Juho Rousu

List of Publications by Year in descending order

74 papers	4,035 citations	218381 26 h-index	138251 58 g-index
86 all docs	86 docs citations	86 times ranked	4812 citing authors

#	Article	IF	Citations
1	Systematic review of computational methods for drug combination prediction. Computational and Structural Biotechnology Journal, 2022, 20, 2807-2814.	1.9	13
2	Strain design optimization using reinforcement learning. PLoS Computational Biology, 2022, 18, e1010177.	1.5	6
3	Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. Nature Biotechnology, 2021, 39, 462-471.	9.4	317
4	Ranking microbial metabolomic and genomic links in the NPLinker framework using complementary scoring functions. PLoS Computational Biology, 2021, 17, e1008920.	1.5	30
5	Modeling drug combination effects via latent tensor reconstruction. Bioinformatics, 2021, 37, i93-i101.	1.8	9
6	Probabilistic framework for integration of mass spectrum and retention time information in small molecule identification. Bioinformatics, 2021, 37, 1724-1731.	1.8	7
7	Substrate specificity of 2-deoxy-D-ribose 5-phosphate aldolase (DERA) assessed by different protein engineering and machine learning methods. Applied Microbiology and Biotechnology, 2020, 104, 10515-10529.	1.7	21
8	Leveraging multi-way interactions for systematic prediction of pre-clinical drug combination effects. Nature Communications, 2020, 11, 6136.	5.8	63
9	Systematic mapping of cancer cell target dependencies using high-throughput drug screening in triple-negative breast cancer. Computational and Structural Biotechnology Journal, 2020, 18, 3819-3832.	1.9	6
10	Improved Small Molecule Identification through Learning Combinations of Kernel Regression Models. Metabolites, 2019, 9, 160.	1.3	13
11	Bayesian metabolic flux analysis reveals intracellular flux couplings. Bioinformatics, 2019, 35, i548-i557.	1.8	19
12	SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. Nature Methods, 2019, 16, 299-302.	9.0	822
13	Principal metabolic flux mode analysis. Bioinformatics, 2018, 34, 2409-2417.	1.8	11
14	A Tutorial on Canonical Correlation Methods. ACM Computing Surveys, 2018, 50, 1-33.	16.1	65
15	Sparse Non-linear CCA through Hilbert-Schmidt Independence Criterion. , 2018, , .		3
16	Liquid-chromatography retention order prediction for metabolite identification. Bioinformatics, 2018, 34, i875-i883.	1.8	52
17	Learning with multiple pairwise kernels for drug bioactivity prediction. Bioinformatics, 2018, 34, i509-i518.	1.8	51
18	Analysis of Fluxomic Experiments with Principal Metabolic Flux Mode Analysis. Methods in Molecular Biology, 2018, 1807, 141-161.	0.4	0

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19	Multi-view kernel completion. Machine Learning, 2017, 106, 713-739.	3.4	38
20	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	2.8	122
21	CamOptimus: a tool for exploiting complex adaptive evolution to optimize experiments and processes in biotechnology. Microbiology (United Kingdom), 2017, 163, 829-839.	0.7	9
22	Computational-experimental approach to drug-target interaction mapping: A case study on kinase inhibitors. PLoS Computational Biology, 2017, 13, e1005678.	1.5	84
23	Selected proceedings of Machine Learning in Systems Biology: MLSB 2016. BMC Bioinformatics, 2016, 17, 437.	1.2	3
24	Soft Kernel Target Alignment for Two-Stage Multiple Kernel Learning. Lecture Notes in Computer Science, 2016, , 427-441.	1.0	2
25	Profiling persistent tubercule bacilli from patient sputa during therapy predicts early drug efficacy. BMC Medicine, 2016, 14, 68.	2.3	55
26	Fast metabolite identification with Input Output Kernel Regression. Bioinformatics, 2016, 32, i28-i36.	1.8	57
27	metaCCA: summary statistics-based multivariate meta-analysis of genome-wide association studies using canonical correlation analysis. Bioinformatics, 2016, 32, 1981-1989.	1.8	138
28	Synthetic Transcription Amplifier System for Orthogonal Control of Gene Expression in Saccharomyces cerevisiae. PLoS ONE, 2016, 11, e0148320.	1.1	31
29	Machine Learning of Protein Interactions in Fungal Secretory Pathways. PLoS ONE, 2016, 11, e0159302.	1.1	7
30	Multilabel classification through random graph ensembles. Machine Learning, 2015, 99, 231-256.	3.4	15
31	Searching molecular structure databases with tandem mass spectra using CSI:FingerID. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12580-12585.	3.3	695
32	Meat Processing Plant Microbiome and Contamination Patterns of Cold-Tolerant Bacteria Causing Food Safety and Spoilage Risks in the Manufacture of Vacuum-Packaged Cooked Sausages. Applied and Environmental Microbiology, 2015, 81, 7088-7097.	1.4	111
33	Identification of drug candidates and repurposing opportunities through compoundâ€“target interaction networks. Expert Opinion on Drug Discovery, 2015, 10, 1333-1345.	2.5	54
34	Canonical Correlation Methods for Exploring Microbe-Environment Interactions in Deep Subsurface. Lecture Notes in Computer Science, 2015, , 299-307.	1.0	1
35	Metabolite identification through multiple kernel learning on fragmentation trees. Bioinformatics, 2014, 30, i157-i164.	1.8	87
36	Comparative Genome-Scale Reconstruction of Gapless Metabolic Networks for Present and Ancestral Species. PLoS Computational Biology, 2014, 10, e1003465.	1.5	84

