

Matthias König



Systems Medicine · Computational Biology · Artificial Intelligence (AI) · Digital Health · Pharmacology

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Carrer Stages & Education

Professor of Metabolic Inflammation and Carcinogenesis of the Liver

 Lübeck University, Germany

Systems Medicine and Digital Twins

06/2026 -

- Lead the **Systems Medicine and Digital Twins** at the University of Lübeck. Development of digital twins, digital pathology methods.

Associate Professor of Pharmacoepidemiology and Data Science

 SDU, Odense, Denmark

Pharmacoepidemiology and Data Science

05/2026

- Lead the **Pharmacoepidemiology and Data Science Group** at the University of Southern Denmark (SDU), advancing research in real-world data analytics, causal inference, and translational data science.

Head of Computational Biomechanics Group

 University of Stuttgart

Coordination Project, DFG Priority Programme SPP 2311

12/2025 - 04/2026

- Lead the **Computational Biomechanics Group** at the University of Stuttgart.
- Coordinate interdisciplinary biomechanics and numerical modeling for robust, translational in silico models.
- Integrate modeling, simulation, and software usability toward clinical applications.
- Promote community building, standardization, and reproducibility within the SPP.

Head of Systems Medicine of the Liver Group

 Humboldt-Universität zu Berlin

DFG Position for Principal Investigators | Systems Medicine of the Liver

06/2021 – Present

- Established and lead the **Systems Medicine of the Liver Group** 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

2010 - 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 – 2009

- 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

- 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.

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.

AI Teaching Certificate (KI-Lehrzertifikat)

HU Berlin, KI-Campus 2.0 & AI Skills Initiative

Higher education didactics qualification on Artificial Intelligence (200 AE)

2025

- Completed: AI Foundations (96%), AI Advanced & Ethics (93%), and AI Didactics in Higher Education (91%).
- Covered core AI topics: machine learning, neural networks, Python/Jupyter, text and image processing, and responsible AI use.
- Training aligned with DGHD standards, including ethics, data and algorithmic governance, and regulatory aspects of AI.
- Focus on AI-supported teaching: generative AI, speech assistants, prompt design, development of AI-based OER teaching units.
- Included a teaching observation and reflective assessments demonstrating competence in designing and implementing AI-enhanced learning scenarios.

Science Communication Certificate Program

ZEWK, TU Berlin

Certificate in Science Communication (120/200 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, and responsible dissemination of results.
- Strengthened understanding of integrity issues in biomedical and translational research.

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.

Skills

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/ Pharmacodynamic (PBPK/PD), Systems Biology, Multiscale Modeling, Machine Learning & Artificial Intelligence, FAIR Data Management, Reproducible Workflows, Computational Simulation, Digital Pathology

Programming

Python, R, Julia, Java, C++, MATLAB, SQL, HTML, JavaScript, PyTorch, TensorFlow, SBML

Tools & Software

git, PyCharm, VS Code, Excel, LaTeX, Typst, Word, PowerPoint, Canva, BioRender, Adobe Illustrator, Inkscape

1.  **Parameter Uncertainty in the Optimization of Pharmacokinetic Models: A Reproducible Bayesian Approach.** Antonio Alavarez (supervisor: **Matthias König**); Master Thesis, April 2026, [Last Author](#)
2.  **A Systems Pharmacology Approach to Rivaroxaban: Physiologically Based Modeling of Pharmacokinetics and Coagulation Dynamics.** Elisabetta Casabianca (supervisor: **Matthias König**); Master Thesis, July 2025, [Last Author](#)
3.  **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, [Last Author](#)
4.  **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, [Last Author](#)
5.  **A physiological-based pharmacokinetic (PBPK) model of the sulfonyleurea glimepiride.** Michelle Elias (supervisor: **Matthias König**); Bachelor Thesis, April 2025, [Last Author](#)
6.  **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, [Last Author](#)
7.  **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, [Last Author](#)
8.  **Enhancing Our Understanding of Enalapril's Pharmacokinetics: A Physiologically Based Modeling Approach.** Master Thesis Shubhankar Palwankar (supervisor: **Matthias König**); Master Thesis, May 2024, [Last Author](#)
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13.  **Computational modelling of omeprazole - pharmacokinetics and pharmacodynamics.** Sükrü Balci (supervisor: **Matthias König**); Bachelor Thesis, October 2021, [Last Author](#)
14.  **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, [Last Author](#)
15.  **Computational Modelling of Simvastatin - Effects on HMG-CoA Reductase Activity and Cholesterol.** Florian Bartsch (supervisor: **Matthias König**); Bachelor Thesis, November 2020, [Last Author](#)
16.  **Computational Modelling of Midazolam Clearance: Effect of Inhibitors and Inducers.** Yannick Duport (supervisor: **Matthias König**); Bachelor Thesis, August 2020, [Last Author](#)

Scientific Results

Ten Selected Publications (total: 66, HF: 26:, i10: 36, citations: 3778,  Google Scholar 08/26)

1.  **A Physiologically Based Pharmacokinetic and Pharmacodynamic (PBPK/PD) Model of Dapagliflozin in Type 2 Diabetes Mellitus: The Effect of Dosing, Hepatorenal Impairment, and Food.** Nike Nemitz, Michelle Elias, **Matthias König**; *Pharmaceutics* 2026, 18(3), 287; <https://doi.org/10.3390/pharmaceutics18030287>, 10.3390/pharmaceutics18030287, IF: **5.5**, [Last Author](#)
2.  **A Digital Twin of the Angiotensin II Receptor Blocker Losartan: Physiologically Based Modeling of Blood Pressure Regulation.** Ennie Tensil, Mariia Myshkina, **Matthias König**; *Pharmaceutics* 2026, 18(2), 262; <https://doi.org/10.3390/pharmaceutics18020262>, 10.3390/pharmaceutics18020262, IF: **5.5**, [Last Author](#)
3.  **A Digital Twin of Glimepiride for Personalized and Stratified Diabetes Treatment.** Michelle Elias, **Matthias König**; *Front. Pharmacol.* 16:1686415., 10.3389/fphar.2025.1686415, IF: **4.8**, [Last Author](#)
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 Klopffleisch, Vaclav Liska, Vladimira Moulisova, Sandra Nickel, Richard Palek, Jachym Rosendorf, Sylvia Saalfeld, Utz Settmacher, Hans-Michael Tautenhahn, **Matthias König**^Δ, Uta Dahmen^Δ (^Δ equal contribution); *Front Pharmacol.* 2024 May 16;15:1404938, 10.3389/fphar.2024.1404938, IF: **5.4**, [Last Equal Author](#)
5.  **A pathway model of glucose-stimulated insulin secretion in the pancreatic β -cell.** Maheshvare MD., Raha S., **König M.**^Δ, and Pal D.^Δ (^Δ equal contribution); *Front. Endocrinol.* 14:1185656, 10.3389/fendo.2023.1185656, IF: **5.7**, [Last Equal Author](#)
6.  **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](#)
7.  **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](#)
8.  **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**, [Last Author](#)
9.  **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**, [Last Author](#)
10.  **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**

