

Prof. Martin Hof Director J. Heyrovský Institute of Physical Chemistry Czech Academy of Sciences

Dolejškova 2155/3, 182 23 Prague 8, Czech Republic Phone: (+420) 775990013 e-mail: hof@jh-inst.cas.cz

http://www.jh-inst.cas.cz/~fluorescence/

May 21, 2019

Model membranes studied by advanced fluorescence techniques and molecular dynamics simulations

Submitted by Mgr. Adéla Melcrová

PhD advisor's opinion on the PhD work

Adéla Melcrová started in October 2013 her PhD studies in my lab. Adéla became first interested in fundamental effects of ions and transmembrane proteins on model biological membranes, and in the later stage in a more medical orientated topic in membrane biophysics, the study of tear lipid film of the human eye. Noteworthy, it was her explicit wish to approach those scientific topics by both, experiments and computer simulations. Honestly, I was in the beginning quite skeptical, since fluorescence methods like the time dependent fluorescence shift approach, fluorescence resonance energy transfer, or fluorescence correlation spectroscopy are quite demanding and usually need the full attention of the student. On the other side, the majority of computational chemists are satisfied when they are able to compare the outcome of their molecular dynamics simulations with experiments provided by other colleagues. As can be documented by her list of publications Adéla managed both, simulations and experiments. For the critical interpretation of the results it turned out to be an advantage that experimental and computational results were done by the same person.

In summary, Adéla Melcrová has proven a high level of adaptability and universality by mastering theoretical approaches when she could not regularly perform the experimental work in laboratory due to her maternal duties. Despite

the limitations in work time in a laboratory, she has already published 8 publications in peer reviewed journals, with her first authorship on 3 of them. The scientific community is receiving her research positively. Her work on the identification and characterization of binding sites for calcium ions in phospholipid membranes has gained 45 citations according to the Web of Science in less than 2,5 years since its release.

There is absolutely no doubt that her PhD thesis should be accepted by the PhD examination board. For the case Mgr. Adéla Melcrová will successfully defend her thesis, she should be awarded with the title PhD.

Sincerely yours,

Martin Hof