S Joshua Swamidass

List of Publications by Year in Descending Order

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	Deep Learning Coordinate-Free Quantum Chemistry. *Journal of Physical Chemistry A*, **2021**, 125, 8978-8986	2.8	0
71	Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. *Nature Communications*, **2021**, 12, 3023	17.4	10
70	Impacts of diphenylamine NSAID halogenation on bioactivation risks. *Toxicology*, **2021**, 458, 152832	4.4	3
69	Black Box to Conversational Machine Learning: Ondansetron Reduces Risk of Hospital-Acquired Venous Thromboembolism. *IEEE Journal of Biomedical and Health Informatics*, **2021**, 25, 2204-2214	7.2	15
68	Modeling the Bioactivation and Subsequent Reactivity of Drugs. *Chemical Research in Toxicology*, **2021**, 34, 584-600	4	3
67	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	5	14
66	XenoNet: Inference and Likelihood of Intermediate Metabolite Formation. *Journal of Chemical Information and Modeling*, **2020**, 60, 3431-3449	6.1	8
65	The Metabolic Rainbow: Deep Learning Phase I Metabolism in Five Colors. *Journal of Chemical Information and Modeling*, **2020**, 60, 1146-1164	6.1	15
64	Dual mechanisms suppress meloxicam bioactivation relative to sudoxicam. *Toxicology*, **2020**, 440, 152478	4.4	8
63	Deep learning quantification of percent steatosis in donor liver biopsy frozen sections. *EBioMedicine*, **2020**, 60, 103029	8.8	12
62	Site-Level Bioactivity of Small-Molecules from Deep-Learned Representations of Quantum Chemistry. *Journal of Physical Chemistry A*, **2020**, 124, 9194-9202	2.8	6
61	Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites. *Journal of Chemical Information and Modeling*, **2020**, 60, 4702-4716	6.1	6
60	CYP2C19 and 3A4 Dominate Metabolic Clearance and Bioactivation of Terbinafine Based on Computational and Experimental Approaches. *Chemical Research in Toxicology*, **2019**, 32, 1151-1164	4	11
59	A Time-Embedding Network Models the Ontogeny of 23 Hepatic Drug Metabolizing Enzymes. *Chemical Research in Toxicology*, **2019**, 32, 1707-1721	4	1
58	Comprehensive kinetic and modeling analyses revealed CYP2C9 and 3A4 determine terbinafine metabolic clearance and bioactivation. *Biochemical Pharmacology*, **2019**, 170, 113661	6	9
57	Precision Medicine in Pancreatic Disease-Knowledge Gaps and Research Opportunities: Summary of a National Institute of Diabetes and Digestive and Kidney Diseases Workshop. *Pancreas*, **2019**, 48, 1250-1258	2.6	6
56	Accounting for proximal variants improves neoantigen prediction. *Nature Genetics*, **2019**, 51, 175-179	36.3	23

55	Standard operating procedure for somatic variant refinement of sequencing data with paired tumor and normal samples. *Genetics in Medicine*, **2019**, 21, 972-981	8.1	31
54	Opportunities and obstacles for deep learning in biology and medicine. *Journal of the Royal Society Interface*, **2018**, 15,	4.1	780
53	Computationally Assessing the Bioactivation of Drugs by N-Dealkylation. *Chemical Research in Toxicology*, **2018**, 31, 68-80	4	19
52	Learning a Local-Variable Model of Aromatic and Conjugated Systems. *ACS Central Science*, **2018**, 4, 52-62	6.8	14
51	Lamisil (terbinafine) toxicity: Determining pathways to bioactivation through computational and experimental approaches. *Biochemical Pharmacology*, **2018**, 156, 10-21	6	11
50	Deep Learning Global Glomerulosclerosis in Transplant Kidney Frozen Sections. *IEEE Transactions on Medical Imaging*, **2018**, 37, 2718-2728	11.7	67
49	Modeling Small-Molecule Reactivity Identifies Promiscuous Bioactive Compounds. *Journal of Chemical Information and Modeling*, **2018**, 58, 1483-1500	6.1	16
48	A deep learning approach to automate refinement of somatic variant calling from cancer sequencing data. *Nature Genetics*, **2018**, 50, 1735-1743	36.3	38
47	Deep Learning to Predict the Formation of Quinone Species in Drug Metabolism. *Chemical Research in Toxicology*, **2017**, 30, 642-656	4	43
46	Computational Approach to Structural Alerts: Furans, Phenols, Nitroaromatics, and Thiophenes. *Chemical Research in Toxicology*, **2017**, 30, 1046-1059	4	24
45	A survey of current trends in computational drug repositioning. *Briefings in Bioinformatics*, **2016**, 17, 2-12	13.4	309
44	Unsupervised detection of cancer driver mutations with parsimony-guided learning. *Nature Genetics*, **2016**, 48, 1288-94	36.3	33
43	A simple model predicts UGT-mediated metabolism. *Bioinformatics*, **2016**, 32, 3183-3189	7.2	39
42	Open Source Drug Discovery with the Malaria Box Compound Collection for Neglected Diseases and Beyond. *PLoS Pathogens*, **2016**, 12, e1005763	7.6	167
41	Inhibition of DNA Methyltransferases Blocks Mutant Huntingtin-Induced Neurotoxicity. *Scientific Reports*, **2016**, 6, 31022	4.9	20
40	Modeling Reactivity to Biological Macromolecules with a Deep Multitask Network. *ACS Central Science*, **2016**, 2, 529-37	16.8	56
39	Education: Initiatives to bridge faith and science. *Nature*, **2015**, 523, 531	50.4	
38	Statistically identifying tumor suppressors and oncogenes from pan-cancer genome-sequencing data. *Bioinformatics*, **2015**, 31, 3561-8	7.2	30

