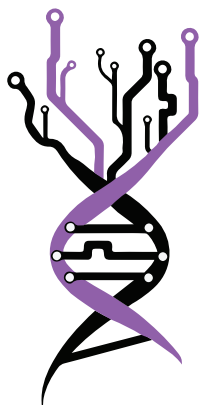


#BelBi2023 • Belgrade, Serbia

BOOK OF ABSTRACTS



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Dr. Ivana Morić

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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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Poster presentation

Comparative study of *in silico* protein design techniques

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Protein design plays a pivotal role in various scientific and industrial applications, such as drug development and biotechnology. With the advancement of computational methods, new tools and algorithms have emerged to facilitate the generation of novel protein designs. This study presents a comparative analysis of Pepspec and RFdiffusion, two prominent methods in protein design, to evaluate their effectiveness in designing peptides with desired properties. Mainly, we aim to design peptides that bind with high affinity and specificity to a desired protein target.

Pepspec is an application native to the Rosetta software package. It relies on Monte Carlo sampling of backbone conformations and residue mutations and a stochastic optimization based on the Rosetta score – a measure approximating the binding free-energy of the complex.

On the other hand, a recently developed tool, RFdiffusion, is a denoising diffusion probabilistic model based on an existing artificial neural network, RoseTTAFold, developed for protein structure estimation. It is trained to remove noise from protein structures on a large database of protein complexes to ultimately be able to generate novel binder designs based on the target structure.

In this study, we aim to compare the efficiency of these two design tools. As it is common in generative ML algorithms, the comparison will be made by evaluating both the design quality and design versatility. The quality will be assessed by using the well-known AlphaFold2 Machine learning tool to estimate the binding affinity of the peptide-protein complex while the versatility will be measured using standard sequence based statistical methods.

RFdiffusion and Pepspec offer distinct approaches to protein design. By assessing the strengths and limitations of each method in this study, we aim to deepen the understanding of these methods and allow leveraging these tools effectively in designing peptides with desired characteristics, contributing to advancements in the field of protein engineering and biotechnology.

Keywords: Rational protein design, AI/ML in biology and medicine, Computational bioengineering



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