List of publications

04 April 2024

Metrics

44 peer-reviewed original research publications; 12 review articles; 5 book chapters; 5 preprint h-index: 25 (Scopus) / 26 (Google Scholar); citations: 2154 (Scopus) / 3063 (Google Scholar) ORCID: 0000-0002-3593-5792 / ResearcherID: P-2469-2019

Peer-reviewed original articles

- Nowrouzi B, Torres-Montero P, Kerkhoven EJ, Martinez JL, Rios-Solis L (2024) Rewiring Saccharomyces cerevisiae metabolism for optimised Taxol® precursors production. Metab Eng Comm. doi:10.1016/j.mec.2023.e00229
- Chen Y, Gustafsson J, Rangel AT, Anton M, Domenzain I, Kittikunapong C, Li F, Yuan L, Nielsen J, Kerkhoven EJ (2024) Reconstruction, simulation and analysis of enzyme-constrained metabolic models using GECKO Toolbox 3.0. Nature Prot. doi:10.1038/s41596-023-00931-7
- Ristinmaa AS, Rangel AT, Idström A, Valenzuela S, Kerkhoven EJ, Pope PB, Hasani M, Larsbrink J (2023)
 Resin acids play key roles in shaping microbial communities during degradation of spruce bark. Nature
 Comm. doi:10.1038/s41467-023-43867-y
- 4. Malcı K, Santibáñez R, Jonguitud-Borrego N, Santoyo-Garcia JH, **Kerkhoven EJ**, Rios-Solis L (2023) Improved production of Taxol® precursors in *S. cerevisiae* using combinatorial in silico design and metabolic engineering. Microb Cell Fact. doi:10.1186/s12934-023-02251-7
- 5. Zaghen S, Konzock O, Fu J, **Kerkhoven EJ** (2023) Abolishing storage lipids induces protein misfolding and stress responses in *Yarrowia lipolytica*. J Ind Microbiol Biotechnol. doi:10.1093/jimb/kuad031
- 6. Reķēna A, Pinheiro MJ, Bonturi N, Belouah I, Tammekivi E, Herodes K, **Kerkhoven EJ**, Lahtvee PJ (2023) Genome-scale metabolic modeling reveals metabolic trade-offs associated with lipid production in *Rhodotorula toruloides*. PLOS Comput Biol. doi:10.1371/journal.pcbi.1011009
- 7. Yuan L, Lu H, Li F, Nielsen J, **Kerkhoven EJ** (2023) HGTphyloDetect: facilitating the identification and phylogenetic analysis of horizontal gene transfer. Brief Bioinform. doi:10.1093/bib/bbad035
- 8. Gustafsson J, Robinson JL, Roshanzamir F, Jörnsten R, **Kerkhoven EJ**, Nielsen J (2023) Generation and analysis of context-specific genome-scale metabolic models derived from single-cell RNA-Seq data. Proc Natl Acad Sci. doi:10.1073/pnas.2217868120
- 9. Konzock O, Zaghen S, Fu J, **Kerkhoven EJ** (2022) Urea is a drop-in nitrogen source alternative to ammonium sulphate in *Yarrowia lipolytica*. iScience doi:10.1016/j.isci.2022.105703
- 10. Lu H, **Kerkhoven EJ**, Nielsen J (2022) A pan-draft metabolic model reflects evolutionary diversity across 332 yeast species. Biomol. doi: 10.3390/biom12111632
- Domenzain I, Sánchez B, Anton M, Kerkhoven EJ, Millán-Oropeza A, Henry C, Siewers V, Morrisey JP, Sonnenschein N, Nielsen J (2022) Reconstruction of a catalogue of genome-scale metabolic models with enzymatic constraints using GECKO 2.0. Nat Comm. doi:10.1038/s41467-022-31421-1
- 12. Li F, Chen Y, Qi Q, Wang Y, Yuan L, Huang M, Elsemman IE, Feizi A, **Kerkhoven EJ**, Nielsen J (2022) Improving recombinant protein production by yeast through genome-scale modeling using proteome constraints. Nat Comm. doi:10.1038/s41467-022-30689-7
- 13. Li F, Yuan L, Lu H, Li G, Chen Y, Engqvist MKM, **Kerkhoven EJ***, Nielsen J (2022) Deep learning based kcat prediction enables improved enzyme constrained model reconstruction. Nat Catalysis. doi: 10.1038/s41929-022-00798-z *corresponding author
- 14. Poorinmohammad N, Fu J, Wabeke B, **Kerkhoven EJ** (2022) Validated growth-rate dependent regulation of lipid metabolism in *Yarrowia lipolytica*. Int J Mol Sci. doi:10.3390/ijms23158517
- 15. Ventorim RZ, de Moura Ferreira MA, de Almeida ELM, **Kerkhoven EJ**, da Silveira WB (2022) Genome-scale metabolic model of oleaginous yeast *Papiliotrema laurentii*. Biochem Eng J. doi:10.1016/j.bej.2022.108353

