

# 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	Microbiome Modelling Toolbox 2.0: efficient, tractable modelling of microbiome communities. <i>Bioinformatics</i> , 2022, 38, 2367-2368.	4.1	18
2	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
3	The gut microbial metabolite formate exacerbates colorectal cancer progression. <i>Nature Metabolism</i> , 2022, 4, 458-475.	11.9	97
4	An international classification of inherited metabolic disorders (<sc>ICIMD</sc>). <i>Journal of Inherited Metabolic Disease</i> , 2021, 44, 164-177.	3.6	146
5	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
6	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
7	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
8	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
9	Dynamic flux balance analysis of whole-body metabolism for type 1 diabetes. <i>Nature Computational Science</i> , 2021, 1, 348-361.	8.0	11
10	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
11	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
12	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
13	Advances in constraint-based modelling of microbial communities. <i>Current Opinion in Systems Biology</i> , 2021, 27, 100346.	2.6	28
14	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
15	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
16	Personalized whole-body models integrate metabolism, physiology, and the gut microbiome. <i>Molecular Systems Biology</i> , 2020, 16, e8982.	7.2	122
17	Parkinson'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
18	Predicting gastrointestinal drug effects using contextualized metabolic models. <i>PLoS Computational Biology</i> , 2019, 15, e1007100.	3.2	16

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19	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
20	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
21	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.	6.4	102
22	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
23	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
24	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
25	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
26	A blood-based signature of cerebrospinal fluid A $\beta$ 42 status. <i>Scientific Reports</i> , 2019, 9, 4163.	3.3	21
27	Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v.3.0. <i>Nature Protocols</i> , 2019, 14, 639-702.	12.0	833
28	The Virtual Metabolic Human database: integrating human and gut microbiome metabolism with nutrition and disease. <i>Nucleic Acids Research</i> , 2019, 47, D614-D624.	14.5	257
29	The Microbiome Modeling Toolbox: from microbial interactions to personalized microbial communities. <i>Bioinformatics</i> , 2019, 35, 2332-2334.	4.1	102
30	Recon3D enables a three-dimensional view of gene variation in human metabolism. <i>Nature Biotechnology</i> , 2018, 36, 272-281.	17.5	520
31	Gut microbiota functions: metabolism of nutrients and other food components. <i>European Journal of Nutrition</i> , 2018, 57, 1-24.	3.9	1,608
32	Modeling metabolism of the human gut microbiome. <i>Current Opinion in Biotechnology</i> , 2018, 51, 90-96.	6.6	122
33	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
34	Reply to "Challenges in modeling the human gut microbiome". <i>Nature Biotechnology</i> , 2018, 36, 686-691.	17.5	12
35	From Network Analysis to Functional Metabolic Modeling of the Human Gut Microbiota. <i>MSystems</i> , 2018, 3, .	3.8	77
36	Finding useful biomarkers for Parkinson's disease. <i>Science Translational Medicine</i> , 2018, 10, .	12.4	125

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37	ReconMap: an interactive visualization of human metabolism. <i>Bioinformatics</i> , 2017, 33, 605-607.	4.1	52
38	Principles of Systems Biology, No. 14. <i>Cell Systems</i> , 2017, 4, 140-143.	6.2	0
39	Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression. <i>Scientific Reports</i> , 2017, 7, 40863.	3.3	30
40	DistributedFBA.jl: high-level, high-performance flux balance analysis in Julia. <i>Bioinformatics</i> , 2017, 33, 1421-1423.	4.1	25
41	Quantitative systems pharmacology and the personalized drug–microbiota–diet axis. <i>Current Opinion in Systems Biology</i> , 2017, 4, 43-52.	2.6	37
42	Leigh map: A novel computational diagnostic resource for mitochondrial disease. <i>Annals of Neurology</i> , 2017, 81, 9-16.	5.3	68
43	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
44	Generation of genome-scale metabolic reconstructions for 773 members of the human gut microbiota. <i>Nature Biotechnology</i> , 2017, 35, 81-89.	17.5	629
45	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
46	BacArena: Individual-based metabolic modeling of heterogeneous microbes in complex communities. <i>PLoS Computational Biology</i> , 2017, 13, e1005544.	3.2	185
47	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
48	CHRR: coordinate hit-and-run with rounding for uniform sampling of constraint-based models. <i>Bioinformatics</i> , 2017, 33, 1741-1743.	4.1	67
49	<i>Metabolic Systems Biology</i> , 2017, , 1-23.		0
50	Editorial: The Human Gutome: Nutrigenomics of Host-Microbiome Interactions. <i>Frontiers in Genetics</i> , 2016, 7, 158.	2.3	7
51	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
52	MetaboTools: A Comprehensive Toolbox for Analysis of Genome-Scale Metabolic Models. <i>Frontiers in Physiology</i> , 2016, 7, 327.	2.8	41
53	Metabolomics enables precision medicine: –A White Paper, Community Perspective–. <i>Metabolomics</i> , 2016, 12, 149.	3.0	434
54	Conditions for duality between fluxes and concentrations in biochemical networks. <i>Journal of Theoretical Biology</i> , 2016, 409, 1-10.	1.7	15