Ten Selected Research Outcomes

1.  **Automated Segmentation of Hepatic Vessels and Lobules in Whole-Slide Images Using U-Net Models.** Mehul Bafna, **Matthias König**, Sylvia Saalfeld, Vladimira Moulisova, Vaclav Liska, Uta Dahmen, Mohamed Albadry; *bioRxiv* 2025.09.08.674181, 10.1101/2025.09.08.674181
2.  **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, [Last Author](#)
3.  Preprint **Assessing the Impact of AI and Digital Twins on Clinical Decision-Making in Hepatology and Hepatobiliary Surgery.** Mariia Myshkina, Elisabetta Casabianca, Anton Schnurpel, Tim Ricken, Hans-Michael Tautenhahn, **Matthias König**; *Preprints* 2025, 10.20944/preprints202509.1164.v1, [Last Author](#)
4.  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.
5.  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.

6.   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.
7.   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.
8.   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.
9.   Software **libsbgpy - Python library for SBGN**. Developed a Python library for working with Systems Biology Graphical Notation (SBGN), supporting standardized visualization and integration of pathway information.
10.   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.

Supervision of Researchers

Over the last 5 years, 1 PhD theses, 4 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 2 PhD, and 2 Internship projects (group members).

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Activities in the Research System

-  **2026: Invited keynote at the Patient Monitoring Roundtable (PMRT)** – Digital Twins and Dashboards for Personalized Drug Treatment at Charité – Universitätsmedizin Berlin.
-  **2026: Interview: Modelle so komplex wie der Körper selbst – Digitale Zwillinge in der Medizin** – Gesellschaft für Informatik interview on digital twins, multi-scale modeling, PBPK, and open, FAIR computational medicine.
-   **2025: Featured in Faces of the Berlin University Alliance** – Highlighted as part of the BUA's 6th-anniversary film series showcasing interdisciplinary collaboration across FU, HU, TU, and Charité.
-  **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.
-  **11/2025: 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 PTab Editor** - Strengthened the PTab standard for parameter estimation problems, ensuring community adoption and long-term sustainability.
-  **2017–2026: Elected COMBINE Coordinator** - Led international coordination of community standards (SBML, SED-ML, PTab, 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: **Participant Lorentz Workshop “Your Dietary Digital Twin”** – Contributed to discussions on integrating mechanistic and data-driven models for personalized nutrition and open science frameworks.
- 2022: **Led X-Student Research Group: Physiologically Based Modeling of Drugs — ACE Inhibitors in Hypertension** - Mentored interdisciplinary student teams.

Funding

- 10/2025 – 04/2026, Recipient, 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.
- 10/2025 – 09/2026, Recipient, 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, Co-Investigator, Circle U., total: 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.
- 01/2024 – 06/2026, Recipient, 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.
- 10/2025 – 9/2027, Recipient, DFG, 219.000€, total: 895.500€, **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 – 09/2023, Recipient, 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.
- 03/2023 – 12/2026, Recipient, BMBF, 311.000€, total: 1530.550€, **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 – 03/2023, Recipient, BMBF, 1.500€, **X-Student Research Group - Physiologically based modeling of drugs: ACE inhibitors in the treatment of high blood pressure**. Project-based teaching initiative on physiologically based pharmacokinetic (PBPK) modeling, focusing on optimizing the use of ACE inhibitors in hypertension therapy.
- 07/2021 – 11/2025, Recipient, DFG, 425.000€, total: 3825.000€, **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.
- 01/2020 – 12/2023, Co-Investigator, DFG, total: 658.942€, **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.
- 06/2020 – 05/2021, Recipient, EOSC-life, 5.000€, total: 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.
- 06/2016 – 05/2022, Recipient, 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

Habilitation Completion Scholarship

Humboldt-Universität zu Berlin

Scholarship supporting the completion of the Habilitation.

11/2025 - 05/2026

- Awarded for the successful finalization of the Habilitation at Humboldt-Universität zu Berlin.

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

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 (2 SWS)	• 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 (2 SWS)	• 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 (2 SWS)	• Guided students in developing PBPK models for lisinopril and ramipril. • Integrated lectures, tutorials, and project-based work to link theory with practice.

Course	Description
	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 (2 SWS) 04/2024 – 09/2024 (2 SWS) 04/2023 – 09/2023 (2 SWS)	- 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 (2 SWS) 10/2020 – 03/2021 (2 SWS) 10/2019 – 03/2020 (2 SWS) 10/2018 – 03/2019 (2 SWS)	- 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 (2 SWS)	- 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

Teaching Qualifications

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.

AI Teaching Certificate (KI-Lehrzertifikat)

HU Berlin, KI-Campus 2.0 & AI Skills Initiative

Higher education didactics qualification on Artificial Intelligence (100/150 AE)

2025 – 2026

- Qualification focused on integrating AI concepts and learning formats into university curricula.
- Training aligned with German Society for Higher Education Didactics (DGHD) standards.
- Emphasis on foundational AI literacy, didactic design, and sustainable curricular implementation.

