

Thermosimfit

Data export
DB4 (core, host model)
DB4 (const, dyn) model
GDN model
IDR model
ixs6

Parameter

Host conc. [M]: 0.000001
Dye conc. [M]: 0.000001
 K_d [LM]: 3000000

Advanced options

Boundaries

K_d value lower boundary [L/M]: 1E-05
 K_d value upper boundary [L/M]: 1e+05
 iD value lower boundary [M]: 0
 iD value upper boundary [M]: 1e+05
 iH value lower boundary [M]: 0
 iH value upper boundary [M]: 1e+05

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization Save result of batch analysis

Found number of replications = 3 and a seed was defined. Only for the first analysis of each dataset respectively, the seed which will be used.

Thermosimfit

Data export
DB4 (core, host model)
DB4 (const, dyn) model
GDN model
IDR model
ixs6

Parameter

Host conc. [M]: 0.000001
Dye conc. [M]: 0.000001
 K_d [LM]: 3000000

Advanced options

Boundaries

K_d value lower boundary [L/M]: 1E-05
 K_d value upper boundary [L/M]: 1e+05
 iD value lower boundary [M]: 0
 iD value upper boundary [M]: 1e+05
 iH value lower boundary [M]: 0
 iH value upper boundary [M]: 1e+05

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization Save result of batch analysis

Found number of replications = 3 and a seed was defined. Only for the first analysis of each dataset respectively, the seed which will be used.

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH}^{(0)}[1/M]$	3000000
Advanced options	+

Boundaries

$k_{dH}^{(0)}$ value lower boundary [1/M]	20
$k_{dH}^{(0)}$ value upper boundary [1/M]	0
$k_{dH}^{(0)}$ value lower boundary [1/M]	1e+08
$k_{dH}^{(0)}$ value upper boundary [1/M]	1e+08
kD value lower boundary [1/M]	0
kD value upper boundary [1/M]	0
kD value lower boundary [1/M]	1e+08
kD value upper boundary [1/M]	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 3; Kd(Kd) = 4.779e+04; (1|0) = 2.547e-05; (1|0) = 1.195e-10; (1|0) = 9.934e-09; Error = 9.227e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 3; Kd(Kd) = 4.779e+04; (1|0) = 2.547e-05; (1|0) = 1.195e-10; (1|0) = 9.934e-09; Error = 9.227e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 3; Kd(Kd) = 1.584e+04; (1|0) = 1.935e-05; (1|0) = 7.979e-09; Error = 1.267e+01
Dataset Nr.: 1; Replication Nr.: 3; Generation = 3; Kd(Kd) = 1.584e+04; (1|0) = 1.935e-05; (1|0) = 7.979e-09; Error = 1.267e+01
Dataset Nr.: 2; Replication Nr.: 2; Generation = 3; Kd(Kd) = 6.118e+04; (2|0) = 2.399e-05; (2|0) = 2.280e-02; (2|0) = 3.480e-02; Error = 9.248e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 3; Kd(Kd) = 6.118e+04; (2|0) = 2.399e-05; (2|0) = 2.280e-02; (2|0) = 3.480e-02; Error = 9.248e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 3; Kd(Kd) = 7.220e+03; (2|0) = 2.094e-05; (2|0) = 1.289e-02; (2|0) = 3.930e-02
```

Found number of replications > 1 and a seed was defined. Only for the first analysis of each dataset respectively, the user defined will be used.

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameter

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	0
1e+00	
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	0
1e+00	
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	0
1e+00	

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

Batch analysis

How often should each dataset be analyzed (using different seeds):

[Start batch analysis](#) [Stop optimization](#) [Save result of batch analysis](#)

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 6; Kac(M) = 4.779e+04; (1|0) = 2.547e-05; (1|0) = 1.150e-10; (1|0) = 0.934e+00; Error = 0.227e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 6; Kac(M) = 4.779e+04; (1|0) = 2.547e-05; (1|0) = 1.150e-10; (1|0) = 0.934e+00; Error = 0.227e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 5; Kac(M) = 2.351e+02; (1|0) = 7.046e-02; (1|0) = 2.813e-05; (1|0) = 0.339e+00; Error = 0.339e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 5; Kac(M) = 2.351e+02; (1|0) = 7.046e-02; (1|0) = 2.813e-05; (1|0) = 0.339e+00; Error = 0.339e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 6; Kac(M) = 3.507e+05; (1|0) = 2.495e-01; (1|0) = 1.240e-05; (1|0) = 0.659e+00; Error = 0.659e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 5; Kac(M) = 4.922e+05; (1|0) = 1.000e-01; (1|0) = 1.120e+00; (1|0) = 2.350e+00; Error = 0.409e+00
```