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37	Reconstructing Gapless Ancestral Metabolic Networks. Communications in Computer and Information Science, 2013, , 126-140.	0.4	1
38	Biomarker Discovery by Sparse Canonical Correlation Analysis of Complex Clinical Phenotypes of Tuberculosis and Malaria. PLoS Computational Biology, 2013, 9, e1003018.	1.5	21
39	Metabolite Identification through Machine Learningâ€" Tackling CASMI Challenge Using FingerID. Metabolites, 2013, 3, 484-505.	1.3	24
40	Metabolite identification and molecular fingerprint prediction through machine learning. Bioinformatics, 2012, 28, 2333-2341.	1.8	143
41	Computing Atom Mappings for Biochemical Reactions without Subgraph Isomorphism. Journal of Computational Biology, 2011, 18, 43-58.	0.8	24
42	Structured Output Prediction of Novel Enzyme Function with Reaction Kernels. Communications in Computer and Information Science, 2011, , 367-379.	0.4	3
43	Multi-task Drug Bioactivity Classification with Graph Labeling Ensembles. Lecture Notes in Computer Science, 2011, , 157-167.	1.0	0
44	Computational methods for metabolic reconstruction. Current Opinion in Biotechnology, 2010, 21, 70-77.	3.3	46
45	Structured Output Prediction of Anti-cancer Drug Activity. Lecture Notes in Computer Science, 2010, , 38-49.	1.0	3
46	Inferring branching pathways in genome-scale metabolic networks. BMC Systems Biology, 2009, 3, 103.	3.0	59
47	FiD: a software for ab initio structural identification of product ions from tandem mass spectrometric data. Rapid Communications in Mass Spectrometry, 2008, 22, 3043-3052.	0.7	116
48	An analytic and systematic framework for estimating metabolic flux ratios from 13C tracer experiments. BMC Bioinformatics, 2008, 9, 266.	1.2	40
49	Towards structured output prediction of enzyme function. BMC Proceedings, 2008, 2, S2.	1.8	32
50	A Computational Method for Reconstructing Gapless Metabolic Networks. Communications in Computer and Information Science, 2008, , 288-302.	0.4	4
51	Probabilistic modeling and machine learning in structural and systems biology. BMC Bioinformatics, 2007, 8, .	1.2	3
52	Planning optimal measurements of isotopomer distributions for estimation of metabolic fluxes. Bioinformatics, 2006, 22, 1198-1206.	1.8	25
53	Practical Approximation of Optimal Multivariate Discretization. Lecture Notes in Computer Science, 2006, , 612-621.	1.0	2
54	Equivalence of Metabolite Fragments and Flow Analysis of Isotopomer Distributions for Flux Estimation. Lecture Notes in Computer Science, 2006, , 198-220.	1.0	0

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55	Isotopomer distribution computation from tandem mass spectrometric data with overlapping fragment spectra. Spectroscopy, 2005, 19, 53-67.	0.8	13
56	Learning hierarchical multi-category text classification models. , 2005, , .		64
57	Finding Feasible Pathways in Metabolic Networks. Lecture Notes in Computer Science, 2005, , 123-133.	1.0	6
58	Approximation Algorithms for Minimizing Empirical Error by Axis-Parallel Hyperplanes. Lecture Notes in Computer Science, 2005, , 547-555.	1.0	2
59	APPLYING MACHINE LEARNING METHODS IN STUDYING RELATIONSHIPS BETWEEN MOUTHFEEL AND MICROSTRUCTURE OF OAT BREAD. Journal of Texture Studies, 2004, 35, 225-250.	1.1	10
60	Efficient Multisplitting Revisited: Optima-Preserving Elimination of Partition Candidates. Data Mining and Knowledge Discovery, 2004, 8, 97-126.	2.4	38
61	Necessary and Sufficient Pre-processing in Numerical Range Discretization. Knowledge and Information Systems, 2003, 5, 162-182.	2.1	11
62	Novel computational tools in bakery process data analysis: a comparative study. Journal of Food Engineering, 2003, 57, 45-56.	2.7	19
63	On Decision Boundaries of NaÃ¯ve Bayes in Continuous Domains. Lecture Notes in Computer Science, 2003, , 144-155.	1.0	3
64	Computing Positional Isotopomer Distributions from Tandem Mass Spectrometric Data. Metabolic Engineering, 2002, 4, 285-294.	3.6	27
65	Linear-Time Preprocessing in Optimal Numerical Range Partitioning. Journal of Intelligent Information Systems, 2002, 18, 55-70.	2.8	0
66	An integrated approach to bioprocess recipe design. Integrated Computer-Aided Engineering, 2001, 8, 363-373.	2.5	4
67	On the Complexity of Optimal Multisplitting. Lecture Notes in Computer Science, 2000, , 552-561.	1.0	0
68	General and Efficient Multisplitting of Numerical Attributes. Machine Learning, 1999, 36, 201-244.	3.4	134
69	Speeding Up the Search for Optimal Partitions. Lecture Notes in Computer Science, 1999, , 89-97.	1.0	3
70	Efficient multisplitting on numerical data. Lecture Notes in Computer Science, 1997, , 178-188.	1.0	1
71	Qualitative knowledge to support reasoning about cases. Lecture Notes in Computer Science, 1997, , 489-498.	1.0	5
72	Adaptation cost as a criterion for solution evaluation. Lecture Notes in Computer Science, 1996, , 354-361.	1.0	5

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73	Towards CBR for bioprocess planning. Lecture Notes in Computer Science, 1996, , 16-27.	1.0	8
74	Computational Methods for Metabolic Networks. Electronic Proceedings in Theoretical Computer Science, EPTCS, 0, 116, 11-11.	0.8	0