Vassily Hatzimanikatis

List of Publications by Year
in descending order

143	9,870	36303	48315
papers	citations	51 h-index	88 g-index

180	180	180	7670
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Expanding biochemical knowledge and illuminating metabolic dark matter with ATLASx. Nature Communications, 2022, 13, 1560.	12.8	19
2	ARBRE: Computational resource to predict pathways towards industrially important aromatic compounds. Metabolic Engineering, 2022, 72, 259-274.	7.0	3
3	Computational tools and resources for designing new pathways to small molecules. Current Opinion in Biotechnology, 2022, 76, 102722.	6.6	12
4	The solubility parameters of carbon dioxide and ionic liquids: Are they an enigma?. Fluid Phase Equilibria, 2021, 527, 112828.	2.5	8
5	Emergence of diauxie as an optimal growth strategy under resource allocation constraints in cellular metabolism. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	23
6	The effects of model complexity and size on metabolic flux distribution and control: case study in Escherichia coli. BMC Bioinformatics, 2021, 22, 134.	2.6	4
7	PhenoMapping: A protocol to map cellular phenotypes to metabolic bottlenecks, identify conditional essentiality, and curate metabolic models. STAR Protocols, 2021, 2, 100280.	1.2	1
8	A computational workflow for the expansion of heterologous biosynthetic pathways to natural product derivatives. Nature Communications, 2021, 12, 1760.	12.8	40
9	NICEpath: Finding metabolic pathways in large networks through atom-conserving substrateâ€“product pairs. Bioinformatics, 2021, 37, 3560-3568.	4.1	10
10	Quantitative modeling of human metabolism: A call for a community effort. Current Opinion in Systems Biology, 2021, 26, 109-115.	2.6	3
11	The influence of the crowding assumptions in biofilm simulations. PLoS Computational Biology, 2021, 17, e1009158.	3.2	3
12	Constraint-based metabolic control analysis for rational strain engineering. Metabolic Engineering, 2021, 66, 191-203.	7.0	12
13	Spatio-temporal modeling of the crowding conditions and metabolic variability in microbial communities. PLoS Computational Biology, 2021, 17, e1009140.	3.2	12
14	NICEdrug.ch, a workflow for rational drug design and systems-level analysis of drug metabolism. ELife, 2021, 10, .	6.0	8
15	A genome-scale metabolic model of Saccharomyces cerevisiae that integrates expression constraints and reaction thermodynamics. Nature Communications, 2021, 12, 4790.	12.8	48
16	Updated ATLAS of Biochemistry with New Metabolites and Improved Enzyme Prediction Power. ACS Synthetic Biology, 2020, 9, 1479-1482.	3.8	34
17	Analysis of human metabolism by reducing the complexity of the genome-scale models using redHUMAN. Nature Communications, 2020, 11, 2821.	12.8	19
18	Large-scale kinetic metabolic models of Pseudomonas putida KT2440 for consistent design of metabolic engineering strategies. Biotechnology for Biofuels, 2020, 13, 33.	6.2	34

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19	MEMOTE for standardized genome-scale metabolic model testing. Nature Biotechnology, 2020, 38, 272-276.	17.5	314
20	The ETFL formulation allows multi-omics integration in thermodynamics-compliant metabolism and expression models. Nature Communications, 2020, 11, 30.	12.8	71
21	Functional and Computational Genomics Reveal Unprecedented Flexibility in Stage-Specific Toxoplasma Metabolism. Cell Host and Microbe, 2020, 27, 290-306.e11.	11.0	81
22	pyTFA and matTFA: a Python package and a Matlab toolbox for Thermodynamics-based Flux Analysis. Bioinformatics, 2019, 35, 167-169.	4.1	75
