

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dye) model

GBA model

IDA model

Info

Parameter

Host conc. [M]

0.00000165

Guest conc. [M]

0.00000132

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

17000000

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]

10000000000

I(0) value lower boundary

0

I(0) 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

Get Status

Save result of optimization

Choose file type:

Excel

Show 10 entries

Search:

	K <sub>a</sub> (HG) [M]	I(0)	I(HD)	I(D)
1	1.25e+6	244	3.32e+9	1.00e-15

Showing 1 to 1 of 1 entries

Previous1Next

Show 10 entries

Search:

Error Metrics: Comparison of in silico signal and seasured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R <sup>2</sup>	R <sup>2</sup> adjusted
1	4,525.20	67.2696	47.9548	0.998895	0.998816

Showing 1 to 1 of 1 entries

Previous1Next

Signal

dye [M]

group measured predicted

dye [M]

Host Conc [M]

dye [M]

Host conc. [M]	0.00000165
Guest conc. [M]	0.00000132
$K_a(\text{HD})$ [1/M]	17000000

+

1e+08

Help

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

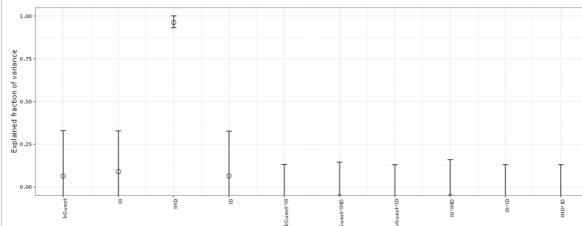
10000000000

1e+08

1e+08

### Sensitivity analysis

Cancel



Explained fraction of variance

