

ICCBIKG 2023

Conference Programme

Thursday 28 September 2023

08:00 - 09:00	Registration of the Participants
09:00 - 09:30 (Hall I)	Opening Ceremony - Welcome speech: Prof. Dr Zoran Marković , Director of the Institute for Information Technologies, Conference Chair, International Organizing Committee. Prof. Dr Nenad Filipović , Rector of the University of Kragujevac, International Scientific Committee, Conference Chair. Prof. Dr Danijela Milošević , Dean of Faculty of Technical Sciences, Republic of Serbia. Prof. Dr Marija Stanić , Dean of Faculty of Science, University of Kragujevac. Chair: Nevena Veselinović
09:30 - 10:00 (Hall I)	Invited speaker: Dr Bartosz Trzaskowski , Full Professor, Centre of New Technologies (CeNT), University of Warsaw, Poland. Topic: Targeting depression via computational approaches to design new coumarin-based serotonin receptor antagonists/agonists and develop reliable models of G protein-coupled receptors Chair: Dr Dejan Milenković
10:00 - 10:30 (Hall I)	Invited speaker: Prof. Dr Miloš Kojić , Full Member of the Serbian Academy of Sciences and Arts, Serbia. Topic: A review of the application of the finite element smeared concept to biomedical engineering problems Chair: Dr Vladimir Simić
10:30 - 11:00	Coffee Break
Session CCMD.T1: 11:00 - 13:00 (Hall I) Chemoinformatics, chemogenomics and molecular design (Oral session) Chair: Dr Nenad Janković	
11:00 - 11:25	Section lecturer: Dr Snežana Zarić , Full Professor, Faculty of Chemistry, Department of General and Inorganic Chemistry, University of Belgrade, Serbia. Topic: Benzene and water – different or similar?

CCMD.T1.1– Combined in silico approach to identify new terpenoid PPAR- α agonists– *Kristina Stevanović, Draginja Radošević, Vladimir Perović, Sanja Glišić.*

CCMD.T1.2– Numerical simulations of the oscillatory dynamics in the Bray-Liebhafsky reaction perturbed by L-tyrosine- *Ana Ivanović-Šašić, Stevan Maćešić, Jelena Maksimović, Željko Čupić, Ljiljana Kolar-Anić.*

CCMD.T1.3– Modeling ion- π interactions of transition metal complexes- *Dušan P. Malenov, Katarina A. Čeranić, Dubravka Z. Vojislavljević-Vasilev, Snežana D. Zarić.*

CCMD.T1.4– Identification of small molecule binding sites using CmDock- *Marko Jukić, Urban Bren.*

CCMD.T1.5– High-throughput screening of novel hydrogen storage materials – ML approach- *Katarina Batalović, Jana Radaković, Bojana Paskaš Mamula, Mirjana Medić Ilić, Bojana Kuzmanović.*

CCMD.T1.6– Anticancer gallium(III) complexes with halogen- and nitroderivatives of 8-hydroxyquinoline- *Ivan Potočnjak, Miroslava Litecká, Jitka Prachařová, Monika Hreusová, Jana Kašpárková.*

Session BE.T1: 11:00 - 12:15 (Hall III)

Biomedical engineering (Oral session)- Part I

Chair: **Dr Miljan Milošević**

11:00 - 11:25	Section lecturer: Dr Marijana Petković , Principal Research Fellow, Vinča Institute of Nuclear Sciences, Belgrade, Serbia. Topic: Application of carbon-based nanocomposite systems as photosensitizers for Photodynamic therapy
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BE.T1.1– Using numerical modeling to analyze the behavior of cancer cells after diverse co-treatments– *Tijana Djukić, Dragana Seklić, Milena Jovanović, Marko Zivanović, Nenad Filipović.*

BE.T1.2– Multiscale Modelling of the Effects of Temperature on Cardiac Twitches– *Momcilo Prodanovic, Srboljub M. Mijailovich.*

BE.T1.3– Application of Machine Learning Algorithms in Medical Data Processing– *Tijana Geroski, Nenad Filipović.*

Session AST.T1: 12:15-13:00 (Hall III)

Applied Science and Technologies (Poster session)

Chair: **Dr Bogdan Milićević**

AST.T1.1– Biocorrosion, biofouling and health risk: biological activity reaction tests of selected brackish groundwater occurrences in Serbia– *Vladimir Šaraba, Jasmina Nikodinović-Runić, Vesna Obradović, Ivica Dimkić, Tamara Janakiev, Veselin Dragišić, Milica Ćirić.*

AST.T1.2– Bacteria in drinking and bathing mineral waters of Serbia with polymer-degrading potential– *Milica Ćirić, Vladimir Šaraba, Clémence Budin, Tjalf de Boer, Jelena Milovanović, Jasmina Nikodinović-Runić.*

AST.T1.3– Potentially toxic elements in the edible part of trout (*Salmo trutta* L.) from the upper reaches of the Raška and Studenica rivers– *Aleksandra M. Milošković, Milena D. Radenković, Simona R. Đuretanović, Nataša M. Kojadinović, Tijana Z. Veličković, Vladica M. Simić.*

AST.T1.4– DRIFT spectroscopy and permutation importance algorithm in quantitative analysis of organic matter in soil model systems– *Branislav D. Jović, Marko N. Panić.*

AST.T1.5– The influence of pyrocatechol added in pre-oscillatory period on the dynamics of the Bray-Liebafsky reaction– *Jelena Maksimović, Kristina Stevanović, Marina Simović-Pavlović, Maja Pagnacco.*

AST.T1.6– Environmental Implications of Financial Development in CEE countries– *Nevena Veselinović, Jelena Živković.*

