MUNI

HABILITATION THESIS REVIEWER'S REPORT

Masaryk University

Applicant	Mgr. David Bednář, Ph.D.
Habilitation thesis	Computational Tools for Analysis and Design of Proteins
Reviewer	doc. RNDr. David Hoksza, Ph.D.
Reviewer's home unit, institution	Department of Software Engineering, Faculty of Mathematics and Physics, Charles University

The thesis covers a relatively wide range of topics from the field of protein engineering, including protein properties prediction, enzyme exploration, and detection and analysis of protein tunnels. The thesis is a compilation of selected publications and is structured to follow division into parts corresponding to the abovementioned topics. The structure is consistent in that each section is divided into a brief introduction to the topic, a description of the state of the art, and a contribution. The text is relatively high-level and easy to follow, even for people outside the covered research fields.

The range of topics covered by the thesis is impressive and proves that Dr. Bednář is an expert in not only a relatively narrow scope of the field but is able to see problems as a part of a bigger picture. The fact that he has been heavily involved in developing the presented tools testifies to the depth of knowledge in the individual fields, as without them, it isn't easy to implement given concepts.

This thesis covers nine publications published in top journals in the bioinformatics field, i.e., Bioinformatics and Nucleic Acids Research. The work of Dr. Bednář has also been published in other leading journals in the field of bioinformatics, computational biology, and biochemistry.

The software tools which are presented in this thesis are widely accepted by the community, as evidenced by the number of citations of the respective publications. I think two factors come into play here: the quality of the methodology behind the tools and the effort made to bring the tools closer to the users who are not experts in bioinformatics. Another aspect that should be emphasized is that the tools are part of the Elixir platform showing engagement in the community efforts.

Reviewer's questions for the habilitation thesis defence (number of questions up to the reviewer)

1. In section 2, protein solubility prediction, pg. 16 it is stated that standardization of mutational data and their FAIR storing would help developers. Therefore, I would like to know what measure are taken in the presented tools toward FAIR storage of the data, especially considering some of the presented contributions are databases.

2. In section 3, prediction of protein stability, pg. 19, it is said that ML-based methods are able to recognize unknown dependencies that are not considered by force fields. Although this somehow intuitively feels true, I would like to know if there are some concrete examples.

3. In section 4, analysis of ligand pathways, pg. 25, parallel heuristics to identify ligand trajectory used with AudoDock Vina are mentioned. How do they work?

Conclusion

The habilitation thesis entitled "Computational Tools for Analysis and Design of Proteins" by David Bednář **fulfils** requirements expected of a habilitation thesis in the field of Environmental Health Sciences.

Date: 28. 2. 2023   Signature: