List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Deep learning in next-generation sequencing. Drug Discovery Today, 2021, 26, 173-180.	6.4	31
2	NOseq: amplicon sequencing evaluation method for RNA m6A sites after chemical deamination. Nucleic Acids Research, 2021, 49, e23-e23.	14.5	25
3	CARE: context-aware sequencing read error correction. Bioinformatics, 2021, 37, 889-895.	4.1	7
4	Learning Molecular Classes from Small Numbers of Positive Examples Using Graph Grammars. Lecture Notes in Computer Science, 2021, , 3-15.	1.3	0
5	Automatic shape detection of ice crystals. Journal of Computational Science, 2021, 54, 101429.	2.9	2
6	Evaluating the microscopic effect of brushing stone tools as a cleaning procedure. Quaternary International, 2020, 569-570, 263-276.	1.5	12
7	A big data approach to metagenomics for all-food-sequencing. BMC Bioinformatics, 2020, 21, 102.	2.6	19
8	Machine learning of reverse transcription signatures of variegated polymerases allows mapping and discrimination of methylated purines in limited transcriptomes. Nucleic Acids Research, 2020, 48, 3734-3746.	14.5	45
9	Polish is quantitatively different on quartzite flakes used on different worked materials. PLoS ONE, 2020, 15, e0243295.	2.5	13
10	Dedicated Bioinformatics Analysis Hardware. , 2019, , 1142-1150.		1
11	Graphical Workflow System for Modification Calling by Machine Learning of Reverse Transcription Signatures. Frontiers in Genetics, 2019, 10, 876.	2.3	10
12	The effect of numerical aperture on quantitative use-wear studies and its implication on reproducibility. Scientific Reports, 2019, 9, 6313.	3.3	22
13	NESSie.jl – Efficient and intuitive finite element and boundary element methods for nonlocal protein electrostatics in the Julia language. Journal of Computational Science, 2018, 28, 193-203.	2.9	2
14	Graph Rewriting Based Search for Molecular Structures: Definitions, Algorithms, Hardness. Lecture Notes in Computer Science, 2018, , 43-59.	1.3	1
15	Next-generation sequencing: big data meets high performance computing. Drug Discovery Today, 2017, 22, 712-717.	6.4	108
16	MetaCache: context-aware classification of metagenomic reads using minhashing. Bioinformatics, 2017, 33, 3740-3748.	4.1	41
17	CoverageAnalyzer (CAn): A Tool for Inspection of Modification Signatures in RNA Sequencing Profiles. Biomolecules, 2016, 6, 42.	4.0	16
18	rapidGSEA: Speeding up gene set enrichment analysis on multi-core CPUs and CUDA-enabled GPUs. BMC Bioinformatics, 2016, 17, 394.	2.6	1

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19	Drug <scp>T</scp> arget <scp>I</scp> nspector: An assistance tool for patient treatment stratification. International Journal of Cancer, 2016, 138, 1765-1776.	5.1	8
20	A computational method for studying the relation between alternative splicing and DNA methylation. Nucleic Acids Research, 2016, 44, e19-e19.	14.5	12
21	CUDA-enabled hierarchical ward clustering of protein structures based on the nearest neighbour chain algorithm. International Journal of High Performance Computing Applications, 2016, 30, 200-211.	3.7	5
22	A novel automated segmentation method for retinal layers in OCT images proves retinal degeneration after optic neuritis. British Journal of Ophthalmology, 2016, 100, 484-490.	3.9	9
23	Integrated quantitative proteomic and transcriptomic analysis of lung tumor and control tissue: a lung cancer showcase. Oncotarget, 2016, 7, 14857-14870.	1.8	17
24	Large oligomeric complex structures can be computationally assembled by efficiently combining docked interfaces. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1887-1899.	2.6	3
25	The reverse transcription signature of <i>N</i> -1-methyladenosine in RNA-Seq is sequence dependent. Nucleic Acids Research, 2015, 43, gkv895.	14.5	163
26	The impact of isolated lesions on white-matter fiber tracts in multiple sclerosis patients. NeuroImage: Clinical, 2015, 8, 110-116.	2.7	31
27	ballaxy: web services for structural bioinformatics. Bioinformatics, 2015, 31, 121-122.	4.1	10
28	SKINK: a web server for string kernel based kink prediction in α-helices. Bioinformatics, 2014, 30, 1769-1770.	4.1	1
29	Efficient computation of root mean square deviations under rigid transformations. Journal of Computational Chemistry, 2014, 35, 765-771.	3.3	9
30	Parallelized Clustering of Protein Structures on CUDA-Enabled GPUs. , 2014, , .		2
31	Competing Salt Effects on Phase Behavior of Protein Solutions: Tailoring of Protein Interaction by the Binding of Multivalent Ions and Charge Screening. Journal of Physical Chemistry B, 2014, 118, 11365-11374.	2.6	35
32	A Greedy Algorithm for Hierarchical Complete Linkage Clustering. Lecture Notes in Computer Science, 2014, , 25-34.	1.3	3
33	NightShift: NMR shift inference by general hybrid model training - a framework for NMR chemical shift prediction. BMC Bioinformatics, 2013, 14, 98.	2.6	1
34	PresentaBALL — A powerful package for presentations and lessons in structural biology. , 2013, , .		4
35	Instruction of haematopoietic lineage choices, evolution of transcriptional landscapes and cancer stem cell hierarchies derived from an <scp>AML</scp> 1― <scp>ETO</scp> mouse model. EMBO Molecular Medicine, 2013, 5, 1804-1820.	6.9	33
36	A dynamic program analysis to find floating-point accuracy problems. , 2012, , .		80

