Curriculum vitae	**Dr. rer. nat. Matthias König**

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Work address	Humboldt-University Berlin
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Academic Education	2016	Junior group leader, Humboldt-University Berlin, Systems Biology and Systems Medicine of the Liver
	2015	Doctorate, Humboldt-University Berlin, Charité University Medicine, Modeling Hepatic Carbohydrate Metabolism
	2008	Diploma biophysics, Humboldt-University Berlin
	2005	Pre-diploma biophysics, Humboldt-University Berlin
	2002	Studies of biophysics, Humboldt-University Berlin

Professional Career	2016–2022	Junior Group Leader, Systems Medicine of the Liver, Institute for Theoretical Biology, Humboldt-University Berlin
	2008–2015	Scientific staff member, Institute of Biochemistry, Computational Systems Biochemistry, Charité University Hospital Berlin

Supervision

Jan Grzegorzewski (PhD Biophysics)	2017–2022	Physiologically based pharmacokinetic (PBPK) modeling for dynamical liver function and CYP phenotyping
Beatrice Stemmer Mallol (Bachelor Biology)	2022	A physiologically based pharmacokinetic (PBPK) of the probe drug talinolol model for the characterization of intestinal P-glycoprotein
Helena Leal Pujol (Bachelor Biology)	2021–2022	A physiologically based model of pravastatin – The role of genotypes and hepatic or renal impairment on the pharmacokinetics of pravastatin
Sükrü Balci (Bachelor Biology)	2021	Computational modelling of omeprazole - pharmacokinetics and pharmacodynamics
Adrian Köller (Bachelor Biophysics)	2020–2021	A Physiologically Based Model of Indocyanine Green Liver Function Tests - Effects of Physiological Factors, Hepatic Disease and Hepatic Surgery
Florian Bartsch (Bachelor Biophysics)	2020	Computational Modelling of Simvastatin – Effects on HMG-CoA Reductase Activity and Cholesterol
Yannick Duport (Bachelor Bioinformatics)	2020	Computational Modelling of Midazolam Clearance: Effect of Inhibitors and Inducers

Teaching

X-Research Group	2022–2023	X-Student Research Group, Physiologically based modeling of drugs: ACE inhibitors in the treatment of high blood pressure funded under the Excellence Strategy of the Federal Government and the Länder by the Berlin University Alliance.
Lecture	2018–2019	Computational models of cellular processes
Course and seminar	2017–2021	Computational models of biological systems
Course	2008–2010	Pre-course in math for freshmen

Third Party Funding

BMBF (311 k€)	2023–2026	ATLAS - AI and Simulation for Tumor Liver ASessment
DFG/BUA (3 k€)	2022–2023	X-Student Research Group - Physiologically based modeling of drugs: ACE inhibitors in the treatment of high blood pressure
DFG (425 k€)	2021–2025	FOR5151 - QuaLiPerF - Quantifying Liver Perfusion-Function Relationship in Complex Resection – A Systems Medicine Approach
DFG (co-applicant)	2020–2023	SPP2311 - SimLivA - SIMulation supported LIVer Assessment for donor organs
EU Horizon (25 k€)	2020–2021	EOSC-Life - Reproducible simulation studies targeting COVID-19
BMBF (723 k€)	2016–2020	LiSyM – Systems Medicine of the Liver – Junior group, Computational modeling of dynamical liver function tests

Scholarships

Google Summer of Code (5 k€)	2015	Scholarship Google Summer of Code for Development of SBML support for Cytoscape
Studienstiftung	2005	Scholarship Studienstiftung des Deutschen Volkes

Conferences

COMBINE2022	2022	Main organizer of the Computational Modeling in Biology (COMBINE) conference in Berlin with > 100 participants as satellite event of the ICSB (https://combine-org.github.io/events/)

Community Outreach

COMBINE Coordinator	2018-2022	Coordinator of the COmputational Modeling in BIology' NEtwork (COMBINE, https://co.mbine.org)
SBML Editor	2018-2020, 2021-2023	Editor of the Systems Biology Markup Language (SBML, https://sbml.org)
SED-ML Editor	2017-2019, 2020-2022	Editor of the Simulation Experiment Description Markup Language (SED-ML, https://sed-ml.org)

