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Unveiling the gating mechanism of ECF Transporter

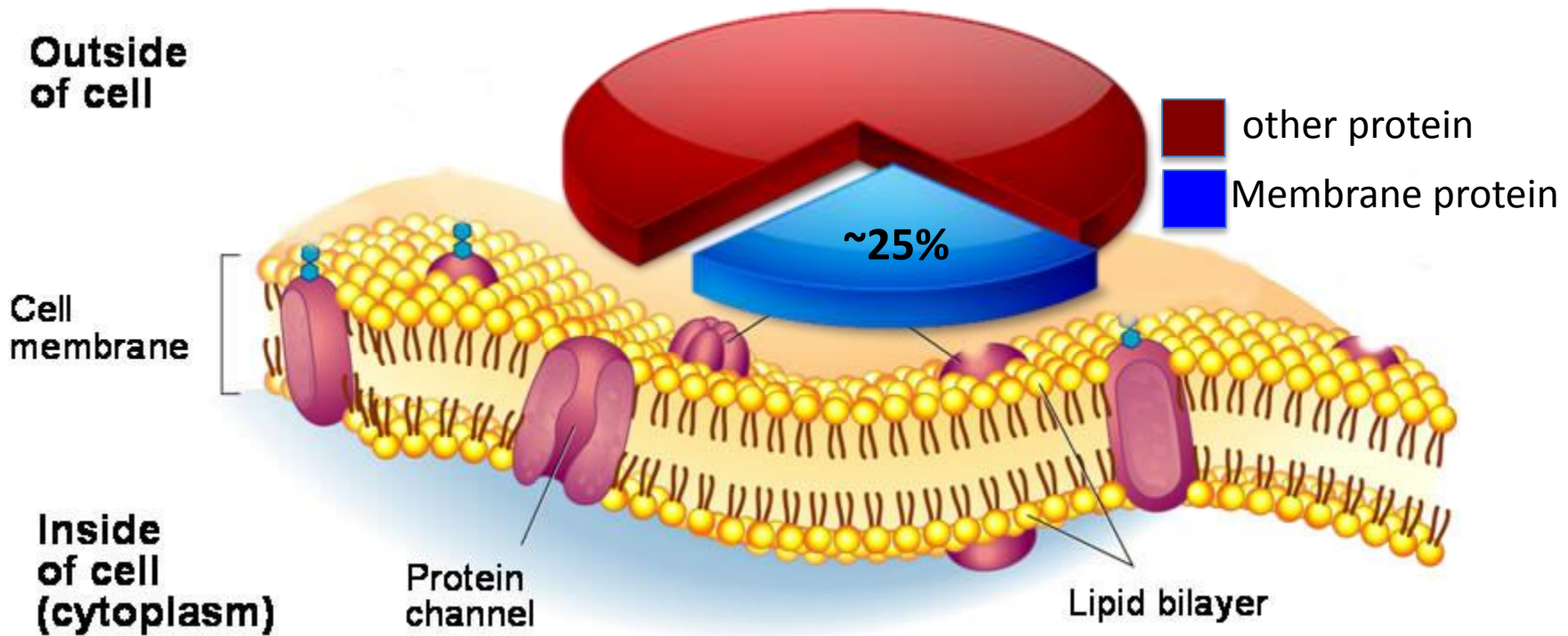
RibU

