Mosbacher Kolloquium "Al-driven (r)evolution in structural biology & protein design"

76

Meeting Secretariat

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Legend - Rooms





We come



Dear Friends and Colleagues,

The traditional spring meeting of the German Society for Biochemistry and Molecular Biology (GBM) is held annually in the picturesque town of Mosbach to promote the exchange of scientific ideas, discuss the latest discoveries and emerging topics and foster the education of young scientists. The topic of the 76th Mosbacher Kolloquium is "Al-based (r)evolution of structural biology and protein design".

Recent Al-driven techniques have become available to explore protein structures, from prediction and analysis to protein design. The availability of a large amount of protein structure data makes the extensive use of ML and Al methods in a wide range possible. The development of AlphaFold and many other tools show the potential but also the challenges in the field not only determined by data handling and storage but also by the integration of data that differ in quality and quantity due to experimental settings. As this multi-disciplinary field is rapidly developing there is a great need for knowledge exchange and discussions bringing together scientists and students from biology, biochemistry, bioinformatics, physics, and computer science.

At the meeting, emerging concepts will be discussed by leading international experts covering the different facets of the field. The topics include theory & tool development, machine learning in structural biology, Albased structure prediction & integrative modeling, and Al-driven protein design. Critical discussions of stateof-the-art research will allow us to together chart future developments at the interface of basic science and applications, while fruitful scientific exchange of ideas will help inspire young scientists in their future research endeavors in this rapidly developing field.

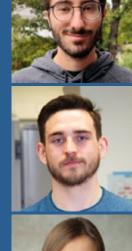
We warmly welcome you!

Janosch Hennig Birte Höcker Ina Koch



Alte Mälzere

Wed., March 19





19:00 - 19:30 **Rainer Rudolph Awards**

16:00

18:00

The Rainer Rudolph Foundation promotes and supports basic and applied research in protein

A short intro to the topic of this year's Mosbacher Kolloquium (delivered by the organizers)

Arrival and registration

Introductory lecture ("Primer")

biochemistry and biotechnology. Every year awards are given to young scientists who have made outstanding advances in these fields.

Davide Amendola /Zürich [DE] The arsenal of a bacterial predator revealed by cryo-electron microscopy

Alexander Braun /Bayreuth [DE] Designing triosephosphate isomerases using generative language models

Britta Lipinski /Darmstadt [DE] Engineering of single domain antibody-based bispecifics

20:00 Welcome reception /Get together

The steering committee of the German Society for Biochemistry and Molecular Biology (GBM) and the city of Mosbach invite you to a welcome reception in the town hall of Mosbach (no registration required)

City hall

We thank the city of Mosbach for the kind hospitality.

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Thu., March 20











latthias Rar



















08:50

Session 1 (09:00 - 12:00) Theory and development (Chair: Clara Schoeder)

by the scientific organizers

David Jones /London [UK]

Opening remarks

- 00:60 The encyclopedia of domains and quickly searching for multi-domain protein structures
- Early career investigator talk 1
- 09:30 Lea Brönnimann /Bern [CH] Exploring antibody repertoires using deep language models
- 09:45 Matthias Rarey /Hamburg [DE]
- Artificial intelligence or intelligent computing? Examples from computer-aided molecular design

Coffee break (10:15 - 10:45)

- Andrea Volkamer /Saarbrücken [DE]
- Hybrid AI and open source for drug design
- 11:15 10:45 Early career investigator talk 2
- David Medina-Ortiz /Halle (Saale) [DE] Integrating geometric deep learning with explainable artificial intelligence to assist protein engineering
- Burkhard Rost /Munich [DE]
- 11:30 Artificial intelligence deciphers the code of life written in proteins?

Lunch break (12:00 - 13:00)



Thu., March 20

nogr

- 2:00 Meet the Industrial Scientist with
 - **Alexander Rives**

(info on page 29)

- 12:00 Meet the Prof with Tanja Kortemme (info on page 29)
- 2:15 Panel discussion "Big Data, Big Challenges -
 - How do we manage research data?" Do you want to organize and store your research data efficiently? Do you wonder how to ensure the reproducibility and integrity of your data? Do you ask yourself how to comply with data management policies and best practices?

