



*Professor Haim J. Wolfson
George and Maritza Pionkowski
Chair in Computer Aided Drug Design*

פרופ' חיים וולפסון
הקתידרה לפיתוח ממוחשב של תרופות
ע"ש ג'ורג' ומריטצה פיונקובסקי

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Prof. Michal Kozubek
Habilitation Committee Chairperson
Faculty of Informatics
Masaryk University
Brno, Czech Republic

Dear Professor Kozubek,

It is my pleasure to evaluate the habilitation thesis "Analysis and Visualization of Biomolecules", which has been submitted by Dr. Barbora Kozlikova.

The thesis deals mainly with algorithms for the analysis of the three dimensional (3D) structures of protein molecules and the graphical visualization of such structures. It particularly focuses on the detection and visualization of the, so called, "tunnels" within protein structures, which are void volumes penetrating into the depth of the protein, where small molecular ligands are transported in order to bind to the protein's functional site.

The work dealing with the analysis of protein 3D structures utilizes advanced Robotics motivated Computational Geometry methods to present solutions to tasks, which are highly relevant for the elucidation of protein function and have the potential to make key contributions to Computer Assisted Drug Design. The major contribution in this regard is the continuous development of the CAVER tunnel detection method, which culminated in the current CAVER 3.0 version, known as one of the best methods for tunnel detection.

Kozlikova has also done impressive work in biomolecular visualization, in particular the visualization of protein tunnels. Her recent work on visualization of tunnels in molecular dynamics simulations is relevant and highly promising.

The thesis includes 23 papers co-authored by Kozlikova. The few introductory chapters preceding the published papers, which introduce the reader to the field of biomolecular visualization and outline the author's contribution are well written and explained. The papers describing Kozlikova's work have been published predominantly in the proceedings of key topical conferences in Computer Graphics and Visualization, as is customary in the informatics field. The major contributions have been also published in established journals in the fields of



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Graphics and Bioinformatics. Notably, almost half of the papers have been published since 2015.

Clearly, the most impressive project, which was co-authored by Kozlikova is CAVER 3.0. This is a *state-of-the-art* tunnel detection technique, which is implemented as a web-server freely available to the biological community. Apparently, this server is widely used by the biological community as evidenced by the numerous citations (more than 300 according to Google Scholar) of the PLOS Computational Biology 2012 paper describing the CAVER 3.0 method (Chovancova et al.).

Notably, the graphical tunnel visualization tool CAVER Analyst 1.0 published in Bioinformatics 2014 (Kozlikova et al.) has also been highly cited (more than 50 times according to GS).

In summary, Dr Barbora Kozlikova has demonstrated innovative research and algorithm design abilities in an interdisciplinary field which applies advanced Computational Geometry and Computer Graphics methodologies for the advancement of Structural Biology and Computer Aided Drug Design research. Her work on protein tunnel discovery and visualization is *state-of-the-art* by international standards. To conclude, the habilitation thesis submitted by Dr. Barbora Kozlikova entitled "Analysis and Visualization of Biomolecules" *meets* the requirements applicable to habilitation theses in the field of Informatics.

Sincerely Yours,

Prof. Haim J. Wolfson