Conference Program

Sunday, June 23rd

13:00–16:00	Registration	
16:00–16:10	Conference opening	
16:10–16:50	**Anna Weinzinger**	Allosteric mechanisms of inward rectifier K^+ channel gating - *Invited speaker* - opening lecture
16:50–17:20	**Denes Berta**	From model building to in silico ligand screening: targetting the SARS-CoV-2 helicase
17:20–17:50	**Nacer 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*

Monday, June 24^{th}

09:00–09:30	**Marco Paolantoni**	Hydration properties of sugars: molecular structure and dynamics - Invited speaker
09:30–10:00	**Christian Schröder**	Computational spectroscopy of water
10:00–10:30	**Ari Paavo Seitsonen**	Vibrational spectroscopies in liquid water: On temperature and coordination effects in Raman and infra-red spectroscopies
10:30–10:50	*Coffee break*	
10:50–11:20	**Esther Heid**	A systematic way of improving machine learning potentials through spatially resolved uncertainty - *Invited speaker*
11:20–11:45	**Marek Štekláč**	Docking power approximations: can molecular docking reproduce experiment?
11:45–12:10	**Berna Dogan**	Predicting Selectivity of Compounds Against HDAC Isoforms Quantitatively Using Deep Learning Approaches
12:10–12:30	**Ján Matúška**	Generalization improvement of the neural network constructed using SchNetPack 2.0
12:30–14:00	*Lunch*	

14:00–14:30	**Zdenek Futera**	Conductance of Solvated Biomolecular Junctions
14:30–15:00	**David Řeha**	Mechanism of carbon dots synthesis from citric acid and ethylenediamine studied by QM calculations
15:00–15:30	**Filip Šebesta**	Electron Transfer via Artificial Tryptophan Pathways
15:30–16:00	**Tibor Kovács**	Development of NMR scaling factors and reaction mechanism computations
16:00–19:00	Sightseeing tour in Piešťany	
19:00	*Dinner*	
20:00	Poster session II.	*odd numbers*

Tuesday, June 25^{th}

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^{2+} 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*	
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*	

14:00–14:30	**Babak Minofar**	Interaction of biomolecules in confined environments
14:30–15:00	**John P. Fetse**	Computational Scoring and Experimental Evaluation of Small Peptide Fragments Targeting PD-L1 for Cancer Immunotherapy - *Invited speaker*
15:00–15:30	**Jaroslav Burda**	Modeling interaction of metals with biomolecules
10:30–10:50	*Coffee break*	
15:50–16:15	**Milan Říha**	From QM to QM/MM: NHC gold(I) complexes as potential cancer therapeutics
16:15–16:40	**Ivan Klbik**	Impact of dimethylsulfoxide on ionic conductance in lipid bilayer-embedded ion channel: implications for cryopreservation
16:40–17:05	**Tamás Horváth**	Investigation of radioactive strontium decorporation by computational analysis of Calcium and strontium ion complexation
18:00–20:00	*Conference dinner*	

Wednesday, June 26^{th}

10:00	Departure

Poster presentations

Sunday, June 23rd

2	Balsam Al-sabea	Carbohydrates-based Hydrogels in Drug Delivery System
4	Christian Fellinger	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

Monday, June 24^{th}

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	Dalal Karad	Theoretical study of the applicability of natural antioxidant additives
9	Natalia Kulik	Application of *in-silico* methods for enzyme engineering of the NtcA protein from *Synechocystis sp.*
11	Julie Mallouhi	Evaluation of *Sargassum*-Derived Activated Carbon and Biochar: Ecotoxicity, and Heavy Metal Adsorption Performance
13	Mike Owen	The Mediation of Amyloid-βDimer Conformations by Gangliosides
15	Ariyo H. Prabowo	Investigation Of Cobalt bioacumulation by *Chlorella Vulgaris*
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