Exp 8. Membrane Protein Analysis

BY YUEJIAN MO

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1 Introduction

To analysis the membrane protein, we can do sequences based analysis to predicte the transmembrane helices and toplogy, or do structure based analysis to know the cross-section and tunnel.

Here I will use some server to predicte membrane protein feature.

2 Methods

1. Predict the transmembrane helices and toplogy of human voltage-gated potassium channel. Compare predcited results with solved potassium channel structure.

2. Load the potassium channel structure (PDB id: 1BL8) to PyMOL and show its surface with electrostatic potential. Analyze its charge distribution features

3. Make cross-section of the structure to show its internal channel. Find out channel at its open or close state.

4. Using previous results by CAVER for the potassium channel structure to further analysis the channel radius versus distance along the channel direction. Find out the narrowest place.

3 Results

3.1 TMHMM

The predicted results and experiment results show below.

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# 1BL8:A|PDBID|CHAIN|SEQUENCE Length: 97
# 1BL8:A|PDBID|CHAIN|SEQUENCE Number of predicted TMHs:  3
# 1BL8:A|PDBID|CHAIN|SEQUENCE Exp number of AAs in TMHs: 51.0683
# 1BL8:A|PDBID|CHAIN|SEQUENCE Exp number, first 60 AAs:  26.70279
# 1BL8:A|PDBID|CHAIN|SEQUENCE Total prob of N-in:        0.59542
# 1BL8:A|PDBID|CHAIN|SEQUENCE POSSIBLE N-term signal sequence
1BL8:A|PDBID|CHAIN|SEQUENCE¯TMHMM2.0¯inside¯     1     6
1BL8:A|PDBID|CHAIN|SEQUENCE¯TMHMM2.0¯TMhelix¯     7    29
1BL8:A|PDBID|CHAIN|SEQUENCE¯TMHMM2.0¯outside¯    30    43
1BL8:A|PDBID|CHAIN|SEQUENCE¯TMHMM2.0¯TMhelix¯    44    66
1BL8:A|PDBID|CHAIN|SEQUENCE¯TMHMM2.0¯inside¯    67    70
1BL8:A|PDBID|CHAIN|SEQUENCE¯TMHMM2.0¯TMhelix¯    71    93
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1BL8:A|PDBID|CHAIN|SEQUENCE¯TMHMM2.0¯outside¯ 94 97

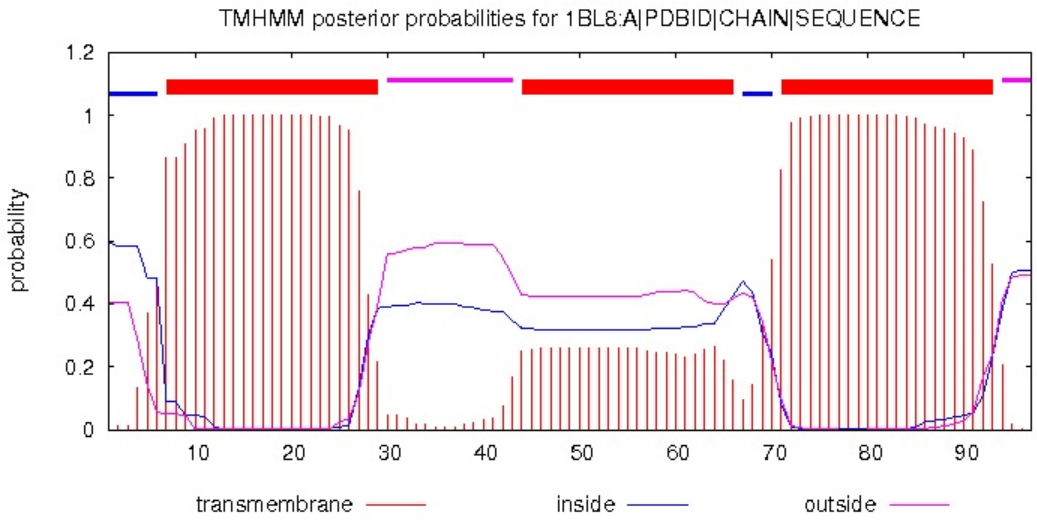

Figure 1. Predicted helices and topology of 1BL8

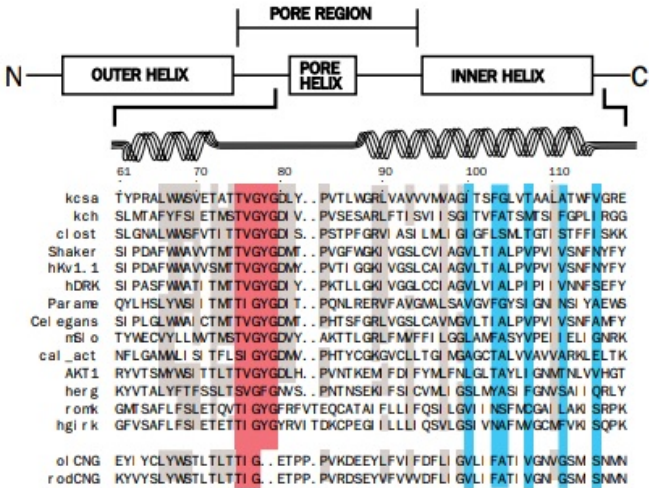

Figure 2. The helices and toplogy from other paper

3.2 Electrostatic Potential Feature

The tunnel of 1BL8 is very postive charged.

