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	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	5.3	123
2	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
3	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
4	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
5	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
6	Ten Simple Rules for Effective Computational Research. PLoS Computational Biology, 2014, 10, e1003506.	3.2	47
7	EasyVVUQ: A Library for Verification, Validation and Uncertainty Quantification in High Performance Computing. Journal of Open Research Software, 2020, 8, 11.	5.9	34
8	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
9	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
10	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
11	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
12	Non-linearity of the collagen triple helix in solution and implications for collagen function. Biochemical Journal, 2017, 474, 2203-2217.	3.7	21
13	Building Confidence in Simulation: Applications of EasyVVUQ. Advanced Theory and Simulations, 2020, 3, 1900246.	2.8	21
14	Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4. Scientific Reports, 2019, 9, 6017.	3.3	18
15	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
16	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
17	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
18	High-throughput binding affinity calculations at extreme scales. BMC Bioinformatics, 2018, 19, 482.	2.6	14

#	Article	IF	Citations
19	Introducing VECMAtk - Verification, Validation and Uncertainty Quantification for Multiscale and HPC Simulations. Lecture Notes in Computer Science, 2019, , 479-492.	1.3	14
20	Mechanism of Drug Efficacy Within the EGF Receptor Revealed by Microsecond Molecular Dynamics Simulation. Molecular Cancer Therapeutics, 2012, 11, 2394-2400.	4.1	13
21	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
22	Hit-to-lead and lead optimization binding free energy calculations for G protein-coupled receptors. Interface Focus, 2020, 10, 20190128.	3.0	11
23	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
24	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
25	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
26	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
27	Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations. , 2018, , .		7
28	Atomistic Modeling of Scattering Curves for Human IgG1/4 Reveals New Structure-Function Insights. Biophysical Journal, 2019, 117, 2101-2119.	0.5	7
29	Global Conformational Dynamics of HIV-1 Reverse Transcriptase Bound to Non-Nucleoside Inhibitors. Biology, 2012, 1, 222-244.	2.8	6
30	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
31	Enabling Trade-offs Between Accuracy and Computational Cost: Adaptive Algorithms to Reduce Time to Clinical Insight. , 2018, , .		5
32	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
33	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
34	The performance of ensemble-based free energy protocols in computing binding affinities to ROS1 kinase. Scientific Reports, 2022, 12, .	3.3	2
35	Towards high-throughput, high-performance computational estimation of binding affinities for patient specific HIV-1 protease sequences. , 2011, , .		0