Jacob D Durrant

List of Publications by Year
in descending order

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Version: 2024-02-01

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	Molecular dynamics simulations and drug discovery. BMC Biology, 2011, 9, 71.	3.8	881
2	NNScore 2.0: A Neural-Network Receptorâ€“Ligand Scoring Function. Journal of Chemical Information and Modeling, 2011, 51, 2897-2903.	5.4	276
3	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
4	BINANA: A novel algorithm for ligand-binding characterization. Journal of Molecular Graphics and Modelling, 2011, 29, 888-893.	2.4	197
5	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
6	POVME: An algorithm for measuring binding-pocket volumes. Journal of Molecular Graphics and Modelling, 2011, 29, 773-776.	2.4	186
7	Emerging Computational Methods for the Rational Discovery of Allosteric Drugs. Chemical Reviews, 2016, 116, 6370-6390.	47.7	176
8	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
9	Computational approaches to mapping allosteric pathways. Current Opinion in Structural Biology, 2014, 25, 98-103.	5.7	122
10	AutoGrow: A Novel Algorithm for Protein Inhibitor Design. Chemical Biology and Drug Design, 2009, 73, 168-178.	3.2	91
11	Mesoscale All-Atom Influenza Virus Simulations Suggest New Substrate Binding Mechanism. ACS Central Science, 2020, 6, 189-196.	11.3	86
12	Computer-aided drug-discovery techniques that account for receptor flexibility. Current Opinion in Pharmacology, 2010, 10, 770-774.	3.5	76
13	HBonanza: A computer algorithm for molecular-dynamics-trajectory hydrogen-bond analysis. Journal of Molecular Graphics and Modelling, 2011, 31, 5-9.	2.4	73
14	A Multidimensional Strategy to Detect Polypharmacological Targets in the Absence of Structural and Sequence Homology. PLoS Computational Biology, 2010, 6, e1000648.	3.2	72
15	AutoGrow4: an open-source genetic algorithm for de novo drug design and lead optimization. Journal of Cheminformatics, 2020, 12, 25.	6.1	68
16	Novel Naphthalene-Based Inhibitors of Trypanosoma brucei RNA Editing Ligase 1. PLoS Neglected Tropical Diseases, 2010, 4, e803.	3.0	64
17	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
18	LipidWrapper: An Algorithm for Generating Large-Scale Membrane Models of Arbitrary Geometry. PLoS Computational Biology, 2014, 10, e1003720.	3.2	60

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19	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
20	Nonâ€Bisphosphonate Inhibitors of Isoprenoid Biosynthesis Identified via Computerâ€Aided Drug Design. Chemical Biology and Drug Design, 2011, 78, 323-332.	3.2	49
21	Machineâ€Learning Techniques Applied to Antibacterial Drug Discovery. Chemical Biology and Drug Design, 2015, 85, 14-21.	3.2	49
22	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
23	ProteinVR: Web-based molecular visualization in virtual reality. PLoS Computational Biology, 2020, 16, e1007747.	3.2	46
24	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
25	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
26	AutoClickChem: Click Chemistry in Silico. PLoS Computational Biology, 2012, 8, e1002397.	3.2	41
27	Computational Identification of Uncharacterized Cruzain Binding Sites. PLoS Neglected Tropical Diseases, 2010, 4, e676.	3.0	40
28	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
29	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
30	Comparative chemical genomics reveal that the spiroindolone antimalarial KAE609 (Cipargamin) is a P-type ATPase inhibitor. Scientific Reports, 2016, 6, 27806.	3.3	38
31	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
32	DeepFrag: a deep convolutional neural network for fragment-based lead optimization. Chemical Science, 2021, 12, 8036-8047.	7.4	36
33	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
34	Novel Cruzain Inhibitors for the Treatment of Chagasâ€™ Disease. Chemical Biology and Drug Design, 2012, 80, 398-405.	3.2	33
35	PARP1: Structural insights and pharmacological targets for inhibition. DNA Repair, 2021, 103, 103125.	2.8	32
36	Neural-Network Scoring Functions Identify Structurally Novel Estrogen-Receptor Ligands. Journal of Chemical Information and Modeling, 2015, 55, 1953-1961.	5.4	31

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37	BlendMol: advanced macromolecular visualization in Blender. Bioinformatics, 2019, 35, 2323-2325.	4.1	31
38	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
39	Rapid Chagas Disease Drug Target Discovery Using Directed Evolution in Drug-Sensitive Yeast. ACS Chemical Biology, 2017, 12, 422-434.	3.4	26
40	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
41	CrystalDock: A Novel Approach to Fragment-Based Drug Design. Journal of Chemical Information and Modeling, 2011, 51, 2573-2580.	5.4	23
42	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
43	Distributed Drug Discovery: Advancing Chemical Education through Contextualized Combinatorial Solid-Phase Organic Laboratories. Journal of Chemical Education, 2015, 92, 819-826.	2.3	23
44	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
45	Capturing the Mechanism Underlying TOP mRNA Binding to LARP1. Structure, 2019, 27, 1771-1781.e5.	3.3	20
46	DeepFrag: An Open-Source Browser App for Deep-Learning Lead Optimization. Journal of Chemical Information and Modeling, 2021, 61, 2523-2529.	5.4	19
47	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
48	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
49	Celastrol inhibits Plasmodium falciparum enoyl-acyl carrier protein reductase. Bioorganic and Medicinal Chemistry, 2014, 22, 6053-6061.	3.0	16
50	LigGrep: a tool for filtering docked poses to improve virtual-screening hit rates. Journal of Cheminformatics, 2020, 12, 69.	6.1	16
51	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
52	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
53	BINANA 2: Characterizing Receptor/Ligand Interactions in Python and JavaScript. Journal of Chemical Information and Modeling, 2022, 62, 753-760.	5.4	12
54	Toward Understanding the Conformational Dynamics of RNA Ligation. Biochemistry, 2009, 48, 709-719.	2.5	11

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55	Characterization of Female Reproductive Proteases in a Butterfly from Functional and Evolutionary Perspectives. Physiological and Biochemical Zoology, 2019, 92, 579-590.	1.5	11
56	Adaptive laboratory evolution in S. cerevisiae highlights role of transcription factors in fungal xenobiotic resistance. Communications Biology, 2022, 5, 128.	4.4	8
57	Tryptophan Contributions to the Empirical Free-Energy Profile in Gramicidin A/M Heterodimer Channels. Biophysical Journal, 2006, 91, 3230-3241.	0.5	7
58	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
59	Scoria: a Python module for manipulating 3D molecular data. Journal of Cheminformatics, 2017, 9, 52.	6.1	6
60	Novel mutation in hexokinase 2 confers resistance to 2-deoxyglucose by altering protein dynamics. PLoS Computational Biology, 2022, 18, e1009929.	3.2	6
61	Towards the development of novel Trypanosoma brucei RNA editing ligase 1 inhibitors. BMC Pharmacology, 2011, 11, 9.	0.4	5
62	MutantHuntWGS: A Pipeline for Identifying Saccharomyces cerevisiae Mutations. G3: Genes, Genomes, Genetics, 2020, 10, 3009-3014.	1.8	5
63	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
64	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
65	Influenza Viral Envelope Simulation Reveals Novel Druggable Pockets on Surface Glycoproteins. Biophysical Journal, 2018, 114, 341a.	0.5	1
66	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. BMC Bioinformatics, 2014, 15, 159.	2.6	0
67	The Do's and Do Not's of a 100 Million Atom Molecular Dynamics Simulation. Biophysical Journal, 2015, 108, 158a.	0.5	0