Ines Thiele

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16,155 49 127 121 h-index g-index citations papers 6.9 139 20,331 9.1 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
121	What is flux balance analysis?. <i>Nature Biotechnology</i> , 2010 , 28, 245-8	44.5	2292
120	The subsystems approach to genome annotation and its use in the project to annotate 1000 genomes. <i>Nucleic Acids Research</i> , 2005 , 33, 5691-702	20.1	1485
119	A protocol for generating a high-quality genome-scale metabolic reconstruction. <i>Nature Protocols</i> , 2010 , 5, 93-121	18.8	1156
118	Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox v2.0. <i>Nature Protocols</i> , 2011 , 6, 1290-307	18.8	1061
117	Global reconstruction of the human metabolic network based on genomic and bibliomic data. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 1777-82	11.5	1060
116	Gut microbiota functions: metabolism of nutrients and other food components. <i>European Journal of Nutrition</i> , 2018 , 57, 1-24	5.2	857
115	A community-driven global reconstruction of human metabolism. <i>Nature Biotechnology</i> , 2013 , 31, 419-	25 _{44.5}	746
114	Reconstruction of biochemical networks in microorganisms. <i>Nature Reviews Microbiology</i> , 2009 , 7, 129-	4 3 2.2	699
113	Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v.3.0. <i>Nature Protocols</i> , 2019 , 14, 639-702	18.8	385
112	Generation of genome-scale metabolic reconstructions for 773 members of the human gut microbiota. <i>Nature Biotechnology</i> , 2017 , 35, 81-89	44.5	368
111	Metabolomics enables precision medicine: "A White Paper, Community Perspective". <i>Metabolomics</i> , 2016 , 12, 149	4.7	327
110	Systematic genome assessment of B-vitamin biosynthesis suggests co-operation among gut microbes. <i>Frontiers in Genetics</i> , 2015 , 6, 148	4.5	313
109	Towards multidimensional genome annotation. <i>Nature Reviews Genetics</i> , 2006 , 7, 130-41	30.1	285
108	Recon3D enables a three-dimensional view of gene variation in human metabolism. <i>Nature Biotechnology</i> , 2018 , 36, 272-281	44.5	283
107	Detailing the optimality of photosynthesis in cyanobacteria through systems biology analysis. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 2678-83	11.5	231
106	A genome-scale metabolic reconstruction of Pseudomonas putida KT2440: iJN746 as a cell factory. <i>BMC Systems Biology</i> , 2008 , 2, 79	3.5	193
105	Expanded metabolic reconstruction of Helicobacter pylori (iIT341 GSM/GPR): an in silico genome-scale characterization of single- and double-deletion mutants. <i>Journal of Bacteriology</i> , 2005 , 187, 5818-30	3.5	193

104	Computationally efficient flux variability analysis. BMC Bioinformatics, 2010, 11, 489	3.6	179
103	Systems-level characterization of a host-microbe metabolic symbiosis in the mammalian gut. <i>Gut Microbes</i> , 2013 , 4, 28-40	8.8	155
102	Three-dimensional structural view of the central metabolic network of Thermotoga maritima. <i>Science</i> , 2009 , 325, 1544-9	33.3	148
101	Genome-scale reconstruction of Escherichia coli's transcriptional and translational machinery: a knowledge base, its mathematical formulation, and its functional characterization. <i>PLoS Computational Biology</i> , 2009 , 5, e1000312	5	143
100	The Virtual Metabolic Human database: integrating human and gut microbiome metabolism with nutrition and disease. <i>Nucleic Acids Research</i> , 2019 , 47, D614-D624	20.1	132
99	Candidate metabolic network states in human mitochondria. Impact of diabetes, ischemia, and diet. <i>Journal of Biological Chemistry</i> , 2005 , 280, 11683-95	5.4	117
98	BacArena: Individual-based metabolic modeling of heterogeneous microbes in complex communities. <i>PLoS Computational Biology</i> , 2017 , 13, e1005544	5	116
