S Joshua Swamidass

List of Publications by Year
in descending order

71	5,196	147801 31	91884 69
papers	citations	h-index	g-index

102	102	102	7417
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	â€˜Black Boxâ€™ to â€˜Conversationalâ€™ Machine Learning: Ondansetron Reduces Risk of Hospital-Acquired Venous Thromboembolism. IEEE Journal of Biomedical and Health Informatics, 2021, 25, 2204-2214.	6.3	24
2	Modeling the Bioactivation and Subsequent Reactivity of Drugs. Chemical Research in Toxicology, 2021, 34, 584-600.	3.3	11
3	Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. Nature Communications, 2021, 12, 3023.	12.8	42
4	Impacts of diphenylamine NSAID halogenation on bioactivation risks. Toxicology, 2021, 458, 152832.	4.2	5
5	Machine learning liver-injuring drug interactions with non-steroidal anti-inflammatory drugs (NSAIDs) from a retrospective electronic health record (EHR) cohort. PLoS Computational Biology, 2021, 17, e1009053.	3.2	33
6	Deep Learning Coordinate-Free Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 8978-8986.	2.5	5
7	Deep learning quantification of percent steatosis in donor liver biopsy frozen sections. EBioMedicine, 2020, 60, 103029.	6.1	32
8	Site-Level Bioactivity of Small-Molecules from Deep-Learned Representations of Quantum Chemistry. Journal of Physical Chemistry A, 2020, 124, 9194-9202.	2.5	7
9	Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites. Journal of Chemical Information and Modeling, 2020, 60, 4702-4716.	5.4	11
10	XenoNet: Inference and Likelihood of Intermediate Metabolite Formation. Journal of Chemical Information and Modeling, 2020, 60, 3431-3449.	5.4	14
11	The Metabolic Rainbow: Deep Learning Phase I Metabolism in Five Colors. Journal of Chemical Information and Modeling, 2020, 60, 1146-1164.	5.4	26
12	Dual mechanisms suppress meloxicam bioactivation relative to sudoxicam. Toxicology, 2020, 440, 152478.	4.2	16
13	A Time-Embedding Network Models the Ontogeny of 23 Hepatic Drug Metabolizing Enzymes. Chemical Research in Toxicology, 2019, 32, 1707-1721.	3.3	6
14	Comprehensive kinetic and modeling analyses revealed CYP2C9 and 3A4 determine terbinafine metabolic clearance and bioactivation. Biochemical Pharmacology, 2019, 170, 113661.	4.4	13
15	CYP2C19 and 3A4 Dominate Metabolic Clearance and Bioactivation of Terbinafine Based on Computational and Experimental Approaches. Chemical Research in Toxicology, 2019, 32, 1151-1164.	3.3	12
16	Precision Medicine in Pancreatic Diseaseâ€”Knowledge Gaps and Research Opportunities. Pancreas, 2019, 48, 1250-1258.	1.1	9
17	Accounting for proximal variants improves neoantigen prediction. Nature Genetics, 2019, 51, 175-179.	21.4	43
18	Standard operating procedure for somatic variant refinement of sequencing data with paired tumor andÂnormal samples. Genetics in Medicine, 2019, 21, 972-981.	2.4	67

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19	Opportunities and obstacles for deep learning in biology and medicine. Journal of the Royal Society Interface, 2018, 15, 20170387.	3.4	1,282
20	Computationally Assessing the Bioactivation of Drugs by N-Dealkylation. Chemical Research in Toxicology, 2018, 31, 68-80.	3.3	30
21	Learning a Local-Variable Model of Aromatic and Conjugated Systems. ACS Central Science, 2018, 4, 52-62.	11.3	18
22	A deep learning approach to automate refinement of somatic variant calling from cancer sequencing data. Nature Genetics, 2018, 50, 1735-1743.	21.4	62
23	Lamisil (terbinafine) toxicity: Determining pathways to bioactivation through computational and experimental approaches. Biochemical Pharmacology, 2018, 156, 10-21.	4.4	17
24	Deep Learning Global Glomerulosclerosis in Transplant Kidney Frozen Sections. IEEE Transactions on Medical Imaging, 2018, 37, 2718-2728.	8.9	119
25	Modeling Small-Molecule Reactivity Identifies Promiscuous Bioactive Compounds. Journal of Chemical Information and Modeling, 2018, 58, 1483-1500.	5.4	28
26	Deep Learning to Predict the Formation of Quinone Species in Drug Metabolism. Chemical Research in Toxicology, 2017, 30, 642-656.	3.3	57
27	Computational Approach to Structural Alerts: Furans, Phenols, Nitroaromatics, and Thiophenes. Chemical Research in Toxicology, 2017, 30, 1046-1059.	3.3	32
28	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. PLoS Pathogens, 2016, 12, e1005763.	4.7	244
29	Inhibition of DNA Methyltransferases Blocks Mutant Huntingtin-Induced Neurotoxicity. Scientific Reports, 2016, 6, 31022.	3.3	28
30	Modeling Reactivity to Biological Macromolecules with a Deep Multitask Network. ACS Central Science, 2016, 2, 529-537.	11.3	76
31	Unsupervised detection of cancer driver mutations with parsimony-guided learning. Nature Genetics, 2016, 48, 1288-1294.	21.4	52
32	A simple model predicts UGT-mediated metabolism. Bioinformatics, 2016, 32, 3183-3189.	4.1	51
33	A survey of current trends in computational drug repositioning. Briefings in Bioinformatics, 2016, 17, 2-12.	6.5	459
34	Securely Measuring the Overlap between Private Datasets with Cryptosets. PLoS ONE, 2015, 10, e0117898.	2.5	6
35	Initiatives to bridge faith and science. Nature, 2015, 523, 531-531.	27.8	0
36	Statistically identifying tumor suppressors and oncogenes from pan-cancer genome-sequencing data. Bioinformatics, 2015, 31, 3561-3568.	4.1	55

