

ISABELL LOUISE GROTHAUS



Computational Biochemist

PERSONAL

married, 1 child
 26.03.1994 in Bünde
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 hmi.grothaus.de
 @IsabellGrothaus
 Isabell Grothaus
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SKILLS

Programming

Python ●●●●●●
Bash ●●●●●●
LaTeX ●●●●●●

Operating systems

Linux ●●●●●●
MacOS ●●●●●●
Windows ●●●●●●

Software & Tools

Visualization ●●●●●●
(e.g. matplotlib, Jupyter)
Data Analysis ●●●●●●
(e.g. pandas, git, mdanalysis)
Machine Learning ●●●●●●
(e.g. scikit-learn)
Pytorch ●●●●●●
MS Office ●●●●●●

Languages

German ●●●●●●
English ●●●●●●
French ●●●●●●

EDUCATION

11/2019 - 12/2023
 University Bremen, Germany

10/2017 - 10/2019
 University Bremen, Germany

09/2014 - 09/2017
 University Bielefeld, Germany

09/2013 - 09/2014
 University Bielefeld, Germany

09/2004 - 07/2013
 Freiherr-vom-Stein Gymnasium,
Bünde, Germany

PhD research degree in engineering
with distinction (summa cum laude)
Topic: Conformational phase spaces of N-glycans
under the computational microscope

Biochemistry and Molecular Biology
Master of Science, Grade: 1.0

Biology (Genetics, Cell biology, Physiology)
Bachelor of Science, Grade: 1.9

Economics

General university entrance qualification, Grade: 1.9

PROFESSIONAL EXPERIENCE

05/2024 - now
 Dioscuri Centre for Modelling of
Posttranslational Modifications
Małopolska Centre of Biotechnology,
Jagiellonian University Krakow

Postdoctoral Researcher

11/2019 - 04/2024
 Hybrid Material Interfaces,
Faculty of Production Engineering,
University Bremen

Research assistant

Supervision of Bachelor and Master students
Giving course on atomistic simulation of macromolecules

11/2017 - 12/2018
 Max-Planck-Institut for
Marine Mikrobiology, Bremen

Student assistant

Mass spectrometry

08/2016 - 10/2016
 Alfred-Wegener-Institut,
Helmholtz-Zentrum for
Polar- und Marine Research,
Bremerhaven

Intern

Working with Arctic Phytoplankton Cultures

TEACHING

2024 - now
 University of Bremen
Master course

Synthetic Biology - Project Proposal

2020 - 2022
2024 - now
 University of Bremen
Master course

Atomistic modelling of biomacromolecules

RESEARCH GRANTS AND SCHOLARSHIPS

07/2022 - 06/2024
 North German Alliance for
High- and Ultracomputing Performance

High performance computing resources
Project ID: hbb00002 at HLRN

06/2020 - 12/2023
 North German Alliance for
High- and Ultracomputing Performance

High performance computing resources
Project ID: hbb00001 at HLRN

- 📅 09/2020 - 10/2020
📍 Trieste
Italy
- 📅 10/2018 - 10/2019
📍 University Bremen
- 📅 10/2016 - 03/2018
📍 Stiftung Studienfonds OWL

HPC-Europa3 transnational access program
Residency and computational fellowship

Deutschlandstipendium

Deutschlandstipendium

FURTHER EDUCATION

- 📅 01/2024 - now
📍 University Bremen
- 📅 09/2022
📍 University Bremen
- 📅 09/2022
📍 University Bremen

plan m - Mentoring in Science

“Fit for Leadership?!”

Self-leadership and self-coaching
for scientists

- 📅 09/2021 - 12/2021
📍 University Bremen

Data Train – Operator Track

“Deep learning”, Quantitative analysis for
data sciences, Evaluation of machine learning and
artificial intelligence algorithms

- 📅 09/2022
📍 University Bremen

Data Train – Starter Track

Data science and “Big Data”, Data and
information management, Statistical approaches,
Fundamentals of computer science for
data science, Programming languages

- 📅 12/2019 - 12/2020
📍 University Bremen

Navigare, Career coaching for
international women in science

EXPERIENCE ABROAD

- 📅 09/2021 - 10/2021
📍 SISSA, Trieste, Italy

Visiting scientist

Research stay in the group of Prof. Dr. Giovanni Bussi
at the SISSA (Scuola Internazionale Superiore di
Studi Avanzati)

