Vassily Hatzimanikatis

List of Publications by Year in Descending Order

156 papers	7,564 citations	48 h-index	84 g-index
180 ext. papers	8,892 ext. citations	7.3 avg, IF	6.29 L-index

#	Paper	IF	Citations
156	Expanding biochemical knowledge and illuminating metabolic dark matter with ATLASx.. *Nature Communications*, **2022**, 13, 1560	17.4	0
155	ARBRE: Computational resource to predict pathways towards industrially important aromatic compounds.. *Metabolic Engineering*, **2022**,	9.7	1
154	Computational tools and resources for designing new pathways to small molecules.. *Current Opinion in Biotechnology*, **2022**, 76, 102722	11.4	0
153	PhenoMapping: a protocol to map cellular phenotypes to metabolic bottlenecks, identify conditional essentiality, and curate metabolic models. *STAR Protocols*, **2021**, 2, 100280	1.4	1
152	A computational workflow for the expansion of heterologous biosynthetic pathways to natural product derivatives. *Nature Communications*, **2021**, 12, 1760	17.4	11
151	Finding metabolic pathways in large networks through atom-conserving substrate-product pairs. *Bioinformatics*, **2021**,	7.2	3
150	Quantitative modeling of human metabolism: A call for a community effort. *Current Opinion in Systems Biology*, **2021**, 26, 109-115	3.2	0
149	Thermodynamics of Metabolic Pathways **2021**, 213-235		
148	Pathway Design **2021**, 237-257		1
147	The influence of the crowding assumptions in biofilm simulations. *PLoS Computational Biology*, **2021**, 17, e1009158	5	1
146	Constraint-based metabolic control analysis for rational strain engineering. *Metabolic Engineering*, **2021**, 66, 191-203	9.7	2
145	The solubility parameters of carbon dioxide and ionic liquids: Are they an enigma?. *Fluid Phase Equilibria*, **2021**, 527, 112828	2.5	3
144	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,	11.5	5
143	The effects of model complexity and size on metabolic flux distribution and control: case study in Escherichia coli. *BMC Bioinformatics*, **2021**, 22, 134	3.6	2
142	Spatio-temporal modeling of the crowding conditions and metabolic variability in microbial communities. *PLoS Computational Biology*, **2021**, 17, e1009140	5	0
141	NICEdrug.ch, a workflow for rational drug design and systems-level analysis of drug metabolism. *ELife*, **2021**, 10,	8.9	4
140	A genome-scale metabolic model of Saccharomyces cerevisiae that integrates expression constraints and reaction thermodynamics. *Nature Communications*, **2021**, 12, 4790	17.4	8

