Report on the thesis of Georgy Derevyanko entitled “Structure-based algorithms for protein-protein interactions” submitted to obtain the degree of PhD from Grenoble University (speciality Physique pour les Sciences du Vivant).

The soluble proteins are the major cogs in the cell biochemical machinery. They are responsible for the integration of transmembrane signals, structural integrity of a cell, maintaining and reproduction of cell components including the proteins themselves. Major body of proteins are working in complexes of several proteins or execute their function by interacting with other proteins. Therefore computational prediction of a protein-protein complex structure from its constituents is an extremely important task both for science and clinics.

The results of the work are presented in 2 sections, devoted to the two new algorithms.

The first of the two (section 2) describes the new approach to perform rigid-body exhaustive search using Hermite functions basis. This algorithm omits one of the two Fourier transform calculations, compared to the commonly used scheme originally proposed by Katchalski-Katzir. The comparison of the speed of the Hermite transform and the Fast Fourier transform was given, that shows clearly that the algorithm is comparable to the well-known industry-grade library even without extensive optimization.

However, the workflow of protein-protein docking includes also the refinement of the sampled conformations and the modeling of the environment.

The next section of Georgy’s thesis is devoted to the development of a new approach to computation of a scoring functions. They are used to filter and refine the conformations yielded by the exhaustive search. The key idea and distinguishing property of the algorithm proposed is that the decoys of a certain structure are discriminated from only its the native structure. This key idea found its implementation in the computational algorithm. Finally, in this section Georgy presents evaluation of the scoring functions obtained using his approach on two protein-protein docking benchmarks. Another application of the algorithm described in this section is the prediction of the positions of water molecules near the binding interface of two proteins.

The results presented in the thesis certainly advanced the corresponding scientific fields, which is evidenced by two scientific publications based on themand one patent.

Consequently, one can say that Georgy Derevyanko conducted a complete study with the needed scientific rigor and in professional manner. The thesis is clearly structured and written, and the results are presented very accessibly. I believe that Georgy deserves granting him a degree of PhD from Grenoble University.