

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 pairs for concentration boundaries: K_a(HG) and I(0) both have lower bounds of 10 and upper bounds of 1e+08; I(HD) and I(D) both have lower bounds of 0 and upper bounds of 1e+08. At the bottom, there are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large 'Sensitivity analysis' dialog box is open, containing a '+/- boundary in [%]' field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A status message 'Initializing...' is shown below the buttons. A pink status bar at the bottom right displays the message 'Registered S3 method overwritten by 'sensitivity': method from print.src.dplyr'. The overall interface is clean with orange and grey accents.

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■ Data import
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■ 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

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' button. The main area is divided into two 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). An 'Advanced options' button is located below these. The 'Boundaries' section contains 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 sections are tabs for 'Optimization', 'Sensitivity analysis' (which is currently selected), and 'Batch processing'. A large red box highlights the 'Sensitivity analysis' section, which 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 status message 'Completed: 1%'. A pink box at the bottom right contains a note about registered methods: 'Registered S3 method overwritten by 'sensitivity': method from print_src dplyr'.

Thermosimfit

☰

■ Data import
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■ 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: 3%

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'. It also displays 'Completed: 3%'. A status message at the bottom right indicates a registered S3 method for 'sensitivity'.

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 shows the Thermosimfit application window. On the left sidebar, there are several model selection buttons: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below these 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). There is also an 'Advanced options' button with a plus sign. The Boundaries section contains six input pairs for lower and upper bounds: K_a(HG) [1/M] (lower: 10, upper: 1e+08); I(0) [1/M] (lower: 0, upper: 1e+08); I(HD) [1/M] (lower: 0, upper: 1e+08); and I(D) [1/M] (lower: 0, upper: 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 4%. The status bar at the bottom right shows a registered S3 method for 'sensitivity'.

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: 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: 7%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a menu icon. On the left, a sidebar lists 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 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 selected), and Batch processing. The 'Sensitivity analysis' section includes a '+/- boundary in [%]' input (15), 'Start Sensitivity analysis' and 'Cancel' buttons, and a progress bar indicating 'Completed: 7%'. 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: 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 progress bar at 0% completion and a large empty rectangular area for results.

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 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 sections are tabs for 'Optimization', 'Sensitivity analysis' (which is currently selected), and 'Batch processing'. The 'Sensitivity analysis' section has a '+/- boundary in [%]' input (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 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] ⓘ 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: 11%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a menu icon. On the left, a sidebar lists 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 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 allows setting boundaries for various parameters like 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 progress bar at 11% completion and a note about +/- boundary in [%] (15%). It includes 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis' buttons.

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 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 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] ⓘ 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: 15%

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 at 15%. 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 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 fields for concentration boundaries: K_a(HG) and I(0) both have lower bounds of 0 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'. A progress bar at the bottom of the 'Sensitivity analysis' section indicates it is 'Completed: 17%'. The bottom right corner of the main window has a large orange rectangular placeholder.

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: 18%



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 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 20%.

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: 21%



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

☰

■ 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: 24%

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 at 24%. 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_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: 26%



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] ⓘ 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: 29%



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: 32%

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 32%.

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: 34%

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 34%.

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: 35%

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 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 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 37%.

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: 38%

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 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 at the bottom indicates the sensitivity analysis is 38% 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]
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: 40%



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

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: 43%

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 43% 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

Completed: 44%

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: 46%



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 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 48%.

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: 49%



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: 50%

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 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

☰

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: 54%



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: 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 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 the 'Sensitivity analysis' task is 57% completed.

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: 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: 60%

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 at the bottom indicates the Sensitivity analysis is 60% 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: 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]
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: 65%

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 65%.

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: 66%

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 section shows a progress bar at 66% completion and a note about +/- boundary in [%] (15%). Buttons for Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis are present.

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 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 68%.

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 different models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below that is an 'Info' link. 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 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 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. A large orange progress bar at the bottom indicates the completion of a Sensitivity analysis task at 71%.

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: 73%



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: 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 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.

At the bottom, there are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A progress bar indicates the Sensitivity analysis is 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]
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: 78%

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 the 'Sensitivity analysis' task is completed at 78%.

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 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. A large orange box highlights the 'Sensitivity analysis' tab and its associated parameters.

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 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 sections are tabs for 'Optimization', 'Sensitivity analysis' (which is currently selected), and 'Batch processing'. The 'Sensitivity analysis' section includes a '+/- boundary in [%]' input (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 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. The 'Sensitivity analysis' section shows '+/- boundary in [%]' 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 box is overlaid on the bottom half of the screen.

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: 0%



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

☰

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

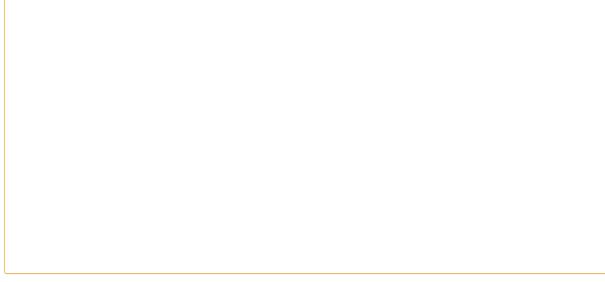
Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 88%



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

☰

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: 91%



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: 92%



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: 94%

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' 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 the 'Sensitivity analysis' task is completed at 94%.

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 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. 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: 97%

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, and IDA model. Below these are links for Info and Advanced options. 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 includes an 'Advanced options' button. The Boundaries section contains six input fields for concentration 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), and I(HD) value upper boundary [1/M] (1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A progress bar at the bottom indicates that the Sensitivity analysis has completed 97%.

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 message indicating the task is completed.

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%

Parameter	Estimated fraction of existence	Lower Boundary	Upper Boundary
K _a (HG)	~0.05	~0.02	~0.08
I(0)	~0.05	~0.02	~0.08
I(HD)	~0.05	~0.02	~0.08
I(D)	~0.05	~0.02	~0.08