Jacob D Durrant

List of Publications by Year in Descending Order

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	Adaptive laboratory evolution in S. cerevisiae highlights role of transcription factors in fungal xenobiotic resistance.. *Communications Biology*, **2022**, 5, 128	6.7	1
65	Novel mutation in hexokinase 2 confers resistance to 2-deoxyglucose by altering protein dynamics.. *PLoS Computational Biology*, **2022**, 18, e1009929	5	0
64	DeepFrag: An Open-Source Browser App for Deep-Learning Lead Optimization. *Journal of Chemical Information and Modeling*, **2021**, 61, 2523-2529	6.1	3
63	PARP1: Structural insights and pharmacological targets for inhibition. *DNA Repair*, **2021**, 103, 103125	4.3	4
62	DeepFrag: a deep convolutional neural network for fragment-based lead optimization. *Chemical Science*, **2021**, 12, 8036-8047	9.4	10
61	Webina: an open-source library and web app that runs AutoDock Vina entirely in the web browser. *Bioinformatics*, **2020**, 36, 4513-4515	7.2	16
60	MutantHuntWGS: A Pipeline for Identifying Mutations. *G3: Genes, Genomes, Genetics*, **2020**, 10, 3009-3014	3.2	1
59	Mesoscale All-Atom Influenza Virus Simulations Suggest New Substrate Binding Mechanism. *ACS Central Science*, **2020**, 6, 189-196	16.8	50
58	ProteinVR: Web-based molecular visualization in virtual reality. *PLoS Computational Biology*, **2020**, 16, e1007747	5	16
57	AutoGrow4: an open-source genetic algorithm for de novo drug design and lead optimization. *Journal of Cheminformatics*, **2020**, 12, 25	8.6	25
56	LigGrep: a tool for filtering docked poses to improve virtual-screening hit rates. *Journal of Cheminformatics*, **2020**, 12, 69	8.6	4
55	PCAViz: An Open-Source Python/JavaScript Toolkit for Visualizing Molecular Dynamics Simulations in the Web Browser. *Journal of Chemical Information and Modeling*, **2019**, 59, 4087-4092	6.1	2
54	Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. *Journal of Cheminformatics*, **2019**, 11, 34	8.6	16
53	Characterization of Female Reproductive Proteases in a Butterfly from Functional and Evolutionary Perspectives. *Physiological and Biochemical Zoology*, **2019**, 92, 579-590	2	5
52	Capturing the Mechanism Underlying TOP mRNA Binding to LARP1. *Structure*, **2019**, 27, 1771-1781.e5	5.2	9
51	Dimorphite-DL: an open-source program for enumerating the ionization states of drug-like small molecules. *Journal of Cheminformatics*, **2019**, 11, 14	8.6	10
50	BlendMol: advanced macromolecular visualization in Blender. *Bioinformatics*, **2019**, 35, 2323-2325	7.2	20

49	Two inhibitors of yeast plasma membrane ATPase 1 (ScPma1p): toward the development of novel antifungal therapies. *Journal of Cheminformatics*, **2018**, 10, 6	8.6	7
48	A Computational Assay that Explores the Hemagglutinin/Neuraminidase Functional Balance Reveals the Neuraminidase Secondary Site as a Novel Anti-Influenza Target. *ACS Central Science*, **2018**, 4, 1570-1577	16.8	20
47	Documenting and harnessing the biological potential of molecules in Distributed Drug Discovery (D3) virtual catalogs. *Chemical Biology and Drug Design*, **2017**, 90, 909-918	2.9	5
46	Rapid Chagas Disease Drug Target Discovery Using Directed Evolution in Drug-Sensitive Yeast. *ACS Chemical Biology*, **2017**, 12, 422-434	4.9	15
45	Scoria: a Python module for manipulating 3D molecular data. *Journal of Cheminformatics*, **2017**, 9, 52	8.6	4
44	Comparative chemical genomics reveal that the spiroindolone antimalarial KAE609 (Cipargamin) is a P-type ATPase inhibitor. *Scientific Reports*, **2016**, 6, 27806	4.9	31
43	Emerging Computational Methods for the Rational Discovery of Allosteric Drugs. *Chemical Reviews*, **2016**, 116, 6370-90	68.1	140
42	Microsecond Molecular Dynamics Simulations of Influenza Neuraminidase Suggest a Mechanism for the Increased Virulence of Stalk-Deletion Mutants. *Journal of Physical Chemistry B*, **2016**, 120, 8590-9	3.4	26
41	Neural-Network Scoring Functions Identify Structurally Novel Estrogen-Receptor Ligands. *Journal of Chemical Information and Modeling*, **2015**, 55, 1953-61	6.1	24
40	Machine-learning techniques applied to antibacterial drug discovery. *Chemical Biology and Drug Design*, **2015**, 85, 14-21	2.9	33
39	Distributed Drug Discovery: Advancing Chemical Education through Contextualized Combinatorial Solid-Phase Organic Laboratories. *Journal of Chemical Education*, **2015**, 92, 819-826	2.4	18
38	A virtual screening approach for identifying plants with anti H5N1 neuraminidase activity. *Journal of Chemical Information and Modeling*, **2015**, 55, 308-16	6.1	36
37	Computational approaches to mapping allosteric pathways. *Current Opinion in Structural Biology*, **2014**, 25, 98-103	8.1	104
36	Celastrol inhibits Plasmodium falciparum enoyl-acyl carrier protein reductase. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 6053-6061	3.4	13
35	POVME 2.0: An Enhanced Tool for Determining Pocket Shape and Volume Characteristics. *Journal of Chemical Theory and Computation*, **2014**, 10, 5047-5056	6.4	164
34	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. *BMC Bioinformatics*, **2014**, 15, 159	3.6	
33	Weighted Implementation of Suboptimal Paths (WISP): An Optimized Algorithm and Tool for Dynamical Network Analysis. *Journal of Chemical Theory and Computation*, **2014**, 10, 511-517	6.4	97
32	LipidWrapper: an algorithm for generating large-scale membrane models of arbitrary geometry. *PLoS Computational Biology*, **2014**, 10, e1003720	5	35

