

# Conference Program

Sunday, June 23<sup>rd</sup>

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13:00–16:00 Registration

16:00–16:10 Conference opening

**Chairman: J. Urban**

16:10–16:50 **Anna Weinzinger** Allosteric mechanisms of inward rectifier K<sup>+</sup> channel gating - *Invited speaker* - opening lecture

16:50–17:20 **Dénes Berta** From model building to in silico ligand screening: targetting the SARS-CoV-2 helicase

17:20–17:50 **Abdenacer Idrissi** Exploring the Interfacial Conformational Changes and Polymorphic Behavior of Curcumin - *Invited speaker*

17:50–18:20 **Béla Fiser** Additives in Action - How to Make 'Greener' Polymers?

18:20–18:50 **László Forgách** Development, In Vitro Characterization & In Vivo Testing of multimodal Prussian Blue nanoparticles in an animal model - *Invited speaker*

19:00 *Dinner Welcome party*

20:30 *Poster session I. even numbers*

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**Monday, June 24<sup>th</sup>**

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**Chairman: A. Idrissi**

09:00–09:30	<b>Marco Paolantoni</b>	Hydration properties of sugars: molecular structure and dynamics - Invited speaker
09:30–10:00	<b>Christian Schröder</b>	Computational spectroscopy of water
10:00–10:30	<b>Ari Paavo Seitsonen</b>	Vibrational spectroscopies in liquid water: On temperature and coordination effects in Raman and infra-red spectroscopies

10:30–10:50 *Coffee break*

**Chairman: Christian Schröder**

10:50–11:20	<b>Esther Heid</b>	A systematic way of improving machine learning potentials through spatially resolved uncertainty - <i>Invited speaker</i>
11:20–11:45	<b>Marek Štekláč</b>	Docking power approximations: can molecular docking reproduce experiment?
11:45–12:10	<b>Berna Dogan</b>	Predicting Selectivity of Compounds Against HDAC Isoforms Quantitatively Using Deep Learning Approaches
12:10–12:30	<b>Ján Matúška</b>	Generalization improvement of the neural network constructed using SchNetPack 2.0

12:30–14:00 *Lunch*

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**Chairman: Jaroslav Burda**

14:00–14:30	<b>Zdenek Futera</b>	Conductance of Solvated Biomolecular Junctions
14:30–15:00	<b>David Řeha</b>	Mechanism of carbon dots synthesis from citric acid and ethylenediamine studied by QM calculations
15:00–15:30	<b>Filip Šebesta</b>	Electron Transfer via Artificial Tryptophan Pathways
15:30–16:00	<b>John P. Fetse</b>	Computational Scoring and Experimental Evaluation of Small Peptide Fragments Targeting PD-L1 for Cancer Immunotherapy - <i>Invited speaker</i>
16:00–19:00	Sightseeing tour in Piešťany	
19:00	<i>Dinner</i>	
20:00	Poster session II.	<i>odd numbers</i>

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**Tuesday, June 25<sup>th</sup>**

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**Chairlady: Jannette. Carey**

- 09:00–09:30     **Rózsa Zsófia Borbála**     Effect of Phospholipid Headgroups on the Permeation of Additives
- 09:30–10:00     **Zoltán Mucsi**     A GFP inspired fluorescent molecular sensor for the detection of Zn<sup>2+</sup> by two-photon microscopy in biology
- 10:00–10:30     **Mohammad Uddin**     An Innovative Dual Action Antibiotic Adjuvant Strategy using Ionic Liquid towards Synergistic Restoration of Activity in MDRO and Enhancing Antimicrobial Activity against MRSA

10:30–10:50     *Coffee break*

**Chairman: Béla Viskolcz**

- 10:50–11:15     **Dalma Dojcsák**     Diagnostic of Pediatric Appendicitis supported by altered serum N-glycome
- 11:15–11:40     **Marion Sappl**     Langevin behavior of the dielectric decrement of amino acids in electrolyte solutions
- 11:40–12:05     **Tímea Gerzsenyi**     Studies on adsorption and antibacterial effect of magnetic nanoparticles
- 12:05–12:30     **Péter Koska**     Bioremediation potential of heavy metal loaded waste water by *C.vulgaris* microalga

