9th Alpbach Workshop on: Repeat Proteins – Biology & Design

Arrivals, Reception and Dinner

MONDAY SEPTEMBER 8

08:50   **Welcome** (**Andrei Lupas and Dek Woolfson**)

09:00 – 10:15   **New developments** (**Andrei Lupas**)

                        Andrei Lupas (Tübingen) – New protein fibers from the dark proteome
                        Joana Pereira (Leuven) – The Protein Universe Atlas: A Lens into Novel Families and Functions Across the Protein Universe
                        Vikram Alva (Tübingen) – Repeat Proteins at the Surface: S-layer Lattices in Archaea and Bacteria

10:15 – 10:45   **Tea break**

10:45 – 12:25   **Software resources** (**Gevorg Grigoryan**)

                        Gevorg Grigoryan (Generate Biomedicines/Dartmouth) – From Protein Design to Programmable Biology and Therapeutic Impact
                        Kaiyu Qiu (Tübingen) – Detecting protein repeats using sequence embeddings from protein language models
                        Christopher Wood (Edinburgh) – CC Central: A Unified Platform for Coiled-Coil Discovery, Analysis, and Design
                        Mohammad ElGamacy (Tübingen) – Synthetic protein design with Damietta

12:30 –   **Lunch - Afternoon free**

17:00 – 17:45   **Flash Presentations for Posters** (**Katarzyna Ożga**)

                        Glenn Carrington (Leeds) – Getting Kinesin Back on Track: TRAK2 as a Mitochondrial Transport Adaptor
                        Melissa Dyson (Bristol) – Installing Functional Metal-Binding Sites into *De Novo* Designed Proteins
                        Gesa Laura Freimann (Tübingen) – Molecular Dynamics Simulations of Af1503 – A Model Protein for Transmembrane Signaling
                        Jesse Gayk (DESY) – A structural chameleon in cryo-EM: cross-α/cross-β amyloids & nanotubes
                        Valeriia Hatskovska (Tübingen) – *De Novo* Design and Characterization of Single-Domain Bivalent Binders for Therapeutic Applications
                        Reece King (Bristol) – Designing cell-permeating peptides to target coil-1A of vimentin intermediate filaments
                        Xiyue Leng (Bristol) – Programmable Three-Helix Bundle Proteins with Controlled Topology and Tunable Stability
                        Holly McKenzie (Bristol) – Blended Domains: A Design Strategy for Constructing Ligand- Responsive Coiled-coil Proteins

Matej Milijaš-Jotić (Tübingen) – Ordering Disorder: A Binder
Design Strategy for BAALC
Leila Motiei (Weizmann) – Chemically Programmable Bacterial
Probes for the Recognition of Cell Surface Proteins
Shai Rahimipour (Bar Ilan Uni) – Targeting Aβ oligomers for early
theranostics of Alzheimer's disease
Lauren A. Rhodes (Bristol) – Design and characterisation of *de
novo* miniproteins to recognise curvature at the plasma
membrane
Britt Rooijakkers (Leiden) – Understanding metal selectivity in *de
novo* designed coiled coil proteins
Alexandra Waldherr (Tübingen) – Non-canonical amino acids and
their inclusion and occurrence in elucidated structures

17:45 – 18:30   **Posters**

18:30 – 20:00   **Dinner**

20:00 – 21:40   **Natural and designed fibres** (**Allon Hochbaum**)

Allon Hochbaum (UC Irvine) –
Matthew J. Harrington (McGill) – Mussels use peculiar coiled coils
to build tough fibers and underwater glues
Caitlin Johnston (CSIRO) – Resolving the structure and assembly
of the honeybee silk heterotetrameric coiled coil
Jordi Bella (Manchester) – Designed, hyperstable recombinant
collagen-like proteins without hydroxyproline

TUESDAY SEPTEMBER 9

09:00 – 10:30   **Design I: structure and dynamics** (**Dek Woolfson**)

Dek Woolfson (Bristol) – Learning to build coiled coil-based
assemblies, structures and functions from scratch
Sarah Berger (Birmingham) – Predictive Structural Analysis of
Coiled Coils Crosslinking Using Computational Tools
Jose M. Martínez-Parra (Santiago de Compostella) – Observing
the internal chirality of non-proteinogenic peptide bundles
Andrey V. Romanyuk (Bristol) – Biomolecular condensation by de
novo designed patchy globular proteins

10:30 – 11:00   **Tea break**

11:00 – 12:15   **Design II: design for function** (**Dek Woolfson**)