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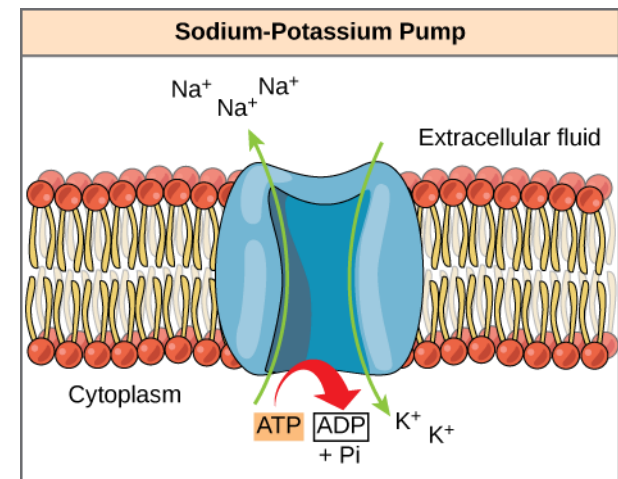
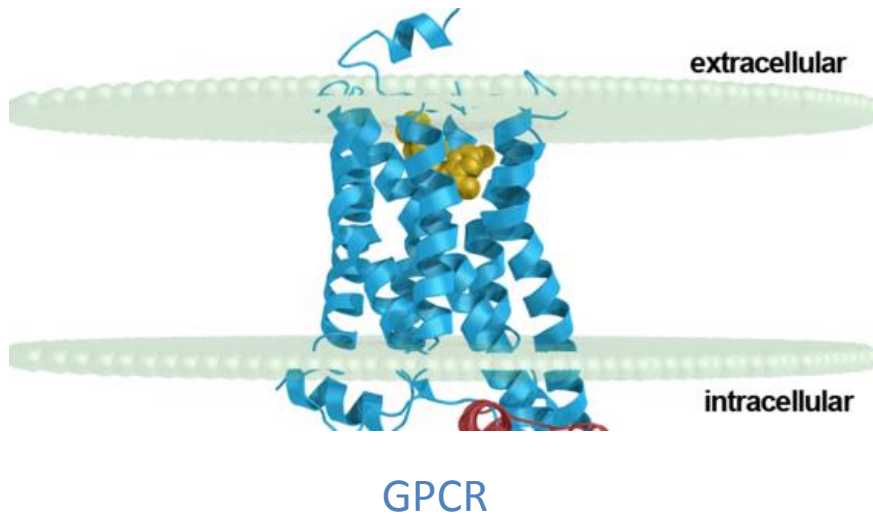
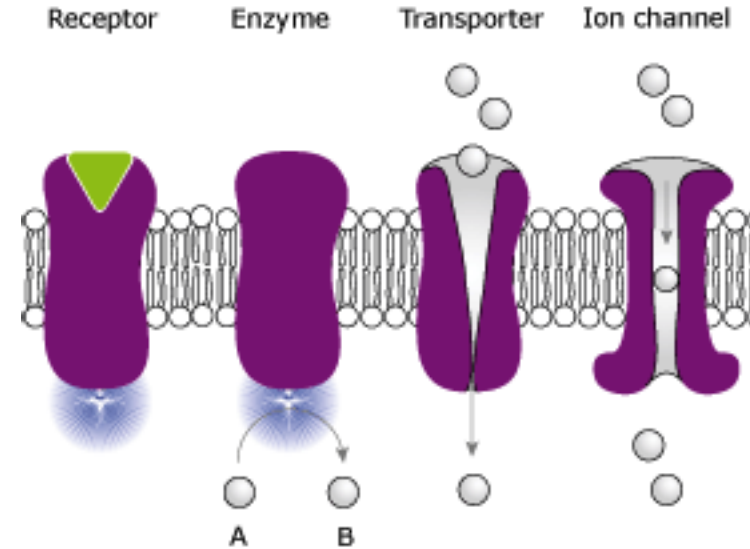
Membrane protein