97	A detailed genome-wide reconstruction of mouse metabolism based on human Recon 1. <i>BMC Systems Biology</i> , 2010 , 4, 140	3.5	114
96	Functional metabolic map of Faecalibacterium prausnitzii, a beneficial human gut microbe. <i>Journal of Bacteriology</i> , 2014 , 196, 3289-302	3.5	109
95	A community effort towards a knowledge-base and mathematical model of the human pathogen Salmonella Typhimurium LT2. <i>BMC Systems Biology</i> , 2011 , 5, 8	3.5	105
94	Systematic assessment of secondary bile acid metabolism in gut microbes reveals distinct metabolic capabilities in inflammatory bowel disease. <i>Microbiome</i> , 2019 , 7, 75	16.6	98
93	Multiscale modeling of metabolism and macromolecular synthesis in E. coli and its application to the evolution of codon usage. <i>PLoS ONE</i> , 2012 , 7, e45635	3.7	87
92	fastGapFill: efficient gap filling in metabolic networks. <i>Bioinformatics</i> , 2014 , 30, 2529-31	7.2	80
91	Metabolic network analysis integrated with transcript verification for sequenced genomes. <i>Nature Methods</i> , 2009 , 6, 589-92	21.6	80
90	Modeling metabolism of the human gut microbiome. <i>Current Opinion in Biotechnology</i> , 2018 , 51, 90-96	11.4	79
89	Systematic prediction of health-relevant human-microbial co-metabolism through a computational framework. <i>Gut Microbes</i> , 2015 , 6, 120-30	8.8	76
88	Anoxic Conditions Promote Species-Specific Mutualism between Gut Microbes In Silico. <i>Applied and Environmental Microbiology</i> , 2015 , 81, 4049-61	4.8	71
87	Monitoring metabolites consumption and secretion in cultured cells using ultra-performance liquid chromatography quadrupole-time of flight mass spectrometry (UPLC-Q-ToF-MS). <i>Analytical and Bioanalytical Chemistry</i> , 2012 , 402, 1183-98	4.4	70

86	A systems biology approach to studying the role of microbes in human health. <i>Current Opinion in Biotechnology</i> , 2013 , 24, 4-12	11.4	70
85	Finding useful biomarkers for Parkinson's disease. Science Translational Medicine, 2018, 10,	17.5	69
84	Systems biology of host-microbe metabolomics. <i>Wiley Interdisciplinary Reviews: Systems Biology and Medicine</i> , 2015 , 7, 195-219	6.6	64
83	Quantitative assignment of reaction directionality in constraint-based models of metabolism: application to Escherichia coli. <i>Biophysical Chemistry</i> , 2009 , 145, 47-56	3.5	64
82	From Network Analysis to Functional Metabolic Modeling of the Human Gut Microbiota. <i>MSystems</i> , 2018 , 3,	7.6	60
81	Association of Altered Liver Enzymes With Alzheimer Disease Diagnosis, Cognition, Neuroimaging Measures, and Cerebrospinal Fluid Biomarkers. <i>JAMA Network Open</i> , 2019 , 2, e197978	10.4	60
8o	Membrane transporters in a human genome-scale metabolic knowledgebase and their implications for disease. <i>Frontiers in Physiology</i> , 2014 , 5, 91	4.6	56
79	A compendium of inborn errors of metabolism mapped onto the human metabolic network. <i>Molecular BioSystems</i> , 2012 , 8, 2545-58		55
78	The human metabolic reconstruction Recon 1 directs hypotheses of novel human metabolic functions. <i>BMC Systems Biology</i> , 2011 , 5, 155	3.5	55
77	von Bertalanffy 1.0: a COBRA toolbox extension to thermodynamically constrain metabolic models. <i>Bioinformatics</i> , 2011 , 27, 142-3	7.2	55
76	Identification of potential pathway mediation targets in Toll-like receptor signaling. <i>PLoS Computational Biology</i> , 2009 , 5, e1000292	5	52
75	Predicting the impact of diet and enzymopathies on human small intestinal epithelial cells. <i>Human Molecular Genetics</i> , 2013 , 22, 2705-22	5.6	51
74	Parkinson's disease-associated alterations of the gut microbiome predict disease-relevant changes in metabolic functions. <i>BMC Biology</i> , 2020 , 18, 62	7.3	50
