David W Wright

List of Publications by Year
in descending order

35 papers	924 citations	567281 15 h-index	454955 30 g-index
35 all docs	35 docs citations	35 times ranked	1363 citing authors

#	Article	IF	Citations
1	Ensemble Simulations and Experimental Free Energy Distributions: Evaluation and Characterization of Isoxazole Amides as SMYD3 Inhibitors. Journal of Chemical Information and Modeling, 2022, 62, 2561-2570.	5.4	6
2	The performance of ensemble-based free energy protocols in computing binding affinities to ROS1 kinase. Scientific Reports, 2022, 12, .	3.3	2
3	Building Confidence in Simulation: Applications of EasyVVUQ. Advanced Theory and Simulations, 2020, 3, 1900246.	2.8	21
4	Hit-to-lead and lead optimization binding free energy calculations for G protein-coupled receptors. Interface Focus, 2020, 10, 20190128.	3.0	11
5	Application of the ESMACS Binding Free Energy Protocol to a Multiâ€Binding Site Lactate Dehydogenase A Ligand Dataset. Advanced Theory and Simulations, 2020, 3, 1900194.	2.8	9
6	EasyVVUQ: A Library for Verification, Validation and Uncertainty Quantification in High Performance Computing. Journal of Open Research Software, 2020, 8, 11.	5.9	34
7	Introducing VECMAtk - Verification, Validation and Uncertainty Quantification for Multiscale and HPC Simulations. Lecture Notes in Computer Science, 2019, , 479-492.	1.3	14
8	Atomistic Modeling of Scattering Curves for Human IgG1/4 Reveals New Structure-Function Insights. Biophysical Journal, 2019, 117, 2101-2119.	0.5	7
9	Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4. Scientific Reports, 2019, 9, 6017.	3.3	18
10	Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations. , 2018, , .		7
11	High-throughput binding affinity calculations at extreme scales. BMC Bioinformatics, 2018, 19, 482.	2.6	14
12	Enabling Trade-offs Between Accuracy and Computational Cost: Adaptive Algorithms to Reduce Time to Clinical Insight. , 2018, , .		5
13	Non-linearity of the collagen triple helix in solution and implications for collagen function. Biochemical Journal, 2017, 474, 2203-2217.	3.7	21
14	Combined Monte Carlo/torsion-angle molecular dynamics for ensemble modeling of proteins, nucleic acids and carbohydrates. Journal of Molecular Graphics and Modelling, 2017, 73, 179-190.	2.4	14
15	Flexibility in Mannan-Binding Lectin-Associated Serine Proteases-1 and -2 Provides Insight on Lectin Pathway Activation. Structure, 2017, 25, 364-375.	3.3	10
16	An Ensemble-Based Protocol for the Computational Prediction of Helixâ€“Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 2254-2270.	5.3	27
17	Rapid, Accurate, Precise, and Reliable Relative Free Energy Prediction Using Ensemble Based Thermodynamic Integration. Journal of Chemical Theory and Computation, 2017, 13, 210-222.	5.3	101
18	Domain structure of human complement C4b extends with increasing NaCl concentration: implications for its regulatory mechanism. Biochemical Journal, 2016, 473, 4473-4491.	3.7	4

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19	Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS). Journal of Applied Crystallography, 2016, 49, 1861-1875.	4.5	67
20	The solution structures of native and patient monomeric human IgA1 reveal asymmetric extended structures: implications for function and IgAN disease. Biochemical Journal, 2015, 471, 167-185.	3.7	22
21	Rapid, Precise, and Reproducible Prediction of Peptideâ€“MHC Binding Affinities from Molecular Dynamics That Correlate Well with Experiment. Journal of Chemical Theory and Computation, 2015, 11, 3346-3356.	5.3	122
22	Structure, Dynamics, and Function of the Hammerhead Ribozyme in Bulk Water and at a Clay Mineral Surface from Replica Exchange Molecular Dynamics. Langmuir, 2015, 31, 2493-2501.	3.5	16
23	Mutation V111I in HIV-2 Reverse Transcriptase Increases the Fitness of the Nucleoside Analogue-Resistant K65R and Q151M Viruses. Journal of Virology, 2015, 89, 833-843.	3.4	15
24	SCT: a suite of programs for comparing atomistic models with small-angle scattering data. Journal of Applied Crystallography, 2015, 48, 953-961.	4.5	30
25	Ten Simple Rules for Effective Computational Research. PLoS Computational Biology, 2014, 10, e1003506.	3.2	47
26	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	5.3	123
27	A Polymorphism at Position 400 in the Connection Subdomain of HIV-1 Reverse Transcriptase Affects Sensitivity to NNRTIs and RNaseH Activity. PLoS ONE, 2013, 8, e74078.	2.5	10
28	Mechanism of Drug Efficacy Within the EGF Receptor Revealed by Microsecond Molecular Dynamics Simulation. Molecular Cancer Therapeutics, 2012, 11, 2394-2400.	4.1	13
29	Thumbs Down for HIV: Domain Level Rearrangements Do Occur in the NNRTI-Bound HIV-1 Reverse Transcriptase. Journal of the American Chemical Society, 2012, 134, 12885-12888.	13.7	22
30	From base pair to bedside: molecular simulation and the translation of genomics to personalized medicine. Wiley Interdisciplinary Reviews: Systems Biology and Medicine, 2012, 4, 585-598.	6.6	11
31	Global Conformational Dynamics of HIV-1 Reverse Transcriptase Bound to Non-Nucleoside Inhibitors. Biology, 2012, 1, 222-244.	2.8	6
32	Quantized Water Access to the HIV-1 Protease Active Site as a Proposed Mechanism for Cooperative Mutations in Drug Affinity. Biochemistry, 2012, 51, 6487-6489.	2.5	3
33	Resolution of Discordant HIV-1 Protease Resistance Rankings Using Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2011, 51, 2636-2649.	5.4	10
34	Towards high-throughput, high-performance computational estimation of binding affinities for patient specific HIV-1 protease sequences. , 2011, , .		0
35	Accurate Ensemble Molecular Dynamics Binding Free Energy Ranking of Multidrug-Resistant HIV-1 Proteases. Journal of Chemical Information and Modeling, 2010, 50, 890-905.	5.4	82