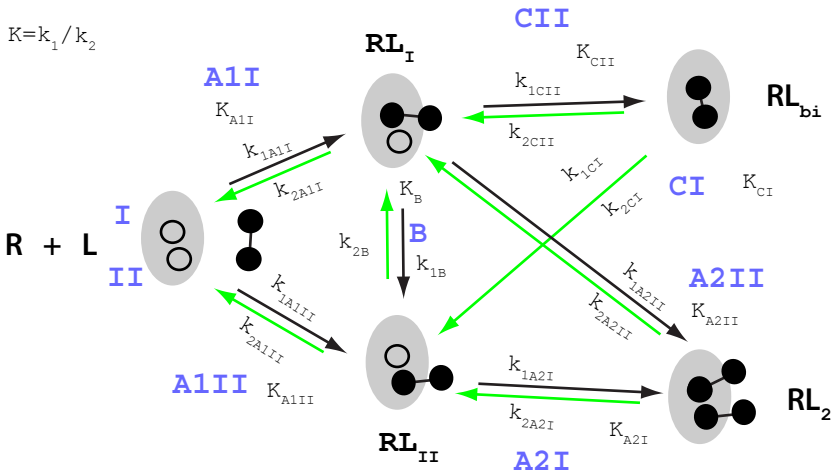
Model code: B-bidentateL-micro

Binding of bi-dentate ligand molecule to R with two binding sites; microscopic constants no conformational change in R itself

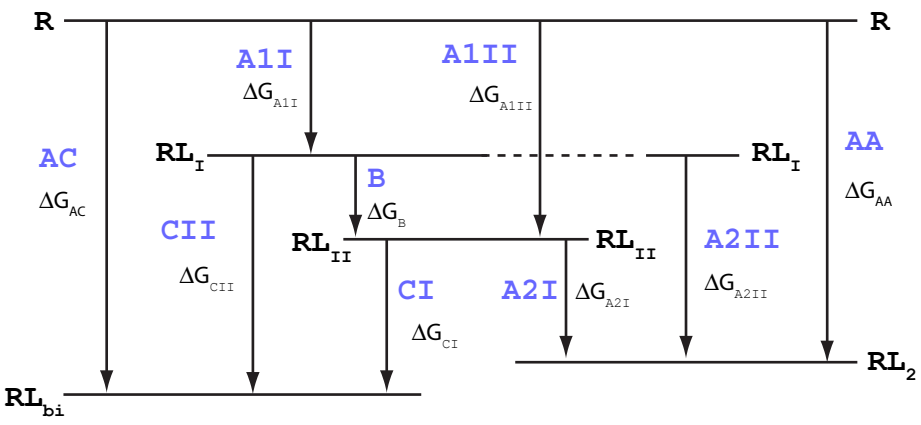
NOTE 1: Capital letters indicate equilibrium constants; lower case letters--kinetic constants.
NOTE 2: I use new naming of the microscopic constants, different from LineShapeKin Simulation.
NOTE 3: Transitions were renamed to match B_micro naming scheme.

Bi-dentate ligand binding

- receptor has two distinct sites I and II;
- ligand has two identical binding motifs;
- ligand-binding transitions "A" are labeled to reflect at which site the binding event occurs;
- "hopping" - the internal isomerization transition "B" occurs inside the "solvent cage";
- "locking" - one-dentate to two-dentate binding transitions are labeled "C".



Standard Gibbs energy diagram
(positions of energy levels are chosen for easy viewing)



Thermodynamic cycles

$\Delta G^o_{AC} = \Delta G^o_{A1I} + \Delta G^o_{CII} = \Delta G^o_{A1II} + \Delta G^o_{CI}$ => $K_{AC} = K_{A1I}K_{CII} = K_{A1II}K_{CI}$

Dependent constants: $\Delta G^o_{CI} = \Delta G^o_{A1I} + \Delta G^o_{CII} - \Delta G^o_{A1II}$ => $K_{CI} = K_{A1I}K_{CII}/K_{A1II}$

$\Delta G^o_{B} = \Delta G^o_{A1II} - \Delta G^o_{A1I}$ => $K_{B} = K_{A1II}/K_{A1I}$

$\Delta G^o_{AA} = \Delta G^o_{A1I} + \Delta G^o_{A2II} = \Delta G^o_{A1II} + \Delta G^o_{A2I}$ => $K_{AA} = K_{A1I}K_{A2II} = K_{A1II}K_{A2I}$

Dependent constants: $\Delta G^o_{A2I} = \Delta G^o_{A1I} + \Delta G^o_{A2II} - \Delta G^o_{A1II}$ => $K_{A2I} = K_{A1I}K_{A2II}/K_{A1II}$