Lei Xie

List of Publications by Year
in descending order

77 papers	4,260 citations	126907 33 h-index	118850 62 g-index
90 all docs	90 docs citations	90 times ranked	5517 citing authors

#	Article	IF	Citations
1	Repurposing ibudilast to mitigate Alzheimerâ€™s disease by targeting inflammation. Brain, 2023, 146, 898-911.	7.6	13
2	Chemical-induced gene expression ranking and its application to pancreatic cancer drug repurposing. Patterns, 2022, 3, 100441.	5.9	9
3	DeepREAL: a deep learning powered multi-scale modeling framework for predicting out-of-distribution ligand-induced GPCR activity. Bioinformatics, 2022, 38, 2561-2570.	4.1	5
4	FAME: Fragment-based Conditional Molecular Generation for Phenotypic Drug Discovery. , 2022, 2022, 720-728.		3
5	Exploration of chemical space with partial labeled noisy student self-training and self-supervised graph embedding. BMC Bioinformatics, 2022, 23, 158.	2.6	3
6	Reinforcement learning for systems pharmacology-oriented and personalized drug design. Expert Opinion on Drug Discovery, 2022, 17, 849-863.	5.0	13
7	A New Weighted Imputed Neighborhood-Regularized Tri-Factorization One-Class Collaborative Filtering Algorithm: Application to Target Gene Prediction of Transcription Factors. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 126-137.	3.0	5
8	TranSynergy: Mechanism-driven interpretable deep neural network for the synergistic prediction and pathway deconvolution of drug combinations. PLoS Computational Biology, 2021, 17, e1008653.	3.2	81
9	A deep learning framework for high-throughput mechanism-driven phenotype compound screening and its application to COVID-19 drug repurposing. Nature Machine Intelligence, 2021, 3, 247-257.	16.0	100
10	MSA-Regularized Protein Sequence Transformer toward Predicting Genome-Wide Chemical-Protein Interactions: Application to GPCRome Deorphanization. Journal of Chemical Information and Modeling, 2021, 61, 1570-1582.	5.4	20
11	COVID-19 Multi-Targeted Drug Repurposing Using Few-Shot Learning. Frontiers in Bioinformatics, 2021, 1, .	2.1	19
12	A cross-level information transmission network for hierarchical omics data integration and phenotype prediction from a new genotype. Bioinformatics, 2021, 38, 204-210.	4.1	9
13	AD-linked R47H- TREM2 mutation induces disease-enhancing microglial states via AKT hyperactivation. Science Translational Medicine, 2021, 13, eabe3947.	12.4	55
14	A Bayesian approach to accurate and robust signature detection on LINCS L1000 data. Bioinformatics, 2020, 36, 2787-2795.	4.1	19
15	The Cancer Microbiome: Distinguishing Direct and Indirect Effects Requires a Systemic View. Trends in Cancer, 2020, 6, 192-204.	7.4	162
16	Machine learning strategies for identifying repurposed drugs for cancer therapy. , 2020, , 55-79.		1
17	Improving Attention Mechanism in Graph Neural Networks via Cardinality Preservation. , 2020, 2020, 1395-1402.		22
18	Pathway-Centric Structure-Based Multi-Target Compound Screening for Anti-Virulence Drug Repurposing. International Journal of Molecular Sciences, 2019, 20, 3504.	4.1	7

