Thursday May 5th 2016

Invitation: **Zdeněk Hostomský, IOCB AS CR director**
Opening: **Jiří Vondrášek IOCB AS CR**

Session 1. (18:00–19:30)
Chairman: Mikael Oliveberg

1.1 18:00–18:45 **Janet Thornton (EMBL-EBI, United Kingdom)**
The Evolution of enzyme function - a model for design

1.2 18:45–19:30 **Alexander Wlodaver (National Cancer Insitute, USA)**
Design of proteins targeting HIV - I

19:30–21:00 **Welcome drink, reception**

Friday May 6th 2016

Session 2 (9:00 - 12:30)
Chairman: Nikolay Dokholyan

2.1 9:00–9:45 **Dek Woolfson (University of Bristol, United Kingdom)**
Exploring new protein folds and functions through de novo design

2.2 9:45–10:30 **Scott Boyken (University of Washington in Seattle, USA)**
Programmable protein interaction specificity

10:30–11:00 **Coffee Break**

2.3 11:00–11:45 **Birte Höcker (Max Planck Institute, Germany)**
Protein Design from subdomain sized fragments

2.4 11:45–12:30 **Pietro Sormanni (Univeristy of Cambridge, United Kingdom)**
A modular design strategy for the rational design of protein interactions

12:30–14:00 **Lunch**

Session 3 (14:00 - 18:30)
Chairman : Alex Wlodawer

3.1 14:00–14:45 **Thomas Schiex (Institute for Agricultural Research, France)**
Guaranteed energetic optimization, exploration and counting of sequence-conformation in Computational Protein Design

3.2 14:45–15:30 **Jiří Damborský (ICRC Brno, Czech Republic)**
Design and evolution of protein tunnels

3.3 15:30–16:15 **Evžen Bouřa (IOCB AS CR, Czech Republic)**
Protein design for macromolecular crystallography

16:15–16:45 **Coffee Break**

3.4 16:45–17:30 **Mikael Oliveberg (Stockholm University, Sweden)**
Protein stability in live cells

3.5 17:30–18:15 **Simon Ebbinghaus (Ruhr-Universitat, Bochum, Germany)**
Proteins in vivo - what determines the folding stability in the cell

18:15–19:00 **Dinner buffet**

19:00–19:30 **Piotr Wardega (NanoTemper)**
Advanced quantitative biomolecular analytics in free solution

19:30–22:00 **Poster Session**

Saturday 7th 2016

Session 4 (9:00–12:30)
Chairman: Barry Honig

4.1 9:00–9:45 **David Eisenberg (University of California Los Angeles, USA)**
Designed inhibitors of amyloid fibrils

4.2 9:45–10:30 **Ingemar André (CPMS Lund, Sweden)**
Computational design of protein and peptide self-assembly

10:30–11:00 **Coffee Break**

4.3 11:00–11:45 **Michele Vendruscolo (Cambridge University, United Kingdom)**
Using rational molecular design to combat protein misfolding diseases

4.4 11:45–12:30 **Barry Honig (Columbia University, USA)**
How adhesion proteins are designed: The molecular basis of specific cell-cell recognition

12:30–14:00 **Lunch**

Session 5 (14:00–18:30)
Chairman: Don Hilvert

5.1 14:00–14:45 **Charlotte M. Deane (University of Oxford, United Kingdom)**
Improving In Silico Therapeutic Antibody Design

5.2 14:45–15:30 **Sarel J. Fleishman (Weizmann Institute of Science, Israel)**
Computational design of novel antibodies and enzymes from fragments of natural ones

5.3 15:30–16:15 **Selected talks from PPS Participants**

5.3.1. 15:30–15:45
Ivan Colluzza (University of Vienna, Austria)
Transferable coarse-grained potential for de novo protein folding and design
5.3.2. 15:45–16:00
Perczel András (Eötvös L. Univ / Lab. Structural Chem&Biol., Hungary)
Hidden folding intermediate by NMR: structural insights of an F I U transition
5.3.3. 16:00–16:15
Kvido Strisovsky (IOCB AS CR, Czech Republic)
Keeping membrane proteins in check – deciphering nature's design of an intramem brane cleaving protease

16:15–16:45 **Coffee Break**

5.4 16:45–17:30 **Jurgen Haas (Swiss Institute of Bioinformatics, Switzerland)**
Keeping Bad Bugs at Bay – Computational Engineering of the Trans-membrane Glycosyl-transferase PglB

5.5 17:30–18:15 **Donald Hilvert (ETH Zurich, Switzerland)**
Nearer to nature: design and optimization of artificial enzymes

20:00–23:00 **Conference Dinner at Strahov Monastery**

Sunday 8th 2016

Session 6 (9:30–11:00)
Chairman: Michele Vendruscolo

6.1 9:30–10:15 **Nikolay Dokholyan (University of North Carolina, Chapel Hill, USA)**
Uncovering mysteries of ALS etiology

6.2 10:15–11:00 **Andrew Lovering (University of Birmingham, United Kingdom)**
Unusual Proteins from the Bacterial Predator Bdellovibrio bacteriovorus

11:00–11:30 **Coffee Break**