

Site1 - Numerical Solution for Interaction Equilibrium

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There are generally two main approaches for solving mathematical problems in the Natural Sciences: analytical solutions and numerical solutions. An *analytical solution* (theoretical model) relies on a function containing one or more independent variables, a dependent variable, and one or more parameters to be determined, which together describe the problem situation. In contrast, a *numerical solution* does not depend on an explicit descriptive equation, but rather on approximations aimed at minimizing a general function ($F(x) = 0$). Numerical methods are employed when the theoretical model is complex, when an explicit solution is not desired, or when such a solution does not exist.

1 Equation:

The *Site1* program numerically solves the quantities involved in a bimolecular interaction equilibrium:



Where:

- R = free receptor (protein, nucleic acid, etc.);
- LR = formed complex;
- k_{on} = association rate constant of the complex;

- k_{off} = dissociation rate constant of the complex.

The equation describing complex formation is:

$$K_d = \frac{[RL]}{[R] + [L]} = \frac{k_{off}}{k_{on}} \quad (2)$$

Where K_d represents the *equilibrium dissociation constant* of the complex. Thus:

$$LR = \frac{L \cdot R}{K_d}$$

Accordingly, for the numerical solution of the theoretical model described above, the minimization functions are defined as:

$$F(x) = 0 : \quad R_0 = R + LR; ; \rightarrow; ; R + \frac{L \cdot R}{K_d} - R_0 = 0$$

$$F(x) = 0 : \quad L_0 = L + LR; ; \rightarrow; ; \frac{L \cdot R}{K_d} - L_0 = 0$$

2 Site1

The program uses the *MSLV* (*Multiple Equation Solver*) command for the simultaneous solution of multiple equations, together with the [MSLV2](#) library, which optimizes its performance. The library can also be loaded onto the calculator from its source code provided by the developer.

Program inputs and outputs are as follows:

```
# Inputs:
  L0, R0, and Kd

# Outputs:
  L x R plot;
  Matrix of L and LR values on the stack;
  Variables (L, R, RL, initial values, and seeds).
```

3 Files:

1. Program
2. Source code

4 Example of use:

```
1. Place on the stack:  
  a. LO = 10;  
  b. RO = 5;  
  c. Kd = 10;  
  
2. Run "Site1".
```

Note:

1. Although fully functional, the program is relatively slow when compared to desktop software. The example above required approximately 16 s to complete graphical output and variable display, whereas the program [Octave](#) required only 1 s.

References

1. Olson, John S. *Numerical analysis of kinetic ligand binding data*. Methods in Enzymology, Vol. 76. Academic Press, 1981, pp. 652–667.

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