



Supervisor statement for supporting thesis defense of MSc. Zeenat Zara

Zeenat Zara was working on her PhD thesis under my supervision since autumn 2018. The topic of her thesis were Bimolecular interaction of Proteins and her first project she started to work on was the computational study of the stability and function of PETase in the presence on ionic liquids. The main idea of the project was to investigate the effect of the ionic liquids on the function and stability of the PETase in order to investigate the possible use of ionic liquids in combination with plastic degrading enzymes, as the ionic liquids can dissolve crystalline form of the plastic, making them easily degradable by the enzyme. The goal of the project was to investigate by means of MD simulations whether PETase would be functional even in the presence of ionic liquids. Zeenat has studied 3 different ionic liquids at different concentrations and the results of her work have been successfully published.

Her second project has been originally the study of possible macrolide antibiotic that overcome the drug resistance. The project has been in the collaboration with experimental group from Institute of Microbiology of CAS and involves molecular docking of possible drug candidates on modified binding site of ribosome followed by MD simulations. Unfortunately the results of this project were not in publishable form on required time, therefore Zeenat has started to work on the additional project. As she has been interested in the project that would involve the membrane protein she started to work on the simulation of GPCRs (in collaboration with experimental work of Dr. Alexey Bondar from our research center), particularly to characterize the interaction interface between 5HT7R receptor and the Gs protein in both active and inactive states of their bound complex. However as the project also involve of the homology modeling (and we have no much experience with homology modeling in our research group) Zeenat has decided to learn the methods during her stay abroad. She has independently found the group of Dr. Antonella Di Pizio from Leibniz-Institute for Food Systems Biology at the Technical University of Munich in Freising, Germany, where she could learn the homology modeling during her stay abroad. Zeenat has successfully modeled the system, performed MD simulation and after analysis her results has been submitted for publication (currently under review).

Apart of her main projects Zeenat has been involved also in few other projects with the member of our research group and our collaborators, resulting in two additional publications with Zeenat as a co-author.

During her PhD study Zeenat has learned the range of the methods of molecular modeling, particularly MD simulation, QM and QM/MM methods, different analysis methods and during her stay abroad also the homology modeling. I can confirm that Zeenat has fulfilled all pre-requirements for finishing her PhD studies. She has published three papers with one paper in impacted journal as the first author and the other of her first authorship paper has been submitted under review. She has passed state exam and all courses required by Ph.D. program. She has also participated at teaching of undergraduate students at annual summer schools at Nove Hradý research center. As she fulfilled all requirements for defending her Ph.D. thesis, I recommend Zeenat to defend her Ph.D. thesis in front of the committee.

Dr. David Řeha, Ph.D.