23	Modeling metabolic networks of individual bacterial agents in heterogeneous and dynamic soil habitats (IndiMeSH). PLoS Computational Biology, 2019, 15, e1007127.	3.2	45
24	Particle-Based Simulation Reveals Macromolecular Crowding Effects on the Michaelis-Menten Mechanism. Biophysical Journal, 2019, 117, 355-368.	0.5	24
25	Genome-Scale Identification of Essential Metabolic Processes for Targeting the Plasmodium Liver Stage. Cell, 2019, 179, 1112-1128.e26.	28.9	92
26	Uncertainty reduction in biochemical kinetic models: Enforcing desired model properties. PLoS Computational Biology, 2019, 15, e1007242.	3.2	20
27	110th Anniversary: From Solubility Parameters to Predictive Equation-of-State Modeling. Industrial & Engineering Chemistry Research, 2019, 58, 12787-12800.	3.7	9
28	Dynamic Radiolabeling of S-Palmitoylated Proteins. Methods in Molecular Biology, 2019, 2009, 111-127.	0.9	3
29	Enhanced flux prediction by integrating relative expression and relative metabolite abundance into thermodynamically consistent metabolic models. PLoS Computational Biology, 2019, 15, e1007036.	3.2	62
30	Control Theory Concepts for Modeling Uncertainty in Enzyme Kinetics of Biochemical Networks. Industrial & Engineering Chemistry Research, 2019, 58, 13544-13554.	3.7	17
31	Investigating the deregulation of metabolic tasks via Minimum Network Enrichment Analysis (MiNEA) as applied to nonalcoholic fatty liver disease using mouse and human omics data. PLoS Computational Biology, 2019, 15, e1006760.	3.2	6
32	Impact of iron reduction on the metabolism of Clostridium acetobutylicum. Environmental Microbiology, 2019, 21, 3548-3563.	3.8	38
33	Enzyme annotation for orphan and novel reactions using knowledge of substrate reactive sites. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7298-7307.	7.1	65
34	Statistical inference in ensemble modeling of cellular metabolism. PLoS Computational Biology, 2019, 15, e1007536.	3.2	14
35	Kinetic models of metabolism that consider alternative steady-state solutions of intracellular fluxes and concentrations. Metabolic Engineering, 2019, 52, 29-41.	7.0	36
36	Discovery and Evaluation of Biosynthetic Pathways for the Production of Five Methyl Ethyl Ketone Precursors. ACS Synthetic Biology, 2018, 7, 1858-1873.	3.8	29

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37	Efficient cleavage of aryl ether Câ€“O linkages by Rhâ€“Ni and Ruâ€“Ni nanoscale catalysts operating in water. Chemical Science, 2018, 9, 5530-5535.	7.4	57
38	Mechanistic Modeling of Genetic Circuits for ArsR Arsenic Regulation. ACS Synthetic Biology, 2017, 6, 862-874.	3.8	18
39	Integration of metabolic, regulatory and signaling networks towards analysis of perturbation and dynamic responses. Current Opinion in Systems Biology, 2017, 2, 59-66.	2.6	13
40	On Lewis acidity/basicity and hydrogen bonding in the equation-of-state approach. Journal of Chemical Thermodynamics, 2017, 110, 3-15.	2.0	13
41	Exploring biochemical pathways for mono-ethylene glycol (MEG) synthesis from synthesis gas. Metabolic Engineering, 2017, 41, 173-181.	7.0	26
42	Reconstruction of biological pathways and metabolic networks from in silico labeled metabolites. Biotechnology Journal, 2017, 12, 1600464.	3.5	14
43	Redefining solubility parameters: Bulk and surface properties from unified molecular descriptors. Journal of Chemical Thermodynamics, 2017, 111, 207-220.	2.0	17
44	Toward a Simple Predictive Molecular Thermodynamic Model for Bulk Phases and Interfaces. Industrial & Engineering Chemistry Research, 2017, 56, 10900-10910.	3.7	18
45	A designâ€“buildâ€“test cycle using modeling and experiments reveals interdependencies between upper glycolysis and xylose uptake in recombinant S. cerevisiae and improves predictive capabilities of large-scale kinetic models. Biotechnology for Biofuels, 2017, 10, 166.	6.2	37