Software

`sbmlutils`	Python utilities for SBML (https://github.com/matthiaskoenig/sbmlutils)
`sbmlsim`	SBML simulation made easy (https://github.com/matthiaskoenig/sbmlsim)
`cysbml`	Cytoscape 3 app for the Systems Biology Markup Language SBML (https://github.com/matthiaskoenig/cy3sbml)
`brendapy`	BRENDA in python (https://github.com/matthiaskoenig/brendapy)
`libsbgnpy`	Python library for SBGN (https://github.com/matthiaskoenig/libsbgn-python)
`roadrunner`	Contributor to the high-performance simulator for SBML (https://github.com/sys-bio/roadrunner/)
`cobrapy`	Contributor to the COBRA python package (https://github.com/opencobra/cobrapy/)
`tellurium`	Contributor to the tellurium simulator (https://github.com/sys-bio/tellurium/)

Publications

1. J. Grzegorzewski, J. Brandhorst, and M. **König**. "Physiologically based pharmacokinetic (PBPK) modeling of the role of CYP2D6 polymorphism for metabolic phenotyping with dextromethorphan". In: *Frontiers In Pharmacology* (2022). DOI: 10.3389/fphar.2022.1029073

2. J. Grzegorzewski, F. Bartsch, A. Köller, and M. **König**. "Pharmacokinetics of Caffeine: A Systematic Analysis of Reported Data for Application in Metabolic Phenotyping and Liver Function Testing". In: *Frontiers in Pharmacology* 12 (2022), p. 752826. DOI: 10.3389/fphar.2021.752826

3. H. Panchiwala, S. Shah, H. Planatscher, M. Zakharchuk, M. **König**, and A. Dräger. "The Systems Biology Simulation Core Library". In: *Bioinformatics* 38.3 (2022). Ed. by J. Xu, pp. 864–865. DOI: 10.1093/bioinformatics/btab669

4. K. Ramachandran, M. **König**, M. Scharm, T. V. N. Nguyen, H. Hermjakob, D. Waltemath, and R. S. Malik Sheriff. *FAIR Sharing of Reproducible Models of Epidemic and Pandemic Forecast*. preprint. Medicine & Pharmacology, 2022. DOI: 10.20944/preprints202206.0137.v1

5. B. Shaikh, L. P. Smith, D. Vasilescu, et al. "BioSimulators: A Central Registry of Simulation Engines and Services for Recommending Specific Tools". In: *Nucleic Acids Research* (2022), gkac331. DOI: 10.1093/nar/gkac331

6. C. Welsh, J. Xu, L. Smith, M. **König**, K. Choi, and H. M. Sauro. "libRoadRunner 2.0: A High-Performance SBML Simulation and Analysis Library". Version 1. In: (2022). DOI: 10.48550/ARXIV.2203.01175

7. J. Grzegorzewski, J. Brandhorst, K. Green, D. Eleftheriadou, Y. Duport, F. Barthorscht, A. Köller, D. Y. J. Ke, S. De Angelis, and M. **König**. "PK-DB: Pharmacokinetics Database for Individualized and Stratified Computational Modeling". In: *Nucleic Acids Research* 49.D1 (2021), pp. D1358–D1364. DOI: 10.1093/nar/gkaa990

8. J. H. Gennari, M. **König**, G. Misirli, M. L. Neal, D. P. Nickerson, and D. Waltemath. "OMEX Metadata Specification (Version 1.2)". In: *Journal of Integrative Bioinformatics* 18.3 (2021). DOI: 10.1515/jib-2021-0020. pmid: 34668356

9. B. Christ, M. Collatz, U. Dahmen, K.-H. Herrmann, S. Höpfl, M. **König**, L. Lambers, M. Marz, D. Meyer, N. Radde, J. R. Reichenbach, T. Ricken, and H.-M. Tautenhahn. "Hepatectomy-Induced Alterations in Hepatic Perfusion and Function - Toward Multi-Scale Computational Modeling for a Better Prediction of Post-hepatectomy Liver Function". In: *Frontiers in Physiology* 12 (2021),

p. 733868. DOI: 10.3389/fphys.2021.733868

10. A. Köller, J. Grzegorzewski, H.-M. Tautenhahn, and M. **König**. "Prediction of Survival After Partial Hepatectomy Using a Physiologically Based Pharmacokinetic Model of Indocyanine Green Liver Function Tests". In: *Frontiers in Physiology* 12 (2021), p. 730418. DOI: 10.3389/fphys.2021.730418

