Jeremy L Jenkins

List of Publications by Year
in descending order

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Version: 2024-02-01

75 papers	6,004 citations	87723 38 h-index	74018 75 g-index
90 all docs	90 docs citations	90 times ranked	6232 citing authors

#	Article	IF	Citations
1	DRUG-seq Provides Unbiased Biological Activity Readouts for Neuroscience Drug Discovery. ACS Chemical Biology, 2022, 17, 1401-1414.	1.6	7
2	CYP27A1-dependent anti-melanoma activity of limonoid natural products targets mitochondrial metabolism. Cell Chemical Biology, 2021, 28, 1407-1419.e6.	2.5	11
3	Learning epistatic gene interactions from perturbation screens. PLoS ONE, 2021, 16, e0254491.	1.1	5
4	CPSF3-dependent pre-mRNA processing as a druggable node in AML and Ewingâ€™s sarcoma. Nature Chemical Biology, 2020, 16, 50-59.	3.9	59
5	Phenotypic landscape of intestinal organoid regeneration. Nature, 2020, 586, 275-280.	13.7	162
6	Systematic Chemogenetic Library Assembly. Cell Chemical Biology, 2020, 27, 1124-1129.	2.5	37
7	Ten simple rules to power drug discovery with data science. PLoS Computational Biology, 2020, 16, e1008126.	1.5	14
8	Benchmarking network algorithms for contextualizing genes of interest. PLoS Computational Biology, 2019, 15, e1007403.	1.5	7
9	Discovery of a ZIP7 inhibitor from a Notch pathway screen. Nature Chemical Biology, 2019, 15, 179-188.	3.9	46
10	Growth-restricting effects of siRNA transfections: a largely deterministic combination of off-target binding and hybridization-independent competition. Nucleic Acids Research, 2018, 46, 9309-9320.	6.5	7
11	DRUG-seq for miniaturized high-throughput transcriptome profiling in drug discovery. Nature Communications, 2018, 9, 4307.	5.8	133
12	Indolyl-Pyridinyl-Propenone-Induced Methuosis through the Inhibition of PIKFYVE. ACS Omega, 2018, 3, 6097-6103.	1.6	22
13	Recurrent ubiquitin B silencing in gynecological cancers establishes dependence on ubiquitin C. Journal of Clinical Investigation, 2017, 127, 4554-4568.	3.9	21
14	Data-Driven Derivation of an â€œInformer Compound Setâ€•for Improved Selection of Active Compounds in High-Throughput Screening. Journal of Chemical Information and Modeling, 2016, 56, 1622-1630.	2.5	14
15	Evidence-Based and Quantitative Prioritization of Tool Compounds in Phenotypic Drug Discovery. Cell Chemical Biology, 2016, 23, 862-874.	2.5	52
16	Identifying compound efficacy targets in phenotypic drug discovery. Drug Discovery Today, 2016, 21, 82-89.	3.2	127
17	Causal Network Models for Predicting Compound Targets and Driving Pathways in Cancer. Journal of Biomolecular Screening, 2014, 19, 791-802.	2.6	23
18	Translation of off-target effects: prediction of ADRs by integrated experimental and computational approach. Toxicology Research, 2014, 3, 433-444.	0.9	11

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19	Using Information from Historical High-Throughput Screens to Predict Active Compounds. Journal of Chemical Information and Modeling, 2014, 54, 1880-1891.	2.5	79
20	Target identification for a Hedgehog pathway inhibitor reveals the receptor GPR39. Nature Chemical Biology, 2014, 10, 343-349.	3.9	53
21	Rethinking cellular drug response. Nature Chemical Biology, 2013, 9, 669-670.	3.9	7
22	Biodiversity of small molecules â€“ a new perspective in screening set selection. Drug Discovery Today, 2013, 18, 674-680.	3.2	51
23	The Multidimensional Perturbation Value: A Single Metric to Measure Similarity and Activity of Treatments in High-Throughput Multidimensional Screens. Journal of Biomolecular Screening, 2013, 18, 367-377.	2.6	30
24	Determination of minimal transcriptional signatures of compounds for target prediction. Eurasip Journal on Bioinformatics and Systems Biology, 2012, 2012, 2.	1.4	7
25	Rethinking Molecular Similarity: Comparing Compounds on the Basis of Biological Activity. ACS Chemical Biology, 2012, 7, 1399-1409.	1.6	181
26	Largeâ€Scale QSAR in Target Prediction and Phenotypic HTS Assessment. Molecular Informatics, 2012, 31, 508-514.	1.4	9
27	Large-scale prediction and testing of drug activity on side-effect targets. Nature, 2012, 486, 361-367.	13.7	782
28	Activity-Aware Clustering of High Throughput Screening Data and Elucidation of Orthogonal Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2011, 51, 3158-3168.	2.5	20
29	From in silico target prediction to multi-target drug design: Current databases, methods and applications. Journal of Proteomics, 2011, 74, 2554-2574.	1.2	243
30	Computational methods for early predictive safety assessment from biological and chemical data. Expert Opinion on Drug Metabolism and Toxicology, 2011, 7, 1497-1511.	1.5	28
31	Recent trends and observations in the design of high-quality screening collections. Future Medicinal Chemistry, 2011, 3, 751-766.	1.1	55
32	A lead discovery strategy driven by a comprehensive analysis of proteases in the peptide substrate space. Protein Science, 2010, 19, 2096-2109.	3.1	7
33	Fishing for neuroactive compounds. Nature Chemical Biology, 2010, 6, 172-173.	3.9	14
34	SPREADâ€”exploiting chemical features that cause differential activity behavior. Statistical Analysis and Data Mining, 2009, 2, 115-122.	1.4	1
35	Chemogenomics: Looking at biology through the lens of chemistry. Statistical Analysis and Data Mining, 2009, 2, 149-160.	1.4	10
36	Plate-Based Diversity Selection Based on Empirical HTS Data to Enhance the Number of Hits and Their Chemical Diversity. Journal of Biomolecular Screening, 2009, 14, 690-699.	2.6	67

