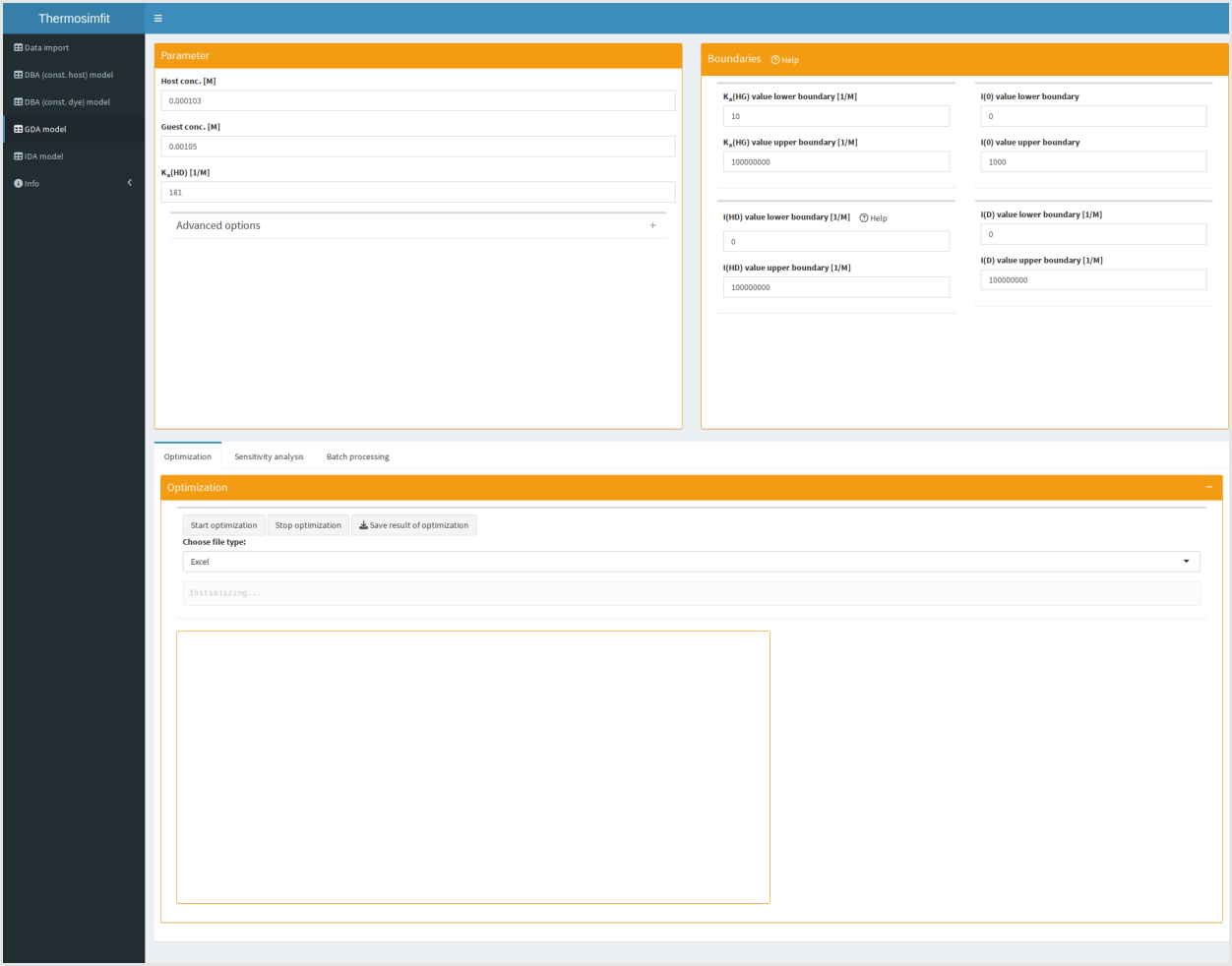
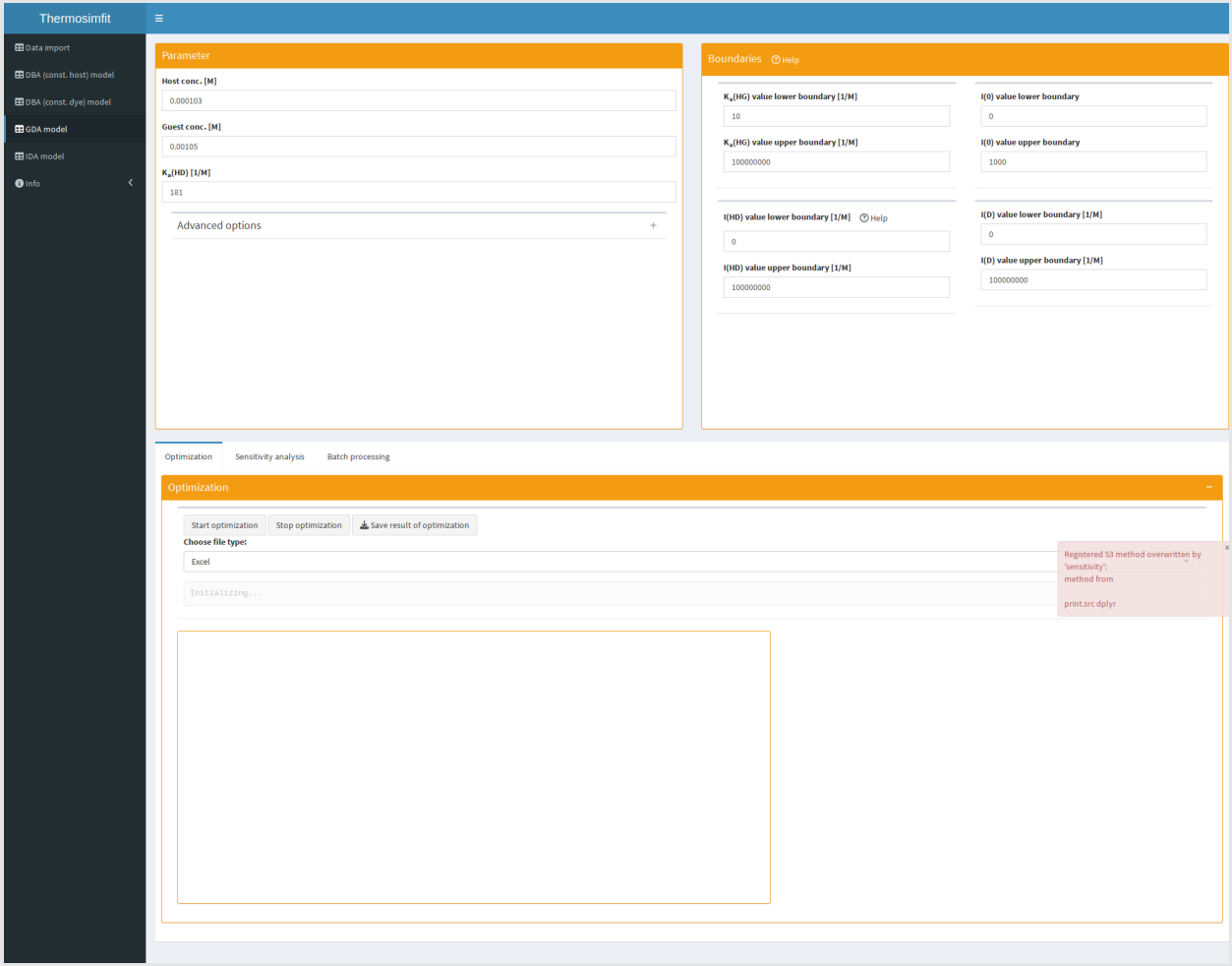