- 16. Malina C, Yu R, Björkeroth J, **Kerkhoven EJ**, Nielsen J (2021) Adaptations in metabolism and protein translation give rise to the Crabtree effect in yeast. PNAS. doi:10.1073/pnas.2112836118
- 17. Malina C, Di Bartolomeo F, **Kerkhoven EJ**, Nielsen J (2021) Constraint-based modeling of yeast mitochondria reveals the dynamics of protein import and iron-sulfur cluster biogenesis. iScience doi: 10.1016/j.isci.2021.103294
- 18. Lu H, Li F, Yuan Le, Domenzain I, Yu R, Wang H, Li G, Chen Y, Ji B, **Kerkhoven EJ**, Nielsen J (2021) Yeast metabolic innovations emerged via expanded metabolic network and gene positive selection. Mol Syst Biol. doi:10.15252/msb.202110427
- 19. Caspeta L, **Kerkhoven EJ**, Martinez A, Nielsen J (2021) The yeastGemMap: A process diagram to assist yeast systems-metabolic studies. Biotechnol Bioeng:10.1002/bit.27943
- 20. Kittikunapong C, Ye S, Magadán-Corpas P, Pérez-Valero Á, Villar CJ, Lombó F, **Kerkhoven EJ** (2021) Reconstruction of a Genome-Scale Metabolic Model of *Streptomyces albus* J1074: Improved Engineering Strategies in Natural Product Synthesis. Metabolites 11:5. doi:10.3390/metabo11050304
- 21. Hapeta P, **Kerkhoven EJ**, Lazar Z (2020) Nitrogen as the major factor influencing gene expression in *Yarrowia lipolytica*. Biotechnol Rep: 27. doi:10.1016/j.btre.2020.e00521
- 22. Sulheim S, Kumelj T, van Dissel D, Salehzadeh-Yazdi A, Du C, Nieselt K, Almaas E, Wentzel A & **Kerkhoven EJ** (2020) Enzyme-constrained models and omics analysis of *Streptomyces coelicolor* reveal metabolic changes that enhance heterologous production. iScience: 23: 9. doi:10.1016/j.isci.2020.101525
- 23. Robinson JL, Kocabaş P, Wang H, Cholley PE, Cook D, Nilsson A, Anton M, Ferreira R, Domenzain I, Billa V, Limeta A, Hedin A, Gustafsson J, **Kerkhoven EJ**, Svensson LT, Palsson BO, Mardinoglu A, Hansson L, Uhlén M, Nielsen J (2020) An atlas of human metabolism. Science Signaling 13: 624. doi:10.1126/scisignal.aaz1482
- 24. Lopes HJS, Bonturi N, **Kerkhoven EJ**, Miranda EA, Lahtvee PJ (2020) C/N ratio and carbon source-dependent lipid production profiling in *Rhodotorula toruloides*. Appl Microbiol Biotechnol. 104: 2639–49. doi:10.1007/s00253-020-10386-5
- 25. Lubuta P, Workman M, **Kerkhoven EJ***, Workman CT* (2019) Investigating the Influence of Glycerol on the Utilization of Glucose in *Yarrowia lipolytica* Using RNA-Seq-Based Transcriptomics. G3 Genes, Genomes, Genet. g3.400469.2019. doi:10.1534/g3.119.400469 *co-corresponding author
- 26. Tiukova IA, Prigent S, Nielsen J, Sandgren M, **Kerkhoven EJ** (2019) Genome-scale model of *Rhodotorula toruloides* metabolism. Biotechnol Bioeng. 116: 3396–3408. doi:10.1002/bit.27162
- 27. Tiukova IA, Brandenburg J, Blomqvist J, Samples S, Mikkelsen N, Skaugen M, Arntzen MØ, Nielsen J, Sandgren M, **Kerkhoven EJ** (2019) Proteome analysis of xylose metabolism in *Rhodotorula toruloides* during lipid production. Biotechnol Biofuels 12: 1–17. doi:10.1186/s13068-019-1478-8
- 28. Johnston K, Kim D-H, **Kerkhoven EJ**, Burchmore R, Barrett MP, Achcar F (2019) Mapping the metabolism of five amino acids in bloodstream form *Trypanosoma brucei* using U-13C-labelled substrates and LC–MS. Biosci Rep. 39: 1–17. doi:10.1042/BSR20181601
- 29. Lu H, Li F, Sánchez BJ, Zhu Z, Li G, Domenzain I, Marcišauskas S, Anton PM, Lappa D, Lieven C, Beber ME, Sonnenschein N, **Kerkhoven EJ**, Nielsen J (2019) A consensus *S. cerevisiae* metabolic model Yeast8 and its ecosystem for comprehensively probing cellular metabolism. Nat Commun. 10: 3586. doi:10.1038/s41467-019-11581-3
- 30. Sánchez BJ, Li F, **Kerkhoven EJ**, Nielsen J (2019) SLIMEr: probing flexibility of lipid metabolism in yeast with an improved constraint-based modeling framework. BMC Syst Biol. 13: 4. doi:10.1186/s12918-018-0673-8
- 31. Pomraning KR, Bredeweg EL, **Kerkhoven EJ**, Barry K, Haridas S, Hundley H, LaButti K, Lipzen A, Yan M, Magnuson JK, Simmons BA, Grigoriev IV, Nielsen J, Baker SE (2018) Regulation of Yeast-to-Hyphae Transition in *Yarrowia lipolytica*. mSphere. 3: 1–18. doi:10.1128/mSphere.00541-18
- 32. Wang H, Marcišauskas S, Sánchez BJ, Domenzain I, Hermansson D, Agren R, Nielsen J, **Kerkhoven EJ** (2018) RAVEN 2.0: A versatile toolbox for metabolic network reconstruction and a case study on *Streptomyces coelicolor*. PLOS Comput Biol. 14: e1006541. doi:10.1371/journal.pcbi.1006541
- 33. Sánchez BJ, Zhang C, Nilsson A, Lahtvee P, **Kerkhoven EJ**, Nielsen J (2017) Improving the phenotype predictions of a yeast genome-scale metabolic model by incorporating enzymatic constraints. Mol Syst Biol. 13: 935. doi:10.15252/msb.20167411