139	Updated ATLAS of Biochemistry with New Metabolites and Improved Enzyme Prediction Power. *ACS Synthetic Biology*, **2020**, 9, 1479-1482	5.7	16
138	Analysis of human metabolism by reducing the complexity of the genome-scale models using redHUMAN. *Nature Communications*, **2020**, 11, 2821	17.4	8
137	Large-scale kinetic metabolic models of KT2440 for consistent design of metabolic engineering strategies. *Biotechnology for Biofuels*, **2020**, 13, 33	7.8	17
136	MEMOTE for standardized genome-scale metabolic model testing. *Nature Biotechnology*, **2020**, 38, 272-276	44.5	121
135	The ETFL formulation allows multi-omics integration in thermodynamics-compliant metabolism and expression models. *Nature Communications*, **2020**, 11, 30	17.4	41
134	Functional and Computational Genomics Reveal Unprecedented Flexibility in Stage-Specific Toxoplasma Metabolism. *Cell Host and Microbe*, **2020**, 27, 290-306.e11	23.4	44
133	Uncertainty reduction in biochemical kinetic models: Enforcing desired model properties. *PLoS Computational Biology*, **2019**, 15, e1007242	5	6
132	110th Anniversary: From Solubility Parameters to Predictive Equation-of-State Modeling. *Industrial & Engineering Chemistry Research*, **2019**, 58, 12787-12800	3.9	7
131	Dynamic Radiolabeling of S-Palmitoylated Proteins. *Methods in Molecular Biology*, **2019**, 2009, 111-127	1.4	2
130	Enhanced flux prediction by integrating relative expression and relative metabolite abundance into thermodynamically consistent metabolic models. *PLoS Computational Biology*, **2019**, 15, e1007036	5	34
129	Control Theory Concepts for Modeling Uncertainty in Enzyme Kinetics of Biochemical Networks. *Industrial & Engineering Chemistry Research*, **2019**, 58, 13544-13554	3.9	9
128	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	5	5
127	Impact of iron reduction on the metabolism of Clostridium acetobutylicum. *Environmental Microbiology*, **2019**, 21, 3548-3563	5.2	17
126	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	11.5	35
125	pyTFA and matTFA: a Python package and a Matlab toolbox for Thermodynamics-based Flux Analysis. *Bioinformatics*, **2019**, 35, 167-169	7.2	26
124	Modeling metabolic networks of individual bacterial agents in heterogeneous and dynamic soil habitats (IndiMeSH). *PLoS Computational Biology*, **2019**, 15, e1007127	5	21
123	Particle-Based Simulation Reveals Macromolecular Crowding Effects on the Michaelis-Menten Mechanism. *Biophysical Journal*, **2019**, 117, 355-368	2.9	13
122	Genome-Scale Identification of Essential Metabolic Processes for Targeting the Plasmodium Liver Stage. *Cell*, **2019**, 179, 1112-1128.e26	56.2	41

121	Statistical inference in ensemble modeling of cellular metabolism. *PLoS Computational Biology*, **2019**, 15, e1007536	5	11
120	Kinetic models of metabolism that consider alternative steady-state solutions of intracellular fluxes and concentrations. *Metabolic Engineering*, **2019**, 52, 29-41	9.7	20
119	Discovery and Evaluation of Biosynthetic Pathways for the Production of Five Methyl Ethyl Ketone Precursors. *ACS Synthetic Biology*, **2018**, 7, 1858-1873	5.7	19
118	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	9.4	41
117	Mechanistic Modeling of Genetic Circuits for ArsR Arsenic Regulation. *ACS Synthetic Biology*, **2017**, 6, 862-874	5.7	12
116	Integration of metabolic, regulatory and signaling networks towards analysis of perturbation and dynamic responses. *Current Opinion in Systems Biology*, **2017**, 2, 59-66	3.2	11
115	On Lewis acidity/basicity and hydrogen bonding in the equation-of-state approach. *Journal of Chemical Thermodynamics*, **2017**, 110, 3-15	2.9	10
114	Exploring biochemical pathways for mono-ethylene glycol (MEG) synthesis from synthesis gas. *Metabolic Engineering*, **2017**, 41, 173-181	9.7	18
113	Reconstruction of biological pathways and metabolic networks from in silico labeled metabolites. *Biotechnology Journal*, **2017**, 12, 1600464	5.6	10
112	Redefining solubility parameters: Bulk and surface properties from unified molecular descriptors. *Journal of Chemical Thermodynamics*, **2017**, 111, 207-220	2.9	16
111	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	20.1	34
110	Bioenergetics-based modeling of Plasmodium falciparum metabolism reveals its essential genes, nutritional requirements, and thermodynamic bottlenecks. *PLoS Computational Biology*, **2017**, 13, e1005397	5	36
109	redGEM: Systematic reduction and analysis of genome-scale metabolic reconstructions for development of consistent core metabolic models. *PLoS Computational Biology*, **2017**, 13, e1005444	5	38
108	lumpGEM: Systematic generation of subnetworks and elementally balanced lumped reactions for the biosynthesis of target metabolites. *PLoS Computational Biology*, **2017**, 13, e1005513	5	25
107	Toward a Simple Predictive Molecular Thermodynamic Model for Bulk Phases and Interfaces. *Industrial & Engineering Chemistry Research*, **2017**, 56, 10900-10910	3.9	13
106	A design-build-test cycle using modeling and experiments reveals interdependencies between upper glycolysis and xylose uptake in recombinant and improves predictive capabilities of large-scale kinetic models. *Biotechnology for Biofuels*, **2017**, 10, 166	7.8	22
105	Thermodynamics-based Metabolite Sensitivity Analysis in metabolic networks. *Metabolic Engineering*, **2017**, 39, 117-127	9.7	17
104	Identification and dynamics of the human ZDHHC16-ZDHHC6 palmitoylation cascade. *ELife*, **2017**, 6,	8.9	53