AST.T1.7– Greenhouse Gas Emissions and Digital Competitiveness in CEE countries– *Jelena Živković, Nevena Veselinović.*

AST.T1.8– Antifreeze with coffee taste– *Milan B. Vraneš, Snežana M. Papović, Jovana J. Panić, Teona Teodora V. Borović, Nikolet A. Cako Baganj, Sanja D. Belić, Sanja Rackov, Slobodan B. Gadžurić.*

AST.T1.9– The hydration and antimicrobial properties of selected imidazole-based ionic liquids with a homologous series of chloride oxyanions– *Jovana J. Panić, Snežana M. Papović, Teona Teodora V. Borović, Nikolet A. Cako Baganj, Sanja D. Belić, Slobodan B. Gadžurić, Milan B. Vraneš.*

AST.T1.10– Influence of the ionic liquids-based electrolytes on the tomato (*Solanum lycopersicum* L.) and cucumber (*Cucumis sativus* L.) growth, development and oxidative stress– *Snežana Papović, Jovana Panić, Teona Teodora Borović, Nikolet Cako Baganj, Sanja Belić, Ivana Maksimović, Marina Putnik Delić, Slobodan Gadžurić, Milan Vraneš.*

AST.T1.11– Solubility and structural organization of taurine molecules in water– *Teona Teodora V. Borović, Snežana M. Papović, Jovana J. Panić, Nikolet A. Cako Baganj, Sanja D. Belić, Slobodan B. Gadžurić, Milan B. Vraneš.*

AST.T1.12– Development of Nanomaterials for Sustainable Food Packaging Applications– *Sanja Rackov, Milan Vraneš, Tamara Erceg, Branka Pilić.*

AST.T1.13– The effect of consumer ethnocentrism on the competitiveness of the economy of the Republic of Serbia– *Ana Spasojević, Stefan Zdravković.*

AST.T1.14– The role of socially responsible business in improving the company's market positioning– *Ana Spasojević, Stefan Zdravković.*

AST.T1.15– Prevalence of radon and metals in natural springs in the Sokobanja area– *Biljana Vučković, Ivana Penjišević, Nataša Todorović, Jovana Nikolov, Ljiljana Gulan, Jelena M. Stajić, Biljana Nikić.*

AST.T1.16– Bioaccumulation potential of 'Meeker' and 'Willamette' raspberry (*Rubus idaeus* L.) fruits towards macro- and microelements and their nutritional evaluation– *Stefan Jevremović, Jasminka Milivojević, Jelena S. Katanić Stanković, Jelena Popović-Đorđević.*

AST.T1.17– In vitro and in silico assessment of anti-inflammatory activity of cocoa powders– *Jelena S. Katanić Stanković, Vanja Todorović, Jelena Đorović Jovanović, Zoran Marković, Sanja Krstić, Nevena Dabetić, Slađana Šobajić, Agnieszka Bartoszek, Zoran Maksimovic, Rudolf Bauer.*

AST.T1.18– Comparison of the luminescence properties of phosphate-tungsten bronze and cerium doped phosphate-tungsten bronze– *Tijana V. Maksimović, Ljubinka G. Joksović, Dimitrije Mara, Rik Van Deun, Zoran P. Nedić, Marina Simović-Pavlović, Maja C. Pagnacco.*

AST.T1.19– The comparison of two methods used to observe a nonlinear system: potentiometry and holography– *Marina Simović Pavlović, Tijana Maksimović, Jelena Maksimović, Maja Pagnacco.*

AST.T1.20– Radioactivity levels and health risks associated with Himalayan salt consumption– *Jelena M. Stajić, Biljana Nikić, Sofija Forkapić, Jan Hansman, Emina Mrkalić.*

AST.T1.21– Modeling of circulating tumor cell (CTC) and platelet interaction in capillaries– *Aleksandar Nikolić, Miljan Milošević, Vladimir Simić, Miloš Kojić.*

AST.T1.22– A computational model of the left ventricle – application in cardiomyopathy disease– *Miljan Milošević, Bogdan Milićević, Vladimir Simić, Miloš Kojić, Nenad Filipović.*

13:00 - 14:00	Buffet Lunch
14:00 - 14:30 (Hall I)	<p style="text-align: center;">Invited speaker: Dr Rudolf Bauer, Full Professor, Institute of Pharmaceutical Sciences, Karl-Franzens University of Graz, Austria. Topic: The Importance of Chemometrics in Drug Discovery from Medicinal Plants Chair: Dr Jelena Katanić Stanković</p>
14:30 - 15:00 (Hall I)	<p style="text-align: center;">Invited speaker: Dr Zlatan Car, Full Professor, Faculty of Engineering, Department of Automation and Electronics, University of Rijeka, Croatia. Topic: Synthetic Data Generation for Biomedical Deep Learning: Methods, Challenges, and Opportunities Chair: Doc. Dr Tijana Geroski</p>

Session CCMD.T2: 15:00-16:15 (Hall I)

Chemoinformatics, chemogenomics and molecular design (Poster session)

Chair: Dr Darko Ašanin

15:00 - 15:25	Section lecturer: Dr Jovana Petrović , Research Professor, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, Topic: Multiparameter monitoring of cardiovascular function
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CCMD.T2.1– 3D-Quantitative Structure-Activity Relationship and design of novel Rho-associated protein kinases-1 (ROCK1) inhibitors– *Milan Beljkas, Jelena Rebić, Milica Radan, Teodora Đikić, Slavica Oljačić, Katarina Nikolić.*

CCMD.T2.2– Virtual Docking, design and in silico ADMET profiling of novel Rho-associated protein kinases-1 (ROCK1) inhibitors – *Milan Beljkas, Jelena Rebić, Milica Radan, Teodora Đikić, Slavica Oljačić, Katarina Nikolić.*