73	rBioNet: A COBRA toolbox extension for reconstructing high-quality biochemical networks. <i>Bioinformatics</i> , 2011 , 27, 2009-10	7.2	50
72	Leigh map: A novel computational diagnostic resource for mitochondrial disease. <i>Annals of Neurology</i> , 2017 , 81, 9-16	9.4	49
71	Prediction of intracellular metabolic states from extracellular metabolomic data. <i>Metabolomics</i> , 2015 , 11, 603-619	4.7	48
7º	Integrated stoichiometric, thermodynamic and kinetic modelling of steady state metabolism. Journal of Theoretical Biology, 2010 , 264, 683-92	2.3	48
69	Functional characterization of alternate optimal solutions of Escherichia coli's transcriptional and translational machinery. <i>Biophysical Journal</i> , 2010 , 98, 2072-81	2.9	46

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68	Comparative Genomic Analysis of the Human Gut Microbiome Reveals a Broad Distribution of Metabolic Pathways for the Degradation of Host-Synthetized Mucin Glycans and Utilization of Mucin-Derived Monosaccharides. <i>Frontiers in Genetics</i> , 2017 , 8, 111	4.5	45
67	The Microbiome Modeling Toolbox: from microbial interactions to personalized microbial communities. <i>Bioinformatics</i> , 2019 , 35, 2332-2334	7.2	45
66	Integrated Analyses of Microbiome and Longitudinal Metabolome Data Reveal Microbial-Host Interactions on Sulfur Metabolism in Parkinson's Disease. <i>Cell Reports</i> , 2019 , 29, 1767-1777.e8	10.6	43
65	Personalized whole-body models integrate metabolism, physiology, and the gut microbiome. <i>Molecular Systems Biology</i> , 2020 , 16, e8982	12.2	43
64	Do genome-scale models need exact solvers or clearer standards?. <i>Molecular Systems Biology</i> , 2015 , 11, 831	12.2	41
63	Candidate states of Helicobacter pylori's genome-scale metabolic network upon application of "loop law" thermodynamic constraints. <i>Biophysical Journal</i> , 2006 , 90, 3919-28	2.9	41
62	From metagenomic data to personalized in silico microbiotas: predicting dietary supplements for Crohn's disease. <i>Npj Systems Biology and Applications</i> , 2018 , 4, 27	5	39
61	Estimation of the number of extreme pathways for metabolic networks. <i>BMC Bioinformatics</i> , 2007 , 8, 363	3.6	38
60	Intracellular metabolite profiling of platelets: evaluation of extraction processes and chromatographic strategies. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2012 , 898, 111-20	3.2	36
59	Genomic Analysis of the Human Gut Microbiome Suggests Novel Enzymes Involved in Quinone Biosynthesis. <i>Frontiers in Microbiology</i> , 2016 , 7, 128	5.7	35
58	Quantitative assignment of reaction directionality in a multicompartmental human metabolic reconstruction. <i>Biophysical Journal</i> , 2012 , 102, 1703-11	2.9	34
57	Metabolic Network Analysis Reveals Altered Bile Acid Synthesis and Metabolism in Alzheimer's Disease. <i>Cell Reports Medicine</i> , 2020 , 1, 100138	18	34
56	CHRR: coordinate hit-and-run with rounding for uniform sampling of constraint-based models. <i>Bioinformatics</i> , 2017 , 33, 1741-1743	7.2	32
55	An international classification of inherited metabolic disorders (ICIMD). <i>Journal of Inherited Metabolic Disease</i> , 2021 , 44, 164-177	5.4	32
54	Integrated In Vitro and In Silico Modeling Delineates the Molecular Effects of a Synbiotic Regimen on Colorectal-Cancer-Derived Cells. <i>Cell Reports</i> , 2019 , 27, 1621-1632.e9	10.6	31
53	MetaboTools: A Comprehensive Toolbox for Analysis of Genome-Scale Metabolic Models. <i>Frontiers in Physiology</i> , 2016 , 7, 327	4.6	31
52	Quantitative systems pharmacology and the personalized drug-microbiota-diet axis. <i>Current Opinion in Systems Biology</i> , 2017 , 4, 43-52	3.2	29
51	ReconMap: an interactive visualization of human metabolism. <i>Bioinformatics</i> , 2017 , 33, 605-607	7.2	29

