Table S1. Table presenting molecular mechanics Poisson Boltzmann surface area and molecular mechanics Generalized Born surface area (MMPBSA-MMGBSA) values of rutin-H^+/K^+-ATPase.

MMGBSA	**Average Values**	**Std. Dev**
VDWAALS	-61.9027	3.1507
EEL	-28.9140	8.5848
EGB	47.3976	7.0177
ESURF	-6.9506	0.2889
ΔG gas	-90.8166	8.9731
ΔG solv	40.4470	7.0278
Δ TOTAL	-50.3696	4.4032
MMPBSA	**Average Values**	**Std. Dev**
VDWAALS	-61.9027	3.1507
EEL	-28.9140	8.5848
EPB	58.4900	6.6887
ENPOLAR	-4.5037	0.1797
ΔG gas	-90.8166	8.9731
ΔG solv	53.9863	6.6765
ΔTOTAL	**-36.8304**	**4.9028**

VDWAALS: van der waals EEL: electrostatic interaction EPB/EGB: the electrostatic contribution to the solvation free energy calculated by PB and GB respectively.
ESURF: non-polar contribution to solvation energy using SASA (solvent accessible surface area) for GB.
ENPOLAR: non-polar contribution to solvation energy from repulsive solute-solvent interactions for PB.
Delta G gas: change in energy in gaseous phase.
Delta G solv: change in energy in solvation phase.

Table S2. Table presenting molecular mechanics Poisson Boltzmann surface area and molecular mechanics Generalized Born surface area (MMPBSA-MMGBSA) values of rutin-voltage gated L-type calcium channel.
VDWAALS: van der waals
EEL: electrostatic interaction

MMGBSA	**Average values**	**Std.Dev**
VDWAALS	-55.6448	4.0571
EEL	-22.6093	8.1912
EGB	34.7234	7.9352
ESURF	-6.3886	0.2655
ΔGgas	-78.2542	9.1786
ΔG solv	28.3348	7.8232
Δ TOTAL	-49.9194	3.9229
MMPBSA	**Average Values**	**Std. Dev**
VDWAALS	-55.6448	4.0571
EEL	-22.6093	8.1912
EPB	45.0120	8.3928
ENPOLAR	-4.3173	0.1342
ΔG gas	-78.2542	9.1786
ΔG solv	40.6947	8.3160
ΔTOTAL	**-37.5595**	**3.4529**

EPB/EGB: the electrostatic contribution to the solvation free energy calculated by PB and GB respectively.
ESURF: non-polar contribution to solvation energy using SASA (solvent accessible surface area) for GB.
ENPOLAR: non-polar contribution to solvation energy from repulsive solute-solvent interactions for PB.
Delta G gas: change in energy in gaseous phase.
Delta G solv: change in energy in solvation phase.