

Monday, 13.09.2021	
9:00 – 9:30	REGISTRATION
9:30 – 9:50	OPENING
9:50 – 10:50	David Leigh <i>Making the Tiniest Machines</i>
10:50 – 11:10	COFFEE BREAK
11:10 – 11:45	Rossen Apostolov <i>Driving European HPC for Biomolecular Research: Advanced Software Applications and Support Structures from BioExcel Centre of Excellence</i>
11:45 – 12:20	<u>Luca Tubiana</u>, Franco Ferrari, Enzo Orlandini <i>Ring-o-rings: Joining the Ends of Poly[n]-Catenanes to Capture Supramolecular Torsion</i>
12:20 – 14:00	LUNCH
14:00 – 14:45	Noam Kaplan <i>Deciphering 3D Genome Organization with Probabilistic Models</i>
14:45 – 15:20	Svetozar Margenov <i>Iterative Solution of Large-Scale Biomedical Problems and Rational Approximation of Fractional Laplacian</i>
15:20 – 15:50	Andrey Brukhno <i>Interscale Simulation: a Novel Combined Methodology to Bridge Between Scales and Methods</i>
15:50 – 16:10	COFFEE BREAK
16:10 – 16:40	<u>Ivan Dimitrov</u>, Mariyana Atanasova and Iринi Doytchinova <i>AllerScreener: a Tool for Allergenicity and Cross-Reactivity Prediction of Proteins</i>
16:40 – 17:10	<u>Meglana Lazarova</u>, Svetoslav Markov, Andrey Vassilev <i>The Reaction Network Approach in Mathematics of Life. Part I – Translation to ODE System</i>
17:10 – 17:40	<u>Meglana Lazarova</u>, <u>Svetoslav Markov</u>, <u>Andrey Vassilev</u> <i>The Reaction Network Approach in Mathematics of Life. Part II – Examples and Numerical Simulations</i>
17:40 – 18:10	Nadezhda Bunzarova and Nina Pesheva <i>Numerical simulations and analytical studies of TASEP – a model of biological transport</i>
18:10 – 18:40	Diana Toneva, Silvia Nikolova, <u>Stanislav Harizanov</u>, Ivaylo Zhelev <i>Applied Mathematics for Forensic Medicine</i>
19:30	WELCOME

Tuesday, 14.09.2021	
9:00 – 9:45	Antti J Niemi <i>Time Crystals and Rotary Molecular Motors</i>
9:45 – 10:30	Franco Ferrari <i>Modeling Polymer Systems in the Presence of Non-Trivial Topological Relations: a Combined Analytical-Numerical Approach</i>
10:30 – 10:50	COFFEE BREAK
10:50 – 11:25	Ivan Coluzza <i>Heteropolymer Design: Learning Protein Evolution by Reverse Engineering</i>
11:25 – 12:00	Raffaello Potestio <i>Optimal Reduced Representations and Multiple Resolution Models of Biomolecules</i>
12:00 – 14:00	LUNCH
14:00 – 14:45	Adam Liwo <i>Theory and Practice of Coarse Graining</i>
14:45 – 15:15	<u>Vlad Sokhan</u>, Michael Seaton, Ilian Todorov <i>Phase Behaviour of Coarse-Grained Fluids</i>
15:15 – 15:45	Julyan Cartwright <i>Topological Aspects to How Life Uses Liquid Crystals</i>
15:45 – 16:15	<u>Bogdan Rangelov</u> and Andrey Milchev <i>Translocation Dynamics of Vesicles Through Narrow Pores</i>
16:15 – 16:35	COFFEE BREAK
16:35 – 17:05	Mateusz Chwastyk <i>Nascent Folding of Proteins Across the Three Domains of Life</i>
17:05 – 17:35	Kristina Kapanova <i>Quantum Analog Computational Device in Life Sciences</i>
17:35 – 18:35	ROUND TABLE DISCUSSION

