Jacob D Durrant

List of Publications by Year
in descending order

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67 papers	4,199 citations	147801 31 h-index	118850 62 g-index
76 all docs	76 docs citations	76 times ranked	5738 citing authors

#	Article	IF	Citations
1	BINANA 2: Characterizing Receptor/Ligand Interactions in Python and JavaScript. Journal of Chemical Information and Modeling, 2022, 62, 753-760.	5.4	12
2	Adaptive laboratory evolution in S. cerevisiae highlights role of transcription factors in fungal xenobiotic resistance. Communications Biology, 2022, 5, 128.	4.4	8
3	Novel mutation in hexokinase 2 confers resistance to 2-deoxyglucose by altering protein dynamics. PLoS Computational Biology, 2022, 18, e1009929.	3.2	6
4	Phosphate position is key in mediating transmembrane ion channel TMEM16Aâ€“phosphatidylinositol 4,5-bisphosphate interaction. Journal of Biological Chemistry, 2022, 298, 102264.	3.4	2
5	DeepFrag: a deep convolutional neural network for fragment-based lead optimization. Chemical Science, 2021, 12, 8036-8047.	7.4	36
6	DeepFrag: An Open-Source Browser App for Deep-Learning Lead Optimization. Journal of Chemical Information and Modeling, 2021, 61, 2523-2529.	5.4	19
7	PARP1: Structural insights and pharmacological targets for inhibition. DNA Repair, 2021, 103, 103125.	2.8	32
8	LigGrep: a tool for filtering docked poses to improve virtual-screening hit rates. Journal of Cheminformatics, 2020, 12, 69.	6.1	16
9	Webina: an open-source library and web app that runs AutoDock Vina entirely in the web browser. Bioinformatics, 2020, 36, 4513-4515.	4.1	64
10	MutantHuntWGS: A Pipeline for Identifying Saccharomyces cerevisiae Mutations. G3: Genes, Genomes, Genetics, 2020, 10, 3009-3014.	1.8	5
11	Mesoscale All-Atom Influenza Virus Simulations Suggest New Substrate Binding Mechanism. ACS Central Science, 2020, 6, 189-196.	11.3	86
12	ProteinVR: Web-based molecular visualization in virtual reality. PLoS Computational Biology, 2020, 16, e1007747.	3.2	46
13	AutoGrow4: an open-source genetic algorithm for de novo drug design and lead optimization. Journal of Cheminformatics, 2020, 12, 25.	6.1	68
14	Characterization of Female Reproductive Proteases in a Butterfly from Functional and Evolutionary Perspectives. Physiological and Biochemical Zoology, 2019, 92, 579-590.	1.5	11
15	Capturing the Mechanism Underlying TOP mRNA Binding to LARP1. Structure, 2019, 27, 1771-1781.e5.	3.3	20
16	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.	5.4	4
17	Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. Journal of Cheminformatics, 2019, 11, 34.	6.1	45
18	Dimorphite-DL: an open-source program for enumerating the ionization states of drug-like small molecules. Journal of Cheminformatics, 2019, 11, 14.	6.1	34

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19	BlendMol: advanced macromolecular visualization in Blender. Bioinformatics, 2019, 35, 2323-2325.	4.1	31
20	Pyrite: A blender plugin for visualizing molecular dynamics simulations using industryâ€standard rendering techniques. Journal of Computational Chemistry, 2018, 39, 748-755.	3.3	13
21	Two inhibitors of yeast plasma membrane ATPase 1 (ScPma1p): toward the development of novel antifungal therapies. Journal of Cheminformatics, 2018, 10, 6.	6.1	17
22	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.	11.3	25
23	Influenza Viral Envelope Simulation Reveals Novel Druggable Pockets on Surface Glycoproteins. Biophysical Journal, 2018, 114, 341a.	0.5	1
24	Documenting and harnessing the biological potential of molecules in Distributed Drug Discovery (D3) virtual catalogs. Chemical Biology and Drug Design, 2017, 90, 909-918.	3.2	6
25	Rapid Chagas Disease Drug Target Discovery Using Directed Evolution in Drug-Sensitive Yeast. ACS Chemical Biology, 2017, 12, 422-434.	3.4	26
26	Scoria: a Python module for manipulating 3D molecular data. Journal of Cheminformatics, 2017, 9, 52.	6.1	6
27	Emerging Computational Methods for the Rational Discovery of Allosteric Drugs. Chemical Reviews, 2016, 116, 6370-6390.	47.7	176
28	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, 8590-8599.	2.6	36
29	Comparative chemical genomics reveal that the spiroindolone antimalarial KAE609 (Cipargamin) is a P-type ATPase inhibitor. Scientific Reports, 2016, 6, 27806.	3.3	38
30	Machineâ€Learning Techniques Applied to Antibacterial Drug Discovery. Chemical Biology and Drug Design, 2015, 85, 14-21.	3.2	49
31	Distributed Drug Discovery: Advancing Chemical Education through Contextualized Combinatorial Solid-Phase Organic Laboratories. Journal of Chemical Education, 2015, 92, 819-826.	2.3	23
32	The Do's and Do Not's of a 100 Million Atom Molecular Dynamics Simulation. Biophysical Journal, 2015, 108, 158a.	0.5	0
33	A Virtual Screening Approach For Identifying Plants with Anti H5N1 Neuraminidase Activity. Journal of Chemical Information and Modeling, 2015, 55, 308-316.	5.4	43
34	Neural-Network Scoring Functions Identify Structurally Novel Estrogen-Receptor Ligands. Journal of Chemical Information and Modeling, 2015, 55, 1953-1961.	5.4	31
35	LipidWrapper: An Algorithm for Generating Large-Scale Membrane Models of Arbitrary Geometry. PLoS Computational Biology, 2014, 10, e1003720.	3.2	60
36	Computational approaches to mapping allosteric pathways. Current Opinion in Structural Biology, 2014, 25, 98-103.	5.7	122