Join the GBM Young Investigators and explore these questions and more with experts from both academia and industry, and learn how to manage your research data effectively!

- Workshop by Thermo Fisher Scientific:
- 13:00 "Empowering Cryo-EM workflows with AI and CryoFlow"
- 3:00 Workshop by Deltablot
- "Demonstrating eLabFTW: A free and opensource electronic laboratory notebook"
- Poster session I

13:00

(even numbers, info on page 30f)

TC

Thu., March 20











Session 2 (14:30 - 16:45) Machine Learning in Structural Biology (Chair: Ora Furman)

- 14:30 Sergey Ovchinnikov /Cambridge [USA]
- Inverting protein structure prediction models for protein design
- 15:00 Noelia Ferruz /Barcelona [ES]
- Optimizing proteins with reinforcement learning

Coffee break (15:30 - 16:00)

- Martin Steinegger /Seoul [KR] Supercharged protein analysis in the era of accurate structure prediction 16:00
- Early career investigator talk 3
- 16:30 Leif Seute /Heidelberg [DE] Learning conformational ensembles of proteins based on backbone geometry

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Thu., March 20





16:45		maceuticals PhD Award				
		endker /Boston [USA] f a protein fractal				
17:00	Karl Lohma (Laudatio: C	nn Prize Ilaus Seidel)				
	Structural in	Tamborrini /Basel [CH] Iral investigation of the relaxed cardiac Ivere by electron cryo-tomography				
17:15	GBM General Meeting (17:15 - 19:30) (for GBM members only)					
19:30	Feodor Lynen Lecture (Laudatio: Birte Höcker)					
1. 10	Tanja Korte	mme /San Francisco [USA] De novo protein design: From new structures to programmable molecular and cellular functions				
T Z		The German Society for Bioche- mistry and Molecular Biology honors Tanja Kortemme with the distinguished Feodor Lynen medal.				

After the prize lecture the GBM invites all participants to join the Lynen Reception.

20:30

Lynen reception & poster session II (even & odd numbers, info on page 30f)

Get Together & Networking



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GESELLSCHAFT FÜR BIOCHEMIE UND MOLEKULARBIOLOGIE E.V.



GBM Compace

Focus on Condensate Biology

Sept 18 - 19, 2025 / Frankfurt am Main

Organization:

Simon Alberti /Dresden Sara Cuylen-Haering /Heidelberg Dorothee Dormann /Mainz Edward A Lemke /Mainz Julia Mahamid /Heidelberg Claus Seidel /Düsseldorf Konstanze Winklhofer /Bochum

77. Mosbacher Kolloquium

More than lipidic barriers -New horizons in membrane biology

March 26 - 28, 2026 / Mosbach (Baden), Germany



Organization Britta Brügger (Universität Heidelberg) || Robert Ernst (Universität des Saarlandes) Andre Nader (MPI CBG Dresden) || Christian Ungermann (Universität Osnabrück)

Fri., March 21

18







ng Zhang



modelling (Chair: Saacnicteh Toledo Patino) Yang Zhang /Singapore [SG] Towards an Al-based solution of protein struc-

Al-based structure prediction & integrative

- 00:60 ture prediction problem
- Early career investigator talk 4

Session 3 (09:00 - 10:15)

- 09:30 Arman Simonyan /Copenhagen [DK] New machine learning-driven approaches for peptide probe and drug discovery
- 09:45 Jan Kosinski /Hamburg [DE]
 - Al-based integrative structural modeling

Coffee break (10:15 - 10:45)

Session 4 (10:45 - 12:00) From protein engineering to AI-based protein design (Chair: Alena Khmelinskaia)

- Possu Huang /Stanford [USA]
- 10:45 SHAPES of protein generative models
- Early career investigator talk 5
- 11:15 Sophie Binder /Bonn [DE] Al-based protein design and validation
- Bruno Correia /Lausanne [CH]
- 11:30 Exploring the structural and functional landscape of proteins by computational design

Lunch break (12:00 - 13:00)

Fri., March 21



















Workshop by Elsevier & Biochemica et

Meet the prof with Matthias Hentze

- I 2:00 Biophysica Acta: How to publish your research in scholarly journals
- Poster session III

13:00

12:00

(odd numbers, info on page 30f)