103	Molecular thermodynamics of metabolism: hydration quantities and the equation-of-state approach. *Physical Chemistry Chemical Physics*, **2016**, 18, 32570-32592	3.6	13
102	ATLAS of Biochemistry: A Repository of All Possible Biochemical Reactions for Synthetic Biology and Metabolic Engineering Studies. *ACS Synthetic Biology*, **2016**, 5, 1155-1166	5.7	97
101	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	9.7	29
100	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	9.7	49
99	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	9.7	56
98	Quantification of Cooperativity in Heterodimer-DNA Binding Improves the Accuracy of Binding Specificity Models. *Journal of Biological Chemistry*, **2016**, 291, 10293-306	5.4	18
97	The SIB Swiss Institute of BioinformaticsSresources: focus on curated databases. *Nucleic Acids Research*, **2016**, 44, D27-37	20.1	41
96	Model-Driven Understanding of Palmitoylation Dynamics: Regulated Acylation of the Endoplasmic Reticulum Chaperone Calnexin. *PLoS Computational Biology*, **2016**, 12, e1004774	5	24
95	Sustainability assessment of succinic acid production technologies from biomass using metabolic engineering. *Energy and Environmental Science*, **2016**, 9, 2794-2805	35.4	67
94	Analysis of Translation Elongation Dynamics in the Context of an Escherichia coli Cell. *Biophysical Journal*, **2016**, 110, 2120-31	2.9	8
93	Solvation quantities from a COSMO-RS equation of state. *Journal of Chemical Thermodynamics*, **2015**, 90, 294-309	2.9	13
92	Design of computational retrobiosynthesis tools for the design of de novo synthetic pathways. *Current Opinion in Chemical Biology*, **2015**, 28, 99-104	9.7	82
91	Metabolic Needs and Capabilities of Toxoplasma gondii through Combined Computational and Experimental Analysis. *PLoS Computational Biology*, **2015**, 11, e1004261	5	71
90	Molecular thermodynamics of metabolism: quantum thermochemical calculations for key metabolites. *Physical Chemistry Chemical Physics*, **2015**, 17, 10438-53	3.6	13
89	Heading in the right direction: thermodynamics-based network analysis and pathway engineering. *Current Opinion in Biotechnology*, **2015**, 36, 176-82	11.4	67
88	Do genome-scale models need exact solvers or clearer standards?. *Molecular Systems Biology*, **2015**, 11, 831	12.2	41
87	Noise analysis of genome-scale protein synthesis using a discrete computational model of translation. *Journal of Chemical Physics*, **2015**, 143, 044109	3.9	4
86	Rites of passage: requirements and standards for building kinetic models of metabolic phenotypes. *Current Opinion in Biotechnology*, **2015**, 36, 146-53	11.4	27

