



**ICCB
2019**

**VIII International Conference on
Computational Bioengineering
4-6 September 2019, Belgrade, Serbia**

ICCB 2019

Proceedings

**8th International Conference on
Computational Bioengineering**

September 4-6, Belgrade, Serbia

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Computational Bioengineering**

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Organizers



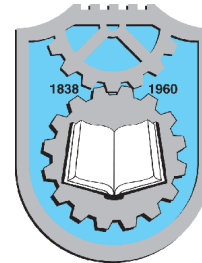
University of Kragujevac



University of Belgrade



**Bioengineering Research and
Development Centre BioIRC**



Faculty of Engineering Kragujevac

Supporting organizations



**The Ministry of Education, Science
and Technological Development of
The Republic of Serbia**



European Society of Biomechanics

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Welcome Message

Dear colleagues and students,

On behalf of the Organizing Committee, it is our great pleasure to welcome you to the *8th International Conference on Computational Bioengineering (ICCB2019)* which is taking place in Belgrade, Serbia, from 4th-6th September, 2019.

The ICCB2019 promotes complementary disciplines that hold great promise for the advancement of research and development in complex medical, biological and computer systems. The main conference includes sixteen sections dealing with topics such as biomechanics, cardiovascular engineering, patient-specific modeling, multiscale modelling, data mining, decision support systems, biomaterials and dental biomechanics, nanomedicine, tissue and cell engineering, computational chemistry, sports bioengineering, etc. Within sixteen sections, we also have seven mini symposia dealing with the issues in the fields of artificial intelligence, machine learning, computational chemistry, risk assessment, computational and experimental physiology, augmented reality and multi-scale modelling. The conference is organized, sponsored and supported by the University of Kragujevac, University of Belgrade, Bioengineering Research and Development Center BioIRC, Ministry of Education, Science and Technological Development of the Republic of Serbia and European Society of Biomechanics.

The ICCB is a large international conference with 16 years of tradition and leading reputation. It follows previous successful conferences held in Spain in 2003, in Portugal in 2005, in Venezuela in 2007, in Italy in 2009, in Belgium in 2013, in Spain in 2015, in France in 2017. ICCB gathers eminent scientists and researchers, as well as students aiming to promote interdisciplinary and multidisciplinary approaches needed for solving complex problems, which requires expertise in the field of biomedical sciences and engineering.

This year, the ICCB 2019 has received more than 150 high-quality research papers and the best papers have been chosen for this Book of Abstracts. Each paper has been reviewed by at least 2 scientists in the program and scientific review committee. As a result of the strict review process and evaluation, the committee has selected papers which will be published as full regular research papers.

We are delighted to announce 10 world renowned scientists as ICCB 2019 keynote speakers:

Dimitrios Fotiadis, University of Ioannina, Greece

Valentin Djonov, University of Bern, Switzerland

Akira Tsuda, HSPH, Harvard University, USA

Marie-Christine Ho Ba Tho, University of Technology of Compiègne, France

Milos Kojic, Houston Methodist Research Institute, USA

Stephane Avril, Center for Biomedical and Healthcare Engineering, France

Nino Russo, Universita della Calabria, Italy

Erik Klein, *University of Technology in Bratislava, Slovakia*

Julien Barthes, *PROTIP MEDICAL, Strasbourg, France*

Atul Bhaskar, *University of Southampton, UK*

We must also say that the conference would certainly not have been so successful without the efforts of many people who were actively engaged in organization of such a major internationally recognized academic event. We give our special gratitude to the members of the program and scientific review committee as well as to all chairs, organizers and committee members for their dedication and support.

This year, ICCB Conference is held in Belgrade, Serbia, a city with rich cultural heritage and extensive and colorful history. We hope that you will find time to explore the city and experience its soul. Serbia already has a number of very good scientists in the area of bioengineering and ICCB2019 is an excellent opportunity to introduce their research and scientific achievements in these challenging areas.

On behalf of the Organizing Committee, we wish you all a pleasant stay in Belgrade and a productive conference.