(info on page 29)

- 13:45 Research funding at the Klaus Tschira
- Foundation

Junior GBM Session (14:30 - 16:00) (Chairs: Frederike Knipp, Marcel Zimmeck)

- 14:30 Alex Rives /New York [USA]
 - Language models at the scale of evolution
- Stanislaw Dunin-Horkawicz /Tübingen [DE]
- 15:00 What can we learn from incorrect AlphaFold2 models? (the case of signal transduction)
- Early career investigator talk 6
- 15:30 Anna Backeberg /Munich [DE]
- De novo design of multiple-geometry forming protein scaffolds
- 15:45 Early career investigator talk 7
- Kateryna Maksymenko /Tübingen [DE] Training-free framework to design protein-based binders

Fri., March 21







Otto Warburg Med

Coffee break (16:00 - 16:30)

Eduard Buchner Prize

6:30 (Laudatio: Janosch Hennig)



Dorothee Kern /La Jolla [USA] The protein dance – from experiments to AI predictions

- 17:30 **Otto Warburg Lecture & Medal**
 - (Laudatio: Volker Haucke)

Matthias Hentze /Heidelberg [DE] From Otto Warburg to riboregulation: a 100 year journey in metabolism

This year the GBM, Elsevier and Biochimica et Biophysica Acta (BBA) will honor Matthias Hentze from the European Molecular Biology Laboratory (EMBL) in recognition of his fundamental contributions to the understanding of gene regulation by RNA-binding proteins and the identification of RNA-binding proteins with the Otto Warburg Medal.

The highest award in Germany for biochemists and molecular biologists promotes outstanding scientific excellence and encourages groundbreaking achievements in the field of fundamental biochemical and molecular biological research.

Since 1963 the Otto Warburg Medal is intended to commemorate the outstanding achievements of Otto Heinrich Warburg. To emphasize the importance of excellent scientific research and motivate young researchers to achieve outstanding results, the prize is endowed with 25.000 Euro. sponsored by



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Sat., March 22









Young Investigator Session (09:00 - 10:15) (Chair: Andrea Hupfeld)

- 00:60 Andrea Thorn /Hamburg [DE]
- The potential of AI for experiments in structural biology
- 09:30 Early career investigator talk 8
 - Marharyta Makarova /Erlangen [DE] A novel rotamer library for nucleic acids enables the design of protein-nucleic acid complexes with the protein design software MUMBO
 - Maximilian Fürst /Groningen [NL]
- 09:45 Big data from wet-lab biochemistry and dry-lab biophysics to advance AI protein design

Coffee break (10:15 - 10:45)

T

Sat., March 22









Session 5 (10:45 - 12:30) Al application in Life Sciences (Chair: N.N.)

- Judith Zaugg /Heidelberg [DE] Mining cryo-electron tomography data with 10:45 self-supervised deep learning models
- Early career investigator talk 9
- 11:15 Salomé Guilbert /Lausanne [CH] In silico design of enzymes to degrade shortchain Per- and Polyfluoroalkyl Substances (PFAS)
- Jens Meiler /Leipzig [DE] How artificial intelligence is reshaping protein structure prediction and therapeutic design from small molecules to new modalities 11:30
- 12:00 Gevorg Grigoryan /Somerville [USA]
- Programmable generative protein design: from molecules to medicines
- 13:00 Poster prizes & closing remarks

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Meet the Prof

This year's guests of the Junior GBM are Tanja Kortemme and Matthias Hentze. The scientists will give insights into their lives as researchers and their personal careers. In addition, you can ask questions in an informal atmosphere that may help you with your personal orientation in research and career or that simply interest you.

Thursday, March 20, 12:00 - 13:00 (Room: Darre) (Chair: Katharina Bachschwöller) **Tanja Kortemme** (University of California UCSF)

Friday, March 21, 12:00 - 13:00 (Room: Darre) (Chair: Philip Müller) Matthias Hentze (EMBL Heidelberg)

The number of participants is limited. A registration is required.

Meet the industrial scientist

The Junior GBM succeeded in winning Alex Rives from EvolutionaryScale for the "Meet the industrial scientist". Similar to the "Meet the Prof" format, the scientist will talk about his work and career and answer your questions.