Thermosimfit

- Data input
- DNA (const. heat model)
- DNA (const. dye model)
- DNA model
- DNA model
- Info

Parameter

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$K_{dH}^{(0)}[1/M]$	3000000
Advanced options	

Boundaries

$K_{dH}^{(0)}$ value lower boundary [1/M]	22
$K_{dH}^{(0)}$ value upper boundary [1/M]	1e+08
$H(D)$ value lower boundary [1/M]	0
$H(D)$ value upper boundary [1/M]	1e+08
$H(D)$ value lower boundary [1/M]	0
$H(D)$ value upper boundary [1/M]	1e+08

Optimization
Sensitivity analysis
Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds):

Start batch analysis Stop optimization

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 9; KdH(0) = 2.0000e+00; 1(0) = 1.0000e+00; 1(10) = 8.451e+00; 1(20) = 2.760e+00; Error = 4.240e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 9; KdH(0) = 2.0000e+00; 1(0) = 1.0000e+00; 1(10) = 8.451e+00; 1(20) = 2.760e+00; Error = 4.240e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 7; KdH(0) = 2.024e+02; 1(0) = 7.044e-02; 1(10) = 1.340e+00; 1(20) = 2.013e+00; Error = 9.350e-02
Dataset Nr.: 1; Replication Nr.: 3; Generation = 7; KdH(0) = 2.024e+02; 1(0) = 7.044e-02; 1(10) = 1.340e+00; 1(20) = 2.013e+00; Error = 9.350e-02
Dataset Nr.: 2; Replication Nr.: 2; Generation = 8; KdH(0) = 1.920e+07; 1(0) = 2.0000e+00; 1(10) = 1.930e+04; 1(20) = 1.900e+05; Error = 8.280e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 8; KdH(0) = 1.920e+07; 1(0) = 2.0000e+00; 1(10) = 1.930e+04; 1(20) = 1.900e+05; Error = 8.280e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 8; KdH(0) = 9.210e+07; 1(0) = 1.0000e+01; 1(10) = 8.830e+07; 1(20) = 2.490e+08; Error = 5.600e+00
```

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	0 1e+00
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	0 1e+00

Optimization
Sensitivity analysis
Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds):

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 12; Ksa(H) = 2.4860e+00; |(0)| = 1.0000e-15; |(0)| = 0.401e+05; |(0)| = 2.768e+04; Error = 4.248e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 12; Ksa(H) = 2.4860e+00; |(0)| = 1.0000e-15; |(0)| = 0.401e+05; |(0)| = 2.768e+04; Error = 4.248e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 18; Ksa(H) = 5.334e+05; |(0)| = 1.0000e-15; |(0)| = 5.349e+05; |(0)| = 1.0000e-15; Error = 0.429e+00
Dataset Nr.: 1; Replication Nr.: 4; Generation = 18; Ksa(H) = 5.334e+05; |(0)| = 1.0000e-15; |(0)| = 5.349e+05; |(0)| = 1.0000e-15; Error = 0.429e+00
Dataset Nr.: 1; Replication Nr.: 5; Generation = 12; Ksa(H) = 1.920e+07; |(0)| = 2.404e-01; |(0)| = 7.303e-04; |(0)| = 1.0000e-15; Error = 0.209e+00
Dataset Nr.: 1; Replication Nr.: 6; Generation = 12; Ksa(H) = 3.320e+08; |(0)| = 1.0000e-15; |(0)| = 9.829e-04; |(0)| = 1.0000e-15; Error = 0.209e+00
```

