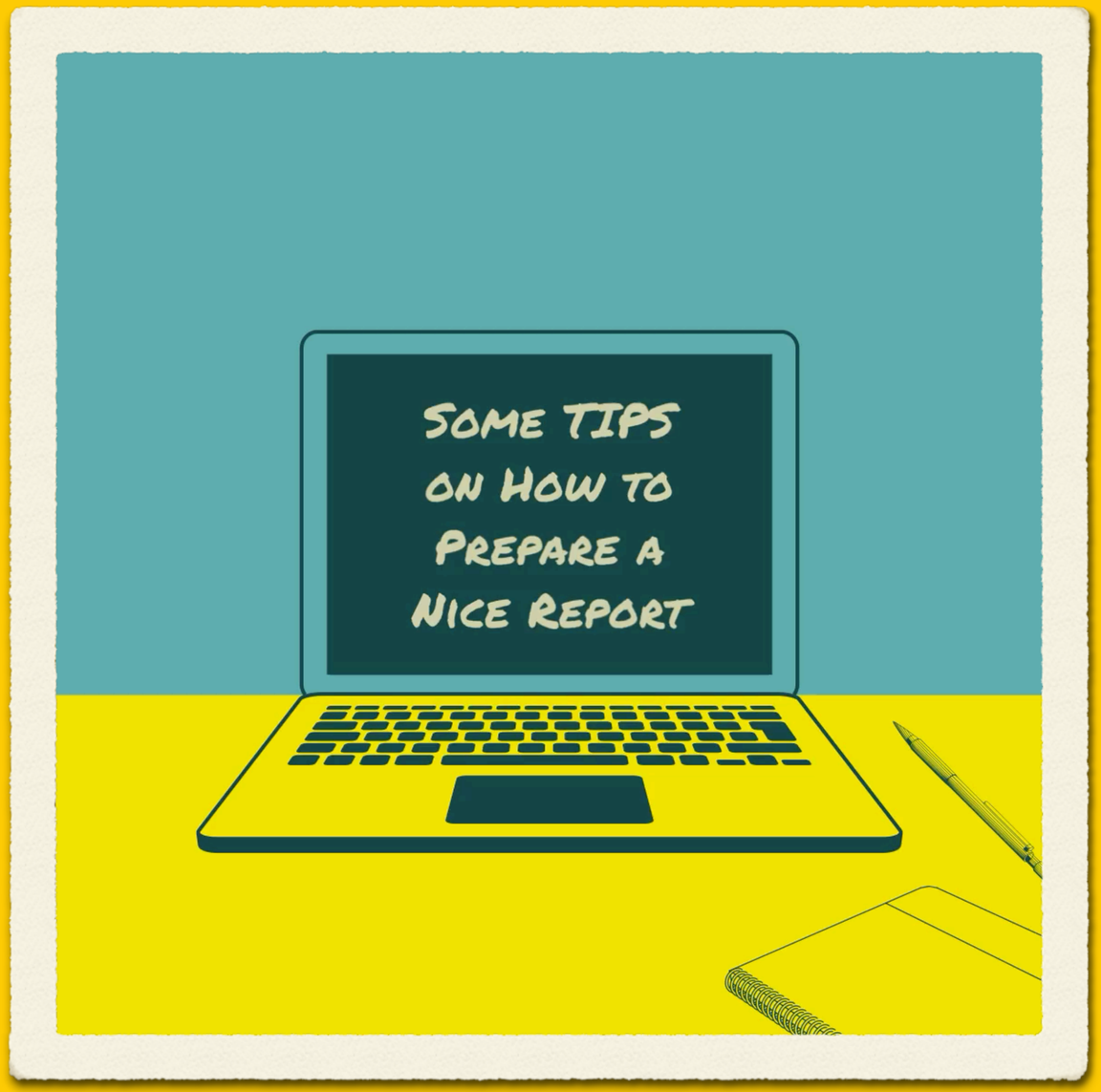
BIOMODELING



MOLECULAR MODELING SECTION (MMS)