Thursday, March 20, 12:00 - 12:45 (Room: Tenne) (Chair: Jens Martin) Alex Rives (EvolutionaryScale)

The number of participants is limited. A registration is required.





Poster Specifications

The posters should be presented in portrait format (DIN A0 resp. \sim 120 x 85 cm).

Session Times

Thursday, 13:00 - 14:30 (even numbers) Thursday, 20:30 - 22:00 (all numbers) Friday, 13:00 - 14:30 (odd numbers)

During the poster sessions the presenting authors are requested to stay near their posters. Posters should be presented throughout the whole meeting.

Poster Abstracts

All poster abstracts are available as pdf-file for down-load on the meeting homepage.

A printed abstract booklet is available for viewing purposes at the registration desk.

Poster Numbers

Please see the poster list on page 40 for poster numbers.

Poster Prizes

The best three posters will be awarded at the end of the meeting with a poster prize by GBM and FEBS Open Bio (300 \in each). In addition, three further posters will be awarded a book voucher worth \in 150, sponsored by Wiley-VCH.

The winners will be announced at the end of the meeting on Saturday. To receive the prize, personal attendance is required.

for GBM stakeholders



19 ר	14:00 - 16:30	(Room: Darre)			
March 19	Sitzung: Arbeitskreis Studium Molekulare Biowissenschaften				
March 19	17:00 - 19:00	(Room: Malzboden)			
	Sitzung: Sprecher der GBN Arbeitskreise	1-Studiengruppen und			
20 ר	12:30 - 14:00	(Room: Malzboden)			
March	Sitzung: GBM-Kontaktpersonen				
March 20	15:15 - 16:30	(Room: Schalander)			
	Meeting of Senior Experts in the GBM				
March 20	17:15 - 19:30	(Lecture hall)			
	GBM-Mitgliederversammlung				
March 21	12:00 - 14:30	(Room: Schalander)			
	Sitzung: Arbeitskreis "Biochemie in der Medizin				
March 21	13:30 - 14:30	(Room: Tenne)			
	Sitzung: Junior GBM Leaders				
March 21 March 21 March 21 March 21 March 20 March 20 March 20	19:00 - 21:00	(Room: Darre)			
	Meeting Postdocs@GBM				
21 ר	19:00 - 21:00	(Lecture hall)			
March	Vollversammlung: Junior (GBM			

Venue

The Kolloquium takes place in the "Alte Mälzerei" in Mosbach/Baden (Germany)

Alte Mälzerei Alte Bergsteige 7 74821 Mosbach/Baden

Internet

There will be a wireless LAN access point in the conference centre.

SSID: GBM Key: gbm-online

Conference Office

Opening hours are

Wednesday:	16.00	19:45
Thursday:	00:80	17:00
Friday:	08:30	16:00
Saturday:	08:30	11:00

none:

+49 69 6605670

Lunch & Coffee Breaks

Coffee, tea and mineral water will be provided for free during the coffee breaks.

Lunch and Dinner is available at your own expense in the conference center or in one of the restaurants in the city of Mosbach.

Please note

Your name badge and the program booklet are available at the registration desk.

We kindly ask to wear your name badge as an entry ticket during the whole meeting.



We thank for the kind support by:







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Please visit the booths of our supporters

Elsevier/BBA (Booth 1a) Walter deGruter (Booth 1b) BMG Labtech (Booth 2) Nikon (Booth 3) Xceltis (Booth 4) Cytiva (Booth 5) xyna.bio (Booth 6) CryoCloud (Booth 7)



0 01

Khadija Aichane-Simon Enforced phosphatase recruitment as a novel strategy in the treatment of acute myeloid leukemia

E 02

Marius Amann Engineering Plasmodium falciparum Proteins for Small-Molecule Drug Discovery: Investigating Stability, Structural Dynamics, and Biophysical Effects

O 02

Varvara Apet Design and optimization of flavoproteins for hyperpolarized EPR methods

E 03

Katharina Bachschwöller Design of functional proteins by fragmentbased chimeragenesis

E 04

Anna Backeberg De novo design of multiple-geometry forming protein scaffolds

A 01

Julian Beck Scaffolding a Kemp eliminase activity into an idealized de novo TIM barrel

