

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Initializing...

Registered S3 method overwritten by 'sensitivity':
method from
print.src.dplyr

The screenshot shows the Thermosimfit application window. On the left, a sidebar lists various models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' button. The main area has two tabs: 'Parameter' and 'Boundaries'. Under 'Parameter', there are three input fields: 'Host conc. [M]' (0.000001), 'Dye conc. [M]' (0.000001), and 'K_a(HD) [1/M]' (3000000). An 'Advanced options' section is partially visible. Under 'Boundaries', there are six input fields for concentration boundaries: K_a(HG) lower (10), K_a(HG) upper (1e+08), I(0) lower (0), I(0) upper (1e+08), I(HD) lower (0), and I(HD) upper (1e+08). Below these tabs are buttons for Optimization, Sensitivity analysis (which is active), and Batch processing. A 'Sensitivity analysis' dialog is open, showing '+/- boundary in [%]' set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A status message 'Initializing...' is displayed. A pink status bar at the bottom right indicates: 'Registered S3 method overwritten by 'sensitivity': method from print.src.dplyr'. The overall interface is clean with orange and grey accents.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 1%

Registered S3 method overwritten by 'sensitivity':
method from
print_src.dplyr

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large central area is labeled 'Sensitivity analysis' and contains a '+/- boundary in [%]' field set to 15, along with 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis' buttons. A progress bar indicates the task is 'Completed: 1%'. A pink status bar at the bottom right provides information about registered methods.

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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 2%

Registered S3 method overwritten by 'sensitivity':
method from
print_src dplyr

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' panel includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these panels are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A 'Sensitivity analysis' dialog is open, showing a '+/- boundary in [%]' field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A status message indicates 'Completed: 2%' and a note about registered methods. The overall interface has a clean, modern design with orange and grey accents.

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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 4%

Registered S3 method overwritten by 'sensitivity':
method from
print_src_dplyr

The screenshot displays the Thermosimfit software interface. On the left, a sidebar lists various models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' link. The main workspace is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains three input fields: 'Host conc. [M]' set to 0.000001, 'Dye conc. [M]' set to 0.000001, and 'K_a(HD) [1/M]' set to 3000000. An 'Advanced options' button is present. The 'Boundaries' section contains six input pairs for concentration boundaries: K_a(HG) with lower at 10 and upper at 1e+08; I(0) with lower at 0 and upper at 1e+08; I(HD) with lower at 0 and upper at 1e+08; and I(D) with lower at 0 and upper at 1e+08. Below these sections are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large progress bar at the bottom indicates the 'Sensitivity analysis' is completed at 4%. A status message above the progress bar states: '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_a(HD) [1/M]
3000000

Advanced options

Boundaries

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 5%

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a menu icon. On the left, a sidebar lists various models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' button. The main workspace is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains three input fields: 'Host conc. [M]' (0.000001), 'Dye conc. [M]' (0.000001), and 'K_a(HD) [1/M]' (3000000). It also features an 'Advanced options' button. The 'Boundaries' section contains six input pairs for concentration boundaries: K_a(HG) and I(0) both have lower bounds of 10 and upper bounds of 1e+08; I(HD) has a lower bound of 0 and an upper bound of 1e+08; and I(D) has a lower bound of 0 and an upper bound of 1e+08. Below these sections are tabs for 'Optimization', 'Sensitivity analysis' (which is currently selected), and 'Batch processing'. The 'Sensitivity analysis' section includes a '+/- boundary in [%]' input (set to 15), a 'Start Sensitivity analysis' button, a 'Cancel' button, a 'Save result of sensitivity analysis' button, and a progress bar indicating 'Completed: 0%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and Info. The main area is divided into two sections: Parameter and Boundaries. The Parameter section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an Advanced options button. The Boundaries section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The Sensitivity analysis section shows a '+/- boundary in [%]' input field set to 15, and buttons for Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis. A progress bar indicates the task is completed at 0%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a '+/- boundary in [%]' input field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates 'Completed: 0%'.

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_a(HD) [1/M]
3000000

Advanced options

Boundaries

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 10%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a sidebar with model selection (Data import, DBA models, GDA model, IDA model) and an 'Info' button. The main workspace is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' section contains ranges for K_a(HG), I(0), I(HD), and I(D). Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a '+/- boundary in [%]' input set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 10%'. A large orange-outlined rectangular area is present in the bottom right of the main workspace.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 12%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar indicates the completion of a sensitivity analysis task at 12%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 13%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a '+/- boundary in [%]' field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 13%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Completed: 14%

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 16%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a '+/- boundary in [%]' input field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 16%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 17%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, having completed 17%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Completed: 1%

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 20%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. The 'Sensitivity analysis' tab shows a progress bar at 20% completion. A large orange rectangular box is overlaid on the bottom half of the screen.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 22%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a '+/- boundary in [%]' input field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 22%'. A large orange-outlined rectangular box is overlaid on the bottom half of the screen.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 23%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 24%



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_a(HD) [1/M]
3000000

Advanced options

Boundaries

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 26%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two main sections: Parameter and Boundaries. The Parameter section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an Advanced options button. The Boundaries section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The Sensitivity analysis section shows a '+/- boundary in [%]' input field set to 15, and buttons for Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis. A progress bar indicates the task is completed at 26%. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 27%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 27%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 28%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ 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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 30%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 31%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two main sections: Parameter and Boundaries.

Parameter Section: Contains fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). An "Advanced options" button is present.

Boundaries Section: Contains boundary settings for K_a(HG), I(0), I(HD), and I(D) values, both for lower and upper bounds.

