List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	Ten simple rules for using entrepreneurship skills to improve research careers and culture. PLoS Computational Biology, 2022, 18, e1009946.	3.2	1
3	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
4	Ten simple rules for improving communication among scientists. PLoS Computational Biology, 2022, 18, e1010130.	3.2	1
5	Ten simple rules for good leadership. PLoS Computational Biology, 2022, 18, e1010133.	3.2	1
6	Harnessing systematic protein–ligand interaction fingerprints for drug discovery. Drug Discovery Today, 2022, 27, 103319.	6.4	19
7	Ten simple rules for starting (and sustaining) an academic data science initiative. PLoS Computational Biology, 2021, 17, e1008628.	3.2	9
8	ls "bioinformatics―dead?. PLoS Biology, 2021, 19, e3001165.	5.6	10
9	IL-13 is a driver of COVID-19 severity. JCI Insight, 2021, 6, .	5.0	80
10	Informatics-enabled citizen science to advance health equity. Journal of the American Medical Informatics Association: JAMIA, 2021, 28, 2009-2012.	4.4	5
11	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
12	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
13	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
14	Evidence for treatment with estradiol for women with SARS-CoV-2 infection. BMC Medicine, 2020, 18, 369.	5.5	106
15	Ten simple rules for writing scientific op-ed articles. PLoS Computational Biology, 2020, 16, e1008187.	3.2	4
16	Computational Prediction of Potential Inhibitors of the Main Protease of SARS-CoV-2. Frontiers in Chemistry, 2020, 8, 590263.	3.6	24
17	Ten simple rules for more objective decision-making. PLoS Computational Biology, 2020, 16, e1007706.	3.2	3
18	Ten simple rules for researchers while in isolation from a pandemic. PLoS Computational Biology, 2020, 16, e1007946.	3.2	5

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19	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
20	Overview of Current Type I/II Kinase Inhibitors. , 2020, , 13-28.		8
21	Ten simple rules for starting research in your late teens. PLoS Computational Biology, 2020, 16, e1008403.	3.2	Ο
22	The <i>Urfold</i> : Structural similarity just above the superfold level?. Protein Science, 2019, 28, 2119-2126.	7.6	9
23	Machine Learning for Classification of Protein Helix Capping Motifs. , 2019, , .		1
24	Ten Simple Rules for avoiding and resolving conflicts with your colleagues. PLoS Computational Biology, 2019, 15, e1006708.	3.2	9
25	Analyzing the symmetrical arrangement of structural repeats in proteins with CE-Symm. PLoS Computational Biology, 2019, 15, e1006842.	3.2	26
26	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
27	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
28	Ten simple rules to aid in achieving a vision. PLoS Computational Biology, 2019, 15, e1007395.	3.2	1
29	Translational Health Disparities Research in a Data-Rich World. Health Equity, 2019, 3, 588-600.	1.9	29
30	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
31	The Small β-Barrel Domain: A Survey-Based Structural Analysis. Structure, 2019, 27, 6-26.	3.3	51
32	Progress with covalent small-molecule kinase inhibitors. Drug Discovery Today, 2018, 23, 727-735.	6.4	154
33	One thousand simple rules. PLoS Computational Biology, 2018, 14, e1006670.	3.2	3
34	Ten simple rules when considering retirement. PLoS Computational Biology, 2018, 14, e1006411.	3.2	1
35	Structural biology meets data science: does anything change?. Current Opinion in Structural Biology, 2018, 52, 95-102.	5.7	14
36	Cloud computing applications for biomedical science: A perspective. PLoS Computational Biology, 2018, 14, e1006144.	3.2	67

