

Ines Thiele

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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

#	Paper	IF	Citations
121	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
120	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
119	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
118	Dynamic flux balance analysis of whole-body metabolism for type 1 diabetes. <i>Nature Computational Science</i> , 2021 , 1, 348-361		2
117	An international classification of inherited metabolic disorders (ICIMD). <i>Journal of Inherited Metabolic Disease</i> , 2021 , 44, 164-177	5.4	32
116	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
115	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
114	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
113	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
112	DEMETER: Efficient simultaneous curation of genome-scale reconstructions guided by experimental data and refined gene annotations. <i>Bioinformatics</i> , 2021 ,	7.2	1
111	Advances in constraint-based modelling of microbial communities. <i>Current Opinion in Systems Biology</i> , 2021 , 27, 100346	3.2	4
110	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
109	Metabolic Network Analysis Reveals Altered Bile Acid Synthesis and Metabolism in Alzheimer's Disease. <i>Cell Reports Medicine</i> , 2020 , 1, 100138	18	34
108	Personalized whole-body models integrate metabolism, physiology, and the gut microbiome. <i>Molecular Systems Biology</i> , 2020 , 16, e8982	12.2	43
107	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
106	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
105	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

104	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
103	A blood-based signature of cerebrospinal fluid A β status. <i>Scientific Reports</i> , 2019 , 9, 4163	4.9	15
102	Predicting gastrointestinal drug effects using contextualized metabolic models. <i>PLoS Computational Biology</i> , 2019 , 15, e1007100	5	11
101	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
100	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
99	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
98	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
97	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
96	The Microbiome Modeling Toolbox: from microbial interactions to personalized microbial communities. <i>Bioinformatics</i> , 2019 , 35, 2332-2334	7.2	45
95	Recon3D enables a three-dimensional view of gene variation in human metabolism. <i>Nature Biotechnology</i> , 2018 , 36, 272-281	44.5	283
94	Gut microbiota functions: metabolism of nutrients and other food components. <i>European Journal of Nutrition</i> , 2018 , 57, 1-24	5.2	857
93	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
92	Reply to "Challenges in modeling the human gut microbiome". <i>Nature Biotechnology</i> , 2018 , 36, 686-691	44.5	8
91	From Network Analysis to Functional Metabolic Modeling of the Human Gut Microbiota. <i>MSystems</i> , 2018 , 3,	7.6	60
90	Finding useful biomarkers for Parkinson's disease. <i>Science Translational Medicine</i> , 2018 , 10,	17.5	69
89	Modeling metabolism of the human gut microbiome. <i>Current Opinion in Biotechnology</i> , 2018 , 51, 90-96	11.4	79
88	Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression. <i>Scientific Reports</i> , 2017 , 7, 40863	4.9	24
87	DistributedFBA.jl: high-level, high-performance flux balance analysis in Julia. <i>Bioinformatics</i> , 2017 , 33, 1421-1423	7.2	14

86	Quantitative systems pharmacology and the personalized drug-microbiota-diet axis. <i>Current Opinion in Systems Biology</i> , 2017 , 4, 43-52	3.2	29
85	Leigh map: A novel computational diagnostic resource for mitochondrial disease. <i>Annals of Neurology</i> , 2017 , 81, 9-16	9.4	49
84	BacArena: Individual-based metabolic modeling of heterogeneous microbes in complex communities. <i>PLoS Computational Biology</i> , 2017 , 13, e1005544	5	116
83	A systems approach reveals distinct metabolic strategies among the NCI-60 cancer cell lines. <i>PLoS Computational Biology</i> , 2017 , 13, e1005698	5	17
82	CHRR: coordinate hit-and-run with rounding for uniform sampling of constraint-based models. <i>Bioinformatics</i> , 2017 , 33, 1741-1743	7.2	32
81	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
80	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
79	Comparative Genomic Analysis of the Human Gut Microbiome Reveals a Broad Distribution of Metabolic Pathways for the Degradation of Host-Synthesized Mucin Glycans and Utilization of Mucin-Derived Monosaccharides. <i>Frontiers in Genetics</i> , 2017 , 8, 111	4.5	45
78	ReconMap: an interactive visualization of human metabolism. <i>Bioinformatics</i> , 2017 , 33, 605-607	7.2	29
77	Computational Modeling of Human Metabolism and Its Application to Systems Biomedicine. <i>Methods in Molecular Biology</i> , 2016 , 1386, 253-81	1.4	24
76	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
75	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
74	MetaboTools: A Comprehensive Toolbox for Analysis of Genome-Scale Metabolic Models. <i>Frontiers in Physiology</i> , 2016 , 7, 327	4.6	31
73	Metabolomics enables precision medicine: "A White Paper, Community Perspective". <i>Metabolomics</i> , 2016 , 12, 149	4.7	327
72	Conditions for duality between fluxes and concentrations in biochemical networks. <i>Journal of Theoretical Biology</i> , 2016 , 409, 1-10	2.3	13
71	Systems biology of bacteria-host interactions 2016 , 113-137		1
70	Anoxic Conditions Promote Species-Specific Mutualism between Gut Microbes In Silico. <i>Applied and Environmental Microbiology</i> , 2015 , 81, 4049-61	4.8	71
69	Systematic prediction of health-relevant human-microbial co-metabolism through a computational framework. <i>Gut Microbes</i> , 2015 , 6, 120-30	8.8	76

