Vassily Hatzimanikatis

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	Thermodynamics-Based Metabolic Flux Analysis. Biophysical Journal, 2007, 92, 1792-1805.	0.5	560
3	Group Contribution Method for Thermodynamic Analysis of Complex Metabolic Networks. Biophysical Journal, 2008, 95, 1487-1499.	0.5	345
4	Exploring the diversity of complex metabolic networks. Bioinformatics, 2005, 21, 1603-1609.	4.1	322
5	MEMOTE for standardized genome-scale metabolic model testing. Nature Biotechnology, 2020, 38, 272-276.	17.5	314
6	Metabolic fluxes in riboflavin-producing Bacillus subtilis. Nature Biotechnology, 1997, 15, 448-452.	17.5	241
7	Kinetic models in industrial biotechnology – Improving cell factory performance. Metabolic Engineering, 2014, 24, 38-60.	7.0	238
8	Metabolic flux analysis of hybridoma cells in different culture media using mass balances. , 1996, 50, 299-318.		226
9	Genome-Scale Thermodynamic Analysis of Escherichia coli Metabolism. Biophysical Journal, 2006, 90, 1453-1461.	0.5	195
10	Analysis and design of metabolic reaction networks via mixed-integer linear optimization. AICHE Journal, 1996, 42, 1277-1292.	3.6	160
11	Metabolic Control Analysis under Uncertainty: Framework Development and Case Studies. Biophysical Journal, 2004, 87, 3750-3763.	0.5	153
12	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
13	Towards kinetic modeling of genomeâ€scale metabolic networks without sacrificing stoichiometric, thermodynamic and physiological constraints. Biotechnology Journal, 2013, 8, 1043-1057.	3.5	141
14	Inverse metabolic engineering: A strategy for directed genetic engineering of useful phenotypes. , 1996, 52, 109-121.		136
15	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
16	Manipulating redox and ATP balancing for improved production of succinate in E. coli. Metabolic Engineering, 2011, 13, 76-81.	7.0	113
17	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
18	Insights into the relation between mRNA and protein expression patterns: I. theoretical considerations. Biotechnology and Bioengineering, 2003, 84, 822-833.	3.3	106

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19	Production of biofuels and biochemicals: in need of an ORACLE. Trends in Biotechnology, 2010, 28, 391-397.	9.3	100
20	Computational framework for predictive biodegradation. Biotechnology and Bioengineering, 2009, 104, 1086-1097.	3.3	96
21	Proteomics: Theoretical and Experimental Considerations. Biotechnology Progress, 1999, 15, 312-318.	2.6	93
22	Sustainability assessment of succinic acid production technologies from biomass using metabolic engineering. Energy and Environmental Science, 2016, 9, 2794-2805.	30.8	93
23	MCA Has More to Say. Journal of Theoretical Biology, 1996, 182, 233-242.	1.7	92
24	Metabolic Needs and Capabilities of Toxoplasma gondii through Combined Computational and Experimental Analysis. PLoS Computational Biology, 2015, 11, e1004261.	3.2	92
25	Genome-Scale Identification of Essential Metabolic Processes for Targeting the Plasmodium Liver Stage. Cell, 2019, 179, 1112-1128.e26.	28.9	92
26	Identification and dynamics of the human ZDHHC16-ZDHHC6 palmitoylation cascade. ELife, 2017, 6, .	6.0	89
27	Inverse metabolic engineering: A strategy for directed genetic engineering of useful phenotypes. Biotechnology and Bioengineering, 2002, 79, 568-579.	3.3	88
28	Effect ofVitreoscilla hemoglobin dosage on microaerobicEscherichia coli carbon and energy metabolism. Biotechnology and Bioengineering, 1996, 49, 139-150.	3.3	87
29	Heading in the right direction: thermodynamics-based network analysis and pathway engineering. Current Opinion in Biotechnology, 2015, 36, 176-182.	6.6	86
30	Dynamical Analysis of Gene Networks Requires Both mRNA and Protein Expression Information. Metabolic Engineering, 1999, 1, 275-281.	7.0	85
31	Mathematical Modeling of the Eukaryotic Heat-Shock Response: Dynamics of the hsp70 Promoter. Biophysical Journal, 2005, 88, 1646-1658.	0.5	83
32	Metabolic networks: enzyme function and metabolite structure. Current Opinion in Structural Biology, 2004, 14, 300-306.	5.7	81
33	Functional and Computational Genomics Reveal Unprecedented Flexibility in Stage-Specific Toxoplasma Metabolism. Cell Host and Microbe, 2020, 27, 290-306.e11.	11.0	81
34	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
35	Optimization of regulatory architectures in metabolic reaction networks. , 1996, 52, 485-500.		77
36	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

