

PERSONAL INFORMATIONEN

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RESEARCH & EDUCATION

Group Leader Junior Research Group 'Computational Structural Biology'
12/2020 – Present University of Leipzig, Institute for Drug Discovery, Leipzig, Germany

Postdoc Vanderbilt University, Center for Structural Biology, Nashville, USA
01/2016 – 11/2020 Computational Structural Biology, Advisor: Prof. Dr. Jens Meiler

- *Development and application of methods for integrative modeling of membrane proteins and biomolecular complexes*
- *Protein structure prediction from sparse NMR data with ROSETTA-NMR*
- *Development of scoring methods for paramagnetic NMR data in ROSETTA-NMR*
- *Structure modeling and molecular dynamics simulations of the voltage-gated K⁺ channel KCNQ1 to study the molecular mechanisms of beta-subunit regulation and the role of mutations in channel dysfunction*

Postdoc University of Leipzig, Institute for Medical Physics & Biophysics, Leipzig, Germany
09/2015 – 12/2015 Biomolecular NMR Spectroscopy, Advisor: Prof. Dr. Daniel Huster

PhD University of Leipzig, Institute for Medical Physics & Biophysics, Leipzig, Germany
10/2010 – 08/2015 Biomolecular NMR Spectroscopy, Advisor: Prof. Dr. Daniel Huster

Thesis: "Interaction of interleukin-10 with glycosaminoglycans studied by NMR spectroscopy", final grade: *summa cum laude*

- *Structure determination of interleukin-10 (IL-10) by solution NMR spectroscopy and X-ray crystallography*
- *Investigation of IL-10–carbohydrate interactions by paramagnetic NMR and saturation transfer difference (STD) NMR spectroscopy*
- *Tagging of IL-10 with lanthanide probes for measurement of pseudocontact shifts and paramagnetic relaxation enhancements*
- *Study of the structure and dynamics of tau amyloids by solid state NMR*

Master University of Leipzig, Leipzig, Germany
10/2008 – 09/2010 MSc. Biochemistry, Major in Biomedicine, final grade: 1.0

Thesis: “Study of the structure and dynamics of the tubulin binding domain K19 of tau bound to phospholipid membranes by ssNMR”, Advisor: Prof. Dr Daniel Huster

09/2009 – 03/2010 University of Cardiff, School of Biosciences, Cardiff, UK

Erasmus student, Advisor: Prof. Dr. Dafydd D. Jones

- Crystal structure determination of an intracellular subtilisin protease from *B. clausii*

Bachelor

University of Leipzig, Leipzig, Germany

10/2005 – 09/2008 BSc. Biochemistry, final grade: 1.0

Thesis: “Study of the binding properties of non-peptide antagonists at Y1 receptor mutants”, Advisor: Prof. Dr. Annette Beck-Sickinger

FELLOWSHIPS & AWARDS

2018 – 2020 Postdoctoral fellowship of the American Heart Association (18POST34080422)

2016 – 2017 Postdoctoral fellowship of the German Research Foundation (KU 3510/1-1)

2011 – 2013 Predoctoral fellowship of the “Verband der Chemischen Industrie e.V.”

2009 – 2010 Erasmus scholarship of the European Union

2007 – 2010 Scholarship of the “Bischöfliche Studienstiftung Cusanuswerk e.V.”

