Jeremy L Jenkins

List of Publications by Year
in descending order

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	Large-scale prediction and testing of drug activity on side-effect targets. Nature, 2012, 486, 361-367.	13.7	782
2	Integrating high-content screening and ligand-target prediction to identify mechanism of action. Nature Chemical Biology, 2008, 4, 59-68.	3.9	332
3	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
4	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
5	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
6	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
7	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
8	Rethinking Molecular Similarity: Comparing Compounds on the Basis of Biological Activity. ACS Chemical Biology, 2012, 7, 1399-1409.	1.6	181
9	Modeling Promiscuity Based on inâ€…vitro Safety Pharmacology Profiling Data. ChemMedChem, 2007, 2, 874-880.	1.6	169
10	Phenotypic landscape of intestinal organoid regeneration. Nature, 2020, 586, 275-280.	13.7	162
11	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
12	Mapping Adverse Drug Reactions in Chemical Space. Journal of Medicinal Chemistry, 2009, 52, 3103-3107.	2.9	156
13	In silico target fishing: Predicting biological targets from chemical structure. Drug Discovery Today: Technologies, 2006, 3, 413-421.	4.0	155
14	DRUG-seq for miniaturized high-throughput transcriptome profiling in drug discovery. Nature Communications, 2018, 9, 4307.	5.8	133
15	Identifying compound efficacy targets in phenotypic drug discovery. Drug Discovery Today, 2016, 21, 82-89.	3.2	127
16	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
17	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
18	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

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19	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
20	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
21	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
22	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
23	Streamlining lead discovery by aligning in silico and high-throughput screening. Current Opinion in Chemical Biology, 2006, 10, 343-351.	2.8	85
24	Using Information from Historical High-Throughput Screens to Predict Active Compounds. Journal of Chemical Information and Modeling, 2014, 54, 1880-1891.	2.5	79
25	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
26	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
27	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
28	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
29	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
30	Binding ofBacillus thuringiensisCry1Ac toxin toManduca sextaaminopeptidase-N receptor is not directly related to toxicity. FEBS Letters, 1999, 462, 373-376.	1.3	57
31	Recent trends and observations in the design of high-quality screening collections. Future Medicinal Chemistry, 2011, 3, 751-766.	1.1	55
32	Target identification for a Hedgehog pathway inhibitor reveals the receptor GPR39. Nature Chemical Biology, 2014, 10, 343-349.	3.9	53
33	Evidence-Based and Quantitative Prioritization of Tool Compounds in Phenotypic Drug Discovery. Cell Chemical Biology, 2016, 23, 862-874.	2.5	52
34	Biodiversity of small molecules â€“ a new perspective in screening set selection. Drug Discovery Today, 2013, 18, 674-680.	3.2	51
35	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
36	Flexible 3D pharmacophores as descriptors of dynamic biological space. Journal of Molecular Graphics and Modelling, 2007, 26, 622-633.	1.3	47

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37	Discovery of a ZIP7 inhibitor from a Notch pathway screen. Nature Chemical Biology, 2019, 15, 179-188.	3.9	46
38	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
39	Systematic Chemogenetic Library Assembly. Cell Chemical Biology, 2020, 27, 1124-1129.	2.5	37
40	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
41	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
42	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
43	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
44	Cleavage of 3â€˜,5â€˜-Pyrophosphate-Linked Dinucleotides by Ribonuclease A and Angioginâ€,â€¡. Biochemistry, 2001, 40, 10262-10272.	1.2	29
45	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
46	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
47	Causal Network Models for Predicting Compound Targets and Driving Pathways in Cancer. Journal of Biomolecular Screening, 2014, 19, 791-802.	2.6	23
48	Indolyl-Pyridinyl-Propenone-Induced Methuosis through the Inhibition of PIKFYVE. ACS Omega, 2018, 3, 6097-6103.	1.6	22
49	Recurrent ubiquitin B silencing in gynecological cancers establishes dependence on ubiquitin C. Journal of Clinical Investigation, 2017, 127, 4554-4568.	3.9	21
50	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
51	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
52	Knowledge-Based Virtual Screening: Application to the MDM4/p53 Proteinâ€“Protein Interaction. Methods in Molecular Biology, 2009, 575, 173-194.	0.4	20
53	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
54	Inhibition of mammalian ribonucleases by endogenous adenosine dinucleotides. Biochemical and Biophysical Research Communications, 2003, 300, 81-86.	1.0	18

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55	Exploring the Mechanism of Action of Insecticidal Proteins by Genetic Engineering Methods. , 2000, 22, 33-54.		17
56	Fishing for neuroactive compounds. Nature Chemical Biology, 2010, 6, 172-173.	3.9	14
57	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
58	Ten simple rules to power drug discovery with data science. PLoS Computational Biology, 2020, 16, e1008126.	1.5	14
59	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
60	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
61	Translation of off-target effects: prediction of ADRs by integrated experimental and computational approach. Toxicology Research, 2014, 3, 433-444.	0.9	11
62	CYP27A1-dependent anti-melanoma activity of limonoid natural products targets mitochondrial metabolism. Cell Chemical Biology, 2021, 28, 1407-1419.e6.	2.5	11
63	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
64	Chemogenomics: Looking at biology through the lens of chemistry. Statistical Analysis and Data Mining, 2009, 2, 149-160.	1.4	10
65	Largeâ€Scale QSAR in Target Prediction and Phenotypic HTS Assessment. Molecular Informatics, 2012, 31, 508-514.	1.4	9
66	Chemogenomic Analysis of Safety Profiling Data. Methods in Molecular Biology, 2009, 575, 207-223.	0.4	9
67	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
68	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
69	Determination of minimal transcriptional signatures of compounds for target prediction. Eurasip Journal on Bioinformatics and Systems Biology, 2012, 2012, 2.	1.4	7
70	Rethinking cellular drug response. Nature Chemical Biology, 2013, 9, 669-670.	3.9	7
71	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
72	Benchmarking network algorithms for contextualizing genes of interest. PLoS Computational Biology, 2019, 15, e1007403.	1.5	7

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73	DRUG-seq Provides Unbiased Biological Activity Readouts for Neuroscience Drug Discovery. ACS Chemical Biology, 2022, 17, 1401-1414.	1.6	7
74	Learning epistatic gene interactions from perturbation screens. PLoS ONE, 2021, 16, e0254491.	1.1	5
75	SPREADâ€”exploiting chemical features that cause differential activity behavior. Statistical Analysis and Data Mining, 2009, 2, 115-122.	1.4	1