

## **Molecular Biotechnology Programme**

Uppsala University School of Engineering

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Title (English)

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## Alignment of protein sequences/structures and its application to predicting protein complex compositions

Title (Swedish)

Abstract

The SALIGN module of MODELLER is a newly developed general protein structure/sequence alignment tool. Described in the first half of this thesis is a web server that accesses SALIGN, to calculate pairwise and multiple alignments of the users' protein structures and/or sequences. The SALIGN server is available at http://salilab.org/salign.

The second half of this thesis presents structure-based predictions of 3,213 binary and 1,234 higher order protein complexes in *S. cerevisiae* involving 750 and 195 proteins, respectively. To generate candidate complexes, comparative models of individual proteins were built and combined together using complexes of known structure as templates. These candidate complexes were then assessed using a specialized statistical potential. Moreover, the predicted complexes were also filtered using functional annotation and sub-cellular localization data. Through integration with MODBASE, the application of the method to proteomes that are less well characterized than that of *S. cerevisiae* will contribute to expansion of the structural and functional coverage of protein interaction space.

Keywords

protein complexes, protein interaction prediction, complex structure assessment sequence alignment, structure alignment, web interface, web server

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