46	Thermodynamics-based Metabolite Sensitivity Analysis in metabolic networks. Metabolic Engineering, 2017, 39, 117-127.	7.0	27
47	Identification and dynamics of the human ZDHHC16-ZDHHC6 palmitoylation cascade. ELife, 2017, 6, .	6.0	89
48	Single-molecule kinetic analysis of HP1-chromatin binding reveals a dynamic network of histone modification and DNA interactions. Nucleic Acids Research, 2017, 45, 10504-10517.	14.5	49
49	Bioenergetics-based modeling of Plasmodium falciparum metabolism reveals its essential genes, nutritional requirements, and thermodynamic bottlenecks. PLoS Computational Biology, 2017, 13, e1005397.	3.2	44
50	redGEM: Systematic reduction and analysis of genome-scale metabolic reconstructions for development of consistent core metabolic models. PLoS Computational Biology, 2017, 13, e1005444.	3.2	61
51	lumpGEM: Systematic generation of subnetworks and elementally balanced lumped reactions for the biosynthesis of target metabolites. PLoS Computational Biology, 2017, 13, e1005513.	3.2	39
52	Model-Driven Understanding of Palmitoylation Dynamics: Regulated Acylation of the Endoplasmic Reticulum Chaperone Calnexin. PLoS Computational Biology, 2016, 12, e1004774.	3.2	37
53	Sustainability assessment of succinic acid production technologies from biomass using metabolic engineering. Energy and Environmental Science, 2016, 9, 2794-2805.	30.8	93
54	Analysis of Translation Elongation Dynamics in the Context of an Escherichia coli Cell. Biophysical Journal, 2016, 110, 2120-2131.	0.5	15

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55	Molecular thermodynamics of metabolism: hydration quantities and the equation-of-state approach. Physical Chemistry Chemical Physics, 2016, 18, 32570-32592.	2.8	18
56	ATLAS of Biochemistry: A Repository of All Possible Biochemical Reactions for Synthetic Biology and Metabolic Engineering Studies. ACS Synthetic Biology, 2016, 5, 1155-1166.	3.8	132
57	A method for analysis and design of metabolism using metabolomics data and kinetic models: Application on lipidomics using a novel kinetic model of sphingolipid metabolism. Metabolic Engineering, 2016, 37, 46-62.	7.0	44
58	iSCHRUNK â€“ In Silico Approach to Characterization and Reduction of Uncertainty in the Kinetic Models of Genome-scale Metabolic Networks. Metabolic Engineering, 2016, 33, 158-168.	7.0	72
59	Identification of metabolic engineering targets for the enhancement of 1,4-butanediol production in recombinant E. coli using large-scale kinetic models. Metabolic Engineering, 2016, 35, 148-159.	7.0	78
60	Quantification of Cooperativity in Heterodimer-DNA Binding Improves the Accuracy of Binding Specificity Models. Journal of Biological Chemistry, 2016, 291, 10293-10306.	3.4	18
61	The SIB Swiss Institute of Bioinformaticsâ€™ resources: focus on curated databases. Nucleic Acids Research, 2016, 44, D27-D37.	14.5	64
62	Do genomeâ€scale models need exact solvers or clearer standards?. Molecular Systems Biology, 2015, 11, 831.	7.2	68
63	Noise analysis of genome-scale protein synthesis using a discrete computational model of translation. Journal of Chemical Physics, 2015, 143, 044109.	3.0	7
64	Rites of passage: requirements and standards for building kinetic models of metabolic phenotypes. Current Opinion in Biotechnology, 2015, 36, 146-153.	6.6	38
65	Solvation quantities from a COSMO-RS equation of state. Journal of Chemical Thermodynamics, 2015, 90, 294-309.	2.0	21
66	Integrative approaches for signalling and metabolic networks. Integrative Biology (United Kingdom), 2015, 7, 844-845.	1.3	4
