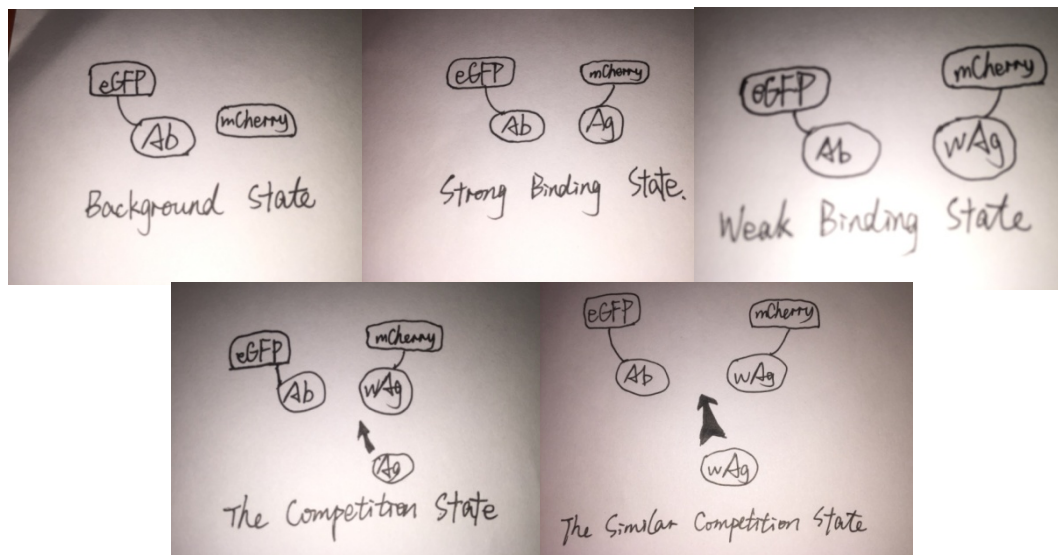# INTRODUCTION

Our Modeling is primarily based on the confirmatory experiments we have designed

Five experimental groups designed in our experiment formed five states which are known as...

Through our experiment, we can know five groups of data about macro binding efficiency. We also can know the occurring probability of the micro FRET in both background state and strong binding state.

Macro binding efficiency depends on FRET micro binding efficiency, the occurring probability of the micro FRET and other variables.

We want to calculate the occurring probability of the micro FRET in weak binding state, the competition state, and the similar competition state when we know FRET occurring probability under the condition of the macro binding efficiency and the strong binding state.

So in this model, our six major variables are the amount of antigen (Ag), the amount of antibody (Ab), the amount of key, the amount of Ab with Ag, the amount of Ab with key and the extend of combination. We will use some differential equation to find out the relationships to between these variables.

Here are also some regular values. Affinity is one of them. We will use the data of affinity to calculate variables.

'k' is related to affinity between one antibody withkey and one antigen. We will start our equation with using the regular value 'k' to work out some differential equations.

By using these equations, we can find out the relationship between these variables.
We can use these variables. We can use these relationships to work out the relationship with these variables and the extend of combination.

Now we know that the extend of combinations is related to six major variables in our equations and 'k'. In the experiment, we can control these variables and use the positive correlation model to calculate the relationship between the extend of combination and affinity.

In the modeling part, we assume that there are some ideal conversion rates when the experiment happening.
: **k** (from Ab-key to Ag and from Ag to Ab-key), **a**(from Ab-Ag to Ag and Ab) and **b**(from Ab-key to Ab and wAg).

And we will use Volterra Model in the part of designing the cycle of injection of Ab-key.

EQUATIONS AND EXPLANATIONS
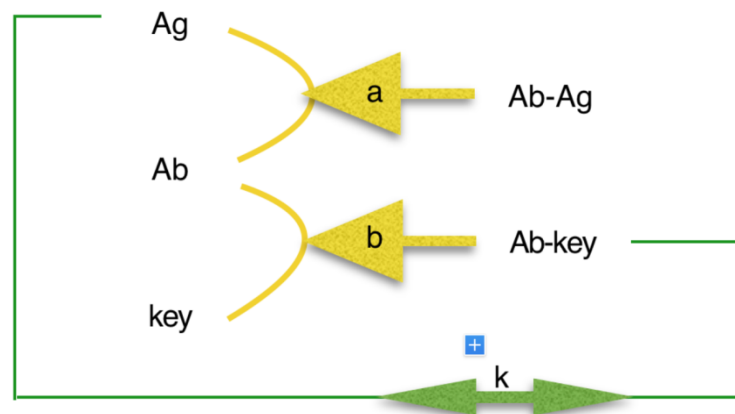
Variable	Description
X1	the amount of Ag
X2	the amount of Ab with Ag
t	time
c	the inchoate value of X1
E	the extend of combination

We have acknowledged that one Ab with key + one Ag coming into one Ab with Ag and one key is irreversible and the amount of this kind of changes is related to X1, X2 and time.

In this picture, we assume that there are some ideal conversion rates when the experiment happening: **k** (from Ab-key to Ag and from Ag to Ab-key), **a**(from Ab-Ag to Ag and Ab) and **b**(from Ab-key to Ab and key).

we can know that

K: —a regular value which is related to affinity(f) between one Ab with key and one Ag which is defined as p,

so we can attain an another equation: k=pf.