Thermosimfit

- Data input
- DSK (const. heat model)
- (DSK (const. dye) model)
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	2
k_{dH} value lower boundary [1/M] <input checked="" type="radio"/> wip	
k_{dH} value upper boundary [1/M]	1e+08
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+08

Optimization
Sensitivity analysis
Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds):

Start batch analysis Stop optimization

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 15; Kaus(H) = 8.777e+00; |(0)| + 1.000e-15; |(0)| = 0.442e+05; |(0)| + 1.000e-15; Error = 3.615e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 15; Kaus(H) = 8.734e+05; |(0)| + 1.000e-15; |(0)| = 5.148e+05; |(0)| + 1.000e-15; Error = 0.429e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 15; Kaus(H) = 8.734e+05; |(0)| + 1.000e-15; |(0)| = 5.148e+05; |(0)| + 1.000e-15; Error = 0.429e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 15; Kaus(H) = 8.734e+05; |(0)| + 1.000e-15; |(0)| = 5.148e+05; |(0)| + 1.000e-15; Error = 0.429e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 15; Kaus(H) = 1.920e+07; |(0)| + 2.400e-01; |(0)| = 7.408e+04; |(0)| + 1.000e-15; Error = 0.209e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 15; Kaus(H) = 3.300e+08; |(0)| + 1.000e-15; |(0)| = 9.829e+04; |(0)| + 1.000e-15; Error = 0.209e+00
```

The screenshot shows a software interface for "Thermosimfit" with a dark theme. The top navigation bar includes a "File" menu with "Import" and "Export" options, and a "Help" menu. On the left, there's a sidebar with a tree view showing project structure: "Data import", "DCA (constant heat) model", "DCA (constant dye) model", "DCA model", and "DO model". A status bar at the bottom indicates "100%".

The main workspace is divided into two main sections:

- Left Section (Parameter Input):** Contains input fields for "Host conc. [M]" (0.000001), "Dye conc. [M]" (0.000001), and "K_d[M] value [M]" (300000). Below these are "Advanced options" and a "Batch processing" section.
- Right Section (Boundary Conditions):** Contains four pairs of input fields for boundary conditions:
 - "K_d[M] value lower boundary 1[M]" (2) and "K_d[M] value upper boundary 1[M]" (1e+00)
 - "K_d[M] value lower boundary 2[M]" (0) and "K_d[M] value upper boundary 2[M]" (1e+00)
 - "K_d[M] value lower boundary 3[M]" (0) and "K_d[M] value upper boundary 3[M]" (1e+00)
 - "K_d[M] value lower boundary 4[M]" (0) and "K_d[M] value upper boundary 4[M]" (1e+00)

Bottom Section (Batch Analysis): This section has tabs for "Optimization", "Sensitivity analysis", and "Batch processing". The "Batch processing" tab is active, showing a progress bar at 0%. It contains a "Batch analysis" section with a dropdown for "How often should each dataset be analyzed (using different seeds)" set to 3, and a "Start batch analysis" button. Below this is a log window displaying results for various datasets and generations:

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 10; Kd[M] = 0.923e+00; I[0] = 1.800e-15; I[0] = 1.047e+00; I[0] = 1.544e+00; Error = 2.556e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 10; Kd[M] = 0.977e+00; I[0] = 1.800e-15; I[0] = 0.842e+00; I[0] = 1.280e+00; Error = 3.616e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 10; Kd[M] = 0.932e+00; I[0] = 1.800e-15; I[0] = 0.842e+00; I[0] = 1.280e+00; Error = 3.616e+00
Dataset Nr.: 2; Replication Nr.: 1; Generation = 10; Kd[M] = 0.923e+00; I[0] = 1.800e-15; I[0] = 1.047e+00; I[0] = 1.544e+00; Error = 2.556e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 10; Kd[M] = 0.977e+00; I[0] = 1.800e-15; I[0] = 0.842e+00; I[0] = 1.280e+00; Error = 3.616e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 10; Kd[M] = 0.932e+00; I[0] = 1.800e-15; I[0] = 0.842e+00; I[0] = 1.280e+00; Error = 3.616e+00
Dataset Nr.: 3; Replication Nr.: 1; Generation = 10; Kd[M] = 0.923e+00; I[0] = 1.800e-15; I[0] = 1.047e+00; I[0] = 1.544e+00; Error = 2.556e+00
Dataset Nr.: 3; Replication Nr.: 2; Generation = 10; Kd[M] = 0.977e+00; I[0] = 1.800e-15; I[0] = 0.842e+00; I[0] = 1.280e+00; Error = 3.616e+00
Dataset Nr.: 3; Replication Nr.: 3; Generation = 10; Kd[M] = 0.932e+00; I[0] = 1.800e-15; I[0] = 0.842e+00; I[0] = 1.280e+00; Error = 3.616e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 18; Kd[M] = 0.893e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 18; Kd[M] = 0.947e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 18; Kd[M] = 0.901e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 2; Replication Nr.: 1; Generation = 18; Kd[M] = 0.893e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 18; Kd[M] = 0.947e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 18; Kd[M] = 0.901e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 3; Replication Nr.: 1; Generation = 18; Kd[M] = 0.893e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 3; Replication Nr.: 2; Generation = 18; Kd[M] = 0.947e+00; I[0] = 6.867e-04; Error = 4.298e+00
Dataset Nr.: 3; Replication Nr.: 3; Generation = 18; Kd[M] = 0.901e+00; I[0] = 6.867e-04; Error = 4.298e+00
```

