

Ines Thiele

List of Publications by Year in descending order

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Version: 2024-02-01

121
papers

23,122
citations

26630

56
h-index

20358

116
g-index

139
all docs

139
docs citations

139
times ranked

20825
citing authors

#	ARTICLE	IF	CITATIONS
1	What is flux balance analysis?. Nature Biotechnology, 2010, 28, 245-248.	17.5	3,233
2	The Subsystems Approach to Genome Annotation and its Use in the Project to Annotate 1000 Genomes. Nucleic Acids Research, 2005, 33, 5691-5702.	14.5	1,806
3	Gut microbiota functions: metabolism of nutrients and other food components. European Journal of Nutrition, 2018, 57, 1-24.	3.9	1,608
4	A protocol for generating a high-quality genome-scale metabolic reconstruction. Nature Protocols, 2010, 5, 93-121.	12.0	1,568
5	Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox v2.0. Nature Protocols, 2011, 6, 1290-1307.	12.0	1,408
6	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, 1777-1782.	7.1	1,259
7	A community-driven global reconstruction of human metabolism. Nature Biotechnology, 2013, 31, 419-425.	17.5	920
8	Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v.3.0. Nature Protocols, 2019, 14, 639-702.	12.0	833
9	Reconstruction of biochemical networks in microorganisms. Nature Reviews Microbiology, 2009, 7, 129-143.	28.6	797
10	Generation of genome-scale metabolic reconstructions for 773 members of the human gut microbiota. Nature Biotechnology, 2017, 35, 81-89.	17.5	629
11	Systematic genome assessment of B-vitamin biosynthesis suggests co-operation among gut microbes. Frontiers in Genetics, 2015, 6, 148.	2.3	565
12	Recon3D enables a three-dimensional view of gene variation in human metabolism. Nature Biotechnology, 2018, 36, 272-281.	17.5	520
13	Metabolomics enables precision medicine: "A White Paper, Community Perspective". Metabolomics, 2016, 12, 149.	3.0	434
14	Towards multidimensional genome annotation. Nature Reviews Genetics, 2006, 7, 130-141.	16.3	321
15	Computationally efficient flux variability analysis. BMC Bioinformatics, 2010, 11, 489.	2.6	267
16	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, 2678-2683.	7.1	266
17	The Virtual Metabolic Human database: integrating human and gut microbiome metabolism with nutrition and disease. Nucleic Acids Research, 2019, 47, D614-D624.	14.5	257
18	A genome-scale metabolic reconstruction of Pseudomonas putida KT2440: iJN746 as a cell factory. BMC Systems Biology, 2008, 2, 79.	3.0	222

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19	Expanded Metabolic Reconstruction of <i>Helicobacter pylori</i> (i IT341 GSM/GPR): an In Silico Genome-Scale Characterization of Single- and Double-Deletion Mutants. <i>Journal of Bacteriology</i> , 2005, 187, 5818-5830.	2.2	220
20	Systematic assessment of secondary bile acid metabolism in gut microbes reveals distinct metabolic capabilities in inflammatory bowel disease. <i>Microbiome</i> , 2019, 7, 75.	11.1	215
21	Systems-level characterization of a host-microbe metabolic symbiosis in the mammalian gut. <i>Gut Microbes</i> , 2013, 4, 28-40.	9.8	210
22	BacArena: Individual-based metabolic modeling of heterogeneous microbes in complex communities. <i>PLoS Computational Biology</i> , 2017, 13, e1005544.	3.2	185
23	Three-Dimensional Structural View of the Central Metabolic Network of <i>Thermotoga maritima</i> . <i>Science</i> , 2009, 325, 1544-1549.	12.6	176
24	Functional Metabolic Map of <i>Faecalibacterium prausnitzii</i> , a Beneficial Human Gut Microbe. <i>Journal of Bacteriology</i> , 2014, 196, 3289-3302.	2.2	173
25	Genome-Scale Reconstruction of <i>Escherichia coli</i> 's Transcriptional and Translational Machinery: A Knowledge Base, Its Mathematical Formulation, and Its Functional Characterization. <i>PLoS Computational Biology</i> , 2009, 5, e1000312.	3.2	161
26	A detailed genome-wide reconstruction of mouse metabolism based on human Recon 1. <i>BMC Systems Biology</i> , 2010, 4, 140.	3.0	147
27	An international classification of inherited metabolic disorders (<scp>ICIMD</scp>). <i>Journal of Inherited Metabolic Disease</i> , 2021, 44, 164-177.	3.6	146
28	Association of Altered Liver Enzymes With Alzheimer Disease Diagnosis, Cognition, Neuroimaging Measures, and Cerebrospinal Fluid Biomarkers. <i>JAMA Network Open</i> , 2019, 2, e197978.	5.9	142
29	Candidate Metabolic Network States in Human Mitochondria. <i>Journal of Biological Chemistry</i> , 2005, 280, 11683-11695.	3.4	138
30	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.	3.0	128
31	Finding useful biomarkers for Parkinsonâ€™s disease. <i>Science Translational Medicine</i> , 2018, 10, .	12.4	125
32	Modeling metabolism of the human gut microbiome. <i>Current Opinion in Biotechnology</i> , 2018, 51, 90-96.	6.6	122
33	Personalized wholeâ€body models integrate metabolism, physiology, and the gut microbiome. <i>Molecular Systems Biology</i> , 2020, 16, e8982.	7.2	122
34	Parkinsonâ€™s disease-associated alterations of the gut microbiome predict disease-relevant changes in metabolic functions. <i>BMC Biology</i> , 2020, 18, 62.	3.8	122
35	<scp>fast</scp>G<scp>ap</scp>F<scp>ill</scp>: efficient gap filling in metabolic networks. <i>Bioinformatics</i> , 2014, 30, 2529-2531.	4.1	105
36	Integrated Analyses of Microbiome and Longitudinal Metabolome Data Reveal Microbial-Host Interactions on Sulfur Metabolism in Parkinsonâ€™s Disease. <i>Cell Reports</i> , 2019, 29, 1767-1777.e8.	6.4	102

