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	Opportunities and obstacles for deep learning in biology and medicine. Journal of the Royal Society Interface, 2018, 15, 20170387.	3.4	1,282
2	A survey of current trends in computational drug repositioning. Briefings in Bioinformatics, 2016, 17, 2-12.	6.5	459
3	Graph kernels for chemical informatics. Neural Networks, 2005, 18, 1093-1110.	5.9	329
4	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. PLoS Pathogens, 2016, 12, e1005763.	4.7	244
5	XenoSite: Accurately Predicting CYP-Mediated Sites of Metabolism with Neural Networks. Journal of Chemical Information and Modeling, 2013, 53, 3373-3383.	5.4	179
6	ChemDB: a public database of small molecules and related chemoinformatics resources. Bioinformatics, 2005, 21, 4133-4139.	4.1	155
7	Kernels for small molecules and the prediction of mutagenicity, toxicity and anti-cancer activity. Bioinformatics, 2005, 21, i359-i368.	4.1	145
8	Modeling Epoxidation of Drug-like Molecules with a Deep Machine Learning Network. ACS Central Science, 2015, 1, 168-180.	11.3	130
9	Deep Learning Global Glomerulosclerosis in Transplant Kidney Frozen Sections. IEEE Transactions on Medical Imaging, 2018, 37, 2718-2728.	8.9	119
10	ChemDB update full-text search and virtual chemical space. Bioinformatics, 2007, 23, 2348-2351.	4.1	117
11	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
12	A CROC stronger than ROC: measuring, visualizing and optimizing early retrieval. Bioinformatics, 2010, 26, 1348-1356.	4.1	88
13	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
14	Mining small-molecule screens to repurpose drugs. Briefings in Bioinformatics, 2011, 12, 327-335.	6.5	85
15	Modeling Reactivity to Biological Macromolecules with a Deep Multitask Network. ACS Central Science, 2016, 2, 529-537.	11.3	76
16	Site of Reactivity Models Predict Molecular Reactivity of Diverse Chemicals with Glutathione. Chemical Research in Toxicology, 2015, 28, 797-809.	3.3	70
17	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
18	XenoSite server: a web-available site of metabolism prediction tool. Bioinformatics, 2015, 31, 1136-1137.	4.1	64

#	Article	IF	Citations
19	A deep learning approach to automate refinement of somatic variant calling from cancer sequencing data. Nature Genetics, 2018, 50, 1735-1743.	21.4	62
20	Mathematical Correction for Fingerprint Similarity Measures to Improve Chemical Retrieval. Journal of Chemical Information and Modeling, 2007, 47, 952-964.	5.4	61
21	Discovery of Power-Laws in Chemical Space. Journal of Chemical Information and Modeling, 2008, 48, 1138-1151.	5.4	58
22	RS-WebPredictor: a server for predicting CYP-mediated sites of metabolism on drug-like molecules. Bioinformatics, 2013, 29, 497-498.	4.1	57
23	Deep Learning to Predict the Formation of Quinone Species in Drug Metabolism. Chemical Research in Toxicology, 2017, 30, 642-656.	3.3	57
24	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
25	Statistically identifying tumor suppressors and oncogenes from pan-cancer genome-sequencing data. Bioinformatics, 2015, 31, 3561-3568.	4.1	55
26	Unsupervised detection of cancer driver mutations with parsimony-guided learning. Nature Genetics, 2016, 48, 1288-1294.	21.4	52
27	A simple model predicts UGT-mediated metabolism. Bioinformatics, 2016, 32, 3183-3189.	4.1	51
28	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
29	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
30	Accounting for proximal variants improves neoantigen prediction. Nature Genetics, 2019, 51, 175-179.	21.4	43
31	Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. Nature Communications, 2021, 12, 3023.	12.8	42
32	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
33	Computational Approach to Structural Alerts: Furans, Phenols, Nitroaromatics, and Thiophenes. Chemical Research in Toxicology, 2017, 30, 1046-1059.	3.3	32
34	Deep learning quantification of percent steatosis in donor liver biopsy frozen sections. EBioMedicine, 2020, 60, 103029.	6.1	32
35	Computationally Assessing the Bioactivation of Drugs by N-Dealkylation. Chemical Research in Toxicology, 2018, 31, 68-80.	3.3	30
36	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

