

# S Joshua Swamidass

## List of Publications by Year in descending order

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Version: 2024-02-01

71  
papers

5,196  
citations

147566

31  
h-index

91712

69  
g-index

102  
all docs

102  
docs citations

102  
times ranked

7417  
citing authors

#	ARTICLE	IF	CITATIONS
1	Opportunities and obstacles for deep learning in biology and medicine. <i>Journal of the Royal Society Interface</i> , 2018, 15, 20170387.	1.5	1,282
2	A survey of current trends in computational drug repositioning. <i>Briefings in Bioinformatics</i> , 2016, 17, 2-12.	3.2	459
3	Graph kernels for chemical informatics. <i>Neural Networks</i> , 2005, 18, 1093-1110.	3.3	329
4	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. <i>PLoS Pathogens</i> , 2016, 12, e1005763.	2.1	244
5	XenoSite: Accurately Predicting CYP-Mediated Sites of Metabolism with Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 3373-3383.	2.5	179
6	ChemDB: a public database of small molecules and related cheminformatics resources. <i>Bioinformatics</i> , 2005, 21, 4133-4139.	1.8	155
7	Kernels for small molecules and the prediction of mutagenicity, toxicity and anti-cancer activity. <i>Bioinformatics</i> , 2005, 21, i359-i368.	1.8	145
8	Modeling Epoxidation of Drug-like Molecules with a Deep Machine Learning Network. <i>ACS Central Science</i> , 2015, 1, 168-180.	5.3	130
9	Deep Learning Global Glomerulosclerosis in Transplant Kidney Frozen Sections. <i>IEEE Transactions on Medical Imaging</i> , 2018, 37, 2718-2728.	5.4	119
10	ChemDB update full-text search and virtual chemical space. <i>Bioinformatics</i> , 2007, 23, 2348-2351.	1.8	117
11	Structure-based inhibitor design of AccD5, an essential acyl-CoA carboxylase carboxyltransferase domain of <i>Mycobacterium tuberculosis</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 3072-3077.	3.3	112
12	A CROC stronger than ROC: measuring, visualizing and optimizing early retrieval. <i>Bioinformatics</i> , 2010, 26, 1348-1356.	1.8	88
13	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, 302-317.	2.5	87
14	Mining small-molecule screens to repurpose drugs. <i>Briefings in Bioinformatics</i> , 2011, 12, 327-335.	3.2	85
15	Modeling Reactivity to Biological Macromolecules with a Deep Multitask Network. <i>ACS Central Science</i> , 2016, 2, 529-537.	5.3	76
16	Site of Reactivity Models Predict Molecular Reactivity of Diverse Chemicals with Glutathione. <i>Chemical Research in Toxicology</i> , 2015, 28, 797-809.	1.7	70
17	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.	1.1	67
18	XenoSite server: a web-available site of metabolism prediction tool. <i>Bioinformatics</i> , 2015, 31, 1136-1137.	1.8	64

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19	A deep learning approach to automate refinement of somatic variant calling from cancer sequencing data. <i>Nature Genetics</i> , 2018, 50, 1735-1743.	9.4	62
20	Mathematical Correction for Fingerprint Similarity Measures to Improve Chemical Retrieval. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 952-964.	2.5	61
21	Discovery of Power-Laws in Chemical Space. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1138-1151.	2.5	58
22	RS-WebPredictor: a server for predicting CYP-mediated sites of metabolism on drug-like molecules. <i>Bioinformatics</i> , 2013, 29, 497-498.	1.8	57
23	Deep Learning to Predict the Formation of Quinone Species in Drug Metabolism. <i>Chemical Research in Toxicology</i> , 2017, 30, 642-656.	1.7	57
24	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, 965-974.	2.5	56
25	Statistically identifying tumor suppressors and oncogenes from pan-cancer genome-sequencing data. <i>Bioinformatics</i> , 2015, 31, 3561-3568.	1.8	55
26	Unsupervised detection of cancer driver mutations with parsimony-guided learning. <i>Nature Genetics</i> , 2016, 48, 1288-1294.	9.4	52
27	A simple model predicts UGT-mediated metabolism. <i>Bioinformatics</i> , 2016, 32, 3183-3189.	1.8	51
28	Influence Relevance Voting: An Accurate And Interpretable Virtual High Throughput Screening Method. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 756-766.	2.5	49
29	Lossless Compression of Chemical Fingerprints Using Integer Entropy Codes Improves Storage and Retrieval. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2098-2109.	2.5	45
30	Accounting for proximal variants improves neoantigen prediction. <i>Nature Genetics</i> , 2019, 51, 175-179.	9.4	43
31	Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. <i>Nature Communications</i> , 2021, 12, 3023.	5.8	42
32	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.	1.5	33
33	Computational Approach to Structural Alerts: Furans, Phenols, Nitroaromatics, and Thiophenes. <i>Chemical Research in Toxicology</i> , 2017, 30, 1046-1059.	1.7	32
34	Deep learning quantification of percent steatosis in donor liver biopsy frozen sections. <i>EBioMedicine</i> , 2020, 60, 103029.	2.7	32
35	Computationally Assessing the Bioactivation of Drugs by N-Dealkylation. <i>Chemical Research in Toxicology</i> , 2018, 31, 68-80.	1.7	30
36	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, 114-125.	1.9	28

