

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_a(\text{HG})$ value lower boundary [1/M]

10

$K_a(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(\text{O})$ value lower boundary

0

$I(\text{O})$ value upper boundary

1000

$I(\text{D})$ value lower boundary [1/M]

0

$I(\text{D})$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Initializing...

Thermosimfit

Data import

DBA (const. host) model

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IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_d(\text{HG})$ value lower boundary [1/M]

10

$K_d(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(\text{O})$ value lower boundary

0

$I(\text{O})$ value upper boundary

1000

$I(\text{D})$ value lower boundary [1/M]

0

$I(\text{D})$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Initializing...

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

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GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(0) value lower boundary

0

I(0) value upper boundary

1000

I(D) value lower boundary [1/M]

0

I(D) value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 2; Ka(HG) = 2.778e+05; I(0) = 8.756e-06; I(HD) = 5.520e+05; I(D) = 7.285e+01; Error = 6.684e+00

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(0) value lower boundary

0

I(0) value upper boundary

1000

I(D) value lower boundary [1/M]

0

I(D) value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 3; Ka(HG) = 2.778e+05; I(0) = 8.756e-06; I(HD) = 5.520e+05; I(D) = 7.285e+01; Error = 6.684e+00

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(0) value lower boundary

0

I(0) value upper boundary

1000

I(D) value lower boundary [1/M]

0

I(D) value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 5; Ka(HG) = 2.778e+05; I(0) = 8.756e-06; I(HD) = 5.520e+05; I(D) = 7.285e+01; Error = 6.684e+00

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_a(\text{HG})$ value lower boundary [1/M]

10

$K_a(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(0)$ value lower boundary

0

$I(0)$ value upper boundary

1000

$I(D)$ value lower boundary [1/M]

0

$I(D)$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 7; $K_a(\text{HG}) = 2.778\text{e}+05$; $I(0) = 8.756\text{e}-06$; $I(\text{HD}) = 5.520\text{e}+05$; $I(D) = 7.285\text{e}+01$; Error = $6.684\text{e}+00$

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

I(D) value lower boundary [1/M]

0

I(D) value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 0; Ka(HG) = 7.398e+05; I(0) = 6.110e-02; I(HD) = 5.060e+05; I(D) = 3.114e+03; Error = 5.283e+00

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

I(D) value lower boundary [1/M]

0

I(D) value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 10; Ka(HG) = 7.198e+05; I(O) = 6.110e-02; I(HD) = 5.066e+05; I(D) = 3.114e+03; Error = 5.283e+00

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

I(D) value lower boundary [1/M]

0

I(D) value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 11; Ka(HG) = 5.318e+06; I(O) = 1.985e-01; I(HD) = 4.272e+05; I(D) = 9.849e+03; Error = 5.843e+09

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_a(\text{HG})$ value lower boundary [1/M]

10

$K_a(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(\text{O})$ value lower boundary

0

$I(\text{O})$ value upper boundary

1000

$I(\text{D})$ value lower boundary [1/M]

0

$I(\text{D})$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 13; $K_a(\text{HG}) = 5.318\text{e}+06$; $I(\text{O}) = 1.985\text{e}-01$; $I(\text{HD}) = 4.272\text{e}+05$; $I(\text{D}) = 9.849\text{e}+03$; Error = 5.843\text{e}+09

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_a(\text{HG})$ value lower boundary [1/M]

10

$K_a(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(\text{O})$ value lower boundary

0

$I(\text{O})$ value upper boundary

1000

$I(\text{D})$ value lower boundary [1/M]

0

$I(\text{D})$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 14; $K_a(\text{HG}) = 1.119\text{e}+07$; $I(\text{O}) = 2.030\text{e}-01$; $I(\text{HD}) = 4.526\text{e}+05$; $I(\text{D}) = 9.497\text{e}+03$; Error = 3.835\text{e}+09

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_a(\text{HG})$ value lower boundary [1/M]

10

$K_a(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(\text{O})$ value lower boundary

0

$I(\text{O})$ value upper boundary

1000

$I(\text{D})$ value lower boundary [1/M]

0

$I(\text{D})$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 16; $K_a(\text{HG}) = 3.382\text{e}+06$; $I(\text{O}) = 1.424\text{e}-01$; $I(\text{HD}) = 5.435\text{e}+05$; $I(\text{D}) = 6.579\text{e}+03$; Error = 3.689\text{e}+09

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_a(\text{HG})$ value lower boundary [1/M]

10

$K_a(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(0)$ value lower boundary

0

$I(0)$ value upper boundary

1000

$I(D)$ value lower boundary [1/M]

0

$I(D)$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 17; $K_a(\text{HG}) = 3.382\text{e}+06$; $I(0) = 1.424\text{e}-01$; $I(\text{HD}) = 5.435\text{e}+05$; $I(D) = 6.579\text{e}+03$; Error = 3.689\text{e}+09

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_d(\text{HD})$ [1/M]

3000000

Advanced options

Boundaries

$K_a(\text{HG})$ value lower boundary [1/M]

10

$K_a(\text{HG})$ value upper boundary [1/M]

100000000

$I(\text{HD})$ value lower boundary [1/M]

0

$I(\text{HD})$ value upper boundary [1/M]

1000000

$I(\text{O})$ value lower boundary

0

$I(\text{O})$ value upper boundary

1000

$I(\text{D})$ value lower boundary [1/M]

0

$I(\text{D})$ value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 19; $K_a(\text{HG}) = 3.382\text{e}+06$; $I(\text{O}) = 1.424\text{e}-01$; $I(\text{HD}) = 5.435\text{e}+05$; $I(\text{D}) = 6.579\text{e}+03$; Error = 3.689\text{e}+09

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dye) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

I(D) value lower boundary [1/M]

0

I(D) value upper boundary [1/M]

1000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 20; Ka(HG) = 3.382e+06; I(O) = 1.424e-01; I(HD) = 5.425e+05; I(D) = 6.579e+03; Error = 3.689e+00

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dye) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_a(HD) [1/M]

3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

100000000

I(HD) value lower boundary [1/M]

0

I(HD) value upper boundary [1/M]

1000000

I(0) value lower boundary

0

I(0) value upper boundary

1000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Showing 1 to 1 of 1 entries

Search:

	K _a (HG) [M]	I(0)	I(HD) [1/M]	I(D) [1/M]
1	3.38e+6	0.142	5.43e+5	6.58e+3

Showing 1 to 1 of 1 entries

Previous

1

Next

Search:

Error Metrics: Comparison of in silico signal and measured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R ²	R ² adjusted
1	0.00349967	0.0591580	0.0316751	0.938013	0.936748

Showing 1 to 1 of 1 entries

Previous

1

Next

Signal [a.u.]

total Guest measured [M]

Dye [M]

total Guest measured [M]

Host-Dye [M]

total Guest measured [M]