List of Publications

Publications

-  **SBML Level 3 Package: Flux Balance Constraints version 3.** Brett G. Olivier, Frank T. Bergmann, Sarah Keating, and Matthias König J Integr Bioinform. 2026; 20260006, 10.1515/jib-2026-0006, IF: **1.5**, Last author
-  **The Parameter Estimation tables (PEtab) format version 2.** Dilan Pathirana, Fabian Fröhlich, Sebastian Persson, Frank T. Bergmann, Matthias König, Paul F. Lang, Severin Bang, Svenja Kemmer, Jan Hasenauer, and Daniel Weindl; J Integr Bioinform. , 10.1515/jib-2026-0004, IF: **1.5**
-  **EFFECT enables reliable and reproducible stochastic simulations across disciplines.** T. J. Sego, Matthias König, Luis L. Fonseca, Dilan Pathirana, Frank T. Bergmann, Hernán E. Grecco, Mauro Silberberg, Subhasis Ray, Baylor Fain, Adam C. Knapp, Krishna Tiwari, Henning Hermjakob, Herbert M. Sauro, James A. Glazier, Reinhard C. Laubenbacher & Rahuman S. Malik-Sheriff; npj Complex (2026), 10.1038/s44260-026-00094-y, IF: **1.6**

4.  **Reproducibility of a Physiologically Based Pharmacokinetic and Pharmacodynamic (PBPK/PD) Model of Dapagliflozin.** Michelle Elias, Mariia Myshkina, Nike Nemitz, Matthias König Physiome. May 13, 2026, 10.36903/physiome.31368556, [Last author](#)
5.  **Automated Segmentation of Hepatic Vessels and Lobules in Whole-Slide Images Using U-Net Models.** Mehul Bafna, Matthias König, Sylvia Saalfeld, Vladimira Moulisova, Vaclav Liska, Uta Dahmen, Mohamed Albadry; Front. Bioinform. 6:1713736, 10.3389/fbinf.2026.1713736, IF: **3.9**
6.  **From FAIR to CURE: Guidelines for Computational Models of Biological Systems.** Herbert M. Sauro, Eran Agmon, Michael L. Blinov, John H. Gennari, Joe Hellerstein, Adel Heydarabadipour, Peter Hunter, Bartholomew E. Jardine, Elebeoba May, David P. Nickerson, Lucian P. Smith, Gary D Bader, Frank Bergmann, Patrick M. Boyle, Andreas Drager, James R. Faeder, Song Feng, Juliana Freire, Fabian Frohlich, James A. Glazier, Thomas E. Gorochofski, Tomas Helikar, Stefan Hoops, Princess Imoukhuede, Sarah M. Keating, Matthias König, Reinhard Laubenbacher, Leslie M. Loew, Carlos F. Lopez, William W. Lytton, Andrew McCulloch, Pedro Mendes, Chris J. Myers, Jerry G. Myers, Lealem Mulugeta, Anna Niarakis, David D. van Niekerk, Brett G. Olivier, Alexander A. Patrie, Ellen M. Quardokus, Nicole Radde, Johann M. Rohwer, Sven Sahle, James C. Schaff, T.J. Sego, Janis Shin, Jacky L. Snoep, Rajanikanth Vadigepalli, H. Steve Wiley, Dagmar Waltemath, Ion Moraru; npj Syst Biol Appl (2026), 10.1038/s41540-026-00651-0, IF: **3.6**
7.  **A Physiologically Based Pharmacokinetic and Pharmacodynamic (PBPK/PD) Model of Dapagliflozin in Type 2 Diabetes Mellitus: The Effect of Dosing, Hepatorenal Impairment, and Food.** Nike Nemitz, Michelle Elias, Matthias König Pharmaceutics 2026, 18(3), 287; <https://doi.org/10.3390/pharmaceutics18030287>, 10.3390/pharmaceutics18030287, IF: **6.9**, [Last author](#)
8.  **A Digital Twin of the Angiotensin II Receptor Blocker Losartan: Physiologically Based Modeling of Blood Pressure Regulation.** Ennie Tensil, Mariia Myshkina, Matthias König Pharmaceutics 2026, 18(2), 262; <https://doi.org/10.3390/pharmaceutics18020262>, 10.3390/pharmaceutics18020262, IF: **6.9**, [Last author](#)
9.  **Reproducibility of a Digital Twin of the Angiotensin II Receptor Blocker Losartan.** Mariia Myshkina, Michelle Elias, Ennie Tensil, Matthias König Physiome. February 2, 2026, 10.36903/physiome.31359823, [Last author](#)
10.  **A Digital Twin of Glimepiride for Personalized and Stratified Diabetes Treatment.** Michelle Elias, Matthias König Front. Pharmacol. 16:1686415., 10.3389/fphar.2025.1686415, IF: **4.8**, [Last author](#)
11.  **Reproducibility of a Digital Twin of Glimepiride for Personalized and Stratified Diabetes Treatment.** Michelle Elias, Matthias König Physiome. October 20, 2025, 10.36903/physiome.28379193, [Last author](#)
12.  **Inflammation and autophagy in peripheral nerves of rodent models with metabolic syndrome and type 2 diabetes mellitus.** Baum P, Ebert T, Klötting 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**
13.  **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**
14.  **Specifications of standards in systems and synthetic biology: status, developments, and tools in 2024.** Martin Golebiewski, Gary Bader, Padraig Gleeson, Thomas E Gorochofski, 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**
15.  **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 Klopffleisch, Vaclav Liska, Vladimira Moulisova, Sandra Nickel, Richard Palek, Jachym Rosendorf, Sylvia Saalfeld, Utz Settmacher, Hans-Michael Tautenhahn, Matthias König^Δ, Uta Dahmen^Δ (^Δ equal contribution); Front Pharmacol. 2024 May 16;15:1404938, 10.3389/fphar.2024.1404938, IF: **5.4**, [Last Equal author](#)
16.  **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, Tauten-

