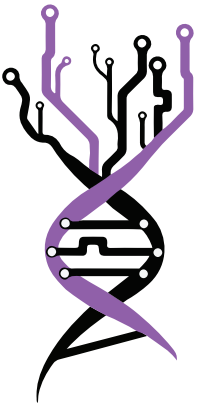
#BelBi2023 • Belgrade, Serbia

BOOK OF ABSTRACTS



4th Belgrade Bioinformatics Conference

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EDITORS
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

An agnostic analysis of the human AlphaFold2 proteome using local protein conformations

Alexandre G. de Brevern[1]

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For more than 30 years, different computational approaches have been implemented to propose 3D structural models of proteins from their amino acid sequence. Using deep Learning, AlphaFold 2 obtained particularly remarkable results; some models were within the uncertainties of the experimental resolution (Jumper et al., *Nature* 2021). AlphaFold 2 code is freely avalaible and EBI provides structural model databases (Tunyasuvunakool et al., *Nature* 2021), i.e. 98.5% of the human proteome is given. 36% of these models are predicted with atomistic quality.
The human protein models provided by AlphaFold were analyzed using its confidence index (pLDDT score), with classic secondary structure and finer analysis of local protein conformation, e.g. γ-turns, β-turns and bends, β-turn types, PolyProline II (PPII), helix curvatures, β-bulges, and a structural alphabet, namely Protein Blocks (PB).
As expected, the large majority of α-helices are well predicted with high pLDDT scores. However, some points are intriguing and could potentially lead to improvements in the future: (i) PPII helices are too often encountered with a low confidence index. They represent 4-5% of all residues and are important in protein-protein interactions; it could so be an issue to be poorly approximated. (ii) In a very surprising way, while β-turns (turns of 4 residues) are well predicted, 55% of γ-turns (3 residues) have very low pLDDT scores. (iii) Even more strikingly, 94.8% of cis ω angles associated with low pLDDT scores, i.e. AlphaFold is clearly unable to propose proper cis ω angles. (iv) β-sheet occurrence is lower than expected, while PB *d* (i.e. β-sheet core geometry) occurrence is completely in accordance with the expected frequencies. There are so potentially β-sheets that were not founded until the end, which would explain this low frequency (de Brevern, *Biochimie* 2023). AlphaFold 2 had impacted the structural modeling area but works remained (Tourlet et al., *BioMedInformatics* 2023)

Keywords: bioinformatics, deep learning, computer science, protein structure, secondary structures.

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