

## PUBLIC LECTURE EVALUATION

### Masaryk University

<b>Faculty</b>	Faculty of Science
<b>Procedure field</b>	Biomolecular Chemistry and Structural Biology
<b>Applicant</b>	doc. RNDr. Karel Berka, Ph.D.
<b>Lecture date</b>	31 <sup>st</sup> October 2024
<b>Lecture topic</b>	Impact of AlphaFold to Structural Biology – What is next in AlphaFoldology
<b>Persons present</b> (number)	51 in person, 15 online (see attached list of attendees)
<b>Designated evaluators</b> (board members)	<p><b>Prof. RNDr. Michaela Wimmerová, Ph.D.</b> <i>National Centre for Biomolecular Research – Faculty of Science, Masaryk University, Brno – in person</i></p> <p><b>Prof. Mgr. Richard Štefl, Ph.D.</b> <i>Centre for Structural Biology – Central European Institute of Technology, National Centre for Biomolecular Research – Faculty of Science, Masaryk University, Brno – in person</i></p> <p><b>Prof. Mgr. Lubomír Rulíšek, CSc. DSc.</b> <i>Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague – in person</i></p> <p><b>Prof. Mgr. Daniel Svozil, Ph.D.</b> <i>Department of Informatics and Chemistry, Faculty of Chemical Technology, University of Chemistry and Technology, Prague – online</i></p> <p><b>Prof. RNDr. MSc. Rudi H. Etrich, Ph.D.</b> <i>Larkin University, Miami, FL, USA – online</i></p>
<b>Board members present online</b>	

Assoc. Prof. Karel Berka delivered his lecture with the title “**Impact of AlphaFold to Structural Biology – What is next in AlphaFoldology**” on 31<sup>st</sup> October 2024. In the lecture, the applicant encompassed the origin of the protein structure prediction problem, the CASP competition and its challenges, and the major breakthrough attributed to AlphaFold 2 in recent years (AF2) program. He has explained the basics of the implementation of AF2, which is a diligent combination of machine learning tools and existing (standard) approaches, such as homology and co-evolution matrices.

In the second half of the lecture, the candidate discussed the broader aspects of this (major) breakthrough in structural biology. Specifically, he used the name “AlphaFoldology” – which is the collection of the innovative tools to study protein structure models. The field developed rapidly since the opening of the AlphaFold code to the public in the summer of 2021. The applicant has shown how he and his team are using AF2, AF3, and related tools in his research of protein structures. Karel Berka clearly demonstrated deep knowledge of the topic and also how to carefully and critically evaluate and utilize AlphaFold and related tools for the research in structural biology. The evaluation board considers the topic to be up-to-date,

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which can be demonstrated by the recent recognition of the AlphaFold program resulting in the Award of this year's Nobel prize in Chemistry.

The lecture stimulated a vivid and broad discussion. All the questions raised by all the members of the evaluation board as well as public revolved around multiple topics concerning the quality of protein model structures, usage for evaluation of macromolecular complexes, analysis of whole proteomes, protocols to use the model structures for drug design, licences of current modelling programs and the OpenFold initiative and about the future of the field. The applicant answered all questions exhaustively, demonstrating a very high degree of his expertise in the field.

## Conclusion

The lecture delivered by Karel Berka, entitled the "Impact of AlphaFold to Structural Biology – What is next in AlphaFoldology" and delivered as part of the professor appointment procedure, **demonstrated** sufficient scholarly qualifications and pedagogical capabilities expected from the applicants participating in a professor appointment procedure in the field of Biomolecular Chemistry and Structural Biology.

The lecture took place in a hybrid form at 2 p.m. The above-mentioned members of the board attended the lecture and provided its evaluation. All designated evaluators are familiar with the text of the evaluation and agree with it.

Date: 31.10.2024

Michaela Wimmerová

Lubomír Rulíšek

Richard Štefl