

Jacob D Durrant

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

66

papers

2,901

citations

26

h-index

53

g-index

76

ext. papers

3,548

ext. citations

6

avg, IF

5.8

L-index

#	Paper	IF	Citations
66	Molecular dynamics simulations and drug discovery. <i>BMC Biology</i> , 2011 , 9, 71	7.3	615
65	NNScore 2.0: a neural-network receptor-ligand scoring function. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2897-903	6.1	173
64	POVME 2.0: An Enhanced Tool for Determining Pocket Shape and Volume Characteristics. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5047-5056	6.4	164
63	POVME: an algorithm for measuring binding-pocket volumes. <i>Journal of Molecular Graphics and Modelling</i> , 2011 , 29, 773-6	2.8	164
62	BINANA: a novel algorithm for ligand-binding characterization. <i>Journal of Molecular Graphics and Modelling</i> , 2011 , 29, 888-93	2.8	142
61	Emerging Computational Methods for the Rational Discovery of Allosteric Drugs. <i>Chemical Reviews</i> , 2016 , 116, 6370-90	68.1	140
60	NNScore: a neural-network-based scoring function for the characterization of protein-ligand complexes. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 1865-71	6.1	135
59	Computational approaches to mapping allosteric pathways. <i>Current Opinion in Structural Biology</i> , 2014 , 25, 98-103	8.1	104
58	Weighted Implementation of Suboptimal Paths (WISP): An Optimized Algorithm and Tool for Dynamical Network Analysis. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 511-517	6.4	97
57	AutoGrow: a novel algorithm for protein inhibitor design. <i>Chemical Biology and Drug Design</i> , 2009 , 73, 168-78	2.9	70
56	A multidimensional strategy to detect polypharmacological targets in the absence of structural and sequence homology. <i>PLoS Computational Biology</i> , 2010 , 6, e1000648	5	61
55	Computer-aided drug-discovery techniques that account for receptor flexibility. <i>Current Opinion in Pharmacology</i> , 2010 , 10, 770-4	5.1	61
54	HBonanza: a computer algorithm for molecular-dynamics-trajectory hydrogen-bond analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2011 , 31, 5-9	2.8	59
53	Mesoscale All-Atom Influenza Virus Simulations Suggest New Substrate Binding Mechanism. <i>ACS Central Science</i> , 2020 , 6, 189-196	16.8	50
52	Novel naphthalene-based inhibitors of Trypanosoma brucei RNA editing ligase 1. <i>PLoS Neglected Tropical Diseases</i> , 2010 , 4, e803	4.8	49
51	Computer-aided identification of Trypanosoma brucei uridine diphosphate galactose 4-epimerase inhibitors: toward the development of novel therapies for African sleeping sickness. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 5025-32	8.3	45
50	Comparing neural-network scoring functions and the state of the art: applications to common library screening. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1726-35	6.1	36

49	AutoGrow 3.0: an improved algorithm for chemically tractable, semi-automated protein inhibitor design. <i>Journal of Molecular Graphics and Modelling</i> , 2013 , 44, 104-12	2.8	36
48	A virtual screening approach for identifying plants with anti H5N1 neuraminidase activity. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 308-16	6.1	36
47	LipidWrapper: an algorithm for generating large-scale membrane models of arbitrary geometry. <i>PLoS Computational Biology</i> , 2014 , 10, e1003720	5	35
46	Applying molecular dynamics simulations to identify rarely sampled ligand-bound conformational states of undecaprenyl pyrophosphate synthase, an antibacterial target. <i>Chemical Biology and Drug Design</i> , 2011 , 77, 412-20	2.9	35
45	AutoClickChem: click chemistry in silico. <i>PLoS Computational Biology</i> , 2012 , 8, e1002397	5	34
44	Non-bisphosphonate inhibitors of isoprenoid biosynthesis identified via computer-aided drug design. <i>Chemical Biology and Drug Design</i> , 2011 , 78, 323-32	2.9	34
43	Computational identification of uncharacterized cruzain binding sites. <i>PLoS Neglected Tropical Diseases</i> , 2010 , 4, e676	4.8	34
42	Machine-learning techniques applied to antibacterial drug discovery. <i>Chemical Biology and Drug Design</i> , 2015 , 85, 14-21	2.9	33
41	Comparative chemical genomics reveal that the spiroindolone antimalarial KAE609 (Cipargamin) is a P-type ATPase inhibitor. <i>Scientific Reports</i> , 2016 , 6, 27806	4.9	31
40	Microsecond Molecular Dynamics Simulations of Influenza Neuraminidase Suggest a Mechanism for the Increased Virulence of Stalk-Deletion Mutants. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8590-9	3.4	26
39	AutoGrow4: an open-source genetic algorithm for de novo drug design and lead optimization. <i>Journal of Cheminformatics</i> , 2020 , 12, 25	8.6	25
38	Neural-Network Scoring Functions Identify Structurally Novel Estrogen-Receptor Ligands. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1953-61	6.1	24
37	Including receptor flexibility and induced fit effects into the design of MMP-2 inhibitors. <i>Journal of Molecular Recognition</i> , 2010 , 23, 173-82	2.6	22
36	Novel cruzain inhibitors for the treatment of Chagas disease. <i>Chemical Biology and Drug Design</i> , 2012 , 80, 398-405	2.9	21
35	BlendMol: advanced macromolecular visualization in Blender. <i>Bioinformatics</i> , 2019 , 35, 2323-2325	7.2	20
34	A Computational Assay that Explores the Hemagglutinin/Neuraminidase Functional Balance Reveals the Neuraminidase Secondary Site as a Novel Anti-Influenza Target. <i>ACS Central Science</i> , 2018 , 4, 1570-1577	16.8	20
33	Distributed Drug Discovery: Advancing Chemical Education through Contextualized Combinatorial Solid-Phase Organic Laboratories. <i>Journal of Chemical Education</i> , 2015 , 92, 819-826	2.4	18
32	CrystalDock: a novel approach to fragment-based drug design. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2573-80	6.1	18