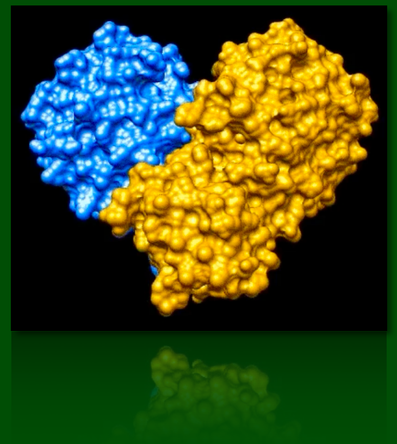
UNIVERSITÀ DEGLI STUDI DI PADOVA

MAHDI HASSANKALHORI

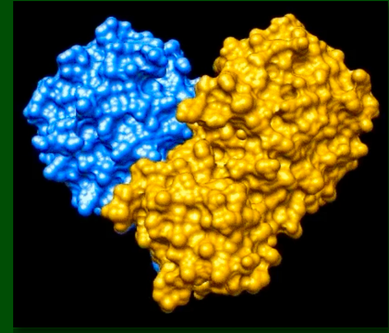
INTRODUCTION

- Comprised of a brief and concise introduction of each protein chain you have in your assigned protein complex PDB file

- Mostly information from biological point of view and physiological roles of each protein and their classification retrieved from papers

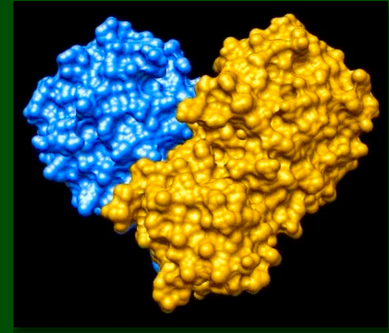


Protein complex characterization



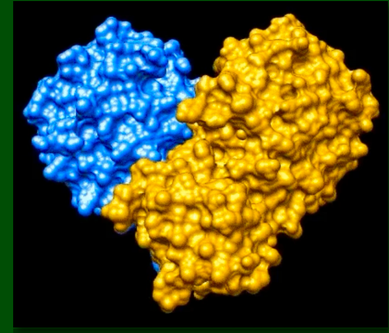
- Title of your assigned PDB, ID, resolution, protein classification and origin
- Important info on the complex from exploring PDB website, and PDB file itself; e.g. number of unique chains, global stoichiometry
- Mentioning present co-crystallized elements such as small molecules, ions and some info about their role in the complex, important interactions with protein chains

Sequence Analysis



- Resulted data from Chimera analysis on the sequence of each unique protein chain: Number of residues, Gap regions, Secondary structure profile

Interaction interface characterization

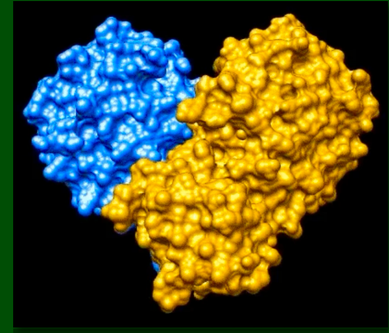


Interface Hydrogen bonds (H-bond) detection

- Brief report of Chimera H-bond calculation

- Discuss on important detected H-bonds with the interacting residues of each chain and relative comparison of the crucial ones in terms of their contribution to the complex free energy and geometrical stabilization based on the H-bond length and position

Interaction interface characterization

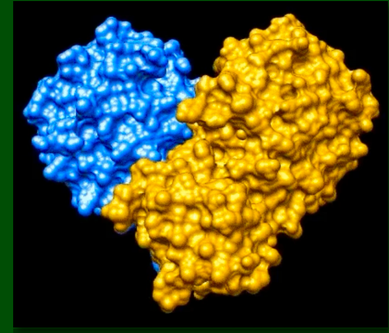


CONTACTS

- Brief report of Chimera contacts calculation

- Scrutinize on the probable hot spot residues with multiple contact sites in each interacting protein chain and their counter-interacting residues in the other chain

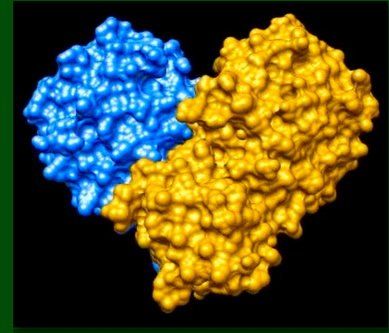
Interaction interface characterization



Clash Points

- Brief report on the sites of clashing points in the complex, if any; the involved residues, the distance

