

PROGRAMME

Wednesday, 14 June 2023

15:00 – 20:00 REGISTRATION

18:00 – 19:00 WELCOME RECEPTION — GARDEN PARTY

OPENING

chairperson: Mateusz Chwastyk

19:00 – 19:10 Mateusz Chwastyk
Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
Welcome address

19:10 – 19:50 George Rose
Department of Biophysics, Johns Hopkins University, USA
Have we been thinking about protein folding "upside down"?

20:00 – 22:00 DINNER AT BONFIRE

Thursday, 15 June 2023

THE INNER LIFE OF THE CELL

chairperson: Anna Niedźwiecka

9:00 – 9:30 Gary Pielak
University of North Carolina, USA
Protein stability in living cells & under crowded conditions in vitro

9:30 – 10:00 Sebastian Glatt
Malopolska Centre of Biotechnology, Jagiellonian University, Poland
tRNAslational Control of Eukaryotic Gene Expression

10:00 – 10:30 Yuji Sugita
Laboratory for Biomolecular Function Simulation, RIKEN
Center for Biosystems Dynamics Research, Japan
How cellular environments are regulated by non-specific molecular interaction

10:30 – 11:00 COFFEE BREAK

MOLECULAR ENGINEERING

chairperson: Mateusz Chwastyk

11:00 – 11:30 Damien Thompson
Department of Physics, University of Limerick, Ireland
Molecular engineering of bio-assemblies: prospects and design rules for sustainable materials for therapeutics and sensing

11:30 – 12:00 Joanna Trylska
Centre of New Technologies, University of Warsaw, Poland
Stapled peptides and peptide nucleic acids as antibacterials

- 12:00 – 12:30 David J. Wales
University of Cambridge, United Kingdom
Energy landscapes: from molecules and nanodevices to machine learning
- 12:30 – 13:00 Piotr Garstecki
Institute of Physical Chemistry, Polish Academy of Sciences, Poland
From idea to a product for medical diagnostics
- 13:00 – 14:30 LUNCH

COVID-19

chairperson: Damien Thompson

- 14:30 – 15:00 Peter Hinterdorfer
Institute of Biophysics, Johannes Kepler University Linz, Austria
Avidity amplification of SARS-Cov-2 spike variants viewed on the single molecule level
- 15:00 – 15:30 Mateusz Sikora
Max Planck Institute of Biophysics, Germany
Protein flexibility and glycan dynamics of the SARS-CoV-2 spike
- 15:30 – 16:00 Mai Suan Li
Institute of Physics, Polish Academy of Sciences, Poland
In silico study of Covid-19
- 16:00 – 16:15 Adolfo Poma
Institute of Fundamental Technological Research, Polish Academy of Sciences, Poland
Nanomechanical investigation of the binding interface stability of SARS-CoV-2 variants with ACE2 receptor
- 16:15 – 16:30 Yoo Jin Oh
Institute of Biophysics, Johannes Kepler University Linz, Austria
Investigation of lectin binding to SARS-CoV-2 spike glycans using single molecule force spectroscopy
- 16:30 – 17:00 COFFEE BREAK

IN MEMORY OF PROF. MAREK CIEPLAK

chairperson: Mariano Carrión-Vázquez

- 17:00 – 17:15 Marta Cieplak, Maja Cieplak-Rotowska, Mateusz Chwastyk
- 17:15 – 17:30 Jayanth Banavar (online)
- 17:30 – 17:45 George Rose
- 17:45 – 18:00 Władek Minor
- 18:00 – 18:15 Anna Niedźwiecka
- 18:15 – 20:00 DINNER
- 20:00 – 22:00 POSTER SESSION I (odd numbers presenting authors)

Friday, 16 June 2023

STRUCTURAL BIOLOGY

chaiperson: Andrzej Kłoczowski

- 9:00 – 9:30 Andrzej Joachimiak
Department of Biochemistry and Molecular Biology, University of Chicago, USA
Dynamic X-ray Crystallography: Time-Resolved β -lactam Cleavage by L1 Metallo- β -Lactamase
- 9:30 – 9:45 Przemyslaw Nogly
Faculty of Biochemistry, Biophysics and Biotechnology, Jagiellonian University, Poland
Time-resolved X-ray crystallography on membrane proteins: watching ions moving in time and space
- 9:45 – 10:15 Mariusz Jaskólski
Faculty of Chemistry, A. Mickiewicz University and Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poland
Stereochemical restraints for nucleic acids revisited
- 10:15 – 10:50 Wlodek Minor
Department of Molecular Physiology and Biological Physics, University of Virginia, USA
Structural biology response to biomedical threats
- 10:50 – 11:10 COFFEE BREAK