37	Modeling Epoxidation of Drug-like Molecules with a Deep Machine Learning Network. *ACS Central Science*, **2015**, 1, 168-80	16.8	102
36	Improved Prediction of CYP-Mediated Metabolism with Chemical Fingerprints. *Journal of Chemical Information and Modeling*, **2015**, 55, 972-82	6.1	10
35	Extending P450 site-of-metabolism models with region-resolution data. *Bioinformatics*, **2015**, 31, 1966-73	7.2	14
34	Subcellular localization and Ser-137 phosphorylation regulate tumor-suppressive activity of profilin-1. *Journal of Biological Chemistry*, **2015**, 290, 9075-86	5.4	17
33	Site of reactivity models predict molecular reactivity of diverse chemicals with glutathione. *Chemical Research in Toxicology*, **2015**, 28, 797-809	4	54
32	XenoSite server: a web-available site of metabolism prediction tool. *Bioinformatics*, **2015**, 31, 1136-7	7.2	44
31	Securely measuring the overlap between private datasets with cryptosets. *PLoS ONE*, **2015**, 10, e0117898	3.7	5
30	Sharing chemical relationships does not reveal structures. *Journal of Chemical Information and Modeling*, **2014**, 54, 37-48	6.1	7
29	Combined Analysis of Phenotypic and Target-Based Screening in Assay Networks. *Journal of Biomolecular Screening*, **2014**, 19, 782-90		11
28	Bigger data, collaborative tools and the future of predictive drug discovery. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 997-1008	4.2	19
27	Managing missing measurements in small-molecule screens. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 469-78	4.2	3
26	RS-WebPredictor: a server for predicting CYP-mediated sites of metabolism on drug-like molecules. *Bioinformatics*, **2013**, 29, 497-8	7.2	45
25	XenoSite: accurately predicting CYP-mediated sites of metabolism with neural networks. *Journal of Chemical Information and Modeling*, **2013**, 53, 3373-83	6.1	135
24	Accounting for noise when clustering biological data. *Briefings in Bioinformatics*, **2013**, 14, 423-36	13.4	14
23	Scaffold network generator: a tool for mining molecular structures. *Bioinformatics*, **2013**, 29, 2655-6	7.2	16
22	Utility-aware screening with clique-oriented prioritization. *Journal of Chemical Information and Modeling*, **2012**, 52, 29-37	6.1	6
21	Automatically detecting workflows in PubChem. *Journal of Biomolecular Screening*, **2012**, 17, 1071-9		6
20	Mining small-molecule screens to repurpose drugs. *Briefings in Bioinformatics*, **2011**, 12, 327-35	13.4	59

19	Probabilistic Substructure Mining From Small-Molecule Screens. *Molecular Informatics*, **2011**, 30, 809-15	3.8	11
18	Enhancing the rate of scaffold discovery with diversity-oriented prioritization. *Bioinformatics*, **2011**, 27, 2271-8	7.2	7
17	A CROC stronger than ROC: measuring, visualizing and optimizing early retrieval. *Bioinformatics*, **2010**, 26, 1348-56	7.2	74
16	An economic framework to prioritize confirmatory tests after a high-throughput screen. *Journal of Biomolecular Screening*, **2010**, 15, 680-6		12
15	Large scale study of multiple-molecule queries. *Journal of Cheminformatics*, **2009**, 1, 7	8.6	23
14	Influence relevance voting: an accurate and interpretable virtual high throughput screening method. *Journal of Chemical Information and Modeling*, **2009**, 49, 756-66	6.1	43
13	Discovery of power-laws in chemical space. *Journal of Chemical Information and Modeling*, **2008**, 48, 1138-51	6.1	53
12	Mathematical correction for fingerprint similarity measures to improve chemical retrieval. *Journal of Chemical Information and Modeling*, **2007**, 47, 952-64	6.1	46
11	Bounds and algorithms for fast exact searches of chemical fingerprints in linear and sublinear time. *Journal of Chemical Information and Modeling*, **2007**, 47, 302-17	6.1	74
10	ChemDB update--full-text search and virtual chemical space. *Bioinformatics*, **2007**, 23, 2348-51	7.2	97
9	Lossless compression of chemical fingerprints using integer entropy codes improves storage and retrieval. *Journal of Chemical Information and Modeling*, **2007**, 47, 2098-109	6.1	41
8	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, 965-74	6.1	49
7	Functional census of mutation sequence spaces: the example of p53 cancer rescue mutants. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2006**, 3, 114-25	3	22
6	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, 3072-7	11.5	105
5	ChemDB: a public database of small molecules and related chemoinformatics resources. *Bioinformatics*, **2005**, 21, 4133-9	7.2	132
4	Graph kernels for chemical informatics. *Neural Networks*, **2005**, 18, 1093-110	9.1	263
3	Kernels for small molecules and the prediction of mutagenicity, toxicity and anti-cancer activity. *Bioinformatics*, **2005**, 21 Suppl 1, i359-68	7.2	125
2	DiffNets: deep learning the structural determinants of proteins biochemical properties by comparing different structural ensembles		1

1 Deep Learning Global Glomerulosclerosis in Transplant Kidney Frozen Sections 2