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37	The Microbiome Modeling Toolbox: from microbial interactions to personalized microbial communities. <i>Bioinformatics</i> , 2019, 35, 2332-2334.	4.1	102
38	Metabolic Network Analysis Reveals Altered Bile Acid Synthesis and Metabolism in Alzheimer's Disease. <i>Cell Reports Medicine</i> , 2020, 1, 100138.	6.5	102
39	Anoxic Conditions Promote Species-Specific Mutualism between Gut Microbes <i>In Silico</i> . <i>Applied and Environmental Microbiology</i> , 2015, 81, 4049-4061.	3.1	101
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.	2.5	100
41	A systems biology approach to studying the role of microbes in human health. <i>Current Opinion in Biotechnology</i> , 2013, 24, 4-12.	6.6	100
42	Systematic prediction of health-relevant human-microbial co-metabolism through a computational framework. <i>Gut Microbes</i> , 2015, 6, 120-130.	9.8	97
43	The gut microbial metabolite formate exacerbates colorectal cancer progression. <i>Nature Metabolism</i> , 2022, 4, 458-475.	11.9	97
44	Metabolic network analysis integrated with transcript verification for sequenced genomes. <i>Nature Methods</i> , 2009, 6, 589-592.	19.0	83
45	Systems biology of host-microbe metabolomics. <i>Wiley Interdisciplinary Reviews: Systems Biology and Medicine</i> , 2015, 7, 195-219.	6.6	80
46	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.	2.3	79
47	From Network Analysis to Functional Metabolic Modeling of the Human Gut Microbiota. <i>MSystems</i> , 2018, 3, .	3.8	77
48	Membrane transporters in a human genome-scale metabolic knowledgebase and their implications for disease. <i>Frontiers in Physiology</i> , 2014, 5, 91.	2.8	76
49	Quantitative assignment of reaction directionality in constraint-based models of metabolism: Application to <i>Escherichia coli</i> . <i>Biophysical Chemistry</i> , 2009, 145, 47-56.	2.8	75
50	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, 1183-1198.	3.7	74
51	A compendium of inborn errors of metabolism mapped onto the human metabolic network. <i>Molecular BioSystems</i> , 2012, 8, 2545.	2.9	69
52	Do genome-scale models need exact solvers or clearer standards?. <i>Molecular Systems Biology</i> , 2015, 11, 831.	7.2	68
53	Leigh map: A novel computational diagnostic resource for mitochondrial disease. <i>Annals of Neurology</i> , 2017, 81, 9-16.	5.3	68
54	CHRR: coordinate hit-and-run with rounding for uniform sampling of constraint-based models. <i>Bioinformatics</i> , 2017, 33, 1741-1743.	4.1	67