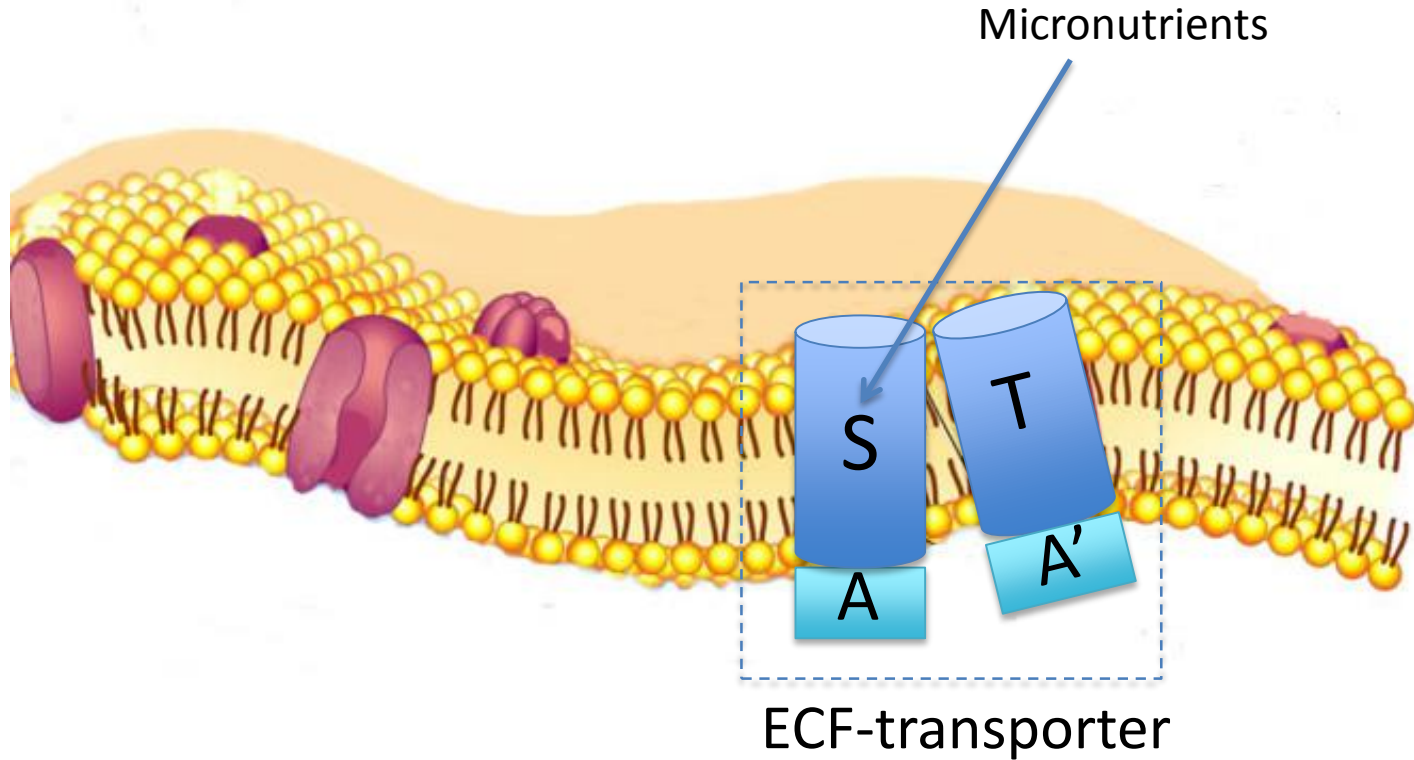
Category of membrane protein

Focus on:

- 1, Membrane receptor:
signal transduction, **GPCR**
- 2, membrane enzymes:
activity, **r-secretase**
- 3, Ion channel:
ions flow, **Na⁺/K⁺ pump**
- 4, Membrane transporter:
molecules, **ECF-transporter**