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19	Prediction of off-target specificity and cell-specific fitness of CRISPR-Cas System using attention boosted deep learning and network-based gene feature. PLoS Computational Biology, 2019, 15, e1007480.	3.2	41
20	Rational discovery of dual-indication multi-target PDE/Kinase inhibitor for precision anti-cancer therapy using structural systems pharmacology. PLoS Computational Biology, 2019, 15, e1006619.	3.2	37
21	Omics Data Integration and Analysis for Systems Pharmacology. Methods in Molecular Biology, 2019, 1939, 199-214.	0.9	7
22	Biological representation of chemicals using latent target interaction profile. BMC Bioinformatics, 2019, 20, 674.	2.6	11
23	Database of adverse events associated with drugs and drug combinations. Scientific Reports, 2019, 9, 20025.	3.3	18
24	Structural Insights into Characterizing Binding Sites in Epidermal Growth Factor Receptor Kinase Mutants. Journal of Chemical Information and Modeling, 2019, 59, 453-462.	5.4	30
25	Heterogeneous Multi-Layered Network Model for Omics Data Integration and Analysis. Frontiers in Genetics, 2019, 10, 1381.	2.3	61
26	ANTENNA, a Multi-Rank, Multi-Layered Recommender System for Inferring Reliable Drug-Gene-Disease Associations: Repurposing Diazoxide as a Targeted Anti-Cancer Therapy. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2018, 15, 1960-1967.	3.0	23
27	A new insight into underlying disease mechanism through semi-parametric latent differential network model. BMC Bioinformatics, 2018, 19, 493.	2.6	7
28	The International Conference on Intelligent Biology and Medicine (ICIBM) 2018: bioinformatics towards translational applications. BMC Bioinformatics, 2018, 19, 492.	2.6	1
29	Target Gene Prediction of Transcription Factor Using a New Neighborhood-regularized Tri-factorization One-class Collaborative Filtering Algorithm. , 2018, 2018, 1-10.		1
30	Predicting serious rare adverse reactions of novel chemicals. Bioinformatics, 2018, 34, 2835-2842.	4.1	18
31	Exploring Landscape of Drug-Target-Pathway-Side Effect Associations. AMIA Summits on Translational Science Proceedings, 2018, 2017, 132-141.	0.4	3
32	JDINAC: joint density-based non-parametric differential interaction network analysis and classification using high-dimensional sparse omics data. Bioinformatics, 2017, 33, 3080-3087.	4.1	24
33	Determining Cysteines Available for Covalent Inhibition Across the Human Kinome. Journal of Medicinal Chemistry, 2017, 60, 2879-2889.	6.4	104
34	Harnessing Big Data for Systems Pharmacology. Annual Review of Pharmacology and Toxicology, 2017, 57, 245-262.	9.4	50
35	Mining FDA resources to compute population-specific frequencies of adverse drug reactions. , 2017, 2017, 1809-1814.		2
36	VariFunNet, an integrated multiscale modeling framework to study the effects of rare non-coding variants in genome-wide association studies: Applied to Alzheimer's disease. , 2017, 2017, 2177-2182.		7

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37	Insights into the binding mode of MEK type-III inhibitors. A step towards discovering and designing allosteric kinase inhibitors across the human kinome. PLoS ONE, 2017, 12, e0179936.	2.5	34
38	Large-Scale Off-Target Identification Using Fast and Accurate Dual Regularized One-Class Collaborative Filtering and Its Application to Drug Repurposing. PLoS Computational Biology, 2016, 12, e1005135.	3.2	65
39	Molecular mechanisms involved in the side effects of fatty acid amide hydrolase inhibitors: a structural phenomics approach to proteome-wide cellular off-target deconvolution and disease association. Npj Systems Biology and Applications, 2016, 2, 16023.	3.0	14
40	Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology. Scientific Reports, 2016, 6, 20441.	3.3	34
41	Toward High-Throughput Predictive Modeling of Protein Binding/Unbinding Kinetics. Journal of Chemical Information and Modeling, 2016, 56, 1164-1174.	5.4	35
42	Delineation of Polypharmacology across the Human Structural Kinome Using a Functional Site Interaction Fingerprint Approach. Journal of Medicinal Chemistry, 2016, 59, 4326-4341.	6.4	39
43	Crowdsourced estimation of cognitive decline and resilience in Alzheimer's disease. Alzheimer's and Dementia, 2016, 12, 645-653.	0.8	72
44	FASCINATE. , 2016, , .		50
45	Improved genome-scale multi-target virtual screening via a novel collaborative filtering approach to cold-start problem. Scientific Reports, 2016, 6, 38860.	3.3	42
46	Proteinâ€fold recognition using an improved singleâ€source <scp>K</scp> diverse shortest paths algorithm. Proteins: Structure, Function and Bioinformatics, 2016, 84, 467-472.	2.6	2
47	Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology. BMC Bioinformatics, 2016, 17, 90.	2.6	45
48	Providing data science support for systems pharmacology and its implications to drug discovery. Expert Opinion on Drug Discovery, 2016, 11, 241-256.	5.0	32
49	PDID: database of molecular-level putative proteinâ€“drug interactions in the structural human proteome. Bioinformatics, 2016, 32, 579-586.	4.1	38
50	Developing multi-target therapeutics to fine-tune the evolutionary dynamics of the cancer ecosystem. Frontiers in Pharmacology, 2015, 6, 209.	3.5	47
51	A new method to improve network topological similarity search: applied to fold recognition. Bioinformatics, 2015, 31, 2106-2114.	4.1	12
52	Zeta Inhibitory Peptide Disrupts Electrostatic Interactions That Maintain Atypical Protein Kinase C in Its Active Conformation on the Scaffold p62. Journal of Biological Chemistry, 2015, 290, 21845-21856.	3.4	33
53	Towards Structural Systems Pharmacology to Study Complex Diseases and Personalized Medicine. PLoS Computational Biology, 2014, 10, e1003554.	3.2	61
54	An integrated workflow for proteome-wide off-target identification and polypharmacology drug design. Tsinghua Science and Technology, 2014, 19, 275-284.	6.1	3