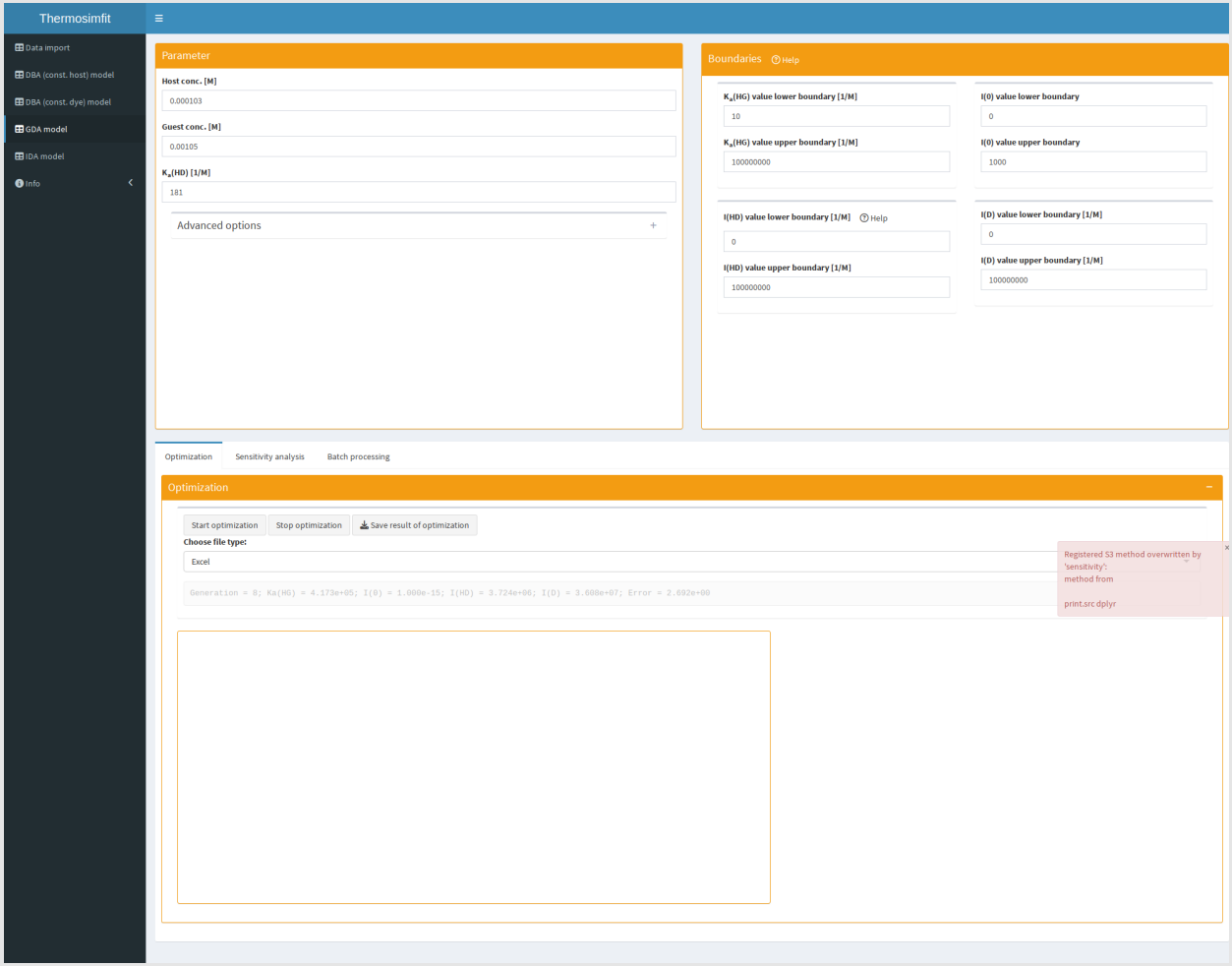
