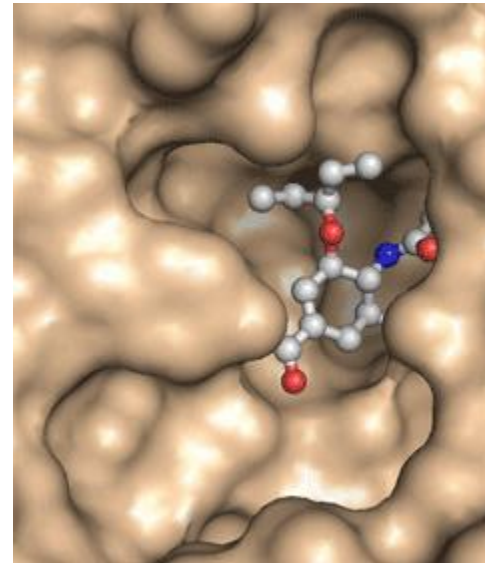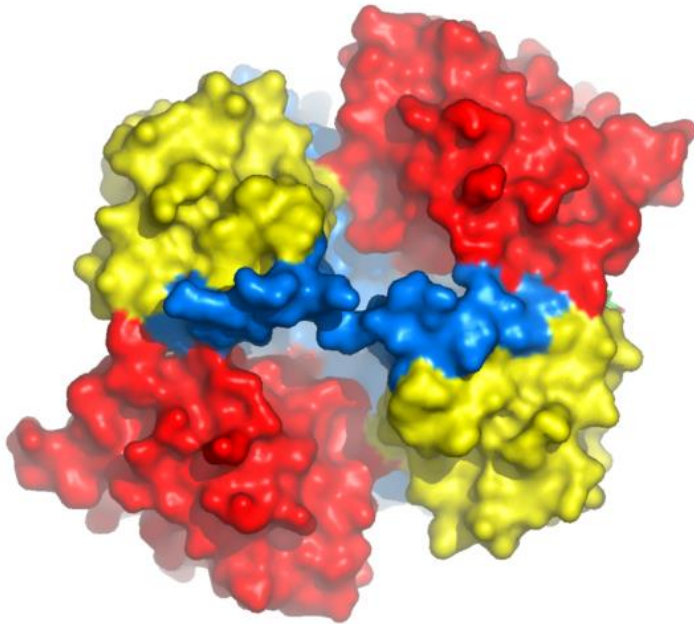# EXPERIMENT 6: SURFACE ANALYSIS
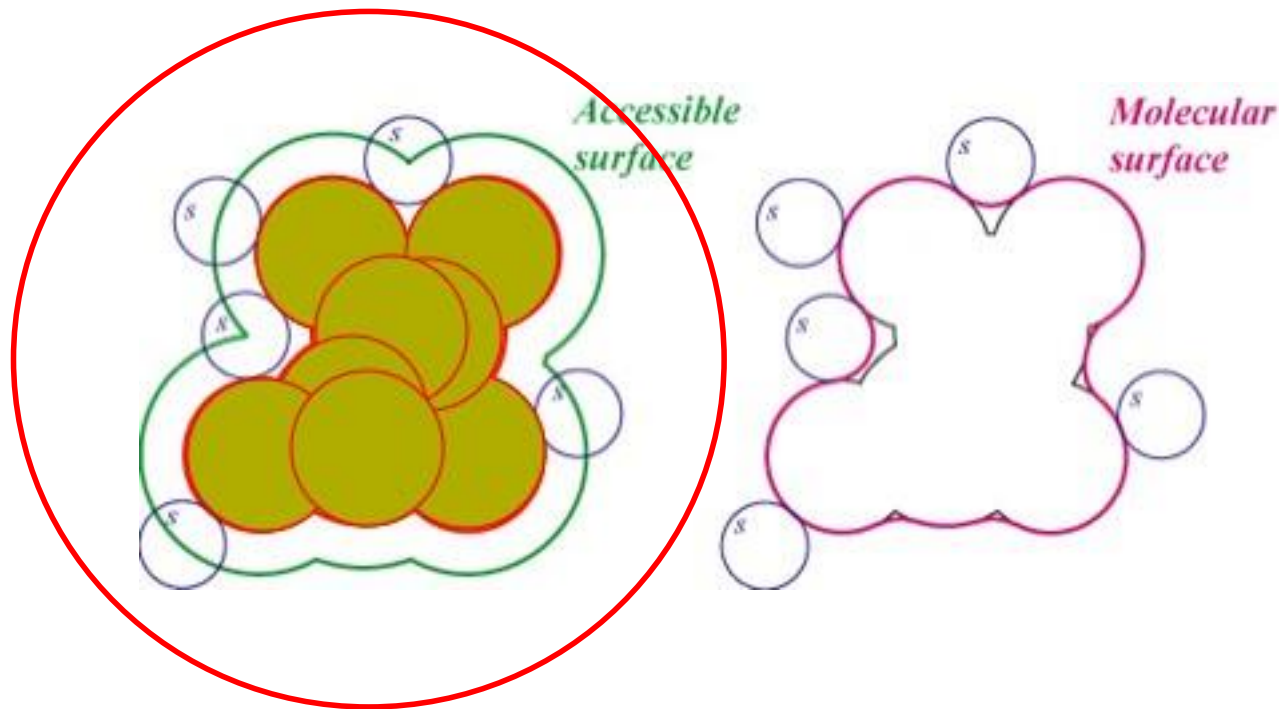
Dr. Zhiyi Wei

