CABS-dock standalone application for protein-peptide docking with large-scale flexibility of the protein receptor

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Protein-peptide interactions may involve large-scale conformational changes of a target protein which are challenging to study both experimentally or computationally[1]. Here we present a new standalone application based on CABS coarse-grained protein model for flexible protein-peptide docking – the CABS-dock[2-4], so far available as a web server[4]. The method performs a blind global search for a binding site combined with an on-the-fly folding of a fully flexible peptide, while the target protein backbone fluctuates around its input conformation (in the default mode). Additionally, users can extend the degree of conformational flexibility of a protein receptor (for chosen regions) and enable large-scale conformational changes. That was the case of the modeling of the MDM2/p53 complex, modeled using CABS-dock with full flexibility of the intrinsically disordered regions of significant length[1]. The obtained CABS-dock results for MDM2/p53 system matched well the experimental data and provided new insights into the possible role of unstructured receptor regions. The standalone CABS-dock application allows for customization of the simulation parameters, providing constraints for user selected protein-peptide contacts, handing large-sized systems and provides a flexible framework for result analysis. CABS-dock is available as a standalone application at http://biocomp.chem.uw.edu.pl/CABSdockApp/ and as a web server at: http://biocomp.chem.uw.edu.pl/CABSdock.

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