

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Initializing...

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

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. 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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 3; Ka(HG) = 2.906e+03; I(O) = 2.405e-01; I(HD) = 1.040e+02; I(D) = 9.564e-03; Error = 9.198e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 5; Ka(HG) = 8.9851e+04; I(O) = 1.0000e-15; I(HD) = 4.984e+05; I(D) = 1.0890e+04; Error = 8.867e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 7; Ka(HG) = 5.912e+04; I(O) = 1.000e-15; I(HD) = 4.529e+05; I(D) = 8.080e+03; Error = 8.461e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 9; K_a(HG) = 5.912e+04; I(O) = 1.000e-15; I(HD) = 4.529e+05; I(D) = 8.089e+03; Error = 8.461e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 12; Ka(HG) = 4.338e+06; I(O) = 1.080e-15; I(HD) = 1.059e+06; I(D) = 6.855e+04; Error = 4.346e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 13; Ka(HG) = 4.338e+06; I(O) = 1.080e-15; I(HD) = 1.050e+06; I(D) = 6.855e+04; Error = 4.346e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 15; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 17; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+00

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

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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 19; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 21; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 23; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 25; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 27; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 29; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 31; Ka(HG) = 0.922e+06; I(O) = 1.000e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 33; Ka(HG) = 7.818e+06; I(O) = 1.000e-15; I(HD) = 8.950e+05; I(D) = 1.631e+05; Error = 1.959e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 36; Ka(HG) = 7.818e+06; I(O) = 1.000e-15; I(HD) = 8.950e+05; I(D) = 1.631e+05; Error = 1.959e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 38; Ka(HG) = 7.818e+06; I(O) = 1.000e-15; I(HD) = 8.950e+05; I(D) = 1.631e+05; Error = 1.959e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 40; Ka(HG) = 7.818e+06; I(O) = 1.000e-15; I(HD) = 8.950e+05; I(D) = 1.631e+05; Error = 1.959e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 41; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 43; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 46; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 48; K_a(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 50; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 53; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 55; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 56; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+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]

1e+08

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

0

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

1e+08

I(O) value lower boundary

0

I(O) value upper boundary

1e+08

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

0

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

1e+08

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 59; Ka(HG) = 1.116e+07; I(O) = 1.000e-15; I(HD) = 1.012e+06; I(D) = 1.720e+05; Error = 1.594e+00

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$K_a(\text{HD})$ [1/M]	3000000

+

10

1e+08

1e+08

1e+08

1e+08

Optimization

Stop optimization

Save result of optimization

Excel

Search:

Search: $I(0)$ $I(0)$

I(HD) [1/M]

I(HD) [1/M]

 $I(D) [1/M]$

1

[Previous](#)

1

Next

Search:

Search:

Error Metrics: Comparison of in silico signal and measured signal

RootMeanSquareError

RootMeanSquareError

MeanAbsoluteError

MeanAbsoluteError

 R^2 R^2

1

[Previous](#)

1

Next

