Bruce R Donald

List of Publications by Year
in descending order

53 papers	2,601 citations	257450 24 h-index	254184 43 g-index
54 all docs	54 docs citations	54 times ranked	2381 citing authors

#	Article	IF	Citations
1	Chiral evasion and stereospecific antifolate resistance in Staphylococcus aureus. PLoS Computational Biology, 2022, 18, e1009855.	3.2	6
2	Minimization-Aware Recursive K*: A Novel, Provable Algorithm that Accelerates Ensemble-Based Protein Design and Provably Approximates the Energy Landscape. Journal of Computational Biology, 2020, 27, 550-564.	1.6	10
3	Novel, provable algorithms for efficient ensemble-based computational protein design and their application to the redesign of the c-Raf-RBD:KRas protein-protein interface. PLoS Computational Biology, 2020, 16, e1007447.	3.2	11
4	Title is missing!. , 2020, 16, e1007447.		0
5	Title is missing!. , 2020, 16, e1007447.		0
6	Title is missing!. , 2020, 16, e1007447.		0
7	Title is missing!. , 2020, 16, e1007447.		0
8	Title is missing!. , 2020, 16, e1007447.		0
9	Title is missing!. , 2020, 16, e1007447.		0
10	Computational Analysis of Energy Landscapes Reveals Dynamic Features That Contribute to Binding of Inhibitors to CFTR-Associated Ligand. Journal of Physical Chemistry B, 2019, 123, 10441-10455.	2.6	9
11	Toward Broad Spectrum Dihydrofolate Reductase Inhibitors Targeting Trimethoprim Resistant Enzymes Identified in Clinical Isolates of Methicillin Resistant Staphylococcus aureus. ACS Infectious Diseases, 2019, 5, 1896-1906.	3.8	16
12	Minimal NMR distance information for rigidity of protein graphs. Discrete Applied Mathematics, 2019, 256, 91-104.	0.9	26
13	BBK* (Branch and Bound Over K*): A Provable and Efficient Ensemble-Based Protein Design Algorithm to Optimize Stability and Binding Affinity Over Large Sequence Spaces. Journal of Computational Biology, 2018, 25, 726-739.	1.6	22
14	OSPREY 3.0: Openâ€source protein redesign for you, with powerful new features. Journal of Computational Chemistry, 2018, 39, 2494-2507.	3.3	56
15	Continuous Interdomain Orientation Distributions Reveal Components of Binding Thermodynamics. Journal of Molecular Biology, 2018, 430, 3412-3426.	4.2	12
16	OSPREY Predicts Resistance Mutations Using Positive and Negative Computational Protein Design. Methods in Molecular Biology, 2017, 1529, 291-306.	0.9	15
17	Parallel Computational Protein Design. Methods in Molecular Biology, 2017, 1529, 265-277.	0.9	4
18	LUTE (Local Unpruned Tuple Expansion): Accurate Continuously Flexible Protein Design with General Energy Functions and Rigid Rotamer-Like Efficiency. Journal of Computational Biology, 2017, 24, 536-546.	1.6	18