67	Design of computational retrobiosynthesis tools for the design of de novo synthetic pathways. Current Opinion in Chemical Biology, 2015, 28, 99-104.	6.1	113
68	Metabolic Needs and Capabilities of Toxoplasma gondii through Combined Computational and Experimental Analysis. PLoS Computational Biology, 2015, 11, e1004261.	3.2	92
69	Molecular thermodynamics of metabolism: quantum thermochemical calculations for key metabolites. Physical Chemistry Chemical Physics, 2015, 17, 10438-10453.	2.8	16
70	Heading in the right direction: thermodynamics-based network analysis and pathway engineering. Current Opinion in Biotechnology, 2015, 36, 176-182.	6.6	86
71	Antihypertensive Drugs Metabolism: An Update to Pharmacokinetic Profiles and Computational Approaches. Current Pharmaceutical Design, 2014, 21, 806-822.	1.9	68
72	Kinetic models in industrial biotechnology â€“ Improving cell factory performance. Metabolic Engineering, 2014, 24, 38-60.	7.0	238

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73	A computational framework for integration of lipidomics data into metabolic pathways. Metabolic Engineering, 2014, 23, 1-8.	7.0	17
74	Constraining the Flux Space Using Thermodynamics and Integration of Metabolomics Data. Methods in Molecular Biology, 2014, 1191, 49-63.	0.9	47
75	Mechanistically Consistent Reduced Models of Synthetic Gene Networks. Biophysical Journal, 2013, 104, 2098-2109.	0.5	1
76	Editorial: Metabolic modeling in biotechnology and medical research. Biotechnology Journal, 2013, 8, 962-963.	3.5	1
77	Towards kinetic modeling of genomeâ€scale metabolic networks without sacrificing stoichiometric, thermodynamic and physiological constraints. Biotechnology Journal, 2013, 8, 1043-1057.	3.5	141
78	Functional genomics of Plasmodium falciparum using metabolic modelling and analysis. Briefings in Functional Genomics, 2013, 12, 316-327.	2.7	16
79	A Genome-Scale Integration and Analysis of Lactococcus lactis Translation Data. PLoS Computational Biology, 2013, 9, e1003240.	3.2	22
80	Tunable reporter signal production in feedbackâ€uncoupled arsenic bioreporters. Microbial Biotechnology, 2013, 6, 503-514.	4.2	25
81	A Novel Pulse-Chase SILAC Strategy Measures Changes in Protein Decay and Synthesis Rates Induced by Perturbation of Proteostasis with an Hsp90 Inhibitor. PLoS ONE, 2013, 8, e80423.	2.5	42
82	Exploration of trade-offs between steady-state and dynamic properties in signaling cycles. Physical Biology, 2012, 9, 045010.	1.8	4
83	A computational framework for the design of optimal protein synthesis. Biotechnology and Bioengineering, 2012, 109, 2127-2133.	3.3	23
84	From network models to network responses: integration of thermodynamic and kinetic properties of yeast genome-scale metabolic networks. FEMS Yeast Research, 2012, 12, 129-143.	2.3	70
85	Integrating computational methods to retrofit enzymes to synthetic pathways. Biotechnology and Bioengineering, 2012, 109, 572-582.	3.3	32
86	Modeling of uncertainties in biochemical reactions. Biotechnology and Bioengineering, 2011, 108, 413-423.	3.3	73
87	Systems biology. Current Opinion in Biotechnology, 2011, 22, 538-540.	6.6	1
88	Manipulating redox and ATP balancing for improved production of succinate in E. coli. Metabolic Engineering, 2011, 13, 76-81.	7.0	113
89	Production of biofuels and biochemicals: in need of an ORACLE. Trends in Biotechnology, 2010, 28, 391-397.	9.3	100
90	DREAMS of metabolism. Trends in Biotechnology, 2010, 28, 501-508.	9.3	44

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91	In silico feasibility of novel biodegradation pathways for 1,2,4-trichlorobenzene. BMC Systems Biology, 2010, 4, 7.	3.0	74
