Alex Dickson

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7008313/publications.pdf

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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	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
2	WExplore: Hierarchical Exploration of High-Dimensional Spaces Using the Weighted Ensemble Algorithm. Journal of Physical Chemistry B, 2014, 118, 3532-3542.	2.6	91
3	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
4	Isothermal Analysis of ThermoFluor Data can readily provide Quantitative Binding Affinities. Scientific Reports, 2019, 9, 2650.	3.3	81
5	Multiple Ligand Unbinding Pathways and Ligand-Induced Destabilization Revealed by WExplore. Biophysical Journal, 2017, 112, 620-629.	0.5	73
6	Enhanced Sampling of Nonequilibrium Steady States. Annual Review of Physical Chemistry, 2010, 61, 441-459.	10.8	71
7	Separating forward and backward pathways in nonequilibrium umbrella sampling. Journal of Chemical Physics, 2009, 131, 154104.	3.0	70
8	Nonequilibrium umbrella sampling in spaces of many order parameters. Journal of Chemical Physics, 2009, 130, 074104.	3.0	68
9	Ligand Release Pathways Obtained with WExplore: Residence Times and Mechanisms. Journal of Physical Chemistry B, 2016, 120, 5377-5385.	2.6	50
10	Native States of Fast-Folding Proteins Are Kinetic Traps. Journal of the American Chemical Society, 2013, 135, 4729-4734.	13.7	46
11	Kinetics of Ligand Binding Through Advanced Computational Approaches: A Review. Current Topics in Medicinal Chemistry, 2017, 17, 2626-2641.	2.1	44
12	A biosensor-based framework to measure latent proteostasis capacity. Nature Communications, 2018, 9, 287.	12.8	43
13	REVO: Resampling of ensembles by variation optimization. Journal of Chemical Physics, 2019, 150, 244112.	3.0	43
14	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
15	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
16	Mapping the Ligand Binding Landscape. Biophysical Journal, 2018, 115, 1707-1719.	0.5	33
17	On Calculating Free Energy Differences Using Ensembles of Transition Paths. Frontiers in Molecular Biosciences, 2020, 7, 106.	3.5	30
18	Multiscale Modeling of a Conditionally Disordered pH-Sensing Chaperone. Journal of Molecular Biology, 2015, 427, 1670-1680.	4.2	27

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19	Efficient in silico exploration of RNA interhelical conformations using Euler angles and WExplore. Nucleic Acids Research, 2014, 42, 12126-12137.	14.5	25
20	Capturing a Dynamic Chaperoneâ€“Substrate Interaction Using NMR-Informed Molecular Modeling. Journal of the American Chemical Society, 2016, 138, 9826-9839.	13.7	25
21	Membrane-Mediated Ligand Unbinding of the PK-11195 Ligand from TSPO. Biophysical Journal, 2021, 120, 158-167.	0.5	25
22	Quantifying Hub-like Behavior in Protein Folding Networks. Journal of Chemical Theory and Computation, 2012, 8, 3044-3052.	5.3	22
23	Coupled folding and binding with 2D Windowâ€Exchange Umbrella Sampling. Journal of Computational Chemistry, 2016, 37, 587-594.	3.3	21
24	Wepy: A Flexible Software Framework for Simulating Rare Events with Weighted Ensemble Resampling. ACS Omega, 2020, 5, 31608-31623.	3.5	21
25	Selectivity, ligand deconstruction, and cellular activity analysis of a BPTF bromodomain inhibitor. Organic and Biomolecular Chemistry, 2019, 17, 2020-2027.	2.8	18
26	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
27	Binding and Folding of the Small Bacterial Chaperone HdeA. Journal of Physical Chemistry B, 2013, 117, 13219-13225.	2.6	16
28	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
29	Markov-State Transition Path Analysis of Electrostatic Channeling. Journal of Physical Chemistry C, 2019, 123, 15284-15292.	3.1	12
30	Long-Range Changes in Neurolysin Dynamics Upon Inhibitor Binding. Journal of Chemical Theory and Computation, 2018, 14, 444-452.	5.3	11
31	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
32	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
33	<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
34	Quantifying Chaperone-Mediated Transitions in the Proteostasis Network of E. coli. PLoS Computational Biology, 2013, 9, e1003324.	3.2	5
35	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
36	Entrainment of a driven oscillator as a dynamical phase transition. Physical Review E, 2011, 84, 061134.	2.1	4

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37	Enhanced Jarzynski free energy calculations using weighted ensemble. Journal of Chemical Physics, 2020, 153, 134116.	3.0	4
38	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
39	Local Ion Densities can Influence Transition Paths of Molecular Binding. Frontiers in Molecular Biosciences, 2022, 9, 858316.	3.5	2
40	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
41	Optimal allosteric stabilization sites using contact stabilization analysis. Journal of Computational Chemistry, 2017, 38, 1138-1146.	3.3	1
42	Incorporating friction and collective shear moves into a lattice gas. Physical Review E, 2010, 81, 051111.	2.1	0
43	Ligand Residence Times and Exit Pathways Obtained in Silico without Biasing Forces. Biophysical Journal, 2016, 110, 203a-204a.	0.5	0
44	NMR-Informed Molecular Modeling Uncovers the Conformational Landscape of Chaperone Binding with Unfolded Substrate. Biophysical Journal, 2016, 110, 369a.	0.5	0
45	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
46	Kinetics and Pathways of Extremely Long Ligand Release Events Revealed by Wexplore and Conformation Space Networks. Biophysical Journal, 2017, 112, 348a.	0.5	0
47	Creating Maps of the Ligand Binding Landscape for Kinetics-Based Drug Discovery. Methods in Molecular Biology, 2022, 2385, 325-334.	0.9	0
48	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