Wednesday, 15.09.2021	
9:00 – 9:45	Pietro Faccioli <i>Pharmacological Protein Inactivation by Targeting Protein Folding Intermediates</i>
9:45 – 10:30	Sarah Harris <i>Understanding the Structure and Dynamics of the SARS-CoV2 Helicase (nsp13) from Molecular Dynamics Simulations</i>
10:30 – 10:50	COFFEE BREAK
10:50 – 11:20	Nevena Ilieva, Peicho Petkov, Miroslav Rangelov, Elena Lilkova, Nadezhda Todorova, and Leandar Litov <i>In silico Study of the Molecular Mechanism of LMWH Antiinflammatory Action Within the COVID-19 Context</i>
11:20 – 11:50	Vasilina Zayats, Agata P. Perlinska, Aleksandra I. Jarmolinska, Borys Jastrzebski, Stanislaw Dunin-Horkawicz, Joanna I. Sulkowska <i>Slipknotted and Unknotted Proteins Might Share a Common Ancestor</i>
11:50 – 12:20	SHORT TALKS – PART I
12:20 – 14:00	LUNCH
14:00 – 14:45	Marek Cieplak <i>Dynamics of Intrinsically Disordered Proteins and their Droplet-like Aggregates</i>
14:45 – 15:15	Piotr Sulkowski <i>Biomolecules and Random Matrices</i>
15:15 – 15:45	Petia Koprinkova-Hristova <i>Spike Timing Neural Network Model of Conscious Visual Perception</i>
15:45 – 16:15	SHORT TALKS – PART II
16:30 – 19:30	CULTURAL PROGRAMME
19:30	SOCIAL DINNER

SHORT TALKS – PART I

- **Pawel Korzeb, Bartosz Gren, Joanna Sulkowska**
Statistical properties of handcuffs in ideal polymers
- **Mateusz Fortunka, Ya-Ming Hou, Adam Stasiulewicz, Agata Perlinska, Joanna Sulkowska**
Understanding the role of YARS2-tRNA complex in MLASA Disease
- **Yadi Cheng, Xubiao Peng, Peicho Petkov, and Nevena Ilieva**
Grafting a Parkinson Inhibitor Peptide on a Cyclotide: a Geometry and Dynamics Study
- **Dessislava Jereva, Maria Angelova, Ivanka Tsakovska, Petko Alov, Ilza Pajeva, Maria A. Miteva, Tania Pencheva**
InterCriteria Analysis Approach to Assess the AMMOS2 Software Platform Performance

SHORT TALKS – PART II

- **Wanda Niemyska, Bartosz A. Gren, Pawel Dabrowski-Tumanski, Joanna I. Sulkowska**
Lasso Proteins – Is this Topology Functional?
- **Bartosz A. Gren, Pawel Dabrowski-Tumanski, Joanna I. Sulkowska**
Statistical properties of lasso polymers and implications for lasso proteins
- **Adam Stasiulewicz, Mai Lan Nguyen, Joanna Sulkowska**
Fighting Antimicrobial Resistance – In Silico Screening for Novel TrmD Inhibitors

SHORT TALKS – PART III

- **Elena Lilkova, Peicho Petkov, Rositsa Marinova, Leandar Litov, Nevena Ilieva**
Enhanced Sampling Molecular Modeling of Peptide-Membrane Interactions: A Case Study
- **Pawel Rubach**
Identification of Protein Topology Using Topoly and the KnotProt Database API

Thursday, 16.09.2021	
9:00 – 9:45	Roumen Anguelov <i>Mathematical Models and Analysis of the Impact of CTCE9908 and Kynurenine Metabolites on the Proliferation and Survival of Tumour Cells</i>
9:45 – 10:15	Rachid Ouifki <i>Mathematical Modeling of the Estrogen Paradox in the Treatment of Breast Cancer</i>
10:15 – 10:45	Anastas Pashov <i>Formal Representation of the Repertoire of IgM Antibody Specificities</i>
10:45 – 11:10	Anastas Pashov, <u>Peter Petrov</u> <i>Topological Approach for a Global Description of the Antibody Repertoire</i>
11:10 – 11:30	SHORT TALKS – PART III
11:30 – 11:40	CLOSING
12:00 – 14:00	LUNCH
14:00	DEPARTURE