CCMD.T2.3– Coumarins as promising PPAR α agonists. Novel in silico insights– *Draginja Radošević, Kristina Stevanović, Vladimir Perović, Sanja Glišić.*

CCMD.T2.4– In silico screening of Solanum lycopersicum carotenoids from Carotenoids Database for candidates PPAR α agonists– *Tamara Drljača, Kristina Stevanović, Draginja Radošević, Jelena Milićević, Nevena Veljković, Sanja Glišić.*

CCMD.T2.5– The assessment of the antioxidant capacity of the selected vanillin-based pyrido-dipyrimidines using DPPH assay: in silico approach – *Svetlana Jeremić, Nenad Janković, Jelena Đorović Jovanović, Zoran Marković.*

CCMD.T2.6– Inhibitory potential of barbarin and its platinum(II) complex towards PBP1a protein – *Svetlana Jeremić, Milan Dekić, Violeta Jakovljević, Enisa Selimović, Amina Gusinac.*

CCMD.T2.7– Substituent effects on stacking interactions of aromatic ligands in organometallic compounds – chemoinformatics and quantum chemical study- *Dušan P. Malenov, Jelena P. Blagojević Filipović, Snežana D. Zarić.*

CCMD.T2.8– Computational study on the interactions of quercetin 3-O-rutinoside with human DPP III- *Dejan Agić, Drago Bešlo, Bono Lučić, Sanja Tomić, Bojana Blagojević, Boris M. Popović.*

CCMD.T2.9– Noncovalent interactions of halogen atoms in halogenated bipyridines- *Bogdan K. Pantelić, Snežana D. Zarić, Jelena M. Živković.*

CCMD.T2.10– Repulsive water-water contacts from Cambridge Structural Database- *Milan R. Milovanović, Jelena M. Živković, Ivana M. Stanković, Dragan B. Ninković, Snežana D. Zarić.*

CCMD.T2.11– Stacking Interactions at Large Horizontal Displacements—Comparison of Various Ring Types- *Jelena P. Blagojević Filipović, Dragan B. Ninković, Snežana D. Zarić.*

CCMD.T2.12– Influence of Coordination on OH/ π and NH/ π Interactions- *Jelena P. Blagojević Filipović, Dubravka Z. Vojislavljević-Vasilev, Snežana D. Zarić.*

CCMD.T2.13– Relativistic DFT calculation and their effect on the accuracy of results- *Marko D. Radovanović, Ignjat Filipović, Maja Djukić, Marija Ristić, Matija Zlatar, Zoran D. Matović.*

CCMD.T2.14– Analysis of prediction of water solubility and lipophilicity of coumarins by free cheminformatics tools- *Drago Bešlo, Dejan Agić, Vesna Rastija, Maja Karnaš, Domagoj Šubarić, Bono Lučić.*

CCMD.T2.15– Influence of phthalimide substitution on the interaction with carbon nanotube- *Sonja S. Zrilić, Jelena M. Živković, Snežana D. Zarić.*

CCMD.T2.16– Interaction energy and decomposition of interaction energy of halo-substituted phthalimide with carbon nanotube- *Sonja S. Zrilić, Jelena M. Živković, Snežana D. Zarić.*

CCMD.T2.17– A comprehensive in silico protocol for fast automated mutagenesis and binding affinity scoring of protein-ligand complexes- *Sebastijan Kralj, Milan Hodošek, Marko Jukić, Urban Bren.*

CCMD.T2.18– Workflow automation of high-throughput inverse docking using Pharammapper- *Aleksa P. Alargić, Bojan D. Levovnik, Miloš M. Svirčev.*

CCMD.T2.19– Investigating the potential inhibitory effect of the megaphone (molecule) on nasopharyngeal cancer growth factor receptors- *Žiko Milanović, Marko Antonijević, Dušica Simijonović, Jelena Đorović Jovanović, Marijana Stanojević Pirković.*

CCMD.T2.20– Chromeno-pyrimidine-type compounds (part II): in vitro evaluation of antioxidant potential- *Edina Avdović, Dušica Simijonović, Žiko Milanović, Sandra Jovičić Milić.*

CCMD.T2.21– Green synthesis of chromeno-pyrimidine derivatives – Part 1- *Dušica Simijonović, Edina Avdović, Žiko Milanović, Dejan Milenković, Zoran Marković.*

Session AST.T2: 15:00-16:15 (Hall III)

Applied Science and Technologies (Oral session)

Chair: **Dr Dušica Simijonović**

15:00 - 15:25	Section lecturer: Dr Jasmina Grbović Novaković , Principal Research Fellow, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, Topic: The hydrogen economy: challenges and prospectives
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AST.T2.1– Entropy dynamics for a propeller-shaped quantum Brownian molecular rotator- *Jasmina Jeknić-Dugić, Igor Petrović, Kristina Kojić, Momir Arsenijević, Miroljub Dugić.*

AST.T2.2– Modeling and simulation of a polymer optical fiber humidity sensor for the skin microenvironment– *Milan S. Kovačević, Marko M. Milošević, Ljubica Kuzmanović, Daniele Tosi, Alexandar Đorđevich.*

AST.T2.3– Selecting critical features for biomedical data classification- *Ulfeta A. Marovac, Lejlja M. Memić, Aldina R. Avdić, Natasa Z. Djordjević, Zana Ć. Dolićanin, Goran M. Babić.*

