List of publications

2021-09-01

Peer-reviewed original articles

1. 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

2. 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

3. 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.101525

4. 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

5. 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

6. 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

7. 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

8. 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

9. 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

10. 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

11. 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

12. 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

13. 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

14. 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

15. **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

16. 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

17. 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

18. **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

19. 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

20. 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

21. 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

22. 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

23. **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

24. 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

25. 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
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Research review articles

1. 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

2. 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

3. 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

4. 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

5. 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

6. 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

7. **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
8. 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

1. 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
2. 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
3. **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
4. 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

1. Li F, Yuan L, Lu H, Li G, Chen Y, Engqvist MKM, **Kerkhoven EJ**, Nielsen J (2021) Deep learning based kcat prediction enables improved enzyme constrained model reconstruction. bioRxiv. doi:10.1101/2021.08.06.455417
2. Zorrilla F, **Kerkhoven EJ** (2021) Reconstruction of genome-scale metabolic model for *Hansenula polymorpha* using RAVEN toolbox. bioRxiv. 10.1101/2021.06.18.448943
3. Domenzain I, Sánchez B, Anton M, **Kerkhoven EJ**, Millán-Oropeza A, Henry C, Siewers V, Morrisey JP, Sonnenschein N, Nielsen J (2021) Reconstruction of a catalogue of genome-scale metabolic models with enzymatic constraints using GECKO 2.0. bioRxiv. doi:10.1101/2021.03.05.433259
4. Lu H, Zhu Z, **Kerkhoven EJ** & Nielsen J (2019) FALCONET: an R package to accelerate automatic visualisation of genome scale metabolic models. bioRxiv: 662056. doi:10.1101/662056