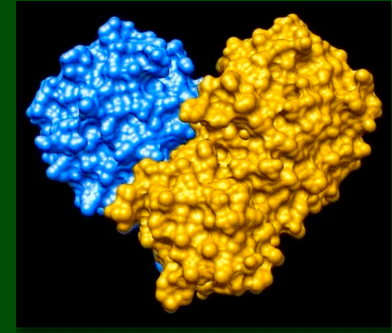
Interaction interface characterization



Surface analysis

- Discuss major surface observations on the interface upon each type of surface representation, i.e. Coulombic, Hydrophobic potential surfaces considering the steric complementarity at the same time; to draw some points on interaction regions of each type and involved residues of essence for the protein-protein recognition and complex formation

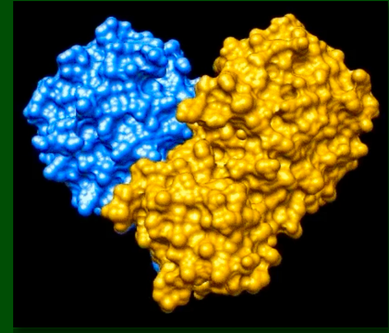
Further analysis



- Further findings from web-based tools; brief intro of the utilized tool and the protocol plus the report of the important findings and the type of information you obtained there, as well as comparison of the resulting data and try to relate with relevant insights inspired by your investigations via Chimera; e.g. hotspot residues

- ANCHOR, and PRODIGY, to name but two; Be curious and try to find more tools that could help you have a better understanding and a more precise analysis of the complex interaction

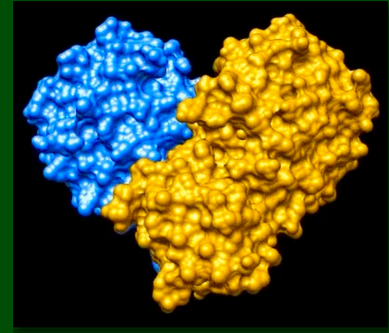
Role of protein-protein recognition and complex formation



- What physiological or pathological events would happen upon recognition and complex formation of the protein chains of interest, and so the complex physiological or pathological role

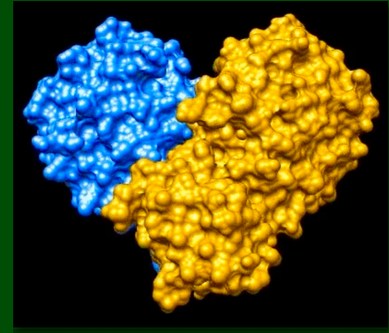
- A concise summary of this kind of data implied from your studies on papers

Mutational speculation



- Some mutational speculations credits from considering their predicted contribution to the binding free energy by ANCHOR web-based tool, the surface and interaction analyses done and represented via Chimera; Hotspots
- “Disrupt” mutations
- “Conservative” mutations based on their similar biochemical properties, charge, hydrophobicity and size with the wild-type residue
- Mentioning the point of mutation residue and the mutant residue e.g. F94A; their supposed effects on the interface interactions (how?) and complex affinity

Protein-Protein interaction Inhibitor

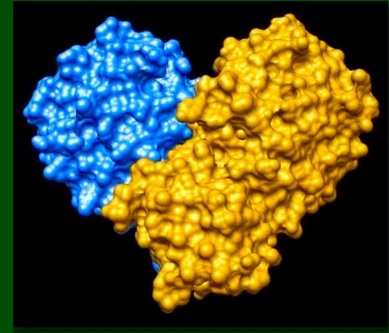


- Discuss if a protein-protein interaction inhibitor of the protein complex can be imagined and designed to be of therapeutic effects