12:30–14:00     *Lunch*

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**Chairman: David Řeha**

14:00–14:30	<b>Babak Minofar</b>	Interaction of biomolecules in confined environments
14:30–15:00	<b>Tibor Kovács</b>	Development of NMR scaling factors and reaction mechanism computations
15:00–15:30	<b>Jaroslav Burda</b>	Modeling interaction of metals with biomolecules
15:30–15:50	<i>Coffee break</i>	

**Chairman: Babak Minofar**

15:50–16:15	<b>Milan Říha</b>	From QM to QM/MM: NHC gold(I) complexes as potential cancer therapeutics
16:15–16:40	<b>Ivan Klbik</b>	Impact of dimethylsulfoxide on ionic conductance in lipid bilayer-embedded ion channel: implications for cryopreservation
16:40–17:05	<b>Tamás Horváth</b>	Investigation of radioactive strontium decorporation by computational analysis of Calcium and strontium ion complexation
17:05–17:30	<b>Jannette Carey</b>	Allostery: Monod's second secret of life
18:00–20:00	<i>Conference dinner</i>	

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**Wednesday, June 26<sup>th</sup>**

10:00                      Departure



# Poster presentations

Sunday, June 23<sup>rd</sup>

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2	Balsam Al-sabea	Carbohydrates-based Hydrogels in Drug Delivery System
4	Christian Fellingner	Binding Affinity Estimation using X-GRADE
6	Márta Gődény	Molecular dynamics simulations of the Influenza M2 proton channel: the role of the protonation state and the polarizability
8	Anikó Jordán	Investigation of polyester-model urethane biodegradation
10	Karina Kécskes	Investigation of the microorganism adsorption capacity of natural-based particles
12	Ádám Lévárdi	Docking Score Prediction of Molecules Using Machine Learning Methods
14	Milan Melicherčík	Chloroquine transport and mutations in PfCRT protein
16	Omid Moghaddam	Interactions of proteins with grafted poly(ethylene oxide) layer in two setups - A Molecular dynamics study
18	Hadeer Waleed Qasim	Experimental and Theoretical Study of Urethane Formation in the Presence of 2,2-dimorpholinodiethylether (DMDEE) and 1,4-dimethylpiperazine (DMP)
20	Jessica Trenkwalder	MD Simulations of SERT for the Analysis of Ligands
22	Adam Vavrečka	QM/MM study of the electron hopping processes of conjugated systems

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**Monday, June 24<sup>th</sup>**

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| 1  | Nesreen Alkanakri  | A Computational Study of Tropocollagen Hexamer and Heptamer   |
| 3  | Marcell D. Csécsi  | Computational and reaction kinetic study of carbodiimide formation  |
| 5  | Fatemeh Heydari    | Development and testing of polymer-encapsulated, amine-functionalized iron-based contrast materials in animal model                     |
| 7  | Ariyo P. Hidayanto | Investigation Of Cobalt bioaccumulation by <i>Chlorella Vulgaris</i>  |
| 9  | Dalal Karad        | Theoretical study of the applicability of natural antioxidant additives   |
| 11 | Natalia Kulik      | Application of <i>in-silico</i> methods for enzyme engineering of the NtcA protein from <i>Synechocystis sp.</i>                        |
| 13 | Julie Mallouhi     | Evaluation of <i>Sargassum</i> -Derived Activated Carbon and Biochar: Ecotoxicity, and Heavy Metal Adsorption Performance               |
| 15 | Mike Owen          | The Mediation of Amyloid- $\beta$ Dimer Conformations by Gangliosides   |
| 17 | Princeton group    | Random proteins bind random ligands   |
| 19 | Ondřej Tichý       | QM/MM study of the electron hopping processes of the Two Lowest Singlet Excited States of Cytosine, its Aza-Derivatives and Carotenoids |
| 21 | László Vanyorek    | Development of antibacterial, core-shell structured transition metal ferrite nanoparticles  |
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