



Habilitation thesis reviewer's report

Masaryk University	
Faculty of Science	
Field of habilitation	Biomolecular chemistry
Applicant	RNDr. Radka Svobodová Vařeková, Ph.D.
Workplace	National Centre for Biomolecular Research Faculty of Science Masaryk University
Habilitation thesis	Analysis of biomacromolecular structural fragments
Reviewer	Dr. Attila Gyenesei
Workplace of reviewer	Vienna Biocenter Core Facilities, Vienna, Austria

Reviewer's report

It is my pleasure to provide my reviewer comments for the habilitation thesis of Dr. Radka Svobodová titled „Analysis of biomacromolecular structural fragments“. The thesis consists of 16 articles published in high-impact scientific journals of which Dr. R. Svobodová appears to have had crucial role in all these papers as first author, corresponding author and co-author. The total impact factor of these papers is 83,659. The publications appeared in both specialist technical journals and more general multidisciplinary journals of excellent reputation and high visibility as well as being easily accessed by the scientific community.

This thesis deals with the challenge of the analysis of biomacromolecular structural fragments such as ligand and metal binding sites, channels and pores as well as supersecondary structure elements. This challenge is inherent in the current development in modern life sciences - the interconnection of structural and chemoinformatics and requires a multidisciplinary approach such as those exemplified in the thesis. To solve these problems, Dr. Svobodová has developed numerous unique methods and original computational tools and has validated their use with real experimental data sets.

This is an excellently presented thesis with very good typesetting and layout. There is a large reference list and these are mostly incorporated well. The scientific English is excellent and written with a very few typos and errors. The thesis is clearly structured, the parts presented in the papers are clearly marked. The actual text is about 50 pages, but together with the 16 papers this is more than adequate.

Dr. Svobodová presents a comprehensive, well motivated and well executed research on the analysis of biomacromolecular structural fragments. Her methods are state-of-the-art, well applied and are excellently integrated with the scientific literature. The developed methods use the powerful combination of chemoinformatics and structural bioinformatics and enable us to produce very beneficial outcome such as information for the classification of biomacromolecules, understanding the relationship between structure and function, predicting their putative functions as well as discovering drug design patterns. The work is timely and important. More importantly, the work can be applied to a large variety of problems and does not discriminate on biological context. Without a doubt, this thesis represents a substantial advancement to our understanding of how the interconnection of structural bioinformatics and



chemoinformatics can bring useful insights into biology, biochemistry and biomolecular chemistry. This work described in this thesis will have a sure and lasting impact for those in this growing field of science.

In summary, I confirm that the thesis by Dr. Radka Svobodová fulfills the criteria of a habilitation dissertation and recommend without reservation to be accepted for the habilitation defence.

Reviewer's questions for the habilitation defence (number of questions up to the reviewer) ...

Although the thesis has described various potential application areas in the field of pharmaceutical research but I am still wondering whether the candidate has exploited this fully. (I would strongly recommend to build collaboration with pharmaceutical companies.)

Conclusion

The habilitation thesis submitted by RNDr. Radka Svobodová Vařeková, Ph.D., entitled „Analysis of biomacromolecular structural fragments“ *meets* the requirements applicable to habilitation theses in the field of Biomolecular chemistry.

In Vienna on 7th of September, 2016