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37	pyTFA and matTFA: a Python package and a Matlab toolbox for Thermodynamics-based Flux Analysis. Bioinformatics, 2019, 35, 167-169.	4.1	75
38	In silico feasibility of novel biodegradation pathways for 1,2,4-trichlorobenzene. BMC Systems Biology, 2010, 4, 7.	3.0	74
39	Computational discovery of biochemical routes to specialty chemicals. Chemical Engineering Science, 2004, 59, 5051-5060.	3.8	73
40	Network thermodynamics in the post-genomic era. Current Opinion in Microbiology, 2010, 13, 350-357.	5.1	73
41	Modeling of uncertainties in biochemical reactions. Biotechnology and Bioengineering, 2011, 108, 413-423.	3.3	73
42	iSCHRUNK – 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
43	The ETFL formulation allows multi-omics integration in thermodynamics-compliant metabolism and expression models. Nature Communications, 2020, 11, 30.	12.8	71
44	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
45	Effects of spatiotemporal variations on metabolic control: Approximate analysis using (log)linear kinetic models. , 1997, 54, 91-104.		68
46	Metabolic engineering under uncertainty. I: Framework development. Metabolic Engineering, 2006, 8, 133-141.	7.0	68
47	Antihypertensive Drugs Metabolism: An Update to Pharmacokinetic Profiles and Computational Approaches. Current Pharmaceutical Design, 2014, 21, 806-822.	1.9	68
48	Do genomeâ€ s cale models need exact solvers or clearer standards?. Molecular Systems Biology, 2015, 11, 831.	7.2	68
49	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
50	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
51	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
52	Metabolic engineering under uncertainty—II: Analysis of yeast metabolism. Metabolic Engineering, 2006, 8, 142-159.	7.0	64
53	The SIB Swiss Institute of Bioinformatics' resources: focus on curated databases. Nucleic Acids Research, 2016, 44, D27-D37.	14.5	64
54	Application of mathematical tools for metabolic design of microbial ethanol production. , 1998, 58, 154-161.		62

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55	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
56	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
57	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
58	Efficient cleavage of aryl ether C–O linkages by Rh–Ni and Ru–Ni nanoscale catalysts operating in water. Chemical Science, 2018, 9, 5530-5535.	7.4	57
59	A Model for Protein Translation: Polysome Self-Organization Leads to Maximum Protein Synthesis Rates. Biophysical Journal, 2007, 92, 717-730.	0.5	50
60	The Origins of Time-Delay in Template Biopolymerization Processes. PLoS Computational Biology, 2010, 6, e1000726.	3.2	49
61	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
62	A genome-scale metabolic model of Saccharomyces cerevisiae that integrates expression constraints and reaction thermodynamics. Nature Communications, 2021, 12, 4790.	12.8	48
63	Constraining the Flux Space Using Thermodynamics and Integration of Metabolomics Data. Methods in Molecular Biology, 2014, 1191, 49-63.	0.9	47
64	Effects of Codon Distributions and tRNA Competition on Protein Translation. Biophysical Journal, 2008, 95, 1018-1033.	0.5	45
65	Thermodynamic analysis of biodegradation pathways. Biotechnology and Bioengineering, 2009, 103, 532-541.	3.3	45
66	Modeling metabolic networks of individual bacterial agents in heterogeneous and dynamic soil habitats (IndiMeSH). PLoS Computational Biology, 2019, 15, e1007127.	3.2	45
67	DREAMS of metabolism. Trends in Biotechnology, 2010, 28, 501-508.	9.3	44
68	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
69	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
70	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
71	An Algorithmic Framework for Genome-Wide Modeling and Analysis of Translation Networks. Biophysical Journal, 2006, 90, 1136-1146.	0.5	41
72	A computational workflow for the expansion of heterologous biosynthetic pathways to natural product derivatives. Nature Communications, 2021, 12, 1760.	12.8	40

