Letter from the PhD. advisor

Prague, August 14, 2014

With great pleasure I am recommending the PhD. thesis of Jana Hladílková (néé Paterová) for defense. Jana has been a PhD. student in my group since 2010. Her undergraduate background has been synthetic organic chemistry, nevertheless, for her PhD. studies she decided to switch fields and focus on computational biochemistry. I recall when Jana interviewed as a potential PhD. candidate I first hesitated a bit given her background, which was very different from that of typical students in my group. But something in the way she courageously and enthusiastically presented her desire to learn computational techniques in biochemistry convinced me to give her a chance. I can safely say today that this was among the best decisions I have ever made concerning student careers.

In the past four years, Jana not only learned state-of-the-art techniques of computer simulations and quantum chemistry, but also played a key role in establishing the molecular basis for understanding specific ion effects on proteins (Hofmeister series). In close collaboration with experimental groups Jana performed pioneering simulations, elucidating the key principles governing interactions of biologically relevant ions with protein backbone and charged side chains. In separate studies, Jana was also able to rationalize the effects of alkali halides on enzymatic activity of haloalkane dehalogenases and to predict the binding site and catalytic action of a potassium cation in the active site of betaine-homocysteine S-methyltransferase. The results presented in Jana’s PhD. thesis, together with a nice introduction relating the calculations to experiments, have been summarized in seven papers published in leading international journals (Jana is the first author of three of them and the first theoretical author of the remaining four). Jana also reported on her results in the form of contributed talks and posters on several international conferences (including Gordon research conferences) and lectures during her research stays abroad (at the Lund University and Tampere University of Technology).

During the last four years, Jana has grown into an independent young scientist, who comes up with her own research ideas, as well as strategies how to address them. After defending PhD. she should thus be perfectly ready for her postdoc experience.

With kindest regards

Prof. Pavel Jungwirth