Exp 6: Surface Analysis

BY YUEJIAN MO

April 18, 2018

Introduction

Here, we will study the surface of Huaman hemoglobin, including hydrophobicity, conservation and electrostatic potential.

Methods

1. Load human hemoglobin structure (PDB id: 4HHB) in PyMOL

   ```
   PyMOL> fetch 4HHB
   ```

2. Create new objecs containing beta-subunit.

   ```
   PyMOL> select beta, chain B
   ```

3. Separate human hemoglobin and hemo group into two objects

4. Generate the surfarces to display the two different properties of the protein

   - Hydrophobicity

     ```
     PyMOL> set surface_color, white, beta,
     PyMOL> show surface, beta
     PyMOL> select hydrophobicity, resn Ala+Val+IIe+Leu+Met+Phe+Tyr+Trp in
     beta
     PyMOL> remove backbone in hydrophobicity
     PyMOL> set surface_color, blue, hydrophobicity
     PyMOL> show surface, hydrophobicity
     PyMOL> set transparency, 0.2
     ```

   - Conservation

5. Generate the electronstatic potential surfaces for the tetrameric hemoglobin

   Action $\longrightarrow$ generate $\longrightarrow$ vacuum electrostatics $\longrightarrow$ protein contact potential (local)

6.

select hydrophobicity, resn Ala+Val+lle+Leu+Met+PheTyr+Trp

set surface_color, green, phobic

set transparency, 0.2

Results

1.

2.

3.

4. Hydrophobicity

   Save the result in Hydrophobicity.pse sence 003. The hole which heme insert is hydrophobicity, in oder to keep heme inside hemoglobin.(Figure 1) Many sunkens surface is hydrophobic(Figure 2), which suggestes show the folding occuar to decrease system energy. However, here are raised surface is hydrophobic.(Figure 3) The hydrophobic environment between subunit interacte edge may explain this exception.

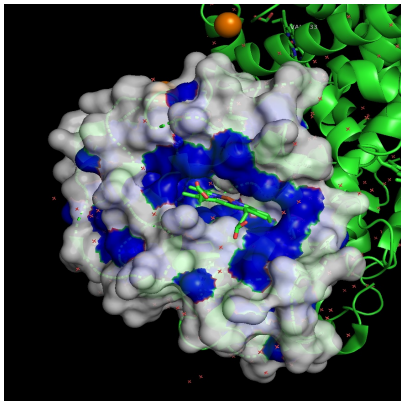

Figure 1. Heme insert to a hydrophobic hole

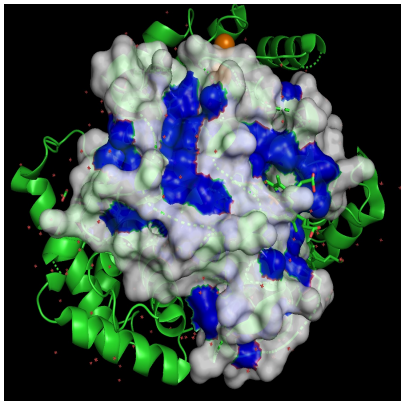

Figure 2. Much sunken surface is hydrophobic

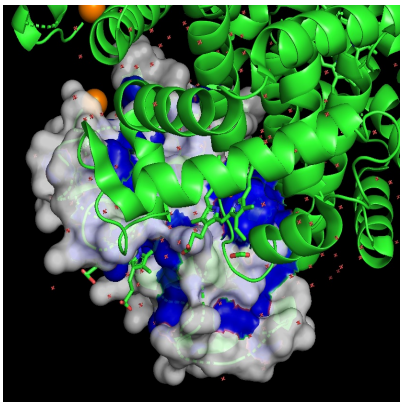

Figure 3. Subunit interacte surface is more hydrophobic

5. Convsersion

6. Electrostatic in vacuum

   Because 2,3-BPG is negative charge, I find a positive charged surface between two β subunits.(Figure 4)(Reference 4)(electrostatic.pse sence 3). I find that four Heme interactioal surface on hemoglobin are positive charged (electrostatic.pse sence 4). However, Heme doesn't show much negative feacture.

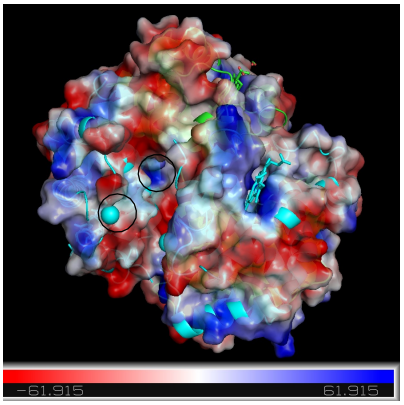

Figure 4. The positive charged pocket for 2,3-BPG binding. Butoom balck circle is a PO^{4-}, and top black circle is responding positive surface to hold PO^{4-}. (Two β subunits are colored by cyans.

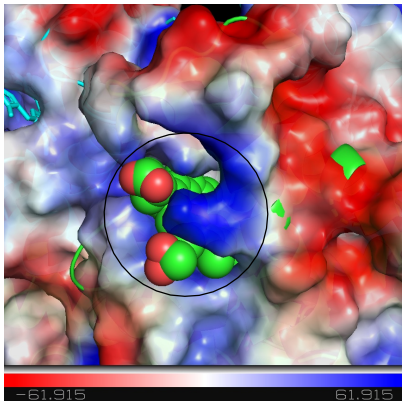

Figure 5. Here are positive charged surface on homoglobin around a Heme (Black circle).

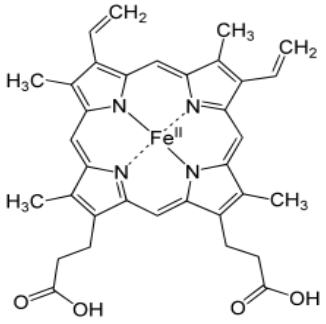

Figure 6. Heme b group (Ref 2)

Conclusions

References

1. https://pymolwiki.org/index.php/Property_Selectors
2. https://en.wikipedia.org/wiki/Heme
3. https://en.wikipedia.org/wiki/2,3-Bisphosphoglyceric_acid
4. http://cbc.chem.arizona.edu/classes/bioc462/462a/NOTES/hemoglobin/hemoglobin_function.htm
5. https://www.rcsb.org/structure/4HHB