- 34. **Kerkhoven EJ**, Kim Y-M, Wei S, Nicora CD, Fillmore TL, Purvine SO, Webb-Robertson BJ, Smith RD, Baker SE, Metz TO, Nielsen J (2017) Leucine Biosynthesis Is Involved in Regulating High Lipid Accumulation in *Yarrowia lipolytica*. MBio. 8: e00857-17. doi:10.1128/mBio.00857-17
- 35. Bredeweg EL, Pomraning KR, Dai Z, Nielsen J, **Kerkhoven EJ**, Baker SE (2017) A molecular genetic toolbox for *Yarrowia lipolytica*. Biotechnol Biofuels. 10: 2. doi:10.1186/s13068-016-0687-7
- 36. Irani ZA, **Kerkhoven EJ**, Shojaosadati SA, Nielsen J (2016) Genome-scale metabolic model of *Pichia pastoris* with native and humanized glycosylation of recombinant proteins. Biotechnol Bioeng. 113: 961–969. doi:10.1002/bit.25863
- 37. **Kerkhoven EJ**, Pomraning KR, Baker SE, Nielsen J (2016) Regulation of amino-acid metabolism controls flux to lipid accumulation in *Yarrowia lipolytica*. NPJ Syst Biol Appl. 2: 16005. doi:10.1038/npjsba.2016.5
- 38. Creek DJ, Mazet M, Achcar F, Anderson J, Kim D-H, Kamour R, Morand P, Millerioux Y, Biran M, **Kerkhoven EJ**, Chokkathukalam A, Weidt SK, Burgess KEV, Breitling R, Watson DG, Bringaud F, Barrett MP (2015) Probing the Metabolic Network in Bloodstream-Form *Trypanosoma brucei* Using Untargeted Metabolomics with Stable Isotope Labelled Glucose. PLOS Pathog. 11: e1004689. doi:10.1371/journal.ppat.1004689
- 39. Hai Y, **Kerkhoven EJ**, Barrett MP, Christianson DW (2015) Crystal Structure of an Arginase-like Protein from *Trypanosoma brucei* That Evolved without a Binuclear Manganese Cluster. Biochemistry. 54: 458–471. doi:10.1021/bi501366a
- 40. Shameer S, Logan-klumpler FJ, Vinson F, Cottret L, Merlet B, Achcar F, Boshart M, Berriman M, Breitling R, Bringaud R, Bütikofer P, Cattanach AM, Bannerman-Chukualim B, Creek DJ, Crouch K, de Koning HP, Denise H, Ebikeme C, Fairlamb AH, Ferguson MAJ, Ginger ML, Hertz-Fowler C, Kerkhoven EJ, Mäaser P, Michels PAM, Nayak A, Nes DW, Nolan DP, Olsen C, Silva-Franco F, Smith TK, Taylor MC, Tielens AGM, Urbaniak MC, van Hellemond JJ, Vincent IM, Wilkinson SR, Wyllie S, Opperdoes FR, Barrett MP, Jourdan F (2015) TrypanoCyc: a community-led biochemical pathways database for *Trypanosoma brucei*. Nucleic Acids Res. 43: D637–D644. doi:10.1093/nar/gku944
- 41. Ledesma-Amaro R, **Kerkhoven EJ**, Revuelta JL, Nielsen J (2014) Genome scale metabolic modeling of the riboflavin overproducer *Ashbya gossypii*. Biotechnol Bioeng. 111: 1191–1199. doi:10.1002/bit.25167
- 42. **Kerkhoven EJ**, Achcar F, Alibu VP, Burchmore RJ, Gilbert IH, Trybiło M, Driessen NN, Gilbert D, Breitling R, Bakker BM, Barrett MP (2013) Handling Uncertainty in Dynamic Models: The Pentose Phosphate Pathway in *Trypanosoma brucei*. PLoS Comput Biol. 9: e1003371. doi:10.1371/journal.pcbi.1003371
- 43. Achcar F, **Kerkhoven EJ**, Bakker BM, Barrett MP, Breitling R (2012) Dynamic modelling under uncertainty: the case of *Trypanosoma brucei* energy metabolism. PLoS Comput Biol. 8: e1002352. doi:10.1371/journal.pcbi.1002352
- 44. Haanstra JR*, **Kerkhoven EJ***, van Tuijl A, Blits M, Wurst M, van Nuland R, Albert MA, Michels PAM, Bouwman J, Clayton C, Westerhoff HV, Bakker BM (2011). A domino effect in drug action: from metabolic assault towards parasite differentiation. Mol Microbiol. 79: 94–108. doi: 10.1111/j.1365-2958.2010.07435.x *contributed equally

