

Protein Electrostatics Belgrade 2018 (PEB2018)

Program

Monday, June 25

9:00 - 10:00 **Registration**

10:00 - 10:20 **Welcome**

The time schedule for the talks includes time for discussions (5 min for long and 3 min for short talks)

Binding and Assembly

10:20 - 10:50 **Paolo Carloni**

Free energy calculations of ligand binding to RNA's

10:50 - 11:20 **Junji Iwahara**

Dynamics equilibria of electrostatic interactions at protein-DNA interfaces: Insight from NMR

11:20 - 11:50 **Coffee break**

11:50 - 12:20 **Jan Antosiewicz**

Electrostatic interaction effects in the kinetics of tri-N acetylglucosamine binding to lysozyme

12:20 - 12:50 **Thomas Simonson**

Accurate PDZ:peptide binding specificity with additive and polarizable free energy simulations

12:50 - 1:05 **Discussion**

1:05 - 3:00 **Lunch break**

Binding and Assembly – Large Complexes

3:00 - 3:30

Alexey Onufriev

Electrostatic Mechanism of the Nucleosome Function

3:30 – 4:00

Emil Alexov

Long-range electrostatic interactions of E-hooks provide guidance and a soft landing for the microtubule binding domain of dynein

4:00 - 4:30

Miljko V. Satrić

How Post-Translational Modifications of C-Termini of Microtubules Impact Intra-Cellular Traffic by motor proteins

4:30 - 5:00

Coffee break

5:00 - 5:30

Holger Gohlke

Molecular determinants of glutamine synthetase deactivation by tyrosine nitration: Impact of a pKa shift

5:30 - 5:45

Yossi Tsfadia

Computational Study of Coronaviruses Interactions with Receptors and Antibodies

5:45 - 6:00

Lorena Zuzic

pH-dependent conformational change in dengue and other flaviviruses

6:00 - 6:15

Nadia Elghobashi-Meinhardt

Niemann-Pick Type C proteins: Insights from molecular dynamics and QM/MM energy calculation

6:15 - 6:30

Discussion

7:00

Dinner at Restaurant "Kolarac", Knez Mihailova 46

Tuesday, June 26

Structural aspects of pK_{as} – Theory

9:00 - 9:30

Adrian Roitberg

Theory and Computation of protonation and electrochemical equilibria guiding experiments: Are we there yet?

9:30 - 10:00

Antonio Baptista

Electrostatics of peptide dendrimers

10:00 - 10:30

Miguel Machuqueiro

Coupling enhanced sampling and biased MD simulations with CpHMD

10:30 - 11:00

Coffee break

11:00 - 11:30

Bernard Brooks

Recent advances in protonation state modeling and constant pH simulations

11:30 - 11:45

Diogo Vila-Viçosa

Development of a pH replica exchange scheme within the stochastic titration CpHMD method

11:45 - 12:15

Ernst Walter Knapp

pK_a computations in different environments: proteins and liquids

12:15 - 12:45

G. Matthias Ullmann

Decomposing the free energy of pH titration

12:45 - 1:00

Discussion

1:00 - 3:00

Lunch break

Theory - Miscellaneous aspects

3:00 - 3:30

Jonathan Essex

How well does the AMOEBA force field reproduce protein electrostatics?

3:30 - 4:00

Duška Janežić

ProBiS Tools at the PDB scale for prediction of protein binding site, the ligand, the sequence variant, and their binding dynamics

4:00 - 4:30

Jim Warwicker

Continuum electrostatics models for mining 'omics data

4:30 - 5:00

Coffee break

5:00 - 5:30

Walter Rocchia

Progresses and first results in the coupled approach between continuum electrostatics and integral equation theory

5:30 – 5:45

Svetoslav Nakov

A posteriori error estimates for the linear Poisson and the fully nonlinear Poisson-Boltzmann equations: reliable adaptive finite element method

5:45 - 6:00

Federico Fogolari

Free Energy from Implicit Solvent End-Point Simulations

6:00 - 6:15

Discussion

7:00

Dinner at "Kalemegdan Terrace", Kalemegdan

Wednesday, June 27

Structural aspects of pK_as – Experiments

9:00 - 9:30

Frans A. A. Mulder

Accurate and individual side chain titrations curves by NMR spectroscopy

9:30 – 10:00

Bertrand Garcia-Moreno

Determinants of pK_a Values of Ionizable Residues Buried in the Hydrophobic Interior of Proteins

10:00 - 10:15

Discussion

Charge/energy transfer

10:15 - 10:30

Michael Shokhen

Rhomboid protease substrate selectivity originates in combined effect of membrane environment and pK_a of catalytic residues

10:30 - 11:00

Coffee break

11:00 - 11:30

Frank Müh

Electrostatic Effects on Optical Spectra of the Photosystem II Reaction Center

11:30 - 12:00

Hiroshi Ishikita

Energetics in both electron transfer pathways in photosynthetic reaction centers

12:00 - 12:30

Thomas Renger

Ab-initio/electrostatic/molecular dynamics description of FRET experiments on proteins

12:30 - 12:45

Discussion

12:45 - 3:30

Lunch at the venue (canapés) and Poster session

Charge/energy transfer – role of water

3:30 – 4:00

Marilyn Gunner

Tracing hydrogen bonding pathways for proton transfer

4:00 – 4:30

Petra Imhof

Hydrogen-bonded network and water dynamics in the proton transfer channels of Cytochrome c Oxidase

4:30 – 5:00

Coffee Break

5:00 - 5:30

Alexei Stuchebrukhov

Dielectric constant of hydrated proteins. Kirkwood-Onsager-Froehlich theory revisited.

5:30 – 5:45

Marco Reidelbach

Reaction Path Prediction in Proton Transfer Systems

5:45 – 6:00

Ekaterina Sobakinskaya

The role of water interior in protein translocation by the SecYEG channel

6:00 - 6:15

Discussion

7:00

Dinner at “Tri šešira” (Three hats), Skadarska 29

Thursday, June 28

Ion conduction/Electric fields

9:00 - 9:30

Maria Kurnikova

Generalized Continuum Theory for Protein Ion Channels

9:30 – 10:00

Benzhuo Lu

Continuum modeling of selective ion permeation in potassium channel

10:00 - 10:30

Ana Damjanović

Constant pH study of a sodium channel

10:30 – 11:00

Coffee break

11:00 - 11:30

Lauren J. Webb

Electrostatics and Electrodynamics in Lipid Bilayer Membranes

11:30 – 12:00

Jack Tuszynski

How tubulin's electrostatic properties determine the conductivity of microtubules

12:00 - 12:15

Frederico Costa

Interactions of specific modulation radiofrequencies with cellular microtubules predicted by biological surrogates in humans

12:15 - 12:30

Discussion

12:30

Announcement of the poster prizes and official farewell