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55	Anti-infectious drug repurposing using an integrated chemical genomics and structural systems biology approach. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2014, , 136-47.	0.7	9
56	Multiscale modeling of the causal functional roles of nsSNPs in a genome-wide association study: application to hypoxia. BMC Genomics, 2013, 14, S9.	2.8	6
57	Antibacterial mechanisms identified through structural systems pharmacology. BMC Systems Biology, 2013, 7, 102.	3.0	23
58	A case-based meta-learning algorithm boosts the performance of structure-based virtual screening. , 2013, , .		0
59	Quantifying Reproducibility in Computational Biology: The Case of the Tuberculosis Drugome. PLoS ONE, 2013, 8, e80278.	2.5	91
60	An integrated workflow for proteome-wide off-target identification and polypharmacology drug design. , 2012, , .		0
61	Raloxifene attenuates Pseudomonas aeruginosa pyocyanin production and virulence. International Journal of Antimicrobial Agents, 2012, 40, 246-251.	2.5	79
62	Structural basis of polypharmacological effects of metformin. , 2012, , .		1
63	Novel Computational Approaches to Polypharmacology as a Means to Define Responses to Individual Drugs. Annual Review of Pharmacology and Toxicology, 2012, 52, 361-379.	9.4	194
64	Discrepancies in purified and cellular PKMÎ¶ inhibition profiles invalidate its proposed role as a mediator of memory. FASEB Journal, 2012, 26, 768.5.	0.5	0
65	Drug Discovery Using Chemical Systems Biology: Weak Inhibition of Multiple Kinases May Contribute to the Anti-Cancer Effect of Nelfinavir. PLoS Computational Biology, 2011, 7, e1002037.	3.2	151
66	A Machine Learning-Based Method To Improve Docking Scoring Functions and Its Application to Drug Repurposing. Journal of Chemical Information and Modeling, 2011, 51, 408-419.	5.4	175
67	Structure-based systems biology for analyzing off-target binding. Current Opinion in Structural Biology, 2011, 21, 189-199.	5.7	131
68	A Multidimensional Strategy to Detect Polypharmacological Targets in the Absence of Structural and Sequence Homology. PLoS Computational Biology, 2010, 6, e1000648.	3.2	72
69	Drug Off-Target Effects Predicted Using Structural Analysis in the Context of a Metabolic Network Model. PLoS Computational Biology, 2010, 6, e1000938.	3.2	183
70	The Mycobacterium tuberculosis Drugome and Its Polypharmacological Implications. PLoS Computational Biology, 2010, 6, e1000976.	3.2	98
71	A unified statistical model to support local sequence order independent similarity searching for ligand-binding sites and its application to genome-based drug discovery. Bioinformatics, 2009, 25, i305-i312.	4.1	89
72	Drug Discovery Using Chemical Systems Biology: Identification of the Protein-Ligand Binding Network To Explain the Side Effects of CETP Inhibitors. PLoS Computational Biology, 2009, 5, e1000387.	3.2	232

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73	Drug Discovery Using Chemical Systems Biology: Repositioning the Safe Medicine Comtan to Treat Multi-Drug and Extensively Drug Resistant Tuberculosis. PLoS Computational Biology, 2009, 5, e1000423.	3.2	283
74	Detecting evolutionary relationships across existing fold space, using sequence order-independent profileâ€“profile alignments. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5441-5446.	7.1	241
75	In Silico Elucidation of the Molecular Mechanism Defining the Adverse Effect of Selective Estrogen Receptor Modulators. PLoS Computational Biology, 2007, 3, e217.	3.2	78
76	A robust and efficient algorithm for the shape description of protein structures and its application in predicting ligand binding sites. BMC Bioinformatics, 2007, 8, S9.	2.6	123
77	The RCSB PDB information portal for structural genomics. Nucleic Acids Research, 2006, 34, D302-D305.	14.5	334