85	Antihypertensive drugs metabolism: an update to pharmacokinetic profiles and computational approaches. *Current Pharmaceutical Design*, **2015**, 21, 806-22	3.3	50
84	Kinetic models in industrial biotechnology - Improving cell factory performance. *Metabolic Engineering*, **2014**, 24, 38-60	9.7	183
83	A computational framework for integration of lipidomics data into metabolic pathways. *Metabolic Engineering*, **2014**, 23, 1-8	9.7	14
82	Constraining the flux space using thermodynamics and integration of metabolomics data. *Methods in Molecular Biology*, **2014**, 1191, 49-63	1.4	31
81	Mechanistically consistent reduced models of synthetic gene networks. *Biophysical Journal*, **2013**, 104, 2098-109	2.9	1
80	Towards kinetic modeling of genome-scale metabolic networks without sacrificing stoichiometric, thermodynamic and physiological constraints. *Biotechnology Journal*, **2013**, 8, 1043-57	5.6	114
79	Functional genomics of Plasmodium falciparum using metabolic modelling and analysis. *Briefings in Functional Genomics*, **2013**, 12, 316-27	4.9	13
78	A genome-scale integration and analysis of Lactococcus lactis translation data. *PLoS Computational Biology*, **2013**, 9, e1003240	5	21
77	Tunable reporter signal production in feedback-uncoupled arsenic bioreporters. *Microbial Biotechnology*, **2013**, 6, 503-14	6.3	23
76	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	3.7	31
75	Integrating computational methods to retrofit enzymes to synthetic pathways. *Biotechnology and Bioengineering*, **2012**, 109, 572-82	4.9	30
74	A computational framework for the design of optimal protein synthesis. *Biotechnology and Bioengineering*, **2012**, 109, 2127-33	4.9	20
73	From network models to network responses: integration of thermodynamic and kinetic properties of yeast genome-scale metabolic networks. *FEMS Yeast Research*, **2012**, 12, 129-43	3.1	60
72	Exploration of trade-offs between steady-state and dynamic properties in signaling cycles. *Physical Biology*, **2012**, 9, 045010	3	3
71	Modeling of uncertainties in biochemical reactions. *Biotechnology and Bioengineering*, **2011**, 108, 413-23	4.9	57
70	Manipulating redox and ATP balancing for improved production of succinate in E. coli. *Metabolic Engineering*, **2011**, 13, 76-81	9.7	104
69	The origins of time-delay in template biopolymerization processes. *PLoS Computational Biology*, **2010**, 6, e1000726	5	38
68	Thermodynamic calculations for biochemical transport and reaction processes in metabolic networks. *Biophysical Journal*, **2010**, 99, 3139-44	2.9	23

67	Network thermodynamics in the post-genomic era. *Current Opinion in Microbiology*, **2010**, 13, 350-7	7.9	61
66	Production of biofuels and biochemicals: in need of an ORACLE. *Trends in Biotechnology*, **2010**, 28, 391-7	15.1	74
65	DREAMS of metabolism. *Trends in Biotechnology*, **2010**, 28, 501-8	15.1	40
64	In silico feasibility of novel biodegradation pathways for 1,2,4-trichlorobenzene. *BMC Systems Biology*, **2010**, 4, 7	3.5	58
63	Discovery and analysis of novel metabolic pathways for the biosynthesis of industrial chemicals: 3-hydroxypropanoate. *Biotechnology and Bioengineering*, **2010**, 106, 462-73	4.9	125
62	Thermodynamic analysis of biodegradation pathways. *Biotechnology and Bioengineering*, **2009**, 103, 532-41	4.9	39
61	Computational framework for predictive biodegradation. *Biotechnology and Bioengineering*, **2009**, 104, 1086-97	4.9	77
60	Discovery of Novel Routes for the Production of Fuels and Chemicals **2009**, 141-148		
59	Group contribution method for thermodynamic analysis of complex metabolic networks. *Biophysical Journal*, **2008**, 95, 1487-99	2.9	294
58	Effects of codon distributions and tRNA competition on protein translation. *Biophysical Journal*, **2008**, 95, 1018-33	2.9	41
57	A model for protein translation: polysome self-organization leads to maximum protein synthesis rates. *Biophysical Journal*, **2007**, 92, 717-30	2.9	45
56	Thermodynamics-based metabolic flux analysis. *Biophysical Journal*, **2007**, 92, 1792-805	2.9	456
55	A model-based optimization framework for the inference of regulatory interactions using time-course DNA microarray expression data. *BMC Bioinformatics*, **2007**, 8, 228	3.6	25
54	A genome-scale metabolic reconstruction for Escherichia coli K-12 MG1655 that accounts for 1260 ORFs and thermodynamic information. *Molecular Systems Biology*, **2007**, 3, 121	12.2	1044
53	Analysis of the maximum theoretical yield for the synthesis of erythromycin precursors in Escherichia coli. *Biotechnology and Bioengineering*, **2006**, 95, 638-44	4.9	19
52	The systems engineering of cellular processes. *Computer Aided Chemical Engineering*, **2006**, 71-80	0.6	
51	An algorithmic framework for genome-wide modeling and analysis of translation networks. *Biophysical Journal*, **2006**, 90, 1136-46	2.9	37
50	Genome-scale thermodynamic analysis of Escherichia coli metabolism. *Biophysical Journal*, **2006**, 90, 1453-61	2.9	176