PUBLICATIONS

Peer-reviewed Publications

28. **Kuenze G**, Huster D, Samsonov S (2021) Investigation of the Structure of Regulatory Proteins Interacting with Glycosaminoglycans by NMR Spectroscopy and Molecular Modeling. **Biol Chem** [Online ahead of print], doi: 10.1515/hsz-2021-0119
27. Chen Z, **Kuenze G**, Wu Y, Meiler J, Canessa CM (2021) Dual effects of TM1 on proton affinity and desensitization uncovers a high-affinity proton-sensor in ASIC channels. **J Gen Physiol** 153(5), e202012802
26. Schoeder CT, Schmitz S, Adolf-Bryfogle J, Sevy AM, Finn JA, Sauer MF, Bozhanova NG, Mueller BK, Sangha AK, Bonet J, Sheehan JH, **Kuenze G**, Marlow B, Smith ST, Woods H, Bender BJ, Martina CE, Del Alamo D, Kodali P, Gulsevin A, Schief WR, Correia BE, Crowe JE Jr, Meiler J, Moretti R (2021) Modeling Immunity with Rosetta: Methods for Antibody and Antigen Design. **Biochemistry** 60(11), 825-846
25. Marlow B, **Kuenze G**, Li B, Sanders CR, Meiler J (2021) Structural determinants of cholesterol recognition in helical integral membrane proteins. **Biophys J** 120(9), 1592-1604
24. Huang H, Chamness LM, Vanoye CG, **Kuenze G**, Meiler J, George AL Jr, Schleich JP, Sanders CR (2021) Disease-linked super-trafficking of a potassium channel. **J Biol Chem** 296, 100423, doi: 10.1016/j.jbc.2021.100423
23. Heiliger J, Matzel T, Çetiner EC, Schwalbe H, **Kuenze G**, Corzilius B (2020) Site-specific dynamic nuclear polarization in a Gd(III)-labeled protein. **Phys Chem Chem Phys** 22(44), 25455-25466

22. **Kuenze G**, Vanoye CG, Desai RR, Adusumilli S, Brewer KR, Woods H, McDonald, EF, George AL Jr, Sanders CR, Meiler J (2020) Allosteric Mechanism for KCNE1 Modulation of KCNQ1 Potassium Channel Activation. *eLife* 9, e57680, doi: 10.7554/eLife.57680
21. Seacrist CD*, **Kuenze G***, Hoffmann RM, Moeller BE, Burke JE, Meiler J, Blind RD (2020) Integrated Structural Modeling of Full-Length LRH-1 Reveals Inter-domain Interactions Contribute to Receptor Structure and Function. *Structure* 28(7), 830-846 (*Authors contributed equally)
20. Brewer KR*, **Kuenze G***, Vanoye CG, George AL Jr, Meiler J, Sanders CR (2020) Structures Illuminate Cardiac Ion Channel Functions in Health and in Long QT Syndrome. *Front Pharmacol.* 11:550 (*Authors contributed equally)
19. Leman JK, Weitzner BD, Lewis SM, Adolf-Bryfogle J, Alam N, Alford RF, Aprahamian M, Baker D, Barlow KA, Barth P, Basanta B, Bender BJ, Blacklock K, Bonet J, Boyken SE, Bradley P, Bystroff C, Conway P, Cooper S, Correia BE, Coventry B, Das R, De Jong RM, DiMaio F, Dsilva L, Dunbrack R, Ford AS, Frenz B, Fu DY, Geniesse C, Goldschmidt L, Gowthaman R, Gray JJ, Gront D, Guffy S, Horowitz S, Huang PS, Huber T, Jacobs TM, Jeliazkov JR, Johnson DK, Kappel K, Karanicolas J, Khakzad H, Khar KR, Khare SD, Khatib F, Khramushin A, King IC, Kleffner R, Koepnick B, Kortemme T, **Kuenze G**, Kuhlman B, Kuroda D, Labonte JW, Lai JK, Lapidoth G, Leaver-Fay A, Lindert S, Linsky T, London N, Lubin JH, Lyskov S, Maguire J, Malmström L, Marcos E, Marcu O, Marze NA, Meiler J, Moretti R, Mulligan VK, Nerli S, Norn C, Ó'Conchúir S, Ollikainen N, Ovchinnikov S, Pacella MS, Pan X, Park H, Pavlovicz RE, Pethe M, Pierce BG, Pilla KB, Raveh B, Renfrew PD, Burman SSR, Rubenstein A, Sauer MF, Scheck A, Schief W, Schueler-Furman O, Sedan Y, Sevy AM, Sgourakis NG, Shi L, Siegel JB, Silva DA, Smith S, Song Y, Stein A, Szegedy M, Teets FD, Thyme SB, Wang RY, Watkins A, Zimmerman L, Bonneau R. (2020) Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nat. Methods* 17(7), 665-680
18. Koehler Leman J, Weitzner BD, Renfrew PD, Lewis SM, Moretti R, Watkins AM, Mulligan VK, Lyskov S, Adolf-Bryfogle J, Labonte JW, Krysz J, **RosettaCommons Consortium**, Bystroff C, Schief W, Gront D, Schueler-Furman O, Baker D, Bradley P, Dunbrack R, Kortemme T, Leaver-Fay A, Strauss CEM, Meiler J, Kuhlman B, Gray JJ, Bonneau R. (2020) Better together: Elements of successful scientific software development in a distributed collaborative community. *PLoS Comput Biol.* 16(5), e1007507
17. Taylor KC, Kang PW, Hou P, Yang ND, **Kuenze G**, Smith JA, Shi J, Huang H, McFarland White K, Peng D, George AL Jr, Meiler J, McFeeters RL, Cui J, Sanders CR (2020) Structure and physiological function of the human KCNQ1 channel voltage sensor intermediate state. *eLife* 9, e53901
16. **Kuenze G**, Bonneau R, Koehler Leman J, Meiler J (2019) Integrative protein modeling in RosettaNMR from sparse paramagnetic restraints. *Structure* 27(11), 1721-1734
15. **Kuenze G**, Duran AM, Woods H, Brewer KR, McDonald EF, Vanoye CG, George AL Jr, Sanders CR, Meiler J (2019) Upgraded molecular models of the human KCNQ1 potassium channel. *PLoS One*, 14(9), e0220415
14. **Kuenze G**, Meiler J (2019) Protein structure prediction using sparse NOE and RDC restraints with Rosetta in CASP13. *Proteins* 87(12), 1341-1350
13. Xia Y, Ledwitch K, **Kuenze G**, Duran AM, Li J, Sanders CR, Manning C, Meiler J (2019) A unified structural model of the mammalian translocator protein (TSPO). *J. Biomol. NMR.* 73, 347-364
12. Huang H, **Kuenze G**, Smith JA, Taylor KC, Duran AM, Hadziselimovic A, Meiler J, Vanoye CG, George AL Jr, Sanders CR (2018) Mechanisms of KCNQ1 channel dysfunction in long QT syndrome involving voltage sensor domain mutations. *Sci. Adv.* 4, eaar2631