- hahn HM, Wei W, Zhao WT, Radde NE.; Bioinformatics. 2024 May 2;40(5):btac312, 10.1093/bioinformatics/btac312, IF: **6.0**
17.  **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](#)
 18.  **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**
 19.  **Eleven Strategies for Making Reproducible Research and Open Science Training the Norm at Research Institutions.** Friederike E Kohrs, Susann Auer, Alexandra Bannach-Brown, Susann Fiedler, Tamarinde Laura Haven, Verena Heise, Constance Holman, Flavio Azevedo, René Bernard, Armin Bleier, Nicole Bössel, Brian Patrick Cahill, Leyla Jael Castro, Adrian Ehrenhofer, Kristina Eichel, Maximillian Frank, Claudia Frick, Malte Frieze, Anne Gärtner, Kerstin Gierend, David Joachim Grüning, Lena Hahn, Maren Hülsemann, Malika Ihle, Sabrina Illius, Laura König, Matthias König, Louisa Kulke, Anton Kutlin, Fritjof Lammers, David MA Mehler, Christoph Miehl, Anett Müller-Alcazar, Claudia Neuendorf, Helen Niemeyer, Florian Pargent, Aaron Peikert, Christina U Pfeuffer, Robert Reinecke, Jan Philipp Röer, Jessica L Rohmann, Alfredo Sánchez-Tójar, Stefan Scherbaum, Elena Sixtus, Lisa Spitzer, Vera Maren Straßburger, Marcel Weber, Clarissa J Whitmire, Josephine Zerna, Dilara Zorbek, Philipp Zumstein, Tracey L Weissgerber; eLife (2023) 12:e89736., 10.7554/eLife.89736, IF: **6.4**
 20.  **A pathway model of glucose-stimulated insulin secretion in the pancreatic β -cell.** Maheshvare MD., Raha S., König M. Δ , and Pal D. Δ (Δ equal contribution); Front. Endocrinol. 14:1185656, 10.3389/fendo.2023.1185656, IF: **5.7**, [Last Equal author](#)
 21.  **Specifications of Standards in Systems and Synthetic Biology: Status and Developments in 2022 and the COMBINE meeting 2022.** M. König, P. Gleeson, M. Golebiewski, T. Gorochowski, M. Hucka, S. Keating, C. Myers, D. Nickerson, F. Schreiber; J Integr Bioinform. 2023 Mar 29;20(1)., 10.1515/jib-2023-0004, IF: **1.5**, [First author](#)
 22.  **libRoadRunner 2.0: A High-Performance SBML Simulation and Analysis Library.** Ciaran Welsh, Jin Xu, Lucian Smith, Matthias König, Kiri Choi, Herbert M. Sauro; Bioinformatics. 2023 Jan 1;39(1):btac770, 10.1093/bioinformatics/btac770, IF: **6.0**
 23.  **Cytochrome p450 enzymes in periportal steatosis: Modulation of drug metabolizing activity but not of pericentral expression pattern.** M. Albadry, S. Höpfl, N. Ehteshamzad, M. König, M. Böttcher, J. Neumann, A. Lupp, O. Dirsch, N. Radde, B. Christ, M. Christ, L.O. Schwen, H. Laue, R. Klopffleisch and Uta Dahmen; Sci Rep. 2022 Dec 17;12(1):21825, 10.1038/s41598-022-26483-6, IF: **3.8**
 24.  **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](#)
 25.  **BioSimulators: a central registry of simulation engines and services for recommending specific tools.** Shaikh B, Smith LP, Vasilescu D, Marupilla G, Wilson M, Agmon E, Agnew H, Andrews SS, Anwar A, Beber ME, Bergmann FT, Brooks D, Bruschi L, Calzone L, Choi K, Cooper J, Detloff J, Drawert B, Dumontier M, Ermentrout GB, Faeder JR, Freiburger AP, Fröhlich F, Funahashi A, Garny A, Gennari JH, Gleeson P, Goelzer A, Haiman Z, Hasenauer J, Hellerstein JL, Hermjakob H, Hoops S, Ison JC, Jahn D, Jakubowski HV, Jordan R, Kalaš M, König M, Liebermeister W, Sherif RSM, Mandal S, McDougal R, Medley JK, Mendes P, Müller R, Myers CJ, Naldi A, Nguyen TVN, Nickerson DP, Olivier BG, Patoliya D, Paulevė L, Petzold LR, Priya A, Rampadarath AK, Rohwer JM, Saglam AS, Singh D, Sinha A, Snoep J, Sorby H, Spangler R, Starruß J, Thomas PJ, van Niekerk D, Weindl D, Zhang F, Zhukova A, Goldberg AP, Schaff JC, Blinov ML, Sauro HM, Moraru II, Karr JR.; Nucleic Acids Res. 2022 May 7;50(W1):W108–14, 10.1093/nar/gkac331, IF: **16.7**
 26.  **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](#)