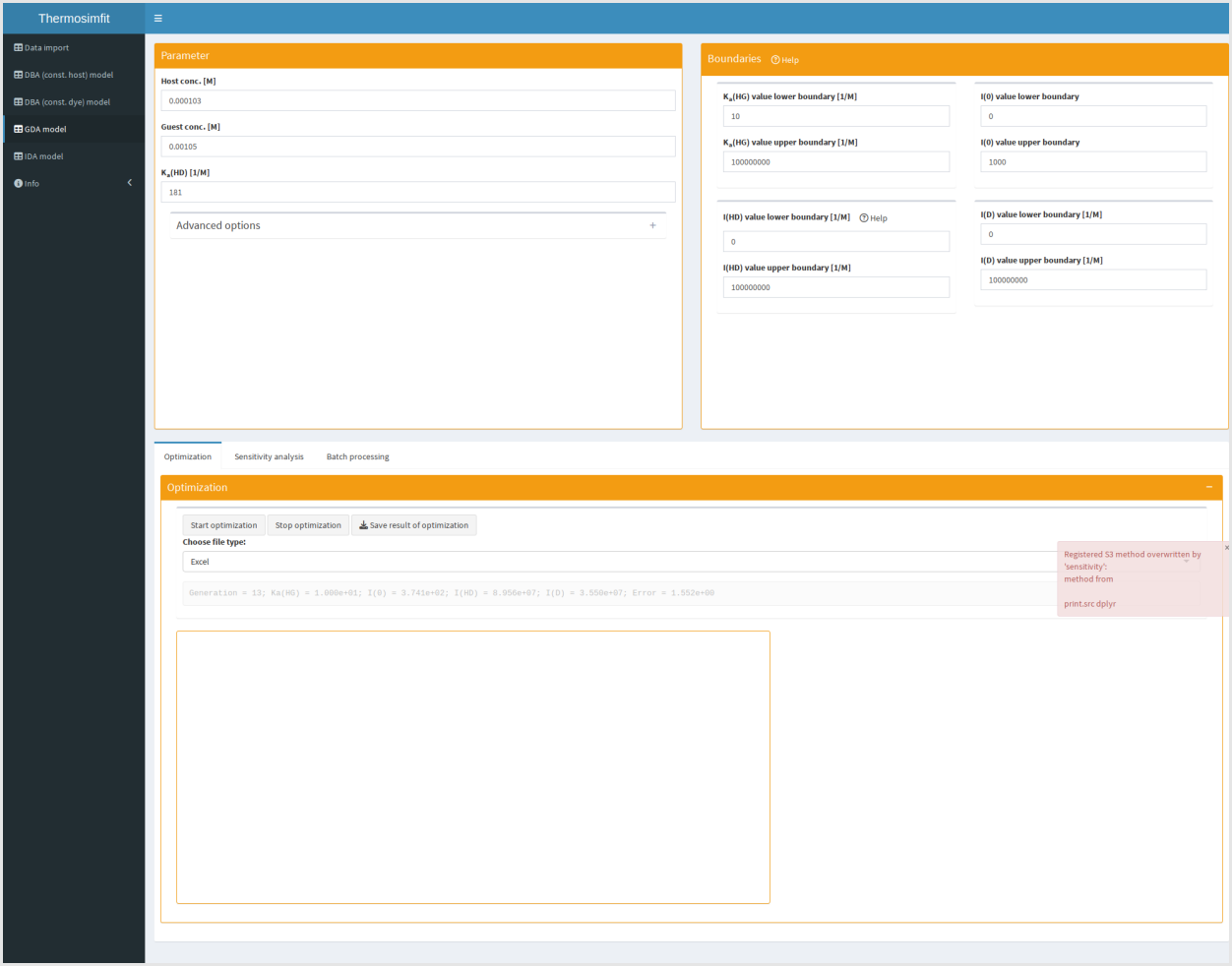
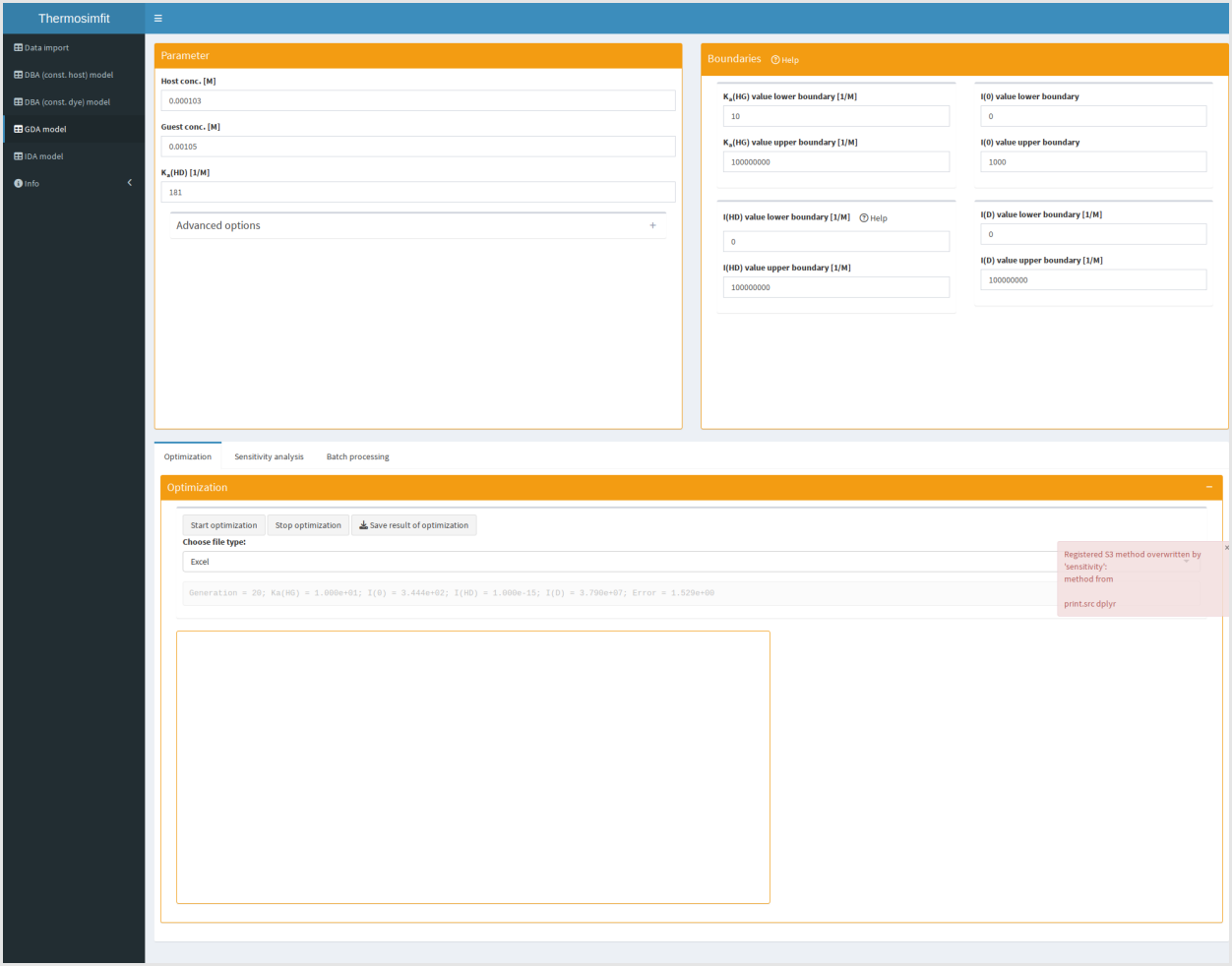