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

$k_{dH} \text{ value lower boundary } [1/\text{M}]$	20	$k_{dH} \text{ value upper boundary }$	0
$k_{dH} \text{ value upper boundary } [1/\text{M}]$	1e+08	$k_{dH} \text{ value lower boundary }$	1e+08
$(\text{Dy}) \text{ value lower boundary } [1/\text{M}]$		$(\text{Dy}) \text{ value upper boundary }$	0
$(\text{Dy}) \text{ value upper boundary } [1/\text{M}]$		$(\text{Dy}) \text{ value lower boundary }$	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 20; Ks(H) = 8.7770e+00; (1|0) + 1.0000e-15; (2|0) = 0.642e+00; (1|0) + 1.0000e-15; (2|0) = 0.415e+00; Error = 3.615e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 18; Ks(H) = 2.370e+00; (1|0) + 1.0000e-15; (2|0) = 9.794e-05; (1|0) + 1.0000e-15; (2|0) = 4.725e+00; Error = 4.725e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 20; Ks(H) = 1.920e+00; (1|0) + 2.400e-01; (2|0) = 7.400e-04; (1|0) + 1.0000e-15; (2|0) = 0.209e+00; Error = 0.209e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 20; Ks(H) = 1.920e+00; (1|0) + 2.400e-01; (2|0) = 7.400e-04; (1|0) + 1.0000e-15; (2|0) = 0.209e+00; Error = 0.209e+00
```

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

$k_{dH} \text{ value lower boundary } [1/\text{M}]$	20	$k_{dH} \text{ value upper boundary }$	0
$k_{dH} \text{ value upper boundary } [1/\text{M}]$	1e+08	$k_{dH} \text{ value lower boundary }$	1e+08
$(\text{Dy}) \text{ value lower boundary } [1/\text{M}]$		$(\text{Dy}) \text{ value upper boundary }$	0
$(\text{Dy}) \text{ value upper boundary } [1/\text{M}]$		$(\text{Dy}) \text{ value lower boundary }$	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```

Dataset Nr.: 1; Replication Nr.: 1; Generation = 23; Kao(H) = 8.777e+00; |(0)| + 1.000e-15; |(0)| = 0.642e+00; |(0)| + 1.000e-15; Error = 3.615e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 23; Kao(H) = 8.777e+00; |(0)| + 1.000e-15; |(0)| = 0.784e+00; |(0)| + 1.000e-15; Error = 4.725e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 23; Kao(H) = 8.777e+00; |(0)| + 1.000e-15; |(0)| = 0.926e+00; |(0)| + 1.000e-15; Error = 5.835e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 22; Kao(H) = 1.929e+01; |(0)| + 2.400e-01; |(0)| = 7.408e+01; |(0)| + 1.000e-15; Error = 9.209e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 22; Kao(H) = 1.929e+01; |(0)| + 2.400e-01; |(0)| = 9.799e+01; |(0)| + 2.400e-01; Error = 2.939e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 22; Kao(H) = 1.929e+01; |(0)| + 2.400e-01; |(0)| = 1.000e+02; |(0)| + 2.400e-01; Error = 2.939e+00