Energy-Coupling-Factor Transporter

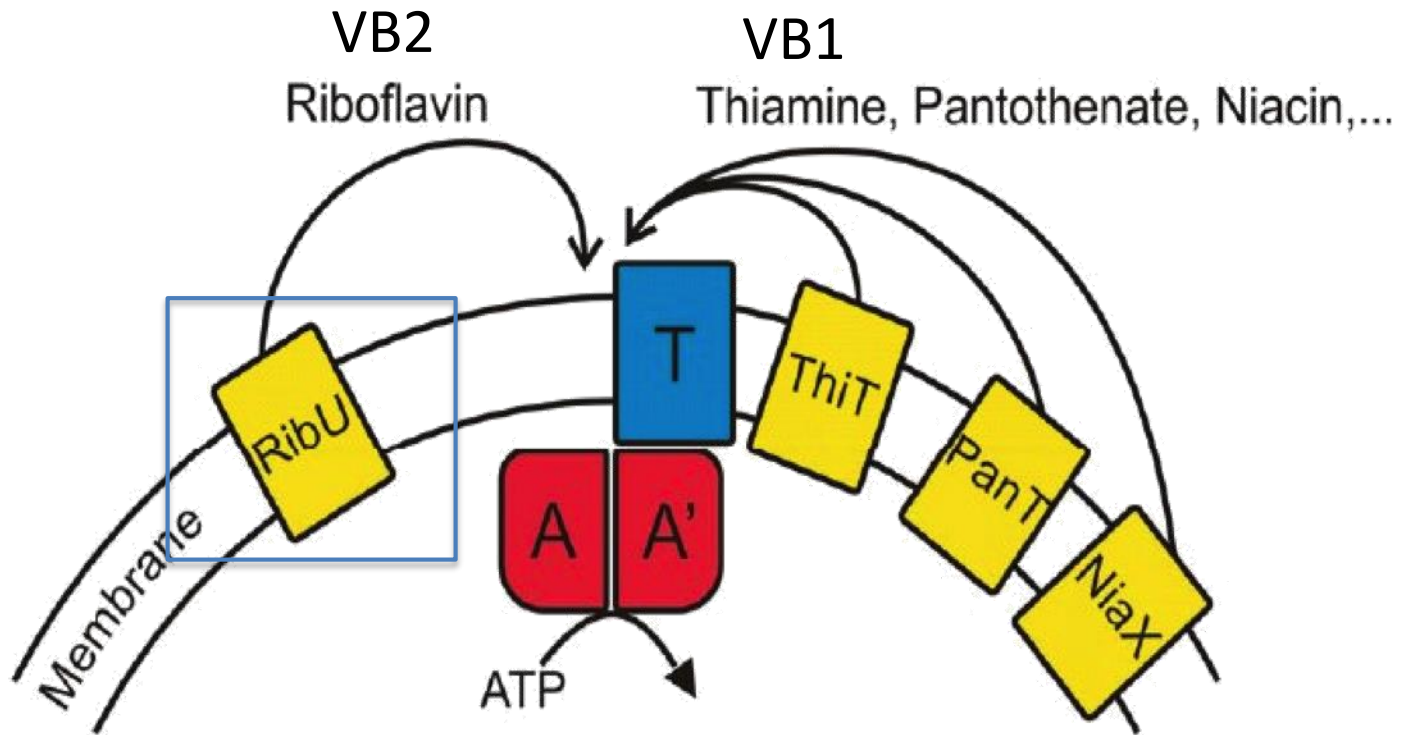


S Component: binding molecules

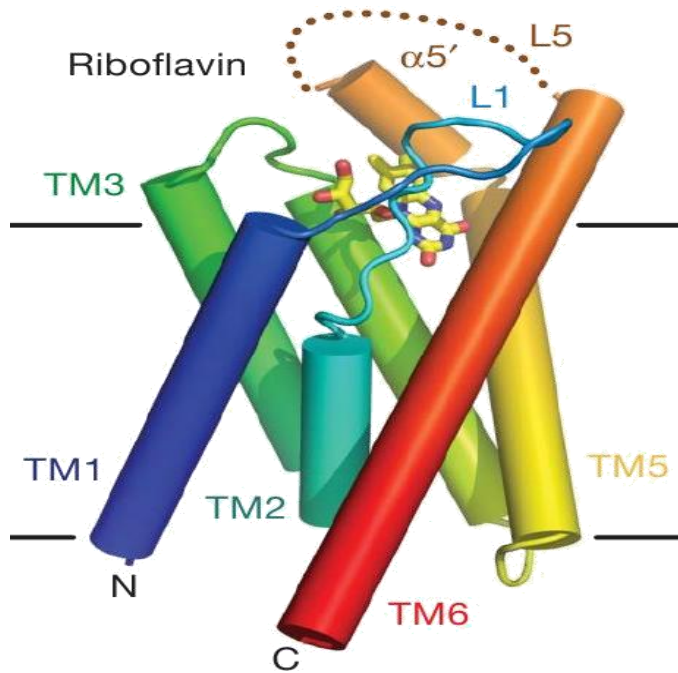
T Component: not clear

A,A' Component: binding ATP

