Matthias **König**

Group Leader - Systems Medicine of Liver · Digital Health · Data Scientist · Computational Modeler

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Carrer Stages & Education

Independent Group Leader   Humboldt-Universität zu Berlin

DFG Position for Principal Investigators | Systems Medicine of the Liver   2021 – Present

- Established and lead the **Systems Medicine of the Liver Lab** at the Institute for Theoretical Biology.
- Secured competitive third-party funding (DFG, EU, BMBF) to advance digital physiology and personalized pharmacotherapy.
- Developed innovative digital twin models integrating physiology, pharmacokinetics, and AI-based decision support.
- Supervised and mentored PhD, Master, and Bachelor students, fostering interdisciplinary and open-science skills.
- Built international collaborations (Virtual Human Twin, EDITH, Lorentz Center) to strengthen systems medicine research.

Junior Group Leader   Humboldt-Universität zu Berlin

BMBF LiSyM Junior Group Leader | Systems Medicine of the Liver   2016 – 2021

- Founded an independent junior research group focused on multiscale computational modeling of liver physiology and disease.
- Developed predictive PBPK/PD models for drug metabolism, liver surgery outcomes, and metabolic disorders.
- Contributed to national flagship program **LiSyM – Liver Systems Medicine** with interdisciplinary and translational projects.
- Initiated and coordinated collaborative projects linking clinical hepatology, surgery, and computational biology.

PhD in Biophysics   Charité – University Medicine Berlin, Humboldt-Universität zu Berlin

Doctorate in Biophysics (magna cum laude) | Computational Modeling of Glucose Metabolism   2015

- Researched and developed detailed kinetic models of hepatic glucose metabolism and whole-body regulation.
- Demonstrated mechanisms underlying glucose homeostasis and hypoglycemia risk in type 2 diabetes.
- Supervisor: Prof. Hermann-Georg Holzhütter (Charité Berlin).

Scientific Staff Member   Charité – University Medicine Berlin

Researcher in HepatoSys and Virtual Liver initiatives   2008 – 2015

- Contributed to two major BMBF-funded consortia (**HepatoSys**, **Virtual Liver**) advancing systems medicine of the liver.
- Built multi-scale models of hepatic metabolism, perfusion, and drug elimination, bridging basic research and clinical application.
- Collaborated closely with experimental and clinical partners to validate models with in vitro, in vivo, and patient data.

Diploma in Biophysics   Humboldt-Universität zu Berlin

Diploma (equivalent to MSc, 1.0 with distinction)   2002 – 2008

- Acquired a strong foundation in biophysics, physiology, and computational modeling.
- Diploma thesis on systems biology modeling of hepatic metabolism, laying the groundwork for doctoral research.

Surgical Support Assistant (Rotational Role)   Bethesda Hospital Stuttgart

Clinical experience prior to academic studies   2001

- Assisted surgical teams with preparation, organization, and post-operative support across multiple departments.
- Coordinated with nurses, anesthesiologists, and surgeons to maintain high standards of patient safety and workflow efficiency.
- Gained early exposure to interdisciplinary teamwork in high-pressure clinical environments.

Training & Certifications

Leadership Certificate Program   ZEWK, TU Berlin

Certificate in Academic Leadership (100 AE)   2025

- Completed a two-stage leadership program designed for junior professors and early-career group leaders.
- Trained in collaborative and respectful teamwork, effective communication, and conflict resolution.
- Strengthened ability to lead within collegial academic structures, balancing autonomy and institutional expectations.
- Enhanced professional skills to take on leadership roles with clarity and confidence.

Science Communication Certificate Program   ZEWK, TU Berlin

Certificate in Science Communication (80/200 AE)   2025 - 2026

- Gained advanced training in effectively communicating research to diverse audiences including the public, media, funding bodies, and scientific peers.

- Acquired skills in media and press work, strategic communication, and legal frameworks in science communication.
- Developed practical competencies in writing, presenting, and visual design through project-based exercises.
- Applied knowledge in real-world communication formats to enhance outreach and visibility of scientific work.

EP PerMed Training on Scientific Integrity
European Partnership for Personalised Medicine

Training on Research Integrity and ELSA (20 AE)   2025

- Participated in international training on ethical, legal, and social aspects (ELSA) of personalised medicine.
- Studied European Code of Conduct guidelines and key principles of research integrity.
- Learned procedures for good research practice, ethics compliance under Horizon Europe, and responsible dissemination of results.
- Strengthened understanding of integrity issues in biomedical and translational research.

Digital Health Professions Educator (DHPE)
Charité – Universitätsmedizin Berlin

Certificate in Digital Teaching for Health Professions (200 AE)   2024 – 2025

- Completed faculty development program focused on digital teaching and innovation in healthcare education.
- Designed and implemented future-oriented teaching scenarios, integrating blended and digital learning.
- Enhanced institutional teaching capacity through innovative, research-based learning formats.
- Applied competencies to improve curriculum development and digitally supported learning in health sciences.

IAR Identify, Assist, Refer
Health & Wellness, University of Toronto

Certificate in Mental Health Assistance and Support (10 AE)   2025

- Completed training on identifying mental health challenges and offering appropriate assistance.
- Gained skills in facilitating help-seeking behavior and providing mental health support in challenging situations.
- Learned strategies for effective communication and crisis intervention.
- Acquired practical knowledge to support individuals experiencing mental health difficulties and refer them to necessary services.