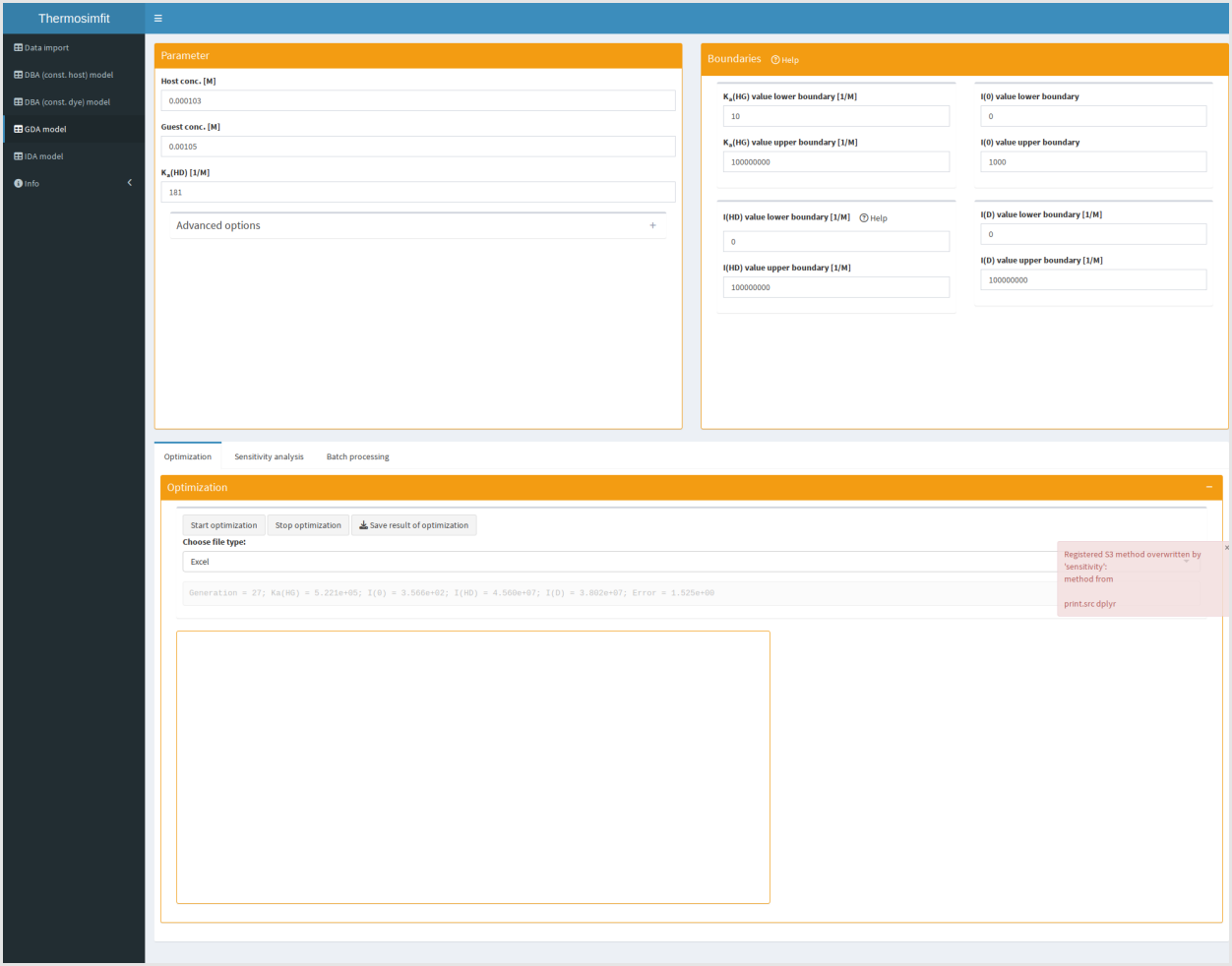