27.  **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**, [Last author](#)
28.  **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**, [Last author](#)
29.  **Specifications of Standards in Systems and Synthetic Biology: Status and Developments in 2021.** F. Schreiber, P. Gleeson, M. Golebiewski, T. Gorochofski, M. Hucka, S. Keating, M. König, C. Myers, D. Nickerson, D. Walthemath; *J Integr Bioinform.* 2021 Oct 22;18(3):20210026, 10.1515/jib-2021-0026, IF: **1.5**
30.  **SBMLWebApp: Web-based Simulation, Steady-State Analysis, and Parameter Estimation of Systems Biology Models.** Takahiro G. Yamada, Kaito Ii, Matthias König, Martina Feierabend, Andreas Dräger, and Akira Funahashi; *Processes* 9, no. 10: 1830, 10.3390/pr9101830, IF: **2.8**
31.  **The simulation experiment description markup language (SED-ML): language specification for level 1 version 4.** Smith, Lucian P., Bergmann, Frank T., Garny, Alan, Helikar, Tomáš, Karr, Jonathan, Nickerson, David, Sauro, Herbert, Waltemath, Dagmar and König, Matthias. *Journal of Integrative Bioinformatics*, vol. 18, no. 3, 2021, pp. 20210021, 10.1515/jib-2021-0021, IF: **1.5**, [Last author](#)
32.  **The Systems Biology Simulation Core Library.** Panchiwala, H.; Shah, S.; Planatscher, H.; Zakharchuk, M.; König, M. Dräger, A.; *Bioinformatics.* 2022 Jan 12;38(3):864-865, 10.1093/bioinformatics/btab669, IF: **6.0**
33.  **OMEX Metadata Specification Version 1.2.** John Gennari, Matthias König, Goskel Misirli, Maxwell Neal, David Nickerson, Dagmar Waltemath; *J Integr Bioinform.* 2021 Oct 20;18(3):20210020, 10.1515/jib-2021-0020, IF: **1.5**
34.  **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**, [Last author](#)
35.  **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, 10.1525/msb.20199110, IF: **8.8**
36.  **Open modeling and exchange (OMEX) metadata specification version 1.0.** Neal ML, Gennari JH, Waltemath D, Nickerson DP, König M *J Integr Bioinform.* 2020 Jun 25;17(2-3):20200020, 10.1515/jib-2020-0020, IF: **1.5**, [Last author](#)
37.  **Specifications of Standards in Systems and Synthetic Biology:Status and Developments in 2020.** F. Schreiber, B. Sommer, G. Bader, P. Gleeson, M. Golebiewski, T. Gorochofski, M. Hucka, S. Keating, M. König, C. Myers, D. Nickerson, D. Walthemath; *J Integr Bioinform.* 2020 Jun 29;17(2-3):20200022, 10.1515/jib-2020-0022, IF: **1.5**
38.  **The first 10 years of the international coordination network for standards in systems and synthetic biology (COMBINE).** D Waltemath, M Golebiewski, M Blinov, P Gleeson, H Hermjakob, E Inau, S Keating, M König, O Krebs, R Malik-Sheriff, D Nickerson, E Oberortner, H Sauro, F Schreiber, L Smith, M Stefan, U Wittig, C Myers; *J Integr Bioinform.* 2020 Jun 29;17(2-3):20200005, 10.1515/jib-2020-0005, IF: **1.5**
39.  **The Distributions Package for SBML Level 3.** L Smith, S Moodie, F Bergmann, C Gillespie, S Keating, M. König, C Myers, M Swat, D Wilkinson, M Hucka; *J Integr Bioinform.* 2020 Jul 20;17(2-3):20200018, 10.1515/jib-2020-0018, IF: **1.5**
40.  **MEMOTE for standardized genome-scale metabolic model testing.** Christian Lieven, Moritz Emanuel Beber, Brett G. Olivier, Frank T. Bergmann, Meric Ataman, Parizad Babaei, Jennifer A. Bartell, Lars M. Blank, Siddharth Chauhan, Kevin Correia, Christian Diener, Andreas Dräger, Birgitta Elisabeth Ebert, Janaka N. Edirisinghe, Jose P. Faria, Adam Feist, Georgios Fengos, Ronan M. T. Fleming, Beatriz Garcia-Jimenez, Vassily Hatzimanikatis, Wout van Helvoirt, Christopher Henry, Henning Hermjakob, Markus J. Herrgard, Hyun Uk

