

PUBLIC LECTURE EVALUATION

Masaryk University

Faculty	Faculty of Science
Procedure field	Physical Chemistry
Applicant	RNDr. Mgr. Jozef Hritz, PhD.
Lecture date	7.10.2021
Lecture topic	Statistical physical chemistry of protein complexes
Persons present (number)	111
Designated evaluators (board members)	prof. RNDr. Radek Marek, Ph.D. (on-site) doc. RNDr. Petr Jurečka, Ph.D. (on-site) doc. Mgr. Lubomír Rulíšek, CSc., DSc. (online)

The public lecture “Statistical Physical Chemistry of Protein Complexes” was given on-site at the Masaryk University Campus Bohunice, Building B11, room 1.32. There was an additional online stream using MS Teams.

The lecture was attended by the following members of the habilitation committee and one reviewer:

prof. Radek Marek (chair)
doc. Petr Jurečka (external member)
doc. Lubomír Rulíšek (external member, online)
Prof. Dr. Bojan Zagrovič (international member, online)
doc. Vojtěch Spiwok (reviewer, online)

Unfortunately, the international reviewers were unable to attend the lecture.

At the beginning of the lecture, the applicant introduced various techniques of molecular modeling used in biomolecular simulations. The applicant provided theoretical introduction to the topic and covered a variety of enhanced sampling and free energy calculation methods developed in the field of biomolecular simulations. He demonstrated his approach to systems with multiple stable conformations separated by high energy barriers. Furthermore, he discussed advantages of Hamiltonian replica-exchange molecular dynamics simulations and his own contributions to this field as well as advantages of the distance field distance restraints method as compared to simple distance restraint replica exchange. He described approaches to calculation of relative free energy differences of protein-ligand binding including alchemical free energy methods. In the last part of the talk, the applicant described challenges in the interpretation of titration NMR experiments of phosphorylated peptides.

The committee found the talk by the applicant very clear, authoritative and competent. At the end of the lecture, there was a long and in-depth discussion about the topic, and the applicant successfully answered all questions of the members of the habilitation committee and the general audience.

Conclusion

The lecture delivered by Dr. Jozef Hritz, entitled “Statistical Physical Chemistry of Protein Complexes” 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 Physical Chemistry.

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: October 7, 2021

Radek Marek

.....
signature

Petr Jurečka

.....
signature