SUSTC

Protein surface

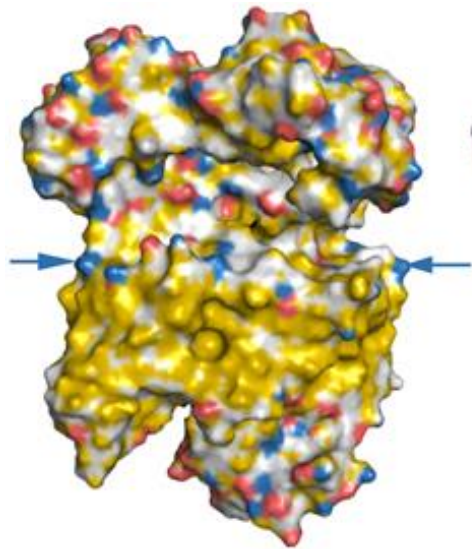# Accessible surface and molecular surface

Methods

- "Surface" in PyMOL
  - http://pymolwiki.org/index.php/Surface
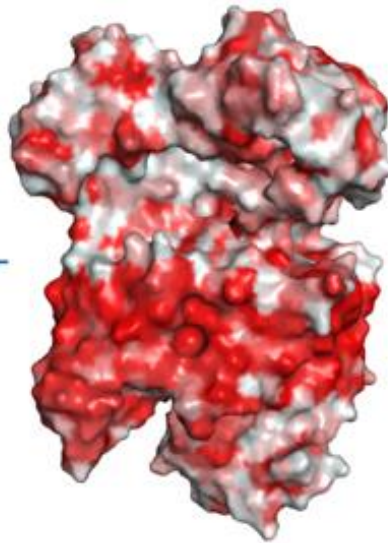- Settings
  - Transparency
  - Quality
  - Probe radius
- Colorings of different properties
  - Conservation
  - Hydrophobicity
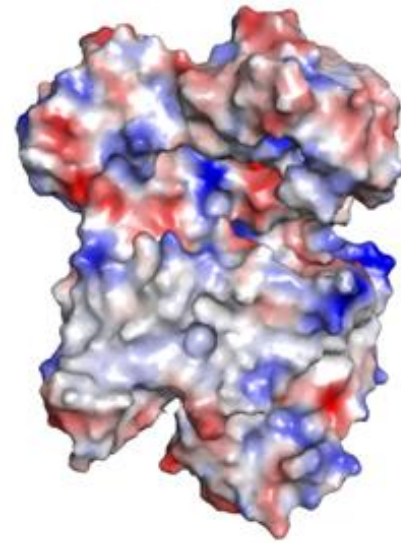 - Electrostatic potential
  - …