Energy-Coupling-Factor Transporter



Structure of S component



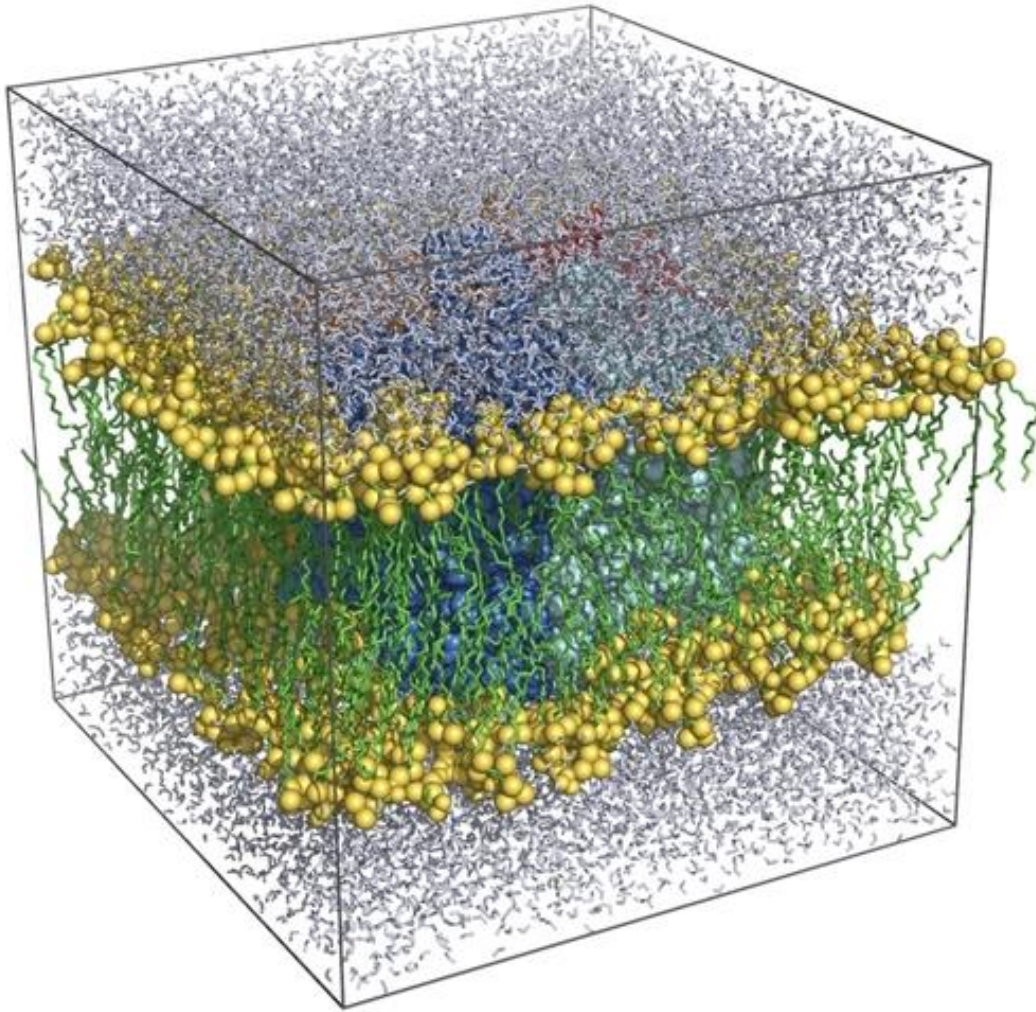
S component RibU

Static structure analysis:

- 1, L1 is used to control the binding of VB2.
- 2, VB2 is transported through RibU