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37	Celastrol inhibits Plasmodium falciparum enoyl-acyl carrier protein reductase. Bioorganic and Medicinal Chemistry, 2014, 22, 6053-6061.	3.0	16
38	POVME 2.0: An Enhanced Tool for Determining Pocket Shape and Volume Characteristics. Journal of Chemical Theory and Computation, 2014, 10, 5047-5056.	5.3	203
39	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. BMC Bioinformatics, 2014, 15, 159.	2.6	0
40	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.	5.3	147
41	Comparing Neural-Network Scoring Functions and the State of the Art: Applications to Common Library Screening. Journal of Chemical Information and Modeling, 2013, 53, 1726-1735.	5.4	40
42	AutoGrow 3.0: An improved algorithm for chemically tractable, semi-automated protein inhibitor design. Journal of Molecular Graphics and Modelling, 2013, 44, 104-112.	2.4	48
43	AutoClickChem: Click Chemistry in Silico. PLoS Computational Biology, 2012, 8, e1002397.	3.2	41
44	The Molecular Dynamics of Trypanosoma brucei UDPâ€Galactose 4â€²â€Epimerase: A Drug Target for African Sleeping Sickness. Chemical Biology and Drug Design, 2012, 80, 173-181.	3.2	14
45	LigMerge: A Fast Algorithm to Generate Models of Novel Potential Ligands from Sets of Known Binders. Chemical Biology and Drug Design, 2012, 80, 358-365.	3.2	17
46	Novel Cruzain Inhibitors for the Treatment of Chagasâ€™ Disease. Chemical Biology and Drug Design, 2012, 80, 398-405.	3.2	33
47	CrystalDock: A Novel Approach to Fragment-Based Drug Design. Journal of Chemical Information and Modeling, 2011, 51, 2573-2580.	5.4	23
48	NNScore 2.0: A Neural-Network Receptorâ€“Ligand Scoring Function. Journal of Chemical Information and Modeling, 2011, 51, 2897-2903.	5.4	276
49	Applying Molecular Dynamics Simulations to Identify Rarely Sampled Ligandâ€bound Conformational States of Undecaprenyl Pyrophosphate Synthase, an Antibacterial Target. Chemical Biology and Drug Design, 2011, 77, 412-420.	3.2	38
50	Pyroneâ€Based Inhibitors of Metalloproteinase Types 2 and 3 May Work as Conformationâ€Selective Inhibitors. Chemical Biology and Drug Design, 2011, 78, 191-198.	3.2	23
51	Nonâ€Bisphosphonate Inhibitors of Isoprenoid Biosynthesis Identified via Computerâ€Aided Drug Design. Chemical Biology and Drug Design, 2011, 78, 323-332.	3.2	49
52	HBonanza: A computer algorithm for molecular-dynamics-trajectory hydrogen-bond analysis. Journal of Molecular Graphics and Modelling, 2011, 31, 5-9.	2.4	73
53	Towards the development of novel Trypanosoma brucei RNA editing ligase 1 inhibitors. BMC Pharmacology, 2011, 11, 9.	0.4	5
54	Molecular dynamics simulations and drug discovery. BMC Biology, 2011, 9, 71.	3.8	881

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55	POVME: An algorithm for measuring binding-pocket volumes. Journal of Molecular Graphics and Modelling, 2011, 29, 773-776.	2.4	186
56	BINANA: A novel algorithm for ligand-binding characterization. Journal of Molecular Graphics and Modelling, 2011, 29, 888-893.	2.4	197
57	Including receptor flexibility and induced fit effects into the design of MMPâ€2 inhibitors. Journal of Molecular Recognition, 2010, 23, 173-182.	2.1	29
58	Potential drug-like inhibitors of Group 1 influenza neuraminidase identified through computer-aided drug design. Computational Biology and Chemistry, 2010, 34, 97-105.	2.3	22
59	A Multidimensional Strategy to Detect Polypharmacological Targets in the Absence of Structural and Sequence Homology. PLoS Computational Biology, 2010, 6, e1000648.	3.2	72
60	Novel Naphthalene-Based Inhibitors of Trypanosoma brucei RNA Editing Ligase 1. PLoS Neglected Tropical Diseases, 2010, 4, e803.	3.0	64
61	NNScore: A Neural-Network-Based Scoring Function for the Characterization of Proteinâ^'Ligand Complexes. Journal of Chemical Information and Modeling, 2010, 50, 1865-1871.	5.4	190
62	Computer-aided drug-discovery techniques that account for receptor flexibility. Current Opinion in Pharmacology, 2010, 10, 770-774.	3.5	76
63	Computational Identification of Uncharacterized Cruzain Binding Sites. PLoS Neglected Tropical Diseases, 2010, 4, e676.	3.0	40
64	Computer-Aided Identification ofTrypanosoma bruceiUridine Diphosphate Galactose 4â€²-Epimerase Inhibitors: Toward the Development of Novel Therapies for African Sleeping Sickness. Journal of Medicinal Chemistry, 2010, 53, 5025-5032.	6.4	56
65	AutoGrow: A Novel Algorithm for Protein Inhibitor Design. Chemical Biology and Drug Design, 2009, 73, 168-178.	3.2	91
66	Toward Understanding the Conformational Dynamics of RNA Ligation. Biochemistry, 2009, 48, 709-719.	2.5	11
67	Tryptophan Contributions to the Empirical Free-Energy Profile in Gramicidin A/M Heterodimer Channels. Biophysical Journal, 2006, 91, 3230-3241.	0.5	7