11. Bhate MP, Lemmin T, **Kuenze G**, Mensa B, Ganguly S, Peters JM, Schmidt N, Pelton JG, Gross CA, Meiler J, DeGrado WF (2018) Structure and function of the transmembrane domain of NsaS, an antibiotic sensing histidine kinase in *Staphylococcus aureus*. *J. Am. Chem. Soc.* 140, 7471-7485
10. Jödicke L*, Mao J*, **Kuenze G***, Reinhart C, Kalavacherla T, Jonker HRA, Richter C, Schwalbe H, Meiler J, Preu J, Michel H, Glaubitz C (2018) The molecular basis of subtype selectivity of human kinin G-protein-coupled receptors. *Nat. Chem. Biol.* 14, 284-290 (*Authors contributed equally)
9. Ruiz-Gómez G, Hawkins JC, Philipp J, **Künze G**, Wodtke R, Löser R, Fahmy K, Pisabarro MT (2016) Rational structure-based rescanning approach to de novo design of interleukin-10 (IL-10) receptor-1 mimetics. *PLoS One* 11, e0154046
8. Köhling S, **Künze G**, Lemmnitzer K, Bermudez M, Wolber G, Schiller J, Huster D, Rademann J (2016) Chemoenzymatic synthesis of nonasulfated tetrahyaluronan with a paramagnetic tag for studying its complex with interleukin-10. *Chemistry* 22, 5563-5574
7. **Künze G**, Köhling S, Vogel A, Rademann J, Huster D (2016) Identification of the glycosaminoglycan binding site of interleukin-10 by NMR spectroscopy. *J. Biol. Chem.* 291, 3100-3113
6. **Künze G**, Gehrcke J-P, Pisabarro MT, Huster D (2014) NMR characterization of the binding properties and conformation of glycosaminoglycans interacting with interleukin-10. *Glycobiology* 24, 1036-1049
5. **Künze G**, Theisgen S, Huster D (2014) Backbone ^1H , ^{15}N , ^{13}C and side chain $^{13}\text{C}\beta$ NMR chemical shift assignment of murine interleukin-10. *Biomol. NMR Assign.* 8, 375-378
4. **Künze G**, Barré P, Scheidt HA, Thomas L, Eliezer D, Huster D (2012) Binding of the three-repeat domain of tau to phospholipid membranes induces an aggregated-like state of the protein. *Biochim. Biophys. Acta* 1818, 2302-2313
3. Gamble M, **Künze G**, Brancale A, Wilson KS, Jones DD (2012) The role of substrate specificity and metal binding in defining the activity and structure of an intracellular subtilisin. *FEBS Open Bio.* 20, 209-215
2. Gamble M, **Künze G**, Dodson E, Wilson KS, Jones DD (2011) Regulation of an intracellular subtilisin protease activity by a short propeptide sequence through an original combined dual mechanism. *Proc. Natl. Acad. Sci.* 108, 3536-3541
1. Vévodová J, Gamble M, **Künze G**, Ariza A, Dodson E, Jones DD, Wilson KS (2010) Crystal structure of an intracellular subtilisin reveals novel structural features unique to this subtilisin family. *Structure* 18, 744-755.

