BCBP4870 Protein Structure Determination

Term Projects 2011

Several protein structures have been determined independently by solution NMR and Xray crystallography. By comparing the same protein solved in the crystalline state and in solution, we can answer some questions about the nature of protein in the aqueous and the crystalline state, and we can answer questions about the strengths and weaknesses of the two methods.

Study two structures

Select a protein whose structure has been solved by both methods. The sequence should be identical or nearly identical in the NMR structure and the crystal structure. Submit your choice for approval by sending us the PDB codes for both.

Use NCBI and RCSB to identify a protein to study.
http://www.ncbi.nlm.nih.gov/
http://www.rcsb.org/
In NCBI search the "structure" database.

Use the CE server to align two PDB structures in 3D.
http://cl.sdsc.edu/ce/ce_align.html
Upload two files, the Xray structure and the NMR structure. (Make sure each file contains only one copy of the protein.)

Use RasMol and/or DeepView to study the structural differences:
http://www.openrasmol.org/doc/
http://ca.expasy.org/spdbv/

Report your findings

For the crystal structure, report the vital statistics: resolution, completeness, number of molecules in the asu, average B-factor, number of waters, R-factor and free R-factor.

For the NMR structure, report the number of structures determined in the NMR structural ensemble, RMSD of the backbone and heavy atoms, Ramanchandran statistics, statistics of NOE, dihedral, hydrogen bond and RDC (if used) constraints. Identify the strategy for isotope labeling for the production of NMR samples.

Find places in the structure where there are differences. Are they near crystal contacts? (You can use DeepView to view crystal contacts). How accurate or precise is the structure in the variable regions? How many NMR distance constraints? How high are the B-factors? Are the differences real? Or are they possible errors? What could have caused the errors? What could have caused the real differences?

Comment on how the two methods provided complementary information about the structure.

Detailed Requirement for Class Project (required for every group):

1. In teams of two.
2. Topic. Choose a protein whose 3D structure has been determined by both X-ray and solution NMR. Compare their structural differences and the functional relevance of such differences. Explore the origin of such differences in methodology.
3. The proposal for the project should include:
    a. Names of the team members.
    b. The title, journal, volume and pages number of the paper describing the X-ray structure and the corresponding pdb code.
    c. The title, journal, volume and pages number of the paper describing the solution NMR structure and the corresponding pdb code.
4. Deadline for proposal Nov. 18th, Thursday. Email submission to both wangc5@rpi.edu and bystrc@rpi.edu is required before or on the Nov. 18th.
5. Due Dec. 6th, Monday. Email slides (PDF or Powerpoint) to both wangc5@rpi.edu and bystrc@rpi.edu before or on Dec. 6^{5h}.

Detailed Requirement for Presentation (required for all students):

1. In teams of two.
2. The presentation will be 15 minutes talk + 5 minutes of Q & A.
3. The powerpoint presentation will include at least 1 slide/minute of talk.
4. Each student is required to ask at least one question and will be graded for the quantity and quality of the questions asked.
5. The presentation of class projects will be held on Dec. 5, Monday and Dec. 8, Thursday.