16:15 - 16:45	Coffee Break
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16:45 - 17:15 (Hall I)	Invited speaker: Dr Janez Konc , Associate Professor, The National Institute of Chemistry, Laboratory for Molecular Modeling, Ljubljana, Slovenia. Topic: Algorithms and web servers for protein binding sites detection in drug discovery Chair: Doc. Dr Svetlana Jeremić
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Session BBMC.T1: 17:15-18:00 (Hall I)

Bioorganic, bioinorganic, and medicinal chemistry (Poster session)

Chair: **Dr Marko Živanović**

BBMC.T1.1– Molecular docking study of ruthenium-p-cymene complexes with isothiazole derivatives as SARS-CoV-2 main protease inhibitors– *Marko Radovanović, Ignjat Filipović, Maja Đukić, Marija Ristić, Ivan Jakovljević, Zoran D. Matović.*

BBMC.T1.2– Structural, spectroscopic and molecular docking analysis of isoprotenerol– *Marija Milosavljević, Aleksandra Rakić, Dušan Dimić.*

BBMC.T1.3– Synthesis, spectroscopic, and quantum-chemical analysis of mononuclear Ru(II)-naphthylhydrazine complex– *Marta Kosanović, Thomas Eichron, Dejan Milenković, Goran Kaluđerović, Jasmina Dimitrić Marković, Dušan Dimić.*

BBMC.T1.4– Synthesis, spectroscopic, and theoretical analysis of Ru(II)-phenylhydrazine complex– *Ana Atanasković, Thomas Eichron, Dejan Milenković, Dušan Dimić, Goran Kaluđerović, Jasmina Dimitrić Marković.*

BBMC.T1.5– DNA/BSA binding study of mononuclear gold(III) complexes with clinically used azoles – *Bojana V. Pantović, Nevena Lj. Stevanović, Tina P. Andrejević, Darko P. Ašanin, Miloš I. Djuran, Biljana Đ. Glišić.*

BBMC.T1.6– DNA/BSA interaction of platinum(II) complexes with phenothiazine and N-methylphenothiazine – *Tina P. Andrejević, Darko P. Ašanin, Bojana V. Pantović, Nevena Lj. Stevanović, Violeta R. Marković, Miloš I. Djuran, Biljana Đ. Glišić.*

BBMC.T1.7– The interaction studies of novel diaminophenazine gold(III) complex and Bovine Serum Albumin (BSA-ibuprofen and BSA-Eozine Y)- *Ana S. Kesić, Snežana R. Radisavljević, Jovana V. Bogojeski, Biljana V. Petrović.*

BBMC.T1.8– The influence of structural modification of Pd(II) pincer-type complexes on the kinetics of substitution reactions- *Snežana Jovanović Stević, Snežana Radisavljević, Aleksandar Mijatović, Biljana Petrović, Ana Kesić.*

BBMC.T1.9– In vitro cytotoxic activity of a monolacunary Wells-Dawson nanocluster against cervical carcinoma HeLa cells- *Mirjana B. Čolović, Jelena J. Žakula, Lela B. Korićanac, Nada Savić, Tatjana Parac-Vogt, Danijela Z. Krstić.*

BBMC.T1.10– The influence of Fe(III) incorporation on anti-cancer potential of a Wells-Dawson nanocluster- *Mirjana B. Čolović, Lela B. Korićanac, Jelena J. Žakula, Nada Savić, Tatjana Parac-Vogt, Danijela Z. Krstić.*

BBMC.T1.11– DFT approach of the redox properties of brimonidine and varenicline- *Marija R. Popović-Nikolić, Katarina Nikolić, Mara Aleksić.*

BBMC.T1.12– Theoretical and experimental study of bilastine ionization- *Marija R. Popović-Nikolić, Gordana Popović, Slavica Oljačić, Katarina Nikolić.*

BBMC.T1.13– New vanadium complexes with potential biological activity- *Miroslava Matiková Mařarová, Alexandra Bilá, Mária Vilková, Erika Samořová, Zuzana Jendželovská, Viktória Bulřková.*

BBMC.T1.14– Synthesis of Schiff bases between some five-membered heterocyclic aldehydes and thiocarbohydrazide (TCH) and optimization of reaction conditions- *Miljan Bigović, Marija Kaluđerović, Jovana Jovanović, Haris Majstorović, Milica Kosović-Perutović.*

BBMC.T1.15– Synthesis, structure and anticancer activity of Zr(IV) complexes with Schiff bases derived from 8-hydroxyquinoline- *Michaela Harmořová, Martin Kello, Mária Vilková, Erika Samořová, Ivan Potočňák.*

BBMC.T1.16– Ionic palladium(II) complexes with nitro and halogen derivatives of 8 hydroxyquinoline- *Martina Kepeňová, Michaela Benediková, Mária Vilková, Miroslava Litecká, Ivan Potočňák.*

BBMC.T1.17– A novel silver complex with 4-hydroxycoumarin derivative: Synthesis, structure, and biological activity- *Jakub Kurjan, Rastislav Jendželovský, Zuzana Jendželovská, Viktória Bulřková, Mária Vilková, Miroslava Litecká, Ivan Potočňák.*

BBMC.T1.18– In silico Drug-Likeness, Pharmacokinetic and other ADME properties of 2-(aminomethyl)cyclopropane-1,1-dicarboxylic acid- *Marina D. Kostić, Jovana S. Marjanović, Sven Mangelinckx, Vera M. Divac.*

BBMC.T1.19– BSA binding of 2-(aminomethyl)cyclopropane-1,1-dicarboxylic acid- *Marina D. Kostić, Vera M. Divac, Sven Mangelinckx, Jovana S. Marjanović.*

BBMC.T1.20– Can three-week administration of methanol extract of wild garlic modulate systemic redox state in hypertensive rats?- *Jovana V. Bradic, Anica M. Petrovic, Vladimir Lj. Jakovljevic.*