Thermosimfit
Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info
Parameter
Host conc. [M]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Initializing...

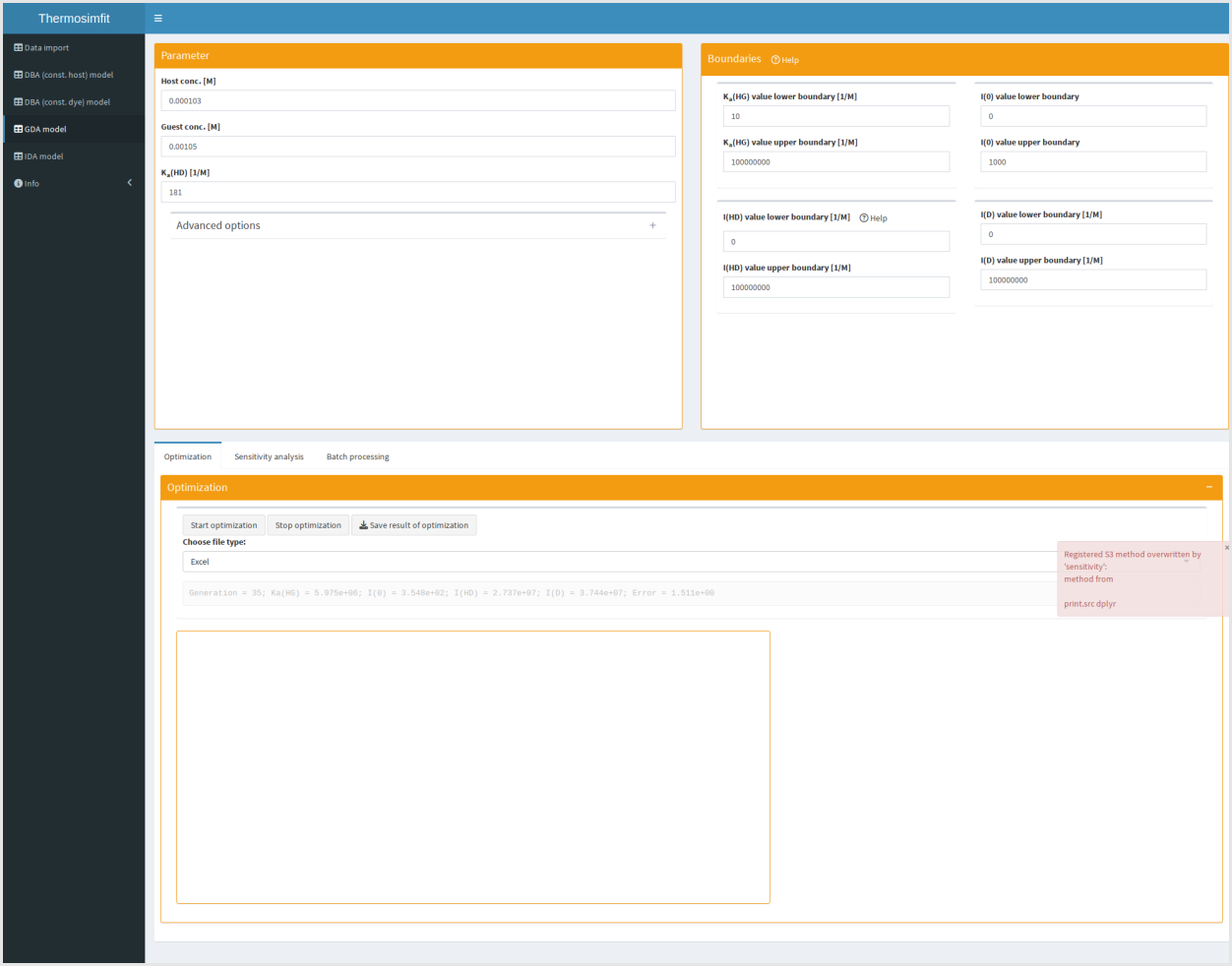

Thermosimfit
Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info
Parameter
Host conc. [M]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
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

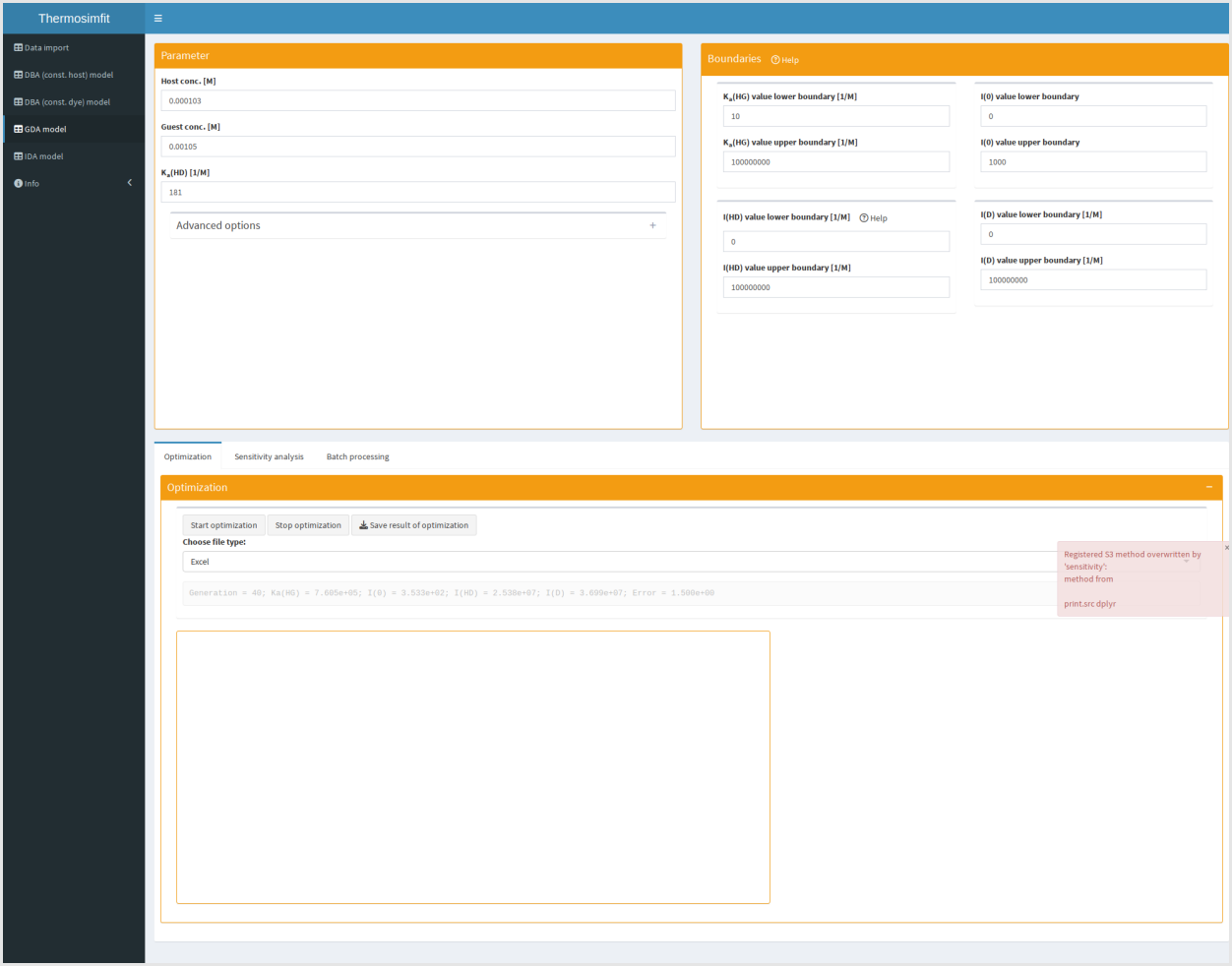

Thermosimfit
Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info
Parameter
Host conc. [M]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 8; Ka(HG) = 4.173e+05; I(0) = 1.000e-15; I(HD) = 3.724e+06; I(D) = 3.608e+07; Error = 2.692e+00
Registered S3 method overwritten by 'sensitivity':
method from
print.src dplyr

