Development of a Software Tool for Protein-Protein Complex Prediction

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Life of all organisms is largely regulated by protein-protein interactions. In particular, immune system reactions are provided by those interactions. When our immune system fails, scientists have to create synthetic molecules to neutralize specific proteins. This requires models of interaction between target protein and its partner. These problems can be solved not only experimentally but also using math modeling. It could be cheaper and faster. We developed the software tool that models optimal geometric and electrostatic docking of two protein molecules. To test this software tool we needed some help of bio-scientists who knew exactly the correct answer of docking. Our supervisors could compare our answer with the real result. So, we tested our tool on some proteins. It means that the tool has been tested in a biotechnology company. We came up with a new fast method of discretisation (simplification molecule to the cubic grid). This method is involved in that biotechnology company. We also implemented the visualization of molecules and the final protein complex (Java3D library is used).

Awards Won: