EXPERIMENT 9: INTERACTION ANALYSIS

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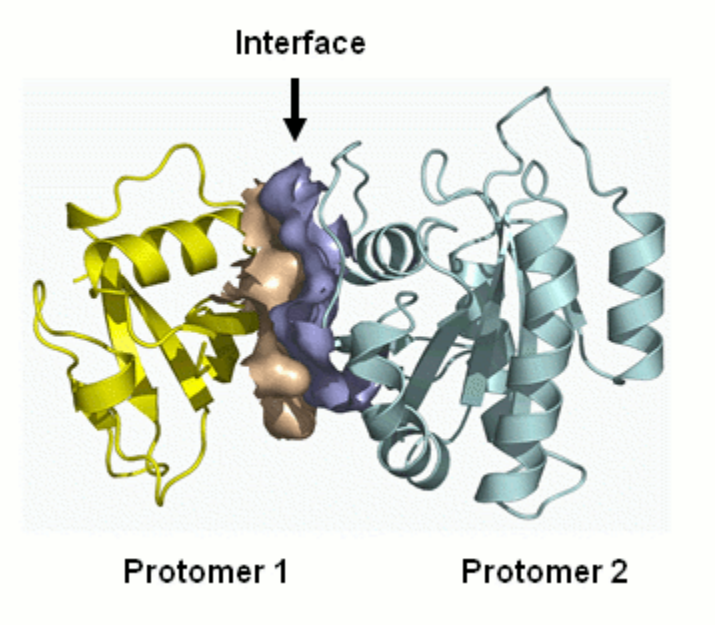
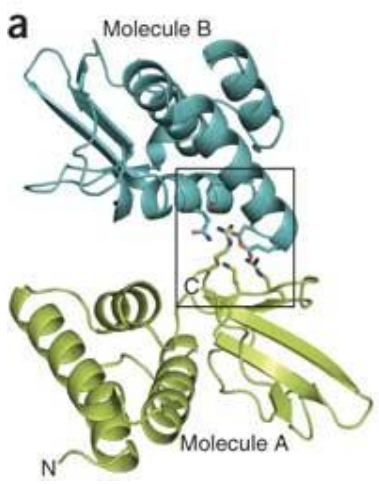
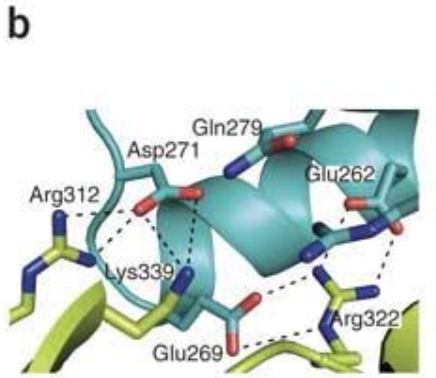
SUSTC

