and Computation, 2020, 16, 3152-3161.	5.3	8
179	Overview of Current Type I/II Kinase Inhibitors. , 2020, , 13-28.		8
180	Integration of open access literature into the RCSB Protein Data Bank using BioLit. BMC Bioinformatics, 2010, 11, 220.	2.6	7

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181	Will Widgets and Semantic Tagging Change Computational Biology?. PLoS Computational Biology, 2010, 6, e1000673.	3.2	7
182	The evolution of the RCSB Protein Data Bank website. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 782-789.	14.6	7
183	Quality assurance for the query and distribution systems of the RCSB Protein Data Bank. Database: the Journal of Biological Databases and Curation, 2011, 2011, bar003-bar003.	3.0	7
184	Receptor Databases and Computational Websites for Ligand Binding. Methods in Molecular Biology, 2012, 897, 1-13.	0.9	7
185	A Turn-Key Approach for Large-Scale Identification of Complex Posttranslational Modifications. Journal of Proteome Research, 2014, 13, 1190-1199.	3.7	7
186	PLoS Computational Biology: A New Community Journal. PLoS Computational Biology, 2005, 1, e4.	3.2	7
187	The Protein Data Bank. Methods of Biochemical Analysis, 2005, , 181-198.	0.2	6
188	Ten Simple Rules for Getting Ahead as a Computational Biologist in Academia. PLoS Computational Biology, 2011, 7, e1002001.	3.2	6
189	Multiscale modeling of the causal functional roles of nsSNPs in a genome-wide association study: application to hypoxia. BMC Genomics, 2013, 14, S9.	2.8	6
190	Structure of a potent neuromuscular blocking agent: Caracurine-II dimethochloride octahydrate, [C40H44N4O2]2+ï¿½2Cl?ï¿½8H2O. Journal of Crystallographic and Spectroscopic Research, 1985, 15, 453-471.	0.2	5
191	PRONUC: a software package for the analysis of protein and nucleic acid sequences. Computer Methods and Programs in Biomedicine, 1987, 24, 27-36.	4.7	5
192	Defining Bioinformatics and Structural Bioinformatics. Methods of Biochemical Analysis, 2005, , 1-14.	0.2	5
193	DOIs for DICOM Raw Images: Enabling Science Reproducibility. Radiology, 2015, 275, 3-4.	7.3	5
194	Ten Simple Rules for Lifelong Learning, According to Hamming. PLoS Computational Biology, 2015, 11, e1004020.	3.2	5
195	Ten simple rules for researchers while in isolation from a pandemic. PLoS Computational Biology, 2020, 16, e1007946.	3.2	5
196	Informatics-enabled citizen science to advance health equity. Journal of the American Medical Informatics Association: JAMIA, 2021, 28, 2009-2012.	4.4	5
197	A Birds-Eye (Re)View of Acid-Suppression Drugs, COVID-19, and the Highly Variable Literature. Frontiers in Pharmacology, 2021, 12, 700703.	3.5	5
198	The structure and heavy-metal-ion-binding sites of horse spleen apoferritin. Biochemical Society Transactions, 1980, 8, 654-655.	3.4	4

#	Article	IF	Citations
199	The Nucleic Acid Database. Methods of Biochemical Analysis, 2005, , 199-216.	0.2	4
200	Resolving a distribution of charge into intrinsic multipole moments: A rankwise distributed multipole analysis. Physical Review E, 2008, 78, 066601.	2.1	4
201	Coarse-graining the electrostatic potential via distributed multipole expansions. Computer Physics Communications, 2011, 182, 1455-1462.	7.5	4
202	Ten Simple Rules for Approaching a New Job. PLoS Computational Biology, 2014, 10, e1003660.	3.2	4
203	Should biomedical research be like Airbnb?. PLoS Biology, 2017, 15, e2001818.	5.6	4
204	Ten simple rules for writing scientific op-ed articles. PLoS Computational Biology, 2020, 16, e1008187.	3.2	4
205	Developing international open science collaborations: Funder reflections on the Open Science Prize. PLoS Biology, 2017, 15, e2002617.	5.6	4
206	Macromolecular Structure Databases: Past Progress and Future Challenges. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1085-1094.	2.5	3
207	Development of Internet-based multimedia applications. Trends in Biochemical Sciences, 1999, 24, 321-324.	7.5	3
208	The New Biology and the Grid. , 0, , 907-922.		3
209	Structural Genomics. Methods of Biochemical Analysis, 2005, , 589-612.	0.2	3
210	All-Atom Contacts: A New Approach to Structure Validation. Methods of Biochemical Analysis, 2005, , 305-320.	0.2	3
211	Fundamentals of Protein Structure. Methods of Biochemical Analysis, 2005, , 15-39.	0.2	3
212	Molecular Visualization. Methods of Biochemical Analysis, 2005, , 135-158.	0.2	3
213	Let's Make Those Book Chapters Open Too!. PLoS Computational Biology, 2013, 9, e1002941.	3.2	3
214	One thousand simple rules. PLoS Computational Biology, 2018, 14, e1006670.	3.2	3
215	Ten simple rules for more objective decision-making. PLoS Computational Biology, 2020, 16, e1007706.	3.2	3
216	Structural Evolution of the Protein Kinase-Like Superfamily. PLoS Computational Biology, 2005, preprint, e49.	3.2	3

