

## Syntax of equation - basic rule

1. In general follow the Excel equation formulation rules.
2. Start with “y=”
3. No space
4. Case sensitive
5. Independent variable (x data) is **x1**.
6. Parameters are **p1, p2, p3**,... (Numbers have to be sequential.)
7. Parameter values are always positive.
8. Maximum parameter count is 8.
9. No differentials

### Examples)

**Polynomial equation:**  $y=p1*x1^2+p2*x1+p3$

**Exponential equation (single exponential decay):**  $y=p1*\exp(-p2*x1)$  [p1 is an initial value, p2 is rate constant, and x1 is usually a time.]

**Michaelis-Menten equation:**  $y=p1*x1/(p2+x1)$  [p1 is Vmax, p2 is Kd, and x1 is a reactant concentration.]

## Syntax of equation - special cases

1. **Using Newton-Raphson method (Please see references for the details about Newton-Raphson method described elsewhere.)**

...Before evaluating sum of square value root value is numerically calculated by real-valued function and is assigned to fitting equation.

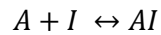
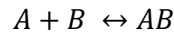
### Syntax)

A root variable: **n1**

Real-valued function (Newton Raphson equation) to find root value: start with “f=” (x:  
 $f(x) = 0$ )

### Example) Competitive Inhibition

Equilibrium binding of reactants (A and B) in the presence of competitive inhibitor (I)



If added A concentration is 20 and added B concentration is 40...

**Real-valued function to find root value:**  $f=20-n1*40/(p1+n1)-n1*x1/p2$

**Fitting equation for evaluating sum of square values:**  $y= n1*40/(p1+n1)$

n1: free A concentration (unknown)

x1: Added I concentration (independent variable: x values)

p1: Dissociation constant (Kd) of (A + B reaction)

p2: Dissociation constant (Ki) of (A + I reaction)

y: Concentration of AB complex (y data values, usually experimentally found by activity and in this case activity of AI complex is assumed to be zero.)

## 2. Equation contains integration.

...rare case when equation contains integral equation parts.

### Syntax)

Integral equation part starts with “I1=”, “I2=”, “I3=”,... (multiple number of integral equation accepted) followed by “lower range number : upper range number : increment:”, then write integrating equation. (Range number part can contain p1, p2,..., x1, x2,..., c1, c2...)

Integration variable: t1, t2, t3....

Calculation speed heavily depends on range values and increments.

### Example)

This is not a real case but ...

$$y = a * x + \int_0^{100} \exp(-bt) dt$$

is written as...

$I1=0:100:1:\exp(-p1*t1)$  ...(\*Increment in this case is 1.)

$y=p2*x1+I1$