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BOOK OF ABSTRACTS



4th Belgrade Bioinformatics Conference

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FOREWORD

Dear colleagues and friends,

The 4th Belgrade Bioinformatics Conference - BelBi2023, where many high-quality scientific contributions were presented, has just ended. With great thanks to all participants, we now proudly present a book of abstracts that both reflects the scientific abundance and diversity of the conference and serves as a reminder of a memorable event.

Several research institutions, faculties, and scientific societies from Serbia joined forces in organizing this international conference, which covered numerous topics in computational biology, bioinformatics, and biomedical and health informatics. The main goal of BelBi2023 was to foster contact between scientists, both early stage career and senior researchers, allowing them to share experiences and latest advances in their fields. We sincerely hope that BelBi2023 has served as a platform for researchers from around the world to meet, initiate new collaborations, and expand professional contacts, and that all of you would become a part of the growing BelBi community.

We are grateful and proud to have welcomed more than 250 researchers from 21 countries. We have had 28 scientific sessions, consisting of more than 60 lectures (including eight Keynote talks), 47 presented posters, as well as three workshops and one satellite event – COST action. We have also organized seven industry lectures, including the NGS Challenge,

two Meet the Expert Sessions, and one Business Coffee Break where ten start-up companies took part. And finally, the future BIO4 campus was presented and first panel on Serbia's resources for storage and analyses of genetic data was organized.

We would like to thank all the members of the International Advisory Board and the International Program Committee for their efforts and help in making this event a success. We are very grateful to the Ministry of Science, Technological Development and Innovation of the Republic of Serbia, SAIGE project, and UNDP-Serbia for their support. Finally, the Local Organizing Committee is very grateful to all the sponsors of the conference - BGI, Illumina & Elta'90MS, PacBio & East Diagnostics, ThermoFisher Scientific & Vivogen, Huawei, Labena, DSP Chromatography, RNIDS, Telekom Srbija, Alfa Genetics, Kefo and Superlab, hoping that they will stay with us for many years to come.

Looking forward to seeing you again at the 5th Belgrade Bioinformatics Conference.

Belgrade, July 2023

Dr. Valentina Đorđević
& *Dr. Ivana Morić,*
On behalf of BelBi2023
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Oral presentation

Computational Modelling of Drug Effects on Cardiomyopathy and Analysis of Myocardial Work

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Analysis of myocardial work is essential in determination of left ventricle ejection fraction (LVEF) and non-invasive assessment of different types of cardiomyopathies. Two major classifications of cardiomyopathy are: dilated (DCM) and hypertrophic (HCM) cardiomyopathy. Although there are clinical improvements in cardiomyopathy risk assessment, patients are still under high risk of severe events. Computational modeling of and computer-aided drug design can significantly advance the understanding of cardiac muscle activity in DCM and HCM cardiomyopathies, speed up the drug discovery and reduce the risk of severe events, aiming to improve the treatment of cardiomyopathy.

The main advantage and novelty of presented study are coupled macro and micro simulations into the integrated Fluid Solid Interaction (FSI) system and its application for examination of heart behavior and drug interactions. In contrary to detailed and patient-specific models where FSI analyses are very time-consuming, our models are parametric and based on dimensions of specific LV components. FSI algorithm within the PAK software is used for modeling the LV with nonlinear material model, together with stretches integration along muscle fibers. The methods are integrated within the SILICOFM platform, and aim to propose an advanced approach for the assessment of work indices and biomechanical characteristics of cardiomyopathies and drugs effects, based on computational modelling.

In this study, simulations of the effect of drugs on improving performance of DCM LV parametric model include the drugs that affect calcium transients (Dygoxin) and changes in kinetic parameters (2-deoxy adenosine triphosphate - dATP). Myocardial work is presented through changes of pressures and volumes (P-V diagrams) for DCM LV model at basic condition (without administered drug) and with using Dygoxin and dATP. Due to increased LV size, the P-V loop for the DCM model without administered drug is shifted toward lower ventricular pressure and larger ventricular volume, with LVEF = 56.83%. Effects of drugs on DCM show an increase in ventricular peak pressures and LVEFs, while the P-V loops are shifted toward decreased volumes, corresponding to healthy hearts.

Computational modeling and drug design approaches can speed up the drug discovery and significantly reduce expenses aiming to improve the treatment of cardiomyopathy.

Keywords: Computational modelling, Myocardial work, Dilated cardiomyopathy, Drug effects

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