[P25] Udock, the Interactive Docking Entertainment System

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Protein–protein interactions play a crucial role in biological processes. Protein docking calculations' goal is to predict, given two proteins of known structures, the associate conformation of the corresponding complex. Here, we present a new interactive protein docking system, Udock [1], that makes use of players' cognitive capabilities added up.

In Udock, the players explore simplified representation of protein structures and tackle protein-protein interfaces conformational space using a gamified interactive docking and scoring on the fly. We assumed that if given appropriate tools, naive user's cognitive capabilities could provide relevant data for 1. the prediction of correct interfaces in binary protein complexes and 2. the identification of the experimental partner in interaction among a set of decoys. To validate the approach, we conducted a two weeks cross-docking playtest where the registered users could perform a cross docking on a dataset constituted of 4 binary protein complexes. The users explored almost all the surface of the proteins that were available in the dataset but favored certain regions that seemed more attractive as potential docking spots. These favored regions were located inside or nearby the experimental binding interface for 5 out of the 8 proteins of the dataset. For most of them, the best scores were obtained with the experimental partner.
The alpha version of Udock is freely accessible at http://www.udock.fr

[1] Levieux G, Tiger G, Natkin S, Zagury JF, Montes M. FD169: Faraday Discuss. 2014, DOI: 10.1039/C3FD00147D