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55	Prediction of intracellular metabolic states from extracellular metabolomic data. <i>Metabolomics</i> , 2015, 11, 603-619.	3.0	66
56	Predicting the impact of diet and enzymopathies on human small intestinal epithelial cells. <i>Human Molecular Genetics</i> , 2013, 22, 2705-2722.	2.9	62
57	The human metabolic reconstruction Recon 1 directs hypotheses of novel human metabolic functions. <i>BMC Systems Biology</i> , 2011, 5, 155.	3.0	60
58	von Bertalanffy 1.0: a COBRA toolbox extension to thermodynamically constrain metabolic models. <i>Bioinformatics</i> , 2011, 27, 142-143.	4.1	59
59	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.	3.0	59
60	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.	6.4	59
61	Functional Characterization of Alternate Optimal Solutions of Escherichia coli's Transcriptional and Translational Machinery. <i>Biophysical Journal</i> , 2010, 98, 2072-2081.	0.5	58
62	Genomic Analysis of the Human Gut Microbiome Suggests Novel Enzymes Involved in Quinone Biosynthesis. <i>Frontiers in Microbiology</i> , 2016, 7, 128.	3.5	56
63	Integrated stoichiometric, thermodynamic and kinetic modelling of steady state metabolism. <i>Journal of Theoretical Biology</i> , 2010, 264, 683-692.	1.7	55
64	rBioNet: A COBRA toolbox extension for reconstructing high-quality biochemical networks. <i>Bioinformatics</i> , 2011, 27, 2009-2010.	4.1	55
65	Reconstruction annotation jamborees: a community approach to systems biology. <i>Molecular Systems Biology</i> , 2010, 6, 361.	7.2	54
66	Identification of Potential Pathway Mediation Targets in Toll-like Receptor Signaling. <i>PLoS Computational Biology</i> , 2009, 5, e1000292.	3.2	52
67	ReconMap: an interactive visualization of human metabolism. <i>Bioinformatics</i> , 2017, 33, 605-607.	4.1	52
68	Candidate States of Helicobacter pylori's Genome-Scale Metabolic Network upon Application of Loop Law Thermodynamic Constraints. <i>Biophysical Journal</i> , 2006, 90, 3919-3928.	0.5	45
69	Systematic genomic analysis reveals the complementary aerobic and anaerobic respiration capacities of the human gut microbiota. <i>Frontiers in Microbiology</i> , 2014, 5, 674.	3.5	45
70	Estimation of the number of extreme pathways for metabolic networks. <i>BMC Bioinformatics</i> , 2007, 8, 363.	2.6	44
71	Quantitative Assignment of Reaction Directionality in a Multicompartmental Human Metabolic Reconstruction. <i>Biophysical Journal</i> , 2012, 102, 1703-1711.	0.5	44
72	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.	3.0	43

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73	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, 111-120.	2.3	42
74	Phenotypic differentiation of gastrointestinal microbes is reflected in their encoded metabolic repertoires. <i>Microbiome</i> , 2015, 3, 55.	11.1	41
75	MetaboTools: A Comprehensive Toolbox for Analysis of Genome-Scale Metabolic Models. <i>Frontiers in Physiology</i> , 2016, 7, 327.	2.8	41
76	A Systems Biology Approach to Drug Targets in <i>Pseudomonas aeruginosa</i> Biofilm. <i>PLoS ONE</i> , 2012, 7, e34337.	2.5	41
77	Quantitative systems pharmacology and the personalized drug-microbiota-diet axis. <i>Current Opinion in Systems Biology</i> , 2017, 4, 43-52.	2.6	37
78	Model-based dietary optimization for late-stage, levodopa-treated, Parkinson's disease patients. <i>Npj Systems Biology and Applications</i> , 2016, 2, 16013.	3.0	34
79	Genome-Scale Metabolic Modeling of the Human Microbiome in the Era of Personalized Medicine. <i>Annual Review of Microbiology</i> , 2021, 75, 199-222.	7.3	33
80	Computational Modeling of Human Metabolism and Its Application to Systems Biomedicine. <i>Methods in Molecular Biology</i> , 2016, 1386, 253-281.	0.9	32
81	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.	7.1	31
82	Toward systems metabolic engineering in cyanobacteria. <i>Bioengineered</i> , 2013, 4, 158-163.	3.2	31
83	Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression. <i>Scientific Reports</i> , 2017, 7, 40863.	3.3	30
84	Modeling the effects of commonly used drugs on human metabolism. <i>FEBS Journal</i> , 2015, 282, 297-317.	4.7	29
85	Advances in constraint-based modelling of microbial communities. <i>Current Opinion in Systems Biology</i> , 2021, 27, 100346.	2.6	28
86	Applying systems biology methods to the study of human physiology in extreme environments. <i>Extreme Physiology and Medicine</i> , 2013, 2, 8.	2.5	26
87	DistributedFBA.jl: high-level, high-performance flux balance analysis in Julia. <i>Bioinformatics</i> , 2017, 33, 1421-1423.	4.1	25
88	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.	6.1	23
89	Comparative evaluation of atom mapping algorithms for balanced metabolic reactions: application to Recon 3D. <i>Journal of Cheminformatics</i> , 2017, 9, 39.	6.1	23
90	Comparative Genomic Analysis Reveals Novel Microcompartment-Associated Metabolic Pathways in the Human Gut Microbiome. <i>Frontiers in Genetics</i> , 2019, 10, 636.	2.3	22