Manuscripts in Revision or Preparation

- Koehler Leman J, Lyskov S, Lewis S, Adolf-Bryfogle J, Alford RF, Barlow K, Ben-Aharon Z, Farrell D, Fell J, Hansen WA, Harmalkar A, Jeliaskov J, **Kuenze G**, Krys JD, Ljubetič A, Loshbaugh AL, Maguire J, Moretti R, Mulligan VK, Nguyen PT, Conchúir SÓ, Roy Burman SS, Smith ST, Teets F, Tiemann JKS, Watkins A, Woods H, Yachnin BJ, Bahl CD, Bailey-Kellogg C, Baker D, Das R, DiMaio F, Khare SD, Kortemme T, Labonte JW, Lindorff-Larsen K, Meiler J, Schief W, Schueler-Furman O, Siegel J, Stein A, Yarov-Yarovoy V, Kuhlman B, Leaver-Fay A, Gront D, Gray JJ, Bonneau R (2021) Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Submitted to Nature Communications [Manuscript # NCOMMS-21-13148]
- Zehnder J, Cadalbert R, Yulikov M, Böckmann, A, Meier BH, **Kuenze G**, Wiegand T (2021) Paramagnetic spin labeling of a bacterial DnaB helicase with nitroxide and lanthanide tags for solid-state NMR studies. [Manuscript in preparation]

- **Kuenze G**, Wilkinson M, Vanoye CG, Desai RR, Sanders CR, George AL Jr, Meiler J (2021) ML277 acts as an allosteric modulator of the KCNQ1 potassium channel. [Manuscript in preparation]

Peer Review Service

I have served as reviewer for the following journals: Nature Structural & Molecular Biology, Journal of Biomolecular NMR, International Journal of Molecular Sciences, Marine Drugs, and PLoS One.

TEACHING ACTIVITIES

16-20.8.2021 **Lecturer**, scientific module „Exploring Biomolecules in 3D: Principles and Applications of Computational Structural Biology“ for SFB1423 and Max-Kade exchange program between University of Leipzig and Vanderbilt University

One-week course that teaches students the theoretical and practical concepts in structural bioinformatics and the use of the ROSETTA software. The course consists of online lectures and practical computer lab exercises.

<https://research.uni-leipzig.de/vanderbilt/16-20-08-2021-module-exploring-biomolecules-in-3d-principles-and-applications-of-computational-structural-biology/>

Spring 2021 **Lecturer**, seminar and lab exercises „Instrumental analytics“ (Module 11-PHA-0401), 2nd year students in pharmaceutical sciences, University of Leipzig

7-18.12.2020 **Lecturer**, scientific module “Solution NMR integrated with computational modeling to study membrane proteins” for SFB1423 and Max-Kade exchange program between University of Leipzig and Vanderbilt University

Two-week online seminar teaching students the theoretical and practical aspects of solution NMR on membrane proteins integrated with computational modeling for the structural elucidation of membrane proteins. The course consisted of online lectures and journal clubs to consolidate the theoretical concepts.