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73	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
74	Metabolic Consequences of Phosphotransferase (PTS) Mutation in a Phenylalanine-Producing Recombinant Escherichia coli. Biotechnology Progress, 1997, 13, 768-775.	2.6	38
75	Rites of passage: requirements and standards for building kinetic models of metabolic phenotypes. Current Opinion in Biotechnology, 2015, 36, 146-153.	6.6	38
76	Impact of iron reduction on the metabolism of <i>Clostridium acetobutylicum</i> . Environmental Microbiology, 2019, 21, 3548-3563.	3.8	38
77	Model-Driven Understanding of Palmitoylation Dynamics: Regulated Acylation of the Endoplasmic Reticulum Chaperone Calnexin. PLoS Computational Biology, 2016, 12, e1004774.	3.2	37
78	A design–build–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
79	Kinetic models of metabolism that consider alternative steady-state solutions of intracellular fluxes and concentrations. Metabolic Engineering, 2019, 52, 29-41.	7.0	36
80	Updated ATLAS of Biochemistry with New Metabolites and Improved Enzyme Prediction Power. ACS Synthetic Biology, 2020, 9, 1479-1482.	3.8	34
81	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
82	Integrating computational methods to retrofit enzymes to synthetic pathways. Biotechnology and Bioengineering, 2012, 109, 572-582.	3.3	32
83	A model-based optimization framework for the inference on gene regulatory networks from DNA array data. Bioinformatics, 2004, 20, 3221-3235.	4.1	31
84	Thermodynamic Calculations for Biochemical Transport and Reaction Processes in Metabolic Networks. Biophysical Journal, 2010, 99, 3139-3144.	0.5	30
85	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
86	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
87	Bistability Explains Threshold Phenomena in Protein Aggregation both In Vitro and In Vivo. Biophysical Journal, 2006, 90, 886-895.	0.5	28
88	Thermodynamics-based Metabolite Sensitivity Analysis in metabolic networks. Metabolic Engineering, 2017, 39, 117-127.	7.0	27
89	Exploring biochemical pathways for mono-ethylene glycol (MEG) synthesis from synthesis gas. Metabolic Engineering, 2017, 41, 173-181.	7.0	26
90	Tunable reporter signal production in feedbackâ€uncoupled arsenic bioreporters. Microbial Biotechnology, 2013, 6, 503-514.	4.2	25

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91	Particle-Based Simulation Reveals Macromolecular Crowding Effects on the Michaelis-Menten Mechanism. Biophysical Journal, 2019, 117, 355-368.	0.5	24
92	A computational framework for the design of optimal protein synthesis. Biotechnology and Bioengineering, 2012, 109, 2127-2133.	3.3	23
93	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
94	A Genome-Scale Integration and Analysis of Lactococcus lactis Translation Data. PLoS Computational Biology, 2013, 9, e1003240.	3.2	22
95	Solvation quantities from a COSMO-RS equation of state. Journal of Chemical Thermodynamics, 2015, 90, 294-309.	2.0	21
96	Nonlinear Metabolic Control Analysis. Metabolic Engineering, 1999, 1, 75-87.	7.0	20
97	Uncertainty reduction in biochemical kinetic models: Enforcing desired model properties. PLoS Computational Biology, 2019, 15, e1007242.	3.2	20
98	Analysis of the maximum theoretical yield for the synthesis of erythromycin precursors inEscherichia coli. Biotechnology and Bioengineering, 2006, 95, 638-644.	3.3	19
99	Analysis of human metabolism by reducing the complexity of the genome-scale models using redHUMAN. Nature Communications, 2020, 11, 2821.	12.8	19
100	Expanding biochemical knowledge and illuminating metabolic dark matter with ATLASx. Nature Communications, 2022, 13, 1560.	12.8	19
101	A mathematical model for the G1/S transition of the mammalian cell cycle. Biotechnology Letters, 1995, 17, 669-674.	2.2	18
102	Studies on glycolysis — I. Multiple steady states in bacterial glycolysis. Chemical Engineering Science, 1997, 52, 2579-2588.	3.8	18
103	Molecular thermodynamics of metabolism: hydration quantities and the equation-of-state approach. Physical Chemistry Chemical Physics, 2016, 18, 32570-32592.	2.8	18
104	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
105	Mechanistic Modeling of Genetic Circuits for ArsR Arsenic Regulation. ACS Synthetic Biology, 2017, 6, 862-874.	3.8	18
106	Toward a Simple Predictive Molecular Thermodynamic Model for Bulk Phases and Interfaces. Industrial & Engineering Chemistry Research, 2017, 56, 10900-10910.	3.7	18
107	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
108	A computational framework for integration of lipidomics data into metabolic pathways. Metabolic Engineering, 2014, 23, 1-8.	7.0	17