49	Metabolic engineering under uncertainty--II: analysis of yeast metabolism. *Metabolic Engineering*, **2006**, 8, 142-59	9.7	54
48	Metabolic engineering under uncertainty. I: framework development. *Metabolic Engineering*, **2006**, 8, 133-41	9.7	56
47	Bistability explains threshold phenomena in protein aggregation both in vitro and in vivo. *Biophysical Journal*, **2006**, 90, 886-95	2.9	24
46	Theoretical considerations and computational analysis of the complexity in polyketide synthesis pathways. *Journal of the American Chemical Society*, **2005**, 127, 9930-8	16.4	54
45	Mathematical modeling of the eukaryotic heat-shock response: dynamics of the hsp70 promoter. *Biophysical Journal*, **2005**, 88, 1646-58	2.9	73
44	Exploring the diversity of complex metabolic networks. *Bioinformatics*, **2005**, 21, 1603-9	7.2	273
43	A model-based optimization framework for the inference on gene regulatory networks from DNA array data. *Bioinformatics*, **2004**, 20, 3221-35	7.2	26
42	Metabolic networks: enzyme function and metabolite structure. *Current Opinion in Structural Biology*, **2004**, 14, 300-6	8.1	69
41	Computational discovery of biochemical routes to specialty chemicals. *Chemical Engineering Science* , **2004**, 59, 5051-5060	4.4	67
40	Metabolic control analysis under uncertainty: framework development and case studies. *Biophysical Journal*, **2004**, 87, 3750-63	2.9	125
39	Insights into the relation between mrna and protein expression patterns: II. Experimental observations in Escherichia coli. *Biotechnology and Bioengineering*, **2003**, 84, 834-41	4.9	67
38	Insights into the relation between mRNA and protein expression patterns: I. Theoretical considerations. *Biotechnology and Bioengineering*, **2003**, 84, 822-33	4.9	91
37	Jay Bailey as mentor--the studentsSperspective. *Biotechnology and Bioengineering*, **2002**, 79, 484-9	4.9	0
36	A memorial review of Jay BaileyS contribution in prokaryotic metabolic engineering. *Biotechnology and Bioengineering*, **2002**, 79, 504-8	4.9	2
35	Inverse metabolic engineering: a strategy for directed genetic engineering of useful phenotypes. *Biotechnology and Bioengineering*, **2002**, 79, 568-79	4.9	84
34	Proteomics: theoretical and experimental considerations. *Biotechnology Progress*, **1999**, 15, 312-8	2.8	73
33	Nonlinear metabolic control analysis. *Metabolic Engineering*, **1999**, 1, 75-87	9.7	20
32	Dynamical analysis of gene networks requires both mRNA and protein expression information. *Metabolic Engineering*, **1999**, 1, 275-81	9.7	74