Structure for simulation



Yellow and green: lipid bilayers

Blue : membrane protein

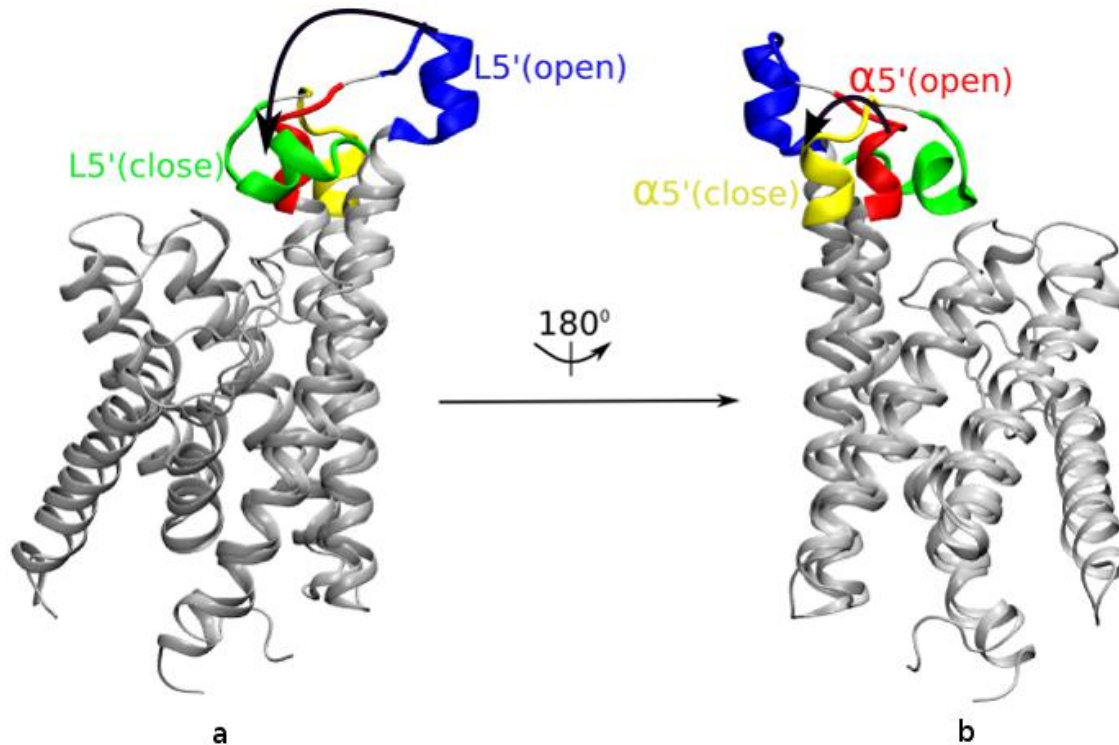
Gray : water

Package: NAMD

Time length: 180 ns

Results

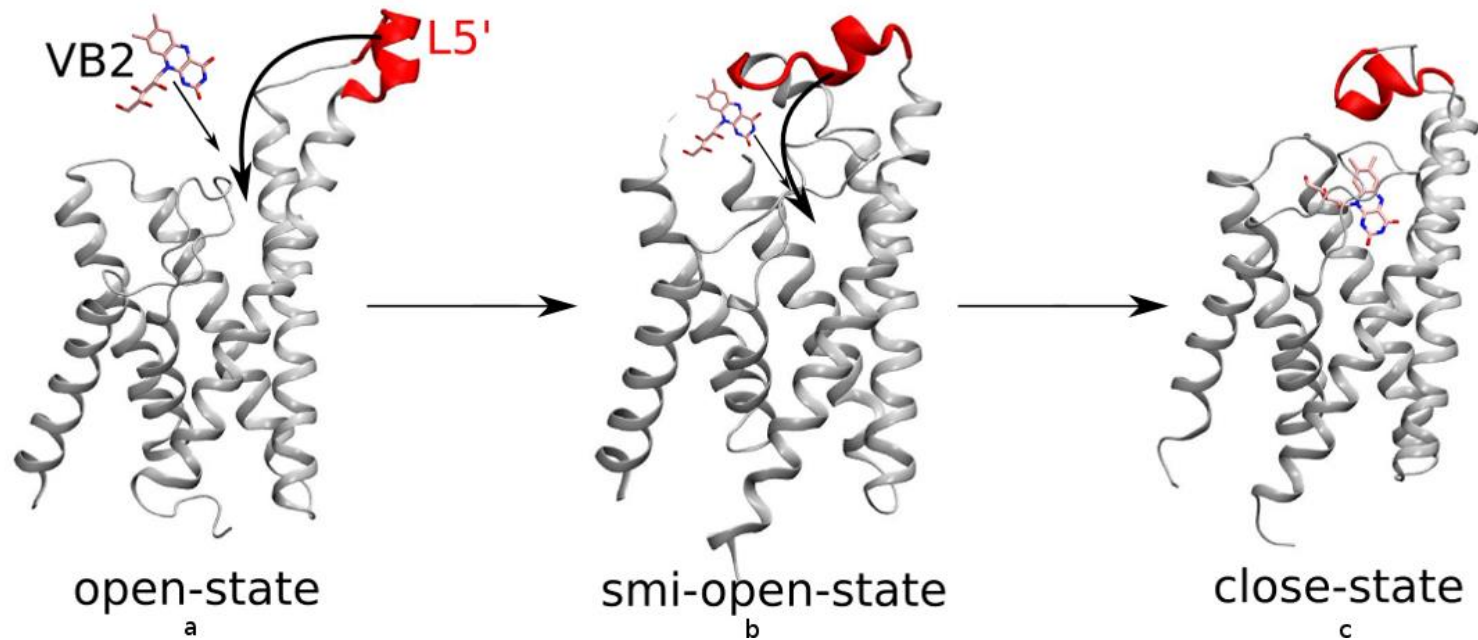
VB2 binding



The conformational changes occurs to L5'. Initially, it is open, but after VB2 binds, it closes. It is regarded that L5' serves as a gate controlling the binding.