Skills

Spoken Languages	**German**, **English**, Spanish (B2)
Teaching & Communication	**University Teaching**, Project-Based Learning, Digital Learning Tools, Science Communication, Mentoring & Supervision, Public Engagement
Research & Modeling	**Physiologically Based Pharmacokinetic (PBPK) Modeling**, **Pharmacodynamics (PD)**, Systems Biology, Multiscale Modeling, Machine Learning, FAIR Data Management, Reproducible Workflows, Computational Simulation
Programming	**Python**, R, Julia, Java, C++, MATLAB, SQL, HTML, JavaScript
Tools & Software	**PyCharm**, **VS Code**, **git**, **Excel**, LaTeX, Typst, Word, PowerPoint, Canva, BioRender, Adobe Illustrator, Inkscape

Scientific Results

Ten Selected Publications (total: 55, HF 25, 🎓 Google Scholar 09/25)

1. **Cross-Species Variability in Lobular Geometry and Cytochrome P450 Hepatic Zonation: Insights into CYP1A2, CYP2E1, CYP2D6 and CYP3A4**. Mohamed Albadry, Jonas Kuettner, Jan Grzegorzewski, Olaf Dirsch, Eva Kindler, Robert Klopfleisch, Vaclav Liska, Vladimira Moulisova, Sandra Nickel, Richard Palek, Jachym Rosendorf, Sylvia Saalfeld, Utz Settmacher, Hans-Michael Tautenhahn, **Matthias König**△, Uta Dahmen△ (△ equal contribution); Front Pharmacol. 2024 May 16;15:1404938, 10.3389/fphar.2024.1404938, IF: **5.4**, Last Equal Author

2. **A pathway model of glucose-stimulated insulin secretion in the pancreatic β-cell**. Maheshvare MD., Raha S., **König M.**△, and Pal D.△ (△ equal contribution); Front. Endocrinol. 14:1185656, 10.3389/fendo.2023.1185656, IF: **5.7**, Last Equal Author

3. **Physiologically based pharmacokinetic (PBPK) modeling of the role of CYP2D6 polymorphism for metabolic phenotyping with dextromethorphan**. Grzegorzewski, J., Brandhorst, J., **König, M.**; Front Pharmacol. 2022 Oct 24;13:1029073, 10.3389/fphar.2022.1029073, IF: **4.4**, Last Author

4. **Pharmacokinetics of caffeine: A systematic analysis of reported data for application in metabolic phenotyping and liver function testing**. Jan Grzegorzewski, Florian Bartsch, Adrian Köller, and **Matthias König**; Frontiers in Pharmacology 2022, Vol12, 10.3389/fphar.2021.752826, IF: **4.4**, Last Author

5. 📄◈ **Prediction of survival after hepatectomy using a physiologically based pharmacokinetic model of indocyanine green liver function tests**. Adrian Köller, Jan Grzegorzewski, Michael Tautenhahn, **Matthias König**; Front. Physiol., 22 November 2021, 10.3389/fphys.2021.730418, IF: **3.2**, <u>Last Author</u>

6. 📄◈ **Physiologically based modeling of the effect of physiological and anthropometric variability on indocyanine green based liver function tests**. Adrian Köller, Jan Grzegorzewski and **Matthias König**; Front Physiol. 2021 Nov 22;12:757293, 10.3389/fphys.2021.757293, IF: **3.2**, <u>Last Author</u>

7. 📄◈ **PK-DB: pharmacokinetics database for individualized and stratified computational modeling**. Grzegorzewski J, Brandhorst J, Green K, Eleftheriadou D, Duport Y, Barthorscht F, Köller A, Ke DYJ, De Angelis S, **König M.**; Nucleic Acids Res. 2021 Jan 8;49(D1):D1358-D1364, 10.1093/nar/gkaa990, IF: **16.7**, <u>Last Author</u>

8. 📄◈ **SBML Level 3: an extensible format for the exchange and reuse of biological models**. SM Keating, D Waltemath, **M König**, F Zhang, A Dräger, C Chaouiya, FT Bergmann, A Finney, CS Gillespie, T Helikar, S Hoops, RS Malik-Sheriff, SL Moodie, II Moraru, CJ Myers, A Naldi, BG Olivier, S Sahle, JC Schaff, LP Smith, MJ Swat, DT, L Watanabe, DJ Wilkinson, ML Blinov, K Begley, JR Faeder, HF Gómez, TM Hamm, Y Inagaki, W Liebermeister, AL Lister, D Lucio, E Mjolsness, CJ Proctor, K Raman, N Rodriguez, CA Shaffer, BE Shapiro, J Stelling, N Swainston, N Tanimura, J Wagner, M Meier-Schellersheim, HM Sauro, B Palsson, H Bolouri, H Kitano, Akira Funahashi, H Hermjakob, JC Doyle M Hucka, and SBML Community members; Mol Syst Biol. 2020;16(8):e9110, 10.15252/msb.20199110, IF: **8.8**

9. 📄 **HEPATOKIN1: A Biochemistry-Based Model of Liver Metabolism Suited for Applications in Medicine and Pharmacology**. Berndt N., Bulik S., Wallach I., Wünsch T., **König M.**, Stockmann M., Meierhofer M., Holzhütter HG.; Nat Commun. 2018 Jun 19;9(1):2386., 10.1038/s41467-018-04720-9, IF: **15.4**