<https://research.uni-leipzig.de/vanderbilt/07-18-12-2020-module-solution-nmr-integrated-with-computational-modeling-to-study-membrane-proteins/>

2016 – 2020 **Lecturer**, ROSETTA Workshop, Vanderbilt University, USA

Biannual, three-day workshop to train academic and industry users on the ROSETTA software. Presented and supervised tutorials on protein folding, homology modeling, protein and ligand docking, and protein design.

<https://structbio.vanderbilt.edu/workshops/rosetta/>

Spring 2019 **Teaching assistant**, Lecture „Thermodynamics and Equilibria“ (CHEM 3310-01), 3rd year chemistry students, Vanderbilt University

One-semester class on physical chemistry for 3rd year undergraduate students. Prepared and taught ten lectures on chemical equilibria, phase equilibria, the Boltzmann distribution, and NMR spectroscopy.

Winter 2013/14 **Teaching assistant**, Exercises in Physics (Module 09-BIO-0103), 1st year bachelor students in biology and biochemistry, University of Leipzig

Winter 2014/15 Weekly exercises in physics to consolidate theoretical concepts learned in class. Topics ranged from classical mechanics, electricity, and optics to applications of physics in medicine such as ultrasound, radioactivity, and X-ray.

- Spring 2014 and Spring 2015 **Teaching assistant**, lab exercises in physics, 1st year medical students, University of Leipzig
- Spring 2015 Weekly lab experiments in physics on topics such as X-ray, radioactivity, optical lenses, ultrasound, heat conductivity, electrical resistors, photometry and polarimetry.

Mentoring Young Scientists

Master Students

- 03/2021 – Present Paul Kluge, Institutes for Drug Discovery and for Bioinformatics, Uni Leipzig
- 03/2017 – 09/2017 Lisa Pankewitz, Institute for Biochemistry, Uni Leipzig

Bachelor Students

- 04/2021 – Present Richy Kümpfel, Institutes for Drug Discovery and for Biochemistry, Uni Leipzig

Undergraduate Students

- 2016 – 2020 Riddhidev Banerjee, Institute for Medical Physics and Biophysics, Uni Leipzig
Elleansar Okwei, Nica Marlow, Hope Woods, Eli McDonald, Kathryn Brewer, Mason Wilkinson, Center for Structural Biology, Vanderbilt University

MEMBERSHIPS

- 2017 – Present American Heart Association (AHA)
- 2017 – Present German Chemical Society (GDCh)
- 2017 – Present German Society for Biochemistry and Molecular Biology (GBM)
- 2019 – Present Biophysical Society (BPS)

SCIENTIFIC COMPETENCES

Scientific Expertise

- Protein structure determination: NMR spectroscopy and X-ray crystallography
- Protein biochemistry: cloning, protein expression and purification
- Protein analytics: NMR, CD, fluorescence, MALDI-MS, DSC
- Structure modeling: *De-Novo*- and homology modeling, docking, MD
- Certified biological safety officer according to §15 GenTSV

Software and Programming

- Rosetta, Amber, Gromacs, VMD, PyMOL, Gaussian, IMP, ATSAS, Jupyter
- C++, Python, Linux Shell

REFERENCES

Jens Meiler (Postdoc advisor)

Distinguished Research Professor

Vanderbilt University Center for Structural Biology, Departments of Chemistry and Pharmacology

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Daniel Huster (PhD advisor)

Research Professor and Director of Institute of Medical Physics and Biophysics

Faculty of Medicine

Leipzig University

Härtelstr. 16-18, 04107 Leipzig, Germany

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Charles R. Sanders (Scientific collaborator)

Associate Dean for Research, Professor of Biochemistry and Medicine, Investigator of Center Molecular Neurosciences, Lyle and Lange Chair of Cardiovascular Research

Vanderbilt University School of Medicine, Department of Biochemistry

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