Protein-Protein Docking:

The Scoring Problem Addressed by Concepts of Information Theory

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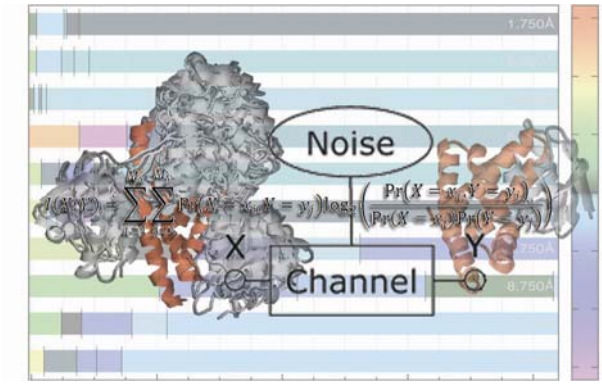
Molecular docking represents a versatile and important computational method for determining the structure of protein-protein complexes. Despite considerable efforts, a general solution to this problem is not yet within reach. One major challenge is the definition of suitable criteria for a scoring function that allows the identification of a good docking solution among many false arrangements.

Our previous work has demonstrated that concepts from information theory can actually be adapted to treat the biological problem of protein-protein docking: the concept of mutual information (MI) can be used to investigate structural features for their information content in protein docking, and the MI-values can be converted into a scoring function [1].



However, these first “proof-of-concepts” also emphasized aspects that have to be improved to result in a robust and widely applicable approach. We present here an extended MI-based approach that relies on a larger dataset and allows a more flexible treatment of structural features in the scoring function.

[1] Othersen et al. *J. Mol. Model.*, **2011**, DOI 10.1007/s00894-011-1157-6.