Protein Interactions: Computational Techniques

Assignment - 1

Corse: BT6320   **Marks: 10**

Questions

1. Get the statistics for the protein-protein complexes from RCSB PDB.
   a. No. of homo and hetero dimers
   b. No. of trimers
   c. No. of tetramers
2. Find a hetero dimer complex from RCSB PDB. (Enter the PDB ID in the excel sheet)
3. Briefly describe the structure and function(s) of the selected complex.
4. Identify the binding site and interaction types using PDB Sum and PDB Param
5. Check the availability of the hetero dimer complex in other databases and provide details of the same.
6. Construct an interaction network for each protein in the hetero dimer complex using STRING. Write your observations.
7. Obtain the thermodynamic information for the selected hetero dimer complex.
8. Identify the binding sites in the hetero dimer complex using
   a. ASA based method
   b. Distance based method
9. Calculate the propensity of the binding site residues (use results from question 8)
10. Identify the top 5 interacting pairs in the hetero dimer complex.
11. Calculate the following for the hetero dimer complex
    a. Binding free energy
    b. Change in binding free energy upon mutation

12. Predict the structure for the given protein-protein complex. Write your observations.

>Subunit1

SGEVQLLESGGGLVQAGGSLRLSCAASDRTFSSYAVGWFRQAPGREREFVAATSWRGDSTYYADSVKGRFTISR
DNAKNTVHLQMNSLKPEDTAVYYCAAKWGPVPTNSVMNYYTREYDYWGQGTQVTVSS

>Subunit2

SGMVSKGEEDNMASLPATHELHIFGSINGVDFDMVGQGTGNPNDGYEELNLKSTKGDLQFSPWILVPHIGYGFH
QYLPYPDGMSPFQAAMVDGSGYQVHRTMQFEDGASLTVNYRYTYEGSHIKGEAQVKGTGFPADGPVMTNSLTAA
DWCRSKKTYPNDKTIISTFKWSYTTGNGKRYRSTARTTYTFAKPMAANYLKNQPMYVFRKTELKHSKTELNFKE
WQKAFTDVMGMDELYK

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