31	Comparing neural-network scoring functions and the state of the art: applications to common library screening. *Journal of Chemical Information and Modeling*, **2013**, 53, 1726-35	6.1	36
30	AutoGrow 3.0: an improved algorithm for chemically tractable, semi-automated protein inhibitor design. *Journal of Molecular Graphics and Modelling*, **2013**, 44, 104-12	2.8	36
29	De Novo Design by Fragment Growing and Docking **2013**, 125-142		2
28	The molecular dynamics of Trypanosoma brucei UDP-galactose 4′-epimerase: a drug target for African sleeping sickness. *Chemical Biology and Drug Design*, **2012**, 80, 173-81	2.9	12
27	LigMerge: a fast algorithm to generate models of novel potential ligands from sets of known binders. *Chemical Biology and Drug Design*, **2012**, 80, 358-65	2.9	13
26	Novel cruzain inhibitors for the treatment of Chagas' disease. *Chemical Biology and Drug Design*, **2012**, 80, 398-405	2.9	21
25	AutoClickChem: click chemistry in silico. *PLoS Computational Biology*, **2012**, 8, e1002397	5	34
24	CrystalDock: a novel approach to fragment-based drug design. *Journal of Chemical Information and Modeling*, **2011**, 51, 2573-80	6.1	18
23	NNScore 2.0: a neural-network receptor-ligand scoring function. *Journal of Chemical Information and Modeling*, **2011**, 51, 2897-903	6.1	173
22	Applying molecular dynamics simulations to identify rarely sampled ligand-bound conformational states of undecaprenyl pyrophosphate synthase, an antibacterial target. *Chemical Biology and Drug Design*, **2011**, 77, 412-20	2.9	35
21	Pyrone-based inhibitors of metalloproteinase types 2 and 3 may work as conformation-selective inhibitors. *Chemical Biology and Drug Design*, **2011**, 78, 191-8	2.9	12
20	Non-bisphosphonate inhibitors of isoprenoid biosynthesis identified via computer-aided drug design. *Chemical Biology and Drug Design*, **2011**, 78, 323-32	2.9	34
19	HBonanza: a computer algorithm for molecular-dynamics-trajectory hydrogen-bond analysis. *Journal of Molecular Graphics and Modelling*, **2011**, 31, 5-9	2.8	59
18	Towards the development of novel Trypanosoma brucei RNA editing ligase 1 inhibitors. *BMC Pharmacology*, **2011**, 11, 9		4
17	Molecular dynamics simulations and drug discovery. *BMC Biology*, **2011**, 9, 71	7.3	615
16	POVME: an algorithm for measuring binding-pocket volumes. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 773-6	2.8	164
15	BINANA: a novel algorithm for ligand-binding characterization. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 888-93	2.8	142
14	A multidimensional strategy to detect polypharmacological targets in the absence of structural and sequence homology. *PLoS Computational Biology*, **2010**, 6, e1000648	5	61

List of Publications

13	Novel naphthalene-based inhibitors of Trypanosoma brucei RNA editing ligase 1. *PLoS Neglected Tropical Diseases*, **2010**, 4, e803	4.8	49
12	NNScore: a neural-network-based scoring function for the characterization of protein-ligand complexes. *Journal of Chemical Information and Modeling*, **2010**, 50, 1865-71	6.1	135
11	Computer-aided drug-discovery techniques that account for receptor flexibility. *Current Opinion in Pharmacology*, **2010**, 10, 770-4	5.1	61
10	Computational identification of uncharacterized cruzain binding sites. *PLoS Neglected Tropical Diseases*, **2010**, 4, e676	4.8	34
9	Computer-aided identification of Trypanosoma brucei uridine diphosphate galactose 4Ʋepimerase inhibitors: toward the development of novel therapies for African sleeping sickness. *Journal of Medicinal Chemistry*, **2010**, 53, 5025-32	8.3	45
8	Including receptor flexibility and induced fit effects into the design of MMP-2 inhibitors. *Journal of Molecular Recognition*, **2010**, 23, 173-82	2.6	22
7	Potential drug-like inhibitors of Group 1 influenza neuraminidase identified through computer-aided drug design. *Computational Biology and Chemistry*, **2010**, 34, 97-105	3.6	16
6	AutoGrow: a novel algorithm for protein inhibitor design. *Chemical Biology and Drug Design*, **2009**, 73, 168-78	2.9	70
5	Toward understanding the conformational dynamics of RNA ligation. *Biochemistry*, **2009**, 48, 709-19	3.2	11
4	Tryptophan contributions to the empirical free-energy profile in gramicidin A/M heterodimer channels. *Biophysical Journal*, **2006**, 91, 3230-41	2.9	7
3	Webina: An Open-Source Library and Web App that Runs AutoDock Vina Entirely in the Web Browser		1
2	Defining the Yeast Resistome through in vitro Evolution and Whole Genome Sequencing		1
1	DeepFrag: A Deep Convolutional Neural Network for Fragment-based Lead Optimization		3