Improved protein docking by predicted interface residues.

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Abstract

Scoring docking solutions is a difficult task, and many methods have been developed for this purpose. In docking, only a handful of the hundreds of thousands of models generated by docking algorithms are acceptable, causing difficulties when developing scoring functions. Today's best scoring functions can significantly increase the number of top-ranked models but still fails for most targets. Here, we examine the possibility of utilising predicted residues on a protein-protein interface to score docking models generated during the scan stage of a docking algorithm. Many methods have been developed to infer the portions of a protein surface that interact with another protein, but most have not been benchmarked using docking algorithms. Different interface prediction methods are systematically tested for scoring >300.000 low-resolution rigid-body template free docking decoys. Overall we find that BIPSPI is the best method to identify interface amino acids and score docking solutions. Further, using BIPSPI provides better docking results than state of the art scoring functions, with >12% of first ranked docking models being acceptable. Additional experiments indicated precision as a high-importance metric when estimating interface prediction quality, focusing on docking constraints production. We also discussed several limitations for the adoption of interface predictions as constraints in a docking protocol.

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