Research review articles

- 1. Chen Y, Gustafsson J, Yang J, Nielsen J, **Kerkhoven EJ** (2024) Single-cell omics analysis with genome-scale metabolic modeling. Curr Opin Biotechnol. doi:10.1016/j.copbio.2024.103078
- de Almeida ELM, Kerkhoven EJ, Silveira WB (2024) Reconstruction of genome-scale metabolic models of non-conventional yeasts: current state, challenges, and perspectives. Biotechnol Bioproc Eng. doi: 10.1007/s12257-024-00009-5
- 3. Han Y, Rangel AT, Pomraning KR, **Kerkhoven EJ**, Kim J (2023) Advances in genome-scale metabolic models of industrially important fungi. Curr Opin Biotechnol. doi:10.1016/j.copbio.2023.103005
- 4. **Kerkhoven EJ** (2022) Advances in constraint-based models: methods for improved predictive power based on resource allocation constraints. Curr Opin Microbiol. doi:10.1016/j.mib.2022.102168
- Lu H, Kerkhoven EJ, Nielsen J (2021) Multiscale models quantifying yeast physiology: towards a whole-cell model. Trends Biotechnol. doi:10.1016/j.tibtech.2021.06.010

- 6. Poorinmohammad N, **Kerkhoven EJ** (2021) Systems-level approaches for understanding and engineering of the oleaginous cell factory *Yarrowia lipolytica*. Biotechnol Bioeng. doi:10.1002/bit.27859
- Domenzain I, Li F, Kerkhoven EJ, Siewers V (2020) Evaluating accessibility, usability and interoperability of genome-scale metabolic models for diverse yeasts species. FEMS Yeast Res. foab002. doi:10.1093/femsyr/foab002
- 8. Doughty T, **Kerkhoven EJ** (2020) Extracting novel hypotheses and findings from RNA-seq data. FEMS Yeast Res. 20: 1–7. doi:10.1093/femsyr/foaa007
- 9. Shi T, Huang H, **Kerkhoven EJ**, Ji X (2018) Advancing metabolic engineering of *Yarrowia lipolytica* using the CRISPR/Cas system. Appl Microbiol Biotechnol. 102: 9541–9548. doi:10.1007/s00253-018-9366-x
- 10. Zhou YJ, **Kerkhoven EJ**, Nielsen J (2018) Barriers and opportunities in bio-based production of hydrocarbons. Nat Energy. 3: 925–35. doi:10.1038/s41560-018-0197-x
- 11. **Kerkhoven EJ**, Lahtvee P-J, Nielsen J (2015). Applications of computational modeling in metabolic engineering of yeast. FEMS Yeast Res. 15: 1–13. doi:10.1111/1567-1364.12199
- 12. Achcar F, **Kerkhoven EJ**, Barrett MP (2014) *Trypanosoma brucei*: meet the system. Curr Opin Microbiol. 20: 162–9. doi:10.1016/j.mib.2014.06.007