10. 📄 **Quantifying the Contribution of the Liver to the Homeostasis of Plasma Glucose: A Detailed Kinetic Model of Hepatic Glucose Metabolism Integrated with the Hormonal Control by Insulin, Glucagon and Epinephrine**. **König M.**, Bulik S. and Holzhütter HG.; PLoS Comput Biol. 2012 Jun;8(6):e1002577. Epub 2012 Jun 21., 10.1371/journal.pcbi.1002577, IF: **4.9**, <u>First Author</u>

Ten Selected Research Outcomes

1. 🗄◈ Database **PK-DB - Pharmacokinetics database**. doi:10.1093/nar/gkaa990 Developed the first FAIR-compliant open database for pharmacokinetics, integrating clinical and pre-clinical trial data. PK-DB enables reproducible PBPK/PD modeling, supports individualized simulations, and has become a key infrastructure for computational pharmacology research.

2. ⚙◈ Software **sbmlutils - Python utilities for SBML**. doi:10.5281/zenodo.597149 Created a versatile Python library to streamline the use of SBML models, providing robust utilities for model handling, analysis, and integration with libSBML. Widely used in reproducible modeling workflows across systems biology.

3. ⚙◈ Software **SBML4Humans - SBML simulation made easy**. Designed an interactive reporting framework that makes SBML models human-readable and accessible, enabling experts and newcomers to explore model content without technical barriers.

4. ⚙◈ Software **sbmlsim - SBML simulation made easy**. Built a lightweight Python package that simplifies simulations of SBML models on top of libRoadRunner, lowering the entry barrier for model testing and teaching.

5. ⚙◈ Software **cysbml - Cytoscape 3 app for the Systems Biology Markup Language**. doi:10.5281/zenodo.597154 Developed and maintained a widely used Cytoscape app for visualization of SBML models in network contexts. cy3sbml has facilitated intuitive exploration of complex models in systems biology and bioinformatics.

6. ⚙◈ Software **brendapy - BRENDA in python**. Authored a Python package providing direct programmatic access to BRENDA enzyme information, enabling large-scale, automated enzyme analysis and integration into computational pipelines.

7. ⚙◈ Software **libsbgnpy - Python library for SBGN**. Developed a Python library for working with Systems Biology Graphical Notation (SBGN), supporting standardized visualization and integration of pathway information.

8. ⚙◈ Software **roadrunner - High-performance simulator for SBML**. Contributed to the development of libRoadRunner, a C/C++ library using LLVM for ultra-fast simulation of SBML models, setting a benchmark for performance in computational biology.

9. ⚙ ◈ Software **COBRApy - COBRA python package**. Advanced COBRApy, the leading Python package for constraint-based reconstruction and analysis, widely adopted in genome-scale metabolic modeling. Provides access to key methods such as flux balance and flux variability analysis.

10. ⚙ ◈ Software **tellurium - systems biology simulation library**. Co-developed Tellurium, a Python-based environment for reproducible dynamical modeling of biological networks. Integrated standard formats with powerful simulation libraries, enabling accessible and transparent modeling.

Supervision of Researchers

Over the last 5 years, 1 PhD theses, 3 Master thesis, 11 Bachelor's theses, 18 Humboldt-Internship students (HIC), and 4 Google Summer of Code (GSOC) students have been supervised. I am currently supervising 1 PhD, 3 Master, and 1 Internship projects (group members).

1. 📄◈ **A Systems Pharmacology Approach to Rivaroxaban: Physiologically Based Modeling of Pharmacokinetics and Coagulation Dynamics**. Elisabetta Casabianca (supervisor: **Matthias König**); Master Thesis, July 2025

2. 📄◈ **A physiological-based pharmacokinetic/ pharmacodynamic (PBPK/PD) model of the angiotensin II receptor blocker (ARB) losartan**. Ennie Tensil (supervisor: **Matthias König**); Bachelor Thesis, July 2025

3. 📄◈ **Physiologically-Based Pharmacokinetic/Pharmacodynamic Modeling of Dapagliflozin: Exploring the Impact of Dosing, Hepatorenal Impairment and Food Intake**. Nike Nemitz (supervisor: **Matthias König**); Bachelor Thesis, June 2025

4. 📄◈ **A physiological-based pharmacokinetic (PBPK) model of the sulfonylurea glimepiride**. Michelle Elias (supervisor: **Matthias König**); Bachelor Thesis, April 2025

5. 📄◈ **Physiologically based pharmacokinetic/pharmacodynamic modeling of the direct renin inhibitor aliskiren: Exploring the impact of hepatorenal impairment and drug-drug interactions**. Bachelor Thesis Yusuf Ali Kulanoglu (supervisor: **Matthias König**); Bachelor Thesis, January 2025

6. 📄◈ **Quantitative Image Analysis of Hepatic Zonation in Cytochrome P450 and Steatosis Using Whole Slide Scans**. Master Thesis Jonas Küttner (supervisor: **Matthias König**); Master Thesis, August 2024

7. 📄◈ **Enhancing Our Understanding of Enalapril's Pharmacokinetics: A Physiologically Based Modeling Approach**. Master Thesis Shubhankar Palwankar (supervisor: **Matthias König**); Master Thesis, May 2024

8. 📄◈ **A systematic overview of protein variability in cytochrome P450 and UDP-glucuronosyltransferase enzymes in the human liver**. Bachelor Thesis Afruja Hossain (supervisor: **Matthias König**); Bachelor Thesis, Jan 2024