E 05

Philipp Becker Past to Protocells: Ancestral Min Proteins and Early Pattern Formation

O 03 Stine Behrmann Predicting structural features of suppressor tRNAs using MD simulations

P 01

Ramachandra M Bhaskara Decoding homeostatic pathways: from data Streams to molecular mechanisms

O 04

Patryk Bielski Bicelles assembled with the G protein-coupled receptor rhodopsin as model lipid-protein system for interaction studies

A 02

Sophie Binder Al-based protein design and validation

A 03 Andreas Blaha A conserved fertilization complex predicted by Alpha-Fold2-Multimer bridges sperm and egg in vertebrates

A 04

Alexander Braun De novo design of triosephosphate isomerases using generative language models

A 05 Breimann Breimann Charting γ-Secretase substrates by explainable AI

O 05 Constanze Breithaupt Multimerization of Grb2 revealed by the Grb2-Gab1(497-528) complex structure

E 07 Adrian Bunzel Al.zymes: A Modular Platform for Evolutionary Enzyme Design

P 02 Grzegorz Chojnowski gapTrick – Structural characterisation of proteinprotein interactions using AlphaFold with multimeric templates

P 03

Sandrine Coquille Mapping of allosteric protein landscapes using Al approaches

O 06

Jan A. Dewald Validation and characterization of a fourth preQ₁ riboswitch class

O 07

Karthikeyan Dhamotharan A core network in SARS-CoV-2 nucleocapsid NTD drives domain stability and RNA recognition.

M 01 Simon Dürr

Predicting interactions of proteins with metals using cofolding methods and AllMetal3D

A 06

Stefan Düsterhöft MaPIN: A computational pipeline to Map Protein Interaction Networks.

O 08

Christoph Elfmann Cutting-edge tools for structural biology: bringing AlphaFold and Foldseek to the people

O 09

Mohammad ElGamacy Design and development of synthetic G-CSFR modulators

A 07

Robert Englmeier

Towards automating cryo-EM data analysis using AI, new algorithms and large scale analysis

M 02

Inken Fender Predicting Molecular Hotspots for Efficient Drug Discovery using Deep Learning

O 10

Anna Franziska Finke Coupling of ribosome biogenesis and translation initiation in human mitochondria

O 11

Karlo Franke

Functional analysis of synthetic cytokine receptors and possible heterodimerisation for optimised intracellular signalling

E 01

Emily Freund Redesigned RNA-binding domains to study their effects on helicases

O 12

Béla Frohn Protein Design For and With Synthetic Cells

O 13

Andreas Gagsteiger Expanding the available structure and sequence space of PET degrading enzymes

A 08

Chiara Gasbarri Al in support of drug off-target effect research: the CavitOmix Copilot

O 14 Florian Gisdon Graph-Theoretical Analysis of Functional Changes in an Open and Closed Conformation of Complex I

E 37

Anastasia Götz Reprogramming self-inserting nanopores for differential transport across synthetic membranes

E 08

Salomé Guilbert In Silico Design of Enzymes to Degrade Shortchain Per- and Polyfluoroalkyl Substances (PFAS)

M 03

Jannik Adrian Gut Synthetic MSAs identify protein conformations

O 15

Jan Hartmann

Severe discrepancies between the newly determined crystal structure of the RNA aptamer B1m15 in complex with the bacterial repressor DasR and the AlphaFold3-predicted structure.

E 09

Noah Ernst Holzleitner Al-guided engineering of CRISPR-Cas proteins

E 10 Stefan Hristov ForceYield2: Validating AI-Assisted Protein Design With In Vivo Selection

A 09

Maxim Janzen

Predicting single residue effects on peptide binding specificities in designed Armadillo repeat proteins

E 11

Michael Adrian Jendrusch Fast and flexible protein structure generation with sparse all-atom denoising (SALAD)

E 12 Alena Khmelinskaia Tales of Dynamic Protein Assembly Design

E 13 Hubert Klein In-silico Design of Foldamer - Protein Interactions

A 10

Sarah Knapp Predicting PARP15 networks with proximity-ligation based mass spectrometry data and MaPIN (Mapping of Protein Interaction Networks)

E 14

Johanna-Sophie Koch Evaluation of cobalamin-binding chimeras designed by fold recombination

E 15

Kerlen Korbeld Enriching Stabilizing Mutations through Analysis of Short Molecular Dynamics Simulations by BoostMut

P 04

Jacqueline Krohn Assessing AI Driven Protein Structure Prediction Methods with Heparanase 2 Splicing Forms

E 16

Georg Künze Computational engineering of a metagenomederived polyester hydrolase for efficient PET depolymerization

P 05

Pasquale Lamagna

Beating viruses at their own game: exploiting structural homology and protein structure predictions to identify new viral host-virus proteinprotein interactions.