BBMC.T1.21– Synthesis and physicochemical characterisation of the Ni(II) complex with 3-(4-chlorophenyl)-1H-pyrazole ligand– *Marijana S. Kostić, Nikola D. Radnović, Ana Radović, David Kočović, Željko Jaćimović, Berta Barta Holló, Mirjana M. Radanović.*

BBMC.T1.22– Pyrazole/tacrine derivatives as potential cholinesterase inhibitors– *Mihajlo J. Krunić, Jelena Z. Penjišević, Slađana Kostić-Rajačić, Vladimir B. Šukalović, Deana B. Andrić, Ivana I. Jevtić.*

BBMC.T1.23- SR FTIR spectroscopy investigation of Pd@S-CD nanocomposite system effects on biomolecules in cervical carcinoma cells- *Vanja Ralić, Maja Nešić, Anamarija Abu el Rub, Tanja Dučić, Branislava Gemović, Manuel Algarra, Milutin Stepić, Lela Korićanac, Jelena Žakula, Marijana Petković.*

BBMC.T1.24- Lichenochemical analysis and in vitro antioxidant activity of extracts and gyrophoric acid from lichen Umbilicaria grisea- *Miroslav Sovrlić, Nedeljko Manojlović, Marijana Kosanić, Aleksandar Kočović, Jovica Tomović, Perica Vasiljević.*

Session BE.T2: 17:15 - 18:00 (Hall III)

Biomedical engineering (Oral session) - Part II

Chair: **Dr Milica Nikolić**

BE.T2.1– A finite element model for structural optimization of parametrized lattice scaffolds– *Jovan Z. Arandžević, Rajko M. Turudija, Nikola D. Korunović, Miloš S. Stojković, Jelena R. Stojković.*

BE.T2.2– Structural simulations predicting protein folding in Alzheimer's disease– *Marios Krokidis, Aristidis Vrahatis, George Dimitrakopoulos, Konstantina Skolariki, Panagiotis Vlamos, Themis Exarchos.*

BE.T2.3– Analytically Computed Fractional Flow Reserve based on Coronary CT Angiography – *Aleksandar Milovanović, Velibor Isailović, Igor Saveljić, Nenad Filipović*

20:00 - 00:00

Gala Dinner, Hall I

Friday 29 September 2023

09:00 - 09:30 (Hall I)	Sponsored presentation: „MC Labor doo Belgrade”
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09:30 - 10:00 (Hall I)	Invited speaker: Prof. Dr Ivan Gutman , Full Member of the Serbian Academy of Sciences and Arts, Serbia. Topic: Vertex degree based topological indices - applications and theory Chair: Prof. Dr Zoran Marković
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Session BBMC.F1: 10:00-11:15 (Hall I) Bioorganic, bioinorganic, and medicinal chemistry (Oral session)- Part I Chair: Dr Dejan Milenković	
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10:00 - 10:25	Section lecturer: Rino Ragno , Full Professor, Pharmacy and Medicine Faculty, Sapienza, University of Rome, Italy. Topic: db.3d-qsar.com. The first 3D QSAR models database
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BBMC.F1.1– Computer-aided design of new drugs against breast cancer– *Milan P. Mladenović, Nevena M. Tomašević, Sanja Lj. Matić, Tamara M. Mladenović, Rino Ragno.*

BBMC.F1.2– The influence of the methanol extract of Galium verum on cardiac oxidative damage in hypertensive rats in a model of global ischemia- *Anica M. Petrovic, Jovana V. Bradić, Vladimir Lj. Jakovljević.*

Session AST.F1: 10:00-11:15 (Hall III) Applied sciences and technologies (Poster session) Chair: Dr Jasmina Obradović	
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10:00 - 10:25	Section lecturer: Dr Dragoslav Nikezić , Full Professor, Department of Natural and Mathematical Sciences, State University Novi Pazar, Serbia. Topic: History of radiological protection and evolution of dosimetric quantities
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AST.F1.1– Investigation of the possibility of interaction between lithium fluoride clusters and boron using LDI MS– *Filip Veljković, Dunja Drakulić, Ana Todorović, Snežana Pejić, Katarina Bobić, Ivana Stajčić, Snežana Pajović, Suzana Veličković.*

AST.F1.2– In vitro biological effects of clonal red wines– *Neda Đorđević, Otilija Keta, Vladana Petković, Nevena Todorović Vukotić, Dalibor Stanković, Vele Tešević, Snežana Pajović.*

AST.F1.3– Applied machine learning in exploring key features of crayfish populations – *Simona R. Đuretanović, Marija M. Jakovljević, Aleksandra M. Milošković, Nataša M. Kojadinović, Milena D. Radenković, Vladica M. Simić, Ivana Maguire.*

AST.F1.4– Dose compensation algorithm in radiotherapy planning– *Neda Milosavljević, Marija Živković Radojević, Darko Stojanović, Marko Spasić.*

AST.F1.5- A protocol for thoracic radiation therapy in patients with cardiac implantable electronic devices– *Neda Milosavljević, Marija Živković Radojević, Darko Stojanović, Katarina Janković, Tatjana B. Miladinović.*

AST.F1.6- Distribution of doses to organs at risk in Cervical Cancer High Dose Rate Brachytherapy using Tandem and Ovoids or Vaginal Cylinder– *Tatjana B. Miladinović, Jasmina Obradović, Marija Živković Radojević, Neda Milosavljević, Aleksandar Miladinović, Milena Živković, Dragana Krstić.*

AST.F1.7- Assessment of radioactivity levels in soil samples on Zlatibor– *Milena P. Živković, Nenad M. Zlatić, Tatjana B. Miladinović, Milan S. Stanković, Dragana Ž. Krstić.*