9. 📄◈ **A physiologically based pharmacokinetic (PBPK) model of the probe drug talinolol for the characterization of intestinal P-glycoprotein**. Bachelor Thesis Beatrice Stemmer Mallol (supervisor: **Matthias König**); Bachelor Thesis, July 2023

10. 📄◈ **Physiologically based pharmacokinetic (PBPK) modeling for dynamical liver function tests and CYP phenotyping**. Jan Grzegorzewski (supervisor: **Matthias König**); PhD Thesis, Jan 2023

11. 📄◈ **A physiologically based model of pravastatin - The role of genotypes and hepatic or renal impairment on the pharmacokinetics of pravastatin**. Helena Leal Pujol (supervisor: **Matthias König**); Bachelor Thesis, May 2022

12. 📄◈ **Computational modelling of omeprazole - pharmacokinetics and pharmacodynamics**. Sükrü Balci (supervisor: **Matthias König**); Bachelor Thesis, October 2021

13. 📄 **A Physiologically Based Model of Indocyanine Green Liver Function Tests - Effects of Physiological Factors, Hepatic Disease and Hepatic Surgery**. Adrian Köller (supervisor: **Matthias König**); Bachelor Thesis, March 2021

14. 📄 **Computational Modelling of Simvastatin - Effects on HMG-CoA Reductase Activity and Cholesterol**. Florian Bartsch (supervisor: **Matthias König**); Bachelor Thesis, November 2020

15. 📄 **Computational Modelling of Midazolam Clearance: Effect of Inhibitors and Inducers**. Yannick Duport (supervisor: **Matthias König**); Bachelor Thesis, August 2020

Activities in the Research System

- ↗ 2025–2026: **Leading X-Student Research Group: Digital Twins in Action — Optimizing Direct Oral Anticoagulant Use** - Supervising students in PBPK modeling and advancing precision medicine.
- ↗ 2025: **Organizing Workshop Open Science & Reproducibility — For Computational Models in Systems Biology & Medicine** - Featuring interactive sessions (LEGO® Serious Play), reproducibility workflows, and open publishing practices.
- ↗ 2025–2026: **Member Research Data Alliance (RDA) Working Group: Building Immune Digital Twins** - Developing standards and methods for Digital Twins.
- ↗ 2018–2023, 2025–2027: **Elected SBML Editor** - Advanced the Systems Biology Markup Language (SBML) standard by coordinating editorial processes, improving specifications, and fostering interoperability.
- ↗ 2024–2026: **Open Science Ambassador, Humboldt-University Berlin** - Promoted reproducibility, FAIR data, and open science practices within the Berlin University Alliance.
- ↗ 2017–2022, 2024–2027: **Elected SED-ML Editor** - Enhanced the Simulation Experiment Description Markup Language to improve reproducibility and exchangeability of simulation experiments.
- ↗ 2023–2026: **Elected PEtab Editor** - Strengthened the PEtab standard for parameter estimation problems, ensuring community adoption and long-term sustainability.
- ↗ 2017–2025: **Elected COMBINE Coordinator** - Led international coordination of community standards (SBML, SED-ML, PEtab, etc.), strengthened collaborations, and organized annual COMBINE meetings.
- ↗ 2025: **Interview: Reproducibility, Open Science, and the Future of Biological Research** - Berlin University Alliance feature highlighting the reproducibility crisis, FAIR data, open standards, and cultural change in academia.
- ↗ 2023: **Led X-Student Research Group: Physiologically Based Digital Twins for Hypertension Therapy** - Focused on ACE inhibitors and diuretics.
- ↗ 2023–2024: **Expert Panel Member: PharmVar CYP1A2 Gene Panel** - Advanced pharmacogenomics standards in drug metabolism.
- ↗ 2023: **Co-authored Open Science Concept: Eleven Strategies for Training Reproducible Research** - Implemented institutional strategies for reproducible research and open science training.
- ↗ 2022: **Organized 13th Computational Modeling in Biology Network (COMBINE) Meeting** - Brought together global experts in modeling standards in Berlin.
- ↗ 2022: **Led X-Student Research Group: Physiologically Based Modeling of Drugs — ACE Inhibitors in Hypertension** - Mentored interdisciplinary student teams.

Funding

- 📷 10/2025 – 2026, BMBF, 1.500€, **X-Student Research Group - Digital Twins in Action: Optimizing Direct Oral Anticoagulant Use.** Project-based teaching initiative on digital twins in medicine, focusing on physiologically based pharmacokinetic (PBPK) modeling to optimize the use of direct oral anticoagulants.
- 📷 2025 – 2026, DFG, 15.000€, **SPP2311 - Startup Funding - SPP-FEMVis: Advancing Open Science with Web-Based FEM Visualization.** Startup funding to develop an open science platform for interactive, web-based visualization of finite element method (FEM) simulations.
- 📷 2024 – 2025, Circle U., 10.000€, **AlgoNomy - Algorithmic Regulation Before Medical Liability - Advancing Doctor-Patient Autonomy in AI-Driven Healthcare.** Building an international academic network to investigate the role of algorithms and AI in medical decision support systems, with a focus on legal, ethical, and patient autonomy implications.
- 📷 2024 – 2025, BUA - BMBF, 4.000€, **Open Science Ambassador.** Supporting the promotion and implementation of open science practices across research communities at Berlin Universities, with a focus on reproducibility, FAIR data, and fostering collaborative exchange.
- 📷 2024 – 2027, DFG, 219.000€, **SPP2311 - SimLivA - SIMulation supported LIVer Assessment for donor organs.** Developing computational models and simulation workflows to assess liver function in donor organs, advancing predictive tools for transplantation and improving clinical decision-making.
- 📷 04/2023 – 2023, BUA - BMBF, 1.500€, **X-Student Research Group - Physiologically based digital twins for the treatment of hypertension with ACE inhibitors and diuretics.** Project-based teaching initiative on