Katerina Maksymenko (Tübingen) – Shape-centric approaches to
protein docking
Adrian Tripp (Graz) – Computational enzyme design via
scaffolding of helical motifs
Rokas Petrenas (Bristol) – Rapid Assessment of Size, Shape, and
Chemical Complementarity of Ligands for Computational
Protein Design

12:30 –	Lunch - Afternoon free

18:30 – 20:00	Dinner

20:00 – 21:20 **AlphaFold successes and failures** (**Stanisław Dunin-Horkawicz**)

Katarzyna Ożga (Copenhagen) – Designing Multidomain Coiled-Coil Proteins: What AlphaFold2 Gets Right and Wrong
Stanisław Dunin-Horkawicz (Tübingen) – Coiled-coil domains hiding in the AlphaFold database
Mikel Martinez Goikoetxea (Tübingen) – CCfrag: A Fragment-Based Framework for Modeling Long Coiled Coils
Grzegorz Chojnowski (Hamburg) – Structural characterisation of protein-protein interactions using AlphaFold

WEDNESDAY SEPTEMBER 10

09:00 – 10:30 **Assemblies and materials** (**Vincent Conticello**)

Vincent Conticello (Emory) – Designable cross-α filaments: Flipping the switch on coiled-coil assembly
Edward H. Egelman (University of Virginia) – Cryo-EM of polymers at near-atomic resolution: from proteins to peptides
Mike Sleutel (VU Brussel) – Auto-crosslinking sporesilk fibers promote endospore and Cry toxin clustering
Maxime Naudé (Copenhagen) – Layers of α-helical barrels for the control of excitons leading to transport of energy

10:30 – 11:00	Tea break

11:00 – 11:40 **Assemblies and materials contd**. (**Vincent Conticello**)

Gabriel A. Frank (Ben Gurion Uni) – A Direct Link Between Evolutionary Pressure and 3D Pattern Formation in Bacterioferritin Assembly
Raz Zarivach (Ben Gurion Uni) – Structural studies of magnetosome-associated protein-mineral interactions

11:45 – 12:45 **Functionalising designed proteins** (**Birte Höcker**)

Birte Höcker (Bayreuth) – Designing for function:Building enzyme and binding sites from scratch
Tanja Kortemme (UCSF) – De novo protein design: From new structures to programmable molecular and cellular functions

12:45 –	Lunch - Afternoon free

17:15 – 18:30 **Natural complex systems I** (**Hadeer ElHabashy**)

Murray Coles (Tübingen) – polyHAMPs
Vera Nazarenko (Tübingen) – Studies of transmembrane signal transduction using a model receptor Af1503

Hadeer ElHabashy (Tübingen/Bayreuth) – Novel insights into the functional landscape of the STAC domain

18:30 – 20:00   **Dinner**

20:00 – 21:15   **Natural complex systems II** (**Jessica Cross**)

Mark Dodding (Bristol) – Control of the activity of the microtubule motor kinesin-1 by its dynamic and multifunctional coiled-coils
Jessica Cross (Bristol) – Hijacking Hinges: Cracking the coiled-coil code to control intracellular transport
Michelle Peckham (Leeds) – How the coiled coil helps keep class 2 myosins switched off

THURSDAY SEPTEMBER 11

09:00 – 10:35   **Repeat-protein Design** (**Andreas Plückthun**)

Andreas Plückthun (Zürich) - Intracellular applications of synthetic repeat proteins
Laura Itzhaki (Cambridge) – Engineering the folding and function of tandem-repeat proteins: Teaching old proteins new tricks
Renko De Vries (Wageningen) – Computational sequence design of α-helical repeat proteins that inhibit ice-crystallization
Zarifa Osmanli (Padova) – GeomeTRe: accurate calculation of geometrical properties of repeat proteins

10:35 – 11:05   **Tea break and Group Photograph**

11:05 – 12:20   **At the membrane** (**Ai Niitsu**)

Ai Niitsu (RIKEN) – Designer membrane proteins towards engineering the signalling frontier
Alexander Kros (Leiden) – Coiled-coil peptide-mediated RNA delivery
Tao Jiang (Xiamen Uni) – On-Cell Assembly of Coiled-Coil Peptides Enables Precise Manipulation of Cell Behaviors

12:30 –   **Lunch - Afternoon Free**

17:30 – 19:30   **The quest for specific binding proteins** (**Dek Woolfson and Andrei Lupas**)

Peter Kim (Stanford) – Adventures with coiled coils, viral membrane fusion, vaccine design, and protein engineering
James Wells (UCSF) – Pirating natural proteins and antibodies for extracellular targeted protein degradation
Bill DeGrado (UCSF) – *De novo* design of functional proteins

20:00 –   **Gourmet Dinner**

FRIDAY SEPTEMBER 12

Departures