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37	Inhibition of DNA Methyltransferases Blocks Mutant Huntingtin-Induced Neurotoxicity. <i>Scientific Reports</i> , 2016, 6, 31022.	1.6	28
38	Modeling Small-Molecule Reactivity Identifies Promiscuous Bioactive Compounds. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1483-1500.	2.5	28
39	The Metabolic Rainbow: Deep Learning Phase I Metabolism in Five Colors. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1146-1164.	2.5	26
40	Large scale study of multiple-molecule queries. <i>Journal of Cheminformatics</i> , 2009, 1, 7.	2.8	24
41	Accounting for noise when clustering biological data. <i>Briefings in Bioinformatics</i> , 2013, 14, 423-436.	3.2	24
42	“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.	3.9	24
43	Combined Analysis of Phenotypic and Target-Based Screening in Assay Networks. <i>Journal of Biomolecular Screening</i> , 2014, 19, 782-790.	2.6	23
44	Subcellular Localization and Ser-137 Phosphorylation Regulate Tumor-suppressive Activity of Profilin-1. <i>Journal of Biological Chemistry</i> , 2015, 290, 9075-9086.	1.6	23
45	Bigger data, collaborative tools and the future of predictive drug discovery. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 997-1008.	1.3	22
46	Scaffold network generator: a tool for mining molecular structures. <i>Bioinformatics</i> , 2013, 29, 2655-2656.	1.8	20
47	Learning a Local-Variable Model of Aromatic and Conjugated Systems. <i>ACS Central Science</i> , 2018, 4, 52-62.	5.3	18
48	Lamisil (terbinafine) toxicity: Determining pathways to bioactivation through computational and experimental approaches. <i>Biochemical Pharmacology</i> , 2018, 156, 10-21.	2.0	17
49	Dual mechanisms suppress meloxicam bioactivation relative to sudoxicam. <i>Toxicology</i> , 2020, 440, 152478.	2.0	16
50	Extending P450 site-of-metabolism models with region-resolution data. <i>Bioinformatics</i> , 2015, 31, 1966-1973.	1.8	15
51	An Economic Framework to Prioritize Confirmatory Tests after a High-Throughput Screen. <i>Journal of Biomolecular Screening</i> , 2010, 15, 680-686.	2.6	14
52	XenoNet: Inference and Likelihood of Intermediate Metabolite Formation. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3431-3449.	2.5	14
53	Improved Prediction of CYP-Mediated Metabolism with Chemical Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 972-982.	2.5	13
54	Comprehensive kinetic and modeling analyses revealed CYP2C9 and 3A4 determine terbinafine metabolic clearance and bioactivation. <i>Biochemical Pharmacology</i> , 2019, 170, 113661.	2.0	13

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55	Probabilistic Substructure Mining From Small-Molecule Screens. <i>Molecular Informatics</i> , 2011, 30, 809-815.	1.4	12
56	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.	1.7	12
57	Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4702-4716.	2.5	11
58	Modeling the Bioactivation and Subsequent Reactivity of Drugs. <i>Chemical Research in Toxicology</i> , 2021, 34, 584-600.	1.7	11
59	Enhancing the rate of scaffold discovery with diversity-oriented prioritization. <i>Bioinformatics</i> , 2011, 27, 2271-2278.	1.8	9
60	Automatically Detecting Workflows in PubChem. <i>Journal of Biomolecular Screening</i> , 2012, 17, 1071-1079.	2.6	9
61	Precision Medicine in Pancreatic Disease—Knowledge Gaps and Research Opportunities. <i>Pancreas</i> , 2019, 48, 1250-1258.	0.5	9
62	Utility-Aware Screening with Clique-Oriented Prioritization. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 29-37.	2.5	7
63	Sharing Chemical Relationships Does Not Reveal Structures. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 37-48.	2.5	7
64	Site-Level Bioactivity of Small-Molecules from Deep-Learned Representations of Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9194-9202.	1.1	7
65	Securely Measuring the Overlap between Private Datasets with Cryptosets. <i>PLoS ONE</i> , 2015, 10, e0117898.	1.1	6
66	A Time-Embedding Network Models the Ontogeny of 23 Hepatic Drug Metabolizing Enzymes. <i>Chemical Research in Toxicology</i> , 2019, 32, 1707-1721.	1.7	6
67	Impacts of diphenylamine NSAID halogenation on bioactivation risks. <i>Toxicology</i> , 2021, 458, 152832.	2.0	5
68	Deep Learning Coordinate-Free Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8978-8986.	1.1	5
69	Managing missing measurements in small-molecule screens. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 469-478.	1.3	3
70	Using economic optimization to design high-throughput screens. <i>Future Medicinal Chemistry</i> , 2013, 5, 9-11.	1.1	2
71	Initiatives to bridge faith and science. <i>Nature</i> , 2015, 523, 531-531.	13.7	0