68	Modeling the effects of commonly used drugs on human metabolism. <i>FEBS Journal</i> , 2015 , 282, 297-317	5.7	25
67	Prediction of intracellular metabolic states from extracellular metabolomic data. <i>Metabolomics</i> , 2015 , 11, 603-619	4.7	48
66	Systems biology of host-microbe metabolomics. <i>Wiley Interdisciplinary Reviews: Systems Biology and Medicine</i> , 2015 , 7, 195-219	6.6	64
65	Do genome-scale models need exact solvers or clearer standards?. <i>Molecular Systems Biology</i> , 2015 , 11, 831	12.2	41
64	Phenotypic differentiation of gastrointestinal microbes is reflected in their encoded metabolic repertoires. <i>Microbiome</i> , 2015 , 3, 55	16.6	27
63	Systematic genome assessment of B-vitamin biosynthesis suggests co-operation among gut microbes. <i>Frontiers in Genetics</i> , 2015 , 6, 148	4.5	313
62	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
61	Functional metabolic map of <i>Faecalibacterium prausnitzii</i> , a beneficial human gut microbe. <i>Journal of Bacteriology</i> , 2014 , 196, 3289-302	3.5	109
60	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
59	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
58	fastGapFill: efficient gap filling in metabolic networks. <i>Bioinformatics</i> , 2014 , 30, 2529-31	7.2	80
57	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
56	Applying systems biology methods to the study of human physiology in extreme environments. <i>Extreme Physiology and Medicine</i> , 2013 , 2, 8		19
55	Consensus and conflict cards for metabolic pathway databases. <i>BMC Systems Biology</i> , 2013 , 7, 50	3.5	9
54	Robust flux balance analysis of multiscale biochemical reaction networks. <i>BMC Bioinformatics</i> , 2013 , 14, 240	3.6	17
53	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
52	Systems-level characterization of a host-microbe metabolic symbiosis in the mammalian gut. <i>Gut Microbes</i> , 2013 , 4, 28-40	8.8	155
51	A community-driven global reconstruction of human metabolism. <i>Nature Biotechnology</i> , 2013 , 31, 419-25	14.5	746

50	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
49	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
48	Toward systems metabolic engineering in cyanobacteria: opportunities and bottlenecks. <i>Bioengineered</i> , 2013 , 4, 158-63	5.7	28
47	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
46	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
45	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
44	Detailing the optimality of photosynthesis in cyanobacteria through systems biology analysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 2678-83	11.5	231
43	A compendium of inborn errors of metabolism mapped onto the human metabolic network. <i>Molecular BioSystems</i> , 2012 , 8, 2545-58		55
42	An in silico re-design of the metabolism in <i>Thermotoga maritima</i> for increased biohydrogen production. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 12205-12218	6.7	23
41	Quantitative assignment of reaction directionality in a multicompartamental human metabolic reconstruction. <i>Biophysical Journal</i> , 2012 , 102, 1703-11	2.9	34
40	Multiscale modeling of metabolism and macromolecular synthesis in <i>E. coli</i> and its application to the evolution of codon usage. <i>PLoS ONE</i> , 2012 , 7, e45635	3.7	87
39	A systems biology approach to drug targets in <i>Pseudomonas aeruginosa</i> biofilm. <i>PLoS ONE</i> , 2012 , 7, e34337	3.7	28
38	Contextualization procedure and modeling of monocyte specific TLR signaling. <i>PLoS ONE</i> , 2012 , 7, e49978	3.7	4
37	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
36	A Systems Biology Approach to the Evolution of Codon Use Pattern. <i>Nature Precedings</i> , 2011 ,		1
35	The human metabolic reconstruction Recon 1 directs hypotheses of novel human metabolic functions. <i>BMC Systems Biology</i> , 2011 , 5, 155	3.5	55
34	A community effort towards a knowledge-base and mathematical model of the human pathogen <i>Salmonella Typhimurium</i> LT2. <i>BMC Systems Biology</i> , 2011 , 5, 8	3.5	105
33	von Bertalanffy 1.0: a COBRA toolbox extension to thermodynamically constrain metabolic models. <i>Bioinformatics</i> , 2011 , 27, 142-3	7.2	55