digital twins in pharmacology, focusing on physiologically based pharmacokinetic (PBPK) modeling to optimize hypertension therapy with ACE inhibitors and diuretics.

- ◉ 2023 – 2026, BMBF, 311.000€, **ATLAS - AI and Simulation for Tumor Liver ASessment.** Developing AI-driven and simulation-based methods to improve the assessment of liver tumors, integrating computational modeling with clinical data to support personalized diagnosis and treatment planning.
- ◉ 10/2022 – 2023, BUA - BMBF, 1.500€, **X-Student Research Group - Physiologically based modeling of drugs: ACE inhibitors in the treatment of high blood pressure.** nan
- ◉ 2021 – 2025, DFG, 425.000€, **FOR5151 - QuaLiPerF - Quantifying Liver Perfusion-Function Relationship in Complex Resection – A Systems Medicine Approach.** Advancing systems medicine by developing computational models to quantify the relationship between liver perfusion and function in complex surgical resections, supporting risk assessment and personalized treatment planning.
- ◉ 2020 – 2023, DFG, **SPP2311 - SimLivA - SIMulation supported LIVer Assessment for donor organs.** Collaborative project developing simulation approaches to assess donor liver function, aiming to improve transplantation outcomes through predictive computational modeling.
- ◉ 2020 – 2021, EOSC-life, 25.000€, **EOSC-Life - Reproducible simulation studies targeting COVID-19.** Developed reproducible computational simulation studies to investigate COVID-19 dynamics, integrating standardized workflows and open science practices for rapid and transparent research dissemination.
- ◉ 2016 – 2022, BMBF, 723.000€, **LiSyM - Systems Medicine of the Liver - Junior group leader - Multi-scale models for the personalized evaluation of liver function.** Led a junior research group developing multi-scale computational models to assess and predict liver function, advancing personalized medicine approaches and translational applications in hepatology.

Academic Distinctions

Michael Stifel Prize
Friedrich Schiller University Jena

Awarded for outstanding interdisciplinary and data-driven research achievements. 2023
- Recognized for contributions advancing computational modeling and systems medicine.

Google Summer of Code Scholarship
Google / Open Source Initiative

Scholarship to develop SBML tools as part of the Google Summer of Code program. 2015
- Advanced open-source infrastructure for systems biology and reproducible modeling.

Scholarship
Studienstiftung des Deutschen Volkes

Awarded a prestigious scholarship from the German National Academic Foundation. 2005
- Selected among top students in Germany for academic excellence and potential.

Teaching

Digital Teaching Project

Course	Description
DHPE-PKPD – An Interactive and Open Course on Pharmacokinetic (PK) and Pharmacodynamic (PD) Modeling Large-scale digital teaching project DHPE (80 AE) Charité – Universitätsmedizin Berlin 10/2024 – 07/2025 ◩ ◈	• Designed and implemented an innovative interactive course integrating theory, simulation practice, and reflection. • Leveraged open-source tools (Jupyter, GitHub, Quarto) to create reproducible, FAIR-compliant teaching materials. • Applied real-world pharmacology case studies and interactive simulations to foster research-oriented learning. • Pioneered blended learning approaches, combining digital resources with in-person tutorials. • Released all course materials openly, promoting accessibility, transparency, and reusability. • Received highly positive student evaluations for interactivity, structure, and practical relevance.

Research Project–Based Teaching

Course	Description
X-Student Research Group: Digital Twins in Action – Optimizing Direct Oral Anticoagulant Use Berlin University Alliance (BUA) 10/2025 – 03/2026	• Leading students in developing a digital twin of apixaban to simulate pharmacokinetics and clinical outcomes. • Combining lectures, tutorials, and hands-on modeling for experiential learning. • Enabling participants to explore personalized dosing strategies and safety aspects in anticoagulant therapy.
X-Student Research Group: Physiologically Based Digital Twins for Hypertension Therapy Berlin University Alliance (BUA) 04/2023 – 09/2023	• Supervised interdisciplinary teams modeling hydrochlorothiazide and lisinopril using PBPK methods. • Trained students in absorption, distribution, metabolism, and excretion (ADME) processes. • Fostered collaboration between STEM and medical students in clinically relevant pharmacology projects.
X-Student Research Group: Physiologically Based Modeling of ACE Inhibitors Berlin University Alliance (BUA) 10/2022 – 03/2023	• Guided students in developing PBPK models for lisinopril and ramipril. • Integrated lectures, tutorials, and project-based work to link theory with practice. • Strengthened student competencies in computational pharmacokinetics and systems medicine.