11. A. Köller, J. Grzegorzewski, and M. **König**. "Physiologically Based Modeling of the Effect of Physiological and Anthropometric Variability on Indocyanine Green Based Liver Function Tests". In: *Frontiers in Physiology* 12 (2021), p. 757293. DOI: 10.3389/fphys.2021.757293

12. M. **König**, J. Grzegorzewski, M. Golebiewski, H. Hermjakob, M. Hucka, B. Olivier, S. Keating, D. Nickerson, F. Schreiber, R. Sheriff, and D. Waltemath. *Ten Simple Rules for FAIR Sharing of Experimental and Clinical Data with the Modeling Community*. preprint. LIFE SCIENCES, 2021. DOI: 10.20944/preprints202108.0303.v2

13. L. P. Smith, F. T. Bergmann, A. Garny, T. Helikar, J. Karr, D. Nickerson, H. Sauro, D. Waltemath, and M. **König**. "The Simulation Experiment Description Markup Language (SED-ML): Language Specification for Level 1 Version 4". In: *Journal of Integrative Bioinformatics* 18.3 (2021), p. 20210021. DOI: 10.1515/jib-2021-0021

14. B. Shaikh, A. P. Freiburger, M. **König**, F. T. Bergmann, D. P. Nickerson, H. M. Sauro, M. L. Blinov, L. P. Smith, I. I. Moraru, and J. R. Karr. *SED-ML Validator: Tool for Debugging Simulation Experiments*. 2021

15. T. G. Yamada, K. Ii, M. **König**, M. Feierabend, A. Dräger, and A. Funahashi. "SBMLWebApp: Web-Based Simulation, Steady-State Analysis, and Parameter Estimation of Systems Biology Models". In: *Processes* 9.10 (2021), p. 1830. DOI: 10.3390/pr9101830

16. S. M. Keating, D. Waltemath, M. **König**, et al. "SBML Level 3: An Extensible Format for the Exchange and Reuse of Biological Models". In: *Molecular Systems Biology* 16.8 (2020). DOI: 10.15252/msb.20199110

17. M. L. Neal, J. H. Gennari, D. Waltemath, D. P. Nickerson, and M. **König**. "Open Modeling and Exchange (OMEX) Metadata Specification Version 1.0". In: *Journal of Integrative Bioinformatics* 17.2-3 (2020), p. 20200020. DOI: 10.1515/jib-2020-0020

18. F. Schreiber, B. Sommer, T. Czauderna, M. Golebiewski, T. E. Gorochowski, M. Hucka, S. M. Keating, M. **König**, C. Myers, D. Nickerson, and D. Waltemath. "Specifications of Standards in Systems and Synthetic Biology: Status and Developments in 2020". In: *Journal of Integrative Bioinformatics* 17.2-3 (2020), p. 20200022. DOI: 10.1515/jib-2020-0022

19. L. P. Smith, S. L. Moodie, F. T. Bergmann, C. Gillespie, S. M. Keating, M. **König**, C. J. Myers, M. J. Swat, D. J. Wilkinson, and M. Hucka. "Systems Biology Markup Language (SBML) Level 3 Package: Distributions, Version 1, Release 1". In: *Journal of Integrative Bioinformatics* 17.2-3 (2020), p. 20200018. DOI: 10.1515/jib-2020-0018

20. D. Waltemath, M. Golebiewski, M. L. Blinov, P. Gleeson, H. Hermjakob, M. Hucka, E. T. Inau, S. M. Keating, M. **König**, O. Krebs, R. S. Malik-Sheriff, D. Nickerson, E. Oberortner, H. M. Sauro, F. Schreiber, L. Smith, M. I. Stefan, U. Wittig, and C. J. Myers. "The First 10 Years of the International Coordination Network for Standards in Systems and Synthetic Biology (COMBINE)". in: *Journal of Integrative Bioinformatics* 17.2-3 (2020), p. 20200005. DOI: 10.1515/jib-2020-0005

