Supporting information

Unveiling the gating mechanism of ECF Transporter RibU

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Figure Captions

Figure S1. Structure of riboflavin (a) and roseoflavin (b). The difference between riboflavin and roseoflavin is that a methyl in riboflavin is replaced by N, N-dimethyl amine in roseoflavin, indicated by the red cycle.

Figure S2. Four hydrogen bonds between the ribityl side chain of riboflavin and RibU in XRD structure

Figure S3. Based on the putative conduction path proposed by Zhang *et al*, helix I-III of RibU are defined as a group and helix IV-VI as another group. The harmonic forces are applied to the center of mass of these two groups in the opposite directions along X-axis, separately. The two black arrows stand for the force direction and the two red ellipses represent the mass center of helix I-III helix IV-VI.

Figure S4. The best structure got from the varied force directions and force constants simulations with lipid molecules (green color) into the pulled channel again.

Figure S5. the boundary between solute and solvent in MM-PB analysis, Interior dielectric constant is set to 1.0, including Protein and lipid bilayer. L stands for lipid bilayer and P represents for protein. Exterior dielectric constant is 80.

Fugure S6. RMSD is plotted for 230 nanoseconds Apo-RibU simulation.

Figure S7. RMSF is calculated for Apo-RibU (red line) and Rbf-RibU (black line).

Figure S8. (a) PCA analysis for Apo-RibU based on the 230 ns simulation trajectory. (b) PCA analysis for Rbf-RibU based on the 170 ns simulation trajectory.

