Alex Dickson

List of Publications by Year
in descending order

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48	1,337	331670	377865
papers	citations	21 h-index	34 g-index

64	64	64	1393
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Creating Maps of the Ligand Binding Landscape for Kinetics-Based Drug Discovery. Methods in Molecular Biology, 2022, 2385, 325-334.	0.9	0
2	Local Ion Densities can Influence Transition Paths of Molecular Binding. Frontiers in Molecular Biosciences, 2022, 9, 858316.	3.5	2
3	The effect of the linker in ureaâ€based soluble epoxide hydrolase inhibitorsâ€™ on their bloodâ€brain penetration ability and drugâ€like properties. FASEB Journal, 2022, 36, .	0.5	0
4	A biosensor of protein foldedness identifies increased â€œholdaseâ€•activity of chaperones in the nucleus following increased cytosolic protein aggregation. Journal of Biological Chemistry, 2022, 298, 102158.	3.4	2
5	Membrane-Mediated Ligand Unbinding of the PK-11195 Ligand from TSPO. Biophysical Journal, 2021, 120, 158-167.	0.5	25
6	<scp>ClassicalGSG</scp>: Prediction of <scp>log</scp>P using classical molecular force fields and geometric scattering for graphs. Journal of Computational Chemistry, 2021, 42, 1006-1017.	3.3	6
7	Predicting partition coefficients for the SAMPL7 physical property challenge using the ClassicalGSG method. Journal of Computer-Aided Molecular Design, 2021, 35, 819-830.	2.9	5
8	Perturbation of ACE2 Structural Ensembles by SARS-CoV-2 Spike Protein Binding. Journal of Chemical Theory and Computation, 2021, 17, 5896-5906.	5.3	3
9	Identification and Characterization of Two Structurally Related Dipeptides that Enhance Catalytic Efficiency of Neurolysin. Journal of Pharmacology and Experimental Therapeutics, 2021, 379, 191-202.	2.5	8
10	Enhanced Jarzynski free energy calculations using weighted ensemble. Journal of Chemical Physics, 2020, 153, 134116.	3.0	4
11	On Calculating Free Energy Differences Using Ensembles of Transition Paths. Frontiers in Molecular Biosciences, 2020, 7, 106.	3.5	30
12	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	2.9	86
13	Wepy: A Flexible Software Framework for Simulating Rare Events with Weighted Ensemble Resampling. ACS Omega, 2020, 5, 31608-31623.	3.5	21
14	REVO: Resampling of ensembles by variation optimization. Journal of Chemical Physics, 2019, 150, 244112.	3.0	43
15	Selectivity, ligand deconstruction, and cellular activity analysis of a BPTF bromodomain inhibitor. Organic and Biomolecular Chemistry, 2019, 17, 2020-2027.	2.8	18
16	Markov-State Transition Path Analysis of Electrostatic Channeling. Journal of Physical Chemistry C, 2019, 123, 15284-15292.	3.1	12
17	Isothermal Analysis of ThermoFluor Data can readily provide Quantitative Binding Affinities. Scientific Reports, 2019, 9, 2650.	3.3	81
18	A Suite of Tutorials for the WESTPA Rare-Events Sampling Software [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	16