31	Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. <i>Journal of Cheminformatics</i> , 2019 , 11, 34	8.6	16
30	Webina: an open-source library and web app that runs AutoDock Vina entirely in the web browser. <i>Bioinformatics</i> , 2020 , 36, 4513-4515	7.2	16
29	ProteinVR: Web-based molecular visualization in virtual reality. <i>PLoS Computational Biology</i> , 2020 , 16, e1007747	5	16
28	Potential drug-like inhibitors of Group 1 influenza neuraminidase identified through computer-aided drug design. <i>Computational Biology and Chemistry</i> , 2010 , 34, 97-105	3.6	16
27	Rapid Chagas Disease Drug Target Discovery Using Directed Evolution in Drug-Sensitive Yeast. <i>ACS Chemical Biology</i> , 2017 , 12, 422-434	4.9	15
26	Celastrol inhibits Plasmodium falciparum enoyl-acyl carrier protein reductase. <i>Bioorganic and Medicinal Chemistry</i> , 2014 , 22, 6053-6061	3.4	13
25	LigMerge: a fast algorithm to generate models of novel potential ligands from sets of known binders. <i>Chemical Biology and Drug Design</i> , 2012 , 80, 358-65	2.9	13
24	The molecular dynamics of Trypanosoma brucei UDP-galactose 4Epimerase: a drug target for African sleeping sickness. <i>Chemical Biology and Drug Design</i> , 2012 , 80, 173-81	2.9	12
23	Pyrone-based inhibitors of metalloproteinase types 2 and 3 may work as conformation-selective inhibitors. <i>Chemical Biology and Drug Design</i> , 2011 , 78, 191-8	2.9	12
22	Toward understanding the conformational dynamics of RNA ligation. <i>Biochemistry</i> , 2009 , 48, 709-19	3.2	11
21	Dimorphite-DL: an open-source program for enumerating the ionization states of drug-like small molecules. <i>Journal of Cheminformatics</i> , 2019 , 11, 14	8.6	10
20	DeepFrag: a deep convolutional neural network for fragment-based lead optimization. <i>Chemical Science</i> , 2021 , 12, 8036-8047	9.4	10
19	Capturing the Mechanism Underlying TOP mRNA Binding to LARP1. <i>Structure</i> , 2019 , 27, 1771-1781.e5	5.2	9
18	Two inhibitors of yeast plasma membrane ATPase 1 (ScPma1p): toward the development of novel antifungal therapies. <i>Journal of Cheminformatics</i> , 2018 , 10, 6	8.6	7
17	Tryptophan contributions to the empirical free-energy profile in gramicidin A/M heterodimer channels. <i>Biophysical Journal</i> , 2006 , 91, 3230-41	2.9	7
16	Documenting and harnessing the biological potential of molecules in Distributed Drug Discovery (D3) virtual catalogs. <i>Chemical Biology and Drug Design</i> , 2017 , 90, 909-918	2.9	5
15	Characterization of Female Reproductive Proteases in a Butterfly from Functional and Evolutionary Perspectives. <i>Physiological and Biochemical Zoology</i> , 2019 , 92, 579-590	2	5
14	Scoria: a Python module for manipulating 3D molecular data. <i>Journal of Cheminformatics</i> , 2017 , 9, 52	8.6	4

13	Towards the development of novel <i>Trypanosoma brucei</i> RNA editing ligase 1 inhibitors. <i>BMC Pharmacology</i> , 2011 , 11, 9		4
12	LigGrep: a tool for filtering docked poses to improve virtual-screening hit rates. <i>Journal of Cheminformatics</i> , 2020 , 12, 69	8.6	4
11	PARP1: Structural insights and pharmacological targets for inhibition. <i>DNA Repair</i> , 2021 , 103, 103125	4.3	4
10	DeepFrag: An Open-Source Browser App for Deep-Learning Lead Optimization. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2523-2529	6.1	3
9	DeepFrag: A Deep Convolutional Neural Network for Fragment-based Lead Optimization		3
8	PCAViz: An Open-Source Python/JavaScript Toolkit for Visualizing Molecular Dynamics Simulations in the Web Browser. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4087-4092	6.1	2
7	De Novo Design by Fragment Growing and Docking 2013 , 125-142		2
6	MutantHuntWGS: A Pipeline for Identifying Mutations. <i>G3: Genes, Genomes, Genetics</i> , 2020 , 10, 3009-3014	2	1
5	Adaptive laboratory evolution in <i>S. cerevisiae</i> highlights role of transcription factors in fungal xenobiotic resistance.. <i>Communications Biology</i> , 2022 , 5, 128	6.7	1
4	Webina: An Open-Source Library and Web App that Runs AutoDock Vina Entirely in the Web Browser		1
3	Defining the Yeast Resistome through in vitro Evolution and Whole Genome Sequencing		1
2	Novel mutation in hexokinase 2 confers resistance to 2-deoxyglucose by altering protein dynamics.. <i>PLoS Computational Biology</i> , 2022 , 18, e1009929	5	0
1	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. <i>BMC Bioinformatics</i> , 2014 , 15, 159	3.6	