92	Discovery and analysis of novel metabolic pathways for the biosynthesis of industrial chemicals: 3â€hydroxypropanoate. Biotechnology and Bioengineering, 2010, 106, 462-473.	3.3	146
93	The Origins of Time-Delay in Template Biopolymerization Processes. PLoS Computational Biology, 2010, 6, e1000726.	3.2	49
94	Thermodynamic Calculations for Biochemical Transport and Reaction Processes in Metabolic Networks. Biophysical Journal, 2010, 99, 3139-3144.	0.5	30
95	Network thermodynamics in the post-genomic era. Current Opinion in Microbiology, 2010, 13, 350-357.	5.1	73
96	Thermodynamic analysis of biodegradation pathways. Biotechnology and Bioengineering, 2009, 103, 532-541.	3.3	45
97	Computational framework for predictive biodegradation. Biotechnology and Bioengineering, 2009, 104, 1086-1097.	3.3	96
98	Discovery of Novel Routes for the Production of Fuels and Chemicals. , 2009, , 141-148.		0
99	Group Contribution Method for Thermodynamic Analysis of Complex Metabolic Networks. Biophysical Journal, 2008, 95, 1487-1499.	0.5	345
100	Effects of Codon Distributions and tRNA Competition on Protein Translation. Biophysical Journal, 2008, 95, 1018-1033.	0.5	45
101	A genomeâ€scale metabolic reconstruction for Escherichia coli Kâ€12 MG1655 that accounts for 1260 ORFs and thermodynamic information. Molecular Systems Biology, 2007, 3, 121.	7.2	1,234
102	A Model for Protein Translation: Polysome Self-Organization Leads to Maximum Protein Synthesis Rates. Biophysical Journal, 2007, 92, 717-730.	0.5	50
103	Thermodynamics-Based Metabolic Flux Analysis. Biophysical Journal, 2007, 92, 1792-1805.	0.5	560
104	A model-based optimization framework for the inference of regulatory interactions using time-course DNA microarray expression data. BMC Bioinformatics, 2007, 8, 228.	2.6	29
105	An Algorithmic Framework for Genome-Wide Modeling and Analysis of Translation Networks. Biophysical Journal, 2006, 90, 1136-1146.	0.5	41
106	Genome-Scale Thermodynamic Analysis of Escherichia coli Metabolism. Biophysical Journal, 2006, 90, 1453-1461.	0.5	195
107	Metabolic engineering under uncertaintyâ€”II: Analysis of yeast metabolism. Metabolic Engineering, 2006, 8, 142-159.	7.0	64
108	Metabolic engineering under uncertainty. I: Framework development. Metabolic Engineering, 2006, 8, 133-141.	7.0	68

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109	Bistability Explains Threshold Phenomena in Protein Aggregation both In Vitro and In Vivo. Biophysical Journal, 2006, 90, 886-895.	0.5	28
110	Analysis of the maximum theoretical yield for the synthesis of erythromycin precursors inEscherichia coli. Biotechnology and Bioengineering, 2006, 95, 638-644.	3.3	19
111	The systems engineering of cellular processes. Computer Aided Chemical Engineering, 2006, , 71-80.	0.5	1
112	Theoretical Considerations and Computational Analysis of the Complexity in Polyketide Synthesis Pathways. Journal of the American Chemical Society, 2005, 127, 9930-9938.	13.7	60
113	Mathematical Modeling of the Eukaryotic Heat-Shock Response: Dynamics of the hsp70 Promoter. Biophysical Journal, 2005, 88, 1646-1658.	0.5	83
114	Exploring the diversity of complex metabolic networks. Bioinformatics, 2005, 21, 1603-1609.	4.1	322
115	A model-based optimization framework for the inference on gene regulatory networks from DNA array data. Bioinformatics, 2004, 20, 3221-3235.	4.1	31
116	Metabolic networks: enzyme function and metabolite structure. Current Opinion in Structural Biology, 2004, 14, 300-306.	5.7	81
117	Computational discovery of biochemical routes to specialty chemicals. Chemical Engineering Science, 2004, 59, 5051-5060.	3.8	73