According to the first equation above, we can know that 'x2=x1+m'.

dx1/dt=dx2/dt=-k*x1*x2'
'k=pf'
'x2=x1+m'

And the program code of matlab is:
dsolve('Dx1=-p*f*x1*(x1+m)','x1(0)=c','t')
ans =m/(exp(m*(log((m + c)/c)/m + f*p*t)) - 1)

x1= m/(exp(m*(log((m + c)/c)/m + f*p*t)) - 1)

'E=(x0-x1)/x1' which is simplified as
'E=1- m/((exp(m*(log((m + c)/c)/m + f*p*t)) - 1)*c)'

Variable	Description
X1	the amount of Ag
X2	the amount of Ab with Ag
X3	the amount of Ab
X4	the amount of key
X5	the amount of Ab with key

Variable	Description
b	the ratio of separability between Ab and key
c	the inchoate value of X1
d	the inchoate value of X2
E	the extend of combination
t	time

We can get:

'dx1/dt=a*x5-k*x1*x2'
'dx2/dt=-b*x2-k*x1*x2'
'dx3/dt=a*x5+b*x2'
'dx4/dt=b*x2+k*x1*x2'
'dx5/dt=-a*x5+k*x1*x2',
by using Volterra Model.

Due to the fact that the amount of Ab,Ag,and key is regular,we can acquire 3 equations:
'x1+x5=c;
x2+x4=d;
x2+x5+x3=d'

We assume that
x3(0)=x4(0)=x5(0)=0.

dsolve('Dx3=a*(c-x1)+b*x2','x3(0)=0','t')
 ans = t*(a*c - a*x1 + b*x2)

So
according the equations above,
x3=x1-x2+d-c.
So
[x1]=dsolve('Dx1=a*(c-x1)-k*x1*x2','x1(0)=c','t')
 x1 = (a*c + c*k*x2*exp(-t*(a + k*x2)))/(a + k*x2)

So we can input the value of x2.

sym x1;
[x1]=solve('(a*c+c*k*(((a*t+1)*x1+d-c-a*c*t)/(b*t+1))*exp(-t*(a+ k*(((a*t
+1)*x1+d-c-a*c*t)/(b*t+1)))))/(a + k*(((a*t+1)*x1+d-c-a*c*t)/(b*t+1)))')
x1 =(c - d + a*c*t - ((b*t + 1)*lambertw(l, a*t*exp(a*t)))/(k*t))/(a*t + 1)
<<NOTE: The solutions are valid under the following conditions: (a*t*exp(a*t)
~= 0 | l == 0) & (lambertw(l, a*t*exp(a*t)) ~= a*t | t ==
0) & t ~= 0 & in(l, 'integer')>>

By inputting k=f*p

As what we have defined above

Variable	Description
X1	the amount of Ag
X2	the amount of Ab with key
b	the possibility of the occurrence of the reaction
c	the ratio of the proliferation of Ab with key
a	the ratio of the proliferation of Ag
E	the extend of combination
K1	the max amount of the Ag in the target realm
K2	the max amount of Ab-key
t	time

By acquiring the 'E' in the target realm ,we can know the exact situation in a short time, and we can know the least dosage in a short time. On the next step we will consider the factor of their own proliferation, but if we still consider the separability, it will increase the complexity of the whole system and won't help the accuracy a lot. By using the model below, we can know the general dosage of Ab-key and we can design the cycle of injection of Ab-key.

We can also combine our modeling system with Volterra model to judge the least dosage because the Ag often has mass poliferation that affects the system a lot. We have acknowledged that one Ab with key + one Ag coming into one Ab with Ag and one key is irreversible and the amount of this kind of changes is related to the amount of Ab with key($x2$) , the amount of Ag ($x1$) and time.

We can acquire b which is related to the affinity(f) between one Ab with key and one Ag which is defined as p,and c and a.

So we can acquire the equations below.
$dx1/dt=a*x1-b*x1*x2$ 1
$dx2/dt=c*x2-b*x1*x2$ 2

Because those are Nonlinear ordinary differential equations, we have to change them into linear equations;
$dx1/dt=a*x1-b*x1*x2=x1*(a-b*x2)=0$ 3
$dx2/dt=c*x2-b*x1*x2=x2*(c-b*x1)=0$ 4

So we have two groups of solutions:
$x1=0,x2=0$ 5
$x1=c/b,x2=a/b$ ......6.

So we can get two linear equation groups:
$dx1/dt=a*x1;$
$dx2/dt=c*x2;$

So we have two groups of solutions:
$x1=0,x2=0;5$
$x1=c/b,x2=a/b;6.$

So we can get two linear equation groups:
$dx1/dt=a*x1;$
$dx2/dt=c*x2;$
The matrix is C1 ;7
$dx1/dt=-c*x2+a*c/b;$
$dx2/dt=-a*x1+ a*c/b;$
The matrix is C2;8

By using the quation' $| \lambda E-C | =0$',we can acquire the eigenroots of the equations.It
is not difficult to find that only the latter group has the eigenroots that are both
below zero,so only the latter group has the stable solutions.

We can also acquire the inchoate amount of the Ag(d)and that of the Ab with key(e).

The Matlab program codes:

'E=(x0-x1)/x1' which is simplified as

We can also acquire the max amount of the Ag in the target realm(K1),and also we can control the max amount of Ab-key(K2)

	(K1 > K2/b*a) Ag can repress Ab-key	(K1 < K2/c*b) Ag can't repress Ab-key
(K2 > K1/b*c) Ab-key can repress Ag	Not sure whether Ag is out of control	Ag is in control
(K2 < K1/a*b) Ab-key can't repress Ag	Ag isn't in control	Ag is in control

$$x1 / dt = a*x1 \ (1 - x1/ K1 - b*c*x2 / K1 = 0 \ldots\ldots\ (1)$$
$$x2/ dt = b*x2 \ (1 - x2 / K2 - a*c*x1/ K2 = 0 \ldots\ldots\ (2)$$

By using the equations above ,we can find the equilibrium point.
'E=(x0-x1)/x1' which is simplified as