Protein-protein interaction





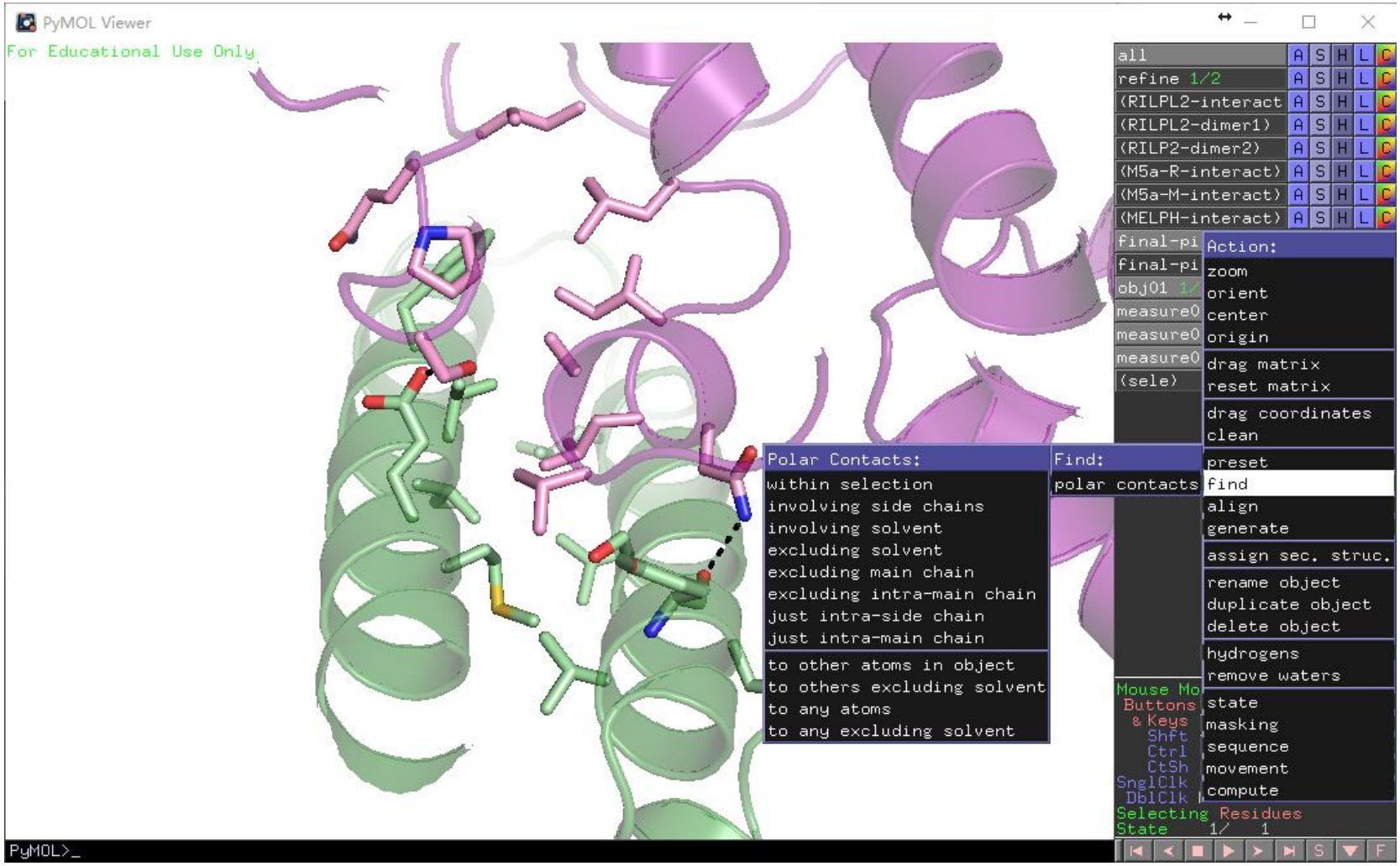


Methods

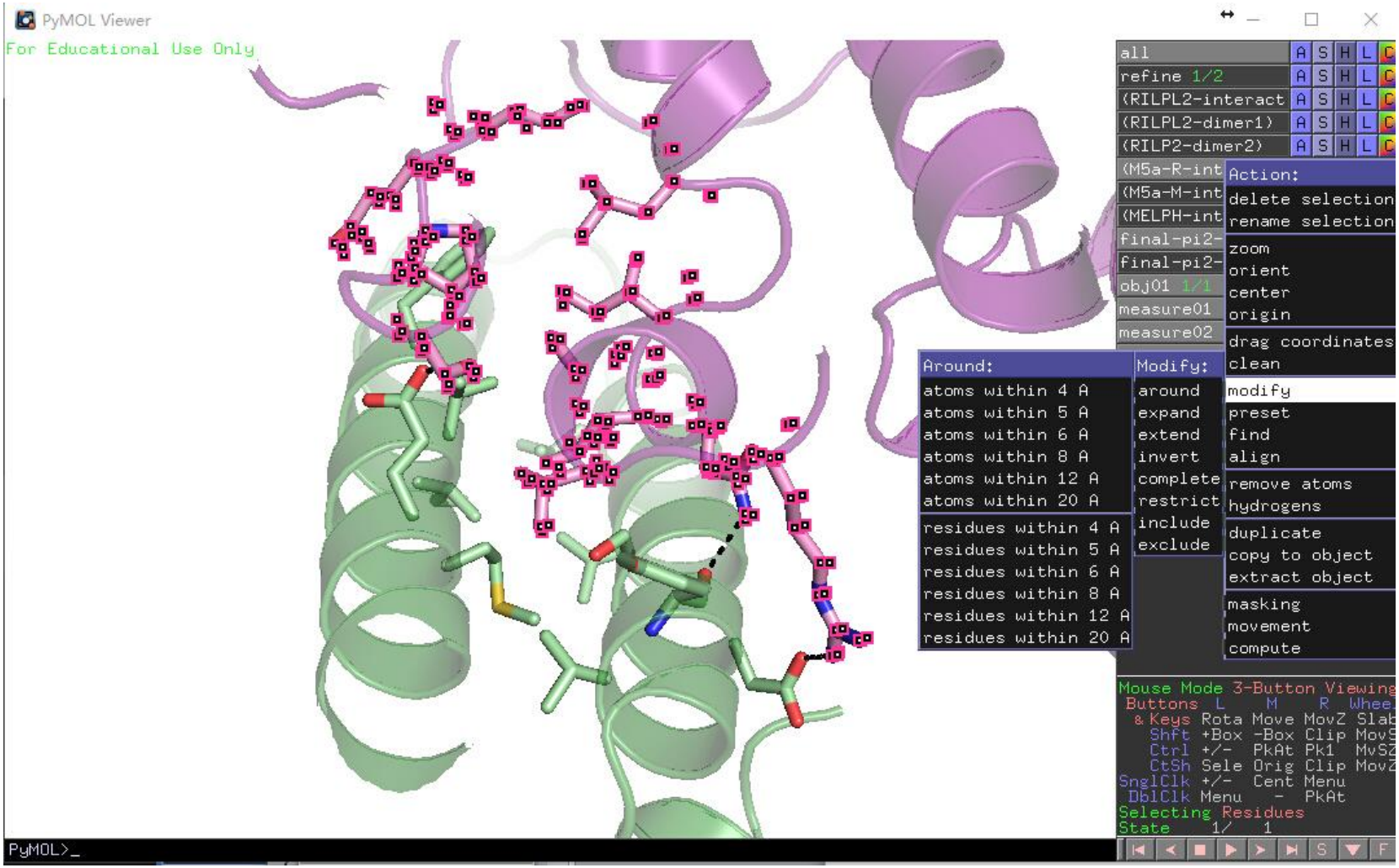
- Quaternary structure analysis
  - Assembly prediction
- Interface analysis
  - Identification of interfaces
  - Calculation of buried area
  - Interface residues

初步的

Preliminary interaction analysis in PyMOL



Preliminary interaction analysis in PyMOL



Automatic interface identification

- The “InterfaceResidues” script in PyMOL
- http://www.pymolwiki.org/index.php/InterfaceResidues

PISA (Proteins, Interfaces, Structures and Assemblies)

- http://www.ebi.ac.uk/msd-srv/prot_int/pistart.html
- Structural and chemical properties of macromolecular surfaces and interfaces
- Probable quaternary structures (assemblies), their structural and chemical properties and probable dissociation pattern
- CCP4 PISA
  - http://www.pymolwiki.org/index.php/Ccp4_pisa
  - Incorporating PISA results into PyMOL

Tasks

1. Open human hemoglobin structure (PDB id: 2HHB) in PyMOL
2. Analyze the interfaces between alpha- and beta-subunit manually in PyMOL
   - Polar interaction
   - Hydrophobic interaction
3. Use “InterfaceResidues” in PyMOL to calculate the interfaces
   - Compare with your own analysis, which one gives better result?
4. Use PISA server to calculate the assembly and interfaces in human hemoglobin
   - Compare the results with those in previous two steps
5. Present the PISA results in PyMOL

Lab report format

- Title
- Your name and student No.
- Introduction
- Methods
- Results
- Conclusions