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37	Use of Ligand Based Models for Protein Domains To Predict Novel Molecular Targets and Applications To Triage Affinity Chromatography Data. Journal of Proteome Research, 2009, 8, 2575-2585.	1.8	20
38	How Similar Are Similarity Searching Methods? A Principal Component Analysis of Molecular Descriptor Space. Journal of Chemical Information and Modeling, 2009, 49, 108-119.	2.5	268
39	Mapping Adverse Drug Reactions in Chemical Space. Journal of Medicinal Chemistry, 2009, 52, 3103-3107.	2.9	156
40	Gaining Insight into Off-Target Mediated Effects of Drug Candidates with a Comprehensive Systems Chemical Biology Analysis. Journal of Chemical Information and Modeling, 2009, 49, 308-317.	2.5	161
41	Knowledge-Based Virtual Screening: Application to the MDM4/p53 Proteinâ€“Protein Interaction. Methods in Molecular Biology, 2009, 575, 173-194.	0.4	20
42	Chemogenomic Analysis of Safety Profiling Data. Methods in Molecular Biology, 2009, 575, 207-223.	0.4	9
43	Blocking binding of Bacillus thuringiensis Cry1Aa to Bombyx mori cadherin receptor results in only a minor reduction of toxicity. BMC Biochemistry, 2008, 9, 3.	4.4	11
44	Integrating high-content screening and ligand-target prediction to identify mechanism of action. Nature Chemical Biology, 2008, 4, 59-68.	3.9	332
45	â€œVirtual Fragment Linkingâ€• An Approach To Identify Potent Binders from Low Affinity Fragment Hits. Journal of Medicinal Chemistry, 2008, 51, 2481-2491.	2.9	39
46	Ligand-Target Prediction Using Winnow and Naive Bayesian Algorithms and the Implications of Overall Performance Statistics. Journal of Chemical Information and Modeling, 2008, 48, 2313-2325.	2.5	92
47	Chemogenomic Data Analysis: Prediction of Small-Molecule Targets and the Advent of Biological Fingerprints. Combinatorial Chemistry and High Throughput Screening, 2007, 10, 719-731.	0.6	97
48	â€œPlate Cherry Pickingâ€• A Novel Semi-Sequential Screening Paradigm for Cheaper, Faster, Information-Rich Compound Selection. Journal of Biomolecular Screening, 2007, 12, 320-327.	2.6	33
49	Analysis of Pharmacology Data and the Prediction of Adverse Drug Reactions and Off-Target Effects from Chemical Structure. ChemMedChem, 2007, 2, 861-873.	1.6	287
50	Clustering and Rule-Based Classifications of Chemical Structures Evaluated in the Biological Activity Space. Journal of Chemical Information and Modeling, 2007, 47, 325-336.	2.5	50
51	Understanding False Positives in Reporter Gene Assays:â€‰ in Silico Chemogenomics Approaches To Prioritize Cell-Based HTS Data. Journal of Chemical Information and Modeling, 2007, 47, 1319-1327.	2.5	66
52	Modeling Promiscuity Based on inâ€…vitro Safety Pharmacology Profiling Data. ChemMedChem, 2007, 2, 874-880.	1.6	169
53	Flexible 3D pharmacophores as descriptors of dynamic biological space. Journal of Molecular Graphics and Modelling, 2007, 26, 622-633.	1.3	47
54	Enrichment of High-Throughput Screening Data with Increasing Levels of Noise Using Support Vector Machines, Recursive Partitioning, and Laplacian-Modified Naive Bayesian Classifiers. Journal of Chemical Information and Modeling, 2006, 46, 193-200.	2.5	110

