

PUBLIC LECTURE EVALUATION

Masaryk University

Faculty	Faculty of Science
Procedure field	Environmental Health Sciences
Applicant	Stanislav Mazurenko, Ph.D.
Lecture date	8.10.2026
Lecture topic	Machine Learning in Protein Engineering
Persons present (number)	44
Designated evaluators (board members)	Prof. RNDr. Robert Vácha, Ph.D. <i>CEITEC and Faculty of Science, Masaryk University</i> Mgr. Tomáš Pluskal, Ph.D. <i>Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences</i> dr hab. Jan Brezovský, Ph.D. <i>Faculty of Biology, Adam Mickiewicz University</i> prof. Sílvia Osuna, Ph.D. <i>Institute of Computational Chemistry and Catalysis, Universitat de Girona</i>

The habilitation lecture of Stanislav Mazurenko was a hybrid event with 34 people present in the lecture room and additional 10 connected online. The chair and all four members of the evaluation board were present.

Stanislav Mazurenko gave a presentation on his habilitation topic, "Machine Learning in Protein Engineering", and presented his significant research contributions to a field that is rapidly developing and has important applications in biotechnology and medicine. He started introducing the basic principles and methods of machine learning and then explained clearly why these approaches are particularly useful in protein research. Only a tiny fraction of known protein sequences are annotated, the number of possible protein mutations is enormous, and molecular simulations generate huge amounts of data. He then showed how his team addresses these challenges using original tools and approaches. These include large-scale mining of sequence databases, zero-shot prediction of how mutations affect enzyme activity, machine-learning analysis of protein dynamics, and generative models such as variational autoencoders. His team used variational autoencoders to design enzyme variants that experiments confirmed to have improved stability and activity. Stanislav also gave a critical and well-balanced view of the current challenges in the field. He discussed limitations related to the quality and quantity of available data, noise in the data, data leakage, data transformation, augmentation, and the ability of models to generalize to new cases.

His presentation demonstrated both deep expertise in his specialised field and an ability to place his research in a broader scientific context. This showed that he is not only an expert in

a specialised area but also someone who sees the problems in a broader context. Stanislav demonstrated that he is a mature, independent scientist and team leader, as well as an experienced lecturer. He presented the results of his interdisciplinary research, which combines mathematics, informatics, biochemistry and molecular biology, in a way that was clear and engaging for a broad audience.

The candidate prepared detailed responses to the reviewers' comments and questions and engaged in a lively discussion with the board members as well as the audience. The discussion covered the integration of physics-based and machine-learning models; approaches to generalization, bias, and overfitting; and the advantages and limitations of protein language models. The participants also discussed whether AI-based generative methods could complement or eventually replace some applications of molecular dynamics simulations. The discussion also addressed the role of independent test sets in models with a limited number of parameters. Ongoing projects and future perspectives were also discussed, including his plans for further involvement in teaching and mentoring junior scientists.

Conclusion

The lecture delivered by Stanislav Mazurenko, entitled "Machine Learning in Protein Engineering" and delivered as part of the habilitation procedure, **demonstrated** sufficient scholarly qualifications and pedagogical capabilities expected of applicants participating in a habilitation procedure in the field of Environmental Health Sciences.

The lecture took place in a hybrid form at 14:00. 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. Since the evaluators apart from the Chair of the board were all present online and are external, the document is signed by the Chair of the board who attended the lecture in person.

Date: 8.10.2026

Prof. RNDr. Robert Vácha, Ph.D.

Digitally signed by
prof. RNDr. Robert Vácha PhD.
08.10.2026
signature