Nov. 30. 2010

Addendum to GST Uebung “Protein Structure Classification”

1. Introduction

Since the SSAP webserver was broken last week, we had to use different structure alignment servers for this Uebung. Substitute these instructions for the ones concerning SSAP. The rest of the Uebung is unaffected by this change.

2. DALI lite

Go to http://www.ebi.ac.uk/Tools/dalilite/index.html. There, you can specify PDB IDs (e.g. 1gxw and 1i1i) for the two structures you are trying to align. Optionally, you can specify certain chains you would like to compare. A few minutes after submitting your query, you are presented with a results page. The table at the top of this page summarizes the input parameters for this alignment. The table in the section “Results of Structure Comparison” contains the results. The link in the “Structural Alignment” column gives you the alignment. As with the SSAP server, you should be able to see that only the second half of 1gxw has been aligned to 1i1i.

The superimposed structures can be downloaded via the links in the final column of the table. Since the second molecule is placed on top of the first one, it is sufficient to download the second molecule (mol2_1.pdb). In order to view the superimposed coordinates of the two proteins, you need to open both the original structure (1gxw) and the file you downloaded (mol2_1.pdb) in chimera. You can download the coordinates for the first molecule as well (mol1_original.pdb), but since that structure is unchanged, the file is identical to 1gxw.pdb. Therefore, downloading the same coordinates again is redundant.

3. CE align

If you chose to use http://cl.sdsc.edu/ce/ce_align.html, you can also specify the PDB IDs of the structures you would like to align. A after submitting the alignment job, you are once again presented with a results page. Here, the resulting alignment is in the center of the page. The alignment scores are at the top of the page. You can download the superimposed coordinates through the link below the alignment. In this case, both proteins are in the same file. When you download the coordinates, give them a meaningful name and change the file name extension from “.txt” to “.pdb”. The alignment is slightly worse than DALI, but it should still lead you to the same conclusions.

Since both structures are in the same file, chimera will give them the same color. To be able to distinguish them use the command `color blue :.A` to give one of them a different color.