Protein Interactions: Computational Techniques
Assignment - 1 (Part B)

Course: BT6320
Questions

1. Consider the protein-protein complex, human growth hormone receptor-human growth hormone (HGH) analyze the following:
    a. Find the complex structure and functional importance from PDB
    b. What is the structural type of the complex (homo/hetero/dimer/trimer etc.)
    c. Obtain binding affinity data for the complex from **SKEMPI**, **PROXiMATE** and **PDBBind** database
    d. Access **PROXiMATE** database and check the number of mutations for the complex with experimentally known binding free energy (ΔΔG).
    e. Identify the mutation, which has the most favorable (highest negative value) and last favorable (highest positive energy value) binding energy
    f. Group the mutations into (i) nonpolar to nonpolar, (ii) nonpolar to polar and (iii) polar to polar and obtain average binding energy [nonpolar: A, C, F, G, I, L, M, V, W, Y]
    g. Obtain the average binding energy at different secondary structures of the mutant, helix, strand and coil
    h. Repeat the same for different ranges of relative ASA, 0-2%, 2-50%, >50%
    i. Identify the binding site residues (interface) using distance based criterion (**use PDBparam**) using a cut off of 5A
    j. Identify the binding site residues (interface) using ASA based criterion (use **GETAREA or DSSP** for ASA values).
    k. Check the common interface residues listed in PDBsum, distance and ASA based criteria
    l. Compute the reduction in accessibility upon complex formation: ASA of HGH, HGH receptor, complex and difference using GETAREA

        Difference =[ASA (HGH) + ASA (HGH receptor)] - ASA (complex)

2. Find the protein–protein interactions in the IntAct **database** for SARS-CoV-2 obtained with ITC.

3. Using the **AbCov database** (https://web.iitm.ac.in/bioinfo2/ab-cov/), for the monoclonal antibody 2B04, find the IC50 value. Find whether it is a neutralizing antibody or not and the source of the antibody.