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55	Computational Modeling of Human Metabolism and Its Application to Systems Biomedicine. <i>Methods in Molecular Biology</i> , 2016, 1386, 253-281.	0.9	32
56	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
57	Systems biology of host-microbe metabolomics. <i>Wiley Interdisciplinary Reviews: Systems Biology and Medicine</i> , 2015, 7, 195-219.	6.6	80
58	Do genome-scale models need exact solvers or clearer standards?. <i>Molecular Systems Biology</i> , 2015, 11, 831.	7.2	68
59	Phenotypic differentiation of gastrointestinal microbes is reflected in their encoded metabolic repertoires. <i>Microbiome</i> , 2015, 3, 55.	11.1	41
60	Systematic genome assessment of B-vitamin biosynthesis suggests co-operation among gut microbes. <i>Frontiers in Genetics</i> , 2015, 6, 148.	2.3	565
61	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
62	Systematic prediction of health-relevant human-microbial co-metabolism through a computational framework. <i>Gut Microbes</i> , 2015, 6, 120-130.	9.8	97
63	Modeling the effects of commonly used drugs on human metabolism. <i>FEBS Journal</i> , 2015, 282, 297-317.	4.7	29
64	Prediction of intracellular metabolic states from extracellular metabolomic data. <i>Metabolomics</i> , 2015, 11, 603-619.	3.0	66
65	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
66	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
67	FAST-GAP: efficient gap filling in metabolic networks. <i>Bioinformatics</i> , 2014, 30, 2529-2531.	4.1	105
68	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
69	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
70	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
71	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
72	Consensus and conflict cards for metabolic pathway databases. <i>BMC Systems Biology</i> , 2013, 7, 50.	3.0	10

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73	Robust flux balance analysis of multiscale biochemical reaction networks. BMC Bioinformatics, 2013, 14, 240.	2.6	21
74	A systems biology approach to studying the role of microbes in human health. Current Opinion in Biotechnology, 2013, 24, 4-12.	6.6	100
75	Systems-level characterization of a host-microbe metabolic symbiosis in the mammalian gut. Gut Microbes, 2013, 4, 28-40.	9.8	210
76	A community-driven global reconstruction of human metabolism. Nature Biotechnology, 2013, 31, 419-425.	17.5	920
77	Inferring the metabolism of human orphan metabolites from their metabolic network context affirms human gluconokinase activity. Biochemical Journal, 2013, 449, 427-435.	3.7	21
78	Predicting the impact of diet and enzymopathies on human small intestinal epithelial cells. Human Molecular Genetics, 2013, 22, 2705-2722.	2.9	62
79	Toward systems metabolic engineering in cyanobacteria. Bioengineered, 2013, 4, 158-163.	3.2	31
80	Mass conserved elementary kinetics is sufficient for the existence of a non-equilibrium steady state concentration. Journal of Theoretical Biology, 2012, 314, 173-181.	1.7	7
81	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
82	A compendium of inborn errors of metabolism mapped onto the human metabolic network. Molecular BioSystems, 2012, 8, 2545.	2.9	69
83	An in silico re-design of the metabolism in Thermotoga maritima for increased biohydrogen production. International Journal of Hydrogen Energy, 2012, 37, 12205-12218.	7.1	31
84	Quantitative Assignment of Reaction Directionality in a Multicompartmental Human Metabolic Reconstruction. Biophysical Journal, 2012, 102, 1703-1711.	0.5	44
85	Multiscale Modeling of Metabolism and Macromolecular Synthesis in E. coli and Its Application to the Evolution of Codon Usage. PLoS ONE, 2012, 7, e45635.	2.5	100
86	Intracellular metabolite profiling of platelets: Evaluation of extraction processes and chromatographic strategies. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2012, 898, 111-120.	2.3	42
87	Monitoring metabolites consumption and secretion in cultured cells using ultra-performance liquid chromatography quadrupole-time of flight mass spectrometry (UPLC-Q-ToF-MS). Analytical and Bioanalytical Chemistry, 2012, 402, 1183-1198.	3.7	74
88	A Systems Biology Approach to Drug Targets in Pseudomonas aeruginosa Biofilm. PLoS ONE, 2012, 7, e34337.	2.5	41
89	Contextualization Procedure and Modeling of Monocyte Specific TLR Signaling. PLoS ONE, 2012, 7, e49978.	2.5	5
90	Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox v2.0. Nature Protocols, 2011, 6, 1290-1307.	12.0	1,408

