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 PhD thesis of Georgy Derevyanko is devoted to the development of novell algorithms for the problem of protein-protein docking and conformations optimization. The protein-protein docking is an old and important research field. The major body of algorithms in this research area consist of two consequent steps: 6D rigid-body exhaustive search and scoring and refinement of the top conformations found. The novel approaches to both of these steps can result in the better understanding of the problem in hand as well as speed and efficiency increase of the new methods.

The thesis consists of an Introduction, two sections devoted to the two main steps of the protein-protein docking algorithms: Hermite fitting and Scoring functions, and a Conclusion and outlook section. The total length of the thesis is 101 pages and the bibliographical reference list consists of 150 references to scientific articles and books.

In the Introduction, the necessary context of the performed studies is given. The author describes the current state of the scientific field and states the rationales behind the presented studies.

The two sections giving the major results of the thesis are:

1. The sections 2 describes the novel approach to 6-dimensional rigid-body exhaustive search using Hermite functions basis. The resulting algorithm is shown to outperform existing ones in terms of sampling efficiency.
2. The section 3 describes the method to obtain the protein-protein scoring potentials. It was applied for both the initial problem of the filtering and refinement of protein-protein complexes conformations. But also it found an application to the prediction of crystallographic water molecules at the interface of the two interacting proteins. The algorithms were validated using the well-known benchmarks and Critical Assessment for Protein Interactions (CAPRI) challenge.

To sum up, the thesis presents a significant amount of work that proposes novel algorithms for all steps in the protein-protein docking workflow.

The results presented in this work are at the basis of 2 scientific publications and one patent.

To conclude, the thesis of Georgy Derevyanko entitled “Structure-based algorithms for protein-protein interactions” presents (not) numerous (un)important results, meets (doesn’t) the requirements for scientific work and its author deserves (doesn’t) granting him a degree of PhD from Grenoble University.