Thermosimfit

- Data import
- DBA (const. host) model
- DBA (const. dye) model
- GDA model
- IDA model
- Info

Parameter

Host conc. [M]

0.00000165

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options +

Boundaries Help

K_a(HG) value lower boundary [1/M]

10

K_a(HG) value upper boundary [1/M]

1e+08

I(0) value lower boundary

0

I(0) value upper boundary

1e+08

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

0

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

10000000000

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

0

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

1e+08

Optimization | Sensitivity analysis

Optimization

Start Optimization | Stop Optimization | Get Status | Save result of optimization

Choose file type:

Excel

```
300/300; kX  =  1.249e+06, I0  =  2.440e+02, IHD  =  3.317e+09, ID  =  1.000e-15 ; Error:  2.986e-01
```

Show 10 entries — Search:

	K_a(HG) [M]	I(0)	I(HD)	I(D)
1	1.25e+6	244	3.32e+9	1.00e-15

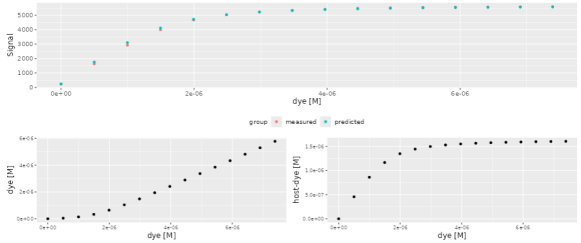
Showing 1 to 1 of 1 entries — Previous 1 Next

Show 10 entries — Search:

Error Metrics: Comparison of in silico signal and seasured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R^2	R^2 adjusted
1	4,525.20	67.2696	47.9548	0.998895	0.998816

Showing 1 to 1 of 1 entries — Previous 1 Next



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10000000000

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

0

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

1e+08

Optimization | Sensitivity analysis

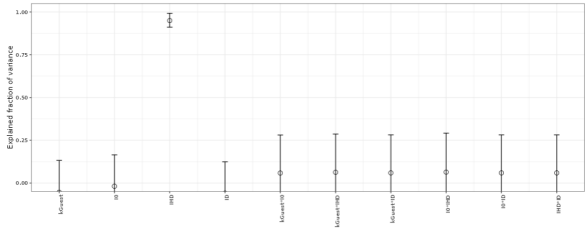
Sensitivity analysis

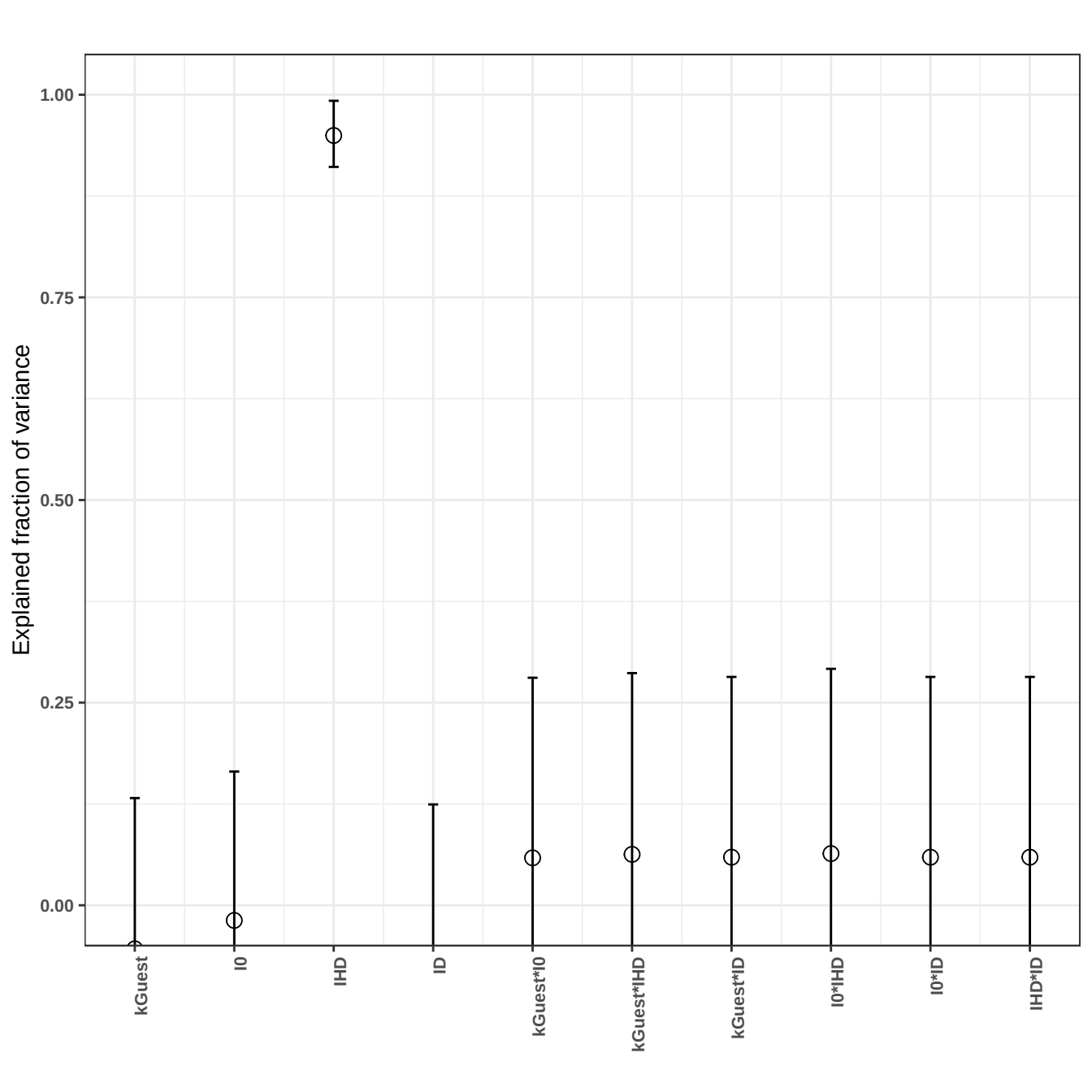
+/- boundary in [%]

15

Start Sensitivity analysis | Cancel | Get Status | Save result of sensitivity analysis

```
Running... 100% Complete
```




Explained fraction of variance
1.00
0.75
0.50
0.25
0.00
kGuest
I0
IHD
ID
kGuest*I0
kGuest*IHD
kGuest*ID
I0*IHD
I0*ID
IHD*ID