O 16

Olive Laprévote Step by step - Engineer Trp Repressor to Walk in a Tandem Gait

E 17

Horst Lechner Developing Machine-Learning-Driven Sequence Design Strategies to Stabilize and Produce Challenging Enzymes

T 01

Jennifer Leclaire BiochemicalAlgorithms.jl -- Rapid application development in Julia

E 18

Bruce Lichtenstein Functional Ligands: Protein design for electrochemical and structural control of ligand properties

P 06

Katja Luck Structural annotation of disease-relevant protein interaction interfaces involving disorder

O 17

Marharyta Makarova

A novel rotamer library for nucleic acids enables the design of protein-nucleic acid complexes with the protein design software MUMBO

A 11

Yelyzaveta Makedon

The role of Beta-2 microglobulin tryptophan mutagenesis in detecting MHC class I heavy chain folding in vitro

P 07

Anja Marquardt

Integrating Artificial Intelligence Based and Classical Structural Biology Methods to Understand the Impact of the β -Actin G74S Mutation on Histidine Methylation

E 20

David Medina-Ortiz

Integrating geometric deep learning with explainable artificial intelligence to assist protein engineering

P 08

Pasquale Miglionico AlphaFold3-based Prediction and Design of GPCR-G protein Coupling

A 12

Johanna Moeller Computational stabilization and functional characterization of single-chain T cell receptors targeting a cancer epitope

A 13

Felix Moorhoff SelectZyme: AI-Based Interactive Protein Space Visualization for Enzyme Discovery, Selection, and Mining

presenting auth

E 21 Lennart Nickel Engineering Cell Type Specific AAVs by Computational Protein Design

E 22

Martin Pacesa Accurate binder design using BindCraft

O 18

Marina Parr Computational analysis of translation elongation factors

O 19

Lars-Oliver Peters Visual dysfunction caused by mutations in the cGMP-signaling protein complex

A 14

Thorsten Pfirrmann CiliAI: A Web-Based Machine Learning Platform for Automated Detection, Analysis, and Signal Densitometry of Primary Cilia in Confocal Microscopy Images

O 20

Agata Raczyńska Enzymes for Polyurethane Degradation: Computational and Experimental Strategies for Design and Discovery

P 10

René Rasche

Pathogenic potential of RalGAP variants explained by combined structural and computational analysis

O 21

Johanna Rathke

Quantitative analysis of Ezrin mutants defective in f-Actin Binding observed with in vitro minimal Actin cortices

E 23

Katharina Rauchenwald-Köchl

Exploring enzymatic active sites using 3D point clouds representing physico-chemical properties of protein cavities

O 22

Johannes Regner Functional and structural characterization of UbiB

P 11

Bianca Reschke FRET-assisted structural modeling of dynamic protein ensembles

P 12

Till Rudack Integration of experiment and theory unveils structure, dynamics, and function of multi-protein complexes

T 02 Jakob Ruickoldt CryoCrane

P 13

Peter Russ Challenges for AI driven structure prediction: The peacock's feather keratin

E 24

Marc Scherer Two-state design enabled the reliable optimisation of dynamic small molecule binding proteins

E 25 Phillip Schlegel From Genome Mining to Enzyme Engineering: A case study one the Phosphoramidon Biosynthetic Pathway

E 26

Lisa Schmidt Analysis and design of protein fold switches

T 03

Clara Schoeder Between sampling and scoring – a fair comparison of self-supervised machine learning methods

M 04

Leif Seute Learning conformational ensembles of proteins based on backbone geometry

A 15

Irina Shevyreva Understanding the catalytic mechanism of bacterial phospholipid N-methyltransferases using AI tools and not only

