

18 June 2019

Tuesday

16:00 Travel and arrival of Conference participants, Check-in and Conference registration  
17:00-18:30 Conference opening, Opening Session

17:15 -18:30 **ANDRÁS PERCZEL**: Achilles heels of proteins  
EOTVOS UNIVERSITY, BUDAPEST, HUNGARY

19:00 Garden Party (Trout skewer)

19 June 2019

Wednesday

7:30 - 9:00 Breakfast

09:00 - 11:00 1st Morning Session  
Chair: Rudi Ettrich

9:00 **MIKAEL LUND**: Ion Specific Effects on Polymer Interactions  
LUND UNIVERSITY, LUND, SWEDEN

10:00 **MICHAEL OWEN**: Validation of Force Fields for the study of amyloid-beta peptide interactions with membrane gangliosides  
UNIVERSITY OF BRNO, BRNO, CZECH REPUBLIC

10:30 **LISA D. MUIZNIKS**: Tuning membrane structure-elasticity to improve lung models at the microscale  
ELVESYS MICROFLUIDICS INNOVATION CENTER, PARIS, FRANCE

11:00 - 11:30 Coffee break

11:30 - 13:00 2nd Morning Session  
Chair: Babak Minofar

11:30 **MOHAMMAD NASIR UDDIN**: Drug formulation development for small molecule drugs and vaccines  
LARKIN UNIVERSITY, MIAMI, US

12:30 **DANIEL BONHENRY**: Activation of STIM calcium sensor  
CNSB, NOVY HRADY, CZECH REPUBLIC

13:00 - 14:30 Lunch

14:30-16:30 1st Afternoon Session  
Chair: Jan Urban

14:30 **CSABA VÁRADI**: Alteration of human serum glycosylation: The challenge of analytical chemistry  
UNIVERSITY OF MISKOLC, MISKOLC, HUNGARY

15:30 **STELLA SCHMODE**: Quinolone derivatives as universal chromophores for standardized dynamic Stokes shift measurements  
UNIVERSITY OF WIEN, WIEN, AUSTRIA

16:00 **DAVID ŘEHA**: Computational study of self-assembly of bacteriochlorophyll in chlorosomes  
CNSB MBU AVCR, NOVY HRADY, CZECH REPUBLIC

16:30 -17:00 Coffee break

17:00-18:30 2nd Afternoon Session  
Chair: Jaroslav Burda

17:00 **ESTHER HEID**: Prediction of electrostatic parameters for a general polarizable force field  
UNIVERSITY OF WIEN, WIEN, AUSTRIA

17:30 **RÉKA ANNA HORVÁTH**: Investigation of Methylamine at Aqueous Surfaces by Computer Simulation Methods  
SEMMELEWEIS UNIVERSITY, BUDAPEST, HUNGARY

18:00 **ZSÓFIA BORBÁLA RÓZSA**: Molecular Dynamics and Metadynamics Insights of 1,4-Dioxane Induced Structural Changes of Biomembrane Model  
UNIVERSITY OF MISKOLC, MISKOLC, HUNGARY

19:00 - 20:00 Conference dinner  
20:00 - 22:00 Poster session, Wine tasting

20 June 2019

Thursday

7:30 Breakfast

09:00 - 11:00 1st Morning Session  
Chair: Milán Szőri

9:00 **JAROSLAV BURDA**: Interaction of hydrated Hg cations with Thymine at various pH; QM/MM MD study  
CHARLES UNIVERSITY, PRAGUE, CZECH REPUBLIC

10:00 **PHILIPP HONEGGER**: Computational spectroscopy of reverse micelles: What can we learn about macromolecular confinement?  
UNIVERSITY OF WIEN, WIEN, AUSTRIA

10:30 **ANITA RÁGYANSZKI**: Modelling Reaction Pathways of Constituents in the Interstellar Medium  
UNIVERSITY OF YORK, TORONTO, CANADA

11:00 - 11:30 Coffee break

11:30 - 13:00 2nd Morning Session  
Chair: Milan Melicherčík

11:00 **RÉGIS POMÈS**: The Liquid State of Proteins  
UNIVERSITY OF TORONTO, MOLECULAR MEDICINE, HOSPITAL FOR SICK CHILDREN, TORONTO, CANADA

12:30 **NATALIA KULIK**: Modeling of protein activity by mutations  
CNSB, NOVY HRADY, CZECH REPUBLIC

13:00 - 14:30 Lunch

14:30 - 16:30 Afternoon Session  
Chair: Mikael Lund

14:30 **MICHELE CASCELLA**: tba.  
UNIVERSITY OF OSLO, OSLO, SWEDEN

15:30 **ANDREA GULJAS**: Significance of  $\pi$ - $\pi$  Interactions in the Phase Separation of Intrinsically Disordered Proteins  
UNIVERSITY OF TORONTO, TORONTO, CANADA

16:00 **MILAN MELICHERČÍK**: Structure and reactivity of aptamers and selected molecular systems in the pathological form of prions  
COMENIUS UNIVERSITY, BRATISLAVA, SLOVAKIA

16:30 - Walk in the Szalajka-valley

20:00 Gala dinner

09:00 - 11:30 Morning Session, Closing remarks  
Chair: Jaroslav Burda

9:00 **RUDI ETTRICH**: Structure and dynamics of a novel domain of the motor subunit of the Type I restriction enzyme EcoR124 involved in complex assembly and DNA binding  
LARKIN UNIVERSITY, MIAMI, F, US

10:00 **BABAK MINOFAR**: Biomolecular interactions in ionic liquids  
CNSB, NOVY HRADY, CZECH REPUBLIC

10:30 **MILÁN SZŐRI**: Glycerol carbonate as a fuel additive for a sustainable future  
UNIVERSITY OF MISKOLC, MISKOLC, HUNGARY

11:00 **BÉLA VISKOLCZ**: Systematic Molecular Design  
UNIVERSITY OF MISKOLC, MISKOLC, HUNGARY

Closing remarks