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37	Inhibition of DNA Methyltransferases Blocks Mutant Huntingtin-Induced Neurotoxicity. Scientific Reports, 2016, 6, 31022.	3.3	28
38	Modeling Small-Molecule Reactivity Identifies Promiscuous Bioactive Compounds. Journal of Chemical Information and Modeling, 2018, 58, 1483-1500.	5.4	28
39	The Metabolic Rainbow: Deep Learning Phase I Metabolism in Five Colors. Journal of Chemical Information and Modeling, 2020, 60, 1146-1164.	5.4	26
40	Large scale study of multiple-molecule queries. Journal of Cheminformatics, 2009, 1, 7.	6.1	24
41	Accounting for noise when clustering biological data. Briefings in Bioinformatics, 2013, 14, 423-436.	6.5	24
42	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
43	Combined Analysis of Phenotypic and Target-Based Screening in Assay Networks. Journal of Biomolecular Screening, 2014, 19, 782-790.	2.6	23
44	Subcellular Localization and Ser-137 Phosphorylation Regulate Tumor-suppressive Activity of Profilin-1. Journal of Biological Chemistry, 2015, 290, 9075-9086.	3.4	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	Scaffold network generator: a tool for mining molecular structures. Bioinformatics, 2013, 29, 2655-2656.	4.1	20
47	Learning a Local-Variable Model of Aromatic and Conjugated Systems. ACS Central Science, 2018, 4, 52-62.	11.3	18
48	Lamisil (terbinafine) toxicity: Determining pathways to bioactivation through computational and experimental approaches. Biochemical Pharmacology, 2018, 156, 10-21.	4.4	17
49	Dual mechanisms suppress meloxicam bioactivation relative to sudoxicam. Toxicology, 2020, 440, 152478.	4.2	16
50	Extending P450 site-of-metabolism models with region-resolution data. Bioinformatics, 2015, 31, 1966-1973.	4.1	15
51	An Economic Framework to Prioritize Confirmatory Tests after a High-Throughput Screen. Journal of Biomolecular Screening, 2010, 15, 680-686.	2.6	14
52	XenoNet: Inference and Likelihood of Intermediate Metabolite Formation. Journal of Chemical Information and Modeling, 2020, 60, 3431-3449.	5.4	14
53	Improved Prediction of CYP-Mediated Metabolism with Chemical Fingerprints. Journal of Chemical Information and Modeling, 2015, 55, 972-982.	5.4	13
54	Comprehensive kinetic and modeling analyses revealed CYP2C9 and 3A4 determine terbinafine metabolic clearance and bioactivation. Biochemical Pharmacology, 2019, 170, 113661.	4.4	13

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55	Probabilistic Substructure Mining From Smallâ€Molecule Screens. Molecular Informatics, 2011, 30, 809-815.	2.5	12
56	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
57	Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites. Journal of Chemical Information and Modeling, 2020, 60, 4702-4716.	5.4	11
58	Modeling the Bioactivation and Subsequent Reactivity of Drugs. Chemical Research in Toxicology, 2021, 34, 584-600.	3.3	11
59	Enhancing the rate of scaffold discovery with diversity-oriented prioritization. Bioinformatics, 2011, 27, 2271-2278.	4.1	9
60	Automatically Detecting Workflows in PubChem. Journal of Biomolecular Screening, 2012, 17, 1071-1079.	2.6	9
61	Precision Medicine in Pancreatic Diseaseâ€"Knowledge Gaps and Research Opportunities. Pancreas, 2019, 48, 1250-1258.	1.1	9
62	Utility-Aware Screening with Clique-Oriented Prioritization. Journal of Chemical Information and Modeling, 2012, 52, 29-37.	5.4	7
63	Sharing Chemical Relationships Does Not Reveal Structures. Journal of Chemical Information and Modeling, 2014, 54, 37-48.	5.4	7
64	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
65	Securely Measuring the Overlap between Private Datasets with Cryptosets. PLoS ONE, 2015, 10, e0117898.	2.5	6
66	A Time-Embedding Network Models the Ontogeny of 23 Hepatic Drug Metabolizing Enzymes. Chemical Research in Toxicology, 2019, 32, 1707-1721.	3.3	6
67	Impacts of diphenylamine NSAID halogenation on bioactivation risks. Toxicology, 2021, 458, 152832.	4.2	5
68	Deep Learning Coordinate-Free Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 8978-8986.	2.5	5
69	Managing missing measurements in small-molecule screens. Journal of Computer-Aided Molecular Design, 2013, 27, 469-478.	2.9	3
70	Using economic optimization to design high-throughput screens. Future Medicinal Chemistry, 2013, 5, 9-11.	2.3	2
71	Initiatives to bridge faith and science. Nature, 2015, 523, 531-531.	27.8	0