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37	Determining Cysteines Available for Covalent Inhibition Across the Human Kinome. Journal of Medicinal Chemistry, 2017, 60, 2879-2889.	6.4	104
38	Harnessing Big Data for Systems Pharmacology. Annual Review of Pharmacology and Toxicology, 2017, 57, 245-262.	9.4	50
39	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
40	BioJava-ModFinder: identification of protein modifications in 3D structures from the Protein Data Bank. Bioinformatics, 2017, 33, 2047-2049.	4.1	8
41	Should biomedical research be like Airbnb?. PLoS Biology, 2017, 15, e2001818.	5.6	4
42	Ten simple rules in considering a career in academia versus government. PLoS Computational Biology, 2017, 13, e1005729.	3.2	8
43	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
44	Developing international open science collaborations: Funder reflections on the Open Science Prize. PLoS Biology, 2017, 15, e2002617.	5.6	4
45	Building the biomedical data science workforce. PLoS Biology, 2017, 15, e2003082.	5.6	25
46	Ten simple rules to consider regarding preprint submission. PLoS Computational Biology, 2017, 13, e1005473.	3.2	77
47	Life is three-dimensional, and it begins with molecules. PLoS Biology, 2017, 15, e2002041.	5.6	2
48	How open science helps researchers succeed. ELife, 2016, 5, .	6.0	449
49	The FAIR Guiding Principles for scientific data management and stewardship. Scientific Data, 2016, 3, 160018.	5.3	8,670
50	Preprints for the life sciences. Science, 2016, 352, 899-901.	12.6	119
51	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
52	Systems biology of the structural proteome. BMC Systems Biology, 2016, 10, 26.	3.0	46
53	Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology. BMC Bioinformatics, 2016, 17, 90.	2.6	45
54	Let's Make Gender Diversity in Data Science a Priority Right from the Start. PLoS Biology, 2015, 13, e1002206.	5.6	11

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55	Ten Years of PLoSâ€; Computational Biology: A Decade of Appreciation and Innovation. PLoS Computational Biology, 2015, 11, e1004317.	3.2	1
56	Developing multi-target therapeutics to fine-tune the evolutionary dynamics of the cancer ecosystem. Frontiers in Pharmacology, 2015, 6, 209.	3.5	47
57	DOIs for DICOM Raw Images: Enabling Science Reproducibility. Radiology, 2015, 275, 3-4.	7.3	5
58	RCSB PDB <i>Mobile</i> : 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
59	Detection of circular permutations within protein structures using CE-CP. Bioinformatics, 2015, 31, 1316-1318.	4.1	12
60	Achievements and challenges in structural bioinformatics and computational biophysics. Bioinformatics, 2015, 31, 146-150.	4.1	24
61	Ten Simple Rules for Lifelong Learning, According to Hamming. PLoS Computational Biology, 2015, 11, e1004020.	3.2	5
62	Toward effective software solutions for big biology. Nature Biotechnology, 2015, 33, 686-687.	17.5	46
63	Confronting the Ethical Challenges of Big Data in Public Health. PLoS Computational Biology, 2015, 11, e1004073.	3.2	9
64	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
65	Perspective: Sustaining the big-data ecosystem. Nature, 2015, 527, S16-S17.	27.8	104
66	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
67	The NIH Big Data to Knowledge (BD2K) initiative. Journal of the American Medical Informatics Association: JAMIA, 2015, 22, 1114-1114.	4.4	68
68	MixGF: Spectral Probabilities for Mixture Spectra from more than One Peptide. Molecular and Cellular Proteomics, 2014, 13, 3688-3697.	3.8	17
69	Ten Simple Rules for Writing a PLOS Ten Simple Rules Article. PLoS Computational Biology, 2014, 10, e1003858.	3.2	16
70	Ten Simple Rules for Better Figures. PLoS Computational Biology, 2014, 10, e1003833.	3.2	90
71	Ten Simple Rules for Approaching a New Job. PLoS Computational Biology, 2014, 10, e1003660.	3.2	4
72	Towards Structural Systems Pharmacology to Study Complex Diseases and Personalized Medicine. PLoS Computational Biology, 2014, 10, e1003554.	3.2	61

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73	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
74	WhatBig Datameans to me. Journal of the American Medical Informatics Association: JAMIA, 2014, 21, 194-194.	4.4	23
75	A Turn-Key Approach for Large-Scale Identification of Complex Posttranslational Modifications. Journal of Proteome Research, 2014, 13, 1190-1199.	3.7	7
76	Systematic Detection of Internal Symmetry in Proteins Using CE-Symm. Journal of Molecular Biology, 2014, 426, 2255-2268.	4.2	44
77	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
78	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
79	Antibacterial mechanisms identified through structural systems pharmacology. BMC Systems Biology, 2013, 7, 102.	3.0	23
80	Communication of Scientific Information: Is It Time to Reassess?. Clinical Chemistry, 2013, 59, 604-611.	3.2	1
81	Biodiversity data should be published, cited, and peer reviewed. Trends in Ecology and Evolution, 2013, 28, 454-461.	8.7	193
82	ANTI-INFECTIOUS DRUG REPURPOSING USING AN INTEGRATED CHEMICAL GENOMICS AND STRUCTURAL SYSTEMS BIOLOGY APPROACH. , 2013, , .		11
83	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
84	Let's Make Those Book Chapters Open Too!. PLoS Computational Biology, 2013, 9, e1002941.	3.2	3
85	Learning How to Run a Lab: Interviews with Principal Investigators. PLoS Computational Biology, 2013, 9, e1003349.	3.2	1
86	Ten Simple Rules for Cultivating Open Science and Collaborative R&D. PLoS Computational Biology, 2013, 9, e1003244.	3.2	26
87	Quantifying Reproducibility in Computational Biology: The Case of the Tuberculosis Drugome. PLoS ONE, 2013, 8, e80278.	2.5	91
88	Ten Simple Rules to Protect Your Intellectual Property. PLoS Computational Biology, 2012, 8, e1002766.	3.2	8
89	Ten Simple Rules for Starting a Company. PLoS Computational Biology, 2012, 8, e1002439.	3.2	2
90	Topic Pages: PLoS Computational Biology Meets Wikipedia. PLoS Computational Biology, 2012, 8, e1002446.	3.2	23