- Kim, Zachary King, Jasper Jan Koehorst, Matthias König, Steffen Klamt, Edda Klipp, Meiyappan Lakshmanan, Nicolas Le Novère, Dong-Yup Lee, Sang Yup Lee, Sunjae Lee, Nathan E. Lewis, Hongwu Ma, Daniel Machado, Radhakrishnan Mahadevan, Paulo Maia, Adil Mardinoglu, Greg L. Medlock, Jonathan Monk, Jens Nielsen, Lars K. Nielsen, Juan Nogales, Intawat Nookaew, Osbaldo Resendis, Bernhard Palsson, Jason A. Papin, Kiran Raosaheb Patil, Mark Poolman, Nathan D. Price, Anne Richelle, Isabel Rocha, Benjamin Sanchez, Peter Schaap, Rahuman S. Malik Sheriff, Saeed Shoaie, Nikolaus Sonnenschein, Bas Teusink, Paulo Vilaca, Jon Olav Vik, Judith A. Wodke, Joana C. Xavier, Qianqian Yuan, Maksim Zakhartsev, Cheng Zhang; Nat Biotechnol. 2020;38(3):272-276, 10.1038/s41587-020-0446-y, IF: **33.1**
41.  **Specifications of Standards in Systems and Synthetic Biology: Status and Developments in 2019.** F Schreiber, G Bader, P Gleeson, M Golebiewski, M Hucka, SM Keating, M König, C Myers, D Nickerson, B Sommer, D Waltemath; J Integr Bioinform. 2019 Jul 13;16(2), 10.1515/jib-2019-0035, IF: **1.5**
 42.   **The Systems Biology Markup Language (SBML): Language Specification for Level 3 Version 2 Core.** M. Hucka, F. Bergmann, C. Chaouiya, A. Dräger, S. Hoops, S. Keating, M. König, N Le Novère, C. Myers, B. Olivier, S. Sahle, J. Schaff, R. Sheriff, L. Smith, D. Waltemath, D. Wilkinson, F. Zhang; J Integr Bioinform. 2019 Jun 20;16(2);, 10.1515/jib-2019-0021, IF: **1.5**
 43.   **Tellurium: An Extensible Python-based Modeling Environment for Systems and Synthetic Biology.** Choi K., Medley K., König M., Stocking K., Smith L., Gu S., and Sauro HM.; Biosystems. 2018 Jul 24. pii: S0303-2647(18)30125-4, 10.1016/j.biosystems.2018.07.006, IF: **2.0**
 44.  **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**
 45.   **Simulation Experiment Description Markup Language (SED-ML) Level 1 Version 3 (L1V3).** Bergmann, FT., Cooper, J., König, M., Moraru, I., Nickerson, D., Le Novère N., Olivier, BG., Sahle, S., Smith, L., Waltemath, D.  corresponding author J Integr Bioinform. 2018 Mar 19;15(1), 10.1515/jib-2017-0086, IF: **1.5**
 46.   **Harmonizing semantic annotations for computational models in biology.** Neal, M.; König, M. Nickerson, D.; Misirli, G.; Kalbasi, R.; Dräger, A.; Atalag, K.; Chelliah, V.; Cooling, M.; Cook, D.; Crook, S.; de Alba, M.; Friedman, S.; Garny, A.; Gennari, J.; Gleeson, P.; Golebiewski, M.; Hucka, M.; Juty, N.; Novère, N. L.; Myers, C.; Olivier, B.; Sauro, H.; Scharm, M.; Snoep, J.; Touré, V.; Wipat, A.; Wolkenhauer, O. & Waltemath, D.; Brief Bioinform. 2019 Mar 22;20(2):540-550, 10.1093/bib/bby087, IF: **7.9**
 47.   **Tellurium Notebooks — An Environment for Reproducible Dynamical Modeling in Systems Biology.** Medley K., Choi K., König M., Smith L., Gu S., Hellerstein J., Sealfon S., and Sauro HM.; PLoS Comput Biol. 2018 Jun 15;14(6):e1006220, 10.1371/journal.pcbi.1006220, IF: **4.5**
 48.   **Toward community standards and software for whole-cell modeling.** Wholecell Consortium (König M.); IEEE Trans Biomed Eng. 2016 Jun 10., 10.1109/TBME.2016.2560762, IF: **4.4**
 49.   **Pathobiochemical signatures of cholestatic liver disease in bile duct ligated mice.** Kerstin A.  König M., Hoppe A., Thomas M., Müller I., Ebert M., Weng H., Holzhütter HG., Zanger UM., Bode J., Vollmar B. and Dooley S. ( equal contribution); BMC Syst Biol. 2015 Nov 20;9(1):83., 10.1186/s12918-015-0229-0, IF: **2.2**, First Equal author
 50.   **LibRoadRunner: a high performance SBML simulation and analysis library.** Somogyi ET., Bouteiller JM., Glazier JA., König M., Medley JK., Swat MH and Sauro HM.; Bioinformatics. 2015 Oct 15;31(20):3315-21, 10.1093/bioinformatics/btv363, IF: **6.0**
 51.   **Modeling function-perfusion behavior in liver lobules including tissue, blood, glucose, lactate and glycogen by use of a coupled two-scale PDE-ODE approach.** Ricken T., Werner D., Holzhütter HG., König M., Dahmen U., Dirsch O.; Biomech Model Mechanobiol. 2015 Jun;14(3):515-36, 10.1007/s10237-014-0619-z, IF: **3.0**
 52.   **Metabolic Gradients as Key Regulators in Zonation of Tumor Energy Metabolism: A Tissue-scale Model Based Study.** König M., Holzhütter HG., Berndt N.; Biotechnol J. 2013 Sep;8(9):1058-69., 10.1002/biot.201200393, IF: **3.7**, First author
 53.   **Kinetic Modeling of Human Hepatic Glucose Metabolism in T2DM Predicts Higher Risk of Hypoglycemic Events in Rigorous Insulin Therapy.** König M. and Holzhütter HG.; J Biol Chem. 2012 Oct 26;287(44):36978-89, 10.1074/jbc.M112.382069, IF: **4.7**, First author

54.  **CySBML: a Cytoscape plugin for SBML.** König M., Dräger A. and Holzhütter HG.; Bioinformatics. 2012 Sep 15;28(18):2402-3, 10.1093/bioinformatics/bts432, IF: **6.0**, [First author](#)
55.  **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**, [First author](#)
56.  **HepatoNet1: a comprehensive metabolic reconstruction of the human hepatocyte for the analysis of liver physiology.** Gille C, Bölling C, Hoppe A, Bulik S, Hoffmann S, Hübner K, Karlstädt A, Ganeshan R, König M, Rother K, Weidlich M, Behre J, Holzhütter HG.; Mol Syst Biol. 2010 Sep 7;6:411, 10.1038/msb.2010.62, IF: **8.6**

Reviews

57.  **Hepatectomy-Induced Alterations in Hepatic Perfusion and Function - Toward Multi-Scale Computational Modeling for a Better Prediction of Post-hepatectomy Liver Function.** Bruno Christ Δ , Maximilian Collatz Δ , Uta Dahmen Δ , Karl-Heinz Herrmann Δ , Sebastian Höpfel Δ , Matthias König Δ , Lena Lambers Δ , Manja Marz Δ , Daria Meyer Δ , Nicole Radde Δ , Jürgen R. Reichenbach Δ , Tim Ricken Δ , and Hans-Michael Tautenhahn Δ (Δ equal contribution); Front Physiol. 2021 Nov 18;12:733868, 10.3389/fphys.2021.733868, IF: **3.2**, [First Equal author](#)
58.  **Computational Modeling in Liver Surgery.** Christ, B. Δ , Dahmen, U. Δ , Herrmann, K.H. Δ , König, M. Δ , Reichenbach, J.R. Δ , Ricken, T. Δ , Schleicher, J. Δ , Ole Schwen, L. Δ , Vlaic, S. Δ and Waschinsky, N. Δ (Δ equal contribution); Front Physiol. 2017 Nov 14;8:906, 10.3389/fphys.2017.00906, IF: **3.2**, [First Equal author](#)
59.  **Enzymatic Features of the Glucose Metabolism in Tumor Cells.** Herling A, König M, Bulik S, Holzhütter HG.; FEBS J. 2011 Jul;278(14):2436-59, 10.1111/j.1742-4658.2011.08174.x, IF: **5.4**

