

S Joshua Swamidass

List of Publications by Citations

Source: <https://exaly.com/author-pdf/8230042/s-joshua-swamidass-publications-by-citations.pdf>

Version: 2024-04-24

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

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

72
papers

3,597
citations

29
h-index

59
g-index

102
ext. papers

4,530
ext. citations

8.5
avg, IF

5.48
L-index

#	Paper	IF	Citations
72	Opportunities and obstacles for deep learning in biology and medicine. <i>Journal of the Royal Society Interface</i> , 2018 , 15,	4.1	780
71	A survey of current trends in computational drug repositioning. <i>Briefings in Bioinformatics</i> , 2016 , 17, 2-12	3.4	309
70	Graph kernels for chemical informatics. <i>Neural Networks</i> , 2005 , 18, 1093-110	9.1	263
69	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. <i>PLoS Pathogens</i> , 2016 , 12, e1005763	7.6	167
68	XenoSite: accurately predicting CYP-mediated sites of metabolism with neural networks. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 3373-83	6.1	135
67	ChemDB: a public database of small molecules and related chemoinformatics resources. <i>Bioinformatics</i> , 2005 , 21, 4133-9	7.2	132
66	Kernels for small molecules and the prediction of mutagenicity, toxicity and anti-cancer activity. <i>Bioinformatics</i> , 2005 , 21 Suppl 1, i359-68	7.2	125
65	Structure-based inhibitor design of AccD5, an essential acyl-CoA carboxylase carboxyltransferase domain of Mycobacterium tuberculosis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006 , 103, 3072-7	11.5	105
64	Modeling Epoxidation of Drug-like Molecules with a Deep Machine Learning Network. <i>ACS Central Science</i> , 2015 , 1, 168-80	16.8	102
63	ChemDB update--full-text search and virtual chemical space. <i>Bioinformatics</i> , 2007 , 23, 2348-51	7.2	97
62	A CROC stronger than ROC: measuring, visualizing and optimizing early retrieval. <i>Bioinformatics</i> , 2010 , 26, 1348-56	7.2	74
61	Bounds and algorithms for fast exact searches of chemical fingerprints in linear and sublinear time. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 302-17	6.1	74
60	Deep Learning Global Glomerulosclerosis in Transplant Kidney Frozen Sections. <i>IEEE Transactions on Medical Imaging</i> , 2018 , 37, 2718-2728	11.7	67
59	Mining small-molecule screens to repurpose drugs. <i>Briefings in Bioinformatics</i> , 2011 , 12, 327-35	13.4	59
58	Modeling Reactivity to Biological Macromolecules with a Deep Multitask Network. <i>ACS Central Science</i> , 2016 , 2, 529-37	16.8	56
57	Site of reactivity models predict molecular reactivity of diverse chemicals with glutathione. <i>Chemical Research in Toxicology</i> , 2015 , 28, 797-809	4	54
56	Discovery of power-laws in chemical space. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 1138-51	5.1	53

55	One- to four-dimensional kernels for virtual screening and the prediction of physical, chemical, and biological properties. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 965-74	6.1	49
54	Mathematical correction for fingerprint similarity measures to improve chemical retrieval. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 952-64	6.1	46
53	RS-WebPredictor: a server for predicting CYP-mediated sites of metabolism on drug-like molecules. <i>Bioinformatics</i> , 2013 , 29, 497-8	7.2	45
52	XenoSite server: a web-available site of metabolism prediction tool. <i>Bioinformatics</i> , 2015 , 31, 1136-7	7.2	44
51	Deep Learning to Predict the Formation of Quinone Species in Drug Metabolism. <i>Chemical Research in Toxicology</i> , 2017 , 30, 642-656	4	43
50	Influence relevance voting: an accurate and interpretable virtual high throughput screening method. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 756-66	6.1	43
49	Lossless compression of chemical fingerprints using integer entropy codes improves storage and retrieval. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 2098-109	6.1	41
48	A simple model predicts UGT-mediated metabolism. <i>Bioinformatics</i> , 2016 , 32, 3183-3189	7.2	39
47	A deep learning approach to automate refinement of somatic variant calling from cancer sequencing data. <i>Nature Genetics</i> , 2018 , 50, 1735-1743	36.3	38
46	Unsupervised detection of cancer driver mutations with parsimony-guided learning. <i>Nature Genetics</i> , 2016 , 48, 1288-94	36.3	33
45	Standard operating procedure for somatic variant refinement of sequencing data with paired tumor and normal samples. <i>Genetics in Medicine</i> , 2019 , 21, 972-981	8.1	31
44	Statistically identifying tumor suppressors and oncogenes from pan-cancer genome-sequencing data. <i>Bioinformatics</i> , 2015 , 31, 3561-8	7.2	30
43	Computational Approach to Structural Alerts: Furans, Phenols, Nitroaromatics, and Thiophenes. <i>Chemical Research in Toxicology</i> , 2017 , 30, 1046-1059	4	24
42	Large scale study of multiple-molecule queries. <i>Journal of Cheminformatics</i> , 2009 , 1, 7	8.6	23
41	Accounting for proximal variants improves neoantigen prediction. <i>Nature Genetics</i> , 2019 , 51, 175-179	36.3	23
40	Functional census of mutation sequence spaces: the example of p53 cancer rescue mutants. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2006 , 3, 114-25	3	22
39	Inhibition of DNA Methyltransferases Blocks Mutant Huntingtin-Induced Neurotoxicity. <i>Scientific Reports</i> , 2016 , 6, 31022	4.9	20
38	Computationally Assessing the Bioactivation of Drugs by N-Dealkylation. <i>Chemical Research in Toxicology</i> , 2018 , 31, 68-80	4	19