32	rBioNet: A COBRA toolbox extension for reconstructing high-quality biochemical networks. <i>Bioinformatics</i> , 2011 , 27, 2009-10	7.2	50
31	What is flux balance analysis?. <i>Nature Biotechnology</i> , 2010 , 28, 245-8	44.5	2292
30	A protocol for generating a high-quality genome-scale metabolic reconstruction. <i>Nature Protocols</i> , 2010 , 5, 93-121	18.8	1156
29	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
28	Computationally efficient flux variability analysis. <i>BMC Bioinformatics</i> , 2010 , 11, 489	3.6	179
27	A detailed genome-wide reconstruction of mouse metabolism based on human Recon 1. <i>BMC Systems Biology</i> , 2010 , 4, 140	3.5	114
26	Integrated stoichiometric, thermodynamic and kinetic modelling of steady state metabolism. <i>Journal of Theoretical Biology</i> , 2010 , 264, 683-92	2.3	48
25	Identification of potential pathway mediation targets in Toll-like receptor signaling. <i>PLoS Computational Biology</i> , 2009 , 5, e1000292	5	52
24	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
23	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
22	Metabolic network analysis integrated with transcript verification for sequenced genomes. <i>Nature Methods</i> , 2009 , 6, 589-92	21.6	80
21	Reconstruction of biochemical networks in microorganisms. <i>Nature Reviews Microbiology</i> , 2009 , 7, 129-43	2.2	699
20	Three-dimensional structural view of the central metabolic network of Thermotoga maritima. <i>Science</i> , 2009 , 325, 1544-9	33.3	148
19	Genome-Scale Reconstruction, Modeling, and Simulation of E. coli's Metabolic Network 2009 , 149-176		1
18	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
17	Estimation of the number of extreme pathways for metabolic networks. <i>BMC Bioinformatics</i> , 2007 , 8, 363	3.6	38
16	Global reconstruction of the human metabolic network based on genomic and bibliomic data. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 1777-82	11.5	1060
15	Bringing Genomes to Life: The Use of Genome-Scale In Silico Models 2007 , 14-36		

14	Candidate states of <i>Helicobacter pylori</i> 's genome-scale metabolic network upon application of "loop law" thermodynamic constraints. <i>Biophysical Journal</i> , 2006 , 90, 3919-28	2.9	41
13	Towards multidimensional genome annotation. <i>Nature Reviews Genetics</i> , 2006 , 7, 130-41	30.1	285
12	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
11	Expanded metabolic reconstruction of <i>Helicobacter pylori</i> (JIT341 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
10	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
9	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
8	Metabolic Network Analysis Reveals Altered Bile Acid Synthesis and Cholesterol Metabolism in Alzheimer's Disease. <i>SSRN Electronic Journal</i> ,	1	2
7	Parkinson's disease-associated alterations of the gut microbiome can invoke disease-relevant metabolic changes		7
6	Identifying differences in bile acid pathways for cholesterol clearance in Alzheimer's disease using metabolic networks of human brain regions		2
5	AGORA2: Large scale reconstruction of the microbiome highlights wide-spread drug-metabolising capacities		6
4	Personalized modeling of the human gut microbiome reveals distinct bile acid deconjugation and biotransformation potential in healthy and IBD individuals		11
3	When metabolism meets physiology: Harvey and Harvatta		12
2	The Microbiome Modeling Toolbox: from microbial interactions to personalized microbial communities		3
1	The Virtual Metabolic Human database: integrating human and gut microbiome metabolism with nutrition and disease		6