

Justin L Maccallum

List of Publications by Year in descending order

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41
papers

4,038
citations

257450

24
h-index

302126

39
g-index

46
all docs

46
docs citations

46
times ranked

5037
citing authors

#	ARTICLE	IF	CITATIONS
1	The Protein-Folding Problem, 50 Years On. <i>Science</i> , 2012, 338, 1042-1046.	12.6	1,231
2	Distribution of Amino Acids in a Lipid Bilayer from Computer Simulations. <i>Biophysical Journal</i> , 2008, 94, 3393-3404.	0.5	486
3	Molecular View of Cholesterol Flip-Flop and Chemical Potential in Different Membrane Environments. <i>Journal of the American Chemical Society</i> , 2009, 131, 12714-12720.	13.7	256
4	Partitioning of Amino Acid Side Chains into Lipid Bilayers: Results from Computer Simulations and Comparison to Experiment. <i>Journal of General Physiology</i> , 2007, 129, 371-377.	1.9	244
5	Thermodynamic Analysis of the Effect of Cholesterol on Dipalmitoylphosphatidylcholine Lipid Membranes. <i>Journal of the American Chemical Society</i> , 2009, 131, 1972-1978.	13.7	157
6	Membrane protein simulations with a united-atom lipid and all-atom protein model: lipid-protein interactions, side chain transfer free energies and model proteins. <i>Journal of Physics Condensed Matter</i> , 2006, 18, S1221-S1234.	1.8	148
7	Computer Simulation of the Distribution of Hexane in a Lipid Bilayer: Spatially Resolved Free Energy, Entropy, and Enthalpy Profiles. <i>Journal of the American Chemical Society</i> , 2006, 128, 125-130.	13.7	135
8	Determining protein structures by combining semireliable data with atomistic physical models by Bayesian inference. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 6985-6990.	7.1	132
9	Structures of Neat and Hydrated 1-Octanol from Computer Simulations. <i>Journal of the American Chemical Society</i> , 2002, 124, 15085-15093.	13.7	113
10	Calculation of the water-cyclohexane transfer free energies of neutral amino acid side-chain analogs using the OPLS all-atom force field. <i>Journal of Computational Chemistry</i> , 2003, 24, 1930-1935.	3.3	101
11	Accelerating molecular simulations of proteins using Bayesian inference on weak information. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 11846-11851.	7.1	88
12	Assessment of protein structure refinement in CASP9. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 74-90.	2.6	87
13	Transfer of Arginine into Lipid Bilayers Is Nonadditive. <i>Biophysical Journal</i> , 2011, 101, 110-117.	0.5	86
14	Hydrophobicity scales: a thermodynamic looking glass into lipid-protein interactions. <i>Trends in Biochemical Sciences</i> , 2011, 36, 653-662.	7.5	81
15	Hydrophobic association of α -helices, steric dewetting, and enthalpic barriers to protein folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 6206-6210.	7.1	78
16	From Inhibition to Degradation: Targeting the Antiapoptotic Protein Myeloid Cell Leukemia 1 (MCL1). <i>Journal of Medicinal Chemistry</i> , 2019, 62, 5522-5540.	6.4	77
17	Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4770-4779.	5.3	76
18	Computed Binding of Peptides to Proteins with MELD-Accelerated Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 870-876.	5.3	68

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19	Blind protein structure prediction using accelerated free-energy simulations. <i>Science Advances</i> , 2016, 2, e1601274.	10.3	57
20	Computer simulation of the KvAP voltage-gated potassium channel: steered molecular dynamics of the voltage sensor. <i>FEBS Letters</i> , 2004, 564, 325-332.	2.8	49
21	Direct Simulation of Transmembrane Helix Association: Role of Asparagines. <i>Biophysical Journal</i> , 2004, 87, 1650-1656.	0.5	37
22	Single Molecule Conformational Memory Extraction: P5ab RNA Hairpin. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6597-6603.	2.6	35
23	Bacterial cyclic diguanylate signaling networks sense temperature. <i>Nature Communications</i> , 2021, 12, 1986.	12.8	35
24	Development of an ultra-sensitive electrochemical sensor for δ^9 -tetrahydrocannabinol (THC) and its metabolites using carbon paper electrodes. <i>Electrochimica Acta</i> , 2019, 307, 351-359.	5.2	34
25	Computing the Relative Stabilities and the Per-Residue Components in Protein Conformational Changes. <i>Structure</i> , 2014, 22, 168-175.	3.3	27
26	The emerging role of physical modeling in the future of structure determination. <i>Current Opinion in Structural Biology</i> , 2018, 49, 145-153.	5.7	21
27	FlexE: Using Elastic Network Models to Compare Models of Protein Structure. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3985-3991.	5.3	20
28	Computer simulations of voltage-gated potassium channel KvAP. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 1071-1078.	2.0	14
29	A Synthetically Accessible Small-Molecule Inhibitor of USP5-Cav3.2 Calcium Channel Interactions with Analgesic Properties. <i>ACS Chemical Neuroscience</i> , 2022, 13, 524-536.	3.5	12
30	High Accuracy Protein Structures from Minimal Sparse Paramagnetic Solid-State NMR Restraints. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 6564-6568.	13.8	11
31	Molecular modeling of biomolecules by paramagnetic NMR and computational hybrid methods. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2017, 1865, 1654-1663.	2.3	9
32	Online Optimization of Total Acceptance in Hamiltonian Replica Exchange Simulations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5448-5457.	2.6	8
33	Correlation between Labeling Yield and Surface Accessibility in Covalent Labeling Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 207-216.	2.8	8
34	Extracting representative structures from protein conformational ensembles. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2671-2680.	2.6	5
35	An Integrative Approach to Determine 3D Protein Structures Using Sparse Paramagnetic NMR Data and Physical Modeling. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 676268.	3.5	4
36	High Accuracy Protein Structures from Minimal Sparse Paramagnetic Solid-State NMR Restraints. <i>Angewandte Chemie</i> , 2019, 131, 6636-6640.	2.0	3

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37	Constraint methods that accelerate free-energy simulations of biomolecules. Journal of Chemical Physics, 2015, 143, 243143.	3.0	1
38	Automatic Protein Structure Determination from Sparse NMR Spectroscopy Data. Biophysical Journal, 2016, 110, 153a.	0.5	1
39	Combining Physics and Knowledge in Blind Protein Structure Prediction. Biophysical Journal, 2016, 110, 345a.	0.5	0
40	Electrochemical Detection of Endotoxins from Gram-Negative Bacteria Using Immobilized TLR4 Immunoproteins. ECS Meeting Abstracts, 2020, MA2020-01, 1889-1889.	0.0	0
41	Towards the Electrochemical Detection of Cannabis Drugs in Human Saliva. ECS Meeting Abstracts, 2020, MA2020-01, 1959-1959.	0.0	0