Exp 9 Interaction Analysis

by Yuejian Mo

11510511
May 24, 2018

Introduction

We will try to find the interaciton surface between chain of 2HHB. Three methods are applied: manual method, pymol script, PISA.

Methods

1. Open human hemoglobin structure (PDB id: 2HHB) in PyMoL

   ```
   PyMOL> fetch 2HHB
   ```

2. Analyze the interfaces between alpha- and beta-subunit manually in PyMOL, including polar interaction and hydrophobic interaction.

3. Use "InterfaceResiduse" in PyMOL to calculate the interfaces. Compare with your own analysis, which one gives better results?

4. Use PISA server to calculate the assembly and interfaces in human hemoglobin. Then compare the results with those in previous two steps.

5. Present the PISA results in PyMOL.

Results

All the results are save in `9_InteractionAnalysis.pse`.

i. Polar interaction and hydrophobic interaction

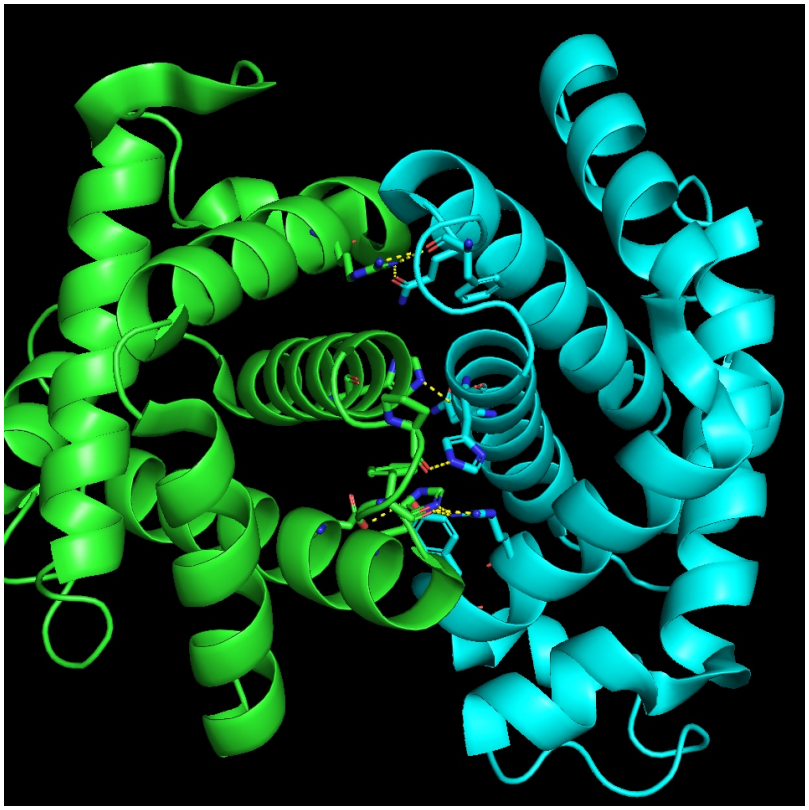

Figure 1. The polar interaction presented by PyMOL (See sence: polar_interaction)