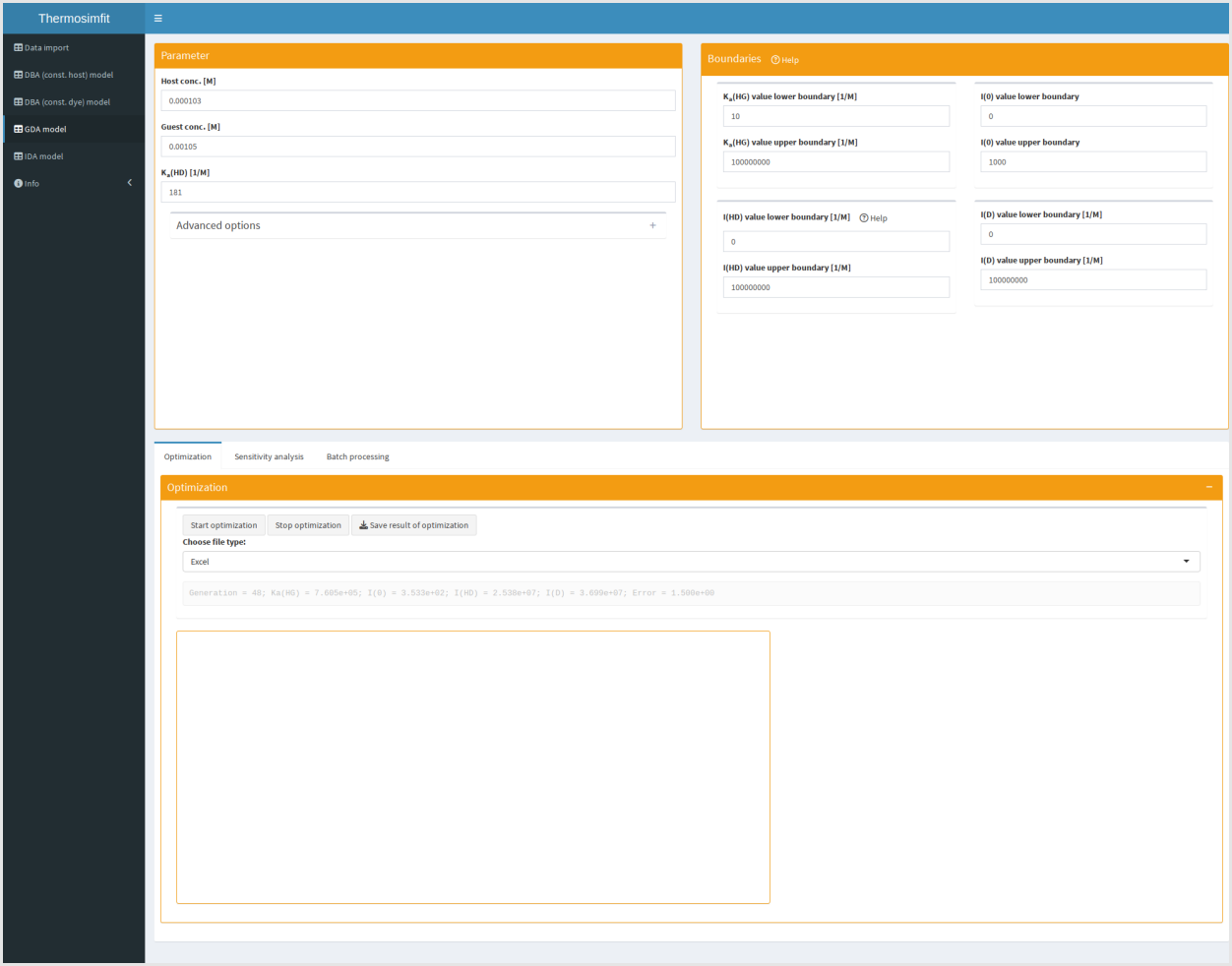

Thermosimfit
Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info
Parameter
Host conc. [M]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 13; Ka(HG) = 1.000e+01; I(0) = 3.741e+02; I(HD) = 8.956e+07; I(D) = 3.550e+07; Error = 1.552e+00
Registered S3 method overwritten by 'sensitivity':
method from
print.src dplyr

