William R Cannon

List of Publications by Year
in descending order

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48 papers	1,884 citations	331670 21 h-index	302126 39 g-index
49 all docs	49 docs citations	49 times ranked	2478 citing authors

#	Article	IF	Citations
1	Integrating machine learning and multiscale modelingâ€”perspectives, challenges, and opportunities in the biological, biomedical, and behavioral sciences. Npj Digital Medicine, 2019, 2, 115.	10.9	319
2	Sulfate Anion in Water: Model Structural, Thermodynamic, and Dynamic Properties. The Journal of Physical Chemistry, 1994, 98, 6225-6230.	2.9	185
3	Multiscale Modeling Meets Machine Learning: What Can We Learn?. Archives of Computational Methods in Engineering, 2021, 28, 1017-1037.	10.2	164
4	Solvation, Reorganization Energy, and Biological Catalysis. Journal of Biological Chemistry, 1998, 273, 26257-26260.	3.4	152
5	Mathematical Modeling of Microbial Community Dynamics: A Methodological Review. Processes, 2014, 2, 711-752.	2.8	152
6	A perspective on biological catalysis. Nature Structural and Molecular Biology, 1996, 3, 821-833.	8.2	148
7	Circadian Proteomic Analysis Uncovers Mechanisms of Post-Transcriptional Regulation in Metabolic Pathways. Cell Systems, 2018, 7, 613-626.e5.	6.2	93
8	A support vector machine model for the prediction of proteotypic peptides for accurate mass and time proteomics. Bioinformatics, 2008, 24, 1503-1509.	4.1	59
9	Multiscale Modeling in the Clinic: Drug Design and Development. Annals of Biomedical Engineering, 2016, 44, 2591-2610.	2.5	50
10	Electrostatic Characterization of Enzyme Complexes:â€‰ Evaluation of the Mechanism of Catalysis of Dihydrofolate Reductase. Journal of the American Chemical Society, 1997, 119, 2386-2395.	13.7	46
11	A nitrogenase-like enzyme system catalyzes methionine, ethylene, and methane biogenesis. Science, 2020, 369, 1094-1098.	12.6	44
12	A support vector machine model for the prediction of proteotypic peptides for accurate mass and time proteomics. Bioinformatics, 2010, 26, 1677-1683.	4.1	39
13	Current trends in computational inference from mass spectrometry-based proteomics. Briefings in Bioinformatics, 2007, 8, 304-317.	6.5	34
14	Sequence optimization as an alternative to de novo analysis of tandem mass spectrometry data. Bioinformatics, 2004, 20, 2296-2304.	4.1	33
15	VESPA: software to facilitate genomic annotation of prokaryotic organisms through integration of proteomic and transcriptomic data. BMC Genomics, 2012, 13, 131.	2.8	31
16	Comparison of Probability and Likelihood Models for Peptide Identification from Tandem Mass Spectrometry Data. Journal of Proteome Research, 2005, 4, 1687-1698.	3.7	28
17	pGraph: Efficient Parallel Construction of Large-Scale Protein Sequence Homology Graphs. IEEE Transactions on Parallel and Distributed Systems, 2012, 23, 1923-1933.	5.6	28
18	Molecular recognition: effect of rotational isomers on host-guest binding. Journal of the American Chemical Society, 1993, 115, 879-884.	13.7	24