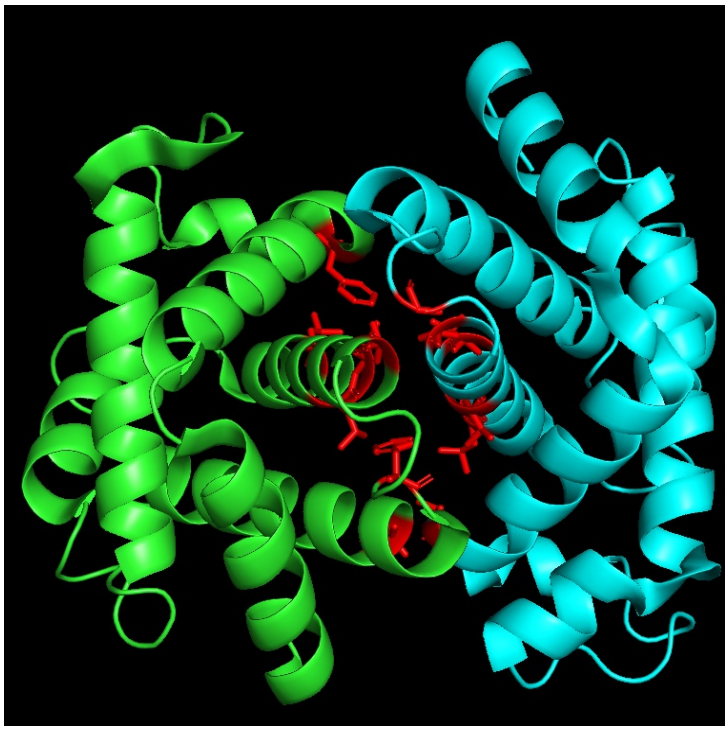

Figure 2. The pydrophobices interaction(see sence: Hydrophobic)

ii. The automatic interface identification script show better than above method manually.

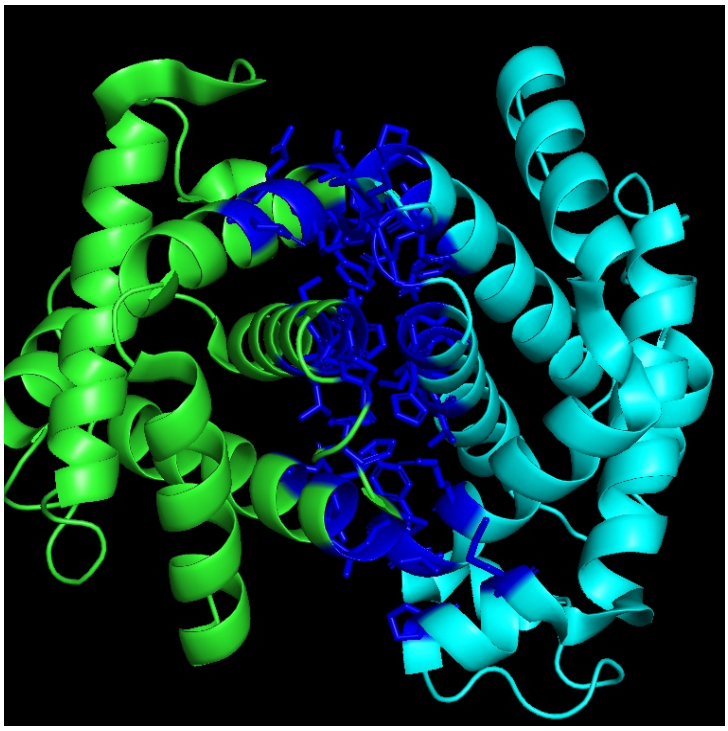

Figure 3. The InterfaceResiduse method (See sence: InteractionScript)

iii. PISA predicte the assebmly to be ACBD[HEM]4[PO4]2, which is most stable. Comparing with above method to find interaction, PISA is more reasonable. Because manual method miss some amino acid and interaction script get more false positive result than PISA.

PQS set		mm	Formula	Composition	Id	Biomol	Stable	Surface	Buried	ΔG^{int},	ΔG^{diss},
NN	«»	Size				R350		area, sq. Å	area, sq. Å	kcal/mol	kcal/mol
1	◉	4	$A_2B_2a_4b_2$	$ACBD[HEM]_4[PO4]_2$	1	1	yes	23970	11610	-102.2	6.7
2	○	2	ABa_2b	$CD[HEM]_2[PO4]$	2	–	yes	13590	4190	-49.2	2.9
	○	2	ABa_2b	$AB[HEM]_2[PO4]$	2	–	yes	13660	4130	-47.5	2.5

Figure 4. The Analysis of protein interfaces suggests the above quaternary structures are stable in solution.(PISA)

Figure 5. The interaction predicted by PISA (See sence: PISA)

Conclusion

Interaction surface alway is compact and spread in one side of helix, which face to another helix.