37	Bigger data, collaborative tools and the future of predictive drug discovery. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 997-1008	4.2	19
36	Subcellular localization and Ser-137 phosphorylation regulate tumor-suppressive activity of profilin-1. <i>Journal of Biological Chemistry</i> , 2015 , 290, 9075-86	5.4	17
35	Modeling Small-Molecule Reactivity Identifies Promiscuous Bioactive Compounds. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1483-1500	6.1	16
34	Scaffold network generator: a tool for mining molecular structures. <i>Bioinformatics</i> , 2013 , 29, 2655-6	7.2	16
33	The Metabolic Rainbow: Deep Learning Phase I Metabolism in Five Colors. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 1146-1164	6.1	15
32	Black Box to Conversational Machine Learning: Ondansetron Reduces Risk of Hospital-Acquired Venous Thromboembolism. <i>IEEE Journal of Biomedical and Health Informatics</i> , 2021 , 25, 2204-2214	7.2	15
31	Extending P450 site-of-metabolism models with region-resolution data. <i>Bioinformatics</i> , 2015 , 31, 1966-73.2	7.2	14
30	Learning a Local-Variable Model of Aromatic and Conjugated Systems. <i>ACS Central Science</i> , 2018 , 4, 52-62.8	6.8	14
29	Accounting for noise when clustering biological data. <i>Briefings in Bioinformatics</i> , 2013 , 14, 423-36	13.4	14
28	Machine learning liver-injuring drug interactions with non-steroidal anti-inflammatory drugs (NSAIDs) from a retrospective electronic health record (EHR) cohort. <i>PLoS Computational Biology</i> , 2021 , 17, e1009053	5	14
27	An economic framework to prioritize confirmatory tests after a high-throughput screen. <i>Journal of Biomolecular Screening</i> , 2010 , 15, 680-6		12
26	Deep learning quantification of percent steatosis in donor liver biopsy frozen sections. <i>EBioMedicine</i> , 2020 , 60, 103029	8.8	12
25	CYP2C19 and 3A4 Dominate Metabolic Clearance and Bioactivation of Terbinafine Based on Computational and Experimental Approaches. <i>Chemical Research in Toxicology</i> , 2019 , 32, 1151-1164	4	11
24	Lamisil (terbinafine) toxicity: Determining pathways to bioactivation through computational and experimental approaches. <i>Biochemical Pharmacology</i> , 2018 , 156, 10-21	6	11
23	Combined Analysis of Phenotypic and Target-Based Screening in Assay Networks. <i>Journal of Biomolecular Screening</i> , 2014 , 19, 782-90		11
22	Probabilistic Substructure Mining From Small-Molecule Screens. <i>Molecular Informatics</i> , 2011 , 30, 809-15	3.8	11
21	Improved Prediction of CYP-Mediated Metabolism with Chemical Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 972-82	6.1	10
20	Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. <i>Nature Communications</i> , 2021 , 12, 3023	17.4	10

19	Comprehensive kinetic and modeling analyses revealed CYP2C9 and 3A4 determine terbinafine metabolic clearance and bioactivation. <i>Biochemical Pharmacology</i> , 2019 , 170, 113661	6	9
18	XenoNet: Inference and Likelihood of Intermediate Metabolite Formation. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 3431-3449	6.1	8
17	Dual mechanisms suppress meloxicam bioactivation relative to sudoxicam. <i>Toxicology</i> , 2020 , 440, 152478-152484	4.4	8
16	Sharing chemical relationships does not reveal structures. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 37-48	6.1	7
15	Enhancing the rate of scaffold discovery with diversity-oriented prioritization. <i>Bioinformatics</i> , 2011 , 27, 2271-8	7.2	7
14	Utility-aware screening with clique-oriented prioritization. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 29-37	6.1	6
13	Automatically detecting workflows in PubChem. <i>Journal of Biomolecular Screening</i> , 2012 , 17, 1071-9		6
12	Site-Level Bioactivity of Small-Molecules from Deep-Learned Representations of Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 9194-9202	2.8	6
11	Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 4702-4716	6.1	6
10	Precision Medicine in Pancreatic Disease-Knowledge Gaps and Research Opportunities: Summary of a National Institute of Diabetes and Digestive and Kidney Diseases Workshop. <i>Pancreas</i> , 2019 , 48, 1250-1258	2.6	6
9	Securely measuring the overlap between private datasets with cryptosets. <i>PLoS ONE</i> , 2015 , 10, e0117898	3.7	5
8	Managing missing measurements in small-molecule screens. <i>Journal of Computer-Aided Molecular Design</i> , 2013 , 27, 469-78	4.2	3
7	Impacts of diphenylamine NSAID halogenation on bioactivation risks. <i>Toxicology</i> , 2021 , 458, 152832	4.4	3
6	Modeling the Bioactivation and Subsequent Reactivity of Drugs. <i>Chemical Research in Toxicology</i> , 2021 , 34, 584-600	4	3
5	Deep Learning Global Glomerulosclerosis in Transplant Kidney Frozen Sections		2
4	A Time-Embedding Network Models the Ontogeny of 23 Hepatic Drug Metabolizing Enzymes. <i>Chemical Research in Toxicology</i> , 2019 , 32, 1707-1721	4	1
3	DiffNets: deep learning the structural determinants of proteins biochemical properties by comparing different structural ensembles		1
2	Deep Learning Coordinate-Free Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 8978-8986	3.6	0

1 Education: Initiatives to bridge faith and science. *Nature*, **2015**, 523, 531

50.4