THE WORLD OF PROTEINS WITH STRUCTURE

chairperson: Mateusz Sikora

- 11:10 – 11:40 Edward O'Brien
Department of Chemistry, Pennsylvania State University, USA
A newly discovered class of protein misfolding explains decades-old biochemical and molecular biology observations
- 11:40 – 11:55 Elisa Rioual
IBS, Université Grenoble Alpes and iLM, Université Claude Bernard Lyon 1, France
Visualizing a Functional Rare State of Human HSP90 ATP Binding Domain
- 11:55 – 12:10 Peter Røgen
Department of Applied Mathematics and Computer Science, Technical University of Denmark, Denmark
Sequence-Similar, Structure- and Topologically-Dissimilar Protein Domain Pairs
- 12:10 – 12:25 Antonio Trovato
Department of Physics and Astronomy, University of Padova and INFN, Italy
Entangled motifs in protein structures
- 12:25 – 12:40 Tomasz Włodarski
University College London, UK
A computational microscope to study co-translational protein folding

12:40 – 14:30	LUNCH
14:30 – 18:30	FREE TIME (EXCURSION)
18:30 – 20:00	DINNER
20:00 – 22:00	POSTER SESSION II (even numbers presenting authors)

Saturday, 17 June 2023

MANAGING BIOLOGICAL PROCESSES chairperson: Joanna Trylska

9:00 – 9:30	Michael Feig <i>Department of Biochemistry and Molecular Biology, Michigan State University, USA</i> Enzyme Function in Crowded Environments
9:30 – 10:00	Dariusz Plewczynski <i>Laboratory of Bioinformatics and Computational Genomics, Warsaw University of Technology, Poland</i> LEM: loop extrusion model of the Human Genome Topology
10:00 – 10:15	Maja Cieplak-Rotowska <i>IMol Polish Academy of Sciences, Poland</i> CwC25's role in choosing the right adenosine as the branch site during the first step of splicing
10:15 – 10:40	COFFEE BREAK

BETWEEN ORDER AND DISORDER chairperson: Adam Liwo

10:40 – 11:10	Yaakov (Koby) Levy <i>Department of Chemical and Structural Biology, Weizmann Institute of Science, Israel</i> Optimized protein function via disordered regions
11:10 – 11:40	Mariano Carrión-Vázquez <i>Instituto Cajal, IC-CSIC, Spain</i> Exploring early amyloidogenesis in search for novel pharmacological targets
11:40 – 12:10	Hisashi Okumura <i>Institute for Molecular Science, The Graduate University for Advanced Studies, Japan</i> Replica-permutation and nonequilibrium molecular dynamics simulations for protein aggregates
12:10 – 12:40	Artem Badasyan <i>University of Nova Gorica, Slovenia</i> Potts spins, protein conformations, and implicit water model
12:40 – 14:30	LUNCH

- 14:30 – 15:00 Nevena Ilieva
Institute of Information and Communication Technologies & Institute of Mathematics and Informatics at the Bulgarian Academy of Sciences, Bulgaria
A new concept of the mechanism of action of antimicrobial peptides
- 15:00 – 15:15 Peter Košovan
Department of Physical and Macromolecular Chemistry, Charles University, Czechia
Exploiting the liquid-liquid phase separation in polyelectrolyte complexes for sequestration of small ions, weak acids and bases
- 15:15 – 15:30 Michał Białobrzewski
Institute of Physics, Polish Academy of Sciences, Poland
Liquid-liquid phase separation of GW182 silencing domain
- 15:30 – 16:15 COFFEE BREAK

SPOTLIGHT ON THE WORLD OF PROTEINS

chairperson: Michael Feig

- 16:15 – 16:45 Christian Kaiser
Department of Biology, Johns Hopkins University, USA
Co-translational stabilization drives folding of a kinetically stable protein
- 16:45 – 17:20 Jayanth Banavar (online)
University of Oregon, USA
A framework for understanding proteins
- 17:20 – 17:50 COFFEE BREAK

CLOSING LECTURE

chairperson: George Rose

- 17:50 – 18:30 Gerhard Hummer
Max Planck Institute of Biophysics, Germany
Molecular simulations in the era of AI and exascale computing
- 19:00 CONFERENCE BANQUET

Sunday, 18 June 2023

Breakfast