Lecture and Course–Based Teaching

Course	Description
Theory, Tools and Methods in Biology – Pharmacokinetic/Pharmacodynamic Modeling Humboldt-Universität zu Berlin (HU) 04/2025 – 09/2025 04/2024 – 09/2024 04/2023 – 09/2023	• Led pharmacokinetic modeling submodule (DHPE-PKPD) • Designed and delivered lectures on drug distribution, clearance, elimination, PBPK modeling, and PD • Integrated clinical applications and drug–drug interaction case studies • Developed submodule as part of the DHPE program
Important Models of Quantitative Biology from the Literature Humboldt-Universität zu Berlin (HU) 10/2021 – 03/2022 10/2020 – 03/2021 10/2019 – 03/2020 10/2018 – 03/2019	• Taught core methods for Boolean and ODE modeling in metabolism and signaling • Supervised student implementation and critical analysis of published models • Fostered analytical skills through structured discussion and group projects
Models of Cellular Processes Humboldt-Universität zu Berlin (HU) 10/2019 – 03/2020	• Introduced constraint-based, Boolean, and ODE models of cellular processes • Taught parameter optimization, stochastic modeling, and sensitivity analysis • Applied methods to real-world biological data examples

List of Publications

Publications

1. 📄 **Inflammation and autophagy in peripheral nerves of rodent models with metabolic syndrome and type 2 diabetes mellitus**. Baum P, Ebert T, Klöting N, Krupka S, **König M**, Paeschke S, Stock P, Bulc M, Blüher M, Palus K, Nowicki M, Kosacka J.; Neurosci Res. 2025 Apr 17:S0168-0102(25)00070-7, 10.1016/j.neures.2025.04.002, IF: **2.4**

2. 📄 **Anti-Endoglin monoclonal antibody prevents the progression of liver sinusoidal endothelial inflammation and fibrosis in MASH**. Eissazadeh S, Fikrova P, Rathouska JU, Nemeckova I, Tripska K, Vasinova M, Havelek R, Mohammadi S, Igreja Sa IC, Theuer C, **König M**, Micuda S, Nachtigal P; Life Sci. 2025 Jan 29:123428, 10.1016/j.lfs.2025.123428, IF: **5.2**

3. 📄 **Specifications of standards in systems and synthetic biology: status, developments, and tools in 2024**. Martin Golebiewski, Gary Bader, Padraig Gleeson, Thomas E Gorochowski, Sarah M Keating, **Matthias König**, Chris J Myers, David P Nickerson, Björn Sommer, Dagmar Waltemath, Falk Schreiber; J Integr Bioinform. 2024 Jul 22, 10.1515/jib-2024-0015, IF: **1.5**

4. 📄◆ **Cross-Species Variability in Lobular Geometry and Cytochrome P450 Hepatic Zonation: Insights into CYP1A2, CYP2E1, CYP2D6 and CYP3A4**. Mohamed Albadry, Jonas Kuettner, Jan Grzegorzewski, Olaf Dirsch, Eva Kindler, Robert Klopfleisch, Vaclav Liska, Vladimira Moulisova, Sandra Nickel, Richard Palek, Jachym Rosendorf, Sylvia Saalfeld, Utz Settmacher, Hans-Michael Tautenhahn, **Matthias König**△, Uta Dahmen△ (△ equal contribution); Front Pharmacol. 2024 May 16;15:1404938, 10.3389/fphar.2024.1404938, IF: **5.4**, Last Equal Author

5. 📄◆ **Bayesian modelling of time series data (BayModTS)-a FAIR workflow to process sparse and highly variable data**. Höpfl S, Albadry M, Dahmen U, Herrmann KH, Kindler EM, **König M**, Reichenbach JR, Tautenhahn HM, Wei W, Zhao WT, Radde NE.; Bioinformatics. 2024 May 2;40(5):btae312, 10.1093/bioinformatics/btae312, IF: **6.0**

6. 📄◆ **The simulation experiment description markup language (SED-ML): language specification for level 1 version 5**. Smith LP, Bergmann FT, Garny A, Helikar T, Karr J, Nickerson D, Sauro H, Waltemath D, **König M.**; J Integr Bioinform. 2024 Apr 15, 10.1515/jib-2024-0008, IF: **1.5**, Last Author

7. 📄 **Quantifying fat zonation in liver lobules: an integrated multiscale in silico model combining disturbed microperfusion and fat metabolism via a continuum biomechanical bi-scale, tri-phasic approach**. Lena Lambers, Navina Waschinsky, Jana Schleicher, **Matthias König**, Hans-Michael Tautenhahn, Mohamed Albadry, Uta Dahmen and Tim Ricken; Biomech Model Mechanobiol. 2024 Feb 25., 10.1007/s10237-023-01797-0, IF: **3.1**

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8. 📄 **Simulation of zonation-function relationships in the liver using coupled multiscale models: Application to drug-induced liver injury**. Steffen Gerhäusser, Lena Lambers, Luis Mandl, Julian Franquinet, Tim Ricken, **Matthias König**; bioRxiv 2024.03.26.586870;, 10.1101/2024.03.26.586870, <u>Last Author</u>

9. 📄◈ **Insights into Intestinal P-glycoprotein Function using Talinolol: A PBPK Modeling Approach**. Beatrice Stemmer Mallol, Jan Grzegorzewski, **Matthias König**; bioRxiv 2023.11.21.568168, 10.1101/2023.11.21.568168, <u>Last Author</u>