Sensitivity Analysis Section: Shows a progress bar at 31% completion. It includes fields for +/- boundary in [%] (15), a Start Sensitivity analysis button, a Cancel button, and a Save result of sensitivity analysis button.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 33%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 33%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Completed: 34%

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ 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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 35%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 37%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 37%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 38%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 39%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 41%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 41%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 42%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Completed: 44%

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 45%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' panel includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these panels are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 45%.

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_a(HD) [1/M]
3000000

Advanced options

Boundaries

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 47%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' panel includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these panels are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a progress bar at 47% completion. At the bottom, there are buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 48%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. The 'Sensitivity analysis' tab shows a progress bar at 48% completion. At the bottom, there are buttons for Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 49%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 49%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 50%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 52%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 53%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 53%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 54%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries, and I(HD) and I(D) lower and upper boundaries, all set to 10 or 1e+08. Below these sections is a navigation bar with Optimization, Sensitivity analysis (which is selected), and Batch processing. The 'Sensitivity analysis' panel shows a '+/- boundary in [%]' field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 54%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 55%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 55%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 57%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, IDA model, and an Info section. The main area is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains three input fields: Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). Below these is a 'Advanced options' button. The 'Boundaries' section contains six input fields for chemical equilibrium constants and initial concentrations. At the bottom, there are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A progress bar indicates that a sensitivity analysis has completed 57%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 58%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 59%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task is 59% completed.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 60%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 62%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_s(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 63%



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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Completed: 64%

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 66%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 66%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 67%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 68%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task is completed at 68%. The overall interface has a clean, modern design with a dark background and orange highlights.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 70%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 70%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis -

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 71%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info section. The main area is divided into two panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' panel contains ranges for K_a(HG), I(0), I(HD), and I(D). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange progress bar at the bottom indicates the completion of a sensitivity analysis at 71%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 72%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' section with a plus sign. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 72%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 74%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange box highlights the 'Sensitivity analysis' section, which shows a progress bar at 74% completion. It includes fields for +/- boundary in [%] (15), buttons for Start Sensitivity analysis and Save result of sensitivity analysis, and a status message.

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_a(HD) [1/M]
3000000

Advanced options

Boundaries

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 75%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' panel includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these panels are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 75%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 76%



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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 77%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M], Dye conc. [M], and K_a(HD) [1/M]. The 'Boundaries' section allows setting lower and upper bounds for K_a(HG), I(0), I(HD), and I(D). Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar at the bottom indicates the sensitivity analysis is 77% completed.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 79%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 79%.

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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M], Dye conc. [M], and K_a(HD) [1/M]. The 'Boundaries' section includes fields for K_a(HG), I(0), I(HD), and I(D) values, both with lower and upper boundaries. Below these sections is a navigation bar with Optimization, Sensitivity analysis, and Batch processing tabs, where the Sensitivity analysis tab is active. The bottom section is titled 'Sensitivity analysis' and features a '+/- boundary in [%]' input field set to 15, a 'Start Sensitivity analysis' button, a 'Cancel' button, a 'Save result of sensitivity analysis' button, and a progress bar indicating 'Completed: 0%'.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a '+/- boundary in [%]' field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 0%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Completed: 0%

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_a(HD) [1/M]
3000000

Advanced options

Boundaries

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 85%

This screenshot shows the Thermosimfit software interface. The left sidebar contains model selection and information buttons. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). The 'Boundaries' section includes ranges for K_a(HG), I(0), I(HD), and I(D). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange progress bar indicates the completion of a sensitivity analysis at 85%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates the completion of a sensitivity analysis task at 0%.

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_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 88%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M], Dye conc. [M], and K_a(HD) [1/M]. The 'Boundaries' section allows setting lower and upper bounds for K_a(HG), I(0), I(HD), and I(D). Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar indicates the completion of a sensitivity analysis at 88%. The bottom of the screen shows a large, empty rectangular area with an orange border.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

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]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 99%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange box highlights the 'Sensitivity analysis' section, which shows a progress bar at 99% completion. It includes fields for +/- boundary in [%] (15), buttons for Start Sensitivity analysis and Save result of sensitivity analysis, and a status message.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_s(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ 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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 92%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ 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]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 93%



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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 95%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task is completed at 95%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 96%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange progress bar at the bottom indicates the Sensitivity analysis is completed at 96%.

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_a(HD) [1/M]
3000000

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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 99%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task is completed at 99%.

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

$K_s(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ 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]
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 Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 99%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and Info. The main area is divided into two sections: Parameter and Boundaries. The Parameter section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and $K_s(HD)$ [1/M] (3000000), with an Advanced options button. The Boundaries section includes fields for $K_s(HG)$ boundaries (lower: 10, upper: 1e+08), $I(0)$ boundaries (lower: 0, upper: 1e+08), $I(HD)$ boundaries (lower: 0, upper: 1e+08), and $I(D)$ boundaries (lower: 0, upper: 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. The Sensitivity analysis tab shows a progress bar at 99% completion. It also features a +/- boundary in [%] input field (15), Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis buttons.

Thermosimfit

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

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

[Advanced options](#)

Boundaries

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]
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](#) [Sensitivity analysis](#) [Batch processing](#)

Sensitivity analysis

+/- boundary in [%]
15

[Start Sensitivity analysis](#) [Cancel](#) [Save result of sensitivity analysis](#)

Completed: 100%

Scale for x is already present.
Adding another scale for x, which will replace the existing scale.

Parameter	Estimated Factor of variance
K _a (HG)	~0.05
K _a (HD)	~0.25
I(0)	~0.15
I(HD)	~0.20
I(D)	~0.25