- 📅 08/2015 - 01/2016
📍 University Uppsala, Sweden

Molecular Biology and Microbiology
Exchange student

- 📅 01/2011 - 04/2011
📍 Sentinal Secondary School
Vancouver, Canada

Exchange Student

SOCIAL ENGAGEMENT

- 📅 10/2021 - 10/2022
📍 University Regensburg, Germany

Project CyberMentor

Mentor for female students in the STEM field




- 📅 05/2018 - 11/2018
📍 University Bremen, Germany


Conference team – „Synthetic Biology -
Turning Science Fiction into reality“

Planning, organization and implementation of a
scientific conference




PUBLICATIONS


Rapid simulation of glycoprotein structures by grafting and steric exclusion of glycan conformer libraries

 Y. Tsai, N. Chang, K. Reuter, H. Chang, T. Yang, S., N. Zerrouki, M. Gecht, C. Penet, **I. L. Grothaus**, L. Colombi Ciacchi, K. Khoo, G. Hummer, S. D. Hsu, C. Hanus, M. Sikora
 2024  Cell 187, 1296-1311





[10.1016/j.cell.2024.01.034](https://doi.org/10.1016/j.cell.2024.01.034)


Modulation of multidrug resistance protein 1-mediated transport processes by the antiviral drug ritonavir in cultured primary astrocytes

 C. Arend*, **I.L. Grothaus***, M. Waespy, L. Colombi Ciacchi, R. Dringen
 2023  Neurochemical Research 49,66-84





[10.1007/s11064-023-04008-5](https://doi.org/10.1007/s11064-023-04008-5)


Exploration, Representation, and Rationalization of the Conformational Phase Space of N Glycans

 **I. L. Grothaus**, G. Bussi & L. Colombi Ciacchi
 2022  Journal of Chemical Information and Modelling 62, 4992-5008





[10.1021/acs.jcim.2c01049](https://doi.org/10.1021/acs.jcim.2c01049)


Identification of a HTT-specific binding motif in DNAJB1 essential for suppression and disaggregation of HTT

 S. M. Ayala Mariscal, M. L. Pigazzini, Y. Richter, M. Özel, **I. L. Grothaus**, J. Protze, K. Ziege, M. Kulke, M. ElBediwi, J. Vermaas, L. Colombi Ciacchi, S. Köppen, F. Liu, J. Kirstein
 2022  Nature Communications 13, 4692





[10.1038/s41467-022-32370-5](https://doi.org/10.1038/s41467-022-32370-5)

N-glycosylation modulates enzymatic activity of Trypanosoma congolense trans-sialidase

 J. Rosenau*, **I.L. Grothaus***, Y. Yang, L. Colombi Ciacchi, S. Kelm, M. Waespy
 2022  Journal of Biological Chemistry 298, 102403


[10.1016/j.jbc.2022.102403](https://doi.org/10.1016/j.jbc.2022.102403)

Corynebacterium glutamicum CrtR and its orthologs in actinobacteria: Conserved function and application as genetically encoded biosensor for detection of geranylgeranyl pyrophosphate

 N.A. Henke, S. Austermeier, **I.L. Grothaus**, S. Götker, M. Persicke, P. Peters-Wendisch, V.F. Wendisch
 2020  International Journal of Molecular Sciences 21, 5482


[10.3390/ijms21155482](https://doi.org/10.3390/ijms21155482)

* Shared co-first authorship

SOFTWARE CODE

GlyCONFORMER - <https://github.com/IsabellGrothaus/GlyCONFORMER>
GlycoSHIELD - <https://dioscuri-biophysics.pages.mpcdf.de/glycoshield-md/>

ACADEMIC PEER REVIEWING



Cell Reports Physical Science

ACADEMIC OUTREACH



"Das Überraschungseiweiß" - Weserkurier 03/2024, [Article](#)

"Faster Drug Discovery with GlycoSHIELD" - Press release by the University of Bremen, 02/2024, [Press release](#)



CONFERENCES

 04/2024
 Hünfeld, Germany



Selected talk: Hünfeld 2024: Workshop on Computer Simulation and Theory of Macromolecules

 02/2024
 Krakow, Polen

Invited talk: Małopolska Centre of Biotechnology, Jagiellonian University Krakow

 02/2023
 San Diego, USA

Poster presentation: Annual meeting - American Biophysical Society

 09/2022
 Lausanne, Switzerland

Selected talk: 20 years of Metadynamics workshop - CECAM

📅 06/2022
📍 Edinburgh, Scotland

Poster presentation: Frontiers in Biomolecular Simulation - 8th Annual meeting of CCPBioSim,

📅 05/2022
📍 Hamburg, Germany

Poster presentation: Biophysics at the Dawn of Exascale Computers - American Biophysical Society

📅 07/2021
📍 Vienna, Austria

Poster presentation: 13th European Biophysics Conference

📅 06/2021
📍 online

Selected talk: Mixed-Gen Session 6, Activated Events - CECAM

📅 11/2020
📍 online

Poster presentation: Annual meeting – Society for Glycobiology