

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

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...

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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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 = 4; K<sub>a</sub>(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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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 = 6; 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 = 9;  $K_a(\text{HG}) = 7.398\text{e}+05$ ;  $I(0) = 6.110\text{e}-02$ ;  $I(\text{HD}) = 5.066\text{e}+05$ ;  $I(D) = 3.114\text{e}+03$ ; Error =  $5.283\text{e}+00$

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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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 = 12; Ka(HG) = 5.318e+06; I(O) = 1.985e-01; I(HD) = 4.272e+05; I(D) = 9.849e+03; Error = 5.843e+09

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

$I(\text{O})$  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 = 15;  $K_a(\text{HG}) = 1.119\text{e}+07$ ;  $I(\text{O}) = 2.030\text{e}-01$ ;  $I(\text{HD}) = 4.526\text{e}+05$ ;  $I(\text{D}) = 9.497\text{e}+03$ ; 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

$I(\text{O})$  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 = 18;  $K_a(\text{HG}) = 3.382\text{e}+06$ ;  $I(\text{O}) = 1.424\text{e}-01$ ;  $I(\text{HD}) = 5.435\text{e}+05$ ;  $I(\text{D}) = 6.579\text{e}+03$ ; 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

$K_d(\text{HD})$  [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 = 20;  $K_a(\text{HG}) = 3.382\text{e}+06$ ;  $I(\text{O}) = 1.424\text{e}-01$ ;  $I(\text{HD}) = 5.435\text{e}+05$ ;  $I(\text{D}) = 6.579\text{e}+03$ ; Error = 3.689\text{e}+00

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 = 22;  $K_a(\text{HG}) = 3.382\text{e}+06$ ;  $I(\text{O}) = 1.424\text{e}-01$ ;  $I(\text{HD}) = 5.435\text{e}+05$ ;  $I(\text{D}) = 6.579\text{e}+03$ ; 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

$I(\text{O})$  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 = 23;  $K_a(\text{HG}) = 3.382\text{e}+06$ ;  $I(\text{O}) = 1.424\text{e}-01$ ;  $I(\text{HD}) = 5.435\text{e}+05$ ;  $I(\text{D}) = 6.579\text{e}+03$ ; 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

Help

$K_d(\text{HG})$  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

Sensitivity analysis

Batch processing

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 25;  $K_d(\text{HG}) = 3.382\text{e}+06$ ;  $I(\text{O}) = 1.424\text{e}-01$ ;  $I(\text{HD}) = 5.435\text{e}+05$ ;  $I(\text{D}) = 6.579\text{e}+03$ ; 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

$I(\text{O})$  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 = 27;  $K_a(\text{HG}) = 3.382\text{e}+06$ ;  $I(\text{O}) = 1.424\text{e}-01$ ;  $I(\text{HD}) = 5.435\text{e}+05$ ;  $I(\text{D}) = 6.579\text{e}+03$ ; 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

$K_d(\text{HD})$  [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 = 28;  $K_a(\text{HG}) = 3.382\text{e}+06$ ;  $I(\text{O}) = 1.424\text{e}-01$ ;  $I(\text{HD}) = 5.435\text{e}+05$ ;  $I(\text{D}) = 6.579\text{e}+03$ ; 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

$I(\text{O})$  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 = 38;  $K_a(\text{HG}) = 1.612\text{e}+07$ ;  $I(\text{O}) = 1.980\text{e}-01$ ;  $I(\text{HD}) = 6.781\text{e}+05$ ;  $I(\text{D}) = 2.824\text{e}+03$ ; Error = 2.385\text{e}+00

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 = 32;  $K_a(\text{HG}) = 1.612\text{e}+07$ ;  $I(\text{O}) = 1.980\text{e}-01$ ;  $I(\text{HD}) = 6.781\text{e}+05$ ;  $I(\text{D}) = 2.824\text{e}+03$ ; Error = 2.385\text{e}+00

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 = 33;  $K_a(\text{HG}) = 1.612\text{e}+07$ ;  $I(\text{O}) = 1.980\text{e}-01$ ;  $I(\text{HD}) = 6.781\text{e}+05$ ;  $I(\text{D}) = 2.824\text{e}+03$ ; Error = 2.385\text{e}+00

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

$K_d(\text{HG})$  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

Generation = 35;  $K_d(\text{HG}) = 1.612\text{e}+07$ ;  $I(\text{O}) = 1.980\text{e}-01$ ;  $I(\text{HD}) = 6.781\text{e}+05$ ;  $I(\text{D}) = 2.824\text{e}+03$ ; Error = 2.385\text{e}+00

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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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 = 36; Ka(HG) = 3.838e+07; I(O) = 1.955e-01; I(HD) = 9.947e+05; I(D) = 9.861e+03; Error = 1.515e+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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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 = 38; Ka(HG) = 3.838e+07; I(O) = 1.955e-01; I(HD) = 9.947e+05; I(D) = 9.861e+03; Error = 1.515e+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 = 48;  $K_a(\text{HG}) = 1.873\text{e}+07$ ;  $I(\text{O}) = 1.975\text{e}-01$ ;  $I(\text{HD}) = 7.549\text{e}+05$ ;  $I(\text{D}) = 1.868\text{e}+04$ ; Error =  $1.287\text{e}+09$

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 = 42;  $K_a(\text{HG}) = 1.873\text{e}+07$ ;  $I(\text{O}) = 1.975\text{e}-01$ ;  $I(\text{HD}) = 7.549\text{e}+05$ ;  $I(\text{D}) = 1.808\text{e}+04$ ; Error =  $1.287\text{e}+09$

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 = 43;  $K_a(\text{HG}) = 1.873\text{e}+07$ ;  $I(\text{O}) = 1.975\text{e}-01$ ;  $I(\text{HD}) = 7.549\text{e}+05$ ;  $I(\text{D}) = 1.808\text{e}+04$ ; Error =  $1.287\text{e}+09$

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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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 = 45; Ka(HG) = 1.873e+07; I(O) = 1.975e-01; I(HD) = 7.549e+05; I(D) = 1.808e+04; Error = 1.287e+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 = 46;  $K_a(\text{HG}) = 1.873\text{e}+07$ ;  $I(\text{O}) = 1.975\text{e}-01$ ;  $I(\text{HD}) = 7.549\text{e}+05$ ;  $I(\text{D}) = 1.868\text{e}+04$ ; Error = 1.287\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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(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

Step optimization

Save result of optimization

Choose file type:

Excel

Show 10 entries

Search:

	K <sub>a</sub> (HG) [M]	I(0)	I(HD) [1/M]	I(D) [1/M]
1	1.83e+7	0.179	8.36e+5	8.42e+3

Showing 1 to 1 of 1 entries

Previous 1 Next

Show 10 entries

Search:

Error Metrics: Comparison of in silico signal and measured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R <sup>2</sup>	R <sup>2</sup> adjusted
1	0.0000343699	0.00586224	0.00500560	0.999833	0.999830

Showing 1 to 1 of 1 entries

Previous 1 Next

Signal [a.u.]

Host-Dye [M]

Dye [M]

total Guest measured [M]

Measured

Predicted

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<sub>a</sub>(HD) [1/M]

3000000

Advanced options

Boundaries

Help

K<sub>a</sub>(HG) value lower boundary [1/M]

-10

K<sub>a</sub>(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

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 21; K<sub>a</sub>(HG) = 2.850e+07; I(0) = 0.000e+00; I(HD) = 1.000e+06; I(D) = 2.020e+05; Error = 1.941e+00