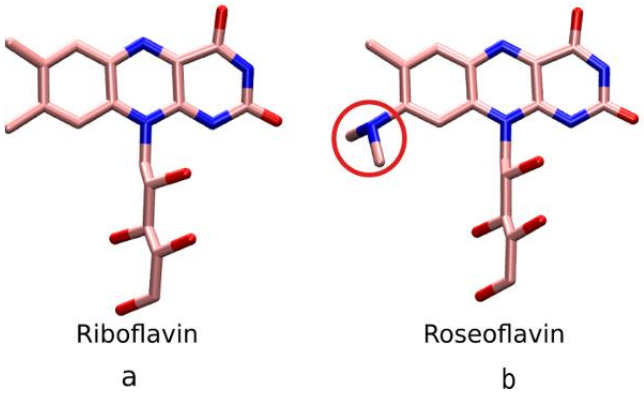

Figure S1

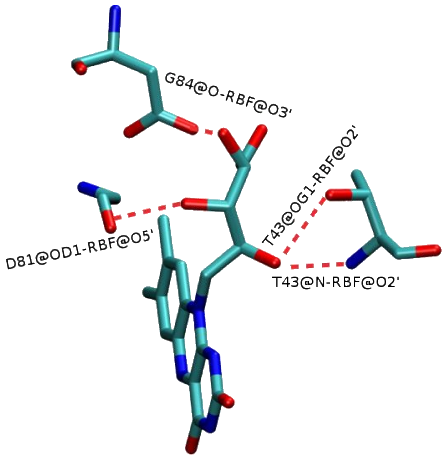

Figure S2

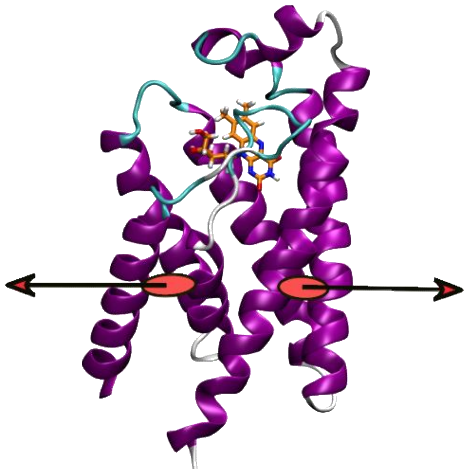

Figure S3

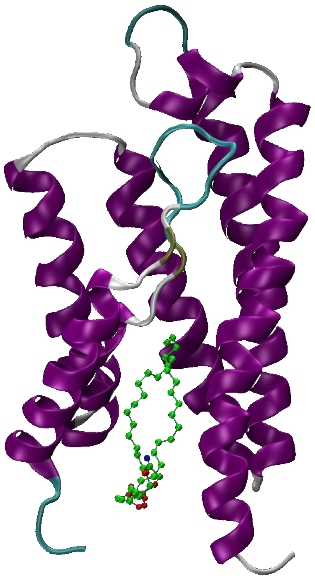

Figure S4

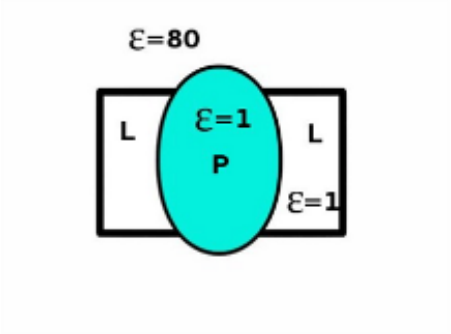

Figure S5

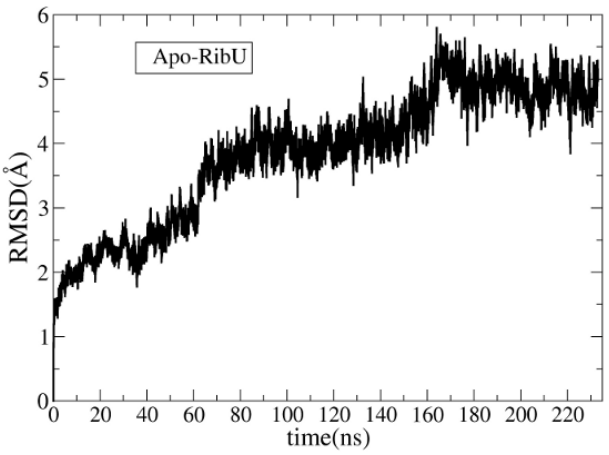
Apo-RibU
RMSD(Å)
time(ns)
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160
180
200
220

Figure S6

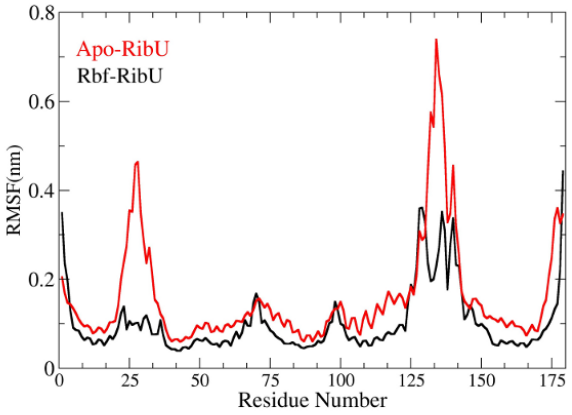
Apo-RibU
Rbf-RibU
RMSF(nm)
Residue Number
0
0.2
0.4
0.6
0.8
0
25
50
75
100
125
150
175

Figure S7

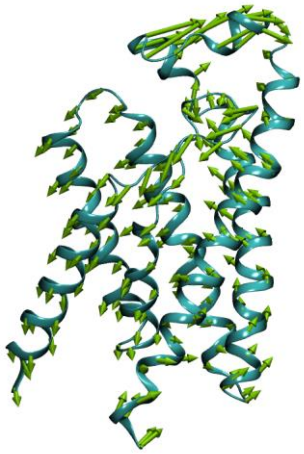

Figure S8a

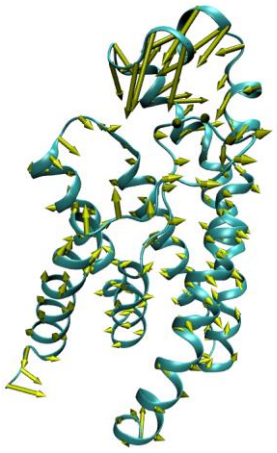

Figure S8b

Table S1 Comparison among different SMD conditions, Force constant is in kcal/mol/Å^2. In condition 4, RibU rotates around z-axis with angular acceleration -1 rad * ps^{-2}.

Force Target	Force Direction	Force Constant
Helix I-III, Helix IV-VI	5°, 15°, 45° with X-axis, vertical to Z-axis	5,10
Helix II	45° with X-axis, vertical to z-axis	20
Helix V	90° with X-axis, vertical to z-axis	5,10,20,50
Riboflavin	An axis parallel to Z-axis	5,10,100
RibU	Rotate around Z-axis	

Table S1 Comparison among different SMD conditions, Force constant is in kcal/mol/Å^2. In condition 4, RibU rotates around z-axis with angular acceleration -1 rad * ps^{-2}.