118	Metabolic Control Analysis under Uncertainty: Framework Development and Case Studies. Biophysical Journal, 2004, 87, 3750-3763.	0.5	153
119	Insights into the relation between mrna and protein expression patterns: ii. Experimental observations inEscherichia coli. Biotechnology and Bioengineering, 2003, 84, 834-841.	3.3	77
120	Insights into the relation between mRNA and protein expression patterns: I. theoretical considerations. Biotechnology and Bioengineering, 2003, 84, 822-833.	3.3	106
121	Jay Bailey as mentor?The students' perspective. Biotechnology and Bioengineering, 2002, 79, 484-489.	3.3	1
122	A memorial review of Jay Bailey's contribution in prokaryotic metabolic engineering. Biotechnology and Bioengineering, 2002, 79, 504-508.	3.3	2
123	Inverse metabolic engineering: A strategy for directed genetic engineering of useful phenotypes. Biotechnology and Bioengineering, 2002, 79, 568-579.	3.3	88
124	Proteomics: Theoretical and Experimental Considerations. Biotechnology Progress, 1999, 15, 312-318.	2.6	93
125	Nonlinear Metabolic Control Analysis. Metabolic Engineering, 1999, 1, 75-87.	7.0	20
126	Dynamical Analysis of Gene Networks Requires Both mRNA and Protein Expression Information. Metabolic Engineering, 1999, 1, 275-281.	7.0	85

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127	A mathematical description of regulation of the G1-S transition of the mammalian cell cycle. Biotechnology and Bioengineering, 1999, 65, 631-637.	3.3	67
128	Modelling molecular mechanisms within their cellular environment. Journal of Biotechnology, 1999, 71, 263-265.	3.8	0
129	Application of mathematical tools for metabolic design of microbial ethanol production. , 1998, 58, 154-161.		62
130	Metabolic fluxes in riboflavin-producing Bacillus subtilis. Nature Biotechnology, 1997, 15, 448-452.	17.5	241
131	Metabolic Consequences of Phosphotransferase (PTS) Mutation in a Phenylalanine-Producing Recombinant Escherichia coli. Biotechnology Progress, 1997, 13, 768-775.	2.6	38
132	The AlkB Monooxygenase of Pseudomonas oleovorans. Synthesis, Stability and Level in Recombinant Escherichia coli and the Native Host. FEBS Journal, 1997, 244, 462-470.	0.2	17
133	Effects of spatiotemporal variations on metabolic control: Approximate analysis using (log)linear kinetic models. , 1997, 54, 91-104.		68
134	Studies on glycolysis â€" I. Multiple steady states in bacterial glycolysis. Chemical Engineering Science, 1997, 52, 2579-2588.	3.8	18
135	Analysis and design of metabolic reaction networks via mixed-integer linear optimization. AIChE Journal, 1996, 42, 1277-1292.	3.6	160
136	Effect ofVitreoscilla hemoglobin dosage on microaerobicEscherichia coli carbon and energy metabolism. Biotechnology and Bioengineering, 1996, 49, 139-150.	3.3	87
137	Metabolic flux analysis of hybridoma cells in different culture media using mass balances. , 1996, 50, 299-318.		226
138	Inverse metabolic engineering: A strategy for directed genetic engineering of useful phenotypes. , 1996, 52, 109-121.		136
139	Optimization of regulatory architectures in metabolic reaction networks. , 1996, 52, 485-500.		77
140	MCA Has More to Say. Journal of Theoretical Biology, 1996, 182, 233-242.	1.7	92
141	Recombinant cyclin E expression activates proliferation and obviates surface attachment of chinese hamster ovary (CHO) cells in protein-free medium. Biotechnology and Bioengineering, 1995, 47, 476-482.	3.3	67
142	A mathematical model for the G1/S transition of the mammalian cell cycle. Biotechnology Letters, 1995, 17, 669-674.	2.2	18
143	A method for pulsed periodic optimization of chemical reaction systems. Chemical Engineering Science, 1993, 48, 789-797.	3.8	14