#	Article	IF	Citations
19	CATS (Coordinates of Atoms by Taylor Series): protein design with backbone flexibility in all locally feasible directions. Bioinformatics, 2017, 33, i5-i12.	4.1	15
20	A critical analysis of computational protein design with sparse residue interaction graphs. PLoS Computational Biology, 2017, 13, e1005346.	3.2	2
21	Fast search algorithms for computational protein design. Journal of Computational Chemistry, 2016, 37, 1048-1058.	3.3	30
22	Algorithms for protein design. Current Opinion in Structural Biology, 2016, 39, 16-26.	5.7	67
23	cOSPREY: A Cloud-Based Distributed Algorithm for Large-Scale Computational Protein Design. Journal of Computational Biology, 2016, 23, 737-749.	1.6	3
24	BWM*: A Novel, Provable, Ensemble-based Dynamic Programming Algorithm for Sparse Approximations of Computational Protein Design. Journal of Computational Biology, 2016, 23, 413-424.	1.6	24
25	<scp>comets</scp>(Constrained Optimization of Multistate Energies by Tree Search): A Provable and Efficient Protein Design Algorithm to Optimize Binding Affinity and Specificity with Respect to Sequence. Journal of Computational Biology, 2016, 23, 311-321.	1.6	30
26	Improved energy bound accuracy enhances the efficiency of continuous protein design. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1151-1164.	2.6	12
27	Fast gap-free enumeration of conformations and sequences for protein design. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1859-1877.	2.6	19
28	Protein design algorithms predict viable resistance to an experimental antifolate. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 749-754.	7.1	48
29	Crystal structure, conformational fixation and entry-related interactions of mature ligand-free HIV-1 Env. Nature Structural and Molecular Biology, 2015, 22, 522-531.	8.2	333
30	Compact Representation of Continuous Energy Surfaces for More Efficient Protein Design. Journal of Chemical Theory and Computation, 2015, 11, 2292-2306.	5.3	25
31	An efficient parallel algorithm for accelerating computational protein design. Bioinformatics, 2014, 30, i255-i263.	4.1	17
32	Enhanced Potency of a Broadly Neutralizing HIV-1 Antibody In Vitro Improves Protection against Lentiviral Infection In Vivo. Journal of Virology, 2014, 88, 12669-12682.	3.4	248
33	osprey. Methods in Enzymology, 2013, 523, 87-107.	1.0	105
34	Deadâ€end elimination with perturbations (DEEPer): A provable protein design algorithm with continuous sidechain and backbone flexibility. Proteins: Structure, Function and Bioinformatics, 2013, 81, 18-39.	2.6	79
35	Planning and control for microassembly of structures composed of stress-engineered MEMS microrobots. International Journal of Robotics Research, 2013, 32, 218-246.	8.5	46
36	Simultaneous determination of subunit and complex structures of symmetric homo-oligomers from ambiguous NMR data. , 2013, , .		0

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37	Computational Design of a PDZ Domain Peptide Inhibitor that Rescues CFTR Activity. PLoS Computational Biology, 2012, 8, e1002477.	3.2	105
38	Protein Design Using Continuous Rotamers. PLoS Computational Biology, 2012, 8, e1002335.	3.2	88
39	NVR-BIP: Nuclear Vector Replacement using Binary Integer Programming for NMR Structure-Based Assignments. Computer Journal, 2011, 54, 708-716.	2.4	11
40	Predicting resistance mutations using protein design algorithms. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 13707-13712.	7.1	113
41	Computational structure-based redesign of enzyme activity. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3764-3769.	7.1	185
42	Automated NMR assignment and protein structure determination using sparse dipolar coupling constraints. Progress in Nuclear Magnetic Resonance Spectroscopy, 2009, 55, 101-127.	7.5	36
43	NVR-BIP: Nuclear vector replacement using binary integer programming for NMR structure-based assignments. , 2009, , .		1
44	The minimized deadâ€end elimination criterion and its application to protein redesign in a hybrid scoring and search algorithm for computing partition functions over molecular ensembles. Journal of Computational Chemistry, 2008, 29, 1527-1542.	3.3	117
45	Planar Microassembly by Parallel Actuation of MEMS Microrobots. Journal of Microelectromechanical Systems, 2008, 17, 789-808.	2.5	135
46	Algorithm for backrub motions in protein design. Bioinformatics, 2008, 24, i196-i204.	4.1	72
47	A HAUSDORFF-BASED NOE ASSIGNMENT ALGORITHM USING PROTEIN BACKBONE DETERMINED FROM RESIDUAL DIPOLAR COUPLINGS AND ROTAMER PATTERNS. , 2008, , .		8
48	Dead-End Elimination with Backbone Flexibility. Bioinformatics, 2007, 23, i185-i194.	4.1	70
49	Allosteric Inhibition of the Protein-Protein Interaction between the Leukemia-Associated Proteins Runx1 and CBFÎ². Chemistry and Biology, 2007, 14, 1186-1197.	6.0	114
50	Redesigning the PheA Domain of Gramicidin Synthetase Leads to a New Understanding of the Enzyme's Mechanism and Selectivityâ€. Biochemistry, 2006, 45, 15495-15504.	2.5	63
51	Improved Pruning algorithms and Divide-and-Conquer strategies for Dead-End Elimination, with application to protein design. Bioinformatics, 2006, 22, e174-e183.	4.1	46
52	A Novel Ensemble-Based Scoring and Search Algorithm for Protein Redesign and Its Application to Modify the Substrate Specificity of the Gramicidin Synthetase A Phenylalanine Adenylation Enzyme. Journal of Computational Biology, 2005, 12, 740-761.	1.6	103
53	A rational rotation method for robust geometric algorithms. , 1992, , .		25