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109	Redefining solubility parameters: Bulk and surface properties from unified molecular descriptors. Journal of Chemical Thermodynamics, 2017, 111, 207-220.	2.0	17
110	Control Theory Concepts for Modeling Uncertainty in Enzyme Kinetics of Biochemical Networks. Industrial & Engineering Chemistry Research, 2019, 58, 13544-13554.	3.7	17
111	Functional genomics of Plasmodium falciparum using metabolic modelling and analysis. Briefings in Functional Genomics, 2013, 12, 316-327.	2.7	16
112	Molecular thermodynamics of metabolism: quantum thermochemical calculations for key metabolites. Physical Chemistry Chemical Physics, 2015, 17, 10438-10453.	2.8	16
113	Analysis of Translation Elongation Dynamics in the Context of an Escherichia coli Cell. Biophysical Journal, 2016, 110, 2120-2131.	0.5	15
114	A method for pulsed periodic optimization of chemical reaction systems. Chemical Engineering Science, 1993, 48, 789-797.	3.8	14
115	Reconstruction of biological pathways and metabolic networks from in silico labeled metabolites. Biotechnology Journal, 2017, 12, 1600464.	3.5	14
116	Statistical inference in ensemble modeling of cellular metabolism. PLoS Computational Biology, 2019, 15, e1007536.	3.2	14
117	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
118	On Lewis acidity/basicity and hydrogen bonding in the equation-of-state approach. Journal of Chemical Thermodynamics, 2017, 110, 3-15.	2.0	13
119	Constraint-based metabolic control analysis for rational strain engineering. Metabolic Engineering, 2021, 66, 191-203.	7.0	12
120	Spatio-temporal modeling of the crowding conditions and metabolic variability in microbial communities. PLoS Computational Biology, 2021, 17, e1009140.	3.2	12
121	Computational tools and resources for designing new pathways to small molecules. Current Opinion in Biotechnology, 2022, 76, 102722.	6.6	12
122	NICEpath: Finding metabolic pathways in large networks through atom-conserving substrate–product pairs. Bioinformatics, 2021, 37, 3560-3568.	4.1	10
123	<i>110th Anniversary</i> : From Solubility Parameters to Predictive Equation-of-State Modeling. Industrial & Engineering Chemistry Research, 2019, 58, 12787-12800.	3.7	9
124	The solubility parameters of carbon dioxide and ionic liquids: Are they an enigma?. Fluid Phase Equilibria, 2021, 527, 112828.	2.5	8
125	NICEdrug.ch, a workflow for rational drug design and systems-level analysis of drug metabolism. ELife, 2021, 10, .	6.0	8
126	Noise analysis of genome-scale protein synthesis using a discrete computational model of translation. Journal of Chemical Physics, 2015, 143, 044109.	3.0	7

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127	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
128	Exploration of trade-offs between steady-state and dynamic properties in signaling cycles. Physical Biology, 2012, 9, 045010.	1.8	4
129	Integrative approaches for signalling and metabolic networks. Integrative Biology (United Kingdom), 2015, 7, 844-845.	1.3	4
130	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
131	Dynamic Radiolabeling of S-Palmitoylated Proteins. Methods in Molecular Biology, 2019, 2009, 111-127.	0.9	3
132	Quantitative modeling of human metabolism: A call for a community effort. Current Opinion in Systems Biology, 2021, 26, 109-115.	2.6	3
133	The influence of the crowding assumptions in biofilm simulations. PLoS Computational Biology, 2021, 17, e1009158.	3.2	3
134	ARBRE: Computational resource to predict pathways towards industrially important aromatic compounds. Metabolic Engineering, 2022, 72, 259-274.	7.0	3
135	A memorial review of Jay Bailey's contribution in prokaryotic metabolic engineering. Biotechnology and Bioengineering, 2002, 79, 504-508.	3.3	2
136	Jay Bailey as mentor?The students' perspective. Biotechnology and Bioengineering, 2002, 79, 484-489.	3.3	1
137	The systems engineering of cellular processes. Computer Aided Chemical Engineering, 2006, , 71-80.	0.5	1
138	Systems biology. Current Opinion in Biotechnology, 2011, 22, 538-540.	6.6	1
139	Mechanistically Consistent Reduced Models of Synthetic Gene Networks. Biophysical Journal, 2013, 104, 2098-2109.	0.5	1
140	Editorial: Metabolic modeling in biotechnology and medical research. Biotechnology Journal, 2013, 8, 962-963.	3.5	1
141	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
142	Modelling molecular mechanisms within their cellular environment. Journal of Biotechnology, 1999, 71, 263-265.	3.8	0
143	Discovery of Novel Routes for the Production of Fuels and Chemicals. , 2009, , 141-148.		0