```

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameter

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	20	k_{dH} value upper boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+08	k_{dH} value lower boundary [1/M]	2e+07
k_{dH} value lower boundary [1/M]		0	k_{dH} value upper boundary [1/M]
k_{dH} value upper boundary [1/M]		1e+08	

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 26; Ks(H) = 8.777e+00; |(0)| + 1.000e-15; |(0)| = 0.642e+05; |(0)| + 1.000e-15; Error = 3.615e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 24; Ks(H) = 2.144e+00; |(0)| + 1.000e-15; |(0)| = 9.479e+05; |(0)| + 1.000e-15; Error = 4.548e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 24; Ks(H) = 2.144e+00; |(0)| + 1.000e-15; |(0)| = 9.479e+05; |(0)| + 1.000e-15; Error = 4.548e+00
Dataset Nr.: 2; Replication Nr.: 1; Generation = 26; Ks(H) = 1.920e+07; |(0)| + 2.400e-01; |(0)| = 7.308e+04; |(0)| + 1.000e-15; Error = 8.209e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 26; Ks(H) = 4.320e+07; |(0)| + 1.000e-15; |(0)| = 1.209e+05; |(0)| + 2.300e-01; Error = 3.989e+00
```

Thermosimfit

☰

File Import
ICO (constant heat) model
ICO (constant dye) model
ICO model
ICO model

134

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_d[M] [1/M]
3000000

Advanced options

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds)?
3

Start batch analysis Stop optimization Save result of batch analysis

Dataset Nr.: 1; Replication Nr.: 1; Generation = 29; $\text{Na}^{+}\text{H}^{+}$ = 0.923e+00; $\text{I}^{(0)}$ = 1.800e-15; $\text{I}^{(0)} = 1.047e+00$; $\text{I}^{(0)} = 1.544e+00$ Error = 2.556e+00

Dataset Nr.: 1; Replication Nr.: 2; Generation = 29; $\text{Na}^{+}\text{H}^{+}$ = 0.377e+00; $\text{I}^{(0)} = 1.800e-15$; $\text{I}^{(0)} = 8.642e+00$; $\text{I}^{(0)} = 1.280e+00$ Error = 3.616e+00

Dataset Nr.: 1; Replication Nr.: 3; Generation = 29; $\text{Na}^{+}\text{H}^{+}$ = 0.923e+00; $\text{I}^{(0)} = 1.800e-15$; $\text{I}^{(0)} = 1.047e+00$; $\text{I}^{(0)} = 1.544e+00$ Error = 2.556e+00

Dataset Nr.: 2; Replication Nr.: 1; Generation = 29; $\text{Na}^{+}\text{H}^{+}$ = 0.923e+00; $\text{I}^{(0)} = 1.800e-15$; $\text{I}^{(0)} = 1.047e+00$; $\text{I}^{(0)} = 1.544e+00$ Error = 2.556e+00

Dataset Nr.: 2; Replication Nr.: 2; Generation = 29; $\text{Na}^{+}\text{H}^{+}$ = 4.290e-07; $\text{I}^{(0)} = 1.800e-15$; $\text{I}^{(0)} = 1.389e+00$; $\text{I}^{(0)} = 2.198e+00$ Error = 1.998e+00

Dataset Nr.: 2; Replication Nr.: 3; Generation = 29; $\text{Na}^{+}\text{H}^{+}$ = 4.290e-07; $\text{I}^{(0)} = 1.800e-15$; $\text{I}^{(0)} = 1.389e+00$; $\text{I}^{(0)} = 2.198e+00$ Error = 1.998e+00

Boundaries ⓘ help

I_d[M] value lower boundary 1[M]
0

I_d[M] value upper boundary 1[M]
1e+00

I_d[M] value lower boundary 2[M]
0

I_d[M] value upper boundary 2[M]
1e+00

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	20
k_{dH} value upper boundary [1/M]	0
k_{dH} value lower boundary [1/M]	1e+08
k_{dH} value upper boundary [1/M]	2e+08
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+08

Optimization
Sensitivity analysis
Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 32; Kao(H) = 2.9326e+00; |(0)| + 1.0000e-15; |(0)| = 7.896e+00; |(0)| = 0.911e+04; Error = 3.689e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 38; Kao(H) = 6.292e+05; |(0)| + 1.0000e-15; |(0)| = 6.987e+05; |(0)| = 1.000e+15; Error = 4.598e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 32; Kao(H) = 1.929e+07; |(0)| + 2.440e-01; |(0)| = 7.308e+04; |(0)| = 1.000e+15; Error = 5.209e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 32; Kao(H) = 4.320e+07; |(0)| + 1.0000e-15; |(0)| = 1.209e+08; |(0)| = 2.009e+08; Error = 5.909e+00
```