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55	Prediction of Biological Targets for Compounds Using Multiple-Category Bayesian Models Trained on Chemogenomics Databases. Journal of Chemical Information and Modeling, 2006, 46, 1124-1133.	2.5	315
56	Chapter 9 Molecular Similarity: Advances in Methods, Applications and Validations in Virtual Screening and QSAR. Annual Reports in Computational Chemistry, 2006, 2, 141-168.	0.9	10
57	Bridging Chemical and Biological Space:Â â€œTarget Fishingâ€•Using 2D and 3D Molecular Descriptors. Journal of Medicinal Chemistry, 2006, 49, 6802-6810.	2.9	184
58	â€œBayes Affinity Fingerprintsâ€•Improve Retrieval Rates in Virtual Screening and Define Orthogonal Bioactivity Space:â€‰ When Are Multitarget Drugs a Feasible Concept?. Journal of Chemical Information and Modeling, 2006, 46, 2445-2456.	2.5	125
59	In silico target fishing: Predicting biological targets from chemical structure. Drug Discovery Today: Technologies, 2006, 3, 413-421.	4.0	155
60	Streamlining lead discovery by aligning in silico and high-throughput screening. Current Opinion in Chemical Biology, 2006, 10, 343-351.	2.8	85
61	A 3D Similarity Method for Scaffold Hopping from Known Drugs or Natural Ligands to New Chemotypes. Journal of Medicinal Chemistry, 2004, 47, 6144-6159.	2.9	126
62	Unexpected Binding Mode for 2â€˜-Phosphoadenosine-Based Nucleotide Inhibitors in Complex with Human Angiogenin Revealed by Heteronuclear NMR Spectroscopyâ€. Biochemistry, 2003, 42, 11137-11149.	1.2	11
63	Identification of Small-Molecule Inhibitors of Human Angiogenin and Characterization of Their Binding Interactions Guided by Computational Dockingâ€. Biochemistry, 2003, 42, 6674-6687.	1.2	34
64	Inhibition of mammalian ribonucleases by endogenous adenosine dinucleotides. Biochemical and Biophysical Research Communications, 2003, 300, 81-86.	1.0	18
65	A small-molecule inhibitor of the ribonucleolytic activity of human angiogenin that possesses antitumor activity. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 10066-10071.	3.3	103
66	Virtual screening to enrich hit lists from high-throughput screening: A case study on small-molecule inhibitors of angiogenin. Proteins: Structure, Function and Bioinformatics, 2002, 50, 81-93.	1.5	75
67	Mutations at the arginine residues in Î±8 loop ofBacillus thuringiensisÎ´-endotoxin Cry1Ac affect toxicity and binding toManduca sextaandLymantria disparaminopeptidase N. FEBS Letters, 2001, 497, 108-112.	1.3	20
68	Cleavage of 3â€˜,5â€˜-Pyrophosphate-Linked Dinucleotides by Ribonuclease A and Angioginâ€‚â€¡. Biochemistry, 2001, 40, 10262-10272.	1.2	29
69	Plasma lipases and lipid transfer proteins increase phospholipid but not free cholesterol transfer from lipid emulsion to high density lipoproteins. BMC Biochemistry, 2001, 2, 1.	4.4	8
70	Binding specificity of Bacillus thuringiensis Cry1Aa for purified, native Bombyx mori aminopeptidase N and cadherin-like receptors. BMC Biochemistry, 2001, 2, 12.	4.4	29
71	Isolation and partial characterization of gypsy moth BTR-270, an anionic brush border membrane glycoconjugate that bindsBacillus thuringiensis Cry1A toxins with high affinity. Archives of Insect Biochemistry and Physiology, 2001, 46, 186-200.	0.6	71
72	Role of two arginine residues in domain II, loop 2 of Cry1Ab and Cry1Ac Bacillus thuringiensis delta-endotoxin in toxicity and binding to Manduca sexta and Lymantria dispar aminopeptidase N. Molecular Microbiology, 2000, 38, 289-298.	1.2	30

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73	Bivalent Sequential Binding Model of a Bacillus thuringiensis Toxin to Gypsy Moth Aminopeptidase N Receptor. Journal of Biological Chemistry, 2000, 275, 14423-14431.	1.6	119
74	Exploring the Mechanism of Action of Insecticidal Proteins by Genetic Engineering Methods. , 2000, 22, 33-54.		17
75	Binding ofBacillus thuringiensisCry1Ac toxin toManduca sextaaminopeptidase-N receptor is not directly related to toxicity. FEBS Letters, 1999, 462, 373-376.	1.3	57