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19	A General System for Studying Proteinâ^'Protein Interactions in Gram-Negative Bacteria. Journal of Proteome Research, 2008, 7, 3319-3328.	3.7	24
20	Prediction of Metabolite Concentrations, Rate Constants and Post-Translational Regulation Using Maximum Entropy-Based Simulations with Application to Central Metabolism of Neurospora crassa. Processes, 2018, 6, 63.	2.8	24
21	Whipple's disease, genomics, and drug therapy. Lancet, The, 2003, 361, 1916.	13.7	23
22	MapReduce implementation of a hybrid spectral library-database search method for large-scale peptide identification. Bioinformatics, 2011, 27, 3072-3073.	4.1	23
23	Consideration of the pH-dependent inhibition of dihydrofolate reductase by methotrexate 1 1Edited by B. Honig. Journal of Molecular Biology, 1997, 271, 656-668.	4.2	22
24	Improved peptide sequencing using isotope information inherent in tandem mass spectra. Rapid Communications in Mass Spectrometry, 2003, 17, 1793-1801.	1.5	20
25	Large Improvements in MS/MS-Based Peptide Identification Rates using a Hybrid Analysis. Journal of Proteome Research, 2011, 10, 2306-2317.	3.7	19
26	Simulating Metabolism with Statistical Thermodynamics. PLoS ONE, 2014, 9, e103582.	2.5	13
27	Statistically Inferring Proteinâ^'Protein Associations with Affinity Isolation LCâ^'MS/MS Assays. Journal of Proteome Research, 2007, 6, 3788-3795.	3.7	11
28	Evaluation of the influence of amino acid composition on the propensity for collision-induced dissociation of model peptides using molecular dynamics simulations. Journal of the American Society for Mass Spectrometry, 2007, 18, 1625-1637.	2.8	10
29	Physicochemical/Thermodynamic Framework for the Interpretation of Peptide Tandem Mass Spectra. Journal of Physical Chemistry C, 2010, 114, 5360-5366.	3.1	9
30	Concepts, Challenges, and Successes in Modeling Thermodynamics of Metabolism. Frontiers in Bioengineering and Biotechnology, 2014, 2, 53.	4.1	9
31	A Scalable Parallel Approach for Peptide Identification from Large-Scale Mass Spectrometry Data. , 2009, , .		6
32	Non-steady state mass action dynamics without rate constants: dynamics of coupled reactions using chemical potentials. Physical Biology, 2017, 14, 055003.	1.8	6
33	Enzyme activities predicted by metabolite concentrations and solvent capacity in the cell. Journal of the Royal Society Interface, 2020, 17, 20200656.	3.4	6
34	Support Vector Machine Classification of Probability Models and Peptide Features for Improved Peptide Identification from Shotgun Proteomics. , 2007, , .		5
35	A model of random sequences for de novo peptide sequencing. , 0, , .		4
36	Comparison of Optimal Thermodynamic Models of the Tricarboxylic Acid Cycle from Heterotrophs, Cyanobacteria, and Green Sulfur Bacteria. Journal of Physical Chemistry B, 2014, 118, 141215120729003.	2.6	4

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37	SEBINI-CABIN: An Analysis Pipeline for Biological Network Inference, with a Case Study in Protein-Protein Interaction Network Reconstruction. , 2007, , .		3
38	Conservative and nonconservative mutations in proteins: Anomalous mutations in a transport receptor analyzed by free energy and quantum chemical calculations. Protein Science, 1995, 4, 387-393.	7.6	3
39	An analysis pipeline for the inference of protein-protein interaction networks. International Journal of Data Mining and Bioinformatics, 2009, 3, 409.	0.1	3
40	Peptide identification via constrained multi-objective optimization: Pareto-based genetic algorithms. Concurrency Computation Practice and Experience, 2005, 17, 1687-1704.	2.2	2
41	Bringing high-performance computing to the biologist's workbench: approaches, applications, and challenges. Journal of Physics: Conference Series, 2008, 125, 012052.	0.4	2
42	On the Reunification of Chemical and Biochemical Thermodynamics: A Simple Example for Classroom Use. Journal of Chemical Education, 2019, 96, 274-284.	2.3	2
43	Applications in Data-Intensive Computing. Advances in Computers, 2010, , 1-70.	1.6	1
44	PROTEOTYPING OF MICROBIAL COMMUNITIES BY OPTIMIZATION OF TANDEM MASS SPECTROMETRY DATA INTERPRETATION. , 2011, , .		1
45	THE CHALLENGE OF PROTEOMIC DATA, FROM MOLECULAR SIGNALS TO BIOLOGICAL NETWORKS AND DISEASE: SESSION INTRODUCTION. , 2005, , .		0
46	Statistically appraising process quality of affinity isolation experiments. Computational Statistics and Data Analysis, 2009, 53, 1720-1726.	1.2	0
47	The formulation of chemical potentials and free energy changes in biochemical reactions. Physical Chemistry Chemical Physics, 2021, 23, 14783-14795.	2.8	0
48	COMPUTATIONAL PROTEOMICS: HIGH-THROUGHPUT ANALYSIS FOR SYSTEMS BIOLOGY â€“ AN INTRODUCTION. , 2006, , .		0