The screenshot shows a software interface for "Thermosimfit" with a dark theme. The top navigation bar includes tabs for "Optimization", "Sensitivity analysis", and "Batch processing". The main workspace is divided into two main sections: "Parameter" and "Boundary".

Parameter Section:

- Host conc. [M]: 0.000001
- Dye conc. [M]: 0.000001
- $K_{dH}^{(0)} \text{ value } [1/\text{M}]$: 3000000

Advanced options button is present.

Boundary Section:

- $I(0)$ value lower boundary [1/M]: 0
- $I(0)$ value upper boundary [1/M]: 1e+00
- $I(D)$ value lower boundary [1/M]: 0
- $I(D)$ value upper boundary [1/M]: 1e+00

Batch analysis Section:

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization Save result of batch analysis

Batch analysis results (Dataset Nr.: 1; Replication Nr.: 1; Generation = 35; 84e-05) + 7.812e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.250e-05; $I(D)$ = 1.633e-05; Error = 1.959e-00

Dataset Nr.: 1; Replication Nr.: 2; Generation = 35; 84e-05 + 4.483e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.704e-05; $I(D)$ = 1.686e-05; Error = 3.713e-00

Dataset Nr.: 1; Replication Nr.: 3; Generation = 35; 84e-05 + 1.318e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.958e-05; $I(D)$ = 1.718e-05; Error = 1.055e-00

Dataset Nr.: 2; Replication Nr.: 1; Generation = 35; 84e-05 + 7.812e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.250e-05; $I(D)$ = 1.633e-05; Error = 1.959e-00

Dataset Nr.: 2; Replication Nr.: 2; Generation = 35; 84e-05 + 4.483e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.704e-05; $I(D)$ = 1.686e-05; Error = 3.713e-00

Dataset Nr.: 2; Replication Nr.: 3; Generation = 35; 84e-05 + 1.318e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.958e-05; $I(D)$ = 1.718e-05; Error = 1.055e-00

Dataset Nr.: 3; Replication Nr.: 1; Generation = 35; 84e-05 + 7.812e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.250e-05; $I(D)$ = 1.633e-05; Error = 1.959e-00

Dataset Nr.: 3; Replication Nr.: 2; Generation = 35; 84e-05 + 4.483e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.704e-05; $I(D)$ = 1.686e-05; Error = 3.713e-00

Dataset Nr.: 3; Replication Nr.: 3; Generation = 35; 84e-05 + 1.318e-05; $I(0)$ = 1.800e-15; $I(0)$ = 8.958e-05; $I(D)$ = 1.718e-05; Error = 1.055e-00

The screenshot shows the Thermosimfit software interface. The left sidebar contains project navigation and model selection. The main area has tabs for Optimization, Sensitivity analysis, and Batch processing, with the Batch processing tab selected. In the Optimization section, parameters like Host conc. [M], Dye conc. [M], and $K_{dH}^{(H)}$ [1/M] are set. Advanced options are available. The Batch processing section shows a list of datasets and their corresponding generation numbers and error values.

