

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

300000

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(D) value lower boundary [1/M]

0

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

1e+08

Optimization

Start Optimization

Stop Optimization

Get Status

Save result of optimization

Choose file type:

Excel

306/306; kX = 1.585e+7, I0 = 1.000e-15, IHD = 9.691e+05, ID = 1.905e+05 ; Error: 5.553e-01

Show 10 entries

Search:

	K <sub>a</sub> (HG) [M]	I(0)	I(HD) [1/M]	I(D) [1/M]
1	1.58e+7	1.00e-15	9.69e+5	1.90e+5

Showing 1 to 1 of 1 entries

Previous1Next

Show 10 entries

Search:

Error Metrics: Comparison of in silico signal and seassured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R <sup>2</sup>	R <sup>2</sup> adjusted
1	0.0000419371	0.00647589	0.00406907	0.998875	0.998852

Showing 1 to 1 of 1 entries

Previous1Next

Signal

guest [M]

group

measured

predicted

4x10<sup>-7</sup>

1e-07

1e-06

1e-05

1e-04

1e-03

1e-02

1e-01

1e-07

1e-06

1e-05

1e-04

1e-03

1e-02

1e-01

1e-07

1e-06

1e-05

1e-04

1e-03

1e-02

1e-01

## Host conc. [M]

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

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

3000000

### Advanced options

+

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

10

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

1e+08

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

0

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

1e+08

I(0) value lower boundary

1

l(0) value upper boundary

1e+08

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

1

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

1e+08

Optimization	Sensitivity analysis	Batch processing
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±/- boundary in [%]

15

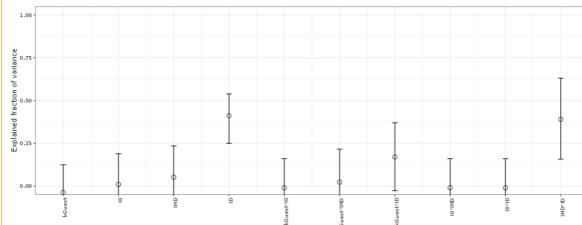
Start Sensitivity analysis

Cancel

Get Status

Save result of sensitivity analysis

Running... 100% Complete



Explained fraction of variance

