

Jacob D Durrant

List of Publications by Year in descending order

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Version: 2024-02-01

67
papers

4,199
citations

147786

31
h-index

118840

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 Receptor-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 Protein-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 of <i>Trypanosoma brucei</i> Uridine Diphosphate Galactose 4 ^ε -Epimerase Inhibitors: Toward the Development of Novel Therapies for African Sleeping Sickness. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 5025-5032.	6.4	56
20	Non- β -Bisphosphonate Inhibitors of Isoprenoid Biosynthesis Identified via Computer-Aided Drug Design. <i>Chemical Biology and Drug Design</i> , 2011, 78, 323-332.	3.2	49
21	Machine-Learning Techniques Applied to Antibacterial Drug Discovery. <i>Chemical Biology and Drug Design</i> , 2015, 85, 14-21.	3.2	49
22	AutoGrow 3.0: An improved algorithm for chemically tractable, semi-automated protein inhibitor design. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 104-112.	2.4	48
23	ProteinVR: Web-based molecular visualization in virtual reality. <i>PLoS Computational Biology</i> , 2020, 16, e1007747.	3.2	46
24	Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. <i>Journal of Cheminformatics</i> , 2019, 11, 34.	6.1	45
25	A Virtual Screening Approach For Identifying Plants with Anti H5N1 Neuraminidase Activity. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 308-316.	5.4	43
26	AutoClickChem: Click Chemistry in Silico. <i>PLoS Computational Biology</i> , 2012, 8, e1002397.	3.2	41
27	Computational Identification of Uncharacterized Cruzain Binding Sites. <i>PLoS Neglected Tropical Diseases</i> , 2010, 4, e676.	3.0	40
28	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, 1726-1735.	5.4	40
29	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, 412-420.	3.2	38
30	Comparative chemical genomics reveal that the spiroindolone antimalarial KAE609 (Cipargamin) is a P-type ATPase inhibitor. <i>Scientific Reports</i> , 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. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8590-8599.	2.6	36
32	DeepFrag: a deep convolutional neural network for fragment-based lead optimization. <i>Chemical Science</i> , 2021, 12, 8036-8047.	7.4	36
33	Dimorphite-DL: an open-source program for enumerating the ionization states of drug-like small molecules. <i>Journal of Cheminformatics</i> , 2019, 11, 14.	6.1	34
34	Novel Cruzain Inhibitors for the Treatment of Chagas [™] Disease. <i>Chemical Biology and Drug Design</i> , 2012, 80, 398-405.	3.2	33
35	PARP1: Structural insights and pharmacological targets for inhibition. <i>DNA Repair</i> , 2021, 103, 103125.	2.8	32
36	Neural-Network Scoring Functions Identify Structurally Novel Estrogen-Receptor Ligands. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1953-1961.	5.4	31

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37	BlendMol: advanced macromolecular visualization in Blender. <i>Bioinformatics</i> , 2019, 35, 2323-2325.	4.1	31
38	Including receptor flexibility and induced fit effects into the design of MMPâ€² inhibitors. <i>Journal of Molecular Recognition</i> , 2010, 23, 173-182.	2.1	29
39	Rapid Chagas Disease Drug Target Discovery Using Directed Evolution in Drug-Sensitive Yeast. <i>ACS Chemical Biology</i> , 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. <i>ACS Central Science</i> , 2018, 4, 1570-1577.	11.3	25
41	CrystalDock: A Novel Approach to Fragment-Based Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2573-2580.	5.4	23
42	Pyroneâ€²Based Inhibitors of Metalloproteinase Types 2 and 3 May Work as Conformationâ€²Selective Inhibitors. <i>Chemical Biology and Drug Design</i> , 2011, 78, 191-198.	3.2	23
43	Distributed Drug Discovery: Advancing Chemical Education through Contextualized Combinatorial Solid-Phase Organic Laboratories. <i>Journal of Chemical Education</i> , 2015, 92, 819-826.	2.3	23
44	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.	2.3	22
45	Capturing the Mechanism Underlying TOP mRNA Binding to LARP1. <i>Structure</i> , 2019, 27, 1771-1781.e5.	3.3	20
46	DeepFrag: An Open-Source Browser App for Deep-Learning Lead Optimization. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2523-2529.	5.4	19
47	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, 358-365.	3.2	17
48	Two inhibitors of yeast plasma membrane ATPase 1 (ScPma1p): toward the development of novel antifungal therapies. <i>Journal of Cheminformatics</i> , 2018, 10, 6.	6.1	17
49	Celastrol inhibits Plasmodium falciparum enoyl-acyl carrier protein reductase. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 6053-6061.	3.0	16
50	LigGrep: a tool for filtering docked poses to improve virtual-screening hit rates. <i>Journal of Cheminformatics</i> , 2020, 12, 69.	6.1	16
51	The Molecular Dynamics of <i>Trypanosoma brucei</i> UDPâ€²Galactose 4â€²â€²Epi-merase: A Drug Target for African Sleeping Sickness. <i>Chemical Biology and Drug Design</i> , 2012, 80, 173-181.	3.2	14
52	Pyrite: A blender plugin for visualizing molecular dynamics simulations using industryâ€²standard rendering techniques. <i>Journal of Computational Chemistry</i> , 2018, 39, 748-755.	3.3	13
53	BINANA 2: Characterizing Receptor/Ligand Interactions in Python and JavaScript. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 753-760.	5.4	12
54	Toward Understanding the Conformational Dynamics of RNA Ligation. <i>Biochemistry</i> , 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. <i>Physiological and Biochemical Zoology</i> , 2019, 92, 579-590.	1.5	11
56	Adaptive laboratory evolution in <i>S. cerevisiae</i> highlights role of transcription factors in fungal xenobiotic resistance. <i>Communications Biology</i> , 2022, 5, 128.	4.4	8
57	Tryptophan Contributions to the Empirical Free-Energy Profile in Gramicidin A/M Heterodimer Channels. <i>Biophysical Journal</i> , 2006, 91, 3230-3241.	0.5	7
58	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.	3.2	6
59	Scoria: a Python module for manipulating 3D molecular data. <i>Journal of Cheminformatics</i> , 2017, 9, 52.	6.1	6
60	Novel mutation in hexokinase 2 confers resistance to 2-deoxyglucose by altering protein dynamics. <i>PLoS Computational Biology</i> , 2022, 18, e1009929.	3.2	6
61	Towards the development of novel <i>Trypanosoma brucei</i> RNA editing ligase 1 inhibitors. <i>BMC Pharmacology</i> , 2011, 11, 9.	0.4	5
62	MutantHuntWGS: A Pipeline for Identifying <i>Saccharomyces cerevisiae</i> Mutations. <i>G3: Genes, Genomes, Genetics</i> , 2020, 10, 3009-3014.	1.8	5
63	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.	5.4	4
64	Phosphate position is key in mediating transmembrane ion channel TMEM16A's phosphatidylinositol 4,5-bisphosphate interaction. <i>Journal of Biological Chemistry</i> , 2022, 298, 102264.	3.4	2
65	Influenza Viral Envelope Simulation Reveals Novel Druggable Pockets on Surface Glycoproteins. <i>Biophysical Journal</i> , 2018, 114, 341a.	0.5	1
66	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. <i>BMC Bioinformatics</i> , 2014, 15, 159.	2.6	0
67	The Do's and Do Not's of a 100 Million Atom Molecular Dynamics Simulation. <i>Biophysical Journal</i> , 2015, 108, 158a.	0.5	0