MUNI

Annex No. 11 to the MU Directive on Habilitation Procedures and Professor Appointment Procedures

PUBLIC LECTURE EVALUATION

Masaryk University	
Faculty	Faculty of Science
Procedure field	Biomolecular Chemistry and Structural Biology
Applicant	doc. RNDr. Radka Svobodová, Ph.D.
Lecture date	November 21, 2024
Lecture topic	What we can learn from protein 3D structures?
Persons present (number)	51
Designated evaluators (board members)	Prof. Mag. Dr. Thomas Rattei, on site prof. Ing. Vojtěch Spiwok, Ph.D. on site prof. Mgr. Lukáš Žídek, Ph.D. on site

On November 21, 2024, doc. RNDr. Radka Svobodová, Ph.D. presented a public lecture at Masaryk University, Faculty of Science. In her lecture, doc. Radka Svobodová introduced the history and the current way of depositing experimental and predicted three-dimensional protein structures and described what can we learn from the deposited structures. The lecture consisted of several sections, related to research areas of doc. Svobodová, to the field of Biomolecular Chemistry and Structural Biology, and also to the courses taught by doc. Svobodová. In these sections, doc. Svobodová discussed the following topics.

(1) History of Protein Data Bank (PDB).

(2) Visualization of protein tertiary structures, secondary structures, and protein families, presenting its history and the benefits of visualization web tools developed with a direct involvement of doc. Svobodová (LiteMol, Mol*, 2DProts).

(3) The need of validation of experimental protein structures in the databases and examples of errors, history, current status and involvement of doc. Svobodová in development of structure validation tools.

(4) Tools developed to identify tunnels, pores, pockets and cavities in protein structures, including those developed with the involvement of doc. Svobodová (MOLE, MOLEonline, ChannelsDB).

(5) Protein properties calculated from protein structures, in particular atomic charge calculations, doc. Svobodová was involved in, and PDB annotations based on them.

(6) Current status, opportunities, and challenges of predicting 3D protein structures, tools of predicting protein properties and structure similarities (AlphaFind).

In the following discussion, doc. Svobodová answered the following questions:

i. What is your opinion on virtual/augmented reality in protein structure visualization? (V. Spiwok) Answer: We collaborate with FI MUNI in this field.

ii. Does AlphaCharges address solvent? (T. Rattei) Answer: There has been a long development in the field of partial atomic charges, from vacuum to solvent or environment of the interest. We follow this development.

iii. What is the relation of lack of structure vs. low confidence in protein structure models? (T. Rattei) Answer: We study this within the development of Alphafind to apply it on complex protein.

iv. What is the procedure of AlphaCharge? (A. Chareshneu) Answer: Structure is retrieved from Alphafold DB, hydrogens are added and various charge types are calculated by previously published methods and visualized by Mol*.

v. What is the future of prediction of protein flexibility by AI? (L. Zidek) Answer: There are limitations of molecular dynamics simulations, but there is a progress towards retrieval of training data for AI.

Conclusion

The lecture delivered by doc. RNDr. Radka Svobodová, Ph.D., entitled "What we can learn from protein 3D structures?" and delivered as part of the professor appointment procedure, **demonstrated** sufficient scholarly qualifications and pedagogical capabilities expected of applicants participating in a professor appointment procedure in the field of Biomolecular Chemistry and Structural Biology.

The lecture took place on-site 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.

Date: November 21, 2024

Prof. Mag. Dr. Thomas Rattei

prof. Ing. Vojtěch Spiwok, Ph.D

prof. Mgr. Lukáš Žídek, Ph.D.