

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]

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<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]

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<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]

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 = 9.190e+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<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]

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<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]

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 = 6; 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<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]

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 = 9; Ka(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<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]

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 = 11; Ka(HG) = 0.382e+05; I(O) = 1.000e-15; I(HD) = 7.298e+05; I(D) = 1.000e-15; Error = 5.968e+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<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]

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<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]

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 = 14; 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<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]

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 = 16; 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<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]

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

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<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]

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<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]

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<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]

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<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]

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<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]

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<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]

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<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]

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<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]

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 = 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<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]

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<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]

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<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]

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 = 42; 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<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]

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 = 45; 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<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]

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<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]

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 = 48; Ka(HG) = 1.116e+07; I(O) = 1.080e-15; I(HD) = 1.012e+06; I(D) = 1.728e+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<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]

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 = 51; 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<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]

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<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]

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<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]

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<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]

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

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dye) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.00001

Dye conc. [M]

0.00001

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

300000

Advanced options

Boundaries

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

10

K<sub>s</sub>(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(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

Showing 1 to 1 of 1 entries

Search:

	K <sub>s</sub> (HG) [M]	I(D)	I(HD) [1/M]	I(D) [1/M]
1	1.12e+7	1.00e-15	1.01e+6	1.73e+5

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 <sup>2</sup>	R <sup>2</sup> adjusted
1	0.000153293	0.0123812	0.00964823	0.992796	0.992649

Showing 1 to 1 of 1 entries

Previous

1

Next

Signal [a.u.]

Dye [M]

Host-Dye [M]

Thermosimfit

Data import

DBA (const., host) model

DBA (const., dye) model

GDA model

DA 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]

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...

Show 10 entries

Search:

	K <sub>a</sub> (HG) [M]	I(O)	I(HD) [1/M]	I(D) [1/M]
1	1.12e+7	1.00e-15	1.01e+6	1.73e+5

Showing 1 to 1 of 1 entries

Previous1Next

Show 10 entries

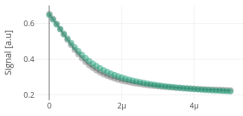
Search:

Error Metrics: Comparison of in silico signal and measured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R <sup>2</sup>	R <sup>2</sup> adjusted
1	0.000153293	0.0123812	0.00964823	0.992796	0.992649

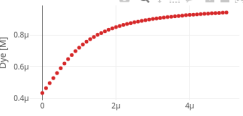
Showing 1 to 1 of 1 entries

Signal [a.u.]



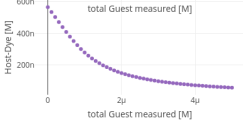
total Guest measured [M]

Dye [M]



total Guest measured [M]

Host-Dye [M]



total Guest measured [M]



Thermosimfit

Data import

DBA (const., host) model

DBA (const., dye) model

GDA model

DA 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]

1

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

0

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

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...

Show 10 entries

Search:

	K <sub>a</sub> (HG) [M]	I(D)	I(HD) [1/M]	I(D) [1/M]
1	1.12e+7	1.00e-15	1.01e+6	1.73e+5

Showing 1 to 1 of 1 entries

Previous1Next

Show 10 entries

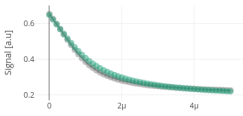
Search:

Error Metrics: Comparison of in silico signal and measured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R <sup>2</sup>	R <sup>2</sup> adjusted
1	0.000153293	0.0123812	0.00964823	0.992796	0.992649

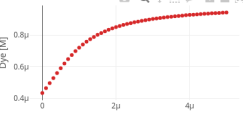
Showing 1 to 1 of 1 entries

Signal [a.u.]



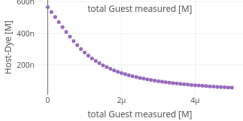
total Guest measured [M]

Dye [M]



total Guest measured [M]

Host-Dye [M]



total Guest measured [M]