

AIM: To find polar interactions after protein-protein docking

The protocol for protein-protein modeling in order **to find the interactions between engineered Encapsulin and protein biomarker MMP9** is as follows -

Docked Structures are retrieved from [ClusPro](#) -

Receptor protein (*Orange*) - Engineered Encapsulin

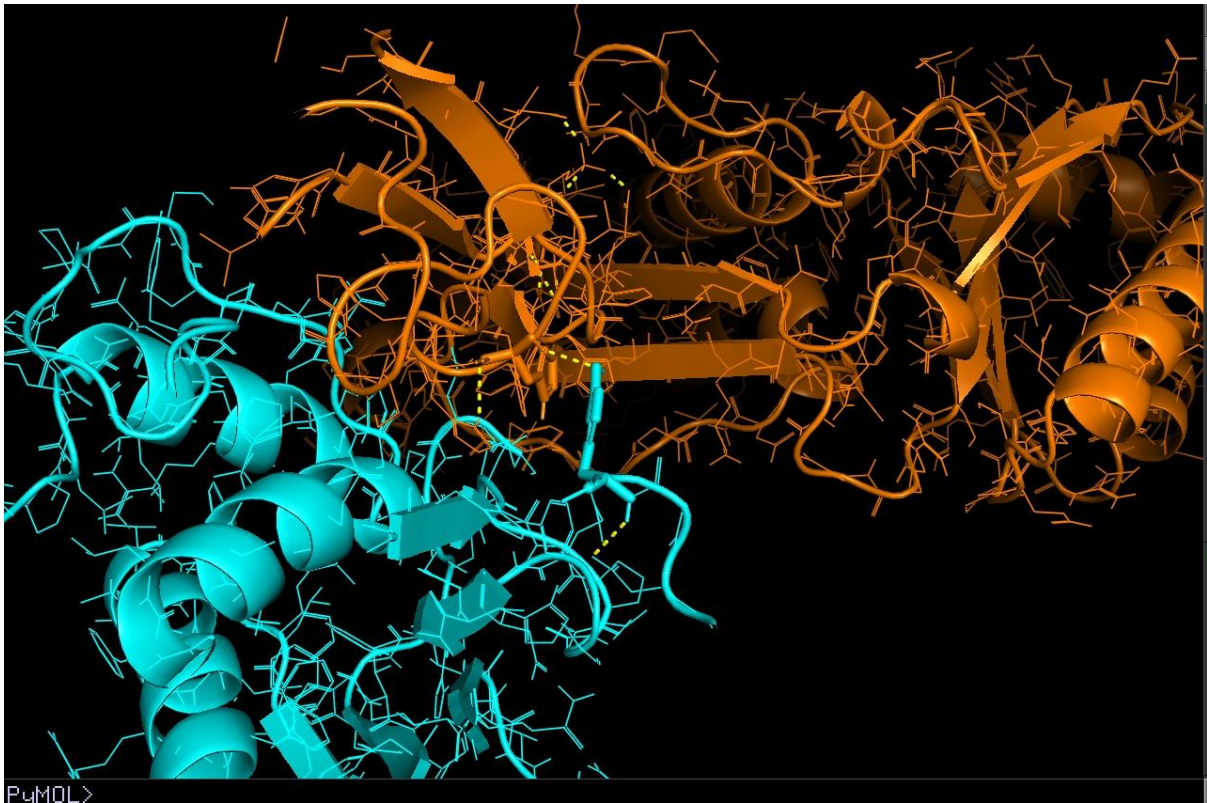
Ligand (*Cyan*) - MMP9 Catalytic Domain

Modelling tool - [PyMol](#)

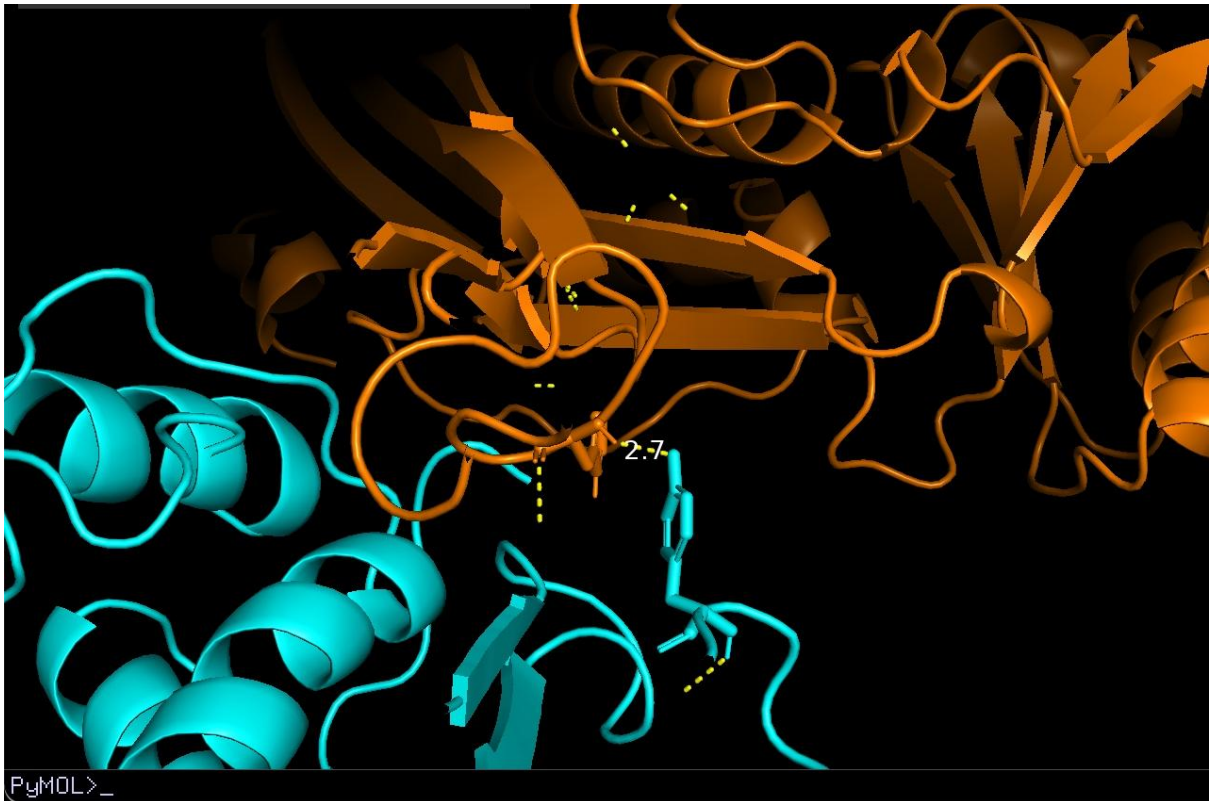
- Select interface residues on receptor → Rename to polar residues



- Choose Action → Find → Polar Contacts → To any atoms
- Choose receptor and ligand individually and choose to 'Show Lines'



- By eyeballing, select the polar interactions (can see in yellow in above diagram)  
→ Rename to ‘interface residues’
- Hide the lines in both receptor and ligand
- Now select the interface residue selection and choose ‘Show sticks’ (‘interface residues’)
- Now repeat the second step of protocol, but for ‘interface residues’: Action → Find → Polar Contacts → To any atoms
- Lastly, to quantify the interactions go to Wizard → Measurement → Select ‘Merge With Previous’



This will help in quantifying the number and distance of the polar contacts between the two proteins. As you can see, the distance between the two polar contacts is 2.7 Angstroms.