21. M. **König**, L. H. Watanabe, J. Grzegorzewski, and C. J. Myers. *Dynamic Flux Balance Analysis Models in SBML*. preprint. Bioinformatics, 2018. DOI: 10.1101/245076

22. N. Berndt, S. Bulik, I. Wallach, T. Wünsch, M. **König**, M. Stockmann, D. Meierhofer, and H.-G. Holzhütter. "HEPATOKIN1 is a biochemistry-based model of liver metabolism for applications in medicine and pharmacology." In: *Nature Communications* 9 (1 2018), p. 2386. DOI: 10.1038/s41467-018-04720-9

23. J. K. Medley, K. Choi, M. **König**, L. Smith, S. Gu, J. Hellerstein, S. C. Sealfon, and H. M. Sauro. "Tellurium notebooks-An environment for reproducible dynamical modeling in systems biology." In: *PLoS Computational Biology* 14 (6 2018), e1006220. DOI: 10.1371/journal.pcbi.1006220

24. K. Abshagen, M. **König**, A. Hoppe, I. Müller, M. Ebert, H. Weng, H.-G. Holzhütter, U. M. Zanger, J. Bode, B. Vollmar, M. Thomas, and S. Dooley. "Pathobiochemical signatures of cholestatic liver

disease in bile duct ligated mice." In: *BMC Systems Biology* 9 (2015), p. 83. DOI: 10.1186/s12918-015-0229-0

25. E. T. Somogyi, J.-M. Bouteiller, J. A. Glazier, M. **König**, J. K. Medley, M. H. Swat, and H. M. Sauro. "libRoadRunner: a high performance SBML simulation and analysis library." In: *Bioinformatics* 31 (20 2015), pp. 3315–3321. DOI: 10.1093/bioinformatics/btv363

26. D. Werner, T. Ricken, U. Dahmen, O. Dirsch, H.-G. Holzhütter, and M. **König**. "On the Influence of Growth in Perfusion Dependent Biological Systems–at the Example of the Human Liver". In: *PAMM* 15.1 (2015), pp. 119–120

27. T. Ricken, D. Werner, H. G. Holzhütter, M. **König**, U. Dahmen, and O. Dirsch. "Modeling function-perfusion behavior in liver lobules including tissue, blood, glucose, lactate and glycogen by use of a coupled two-scale PDE-ODE approach." In: *Biomechanics and Modeling in Mechanobiology* 14 (3 2015), pp. 515–536. DOI: 10.1007/s10237-014-0619-z

28. M. **König**, H.-G. Holzhütter, and N. Berndt. "Metabolic gradients as key regulators in zonation of tumor energy metabolism: a tissue-scale model-based study." In: *Biotechnology Journal* 8 (9 2013), pp. 1058–1069. DOI: 10.1002/biot.201200393

29. M. **König** and H.-G. Holzhütter. "Kinetic Modeling of Human Hepatic Glucose Metabolism in Type 2 Diabetes Mellitus Predicts Higher Risk of Hypoglycemic Events in Rigorous Insulin Therapy." In: *The Journal of biological chemistry* 287.44 (2012), pp. 36978–36989. DOI: 10.1074/jbc.M112.382069. pmid: 22977253

30. M. **König**, S. Bulik, and H.-G. Holzhütter. "Quantifying the contribution of the liver to glucose home-ostasis: a detailed kinetic model of human hepatic glucose metabolism." In: *PLoS Computational Biology* 8 (6 2012), e1002577. DOI: 10.1371/journal.pcbi.1002577

31. M. **König**, A. Dräger, and H.-G. Holzhütter. "CySBML: a Cytoscape plugin for SBML.". In: *Bioinformatics (Oxford, England)* 28 (18 2012), pp. 2402–2403. DOI: 10.1093/bioinformatics/bts432

32. C. Gille, C. Bölling, A. Hoppe, S. Bulik, S. Hoffmann, K. Hübner, A. Karlstädt, R. Ganeshan, M. **König**, K. Rother, M. Weidlich, J. Behre, and H.-G. Holzhütter. "HepatoNet1: a comprehensive metabolic reconstruction of the human hepatocyte for the analysis of liver physiology." In: *Molecular Systems Biology* 6 (2010), p. 411. DOI: 10.1038/msb.2010.62