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19	A biosensor-based framework to measure latent proteostasis capacity. Nature Communications, 2018, 9, 287.	12.8	43
20	Unbiased Molecular Dynamics of 11 min Timescale Drug Unbinding Reveals Transition State Stabilizing Interactions. Journal of the American Chemical Society, 2018, 140, 618-628.	13.7	107
21	Long-Range Changes in Neurolysin Dynamics Upon Inhibitor Binding. Journal of Chemical Theory and Computation, 2018, 14, 444-452.	5.3	11
22	Mapping the Ligand Binding Landscape. Biophysical Journal, 2018, 115, 1707-1719.	0.5	33
23	Predicting ligand binding affinity using on- and off-rates for the SAMPL6 SAMPLing challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1001-1012.	2.9	38
24	Structural insights into lethal contractural syndrome type 3 (LCCS3) caused by a missense mutation of PIP5Kî³. Biochemical Journal, 2018, 475, 2257-2269.	3.7	7
25	How Does a Ligand Explore the Deep Channel of Neurolysin? A Conformational Dynamics Study with Wexplore and Elastic Network Modeling. Biophysical Journal, 2017, 112, 355a.	0.5	0
26	Multiple Ligand Unbinding Pathways and Ligand-Induced Destabilization Revealed by WExplore. Biophysical Journal, 2017, 112, 620-629.	0.5	73
27	Kinetics and Pathways of Extremely Long Ligand Release Events Revealed by Wexplore and Conformation Space Networks. Biophysical Journal, 2017, 112, 348a.	0.5	0
28	Optimal allosteric stabilization sites using contact stabilization analysis. Journal of Computational Chemistry, 2017, 38, 1138-1146.	3.3	1
29	Kinetics of Ligand Binding Through Advanced Computational Approaches: A Review. Current Topics in Medicinal Chemistry, 2017, 17, 2626-2641.	2.1	44
30	Ligand Residence Times and Exit Pathways Obtained in Silico without Biasing Forces. Biophysical Journal, 2016, 110, 203a-204a.	0.5	0
31	Capturing a Dynamic Chaperoneâ€“Substrate Interaction Using NMR-Informed Molecular Modeling. Journal of the American Chemical Society, 2016, 138, 9826-9839.	13.7	25
32	Ligand Release Pathways Obtained with WExplore: Residence Times and Mechanisms. Journal of Physical Chemistry B, 2016, 120, 5377-5385.	2.6	50
33	NMR-Informed Molecular Modeling Uncovers the Conformational Landscape of Chaperone Binding with Unfolded Substrate. Biophysical Journal, 2016, 110, 369a.	0.5	0
34	Coupled folding and binding with 2D Windowâ€Exchange Umbrella Sampling. Journal of Computational Chemistry, 2016, 37, 587-594.	3.3	21
35	pH-Dependent Transient Conformational States Control Optical Properties in Cyan Fluorescent Protein. Journal of the American Chemical Society, 2015, 137, 2892-2900.	13.7	17
36	Multiscale Modeling of a Conditionally Disordered pH-Sensing Chaperone. Journal of Molecular Biology, 2015, 427, 1670-1680.	4.2	27

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37	Efficient in silico exploration of RNA interhelical conformations using Euler angles and WExplore. Nucleic Acids Research, 2014, 42, 12126-12137.	14.5	25
38	WExplore: Hierarchical Exploration of High-Dimensional Spaces Using the Weighted Ensemble Algorithm. Journal of Physical Chemistry B, 2014, 118, 3532-3542.	2.6	91
39	Native States of Fast-Folding Proteins Are Kinetic Traps. Journal of the American Chemical Society, 2013, 135, 4729-4734.	13.7	46
40	Binding and Folding of the Small Bacterial Chaperone HdeA. Journal of Physical Chemistry B, 2013, 117, 13219-13225.	2.6	16
41	Quantifying Chaperone-Mediated Transitions in the Proteostasis Network of E. coli. PLoS Computational Biology, 2013, 9, e1003324.	3.2	5
42	Quantifying Hub-like Behavior in Protein Folding Networks. Journal of Chemical Theory and Computation, 2012, 8, 3044-3052.	5.3	22
43	Flow-Dependent Unfolding and Refolding of an RNA by Nonequilibrium Umbrella Sampling. Journal of Chemical Theory and Computation, 2011, 7, 2710-2720.	5.3	36
44	Entrainment of a driven oscillator as a dynamical phase transition. Physical Review E, 2011, 84, 061134.	2.1	4
45	Enhanced Sampling of Nonequilibrium Steady States. Annual Review of Physical Chemistry, 2010, 61, 441-459.	10.8	71
46	Incorporating friction and collective shear moves into a lattice gas. Physical Review E, 2010, 81, 051111.	2.1	0
47	Nonequilibrium umbrella sampling in spaces of many order parameters. Journal of Chemical Physics, 2009, 130, 074104.	3.0	68
48	Separating forward and backward pathways in nonequilibrium umbrella sampling. Journal of Chemical Physics, 2009, 131, 154104.	3.0	70