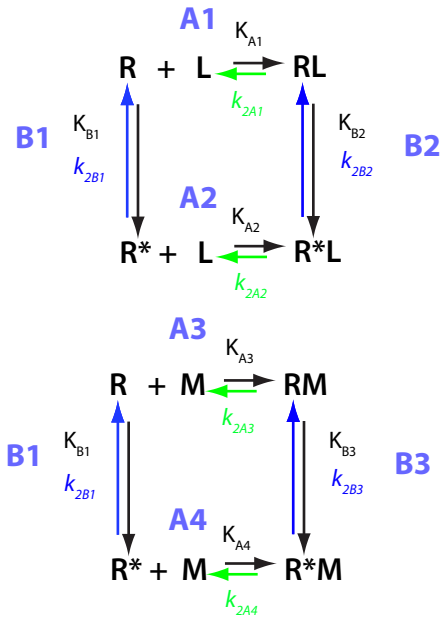


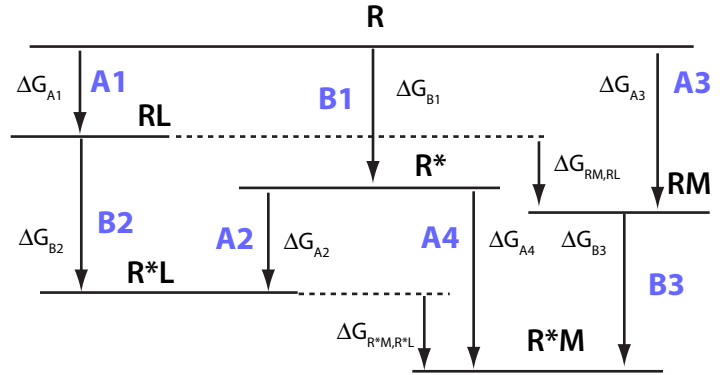
U-R-RL-RM

Binding of two mutually exclusive ligands coupled with intramolecular isomerization of the receptor (competitive ligand binding)

Reaction scheme



Free-energy diagram (positions of energy levels are chosen for easy viewing)



Thermodynamic cycles

$$\Delta G_{B1}^{\circ} + \Delta G_{A2}^{\circ} = \Delta G_{A1}^{\circ} + \Delta G_{B2}^{\circ}, \quad K_{B1}K_{A2} = K_{A1}K_{B2}$$

$$\Delta G_{B1}^{\circ} + \Delta G_{A4}^{\circ} = \Delta G_{A3}^{\circ} + \Delta G_{B3}^{\circ}, \quad K_{B1}K_{A4} = K_{A3}K_{B3}$$

For calculations I will assume that I know equilibrium constants for B1, B2, B3, A1 and A3. Dependent constants then correspond to A2 and A4:

$$K_{A2} = K_{A1}K_{B2}/K_{B1}$$

$$K_{A4} = K_{A3}K_{B3}/K_{B1}$$

Additional equilibrium constants between alternative forms of R and R* may be determined as:

Relationship between concentrations of bound forms of R:

$$K_{RM,RL} = [RM][L] / \{[RL][M]\}$$

$$\Delta G_{A3}^{\circ} - \Delta G_{A1}^{\circ} = \Delta G_{RM,RL}^{\circ}$$

$$K_{RM,RL} = K_{A3}/K_{A1}$$

Relationship between concentrations of bound forms of R*:

$$K_{R^*M,R^*L} = [R^*M][L] / \{[R^*L][M]\}$$

$$\Delta G_{A3}^{\circ} + \Delta G_{B3}^{\circ} - \Delta G_{A1}^{\circ} - \Delta G_{B2}^{\circ} = \Delta G_{R^*M,R^*L}^{\circ}$$

$$K_{R^*M,R^*L} = K_{A3}K_{B3}/(K_{A1}K_{B2})$$