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91	Seven Years; It's Time for a Change. PLoS Computational Biology, 2012, 8, e1002728.	3.2	Ο
92	Ten Simple Rules To Commercialize Scientific Research. PLoS Computational Biology, 2012, 8, e1002712.	3.2	14
93	SuperTarget goes quantitative: update on drug-target interactions. Nucleic Acids Research, 2012, 40, D1113-D1117.	14.5	174
94	An integrated workflow for proteome-wide off-target identification and polypharmacology drug design. , 2012, , .		0
95	The RCSB Protein Data Bank: new resources for research and education. Nucleic Acids Research, 2012, 41, D475-D482.	14.5	418
96	BioJava: an open-source framework for bioinformatics in 2012. Bioinformatics, 2012, 28, 2693-2695.	4.1	160
97	Immune epitope database analysis resource. Nucleic Acids Research, 2012, 40, W525-W530.	14.5	446
98	Raloxifene attenuates Pseudomonas aeruginosa pyocyanin production and virulence. International Journal of Antimicrobial Agents, 2012, 40, 246-251.	2.5	79
99	Receptor Databases and Computational Websites for Ligand Binding. Methods in Molecular Biology, 2012, 897, 1-13.	0.9	7
100	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
101	A Review of 2011 for PLoS Computational Biology. PLoS Computational Biology, 2012, 8, e1002387.	3.2	Ο
102	Discrepancies in purified and cellular PKMζ inhibition profiles invalidate its proposed role as a mediator of memory. FASEB Journal, 2012, 26, 768.5.	0.5	0
103	IEDB-3D: structural data within the immune epitope database. Nucleic Acids Research, 2011, 39, D1164-D1170.	14.5	59
104	Teaching Bioinformatics at the Secondary School Level. PLoS Computational Biology, 2011, 7, e1002242.	3.2	13
105	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
106	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
107	Peptide Identification by Database Search of Mixture Tandem Mass Spectra. Molecular and Cellular Proteomics, 2011, 10, M111.010017.	3.8	25
108	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

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109	Structure-based systems biology for analyzing off-target binding. Current Opinion in Structural Biology, 2011, 21, 189-199.	5.7	131
110	The evolution of the RCSB Protein Data Bank website. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 782-789.	14.6	7
111	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
112	Coarse-graining the electrostatic potential via distributed multipole expansions. Computer Physics Communications, 2011, 182, 1455-1462.	7.5	4
113	PROMISCUOUS: a database for network-based drug-repositioning. Nucleic Acids Research, 2011, 39, D1060-D1066.	14.5	203
114	The RCSB Protein Data Bank: redesigned web site and web services. Nucleic Acids Research, 2011, 39, D392-D401.	14.5	549
115	Cobweb: a Java applet for network exploration and visualisation. Bioinformatics, 2011, 27, 1725-1726.	4.1	8
116	A Review of 2010 for PLoS Computational Biology. PLoS Computational Biology, 2011, 7, e1002003.	3.2	0
117	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
118	Ten Simple Rules for Building and Maintaining a Scientific Reputation. PLoS Computational Biology, 2011, 7, e1002108.	3.2	33
119	Ten Simple Rules for Getting Ahead as a Computational Biologist in Academia. PLoS Computational Biology, 2011, 7, e1002001.	3.2	6
120	Digital research/analog publishing – one scientist's view. Serials, 2011, 24, 119-122.	0.5	0
121	Integration of open access literature into the RCSB Protein Data Bank using BioLit. BMC Bioinformatics, 2010, 11, 220.	2.6	7
122	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
123	Save the tree of life or get lost in the woods. Biology Direct, 2010, 5, 44.	4.6	8
124	SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison. Nucleic Acids Research, 2010, 38, W441-W444.	14.5	59
125	A Multidimensional Strategy to Detect Polypharmacological Targets in the Absence of Structural and Sequence Homology. PLoS Computational Biology, 2010, 6, e1000648.	3.2	72
126	What Do I Want from the Publisher of the Future?. PLoS Computational Biology, 2010, 6, e1000787.	3.2	18

