EXPERIMENT 10: INTERACTION ANALYSIS 2

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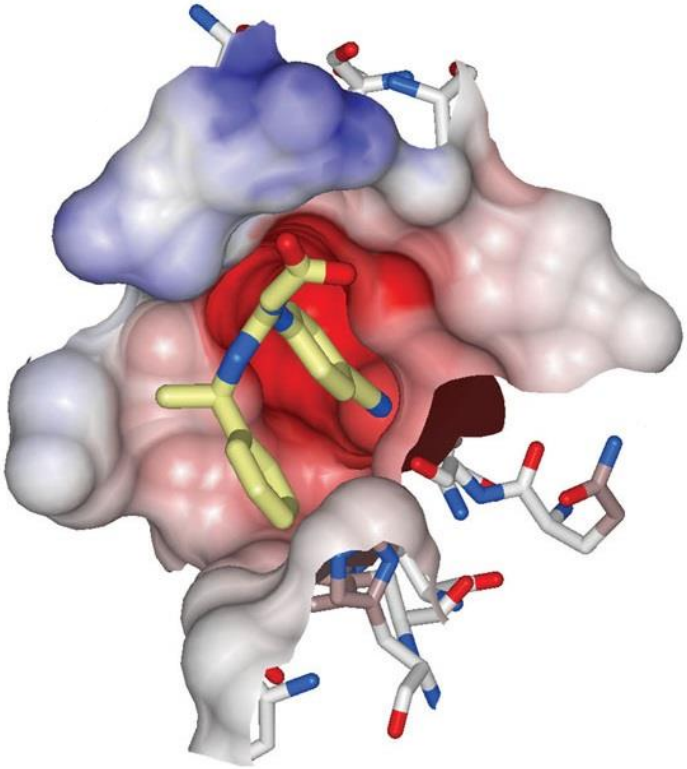
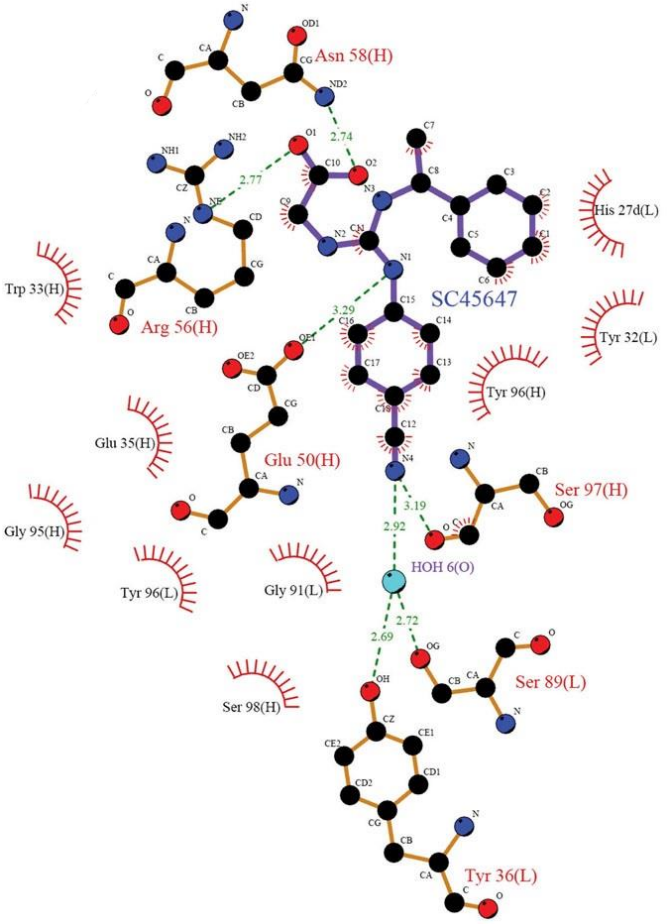
SUSTC