31	A mathematical description of regulation of the G1-S transition of the mammalian cell cycle. *Biotechnology and Bioengineering*, **1999**, 65, 631-7	4.9	55
30	Modelling molecular mechanisms within their cellular environment. *Journal of Biotechnology*, **1999**, 71, 263-265	3.7	
29	Application of mathematical tools for metabolic design of microbial ethanol production. *Biotechnology and Bioengineering*, **1998**, 58, 154-61	4.9	54
28	Metabolic fluxes in riboflavin-producing Bacillus subtilis. *Nature Biotechnology*, **1997**, 15, 448-52	44.5	221
27	Metabolic consequences of phosphotransferase (PTS) mutation in a phenylalanine-producing recombinant Escherichia coli. *Biotechnology Progress*, **1997**, 13, 768-75	2.8	32
26	The AlkB monooxygenase of Pseudomonas oleovorans--synthesis, stability and level in recombinant Escherichia coli and the native host. *FEBS Journal*, **1997**, 244, 462-70		14
25	Effects of spatiotemporal variations on metabolic control: approximate analysis using (log)linear kinetic models. *Biotechnology and Bioengineering*, **1997**, 54, 91-104	4.9	54
24	Studies on glycolysis □. Multiple steady states in bacterial glycolysis. *Chemical Engineering Science* , **1997**, 52, 2579-2588	4.4	17
23	Analysis and design of metabolic reaction networks via mixed-integer linear optimization. *AICHE Journal*, **1996**, 42, 1277-1292	3.6	134
22	Effect of Vitreoscilla hemoglobin dosage on microaerobic Escherichia coli carbon and energy metabolism. *Biotechnology and Bioengineering*, **1996**, 49, 139-50	4.9	83
21	Metabolic flux analysis of hybridoma cells in different culture media using mass balances. *Biotechnology and Bioengineering*, **1996**, 50, 299-318	4.9	200
20	Inverse metabolic engineering: A strategy for directed genetic engineering of useful phenotypes. *Biotechnology and Bioengineering*, **1996**, 52, 109-21	4.9	122
19	Optimization of regulatory architectures in metabolic reaction networks. *Biotechnology and Bioengineering*, **1996**, 52, 485-500	4.9	64
18	MCA has more to say. *Journal of Theoretical Biology*, **1996**, 182, 233-42	2.3	78
17	A mathematical model for the G1/S transition of the mammalian cell cycle. *Biotechnology Letters*, **1995**, 17, 669-674	3	15
16	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, 476-82	4.9	61
15	A method for pulsed periodic optimization of chemical reaction systems. *Chemical Engineering Science*, **1993**, 48, 789-797	4.4	12
14	Symbolic Kinetic Models in Python (SKiMpy): Intuitive modeling of large-scale biological kinetic models		1

13	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	1
12	Particle-based simulation reveals macromolecular crowding effects on the Michaelis-Menten mechanism	1
11	Emergence of diauxie as an optimal growth strategy under resource allocation constraints in cellular metabolism	3
10	Finding metabolic pathways in large networks through atom-conserving substrate-product pairs	3
9	Assigning enzyme sequences to orphan and novel reactions using knowledge of substrate reactive sites	1
8	Memote: A community driven effort towards a standardized genome-scale metabolic model test suite	26
7	The architecture of the endoplasmic reticulum is regulated by the reversible lipid modification of the shaping protein CLIMP-63	2
6	Enhanced flux prediction by integrating relative expression and relative metabolite abundance into thermodynamically consistent metabolic models	2
5	TEX-FBA: A constraint-based method for integrating gene expression, thermodynamics, and metabolomics data into genome-scale metabolic models	4
4	Large-scale kinetic metabolic models ofPseudomonas putidafor a consistent design of metabolic engineering strategies	1
3	ETFL: A formulation for flux balance models accounting for expression, thermodynamics, and resource allocation constraints	2
2	The effects of model complexity and size on metabolic flux distribution and control. Case study inE. coli	1
1	ATLASx: a computational map for the exploration of biochemical space	2