Prof. Nenad Filipović, *Conference Program Chair*

Organization and Committees

Local Organization Committee

Nenad Filipovic, University of Kragujevac, (Chairperson)

Milos Kojic, BioIRC - University of Kragujevac

Veljko Milutinovic, University of Belgrade

Miroslav Trajanovic, University of Nis

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P. Vena, Italy
A. Bhaskar, UK
O. Altwijri, Saudi Arabia
M. Viceconti, UK
Yang GZ, UK
Zervakis M, Greece

Program at a Glance

| Wednesday 04 September 2019 | | | |
|----------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|
| 08:45 - 09:15 | <p>Opening Ceremony - Welcome speech:</p> <p>Dr. Nenad Filipovic, rector of the University of Kragujevac, Conference Chair Dr. Viktor Nedovic, State Secretary, Ministry of Education, Science and Technological Development Dr. Berislav Vekic, State Secretary, Ministry of Health</p> | | |
| 09:15- 09:45 | <p>Keynote speaker:</p> <p>Topic: Angiogenesis modeling Prof. Valentin Djonov, University of Bern, Switzerland</p> | | |
| 09:45 - 10:30 | <p>Session W.1 Mini-Symposia 4: COMPUTATIONAL AND EXPERIMENTAL PHYSIOLOGY: NOVEL POTENTIAL ANTINEOPLASTIC COMPOUNDS AND CARDIOVASCULAR SYSTEM</p> | | |
| 10:30 - 11:00 | Coffee Break | | |
| 11:00 - 11:30 | <p>Keynote speaker:</p> <p>Topic: Nanoparticles, pulmonary medicine Prof. Akira Tsuda, Harvard School of Public Health, Boston, MA, USA</p> | | |
| 11:30 – 13:00 | <p>Session W.2 Mini-Symposia 6: MULTISCALE IN-SILICO MODELING OF CARDIOMYOPATHY FROM GENO TYPE TO PHENO TYPE</p> | | |
| 13:00 - 14:00 | Buffet Lunch | | |
| 14:00 - 15:00 | <p>Session W.3 Biomedical Decision Support System</p> | | |
| 15:00 - 15:30 | <p>Keynote speaker:</p> <p>Topic: In silico and in vitro tissue models for biomaterial risk assessment and tissue engineering Julien Barthes, PROTIP MEDICAL, Strasbourg, France</p> | | |
| 15:30 - 16:30 | <p>Session W.4 Mini-Symposia 7: MULTISCALE MODELLING OF EXPERIMENTAL DATA RELATED TO BIOMATERIAL RISK ASSESSMENT (part I)</p> | | |
| 16:30 - 17:00 | Coffee Break | | |
| 17:00 - 17:45 | <p>Session W.5 Mini-Symposia 7: MULTISCALE MODELLING OF EXPERIMENTAL DATA RELATED TO BIOMATERIAL RISK ASSESSMENT (part II)</p> | | |
| 17:45 – 18:30 | <table border="0" style="width: 100%;"> <tr> <td style="width: 50%; text-align: center;"> <p>Session W.6.1 Gene Expression Analysis and Engineering</p> </td> <td style="width: 50%; text-align: center;"> <p>Session W.6.2 Mini-Symposia 3: RISK ASSESSMENT IN CARDIOVASCULAR DISEASES</p> </td> </tr> </table> | <p>Session W.6.1 Gene Expression Analysis and Engineering</p> | <p>Session W.6.2 Mini-Symposia 3: RISK ASSESSMENT IN CARDIOVASCULAR DISEASES</p> |
| <p>Session W.6.1 Gene Expression Analysis and Engineering</p> | <p>Session W.6.2 Mini-Symposia 3: RISK ASSESSMENT IN CARDIOVASCULAR DISEASES</p> | | |

| Thursday 05 September 2019 | | |
|----------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------|
| 08:30 - 09:00 | Keynote speaker: Topic: Multiscale modeling Prof. Dimitrios I. Fotiadis, <i>University of Ioannina, Greece</i> | |
| 09:00 – 09:30 | Keynote speaker: Topic: Smeared multiscale finite element models for drug delivery and in electrophysiology Prof. Milos Kojic, <i>Houston Methodist Research Institute, USA</i> | |
| 09:30 - 11:00 | Session T.1 Computational Modeling | |
| 11:00 - 11:30 | Coffee Break | |
| 11:30 – 12:00 | Keynote speaker: Topic: Inverse problems in cardiovascular continuum mechanics and medical applications Prof. Stephane Avril, <i>Center for Biomedical and Healthcare Engineering, France</i> | |
| 12:00 – 13:00 | Session T.2 Cardiovascular Engineering | |
| 13:00 - 14:00 | Buffet Lunch | |
| 14:00 – 16:00 | Session T.3.1 Biomechanics (part I) | Session T.3.2 InSilc Workshop |
| 16:00 - 16:30 | Coffee Break | |
| 16:30 - 17:00 | Keynote speaker: Topic: Theoretical Study of Radical Scavenging Activity of Para-Substituted Phenols Prof. Erik Klein, <i>University of Technology in Bratislava, Slovakia</i> | |
| 17:00 - 18:45 | Session T.4 Mini-Symposia 2: APPLIED COMPUTATIONAL CHEMISTRY (part I) | |
| 20:00 - 23:00 | Gala Dinner | |