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91	A Systems Biology Approach to the Evolution of Codon Use Pattern. Nature Precedings, 2011, , .	0.1	2
92	The human metabolic reconstruction Recon 1 directs hypotheses of novel human metabolic functions. BMC Systems Biology, 2011, 5, 155.	3.0	60
93	A community effort towards a knowledge-base and mathematical model of the human pathogen Salmonella Typhimurium LT2. BMC Systems Biology, 2011, 5, 8.	3.0	128
94	von Bertalanffy 1.0: a COBRA toolbox extension to thermodynamically constrain metabolic models. Bioinformatics, 2011, 27, 142-143.	4.1	59
95	rBioNet: A COBRA toolbox extension for reconstructing high-quality biochemical networks. Bioinformatics, 2011, 27, 2009-2010.	4.1	55
96	Computationally efficient flux variability analysis. BMC Bioinformatics, 2010, 11, 489.	2.6	267
97	A detailed genome-wide reconstruction of mouse metabolism based on human Recon 1. BMC Systems Biology, 2010, 4, 140.	3.0	147
98	Integrated stoichiometric, thermodynamic and kinetic modelling of steady state metabolism. Journal of Theoretical Biology, 2010, 264, 683-692.	1.7	55
99	What is flux balance analysis?. Nature Biotechnology, 2010, 28, 245-248.	17.5	3,233
100	A protocol for generating a high-quality genome-scale metabolic reconstruction. Nature Protocols, 2010, 5, 93-121.	12.0	1,568
101	Functional Characterization of Alternate Optimal Solutions of Escherichia coli's Transcriptional and Translational Machinery. Biophysical Journal, 2010, 98, 2072-2081.	0.5	58
102	Reconstruction annotation jamborees: a community approach to systems biology. Molecular Systems Biology, 2010, 6, 361.	7.2	54
103	Identification of Potential Pathway Mediation Targets in Toll-like Receptor Signaling. PLoS Computational Biology, 2009, 5, e1000292.	3.2	52
104	Genome-Scale Reconstruction of Escherichia coli's Transcriptional and Translational Machinery: A Knowledge Base, Its Mathematical Formulation, and Its Functional Characterization. PLoS Computational Biology, 2009, 5, e1000312.	3.2	161
105	Quantitative assignment of reaction directionality in constraint-based models of metabolism: Application to Escherichia coli. Biophysical Chemistry, 2009, 145, 47-56.	2.8	75
106	Metabolic network analysis integrated with transcript verification for sequenced genomes. Nature Methods, 2009, 6, 589-592.	19.0	83
107	Reconstruction of biochemical networks in microorganisms. Nature Reviews Microbiology, 2009, 7, 129-143.	28.6	797
108	Three-Dimensional Structural View of the Central Metabolic Network of Thermotoga maritima. Science, 2009, 325, 1544-1549.	12.6	176

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109	Genome-Scale Reconstruction, Modeling, and Simulation of <i>E. coli</i> 's Metabolic Network. , 2009, , 149-176.		1
110	A genome-scale metabolic reconstruction of <i>Pseudomonas putida</i> KT2440: iJN746 as a cell factory. <i>BMC Systems Biology</i> , 2008, 2, 79.	3.0	222
111	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, 1777-1782.	7.1	1,259
112	Estimation of the number of extreme pathways for metabolic networks. <i>BMC Bioinformatics</i> , 2007, 8, 363.	2.6	44
113	Bringing Genomes to Life: The Use of Genome-Scale In Silico Models. , 2007, , 14-36.		0
114	Candidate States of <i>Helicobacter pylori</i> 's Genome-Scale Metabolic Network upon Application of $\Delta\epsilon$ Loop Law's Thermodynamic Constraints. <i>Biophysical Journal</i> , 2006, 90, 3919-3928.	0.5	45
115	Towards multidimensional genome annotation. <i>Nature Reviews Genetics</i> , 2006, 7, 130-141.	16.3	321
116	Expanded Metabolic Reconstruction of <i>Helicobacter pylori</i> ( iIT341 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
117	Candidate Metabolic Network States in Human Mitochondria. <i>Journal of Biological Chemistry</i> , 2005, 280, 11683-11695.	3.4	138
118	The Subsystems Approach to Genome Annotation and its Use in the Project to Annotate 1000 Genomes. <i>Nucleic Acids Research</i> , 2005, 33, 5691-5702.	14.5	1,806
119	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
120	Metabolic Network Analysis Reveals Altered Bile Acid Synthesis and Cholesterol Metabolism in Alzheimer's Disease. <i>SSRN Electronic Journal</i> , 0, , .	0.4	6
121	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