**Modelling membrane and transmembrane protein in computer**

1. Use ‘input generator’ panel to access ‘membrane builder’. Use ‘bilayer builder’ there Prepare a system of 128-copy DOPC lipid bilayer (64 in each leaflet) with a water thickness of 22.5 Angstrom along Z… Visualise the structure and Generate gromacs formatted files. Use ‘membrane-only’ option

2. Prepare a system of 128-copy DOPC lipid + 15 % cholesterol… Visualise the structure and generate gromacs formatted files. ‘Use membrane-only’ option.

3. Finally place a truncated part (12-residue) of short peptide called WALP19 (pdb id: 2LCN) in the water phase of DOPC bilayer. Use ‘membrane/protein’ option. Use ‘orientation’ and ‘translate’ option.

Due to compute-intensive nature, only few set of MD simulations will be run at a time. So, please coordinate among each other and run the simulation in class one person at a time.