Book chapters

- Zorrilla F, Kerkhoven EJ (2022) Reconstruction of genome-scale metabolic model for Hansenula polymorpha using RAVEN. In: Mapelli V, Bettiga M, editors. Yeast Metabolic Engineering. Springer. doi: 10.1007/978-1-0716-2399-2 16
- Lu H, Chen Y, Nielsen J, Kerkhoven EJ (2021) Kinetic Models of Metabolism. In: Nielsen J, Stephanopoulos G, Lee SY, editors. Metabolic Engineering: Concepts and Applications. Vol 13a. Wiley-VCH GmbH. doi:10.1002/9783527823468.ch5
- Chen Y, Nielsen J, Kerkhoven EJ (2021) Proteome Constraints in Genome-Scale Models. In: Nielsen J, Stephanopoulos G, Lee SY, editors. Metabolic Engineering: Concepts and Applications. Vol 13a. Wiley-VCH GmbH. doi:10.1002/9783527823468.ch4
- 4. **Kerkhoven EJ** (2019) Modeling Lipid Metabolism in Yeast. In: Geiger O, editor. Biogenesis of Fatty Acids, Lipids and Membranes Handbook of Hydrocarbon and Lipid Microbiology. Springer International Publishing; pp. 375–388. doi:10.1007/978-3-319-50430-8 9
- Achcar F, Fadda A, Haanstra JR, Kerkhoven EJ, Kim D-H, Leroux AE, Papamarkou T, Rojas F, Bakker BM, Barrett MP, Clayton C, Girolami M, Krauth-Siegel RL, Matthews KR, Breitling R (2014). The silicon trypanosome: a test case of iterative model extension in systems biology. In: Poole RK, editor. Advances in microbial physiology. 1st ed. Elsevier Ltd.; pp. 115–43. doi:10.1016/B978-0-12-800143-1.00003-8

Preprints

- Zhang C, Sánchez BJ, Li F, Eiden CWQ, Scott WT, Liebal UW, Blank LM, Mengers HG, Anton M, Rangel AT, Mendoza SN, Zhang L, Nielsen J, Lu H, **Kerkhoven EJ** (2023) Yeast9: a consensus yeast metabolic model enables quantitative analysis of cellular metabolism by incorporating big data. bioRxiv. doi:10.1101/2023.12.03.569754
- Fu J, Zaghen S, Lu H, Konzock O, Poorinmohammad N, Kornberg A, Koseto D, Wentzel A, Di Bartolomeo F, Kerkhoven EJ (2023) Reprogramming *Yarrowia lipolytica* metabolism for efficient synthesis of itaconic acid from flask to semi-pilot scale. bioRxiv. doi:10.1101/2023.07.17.549194
- 3. Peri KVR, Yuan L, Oliveira FF, Persson K, Alalam HD, Olsson L, Larsbrink J, **Kerkhoven EJ**, Geijer C. (2023) Regulation of lactose and galactose growth: Insights from a unique metabolic gene cluster in *Candida intermedia*. bioRxiv. doi:10.1101/2023.12.19.572343
- 4. Anton M, Almaas E, Benfeitas R, Benito-Vaquerizo S, Blank LM, Dräger A, Hancock JM, Kittikunapong C, König M, Li F, Liebal UW, Lu H, Ma H, Mahadevan R, Mardinoglu A, Nielsen J, Nogales J, Pagni M, Papin JA, Patil KR, Price ND, Robinson JL, Sánchez BJ, Diez MS, Sulheim S, Svensson LT, Teusink B, Vongsangnak W,

- Wang H, Zeidan AA, **Kerkhoven EJ** (2023) standard-GEM: standardization of open-source genome-scale metabolic models. bioRxiv. doi:10.1101/2023.03.21.512712
- 5. Lu H, Zhu Z, **Kerkhoven EJ** & Nielsen J (2019) FALCONET: an R package to accelerate automatic visualisation of genome scale metabolic models. bioRxiv. doi:10.1101/662056