Protein-ligand interaction



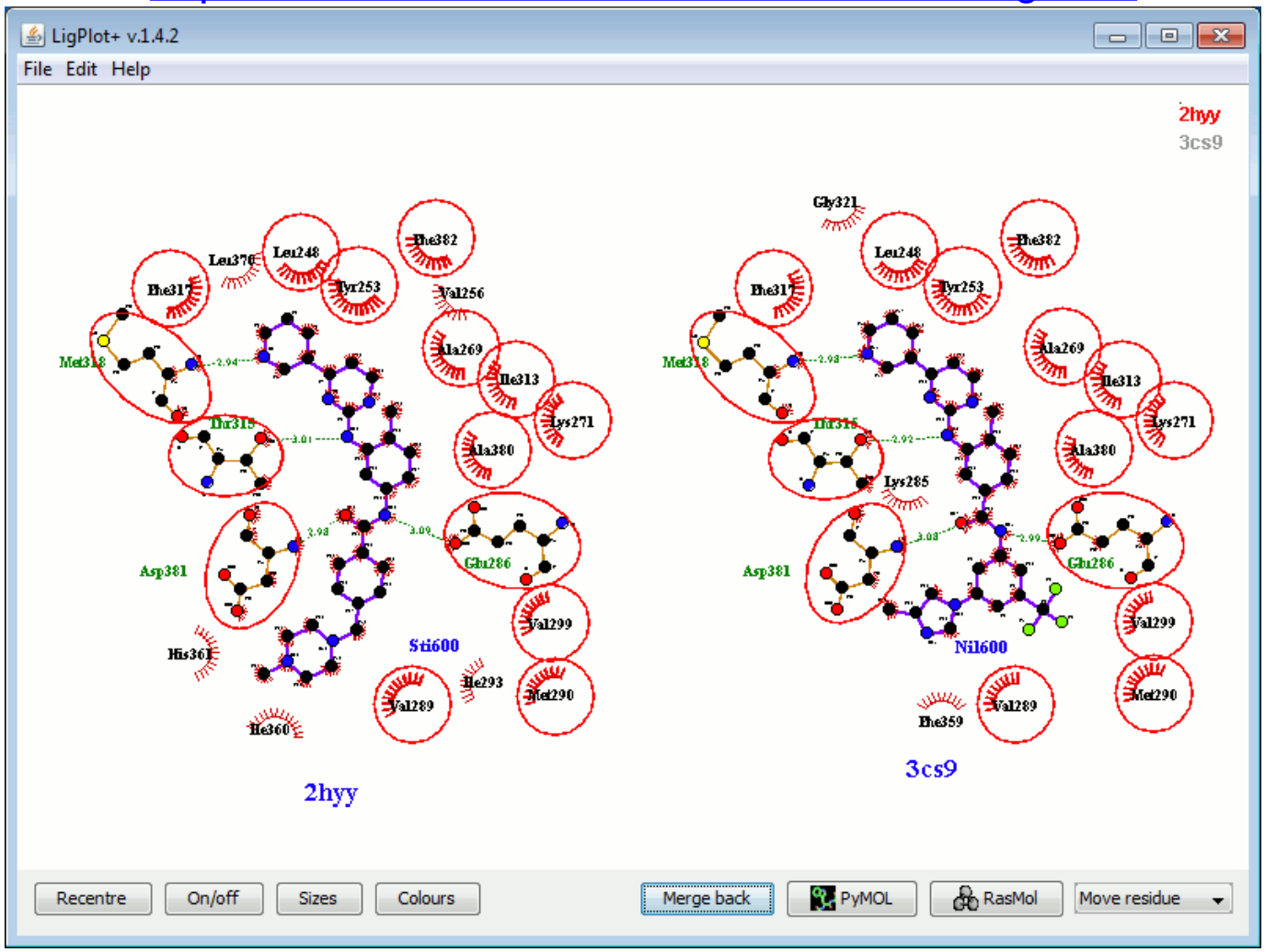


Methods

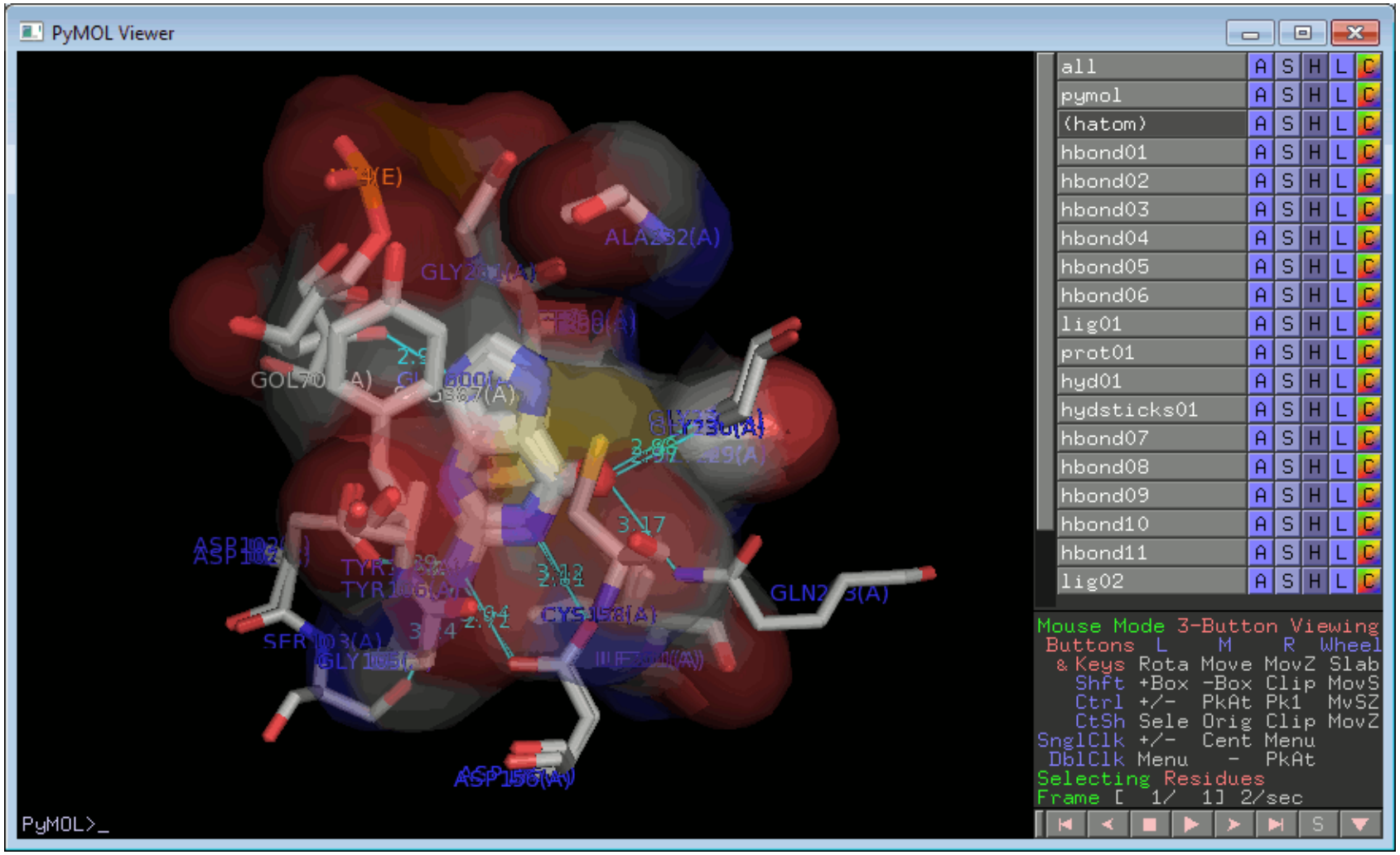
- Interface analysis
  - Identification of interfaces
  - Calculation of buried area
  - Interface residues
- 2D ligand-protein interaction analysis

Ligplot+

http://www.ebi.ac.uk/thornton-srv/software/LigPlus/



Viewing Ligplot results in PyMOL



Tasks

1. Open human hemoglobin structure (PDB id: 2HHB) in PyMOL
2. Analyze the interfaces between heme group and beta-subunit manually in PyMOL
   - Polar interaction
   - Hydrophobic interaction
3. Use Ligplot+ to analyze the heme/globin interactions
   - Compare the heme/alpha-globin and heme/beta-globin interactions
4. Present the Ligplot results in PyMOL

Lab report format

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