AST.F1.8- Influence of different production systems and tomato genotypes on the content of macroelements in tomato fruits– *Vojin Cvijanović, Beka Sarić, Marija Bajagić, Petar B. Stanić, Nenad Đurić, Gordana Dozet, Gorica Cvijanović.*

AST.F1.9- Challenges in radiotherapy planning in patients with synchronous rectal and prostate cancer and hip prosthesis – *Marija Živković Radojević, Neda Milosavljević, Slađana Aćimović Talijan, Tatjana B. Miladinović, Aleksandar Miladinović, Miloš Grujić.*

AST.F1.10- Exploring the Pharmacokinetic Properties of (NH₄)₄[Fe(idadtc)₂]: In Silico Biological screening and ADMET analysis – *Marko Antonijević, Milica Kosović Perutović, Zorica Leka, Zoran Marković.*

AST.F1.11- The influence of different plasticizers on the mechanical properties of active edible bilayer films – *Tamara Erceg, Olja Šovljanski, Ana Tomić, Nevena Vukić, Dejan Kojić, Senka Popović, Vesna Teofilović.*

AST.F1.12- Patch clamp pipette giga seal forming success on the nanosurgery-obtained filamentous fungi protoplasts – *Katarina Stevanović, Tanja Pajić, Aleksandar Krmpot, Mihailo Rabasović, Milan Žižić, Miroslav Živić, Nataša V Todorović.*

AST.F1.13- Analysis of heavy metals in the soil in the Ibar river valley in the district of Kosovska Mitrovica – *Svetlana Belošević, Maja Đukić, Marija Ristić, Ljubomir Milentijević, Slavica Jovanović, Katarina Mačenovski Gagnon, Jakov Danilović.*

AST.F1.14- Water quality analysis in the district of Kosovska Mitrovica – *Svetlana Belošević, Maja Đukić, Marija Ristić, Ljubomir Milentijević, Slavica Jovanović, Katarina Mačenovski Gagnon, Jakov Danilović.*

AST.F1.15- Chemometric approach to the investigation of microelements and potentially toxic elements in the soil – *Jelena Božović, Zoran Miletić, Ilija Đorđević, Dragana Živojinović.*

AST.F1.16- Application of chemometrics in monitoring of spatial and temporal variations in river water quality and water classification – *Dragana Živojinović, Dušan Trajković, Jelena Božović.*

AST.F1.17- Mechanochemistry: optimization of the synthesis of dithiocarbamate derivatives – *Milica Kosović Perutović, Zorica Leka, Miljan Bigović, Jana Mišurović, V. Medojević.*

AST.F1.18- Capacitive behaviour of biomass-derived activated carbon in Al-ion-containing electrolytes – *Jana Mišurović, Aleksandra Gezović, Veselinka Grudić, Milica Vujković.*

AST.F1.19- The interdependence of structural properties and pseudocapacitive behavior of biomass-derived activated carbon– *Minea Kapidžić, Sonja Kastratović, Milica Vujković, Veselinka Grudić, Jana Mišurović.*

AST.F1.20- Numerical modeling of new 4,7-dihydroxycoumarin derivative diffusion within finite element liver model– *Vladimir Simić, Miljan Milošević, Žiko Milanović, Miloš Kojić.*

AST.F1.21- Overview of Left Ventricular Segmentation in Ultrasound Images– *Bogdan Milićević, Miljan Milošević, Mina Vasković Jovanović, Vladimir Milovanović, Nenad Filipović, Miloš Kojić.*

AST.F1.22– UV-blocking sustainable food packaging based on polyhydroxyalkanoate and bacterial pigment prodigiosin– *Marijana Ponjavić, Ivana Malagurski, Ana Salević-Jelić, Jelena Lazić, Jasmina Nikodinović-Runić.*

AST.F1.23– Finite element analysis of stress distribution in 3D tooth model with extensive cavities restored with direct and indirect composite restoration– *Ivana R. Kantardžić, Bojana D. Ramić, Karolina Vukoje, Tijana Z. Lainović, Darko M. Vasiljević, Larisa Blažić.*

11:15 - 11:45	Coffee Break
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<p>Session BAB.F1: 11:45-13:00 (Hall I)</p> <p>Bioinformatics and applied biology (Poster session)</p> <p>Chair: Dr Marina Kostić</p>
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11:45 - 12:10	<p>Section lecturer:</p> <p>Dr Ralph Puchta, Assistant Professor, Department of Chemistry and Pharmacy, Friedrich- Alexander University, Erlangen, Nuremberg.</p> <p>Topic: IRM@Be2+ - quantum chemistry between Bavaria and Šumadija</p>
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BAB.F1.1– Abundance, species richness and diversity of earthworms (Lumbricidae) in several habitats of the northern part of Jastrebac Mountain– *Filip J. Popović, Tanja B. Trakić, Mirjana M. Stojanović, Jovana M. Sekulić.*

BAB.F1.2– A new record of *Dendrobaena serbica* Karaman, 1973 (Clitellata; Lumbricidae) from Serbia – *Filip J. Popović, Tanja B. Trakić, Mirjana M. Stojanović, Jovana M. Sekulić.*

BAB.F1.3– Comparison of organic substance content in peloids from Sutomore and Igalo (Montenegro)– *Miljan Bigović, Marija Kaluđerović, Jovana Jovanović, Dijana Đurović, Željko Jaćimović.*

BAB.F1.4– Diet composition and feeding habits of common bleak (*Alburnus alburnus* L.) in the Gruža and Gazivode reservoirs– *Milena D. Radenković, Aleksandra M. Milošković, Nataša M. Kojadinović, Simona R. Đuretanović, Tijana Z. Veličković, Marija M. Jakovljević, Vladica M. Simić.*

