

Structural Bioinformatics 2002-03 Semester B

Project

Submission date August 15 2003

Flexible Sequence Order Independent Structural Alignment.

- The task is to write a program that performs flexible structural alignment of two protein molecules.
 - Alignment is sequence order independent.
 - Hinge position is unknown. Make an efficient search for a hinge. To fasten the search for a hinge position any kind of information can be applied, for example knowledge about secondary structures.
- Pay attention to the programming style. See examples from the GAMB library.
- Write a good concise description of the project and its application on “real” molecules. Do not exceed 5 pages.
- This is a contest. The best result (measured by alignment quality and program speed) will be awarded 7 bonus points in addition to the project grade.
- As in the previous assignment the project should be implemented in C/C++ and compiled under Linux.
- You should submit
 - Printed code and documentation
 - Email with directory name where the executable and the source code are and your ID number.
- A meeting and oral exam on the project and background material related to it will be scheduled individually after the submission.
- Additional comments will be sent to the listserver.
- References:
 1. Wolfson, H. J., Generalizing the Generalized Hough Transform, Pattern Recognition Letters, vol. 12(9), pp. 565 - 573, (1991).
 2. Verbitsky, G., Nussinov, R., and Wolfson, H.J., Structural Comparison Allowing Hinge Bending, Swiveling Motions, PROTEINS, vol. 34, pp. 232–254, (1999).