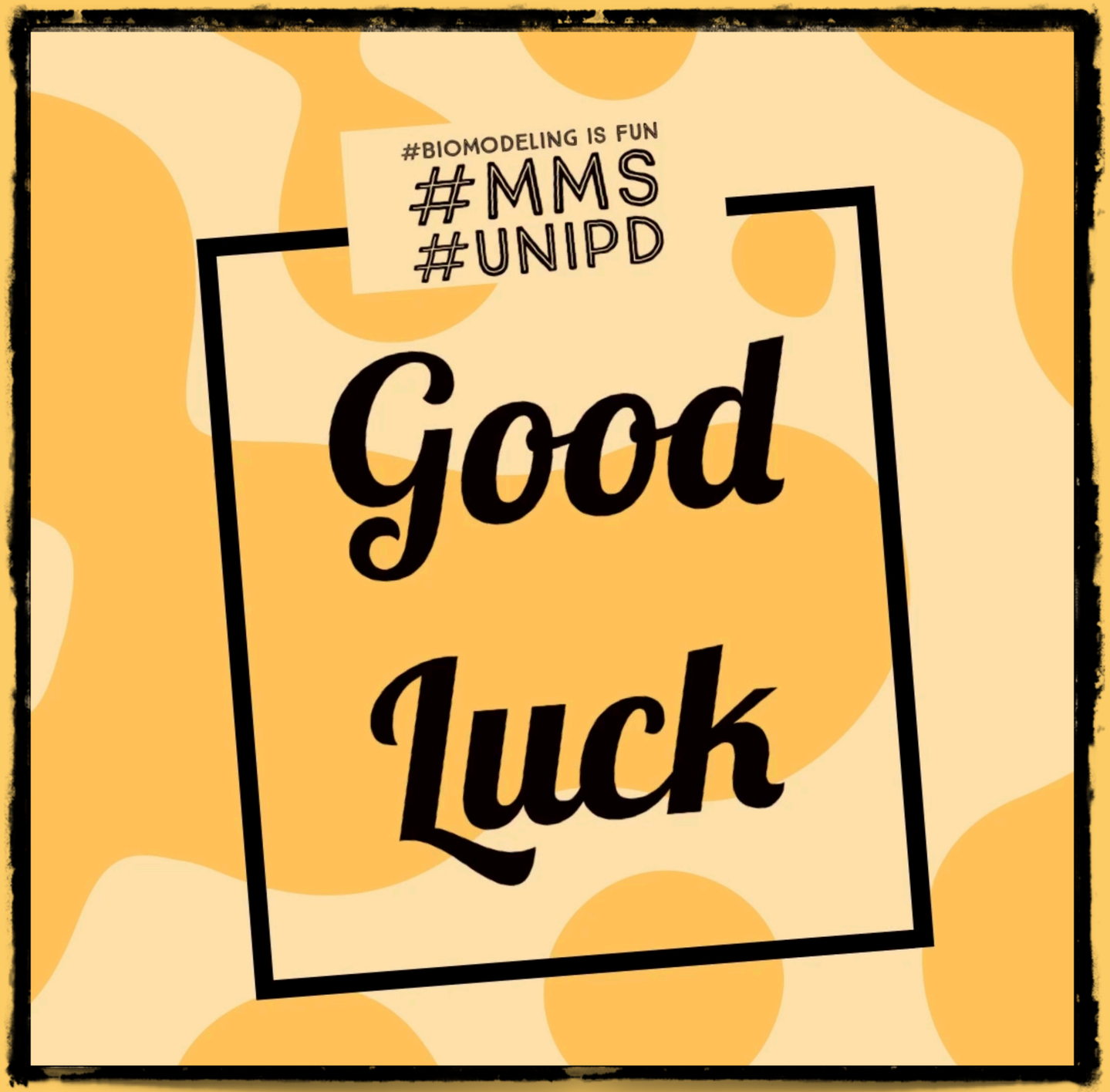
- What would be the importance of having such an Inhibitor

- Which protein chain is better to be the target of the suggested inhibitor to have the desired therapeutic effects

The list of References and the Figures



- References to the studied papers, the utilized tools and softwares
- Captured representations of the data generated via Chimera, or other tools along with a clear caption describing what exactly can be seen and inferred by the very figure
- Only include informative figures supporting your statements and findings and not just any random figure


#BIOMODELING IS FUN
#MMS
#UNIPD
Good
Luck