#	Article	IF	Citations
217	Selecting a processor for computations in molecular biophysics. Computers in Biology and Medicine, 1988, 18, 341-349.	7.0	2
218	A CPU benchmark for protein crystallographic refinement. Computers in Biology and Medicine, 1990, 20, 219-230.	7.0	2
219	STATISTICAL AND VISUAL MORPH MOVIE ANALYSIS OF CRYSTALLOGRAPHIC MUTANT SELECTION BIAS IN PROTEIN MUTATION RESOURCE DATA. Journal of Bioinformatics and Computational Biology, 2004, 02, 61-75.	0.8	2
220	Overview of Structural Bioinformatics. , 2005, , 15-44.		2
221	Fundamentals of DNA and RNA Structure. Methods of Biochemical Analysis, 2005, , 41-73.	0.2	2
222	Protein Structure Evolution and the Scop Database. Methods of Biochemical Analysis, 2005, , 237-248.	0.2	2
223	Ten Simple Rules for Starting a Company. PLoS Computational Biology, 2012, 8, e1002439.	3.2	2
224	Life is three-dimensional, and it begins with molecules. PLoS Biology, 2017, 15, e2002041.	5.6	2
225	Structure comparison and alignment. Methods of Biochemical Analysis, 2003, 44, 321-37.	0.2	2
226	Other Structure-Based Databases. Methods of Biochemical Analysis, 2005, , 217-236.	0.2	1
227	Communication of Scientific Information: Is It Time to Reassess?. Clinical Chemistry, 2013, 59, 604-611.	3.2	1
228	The reaming of life: based on the 2010 Jim Gray eScience Award Lecture. Concurrency Computation Practice and Experience, 2013, 25, 445-453.	2.2	1
229	Learning How to Run a Lab: Interviews with Principal Investigators. PLoS Computational Biology, 2013, 9, e1003349.	3.2	1
230	Ten Years of PLoSâ€¡ Computational Biology: A Decade of Appreciation and Innovation. PLoS Computational Biology, 2015, 11, e1004317.	3.2	1
231	Ten simple rules when considering retirement. PLoS Computational Biology, 2018, 14, e1006411.	3.2	1
232	Machine Learning for Classification of Protein Helix Capping Motifs. , 2019, , .		1
233	Ten simple rules to aid in achieving a vision. PLoS Computational Biology, 2019, 15, e1007395.	3.2	1
234	Using the Structural Kinome to Systematize Kinase Drug Discovery. Biochemistry, 0, , .	1.2	1

#	Article	IF	Citations
235	Ten simple rules for using entrepreneurship skills to improve research careers and culture. PLoS Computational Biology, 2022, 18, e1009946.	3.2	1
236	Ten simple rules for improving communication among scientists. PLoS Computational Biology, 2022, 18, e1010130.	3.2	1
237	Ten simple rules for good leadership. PLoS Computational Biology, 2022, 18, e1010133.	3.2	1
238	Computational Aspects of High-Throughput Crystallographic Macromolecular Structure Determination. Methods of Biochemical Analysis, 2005, 44, 75-87.	0.2	0
239	A Systematic Approach to Identifying Protein-Ligand Binding Profiles on a Proteome Scale. Nature Precedings, 2008, , .	0.1	0
240	Changes in Scholarly Communication and the Potential Impact on Biocuration. Nature Precedings, 2009, , .	0.1	0
241	The Rankwise Distributed Multipole Analysis (RWDMA) of the Electrostatic Field of Large Biomolecules. Biophysical Journal, 2009, 96, 303a.	0.5	0
242	A Review of 2009 for PLoS Computational Biology. PLoS Computational Biology, 2010, 6, e1000687.	3.2	0
243	A Review of 2010 for PLoS Computational Biology. PLoS Computational Biology, 2011, 7, e1002003.	3.2	0
244	Seven Years; It's Time for a Change. PLoS Computational Biology, 2012, 8, e1002728.	3.2	0
245	An integrated workflow for proteome-wide off-target identification and polypharmacology drug design. , 2012, , .		0
246	Protein Data Resources. , 2004, , 478-483.		0
247	Session Introduction. , 2004, , .		0
248	Functional Coverage of the Human Genome by Existing Structures, Structural Genomics Targets and Homology Models. PLoS Computational Biology, 2005, preprint, e31.	3.2	0
249	In Silico Elucidation of the Molecular Mechanism Defining the Adverse Effect of Selective Estrogen Receptor Modulators. PLoS Computational Biology, 2005, preprint, e217.	3.2	0
250	Digital research/analog publishing â€“ one scientist's view. Serials, 2011, 24, 119-122.	0.5	0
251	A Review of 2011 for PLoS Computational Biology. PLoS Computational Biology, 2012, 8, e1002387.	3.2	0
252	Discrepancies in purified and cellular PKMÎ¶ inhibition profiles invalidate its proposed role as a mediator of memory. FASEB Journal, 2012, 26, 768.5.	0.5	0

#	Article	IF	Citations
253	Ten simple rules for starting research in your late teens. PLoS Computational Biology, 2020, 16, e1008403.	3.2	0