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37	Modeling Epoxidation of Drug-like Molecules with a Deep Machine Learning Network. ACS Central Science, 2015, 1, 168-180.	11.3	130
38	Improved Prediction of CYP-Mediated Metabolism with Chemical Fingerprints. Journal of Chemical Information and Modeling, 2015, 55, 972-982.	5.4	13
39	Extending P450 site-of-metabolism models with region-resolution data. Bioinformatics, 2015, 31, 1966-1973.	4.1	15
40	Subcellular Localization and Ser-137 Phosphorylation Regulate Tumor-suppressive Activity of Profilin-1. Journal of Biological Chemistry, 2015, 290, 9075-9086.	3.4	23
41	Site of Reactivity Models Predict Molecular Reactivity of Diverse Chemicals with Glutathione. Chemical Research in Toxicology, 2015, 28, 797-809.	3.3	70
42	XenoSite server: a web-available site of metabolism prediction tool. Bioinformatics, 2015, 31, 1136-1137.	4.1	64
43	Sharing Chemical Relationships Does Not Reveal Structures. Journal of Chemical Information and Modeling, 2014, 54, 37-48.	5.4	7
44	Combined Analysis of Phenotypic and Target-Based Screening in Assay Networks. Journal of Biomolecular Screening, 2014, 19, 782-790.	2.6	23
45	Bigger data, collaborative tools and the future of predictive drug discovery. Journal of Computer-Aided Molecular Design, 2014, 28, 997-1008.	2.9	22
46	Managing missing measurements in small-molecule screens. Journal of Computer-Aided Molecular Design, 2013, 27, 469-478.	2.9	3
47	RS-WebPredictor: a server for predicting CYP-mediated sites of metabolism on drug-like molecules. Bioinformatics, 2013, 29, 497-498.	4.1	57
48	XenoSite: Accurately Predicting CYP-Mediated Sites of Metabolism with Neural Networks. Journal of Chemical Information and Modeling, 2013, 53, 3373-3383.	5.4	179
49	Accounting for noise when clustering biological data. Briefings in Bioinformatics, 2013, 14, 423-436.	6.5	24
50	Using economic optimization to design high-throughput screens. Future Medicinal Chemistry, 2013, 5, 9-11.	2.3	2
51	Scaffold network generator: a tool for mining molecular structures. Bioinformatics, 2013, 29, 2655-2656.	4.1	20
52	Automatically Detecting Workflows in PubChem. Journal of Biomolecular Screening, 2012, 17, 1071-1079.	2.6	9
53	Utility-Aware Screening with Clique-Oriented Prioritization. Journal of Chemical Information and Modeling, 2012, 52, 29-37.	5.4	7
54	Mining small-molecule screens to repurpose drugs. Briefings in Bioinformatics, 2011, 12, 327-335.	6.5	85

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55	Probabilistic Substructure Mining From Smallâ€Molecule Screens. Molecular Informatics, 2011, 30, 809-815.	2.5	12
56	Enhancing the rate of scaffold discovery with diversity-oriented prioritization. Bioinformatics, 2011, 27, 2271-2278.	4.1	9
57	A CROC stronger than ROC: measuring, visualizing and optimizing early retrieval. Bioinformatics, 2010, 26, 1348-1356.	4.1	88
58	An Economic Framework to Prioritize Confirmatory Tests after a High-Throughput Screen. Journal of Biomolecular Screening, 2010, 15, 680-686.	2.6	14
59	Large scale study of multiple-molecule queries. Journal of Cheminformatics, 2009, 1, 7.	6.1	24
60	Influence Relevance Voting: An Accurate And Interpretable Virtual High Throughput Screening Method. Journal of Chemical Information and Modeling, 2009, 49, 756-766.	5.4	49
61	Discovery of Power-Laws in Chemical Space. Journal of Chemical Information and Modeling, 2008, 48, 1138-1151.	5.4	58
62	ChemDB update full-text search and virtual chemical space. Bioinformatics, 2007, 23, 2348-2351.	4.1	117
63	Lossless Compression of Chemical Fingerprints Using Integer Entropy Codes Improves Storage and Retrieval. Journal of Chemical Information and Modeling, 2007, 47, 2098-2109.	5.4	45
64	One- to Four-Dimensional Kernels for Virtual Screening and the Prediction of Physical, Chemical, and Biological Properties. Journal of Chemical Information and Modeling, 2007, 47, 965-974.	5.4	56
65	Mathematical Correction for Fingerprint Similarity Measures to Improve Chemical Retrieval. Journal of Chemical Information and Modeling, 2007, 47, 952-964.	5.4	61
66	Bounds and Algorithms for Fast Exact Searches of Chemical Fingerprints in Linear and Sublinear Time. Journal of Chemical Information and Modeling, 2007, 47, 302-317.	5.4	87
67	Functional Census of Mutation Sequence Spaces: The Example of p53 Cancer Rescue Mutants. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2006, 3, 114-125.	3.0	28
68	Structure-based inhibitor design of AccD5, an essential acyl-CoA carboxylase carboxyltransferase domain of Mycobacterium tuberculosis. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 3072-3077.	7.1	112
69	Graph kernels for chemical informatics. Neural Networks, 2005, 18, 1093-1110.	5.9	329
70	Kernels for small molecules and the prediction of mutagenicity, toxicity and anti-cancer activity. Bioinformatics, 2005, 21, i359-i368.	4.1	145
71	ChemDB: a public database of small molecules and related chemoinformatics resources. Bioinformatics, 2005, 21, 4133-4139.	4.1	155