50	Toward systems metabolic engineering in cyanobacteria: opportunities and bottlenecks. <i>Bioengineered</i> , 2013 , 4, 158-63	5.7	28
49	A systems biology approach to drug targets in Pseudomonas aeruginosa biofilm. <i>PLoS ONE</i> , 2012 , 7, e3	43 <i>3</i> 7	28
48	Phenotypic differentiation of gastrointestinal microbes is reflected in their encoded metabolic repertoires. <i>Microbiome</i> , 2015 , 3, 55	16.6	27
47	Modeling the effects of commonly used drugs on human metabolism. FEBS Journal, 2015, 282, 297-317	5.7	25
46	Systematic genomic analysis reveals the complementary aerobic and anaerobic respiration capacities of the human gut microbiota. <i>Frontiers in Microbiology</i> , 2014 , 5, 674	5.7	25
45	Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression. <i>Scientific Reports</i> , 2017 , 7, 40863	4.9	24
44	Computational Modeling of Human Metabolism and Its Application to Systems Biomedicine. <i>Methods in Molecular Biology</i> , 2016 , 1386, 253-81	1.4	24
43	Model-based dietary optimization for late-stage, levodopa-treated, Parkinson's disease patients. <i>Npj Systems Biology and Applications</i> , 2016 , 2, 16013	5	24
42	An in silico re-design of the metabolism in Thermotoga maritima for increased biohydrogen production. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 12205-12218	6.7	23
41	Applying systems biology methods to the study of human physiology in extreme environments. <i>Extreme Physiology and Medicine</i> , 2013 , 2, 8		19
40	Inferring the metabolism of human orphan metabolites from their metabolic network context affirms human gluconokinase activity. <i>Biochemical Journal</i> , 2013 , 449, 427-35	3.8	18
39	A systems approach reveals distinct metabolic strategies among the NCI-60 cancer cell lines. <i>PLoS Computational Biology</i> , 2017 , 13, e1005698	5	17
38	Robust flux balance analysis of multiscale biochemical reaction networks. <i>BMC Bioinformatics</i> , 2013 , 14, 240	3.6	17
37	Comparative Genomic Analysis Reveals Novel Microcompartment-Associated Metabolic Pathways in the Human Gut Microbiome. <i>Frontiers in Genetics</i> , 2019 , 10, 636	4.5	16
36	Comparative evaluation of open source software for mapping between metabolite identifiers in metabolic network reconstructions: application to Recon 2. <i>Journal of Cheminformatics</i> , 2014 , 6, 2	8.6	16
35	A blood-based signature of cerebrospinal fluid Alatatus. Scientific Reports, 2019, 9, 4163	4.9	15
34	Comparative evaluation of atom mapping algorithms for balanced metabolic reactions: application to Recon 3D. <i>Journal of Cheminformatics</i> , 2017 , 9, 39	8.6	15
33	DistributedFBA.jl: high-level, high-performance flux balance analysis in Julia. <i>Bioinformatics</i> , 2017 , 33, 1421-1423	7.2	14

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32	Metabolic modelling reveals broad changes in gut microbial metabolism in inflammatory bowel disease patients with dysbiosis. <i>Npj Systems Biology and Applications</i> , 2021 , 7, 19	5	13
31	Conditions for duality between fluxes and concentrations in biochemical networks. <i>Journal of Theoretical Biology</i> , 2016 , 409, 1-10	2.3	13
30	When metabolism meets physiology: Harvey and Harvetta		12
29	Predicting gastrointestinal drug effects using contextualized metabolic models. <i>PLoS Computational Biology</i> , 2019 , 15, e1007100	5	11
28	Personalized modeling of the human gut microbiome reveals distinct bile acid deconjugation and biotransformation potential in healthy and IBD individuals		11
27	Dynamic genome-scale cell-specific metabolic models reveal novel inter-cellular and intra-cellular metabolic communications during ovarian follicle development. <i>BMC Bioinformatics</i> , 2019 , 20, 307	3.6	9
