















PROGRAMME

MONDAY, JUNE 7






9:30 – 10:00	REGISTRATION	
CHAIR: Hrvoj Vančik		
10:00 – 11:00	Jerzy Cioslowski: <i>Reverse Engineering in Quantum Chemistry: How to Reveal the Fifth-Order Off-Diagonal Cusp in the One-Electron Reduced Density Matrix Without Actually Calculating it</i>	
11:00 – 12:00	Filip Prątnicki: <i>Uniform Description of the Helium Isoelectronic Series Down to the Critical Nuclear Charge</i>	
12:00 – 12:15	COFFEE BREAK	
12:15 – 13:15	Gabriela Herrero-Saboya: <i>Linking Atomistic Modelling with Experimental Data: General Jahn-Teller Models for Defects in Semiconductors</i>	
13:15 – 14:15	Xabier Telleria-Allika: <i>Few Electron Systems Confined in Gaussian Potential Wells: Connection to Hooke Atoms and Introduction to Gaussian Molecular Structure</i>	
14:15 – 16:00	LUNCH BREAK	
CHAIR: Urban Bren		
16:00 – 17:00	Claudiu N. Lungu: <i>Big data analysis and QSAR – Finding Needles in a Haystack: Determining Key Molecular Descriptors Associated With the Blood-Brain Barrier Entry of Chemical Compounds Using ML</i>	
17:00 – 18:00	Oleg Miloserdov: <i>QSPR Method for Prediction of Sorption Parameters of Light Gases in Glassy Polymers</i>	

TUESDAY, JUNE 8

CHAIR: Bono Lučić		
9:00 – 10:00	Miha Gunde: <i>A Shape Matching Algorithm for Off-lattice Atom Resolved Kinetic Monte Carlo</i>	
10:00 – 11:00	Matic Poberžnik: <i>ARTn as a Plugin for Electronic Structure Calculation and Molecular Dynamics Codes</i>	
11:00 – 12:00	Tomica Hrenar: <i>Machine Learning Multivariate Linear Regression: Evaluating all Possible Regression Models</i>	
12:00 – 12:15	COFFEE BREAK	
12:15 – 13:15	Xiang Xu: <i>Analysis of Dynamic and Nondynamic Correlation Diagnostics</i>	
13:15 – 13:45	R. B. Mallion: <i>Postscript on Viable Ground-States for Calculating Topological π-Electron Ring-currents Using the Hückel–London–Pople–Mcweeny Model</i>	
13:45 – 15:30	LUNCH BREAK	
CHAIR: Sanja Tomić		
15:30 – 16:30	Bono Lučić: <i>The Derivation of Formulas for Calculation of Characteristic Values of Statistical Parameters Used in Model Quality Estimation</i>	
16:30 – 17:30	Urban Bren: <i>Polyphenols as Natural Scavengers of Chemical Carcinogens: a Computational Approach</i>	
17:30 – 18:30	Marjana Novič: <i>Randić Connectivity Index and its Variations for QSPR Modelling of Aqueous Solubility</i>	





WEDNESDAY, JUNE 9

Session in honor of Milan Randić

9:30 – 10:00	Marjana Noviĉ: A few words in honor of Milan Randić	
CHAIR: Jerzy Cioslowski		
10:00 – 11:00	Xueliang Li: <i>Spectral Extremal Trees With Degree-Based Weights</i>	
11:00 – 12:00	Juraj Kolĉák: <i>Efficient Application of Modular Graph Transformation Rules</i>	
12:00 – 12:15	COFFEE BREAK	
12:15 – 13:15	Mehmet Aziz Yirik: <i>MAYGEN - an Open-Source Chemical Graph Generator Based on the Orderly Generation Principle</i>	
13:15 – 14:15	Bünyamin Şahin: <i>On Marginal Entropy of Graphs</i>	[•REC]
14:15 – 16:00	LUNCH BREAK	
16:00 – 18:00	Igor Ronĉević: <i>Modelling Reactions at Metal-organic Interfaces</i>	






THURSDAY, JUNE 10

CHAIR: Filip Prażnicki

10:00 – 11:00	Snjeřana Majstorović: <i>Trees with Extremal Graovac-Ghorbani Indices</i>	
11:00 – 12:00	Abdulgani Şahin: <i>On ve-Degree Irregularity Indices of Some Molecular Structures</i>	
12:00 – 12:15	COFFEE BREAK	
12:15 – 13:15	Ana Amiĉ: <i>Contribution of C-ring Hydrogens to Free Radical Scavenging by Equol</i>	
13:15 – 14:15	POSTER SESSION	
	CONFERENCE DINNER	

FRIDAY, JUNE 11

Session in honor of Mircea Diudea

9:30 – 10:00	Vladimir Rosenfeld: A few words in honor of Mircea Diudea	
CHAIR: Igor Ronĉević		
10:00 – 11:00	Ana Mikeliĉ: <i>Multi-target Antimicrobial Activity Model of Cinchona Alkaloids Established by Machine Learning</i>	
11:00 – 12:00	Sanja Tomić: <i>Inhibitory Zinc Ion Binding Site and The Metal Exchange Mechanism in Human DPP III</i>	
12:00 – 12:15	COFFEE BREAK	
12:15 – 13:15	Miquel Solà: <i>Nido Cage...π Non-covalent Interactions</i>	
13:15 – 14:15	Berislav Perić: <i>Mer-Coordination of a Mixed Iminoacetamide / (2-Picoyl)amine Ligand to the Zn²⁺ Cation: X-ray and NMR Study</i>	
14:15 – 14:45	CLOSING	