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127	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
128	Will Widgets and Semantic Tagging Change Computational Biology?. PLoS Computational Biology, 2010, 6, e1000673.	3.2	7
129	The Mycobacterium tuberculosis Drugome and Its Polypharmacological Implications. PLoS Computational Biology, 2010, 6, e1000976.	3.2	98
130	Pre-calculated protein structure alignments at the RCSB PDB website. Bioinformatics, 2010, 26, 2983-2985.	4.1	183
131	A Review of 2009 for PLoS Computational Biology. PLoS Computational Biology, 2010, 6, e1000687.	3.2	0
132	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
133	Limitations of Ab Initio Predictions of Peptide Binding to MHC Class II Molecules. PLoS ONE, 2010, 5, e9272.	2.5	45
134	Changes in Scholarly Communication and the Potential Impact on Biocuration. Nature Precedings, 2009, , .	0.1	0
135	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
136	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
137	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
138	Structural analysis of polarizing indels: an emerging consensus on the root of the tree of life. Biology Direct, 2009, 4, 30.	4.6	27
139	The Rankwise Distributed Multipole Analysis (RWDMA) of the Electrostatic Field of Large Biomolecules. Biophysical Journal, 2009, 96, 303a.	0.5	0
140	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
141	The Evolutionary History of Protein Domains Viewed by Species Phylogeny. PLoS ONE, 2009, 4, e8378.	2.5	79
142	Rethinking Proteasome Evolution: Two Novel Bacterial Proteasomes. Journal of Molecular Evolution, 2008, 66, 494-504.	1.8	30
143	ElliPro: a new structure-based tool for the prediction of antibody epitopes. BMC Bioinformatics, 2008, 9, 514.	2.6	1,076
144	Immune epitope database analysis resource (IEDB-AR). Nucleic Acids Research, 2008, 36, W513-W518.	14.5	304

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145	Superimpose: a 3D structural superposition server. Nucleic Acids Research, 2008, 36, W47-W54.	14.5	31
146	Detecting evolutionary relationships across existing fold space, using sequence order-independent profile–profile alignments. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5441-5446.	7.1	241
147	Computational Biology Resources Lack Persistence and Usability. PLoS Computational Biology, 2008, 4, e1000136.	3.2	26
148	BioLit: integrating biological literature with databases. Nucleic Acids Research, 2008, 36, W385-W389.	14.5	30
149	I Am Not a Scientist, I Am a Number. PLoS Computational Biology, 2008, 4, e1000247.	3.2	9
150	Open Access: Taking Full Advantage of the Content. PLoS Computational Biology, 2008, 4, e1000037.	3.2	16
151	Resolving a distribution of charge into intrinsic multipole moments: A rankwise distributed multipole analysis. Physical Review E, 2008, 78, 066601.	2.1	4
152	A Systematic Approach to Identifying Protein-Ligand Binding Profiles on a Proteome Scale. Nature Precedings, 2008, , .	0.1	0
153	Analysis of the Human Kinome Using Methods Including Fold Recognition Reveals Two Novel Kinases. PLoS ONE, 2008, 3, e1597.	2.5	9
154	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
155	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
156	SuperTarget and Matador: resources for exploring drug-target relationships. Nucleic Acids Research, 2007, 36, D919-D922.	14.5	518
157	Ten Simple Rules for a Good Poster Presentation. PLoS Computational Biology, 2007, 3, e102.	3.2	62
158	Ten Simple Rules for Graduate Students. PLoS Computational Biology, 2007, 3, e229.	3.2	12
159	Con-Struct Map: a comparative contact map analysis tool. Bioinformatics, 2007, 23, 2491-2492.	4.1	12
160	Ten Simple Rules for Making Good Oral Presentations. PLoS Computational Biology, 2007, 3, e77.	3.2	46
161	Ten Simple Rules for a Successful Collaboration. PLoS Computational Biology, 2007, 3, e44.	3.2	77
162	Antibody-protein interactions: benchmark datasets and prediction tools evaluation. BMC Structural Biology, 2007, 7, 64.	2.3	195