O 23

Ingrid Span Exploring the gas channel in [FeFe] hydrogenases

P 15

Simon Straß Analytical high-throughput assays for generation of validated datasets to train ML models for cellulase optimization

P 16

Milton T. Stubbs Modelling conformational transitions in macromolecular interactions

E 27

Andrey Sysoev Protein Design Yielding Complex Functions in Synthetic Cells

P 17

Tomer Tsaban Moonlighting signal peptides of protein isoforms discovered by deep learning

O 24

Pascal Vielberth

Analysis of Interactions between the $\gamma\text{-Tubulin}$ Ring Complex with the Centrosomal Proteins CDK5RAP2 and CP148 in Dictyostelium discoideum

E 28

Vsevolod Viliuga Flexibility-conditioned protein structure design

E 29

Leo von Bank A multifaceted approach for efficient protein translocation and direct purification of in vitro synthesized protein

O 25

Srdan Vujinovic Non-canonical G protein signaling in magnetoreception of European robin

E 30

Simon Wagner Generating Highly Designable Proteins with Geometric Algebra Flow Matching

A 16

Daniel Wedemeyer Protein half-lives and destabilizing regions via language models

E 31 Jonas Wepfer Computational design of sequence-specific peptide binders using AF2

E 32

Timothy Whitehead Computational design of biosensors and point of care diagnostics for emerging synthetic opioids

O 26

Nex Maris Winkler Elucidating the structural basis for phenotypical variations caused by naturally occurring YUC-CA8 proteoforms in Arabidopsis thaliana

E 33

Benedict Wolf Rational engineering of allosteric protein switches by in silico prediction of domain insertion sites

E 34

Tobias Wörtwein Damietta protein design toolkit

E 35

Christina Wüst Al-Driven Design of Chimeric Antigen Receptor Binders

M 06

Max Dongsheng Yin Structural Insights into an Anaerobic CO₂ Fixation Complex

P 14

Büsra Yüksel Model of the inactive dimeric conformation of TAp63α

E 36

Cathleen Zeymer Al-based redesign improves catalytic efficiency and enantioselectivity of an artificial photoenzyme

M 05

Hanne Zillmer Towards a comprehensive view of the pocketome universe – biological implications and algorithmic challenges

E 19

Anna Zink Designing Protein Extensions: Key Puzzle Pieces for Artificial Molecular Motors

A 17

Aleksandr Zlobin Towards robust computational activity assays for enzyme study and design

A 01 Julian Beck Scaffolding a Kemp eliminase activity into an idealized de novo TIM barrel

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Robert Englmeier Towards automating cryo-EM data analysis using AI, new algorithms and large scale analysis

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Computational stabilization and functional characterization of single-chain T cell receptors targeting a cancer epitope

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Felix Moorhoff SelectZyme: Al-Based Interactive Protein Space Visualization for Enzyme Discovery, Selection, and Mining

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CiliAI: A Web-Based Machine Learning Platform for Automated Detection, Analysis, and Signal Densitometry of Primary Cilia in Confocal Microscopy Images

A 15

Irina Shevyreva

Understanding the catalytic mechanism of bacterial phospholipid N-methyltransferases using AI tools and not only

A 16 Daniel Wedemeyer Protein half-lives and destabilizing regions via language models

A 17

Aleksandr Zlobin Towards robust computational activity assays for enzyme study and design

E 01 Emily Freund Redesigned RNA-binding domains to study their effects on helicases

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Marius Amann Engineering Plasmodium falciparum Proteins for Small-Molecule Drug Discovery: Investigating Stability, Structural Dynamics, and Biophysical Effects

E 03 Katharina Bachschwöller Design of functional proteins by fragmentbased chimeragenesis

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Anna Backeberg De novo design of multiple-geometry forming protein scaffolds

E 05 Philipp Becker Past to Protocells: Ancestral Min Proteins and Early Pattern Formation

E 07 Adrian Bunzel Al.zymes: A Modular Platform for Evolutionary Enzyme Design E 08 Salomé Guilbert In Silico Design of Enzymes to Degrade Short-chain Per- and Polyfluoroalkyl Substances (PFAS)

E 09 Noah Ernst Holzleitner Al-guided engineering of CRISPR-Cas proteins

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