10. 📄◈ **A physiologically based pharmacokinetic model for CYP2E1 phenotyping via chlorzoxazone**. J. Küttner, J. Grzegorzewski, HM. Tautenhahn, **M. König**; bioRxiv 2023.04.12.536571, 10.1101/2023.04.12.536571, <u>Last Author</u>

11. 📄◈ **standard-GEM: standardization of open-source genome-scale metabolic models**. Mihail Anton, Eivind Almaas, Rui Benfeitas, Sara Benito-Vaquerizo, Lars M. Blank, Andreas Dräger, John M. Hancock, Cheewin Kittikunapong, **Matthias König**, Feiran Li, Ulf W. Liebal, Hongzhong Lu, Hongwu Ma, Radhakrishnan Mahadevan, Adil Mardinoglu, Jens Nielsen, Juan Nogales, Marco Pagni, Jason A. Papin, Kiran Raosaheb Patil, Nathan D. Price, Jonathan L. Robinson, Benjamín J. Sánchez, Maria Suarez-Diez, Snorre Sulheim, L. Thomas Svensson, Bas Teusink, Wanwipa Vongsangnak, Hao Wang, Ahmad A. Zeidan, Eduard J. Kerkhoven; bioRxiv 2023.03.21.512712, 10.1101/2023.03.21.512712

12. 📄◈ **Simvastatin therapy in different subtypes of hypercholesterolemia - a physiologically based modelling approach**. F. Bartsch, J. Grzegorzewski, H. Pujol, HM. Tautenhahn, **M. König**; medRxiv 2023.02.01.23285358, 10.1101/2023.02.01.23285358, <u>Last Author</u>

13. 📄◈ **FAIR Sharing of Reproducible Models of Epidemic and Pandemic Forecast**. Ramachandran, K.△; **König, M.**△; Scharm, M.; Nguyen, T.V.N.; Hermjakob, H.; Waltemath, D.; Malik Sheriff, R.S. (△ equal contribution); Preprints 2022, 2022060137, 10.20944/preprints202206.0137.v1, <u>First Equal Author</u>

14. 📄◈ **Dynamic Flux Balance Analysis Models in SBML**. **Matthias König**△, Leandro H. Watanabe△, Jan Grzegorzewski, and Chris J. Myers. (△ equal contribution); bioRxiv 245076, 10.1101/245076, <u>First Equal Author</u>

15. 📄 **Ten Simple Rules for FAIR Sharing of Experimental and Clinical Data with the Modeling Community**. **Matthias König**△, Jan Grzegorzewski, Martin Golebiewski, Henning Hermjakob, Mike Hucka, Brett Olivier, Sarah M. Keating, David Nickerson, Falk Schreiber, Rahuman Sheriff, Dagmar Waltemath; Preprints 2021, 2021080303, 10.20944/preprints202108.0303.v2, <u>First Author</u>

16. 📄◈ **SED-ML Validator: tool for debugging simulation experiments**. Bilal Shaikh, Andrew Philip Freiburger, **Matthias König**, Frank T. Bergmann, David P. Nickerson, Herbert M. Sauro, Michael L. Blinov, Lucian P. Smith, Ion I. Moraru, Jonathan R. Karr; arXiV, 2021, 10.48550/arXiv.2106.00844

17. 📄◈ **Executable Simulation Model of the Liver**. **Matthias König**; bioRxiv 2020.01.04.894873, 10.1101/2020.01.04.894873v1, <u>First Author</u>

18. 📄◈ **cy3sabiork: A Cytoscape app for visualizing kinetic data from SABIO-RK**. **König M.**; [version 1; referees: awaiting peer review]. F1000Research 2016, 5:1736, 10.12688/f1000research.9211.1, <u>First Author</u>

Selected Presentations

1. 📄 **Reproducibility of a Digital Twin of Glimepiride for Personalized and Stratified Diabetes Treatment**. Michelle Elias and **Matthias König**; *Institute for Theoretical Biology, Institute Seminar*, 2025-09-10, <u>Invited Talk</u>

2. 📄 **Reproducible Digital Twins for Studying the Effect of Disease on Pharmacokinetics**. **Matthias König**; *17th International Conference on Systems Biology of Human Disease (SBHD2025)*, 2025-06-16, <u>Selected Talk</u>

3. 📄 **Digital Twins of the Liver in Pharmacokinetics**. **Matthias König**; *Camo Seminar, KIT Institute of Biomedical Engineering, Computational Cardiac Modeling*, 2025-04-24, <u>Invited Talk</u>

4. 📄 **Reproducible Digital Twins in Pharmacokinetics**. **Matthias König**; *9th Disease Maps Community Meeting (DMCM2025)*, 2025-04-17, <u>Selected Talk</u>

5. 📄 **Reproducible digital twins for personalized drug pharmacokinetics**. **Matthias König**; *Disease Maps Meeting*, 2025-02-05, <u>Invited Talk</u>

6. **Reproducible digital twins for personalized liver function assessment**. **Matthias König**; *University of Darmstadt, Institute for Mechanics, Institute Seminar*, 2025-02-05, <u>Invited Talk</u>

7. 📄 **Reproducible digital twins for personalized liver function assessment**. **Matthias König**; *COMBINE 2024 Stuttgart*, 2024-09-02, <u>Selected Talk</u>

8. 📑📄 **Reproducible digital twins for personalized liver function assessment**. **Matthias König**; *e:Med Meeting 2023 on Systems Medicine*, 2023-10-10, <u>Selected Talk</u>