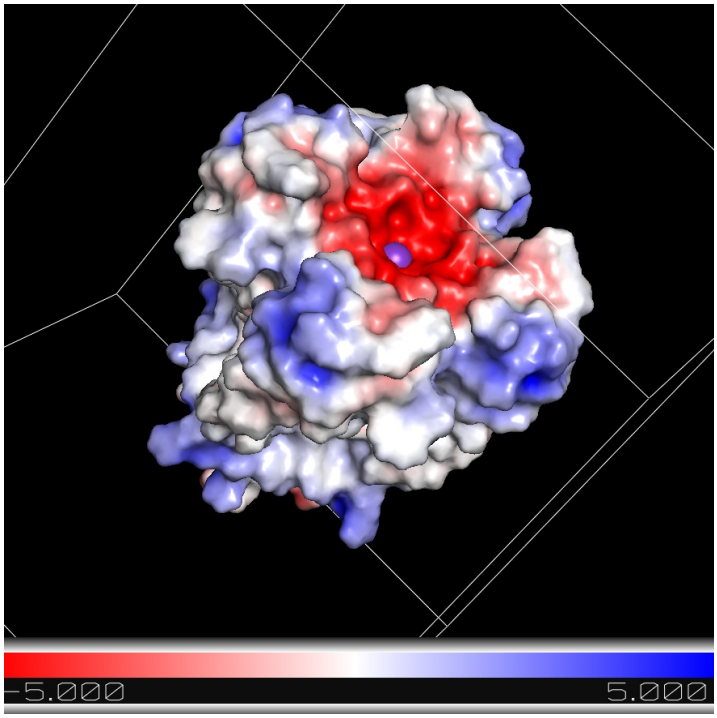

Figure 3. The electrostatic surface using APBS

3.3 The cross-section of 1BL8

Show that this channel is in close state.

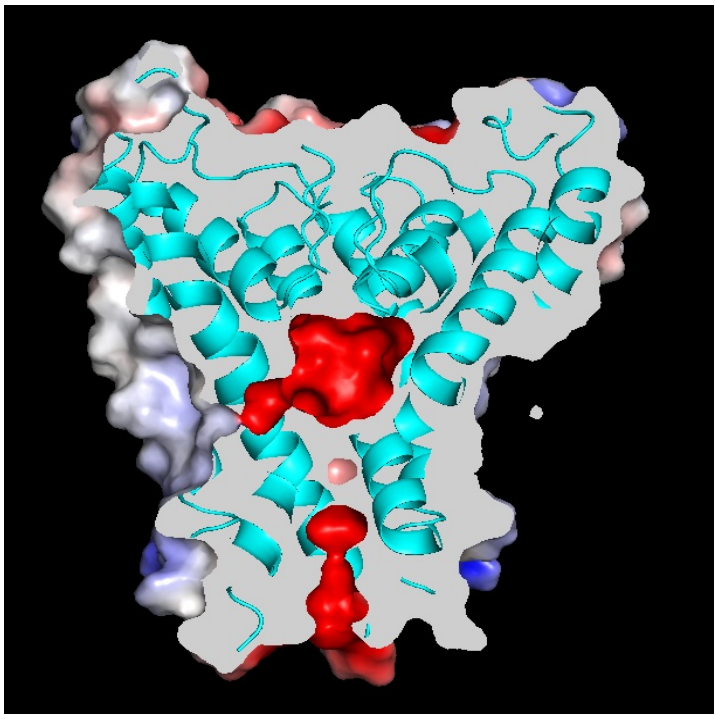

Figure 4. The cross setion of 1BL8

3.4 Find out the narrowest place in the channel

The narrowest place is in gate. Because gate narrowest must can block the potassium rather than filter.

4 Conclusions

Based on sequences and structure analysis, we can glon on how the structure act on the biological function.

5 References

- G.E Tusnády and I. Simon (1998) *J. Mol. Biol.* **283**, 489-506.
- G.E Tusnády and I. Simon (2001) *Bioinformatics* **17**, 849-850.
- Chovancova, E., Pavelka, A., Benes, P., Strnad, O., Brezovsky, J., Kozlikova, B., Gora, A., Sustr, V., Klvana, M., Medek, P., Biedermannova, L., Sochor, J. Damborsky, J. (2012) CAVER 3.0: A Tool for the Analysis of Transport Pathways in Dynamic Protein Structures. PLoS Comput Biol 8: e1002708. doi:10.1371/journal.pcbi.1002708