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163	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
164	High-throughput identification of interacting protein-protein binding sites. BMC Bioinformatics, 2007, 8, 223.	2.6	10
165	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
166	INTRINSIC EVALUATION OF TEXT MINING TOOLS MAY NOT PREDICT PERFORMANCE ON REALISTIC TASKS. , 2007, , .		12
167	Ten Simple Rules for Doing Your Best Research, According to Hamming. PLoS Computational Biology, 2007, 3, e213.	3.2	16
168	Partitioning Protein Structures into Domains: Why Is it so Difficult?. Journal of Molecular Biology, 2006, 361, 562-590.	4.2	100
169	Outcome of a Workshop on Archiving Structural Models of Biological Macromolecules. Structure, 2006, 14, 1211-1217.	3.3	60
170	The RCSB PDB information portal for structural genomics. Nucleic Acids Research, 2006, 34, D302-D305.	14.5	334
171	Wiggle—Predicting Functionally Flexible Regions from Primary Sequence. PLoS Computational Biology, 2006, 2, e90.	3.2	26
172	Ten Simple Rules for Selecting a Postdoctoral Position. PLoS Computational Biology, 2006, 2, e121.	3.2	20
173	Ten Simple Rules for Getting Grants. PLoS Computational Biology, 2006, 2, e12.	3.2	33
174	Ten Simple Rules for Reviewers. PLoS Computational Biology, 2006, 2, e110.	3.2	30
175	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
176	Structural Genomics. Methods of Biochemical Analysis, 2005, , 589-612.	0.2	3
177	All-Atom Contacts: A New Approach to Structure Validation. Methods of Biochemical Analysis, 2005, , 305-320.	0.2	3
178	Identifying Structural Domains in Proteins. Methods of Biochemical Analysis, 2005, , 365-385.	0.2	8
179	Ab Initio Methods. Methods of Biochemical Analysis, 2005, 44, 547-557.	0.2	15
180	Structural Quality Assurance. Methods of Biochemical Analysis, 2005, , 273-303.	0.2	23

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181	Secondary Structure Assignment. Methods of Biochemical Analysis, 2005, , 339-363.	0.2	13
182	The Cath Domain Structure Database. Methods of Biochemical Analysis, 2005, 44, 249-271.	0.2	50
183	Prediction of Protein-Protein Interactions from Evolutionary Information. Methods of Biochemical Analysis, 2005, , 409-426.	0.2	20
184	CASP and CAFASP Experiments and Their Findings. Methods of Biochemical Analysis, 2005, , 499-507.	0.2	16
185	Prediction in 1D: Secondary Structure, Membrane Helices, and Accessibility. Methods of Biochemical Analysis, 2005, , 559-587.	0.2	25
186	Fold Recognition Methods. Methods of Biochemical Analysis, 2005, 44, 525-546.	0.2	78
187	The Molecular Biology Toolkit (MBT): a modular platform for developing molecular visualization applications. BMC Bioinformatics, 2005, 6, 21.	2.6	257
188	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
189	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
190	Exploiting sequence and structure homologs to identify protein-protein binding sites. Proteins: Structure, Function and Bioinformatics, 2005, 62, 630-640.	2.6	79
191	Structural Evolution of the Protein Kinase–Like Superfamily. PLoS Computational Biology, 2005, 1, e49.	3.2	234
192	Functional Coverage of the Human Genome by Existing Structures, Structural Genomics Targets, and Homology Models. PLoS Computational Biology, 2005, 1, e31.	3.2	63
193	Will a Biological Database Be Different from a Biological Journal?. PLoS Computational Biology, 2005, 1, e34.	3.2	87
194	Overview of Structural Bioinformatics. , 2005, , 15-44.		2
195	Homology Modeling. Methods of Biochemical Analysis, 2005, 44, 509-523.	0.2	142
196	Principles and Methods of Docking and Ligand Design. Methods of Biochemical Analysis, 2005, , 441-476.	0.2	10
197	Electrostatic Interactions. Methods of Biochemical Analysis, 2005, , 427-440.	0.2	10
198	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

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199	Structure Comparison and Alignment. Methods of Biochemical Analysis, 2005, , 321-337.	0.2	15
200	Inferring Protein Function from Structure. Methods of Biochemical Analysis, 2005, , 387-407.	0.2	19
201	Ten Simple Rules for Getting Published. PLoS Computational Biology, 2005, 1, e57.	3.2	54
202	Structural Bioinformatics in Drug Discovery. Methods of Biochemical Analysis, 2005, 44, 477-497.	0.2	9
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