

# Exp 6: Surface Analysis

BY YUEJIAN MO

April 14, 2018

## 1 Introduction

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

## 2 Methods

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

```
PyMOL> fetch 4HHB
```

2. Create new objects containing beta-subunit.

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

3. Separate human hemoglobin and hemo group into two objects

4. Generate the surfaces 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+Ile+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 electrostatic potential surfaces for the tetrameric hemoglobin

- 6.

```
select hydrophobicity, resn Ala+Val+Ile+Leu+Met+PheTyr+Trp
```

```
set surface_color, green, phobic
```

```
set transparency, 0.2
```

## 3 Results

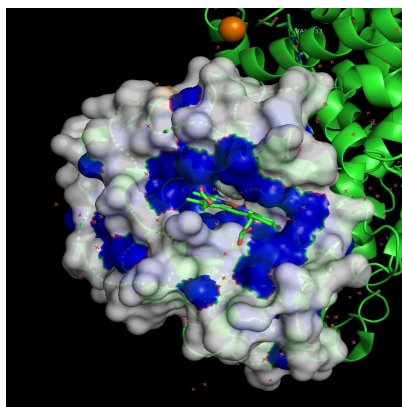
- 1.

2.

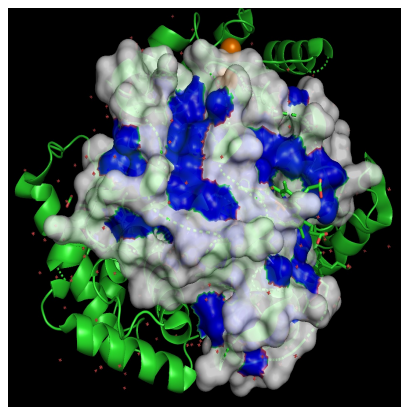
3.

#### 4. Hydrophobicity

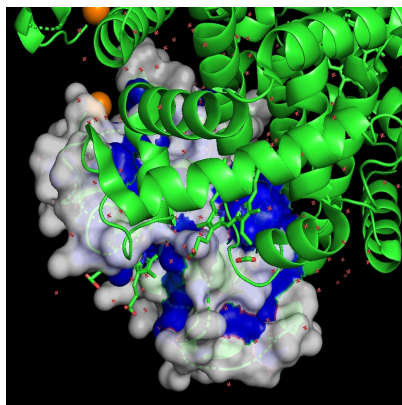
Save the result in Hydrophobicity.pse since 003. The hole which heme insert is hydrophobic, in order to keep heme inside hemoglobin.(Figure 1) Many sunken surface is hydrophobic(Figure 2), which suggests show the folding occur to decrease system energy. However, here are raised surface is hydrophobic.( Figure 3) The hydrophobic environment between subunit interact edge may explain this exception.



**Figure 1.** Hem insert to a hydrophobic hole



**Figure 2.** Much sunken surface is hydrophobic



**Figure 3.** Subunit interact surface is more hydrophobic

5.

## 4 Conclusions

## 5 References

- [https://pymolwiki.org/index.php/Property\\_Selectors](https://pymolwiki.org/index.php/Property_Selectors)
- <https://en.wikipedia.org/wiki/Heme>