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91	Integration of constraint-based modeling with fecal metabolomics reveals large deleterious effects of <i>Fusobacterium</i> spp. on community butyrate production. <i>Gut Microbes</i> , 2021, 13, 1-23.	9.8	22
92	Robust flux balance analysis of multiscale biochemical reaction networks. <i>BMC Bioinformatics</i> , 2013, 14, 240.	2.6	21
93	Inferring the metabolism of human orphan metabolites from their metabolic network context affirms human gluconokinase activity. <i>Biochemical Journal</i> , 2013, 449, 427-435.	3.7	21
94	A blood-based signature of cerebrospinal fluid A β 1-42 status. <i>Scientific Reports</i> , 2019, 9, 4163.	3.3	21
95	Rare genetic variants affecting urine metabolite levels link population variation to inborn errors of metabolism. <i>Nature Communications</i> , 2021, 12, 964.	12.8	20
96	A systems approach reveals distinct metabolic strategies among the NCI-60 cancer cell lines. <i>PLoS Computational Biology</i> , 2017, 13, e1005698.	3.2	19
97	Microbiome Modelling Toolbox 2.0: efficient, tractable modelling of microbiome communities. <i>Bioinformatics</i> , 2022, 38, 2367-2368.	4.1	18
98	Predicting gastrointestinal drug effects using contextualized metabolic models. <i>PLoS Computational Biology</i> , 2019, 15, e1007100.	3.2	16
99	Conditions for duality between fluxes and concentrations in biochemical networks. <i>Journal of Theoretical Biology</i> , 2016, 409, 1-10.	1.7	15
100	Arterio-venous metabolomics exploration reveals major changes across liver and intestine in the obese Yucatan minipig. <i>Scientific Reports</i> , 2019, 9, 12527.	3.3	14
101	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.	2.6	13
102	DEMETER: efficient simultaneous curation of genome-scale reconstructions guided by experimental data and refined gene annotations. <i>Bioinformatics</i> , 2021, 37, 3974-3975.	4.1	13
103	Reply to "Challenges in modeling the human gut microbiome". <i>Nature Biotechnology</i> , 2018, 36, 686-691.	17.5	12
104	Dynamic flux balance analysis of whole-body metabolism for type 1 diabetes. <i>Nature Computational Science</i> , 2021, 1, 348-361.	8.0	11
105	NMR Metabolomics Reveal Urine Markers of Microbiome Diversity and Identify Benzoate Metabolism as a Mediator between High Microbial Alpha Diversity and Metabolic Health. <i>Metabolites</i> , 2022, 12, 308.	2.9	11
106	Consensus and conflict cards for metabolic pathway databases. <i>BMC Systems Biology</i> , 2013, 7, 50.	3.0	10
107	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.	3.2	9
108	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, 12682.	4.1	8

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109	Mass conserved elementary kinetics is sufficient for the existence of a non-equilibrium steady state concentration. <i>Journal of Theoretical Biology</i> , 2012, 314, 173-181.	1.7	7
110	Genome-Scale Methods Converge on Key Mitochondrial Genes for the Survival of Human Cardiomyocytes in Hypoxia. <i>Circulation: Cardiovascular Genetics</i> , 2014, 7, 407-415.	5.1	7
111	Editorial: The Human Gutome: Nutrigenomics of Host-Microbiome Interactions. <i>Frontiers in Genetics</i> , 2016, 7, 158.	2.3	7
112	Methanogenic granule growth and development is a continual process characterized by distinct morphological features. <i>Journal of Environmental Management</i> , 2021, 286, 112229.	7.8	7
113	Metabolic Network Analysis Reveals Altered Bile Acid Synthesis and Cholesterol Metabolism in Alzheimer's Disease. <i>SSRN Electronic Journal</i> , 0, , .	0.4	6
114	Contextualization Procedure and Modeling of Monocyte Specific TLR Signaling. <i>PLoS ONE</i> , 2012, 7, e49978.	2.5	5
115	A Systems Biology Approach to the Evolution of Codon Use Pattern. <i>Nature Precedings</i> , 2011, , .	0.1	2
116	Integrated Analyses of Microbiome and Longitudinal Metabolome Data Reveal Microbial-Host Interactions on Sulfur Metabolism in Parkinson's Disease. <i>SSRN Electronic Journal</i> , 0, , .	0.4	2
117	Genome-Scale Reconstruction, Modeling, and Simulation of <i>E. coli</i> 's Metabolic Network. , 2009, , 149-176.		1
118	Principles of Systems Biology, No. 14. <i>Cell Systems</i> , 2017, 4, 140-143.	6.2	0
119	Metabolic Systems Biology. , 2017, , 1-23.		0
120	Integrated in Vitro and in Silico Modelling Delineates the Molecular Effects of a Symbiotic Regimen on Colorectal Cancer-Derived Cells. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
121	Bringing Genomes to Life: The Use of Genome-Scale In Silico Models. , 2007, , 14-36.		0