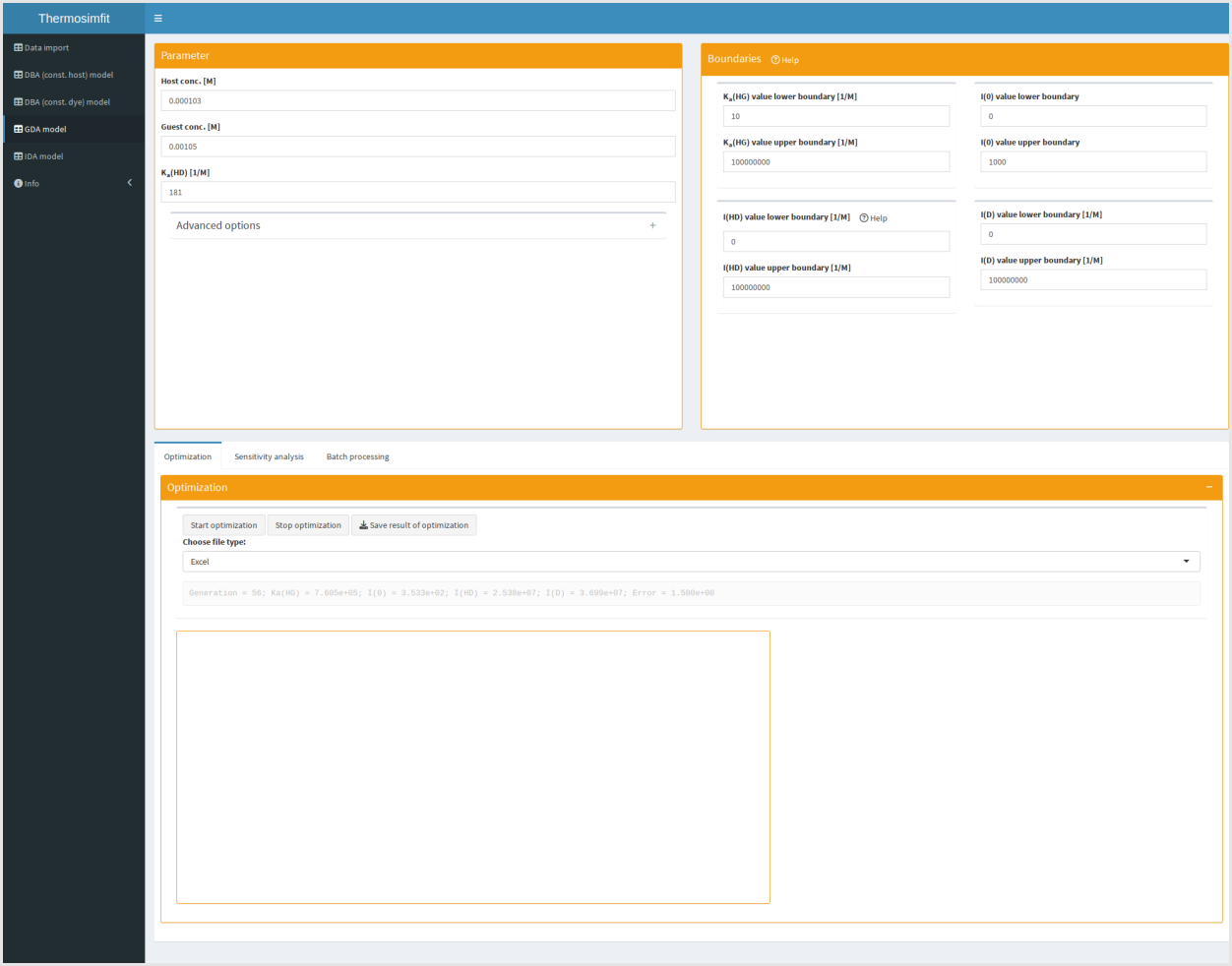

Thermosimfit
Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info
Parameter
Host conc. [M]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 20; Ka(HG) = 1.000e+01; I(0) = 3.444e+02; I(HD) = 1.000e-15; I(D) = 3.790e+07; Error = 1.529e+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]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 27; Ka(HG) = 5.221e+05; I(0) = 3.566e+02; I(HD) = 4.560e+07; I(D) = 3.802e+07; Error = 1.525e+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]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 35; Ka(HG) = 5.975e+06; I(0) = 3.548e+02; I(HD) = 2.737e+07; I(D) = 3.744e+07; Error = 1.511e+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]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 40; Ka(HG) = 7.605e+05; I(0) = 3.533e+02; I(HD) = 2.538e+07; I(D) = 3.699e+07; Error = 1.500e+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]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 48; Ka(HG) = 7.605e+05; I(0) = 3.533e+02; I(HD) = 2.538e+07; I(D) = 3.699e+07; Error = 1.500e+00


Thermosimfit
Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info
Parameter
Host conc. [M]
0.000103
Guest conc. [M]
0.00105
K_a(HD) [1/M]
181
Advanced options
Boundaries
Help
K_a(HG) value lower boundary [1/M]
10
K_a(HG) value upper boundary [1/M]
100000000
I(0) value lower boundary
0
I(0) value upper boundary
1000
I(HD) value lower boundary [1/M]
Help
0
I(HD) value upper boundary [1/M]
100000000
I(D) value lower boundary [1/M]
0
I(D) value upper boundary [1/M]
100000000
Optimization
Sensitivity analysis
Batch processing
Optimization
Start optimization
Stop optimization
Save result of optimization
Choose file type:
Excel
Generation = 56; Ka(HG) = 7.605e+05; I(0) = 3.533e+02; I(HD) = 2.538e+07; I(D) = 3.699e+07; Error = 1.500e+00

Thermosimfit

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

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K_a(HD) [1/M]

181

Advanced options +

Boundaries Help

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

10

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

100000000

I(0) value lower boundary

0

I(0) value upper boundary

1000

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

0

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

100000000

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

0

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

100000000

Optimization | Sensitivity analysis | Batch processing

Optimization

Start optimization | Stop optimization | Save result of optimization

Choose file type:

Excel

Show 10 entries Search:

	K_a(HG) [M]	I(0)	I(HD) [1/M]	I(D) [1/M]
1	7.61e+5	353	2.54e+7	3.70e+7

Showing 1 to 1 of 1 entries Previous 1 Next

Show 10 entries Search:

Error Metrics: Comparison of in silico signal and measured signal

	MeanSquareError	RootMeanSquareError	MeanAbsoluteError	R^2	R^2 adjusted
1	3.44841e+6	1,856.99	1,492.01	0.956781	0.952459

Showing 1 to 1 of 1 entries Previous 1 Next