Colorings of different properties
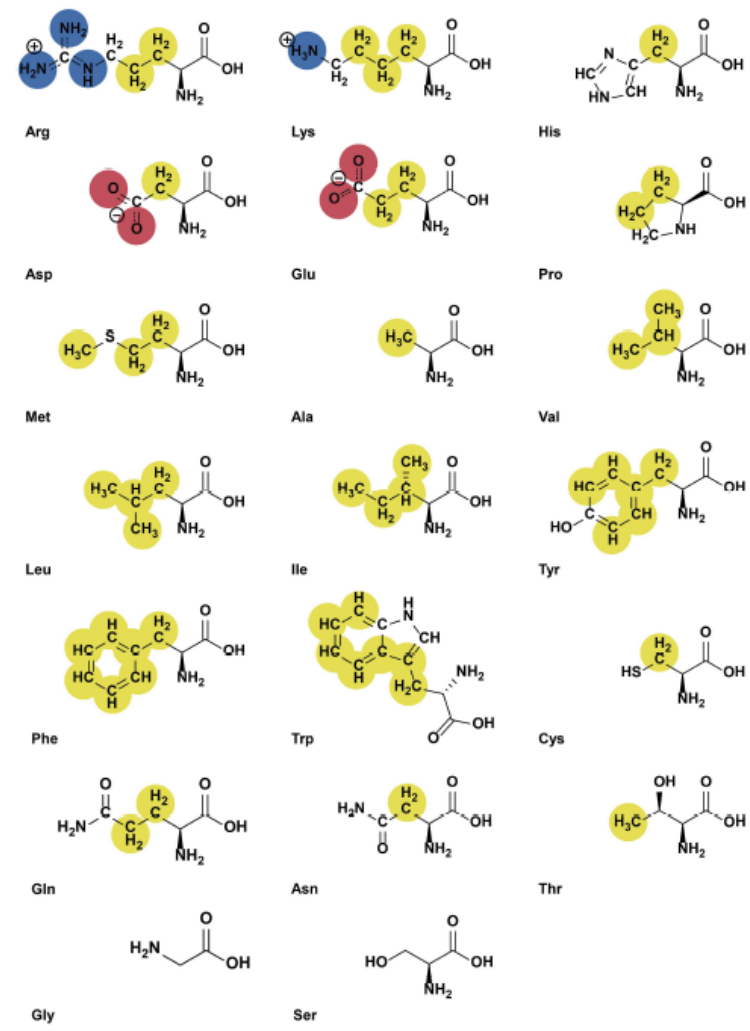

Hydrophobicity   Conservation   Electrostatic potential

Color settings for presenting hydrophobicity

Color settings for presenting conservation

- Based on multi-sequence alignment

- Identical residues (dark red)

- Highly similar residues (red)

- Similar residues (light red)

- Dissimilar residues (white)

Color settings for presenting electrostatic potential

- Positive charge (blue)

- Negative charge (red)

- Macromolecular electrostatics calculation

  - Simple calculation (assume vacuum environment) by PyMOL

  - APBS (http://www.pymolwiki.org/index.php/APBS)

    - Involving solvent

    - More accurate

Tasks

1. Open human hemoglobin structure (PDB id: 4HHB) in PyMOL
2. Create new objects containing beta-subunit
3. Separate the protein and the heme group into two objects
4. Generate the surfaces to display the two different properties of the protein
   - Hydrophobicity
     - Which parts of surface are more hydrophobic? Why?
   - Conservation
     - Which parts of surface are conserved? Why?
5. Generate the electrostatic potential surfaces for the tetrameric hemoglobin
   - Where is the positive charged pocket for allosteric effector (2,3-BPG) binding?
6. Use the APBS program to calculate the electrostatic potential surface (Do it @home)
   - Compare the APBS surface with the one generated by simple calculation
7. Analyze the sickle-cell mutation (E6V)
   - How this mutation affect the protein surface properties?

Lab report format

- Title

- Your name and student No.

- Introduction

- Methods

- Results

- Conclusions