Dr. Ratna Singh

MAPPING CONSERVED RESIDUES ON THE STRUCTURE

Conserved residues on your generated structure

Two options

1)) map conserved residues based on server generated MSA alignment

2) provide you own MSA alignment file for mapping conserved residues

Consurf http://consurf.tau.ac.il/ → amino acids → Is there any protein structure known →yes → enter pdb code (e.g 2IW0.pdb) → chain identifier select "A"→MSA file to upload YES/NO → In case of " YES" → mention the query sequence name e.g 2IWO (exactly same name of query sequence as in alignment file) → tree file to upload NO

Wait for the results

Final results→

1) For MSA sequence (color code conserved residue in alignment file)

Multiple Sequence Alignment Color-Coded by Conservation → Amino Acid Conservation Scores, Confidence Intervals and Conservation Colors

2) Structure (conserved residues on structure)

Go to create high resolution figures → Follow the instructions to produce a PyMol figure (For users of PyMol)

Download → PDB_FILE hiding Insufficient Data → Download the file consurf_new.py.

Open pymol→ load downloaded pdb file

Pymol → file → run →consurf_new.py. (change the representation according to you)