QASDOM: A META-SERVER FOR SCORING, ANALYSIS AND RANKING OF PROTEIN-PROTEIN DOCKING MODELS

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QASDOM Server (Quality ASsessment of Docking Models) is a simple and efficient tool for real-time simultaneous analysis, scoring and ranking of datasets of receptor-ligand models built by global docking techniques. Modeling with multiple servers that use different algorithms for docking results in more reliable predictions of interaction sites. However, the scoring and comparison of all models by the an expert is time-consuming and is not feasible for large volumes of data generated by such modeling. This meta-server is designed for users who need to analyze large datasets of docking models, built by different algorithms and prediction tools, in order to estimate the probability of specific residues and clusters of residues being involved in the process of receptor-ligand recognition, to rank the models by quality criteria, and to select the best model. The server allows visualizing resodies forming interaction sites in the receptor and ligand sequence, and displays three-dimensional model structures of the receptor-ligand complexes.

Each model is assigned two independent scores characterizing the quality of the model in a given set of docking models. As input data QASDOM server accepts docking models in PDB format built by the servers Hex, SwarmDock, ClusPro, Gramm-X, Zdock, as well as any other models of complexes in the PDB format, archived with zip, tar, tar.gz or without archiving. Molecules with various chemical structure can be present as a ligand and receptor in complexes, including proteins and nucleic acids. Chemical modifications are allowed as part of a receptor or a ligand. The server was used for the study of models of protein-protein complexes in [1] and [2].

Bibliography
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