BAB.F1.5– Edible mushrooms as promising antioxidants– *Jovana D. Todorović, Aleksandra D. Vesić, Nevena N. Petrović, Marijana M. Kosanić.*

BAB.F1.6– Antimicrobial potential of mushrooms *Macrolepiota procera* and *Chlorophyllum rhacodes*– *Jovana D. Todorović, Aleksandra D. Vesić, Nevena N. Petrović, Marijana M. Kosanić.*

BAB.F1.7– Obesity as a risk factor for Covid-19 mortality: an overview of published meta-analyses– *Jasmina Obradović, Jelena Mladenović, Vladimir Jurišić.*

BAB.F1.8– Classification and analysis of key parameters in predicting the state of facultative oligotrophs in two different reservoirs– *Ivana Radojević, Nenad Stefanović, Aleksandar Ostojić.*

BAB.F1.9– Ecological applications based on bacterial community abundance in reservoirs using an artificial neural network approach – *Ivana Radojević, Aleksandar Ostojić, Vesna Ranković.*

BAB.F1.10– Oxidative DNA damage preventive activity of essential oils of three *Pinus* species: *P. mugo*, *P. sibirica*, and *P. silvestre*– *Sanja Lj. Matić, Tamara M. Mladenović, Milan P. Mladenović, Nevena M. Tomašević, Roberto Capobianco, Alessio Ragno, Filippo U. Sapienza, Roberta Astolfi, Rino Ragno.*

BAB.F1.11– Comparative assessment of fish diversity indices in protected Vlasina Reservoir and unprotected Gruža Reservoir– *Marija M. Jakovljević, Simona R. Đuretanić, Marijana D. Nikolić, Nataša M. Kojadinović, Milena D. Radenković, Predrag M. Simović, Vladica M. Simić.*

BAB.F1.12– Assessment of different machine learning tools employed in lipidomics– *David Pirić, Romana Masnikosa.*

BAB.F1.13– Slight cooling during growth induced changes in filamentous fungi hypha mitochondrial morphology– *Aleksandra Vitkovic, Tanja Pajić, Marta Bukumira, Marina Stanić, Mihailo Rabasović, Nataša Todorović.*

Session BBMC.F2: 11:45-13:00 (Hall III)

Bioorganic, bioinorganic, and medicinal chemistry (Oral session) - Part II

Chair: **Dr Dejan Milenković**

BBMC.F2.1- A metric for pairwise similarity analysis of binary cheminformatics data- *Izudin Redžepović.*

BBMC.F2.2- Investigation of binding mode of novel 2,4-diketo esters to BSA- *Emilija Milović, Kristina Mihajlović, Nenad Joksimović, Jelena Petronijević, Nenad Janković.*

BBMC.F2.3– Thrombophilia Prediction Using Machine Learning Algorithms- *Aldina R. Avdić, Natasa Z. Djordjević, Ulfeta A. Marovac, Lejlja M. Memić, Zana Ć. Dolićanin, Goran M. Babić.*

13:00 - 14:30	Buffet Lunch
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14:30 - 15:00 (Hall I)	Invited speaker: Dr Henryk Witek , Full Professor, National Yang Ming Chiao Tung University, Taiwan. Topic: Toward quantitative Raman spectroscopy Chair: Dr Dejan Milenković
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Session BAB.F2: 15:00-17:00 (Hall III)

Bioinformatics and applied biology (Oral session)

Chair: **Marko Antonijević**

15:00 - 15:25	Section lecturer: Dr Bono Lučić , Senior Research Associate, Ruđer Bošković Institute, Croatia. Topic: Confusion about the choice of evaluation metrics for model performance assesment in chemoinformatics, bioinformatics and in general
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BAB.F2.1– Identification of protein target molecules for [Pd(dach)Cl₂] complex in HeLa cervical carcinoma cells– *Vanja Ralić, Branislava Gemović, Maja D. Nešić, Iva Popović, Milutin Stepić, Marijana Petković.*

BAB.F2.2– A Machine Learning approach combining omics data for Alzheimer's Disease analysis– *Georgios N. Dimitrakopoulos, Konstantinos Lazaros, Aristidis G. Vrahatis, Marios Krokidis, Konstantina Skolariki, Panagiotis Vlamos, Themis Exarchos.*

BAB.F2.3– Elucidating Health-Enhancing Properties of Natural Products: A Journey from Extract Isolation to Quantum Mechanics (QM) Calculations– *Gregor Hostnik, Anja Petek, Sara Štumpf, Franjo Frešer, Zala Kolenc, Matej Keber, Jelena Tošović, Urban Bren.*

BAB.F2.4– Status and quality of life of people with celiac and people on a gluten-free diet– *Jasna Frljak, Senita Isaković, Enver Karahmet, Almir Toroman, Ervina Bečić, Fahir Bečić, Zoran Marković.*

BAB.F2.5– Simulation of DNA damage using the “molecularDNA” example application of Geant4-DNA- *Milos Dordević, Konstantinos Chatzipapas, Ngoc Hoang Tran, Dousatsu Sakata, Ivan Petrović, Aleksandra Ristić-Fira, Sara Zein, Jeremy M.C. Brown, Ioanna Kyriakou, Dimitris Emfietzoglou, Susanna Guatelli, Sebastien Incerti.*

Session BBMC.F3: 15:00-15:45 (Hall I)

Bioorganic, bioinorganic, and medicinal chemistry (Poster session)