9. 📑📄 **Reproducible digital twins for personalized liver function assessment**. **Matthias König**; *Institute for Theoretical Biology Meeting*, 2023-10-10, <u>Invited Talk</u>

10. 📄 **Studying the impact of drug metabolism on the liver tissue: An integrated biomechanical modeling approach**. **Matthias König**, Steffen Gerhäusser, Luis Mandl, Lena Lambers, Uta Dahmen, Hans-Michael Tautenhahn, Tim Ricken; *X International Conference on Computational Bioengineering*, 2023-09-22, <u>Selected Talk</u>

11. 📄 **Digital twins for liver function & metabolic phenotyping**. **Matthias König**; *AstraZeneca seminar*, 2023-09-01, <u>Invited Talk</u>

12. 📄 **Advancing Liver Function Assessment: Personalized and Stratified Approaches with Standardized Computational Models and Data**. **Matthias König**; *Workshop on Computational Models in Biology and Medicine 2023*, 2023-06-19, <u>Invited Talk</u>

13. 📄 **Digital twins for liver function & metabolic phenotyping**. **Matthias König**; *Workshop on Modelling in Biology and Medicine*, 2023-05-22, <u>Invited Talk</u>

14. 📑📄 **Developing computational models with SBML - sbmlutils & cy3sbml**. **Matthias König**; *CRBM Network Modeling Virtual Symposium*, 2022-07-22, <u>Selected Talk</u>

Selected Panels

1. **Real Work Experiences for a Real Career: What Learnings and Skills Really Matter?**. **Matthias König**; *HIC conference 2025, Humboldt Internship Program Day*, 2025-07-07, <u>Panelist</u>

2. **Methods of Inclusion: Designing Research for a Plural World**. **Matthias König**, Fariha Azad, Lara Bister, Michaela Kreyenfeld; *Berlin University Alliance Fellows Forum with Einstein Center Population Diversity*, 2025-06-11, <u>Panelist</u>

3. **AI as a medical device - Challenges and regulatory perspective**. **Matthias König**, Valentina Calderai; *Festival della Robotica 2025*, 2025-05-11, <u>Panelist</u>
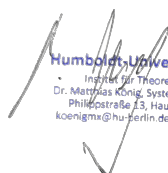
Selected Posters

1. 📄 **A Physiologically Based Pharmacokinetic and Pharmacodynamic Model of Lixisenatide**.
   Olivia Yau[2], **Matthias König**[1]
   [1]Humboldt-Universität zu Berlin, Institute for Theoretical Biology, Berlin, Germany, [2]University of Toronto, Dept. of Pharmacology and Toxicology, Toronto, Canada
   HIC conference 2025, Humboldt Internship Program Day, Berlin, 7 July 2025; 2025-07-07

2. 📄 **A Physiologically Based Pharmacokinetic Model of Dulaglutide**.
   Kim Minjun[2], **Matthias König**[1]
   [1]Humboldt-Universität zu Berlin, Institute for Theoretical Biology, Berlin, Germany, [2]National University of Singapore, Singapore
   HIC conference 2025, Humboldt Internship Program Day, Berlin, 7 July 2025; 2025-07-07

3. 📄 **A Physiologically-Based Pharmacokinetic and Pharmacodynamic Model of Liraglutide**.
   Isabella Tan[2], **Matthias König**[1]
   [1]Humboldt-Universität zu Berlin, Institute for Theoretical Biology, Berlin, Germany, [2]University of Toronto, Dept. Pharmacology & Biomedical Toxicology, Toronto, Canada
   HIC conference 2025, Humboldt Internship Program Day, Berlin, 7 July 2025; 2025-07-07

4. 📄 **PK-LLM : Large Language Model (LLM) for Pharmacokinetic (PK) Data Curation**.
   Prerna Parakkat[2], **Matthias König**[1]
   [1]Humboldt-University of Berlin, Institute for Theoretical Biology, Berlin, Germany, [2]Vellore Institute of Technology, Chennai, India
   HIC conference 2024, Humboldt Internship Program Day, Berlin, 18 July 2024; 2024-07-18

5. 📄 **Canagliflozin**.
   Vera Tereshchuk[1], **Matthias König**[2]
   [1]Moscow Institute of Physics and Technology, [2]Humboldt-University of Berlin, Institute for Theoretical Biology, Berlin, Germany
   HIC conference 2024, Humboldt Internship Program Day, Berlin, 18 July 2024; 2024-07-18

6. 📄 **A physiologically based pharmacokinetic model of morphine**.
Deepa Maheshvare M.[2], Rohini Chakraborty[2], Rohit Chakraborty[2], **Matthias König**[1]
[2]Humboldt-University of Berlin, Institute for Theoretical Biology, Berlin, Germany, [2]Indian Institute of Science, Bengaluru, India
HIC conference 2024, Humboldt Internship Program Day, Berlin, 18 July 2024; 2024-07-18

7. 📄 **Captopril in Focus: Establishing an Open Pharmacokinetic Dataset and PBPK Modeling**.
Mariia Myshkina[1], **Matthias König**[1]
[1]Humboldt-University of Berlin, Institute for Theoretical Biology, Berlin, Germany
PAGE2024 - Population Approach Group Europe, Rome, 26-28 June 2024; 2024-06-26

Dr. Matthias König
Berlin, 15. September 2025

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