Proceedings

60.  **SimLivA – Modelling ischemia reperfusion injury in the liver: A first step towards a clinical decision support tool.** Hans-Michael Tautenhahn, Tim Ricken, Uta Dahmen, Luis Mandl, Laura Bütow, Steffen Gerhäuser, Lena Lambers, Xinpei Chen, Elina Lehmann, Olaf Dirsch, Matthias König GAMM-Mitteilungen. (2024), e202370003, 10.1002/gamm.202370003, [Last author](#)
61.  **QualiPerF – Multi-X Liver Modelling.** Tim Ricken, Lena Lambers, Bruno Christ, Uta Dahmen, Karl-Heinz Herrmann, Matthias König, Manja Marz, Nicole Radde, Jürgen R. Reichenbach, Lars Ole Schwen & Hans-Michael Tautenhahn; GACM - German Association for Computational Mechanics Report, winter 2020: No. 13
62.  **Model Order Reduction (MOR) of Function-Perfusion-Growth Simulation in the Human Fatty Liver via Artificial Neural Network (ANN).** Lambers L., Ricken T., and König M. Proceedings in Applied Mathematics & Mechanics, PAMM, 2019, 10.1002/pamm.201900429, [Last author](#)
63.  **Challenges and opportunities for system biology standards and tools in medical research.** König M. Δ , Oellrich A. Δ , Waltemath D. Δ , Dobson R., Hubbard T., and Wolkenhauer O. (Δ equal contribution); ODLs, p1-6, 2016, [First Equal author](#)
64. **On the Influence of Growth in Perfusion Dependent Biological Systems - at the Example of the Human Liver.** Werner D., Ricken T., Dahmen U., Dirsch O., Holzhütter HG., König M. PAMM 15 (1), 119-120, 2015, 10.1002/pamm.201510050, [Last author](#)
65.  **Homeostasis of blood glucose - Computer simulations of central liver functions.** König M. and Holzhütter HG.; systembiologie.de 2014; 8:p.53-57, [First author](#)
66.  **FluxViz - Cytoscape Plug-in for Visualization of Flux Distributions in Networks.** König M. and Holzhütter HG.; Genome Informatics 2010, Vol.24, p.96-103, [First author](#)

Preprints

1.  **A Physiologically Based Pharmacokinetic/Pharmacodynamic Model of the Diuretic Hydrochlorothiazide.** Amanda Schwaiger, Matthias König Preprints 2026, 10.20944/preprints202607.0306.v1, 10.20944/preprints202607.0306.v1, [Last author](#)
2.  **TabularQual: A spreadsheet-based format for annotating and curating logical models in SBML-qual.** Luna Xingyu Li, Carissa Bleker, Sylvain Soliman, Laurence Calzone, Noriko Hiroi, Tomas Helikar, Matthias König, Luiz Ladeira, Pedro Tiago Monteiro, Vincent Noel, Samuel Pastva, Albin Salazar,

3.  **A PBPK Digital Twin of Rapamycin for Predicting Dose-Exposure Relationships, Organ Impairment Effects, and Drug-Drug Interactions.** Monika Jesionek, Matthias König Preprints 2026, 10.20944/preprints202605.0249.v1, 10.20944/preprints202605.0328.v1, [Last author](#)
4.  **An Open and Reproducible Digital Twin for Personalised Anticoagulant Therapy: Modelling Apixaban Pharmacokinetics and Pharmacodynamics.** Mariia Myshkina, Mariia Babaeva, Linh Chang Nguyen, Shelee Bedón, Johannes Metternich, Michelle Elias, Matthias König Preprints 2026, 10.20944/preprints202605.0249.v1, 10.20944/preprints202605.0249.v1, [Last author](#)
5.  **A Digital Twin of Empagliflozin Pharmacokinetics and Pharmacodynamics.** Jennessé Alejandro, Michelle Elias, Mariia Babaeva, Matthias König Preprints 2026, 10.20944/preprints202603.1559.v1, 10.20944/preprints202603.1559.v1, [Last author](#)
6.  **User-driven development and evaluation of an agentic framework for analysis of large pathway diagrams.** Marie Corradi, Ivo Djidrovski, Luiz Ladeira, Bernard Staumont, Anouk Verhoeven, Julien Sanz Serrano, Adrien Rougny, Ahmad Vaez, Ahmed Hemedan, Alexander Mazein, Anna Niarakis, Arthur de Carvalho e Silva, Charles Auffray, Egon Wilighagen, Eliska Kuchovska, Falk Schreiber, Irina Balaur¹⁷, Laurence Calzone, Lisa Matthews, Lorenzo Veschini, Marc E Gillespie, Martina Kutmon, Matthias König, Matti van Welzen, Noriko Hiroi, Oxana Lopata, Pierre Klemmer, Rupert Overall, Tim Hofer, Venkata Satagopam, Reinhard Schneider, Marc Teunis, Liesbet Geris, Marek Ostaszewski; bioRxiv 2026.03.10.710813, 10.64898/2026.03.10.710813
7.  **A Digital Twin of Canagliflozin Pharmacokinetics and Pharmacodynamics in Type 2 Diabetes Mellitus.** Vera Tereshchuk, Michelle Elias, Matthias König Preprints 2026, 10.20944/preprints202601.2095.v1, 10.20944/preprints202601.2095.v1, [Last author](#)
8.  **Assessing the Impact of AI and Digital Twins on Clinical Decision-Making in Hepatology and Hepatobiliary Surgery.** Mariia Myshkina, Elisabetta Casabianca, Anton Schnurpel, Tim Ricken, Hans-Michael Tautenhahn, Matthias König Preprints 2025, 10.20944/preprints202509.1164.v1, [Last author](#)
9.  **A Systems Pharmacology Approach to Rivaroxaban: Physiologically Based Modeling of Pharmacokinetics and Coagulation Dynamics.** Elisabetta Casabianca, Mariia Myshkina, Matthias König Preprints 2025, 202507.1945., 10.20944/preprints202507.1945.v1, [Last author](#)
10.  **FAIRification of computational models in biology.** Irina Balaur, David P. Nickerson, Danielle Welter, Judith A.H. Wodke, Francois Ancien, Tom Gebhardt, Valentin Grouès, Henning Hermjakob, Matthias König, Nicole Radde, Adrien Rougny, Reinhard Schneider, Rahuman S. Malik-Sheriff, Kirubel Biruk Shiferaw, Melanie Stefan, Venkata Satagopam, Dagmar Waltemath; bioRxiv 2025.03.21.644517, 10.1101/2025.03.21.644517
11.  **FROG Analysis Ensures the Reproducibility of Genome Scale Metabolic Models.** Karthik Raman, Miroslav Kratochvil, Brett G. Olivier, Matthias König, Pratyay Sengupta, Dinesh Kumar Kuppa Baskaran, Tung V N Nguyen, Daniel Lobo, St Elmo Wilken, Krishna Kumar Tiwari, Aswathy K. Raghu, Indumathi Palanikumar, Lavanya Raajaraam, Maziya Ibrahim, Sanjaay Balakrishnan, Shreyansh Umale, Frank Bergmann, Tanisha Malpani, Venkata P Satagopam, Reinhard Schneider, Moritz E. Beber, Sarah Keating, Mihail Anton, Alina Renz, Meiyappan Lakshmanan, Dong-Yup Lee, Lokanand Koduru, Reihaneh Mostolizadeh, Oscar Dias, Emanuel Cunha, Alexandre Oliveira, Yi Qing Lee, Karsten Zengler, Rodrigo Santibanez-Palominos, Manish Kumar, Matteo Barberis, Bhanwar Lal Puniya, Tomas Helikar, Hoang V. Dinh, Patrick F. Suthers, Costas D. Maranas, Isabella Casini, Seyed Babak Loghmani, Nadine Veith, Nantia Leonidou, Feiran Li, Yu Chen, Jens Nielsen, GaRyoung Lee, Sang Mi Lee, Gi Bae Kim, Pedro T. Monteiro, Miguel C. Teixeira, Hyun Uk Kim, Sang Yup Lee, Ulf W. Liebal, Lars M. Blank, Christian Lieven, Chaimaa Tarzi, Claudio Angione, Manga Enuh Blaise, Celik Pinar Aytar, Mikhail Kulyashov, Ilya Akberdin, Dohyeon Kim, Sung Ho Yoon, Zhaohui Xu, Jyotshana Gautam, William T. Scott Jr., Peter J. Schaap, Jasper J. Koehorst, Cristal Zuniga, Gabriela Canto-Encalada, Sara Benito-Vaquerizo, Ivette Parera Olm, Maria Suarez-Diez, Qianqian Yuan, Hongwu Ma, Mohammad Mazharul Islam, Jason A. Papin, Francisco Zorrilla, Kiran Raosaheb Patil, Arianna Basile, Juan Nogales, Granado San Leon, Freddy Castillo-Alfonso, Roberto Olivares-Hernandez, Gabriel Vigueras-Ramirez, Henning Hermjakob, Andreas Dräger, Rahuman S Malik-Sheriff; bioRxiv 2024.09.24.614797, 10.1101/2024.09.24.614797
12.  **Simulation of zonation-function relationships in the liver using coupled multiscale models: Application to drug-induced liver injury.** Steffen Gerhäuser, Lena Lambers, Luis Mandl, Julian Franquinet, Tim Ricken, Matthias König bioRxiv 2024.03.26.586870; 10.1101/2024.03.26.586870, [Last author](#)