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37	CellLineNavigator: a workbench for cancer cell line analysis. Nucleic Acids Research, 2012, 41, D942-D948.	14.5	15
38	ProteinScanAR - An Augmented Reality Web Application for High School Education in Biomolecular Life Sciences. , 2012, , .		14
39	On the Applicability of Elastic Network Normal Modes in Small-Molecule Docking. Journal of Chemical Information and Modeling, 2012, 52, 844-856.	5.4	27
40	lsotope pattern deconvolution for peptide mass spectrometry by non-negative least squares/least absolute deviation template matching. BMC Bioinformatics, 2012, 13, 291.	2.6	14
41	A dynamic program analysis to find floating-point accuracy problems. ACM SIGPLAN Notices, 2012, 47, 453-462.	0.2	35
42	String Kernels and High-Quality Data Set for Improved Prediction of Kinked Helices in α-Helical Membrane Proteins. Journal of Chemical Information and Modeling, 2011, 51, 3017-3025.	5.4	15
43	Automated bond order assignment as an optimization problem. Bioinformatics, 2011, 27, 619-625.	4.1	13
44	A fast solver for nonlocal electrostatic theory in biomolecular science and engineering. , 2011, , .		5
45	BALL - biochemical algorithms library 1.3. BMC Bioinformatics, 2010, 11, 531.	2.6	62
46	A new numerical method for nonlocal electrostatics in biomolecular simulations. Journal of Computational Physics, 2010, 229, 4059-4074.	3.8	28
47	Universality of protein reentrant condensation in solution induced by multivalent metal ions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3450-3457.	2.6	106
48	Characterization of metalâ€labelled peptides by matrixâ€assisted laser desorption/ionization mass spectrometry and tandem mass spectrometry. Rapid Communications in Mass Spectrometry, 2010, 24, 3279-3289.	1.5	13
49	Human SAP18 mediates assembly of a splicing regulatory multiprotein complex via its ubiquitin-like fold. Rna, 2010, 16, 2442-2454.	3.5	40
50	Measuring properties of molecular surfaces using ray casting. , 2010, , .		9
51	Real-Time Ray Tracing of Complex Molecular Scenes. , 2010, , .		7
52	Signal Processing in Proteomics. Methods in Molecular Biology, 2010, 604, 145-161.	0.9	2
53	Highly accelerated feature detection in proteomics data sets using modern graphics processing units. Bioinformatics, 2009, 25, 1937-1943.	4.1	36
54	A consensus line search algorithm for molecular potential energy functions. Journal of Computational Chemistry, 2009, 30, 1499-1509.	3.3	3

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55	Revisiting Automated G-Protein Coupled Receptor Modeling: The Benefit of Additional Template Structures for a Neurokinin-1 Receptor Model. Journal of Medicinal Chemistry, 2009, 52, 3166-3173.	6.4	30
56	OpenMS – An open-source software framework for mass spectrometry. BMC Bioinformatics, 2008, 9, 163.	2.6	556
57	Computational Quantification of Peptides from LC-MS Data. Journal of Computational Biology, 2008, 15, 685-704.	1.6	12
58	Reentrant Condensation of Proteins in Solution Induced by Multivalent Counterions. Physical Review Letters, 2008, 101, 148101.	7.8	184
59	Electrostatic potentials of proteins in water: a structured continuum approach. Bioinformatics, 2007, 23, e99-e103.	4.1	41
60	Efficient Analysis of Mass Spectrometry Data Using the Isotope Wavelet. AIP Conference Proceedings, 2007, , .	0.4	6
61	A Fast and Accurate Algorithm for the Quantification of Peptides from Mass Spectrometry Data. Lecture Notes in Computer Science, 2007, , 473-487.	1.3	9
62	BN++ – A Biological Information System. Journal of Integrative Bioinformatics, 2006, 3, 148-161.	1.5	17
63	A minimally invasive multiple marker approach allows highly efficient detection of meningioma tumors. BMC Bioinformatics, 2006, 7, 539.	2.6	26
64	Glycosylation patterns of human chorionic gonadotropin revealed by liquid chromatography-mass spectrometry and bioinformatics. Electrophoresis, 2006, 27, 2734-2746.	2.4	35
65	BALLView: a tool for research and education in molecular modeling. Bioinformatics, 2006, 22, 365-366.	4.1	53
66	High-accuracy peak picking of proteomics data using wavelet techniques. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2006, , 243-54.	0.7	22
67	BALLView: An object-oriented molecular visualization and modeling framework. Journal of Computer-Aided Molecular Design, 2005, 19, 791-800.	2.9	40
68	Complex humoral immune response against a benign tumor: Frequent antibody response against specific antigens as diagnostic targets. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 9601-9606.	7.1	73
69	Novel Formulation of Nonlocal Electrostatics. Physical Review Letters, 2004, 93, 108104.	7.8	83
70	Structure prediction of protein complexes by an NMR-based protein docking algorithm. Journal of Biomolecular NMR, 2001, 20, 15-21.	2.8	16
71	Modeling Protein-Protein and Protein-DNA Docking. , 0, , 601-650.		2