Justin L Maccallum

List of Publications by Year
in descending order

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	A Synthetically Accessible Small-Molecule Inhibitor of USP5-Cav3.2 Calcium Channel Interactions with Analgesic Properties. ACS Chemical Neuroscience, 2022, 13, 524-536.	3.5	12
2	Bacterial cyclic diguanylate signaling networks sense temperature. Nature Communications, 2021, 12, 1986.	12.8	35
3	An Integrative Approach to Determine 3D Protein Structures Using Sparse Paramagnetic NMR Data and Physical Modeling. Frontiers in Molecular Biosciences, 2021, 8, 676268.	3.5	4
4	Correlation between Labeling Yield and Surface Accessibility in Covalent Labeling Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2020, 31, 207-216.	2.8	8
5	Electrochemical Detection of Endotoxins from Gram-Negative Bacteria Using Immobilized TLR4 Immunoproteins. ECS Meeting Abstracts, 2020, MA2020-01, 1889-1889.	0.0	0
6	Towards the Electrochemical Detection of Cannabis Drugs in Human Saliva. ECS Meeting Abstracts, 2020, MA2020-01, 1959-1959.	0.0	0
7	From Inhibition to Degradation: Targeting the Antiapoptotic Protein Myeloid Cell Leukemia 1 (MCL1). Journal of Medicinal Chemistry, 2019, 62, 5522-5540.	6.4	77
8	High Accuracy Protein Structures from Minimal Sparse Paramagnetic Solidâ€State NMR Restraints. Angewandte Chemie - International Edition, 2019, 58, 6564-6568.	13.8	11
9	Development of an ultra-sensitive electrochemical sensor for Î”9-tetrahydrocannabinol (THC) and its metabolites using carbon paper electrodes. Electrochimica Acta, 2019, 307, 351-359.	5.2	34
10	High Accuracy Protein Structures from Minimal Sparse Paramagnetic Solidâ€State NMR Restraints. Angewandte Chemie, 2019, 131, 6636-6640.	2.0	3
11	Online Optimization of Total Acceptance in Hamiltonian Replica Exchange Simulations. Journal of Physical Chemistry B, 2018, 122, 5448-5457.	2.6	8
12	The emerging role of physical modeling in the future of structure determination. Current Opinion in Structural Biology, 2018, 49, 145-153.	5.7	21
13	Computed Binding of Peptides to Proteins with MELD-Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 870-876.	5.3	68
14	Molecular modeling of biomolecules by paramagnetic NMR and computational hybrid methods. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1654-1663.	2.3	9
15	Blind protein structure prediction using accelerated free-energy simulations. Science Advances, 2016, 2, e1601274.	10.3	57
16	Automatic Protein Structure Determination from Sparse NMR Spectroscopy Data. Biophysical Journal, 2016, 110, 153a.	0.5	1
17	Combining Physics and Knowledge in Blind Protein Structure Prediction. Biophysical Journal, 2016, 110, 345a.	0.5	0
18	Constraint methods that accelerate free-energy simulations of biomolecules. Journal of Chemical Physics, 2015, 143, 243143.	3.0	1

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19	Determining protein structures by combining semireliable data with atomistic physical models by Bayesian inference. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6985-6990.	7.1	132
20	Accelerating molecular simulations of proteins using Bayesian inference on weak information. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 11846-11851.	7.1	88
21	Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations. Journal of Chemical Theory and Computation, 2015, 11, 4770-4779.	5.3	76
22	Extracting representative structures from protein conformational ensembles. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2671-2680.	2.6	5
23	Computing the Relative Stabilities and the Per-Residue Components in Protein Conformational Changes. Structure, 2014, 22, 168-175.	3.3	27
24	Single Molecule Conformational Memory Extraction: P5ab RNA Hairpin. Journal of Physical Chemistry B, 2014, 118, 6597-6603.	2.6	35
25	The Protein-Folding Problem, 50 Years On. Science, 2012, 338, 1042-1046.	12.6	1,231
26	FlexE: Using Elastic Network Models to Compare Models of Protein Structure. Journal of Chemical Theory and Computation, 2012, 8, 3985-3991.	5.3	20
27	Transfer of Arginine into Lipid Bilayers Is Nonadditive. Biophysical Journal, 2011, 101, 110-117.	0.5	86
28	Hydrophobicity scales: a thermodynamic looking glass into lipidâ€“protein interactions. Trends in Biochemical Sciences, 2011, 36, 653-662.	7.5	81
29	Assessment of protein structure refinement in CASP9. Proteins: Structure, Function and Bioinformatics, 2011, 79, 74-90.	2.6	87
30	Molecular View of Cholesterol Flip-Flop and Chemical Potential in Different Membrane Environments. Journal of the American Chemical Society, 2009, 131, 12714-12720.	13.7	256
31	Thermodynamic Analysis of the Effect of Cholesterol on Dipalmitoylphosphatidylcholine Lipid Membranes. Journal of the American Chemical Society, 2009, 131, 1972-1978.	13.7	157
32	Distribution of Amino Acids in a Lipid Bilayer from Computer Simulations. Biophysical Journal, 2008, 94, 3393-3404.	0.5	486
33	Hydrophobic association of Â-helices, steric dewetting, and enthalpic barriers to protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6206-6210.	7.1	78
34	Partitioning of Amino Acid Side Chains into Lipid Bilayers: Results from Computer Simulations and Comparison to Experiment. Journal of General Physiology, 2007, 129, 371-377.	1.9	244
35	Computer Simulation of the Distribution of Hexane in a Lipid Bilayer:Â Spatially Resolved Free Energy, Entropy, and Enthalpy Profiles. Journal of the American Chemical Society, 2006, 128, 125-130.	13.7	135
36	Membrane protein simulations with a united-atom lipid and all-atom protein model: lipidâ€“protein interactions, side chain transfer free energies and model proteins. Journal of Physics Condensed Matter, 2006, 18, S1221-S1234.	1.8	148

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37	Computer simulations of voltage-gated potassium channel KvAP. International Journal of Quantum Chemistry, 2004, 100, 1071-1078.	2.0	14
38	Direct Simulation of Transmembrane Helix Association: Role of Asparagines. Biophysical Journal, 2004, 87, 1650-1656.	0.5	37
39	Computer simulation of the KvAP voltage-gated potassium channel: steered molecular dynamics of the voltage sensor. FEBS Letters, 2004, 564, 325-332.	2.8	49
40	Calculation of the water-cyclohexane transfer free energies of neutral amino acid side-chain analogs using the OPLS all-atom force field. Journal of Computational Chemistry, 2003, 24, 1930-1935.	3.3	101
41	Structures of Neat and Hydrated 1-Octanol from Computer Simulations. Journal of the American Chemical Society, 2002, 124, 15085-15093.	13.7	113