26	Consensus and conflict cards for metabolic pathway databases. BMC Systems Biology, 2013, 7, 50	3.5	9
25	Reply to "Challenges in modeling the human gut microbiome". <i>Nature Biotechnology</i> , 2018 , 36, 686-691	44.5	8
24	Arterio-venous metabolomics exploration reveals major changes across liver and intestine in the obese Yucatan minipig. <i>Scientific Reports</i> , 2019 , 9, 12527	4.9	7
23	Mass conserved elementary kinetics is sufficient for the existence of a non-equilibrium steady state concentration. <i>Journal of Theoretical Biology</i> , 2012 , 314, 173-81	2.3	7
22	Parkinson disease-associated alterations of the gut microbiome can invoke disease-relevant metabolic changes		7
21	Genome-scale methods converge on key mitochondrial genes for the survival of human cardiomyocytes in hypoxia. <i>Circulation: Cardiovascular Genetics</i> , 2014 , 7, 407-15		6
20	AGORA2: Large scale reconstruction of the microbiome highlights wide-spread drug-metabolising capa	cities	6
19	The Virtual Metabolic Human database: integrating human and gut microbiome metabolism with nutrition and disease		6
18	Integration of constraint-based modeling with fecal metabolomics reveals large deleterious effects of spp. on community butyrate production. <i>Gut Microbes</i> , 2021 , 13, 1-23	8.8	5
17	Contextualization procedure and modeling of monocyte specific TLR signaling. <i>PLoS ONE</i> , 2012 , 7, e499	7387	4
16	Rare genetic variants affecting urine metabolite levels link population variation to inborn errors of metabolism. <i>Nature Communications</i> , 2021 , 12, 964	17.4	4
15	Advances in constraint-based modelling of microbial communities. <i>Current Opinion in Systems Biology</i> , 2021 , 27, 100346	3.2	4

14	The Microbiome Modeling Toolbox: from microbial interactions to personalized microbial communities		3
13	Metabolic Network Analysis Reveals Altered Bile Acid Synthesis and Cholesterol Metabolism in Alzheimer Disease. SSRN Electronic Journal,	1	2
12	Identifying differences in bile acid pathways for cholesterol clearance in Alzheimer disease using metabolic networks of human brain regions		2
11	Methanogenic granule growth and development is a continual process characterized by distinct morphological features. <i>Journal of Environmental Management</i> , 2021 , 286, 112229	7.9	2
10	Dynamic flux balance analysis of whole-body metabolism for type 1 diabetes. <i>Nature Computational Science</i> , 2021 , 1, 348-361		2
9	Integration of a physiologically-based pharmacokinetic model with a whole-body, organ-resolved genome-scale model for characterization of ethanol and acetaldehyde metabolism. <i>PLoS Computational Biology</i> , 2021 , 17, e1009110	5	2
8	A Systems Biology Approach to the Evolution of Codon Use Pattern. <i>Nature Precedings</i> , 2011 ,		1
7	Early-Life Adversity Leaves Its Imprint on the Oral Microbiome for More Than 20 Years and Is Associated with Long-Term Immune Changes. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	1
6	Integrated Analyses of Microbiome and Longitudinal Metabolome Data Reveal Microbial-Host Interactions on Sulfur Metabolism in Parkinson's Disease. <i>SSRN Electronic Journal</i> ,	1	1
5	Systems biology of bacteria-host interactions 2016 , 113-137		1
4	Genome-Scale Metabolic Modeling of the Human Microbiome in the Era of Personalized Medicine. <i>Annual Review of Microbiology</i> , 2021 , 75, 199-222	17.5	1
3	DEMETER: Efficient simultaneous curation of genome-scale reconstructions guided by experimental data and refined gene annotations. <i>Bioinformatics</i> , 2021 ,	7.2	1
2	Genome-Scale Reconstruction, Modeling, and Simulation of E. coli?s Metabolic Network 2009 , 149-176		1
1	Bringing Genomes to Life: The Use of Genome-Scale In Silico Models 2007 , 14-36		