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	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
2	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
3	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
4	Planar Microassembly by Parallel Actuation of MEMS Microrobots. Journal of Microelectromechanical Systems, 2008, 17, 789-808.	2.5	135
5	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
6	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
7	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
8	Computational Design of a PDZ Domain Peptide Inhibitor that Rescues CFTR Activity. PLoS Computational Biology, 2012, 8, e1002477.	3.2	105
9	osprey. Methods in Enzymology, 2013, 523, 87-107.	1.0	105
10	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
11	Protein Design Using Continuous Rotamers. PLoS Computational Biology, 2012, 8, e1002335.	3.2	88
12	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
13	Algorithm for backrub motions in protein design. Bioinformatics, 2008, 24, i196-i204.	4.1	72
14	Dead-End Elimination with Backbone Flexibility. Bioinformatics, 2007, 23, i185-i194.	4.1	70
15	Algorithms for protein design. Current Opinion in Structural Biology, 2016, 39, 16-26.	5.7	67
16	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
17	OSPREY 3.0: Openâ€source protein redesign for you, with powerful new features. Journal of Computational Chemistry, 2018, 39, 2494-2507.	3.3	56
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	Fast search algorithms for computational protein design. Journal of Computational Chemistry, 2016, 37, 1048-1058.	3.3	30
23	<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
24	Minimal NMR distance information for rigidity of protein graphs. Discrete Applied Mathematics, 2019, 256, 91-104.	0.9	26
25	A rational rotation method for robust geometric algorithms. , 1992, , .		25
26	Compact Representation of Continuous Energy Surfaces for More Efficient Protein Design. Journal of Chemical Theory and Computation, 2015, 11, 2292-2306.	5.3	25
27	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
28	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
29	Fast gap-free enumeration of conformations and sequences for protein design. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1859-1877.	2.6	19
30	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
31	An efficient parallel algorithm for accelerating computational protein design. Bioinformatics, 2014, 30, i255-i263.	4.1	17
32	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
33	OSPREY Predicts Resistance Mutations Using Positive and Negative Computational Protein Design. Methods in Molecular Biology, 2017, 1529, 291-306.	0.9	15
34	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
35	Improved energy bound accuracy enhances the efficiency of continuous protein design. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1151-1164.	2.6	12
36	Continuous Interdomain Orientation Distributions Reveal Components of Binding Thermodynamics. Journal of Molecular Biology, 2018, 430, 3412-3426.	4.2	12

#	Article	IF	Citations
37	NVR-BIP: Nuclear Vector Replacement using Binary Integer Programming for NMR Structure-Based Assignments. Computer Journal, 2011, 54, 708-716.	2.4	11
38	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
39	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
40	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
41	A HAUSDORFF-BASED NOE ASSIGNMENT ALGORITHM USING PROTEIN BACKBONE DETERMINED FROM RESIDUAL DIPOLAR COUPLINGS AND ROTAMER PATTERNS. , 2008, , .		8
42	Chiral evasion and stereospecific antifolate resistance in Staphylococcus aureus. PLoS Computational Biology, 2022, 18, e1009855.	3.2	6
43	Parallel Computational Protein Design. Methods in Molecular Biology, 2017, 1529, 265-277.	0.9	4
44	cOSPREY: A Cloud-Based Distributed Algorithm for Large-Scale Computational Protein Design. Journal of Computational Biology, 2016, 23, 737-749.	1.6	3
45	A critical analysis of computational protein design with sparse residue interaction graphs. PLoS Computational Biology, 2017, 13, e1005346.	3.2	2
46	NVR-BIP: Nuclear vector replacement using binary integer programming for NMR structure-based assignments. , 2009, , .		1
47	Simultaneous determination of subunit and complex structures of symmetric homo-oligomers from ambiguous NMR data. , 2013, , .		0
48	Title is missing!. , 2020, 16, e1007447.		0
49	Title is missing!. , 2020, 16, e1007447.		0
50	Title is missing!. , 2020, 16, e1007447.		0
51	Title is missing!. , 2020, 16, e1007447.		0
52	Title is missing!. , 2020, 16, e1007447.		0
53	Title is missing!. , 2020, 16, e1007447.		0