Chair: **Dr Žiko Milanović**

BBMC.F3.1–The effects of a selected methoxy substituted chalcone in human melanoma cells irradiated with γ -rays– *Otilija Keta, Vladana Petković, Neda Đorđević, Miloš Đorđević, Branka Ivković, Vladimir Dobričić.*

BBMC.F3.2–In silico estimation of COX-2 and 5-LOX inhibitory potential of some novel thiourea derivatives of naproxen– *Nikola V. Nedeljković, Vladimir D. Dobričić, Marina Ž. Vesović, Ana S. Živanović, Gordana P. Radić, Zorica B. Vujić, Miloš V. Nikolić.*

BBMC.F3.3–Molecular docking study of designed N-myristoyl transferase inhibitors– *Anđela D. Gogić, Marina Ž. Vesović, Miloš V. Nikolić, Andriana M. Bukonjić, Dušan Lj. Tomović, Nikola V. Nedeljković.*

BBMC.F3.4–Platinum(II) complexes with epoxide derivative of 1,10-phenanthroline in interaction with human serum albumin– *Anđela A. Franich, Marija D. Živković, Snežana Rajković.*

BBMC.F3.5–Analytical values of beeswax from Montenegro and detection of adulteration– *Vlatko Kastratović, Minea Kapidžić, Bojana Knežević.*

BBMC.F3.6–Phenolic N-acyl hydrazone derivatives: In silico assessment of potential antibacterial activity against selected G+ and G- strains– *Jovica Branković, Zorica D. Petrović, Vladimir P. Petrović.*

BBMC.F3.7– In silico antibiofilm potency of phenolic N-acyl hydrazones against selected bacterial strains– *Jovica Branković, Zorica D. Petrović, Vladimir P. Petrović.*

BBMC.F3.8– TiO₂ nanoparticles and TiO₂ nanoparticles surface modified with salicylic acid affect neurological functions and oxidative stress markers in the eyes of adult rats– *Katarina Bobić, Ana Todorović, Snežana Pejić, Filip Veljković, Suzana Veličković, Snežana Pajović, Dunja Drakulić.*

BBMC.F3.9– Synthesis and cytotoxic activity of selected dual COX-2 and 5-LOX inhibitors in HeLa and MIA PaCa-2 human cancer cell lines– *Otilija Keta, Jelena Bošković, Vladana Petković, Neda Đorđević, Vladimir Dobričić, Olivera Čudina, Snežana B. Pajović.*

BBMC.F3.10– Synthesis, characterization and HSA interactions of a new piano-stool ruthenium(II) complex containing a thioamide-type ligand– *Danijela Stojković, Maja Đukić, Marija Ristić, Marina Ćendić Serafinović, Svetlana Belošević, Emina Mrkalić, Ivan Jakovljević.*

BBMC.F3.11– HPLC/UV profile and determination of total phenolic and flavonoid contents of lichen Umbilicaria crustulosa growing in Serbia– *Jovica Tomović, Perica Vasiljević, Aleksandar Kočović, Nedeljko Manojlović.*

BBMC.F3.12– Biological activity of thienyl-terpyridine Ru(II) complex in the presence of biocompatible ionic liquids– *Ana Rilak Simović, Milica Međedović, Dejan Lazić, Milan Vraneš, Ghodrat Mahmoudi, Biljana Petrović.*

BBMC.F3.13– Kinetic studies of the Ru(II) polypyridyl complex with biologically relevant ligands– *Milica Međedović, Dejan Lazić, Milan Vraneš, Ghodrat Mahmoudi, Biljana Petrović, Ana Rilak Simović.*

BBMC.F3.14– Normal and Reversed Phases Thin-Layer Chromatography of Arylidene 2-Thiohydantoin Derivatives– *Petar B. Stanić, Biljana Šmit, Jovana Muškinja, Tanja Soldatović, Marko Ilić, Kristian Pastor, Marijana Ačanski.*

BBMC.F3.15– Investigation of the anticancer activity of 2-amino-6-methylbenzothiazole and corresponding Pd(II) complex using molecular docking simulations– *Sandra S. Jovičić Milić, Marko Antonijević, Đorđe S. Petrović, Verica V. Jevtić, Danijela Lj. Stojković.*

BBMC.F3.16– DNA binding and molecular docking of four palladium(II) complexes with O,O'-dialkyl esters of (S,S)-propylenediamine-N,N'-di-2-(2-benzyl) acetic acid– *Đorđe Petrović, Maja Đukić, Edina Avdović, Danijela Stojković, Verica Jevtić, Sandra Jovičić Milić, Marina Vesović.*

BBMC.F3.17– Macro and microelements in the leaf and extract of nettle from different localities of Montenegro– *Bojana Knežević, Nataša Bošković, Marija Zorić, Zorica B. Leka.*

BBMC.F3.18– Synthesis and antioxidant activity of novel vanillin-based ferrocenyl chalcones– *Violeta R. Marković, Jovana M. Muškinja, Tamara Lj. Todorović.*

BBMC.F3.19– A contribution to the knowledge of the species *Dipsacus sylvestris* Huds– *Milica Pavlović, Vesna Velicković, Gorica Đelić.*

BBMC.F3.20– Qualitative content of selected phenolic compounds in different extracts of plant species *Iris pumila* L.– *Gorica Đelić, Milica Pavlović, Vesna Veličković.*

BBMC.F3.21– Building a 3D QSAR model with isopropylidene analogs of cytotoxic styryl-lactones– *Bojan D. Levovnik, Aleksa P. Alargić, Miloš M. Svirčev, Goran I. Benedeković.*

BBMC.F3.22– Validation of gravimetric method for determination of clay in soil– *Marina Udilanović, Andrija Ćirić.*

17:00 - 17:30 (Hall I)	Closing Ceremony
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