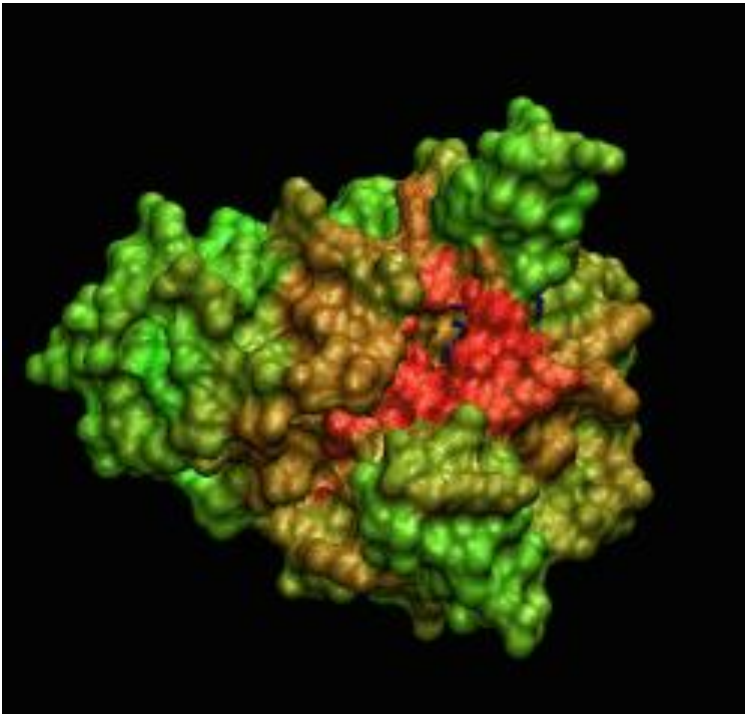# EXPERIMENT 7:
IDENTIFICATION OF FUNCTIONAL SITES

**Dr. Zhiyi Wei**

SUSTC

Methods

- Sequence based analysis
  - Sequence profiling
  - Sequence motif search
- **Structure based analysis**
  - Structural comparison
    - Identify structural motif
  - Surface property analysis
    - Conservation
    - Hydrophobicity
    - Electrostatic potential
    - Surface geometry
- Combination of sequence and structure

Surface geometry

- Concavity
- Tunnel

Cavity and Tunnel Detection

CASTp   MolAxis
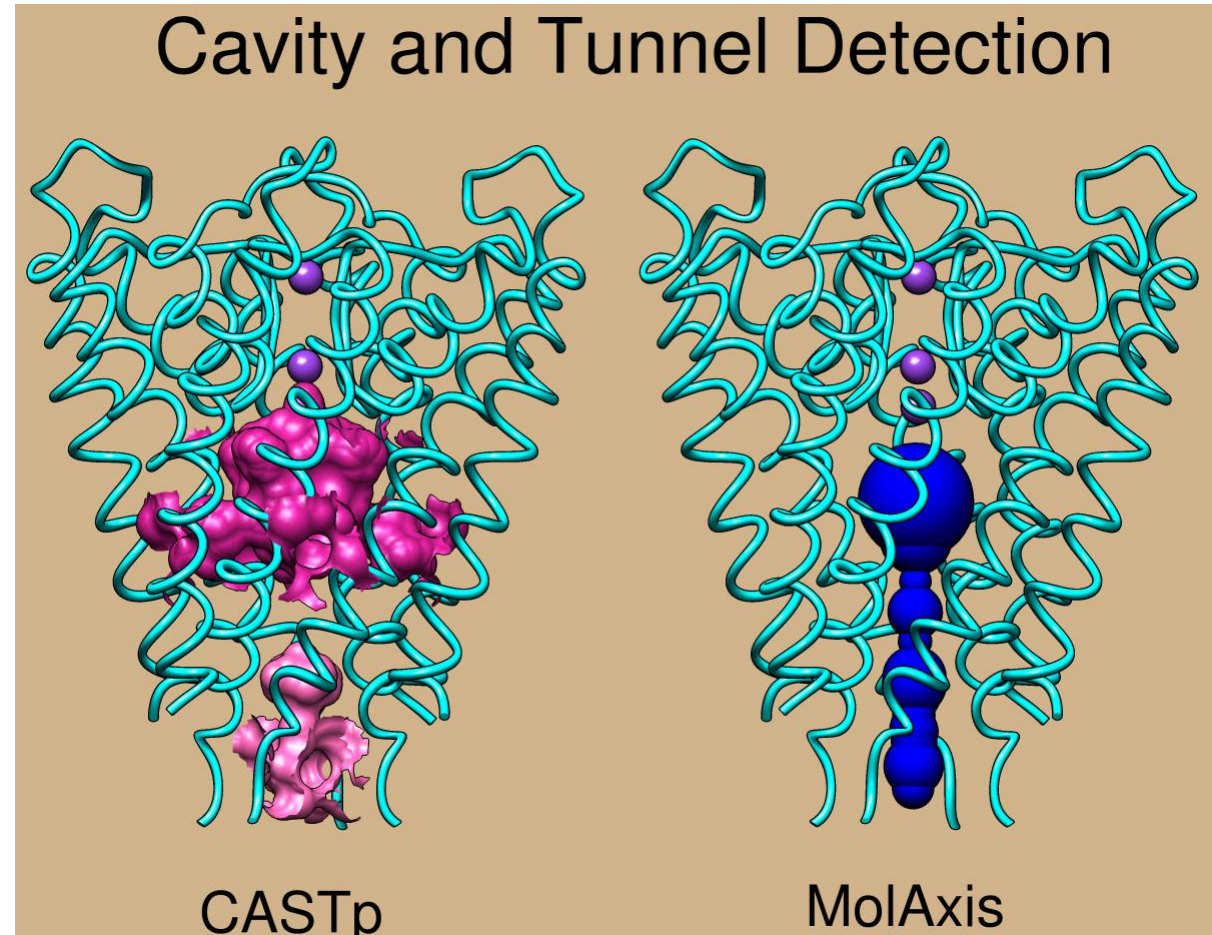
Tasks

1. Open human hemoglobin structure with 2,3-BPG bound (PDB id: 1B86) in PyMOL

2. Base on your previous surface property analysis, explain following questions

    • What is the Heme group binding environment, why?

    • What is the 2,3-BPG molecule binding environment, why?

    • Why does the sickle-cell mutation (E6V) lead to filament assembly?

3. Use POCASA server to predict pockets in 1B86

    • http://altair.sci.hokudai.ac.jp/g6/Research/POCASA_e.html

4. Use CAVER to predict tunnel in potassium channel (PDB id: 1BL8) @home

    • http://www.caver.cz/index.php?sid=121

Lab report format

- Title

- Your name and student No.

- Introduction

- Methods

- Results

- Conclusions