| Friday 06 September 2019 | |
|--------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 08:30 - 09:00 | <p>Keynote speaker: Topic: Musculoskeletal system Prof. Marie-Christine Ho Ba Tho, <i>University of Technology of Compiègne, France</i></p> |
| 09:00 – 11:00 | <p>Session F.1 Biomechanics (part II)</p> |
| 11:00 - 11:30 | Coffee Break |
| 11:30 – 12:30 | <p>Session F.2 Mini-Symposia 1: ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN BIOENGINEERING</p> |
| 12:30 - 13:00 | <p>Keynote speaker: Topic: Computational mechanics of implants and scaffolds Prof. Atul Bhaskar, <i>University of Southampton, UK</i></p> |
| 13:00 – 14:00 | Buffet Lunch |
| 14:00 - 14:30 | <p>Keynote speaker: Topic: Metals in cancer therapy. A computational viewpoint Prof. Nino Russo, <i>Universita della Calabria, Italy</i></p> |
| 14:30 - 16:15 | <p>Session F.3 Mini-Symposia 2: APPLIED COMPUTATIONAL CHEMISTRY (part II)</p> |
| 16:15 – 17:15 | <p>Session F.4 Signal Processing</p> |
| 17:15 – 17:45 | <p>Session F.5 Mini-Symposia 5: HOLOGRAM AND AUGMENTED REALITY BIOMECHANICAL MODELS OF A VIRTUAL BALANCE PHYSIOTHERAPIST AND COGNITIVE TRAINING GAMES</p> |
| 17:45 - 18:15 | Closing Ceremony |

F.3.1 – Combined 3D-QSAR modeling, molecular dynamics and molecular docking studies in rational drug design of novel 5-HT_{2A} antagonists - Milica Radan¹, Mirjana Antonijevic¹, Teodora Djikic¹, Dusan Ruzic¹ and Katarina Nikolic^{1*}

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Abstract:

Serotonin 5-HT_{2A} receptors are widely distributed in the human brain where they play a key role in many physiological functions. Numerous neurological disorders caused by 5-HT_{2A} malfunction have made it a very attractive target. Therefore, analysis of 3D-structure of the pharmacophore as well as binding kinetics of 5-HT_{2A} antagonists would be beneficial for future rational drug design. Three-dimensional quantitative structure-activity relationship (3D-QSAR) study was combined with molecular docking and molecular dynamic (MD) simulation in order to find crucial structural features responsible for high binding affinity and selectivity of 5-HT_{2A} antagonists. This study was performed on wide range of structurally diverse antagonists that were divided into three different clusters: clozapine, ziprasidone, and ChEMBL240876 derivatives. We have used 50ns MD simulations to obtain inactive, antagonist-bound, conformations of each cluster representative. Subsequently, these conformations were used as templates for docking studies in order to find virtually bioactive conformations of examined compounds. Selected virtually bioactive conformations were used for generation of specific molecular descriptors (Grid Independent Descriptors- GRIND) and 3D-QSAR model building. The 3D-QSAR approach was used to identify the most important structural determinants responsible for the antagonistic activity and to propose structural modifications for novel antagonists of serotonin 5-HT_{2A} receptors. Furthermore, diverse internal and external validation methods were applied. Obtained statistical parameters indicated the reliability and good predictive potential of the created model. Following these findings we have identified differences and similarities in the binding mode and pharmacophores of structurally diverse 5-HT_{2A} antagonists as well as conformational changes they provoke.

Keywords: 3D-QSAR, molecular docking, MD simulation, pharmacophore, antagonists of serotonin 5-HT_{2A} receptors

F.3.2 – Vibrational spectroscopy study of coumarine-derived ligand 3-(1-(o-toluidino)ethylidene)-chroman-2,4-dione: A combined theoretical and experimental investigation - Zoran S. Marković^{1,2}, Edina H. Avdović^{3*}, Žiko B. Milanović², Dejan Milenković², Svetlana Jeremić¹, Srećko R. Trifunović³

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