

Exp 10 Interaction Analysis 2

BY YUEJIAN MO

11510511

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Introduction

We will focus on quantitative interface analysis and 2D ligand-protein interaction analysis. Identification of interfaces and interface residues, calculation of buried area are trained in 2HHB.

Methods

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

Results

I failed to find meaningful polar interfaces between heme and globin. So I get rid to find hydrophobic interfaces. It is not easy to clear the polar and hydrophobic interaction, so I just calculate the buried area as following table. Interesting, here are negative buried area, which suggest that the interaction enlarges the surface.

	Area
Heme in chain A	1512.364 Angstroms ²
Chain A	13761.944 Angstroms ²
Chain A with heme	16480.143 Angstroms ²
Buried area	12594.165 Angstroms²
Heme in chain B	14462.859 Angstroms ²
Chain B	1512.364 Angstroms ²
Chain B with heme	16008.861 Angstroms ²
Buried area	-33.638

Table 1. The buried area

The Ligplot+ show that heme is more interaction with beta-globin(Figure 2) than alpha-globin(Figure 2). The interaction between His 45 and heme may result in the difference. Phe48

and Val67 also contribute to the difference.

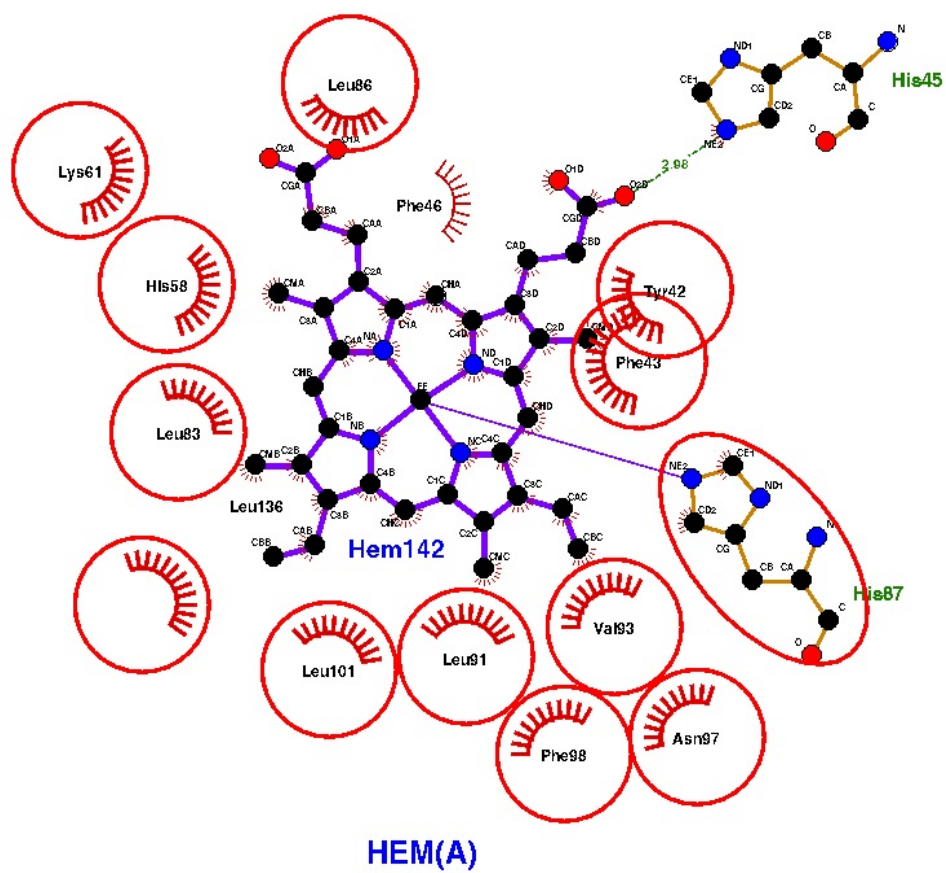


Figure 1. The Heme-hemoglobin subunit A

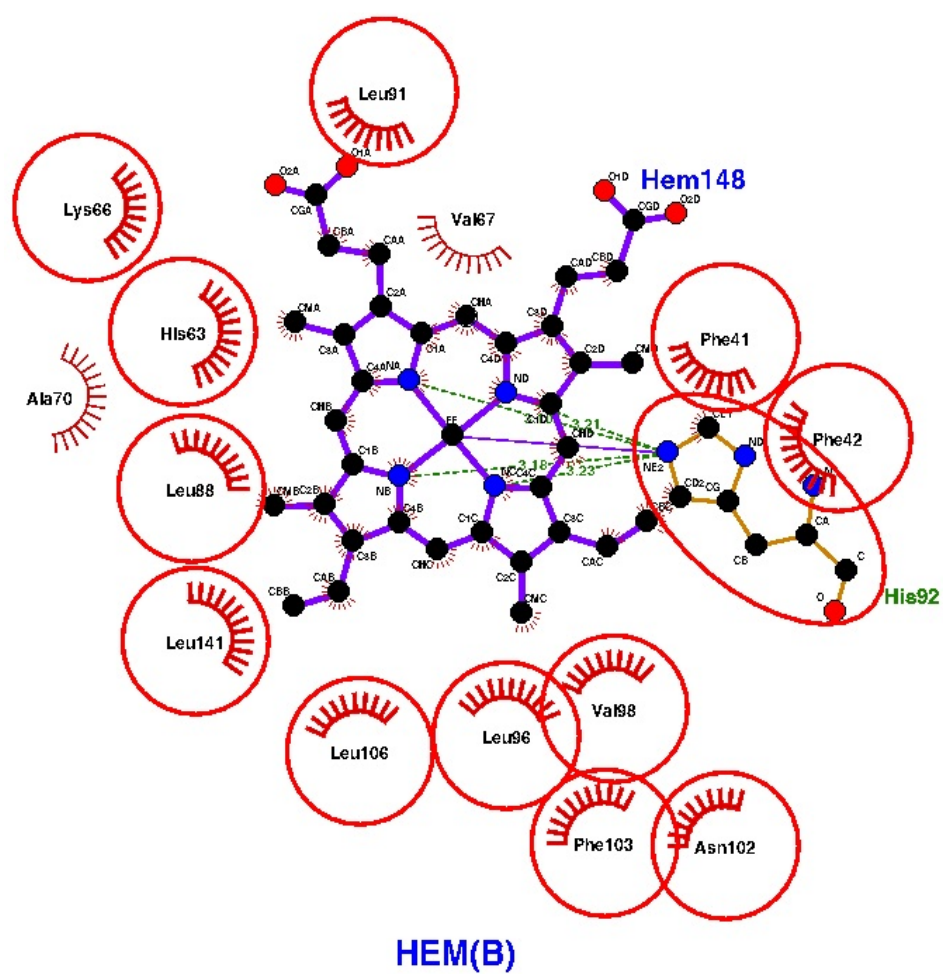


Figure 2. The Heme-hemoglobin subunit B interaction.

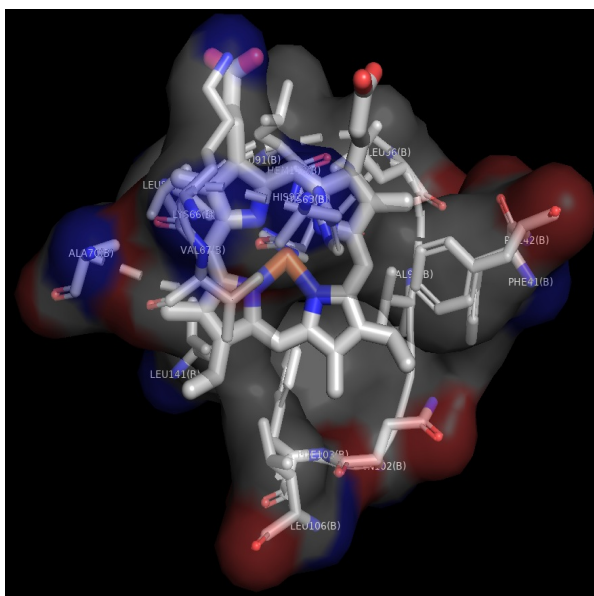


Figure 3. Representation of interaction between heme and beta-globin(chain B)
(some feature is miss)

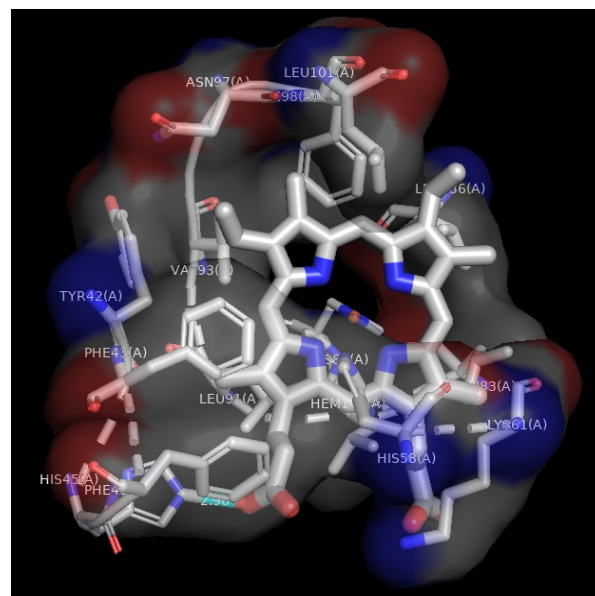


Figure 4. Representation of interaction between heme and alpha-globin (chain A)
(some feature is miss)

Conclusion

Ligplot+ is powerful tool to find out the ligand-protein interaction.