13.  **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, [Last author](#)
14.  **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, [Last author](#)
15.  **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
16.  **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, [Last author](#)
17.  **FAIR Sharing of Reproducible Models of Epidemic and Pandemic Forecast.** Ramachandran, K.Δ; König, M.Δ Scharm, M.; Nguyen, T.V.N.; Hermjakob, H.; Waltemath, D.; Malik Sherif, R.S. (Δ equal contribution); Preprints 2022, 2022060137, 10.20944/preprints202206.0137.v1, [First Equal author](#)
18.  **Dynamic Flux Balance Analysis Models in SBML.** Matthias KönigΔ, Leandro H. WatanabeΔ, Jan Grzegorzewski, and Chris J. Myers. (Δ equal contribution); bioRxiv 245076, 10.1101/245076, [First Equal author](#)
19.  **Ten Simple Rules for FAIR Sharing of Experimental and Clinical Data with the Modeling Community.** Matthias KönigΔ, Jan Grzegorzewski, Martin Golebiewski, Henning Hermjakob, Mike Hucka, Brett Olivier, Sarah M. Keating, David Nickerson, Falk Schreiber, Rahuman Sherif, Dagmar Waltemath; Preprints 2021, 2021080303, 10.20944/preprints202108.0303.v2, [First author](#)
20.  **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
21.  **Executable Simulation Model of the Liver.** Matthias König bioRxiv 2020.01.04.894873, 10.1101/2020.01.04.894873, [First author](#)
22.  **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, [First author](#)

Thesis

1.  **Parameter Uncertainty in the Optimization of Pharmacokinetic Models: A Reproducible Bayesian Approach.** Antonio Alvarez (supervisor: Matthias König); Master Thesis, April 2026, [Last author](#)
2.  **A Systems Pharmacology Approach to Rivaroxaban: Physiologically Based Modeling of Pharmacokinetics and Coagulation Dynamics.** Elisabetta Casabianca (supervisor: Matthias König); Master Thesis, July 2025, [Last author](#)
3.  **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, [Last author](#)
4.  **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, [Last author](#)
5.  **A physiological-based pharmacokinetic (PBPK) model of the sulfonylurea glimepiride.** Michelle Elias (supervisor: Matthias König); Bachelor Thesis, April 2025, [Last author](#)
6.  **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, [Last author](#)

7.   **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, [Last author](#)
8.   **Enhancing Our Understanding of Enalapril's Pharmacokinetics: A Physiologically Based Modeling Approach.** Master Thesis Shubhankar Palwankar (supervisor: Matthias König); Master Thesis, May 2024, [Last author](#)
9.   **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, [Last author](#)
10.   **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, [Last author](#)
11.   **Physiologically based pharmacokinetic (PBPK) modeling for dynamical liver function tests and CYP phenotyping.** Jan Grzegorzewski (supervisor: Matthias König); PhD Thesis, Jan 2023, [Last author](#)
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14.   **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, [Last author](#)
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16.   **Computational Modelling of Midazolam Clearance: Effect of Inhibitors and Inducers.** Yannick Duport (supervisor: Matthias König); Bachelor Thesis, August 2020, [Last author](#)

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