Results

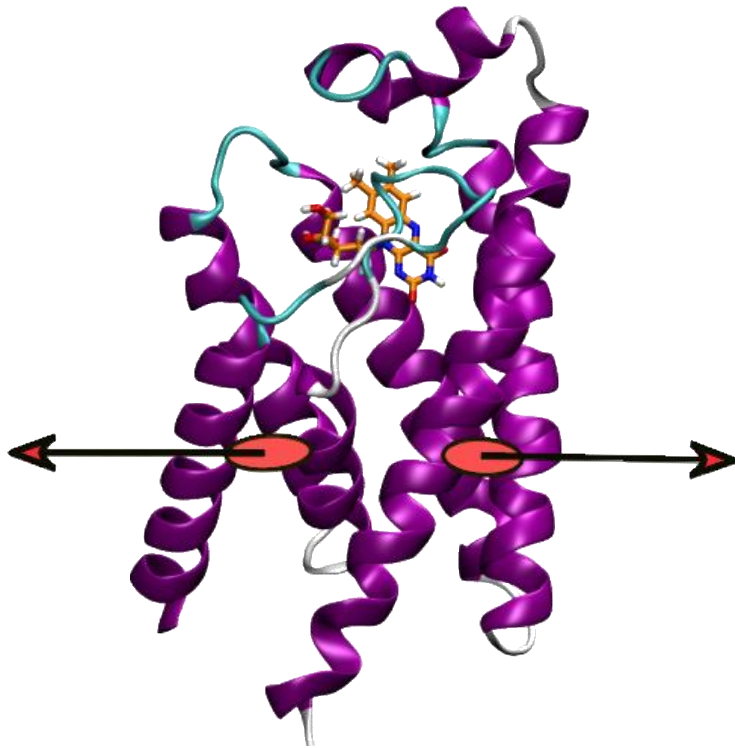
L5' binding mechanism



As vitamin B2 comes near to the binding pocket, L5' closes slowly and slowly.

Results

Transport mechanism



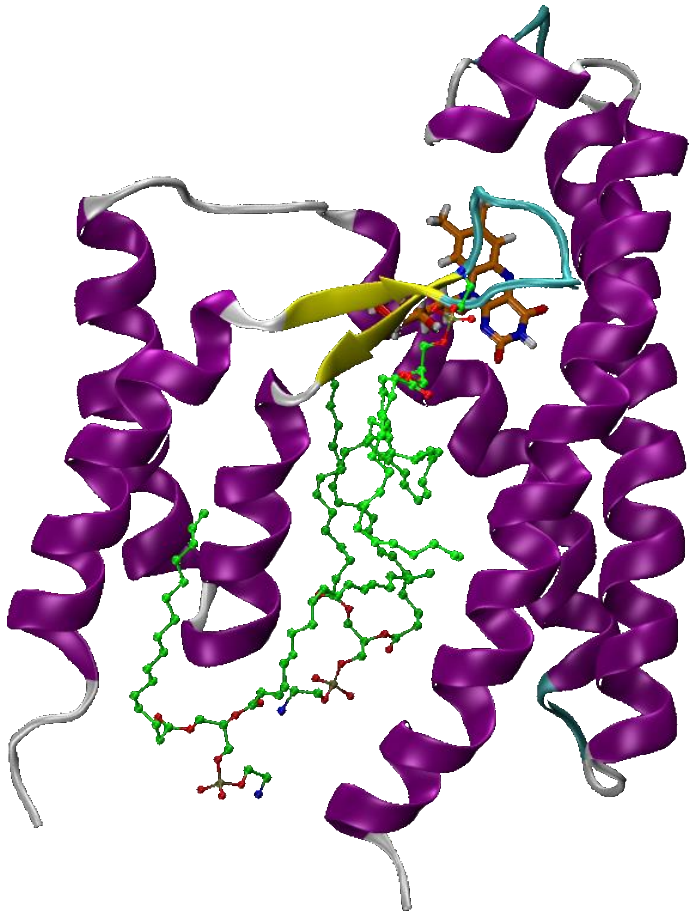
Left handle: TM1, TM2, TM3

Right handle: TM4, TM5, TM6

Force the two handles away from each other

Results

Transport mechanism



Green: lipid molecule

Purple: RibU

Lipids go through the pulled channel
and prevent the transporting of VB2

movie

Conclusion

- 1, L5' is a gate controlling the binding of Vitamin B2, not L1.
- 2, RibU alone is not able to transport riboflavin through lipid bilayers
The transport channel should be between S component and T component.

Thank you!