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{dH}^{(H)}$ [1/M]
3000000

Advanced options

Batch analysis

How often should each dataset be analyzed (using different seeds)?
3

Start batch analysis Stop optimization

Dataset Nr.	Replication Nr.	Generation	Error
Dataset Nr.: 1	1; Replication Nr.: 1;	Generation = 38; 94(M)	$7.810e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 1	1; Replication Nr.: 2;	Generation = 38; 94(M)	$7.717e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 3.294e+00
Dataset Nr.: 1	1; Replication Nr.: 3;	Generation = 38; 94(M)	$7.717e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 3.294e+00
Dataset Nr.: 2	1; Replication Nr.: 1;	Generation = 37; 94(M)	$7.810e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	1; Replication Nr.: 2;	Generation = 37; 94(M)	$7.810e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	1; Replication Nr.: 3;	Generation = 38; 94(M)	$7.810e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	2; Replication Nr.: 1;	Generation = 38; 94(M)	$7.832e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	2; Replication Nr.: 2;	Generation = 38; 94(M)	$7.832e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	2; Replication Nr.: 3;	Generation = 38; 94(M)	$7.832e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	3; Replication Nr.: 1;	Generation = 38; 94(M)	$7.832e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	3; Replication Nr.: 2;	Generation = 38; 94(M)	$7.832e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00
Dataset Nr.: 2	3; Replication Nr.: 3;	Generation = 38; 94(M)	$7.832e+00$; $I(0) = 1.800e-15$; $I(H) = 0.250e+01$; $I(D) = 1.632e+00$; Error = 1.059e+00

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}$	3000000
3000000	

Advanced options

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	0
k_{dH} value lower boundary [1/M]	1e+00
k_{dH} value upper boundary [1/M]	2e+00
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+00
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+00

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

Batch analysis

How often should each dataset be analyzed (using different seeds):

[Start batch analysis](#) [Stop optimization](#) [Save result of batch analysis](#)

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 48; Kao(H) = 3.731e+00; |(0)| + 1.0000e-15; |(0)| = 7.222e+05; |(0)| + 1.0000e-15; Error = 3.258e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 48; Kao(H) = 6.230e+00; |(0)| + 1.0000e-15; |(0)| = 9.834e+05; |(0)| + 1.0000e-15; Error = 2.493e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 48; Kao(H) = 1.0000e+01; |(0)| + 1.0000e-15; |(0)| = 1.571e+06; |(0)| + 1.0000e-15; Error = 4.978e+00
Dataset Nr.: 2; Replication Nr.: 1; Generation = 48; Kao(H) = 1.920e+07; |(0)| + 2.4000e-01; |(0)| = 7.308e+04; |(0)| + 1.0000e-15; Error = 9.209e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 48; Kao(H) = 1.932e+07; |(0)| + 1.0000e-15; |(0)| = 8.730e+04; |(0)| + 1.0000e-15; Error = 1.762e+00
```

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	0
k_{dH} value lower boundary [1/M]	1e+08
k_{dH} value upper boundary [1/M]	2e+08
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+08

Optimization
Sensitivity analysis
Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 44; Kao(H) = 3.731e+00; |(0)| + 1.0000e-15; |(0)| = 7.222e+05; |(0)| + 1.022e+05; Error = 3.258e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 42; Kao(H) = 6.150e+00; |(0)| + 1.0000e-15; |(0)| = 9.834e+05; |(0)| + 1.089e+05; Error = 2.493e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 43; Kao(H) = 1.0000e+01; |(0)| + 2.440e-01; |(0)| = 1.703e+06; |(0)| + 1.762e+06; Error = 4.289e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 41; Kao(H) = 1.929e+01; |(0)| + 2.440e-01; |(0)| = 7.408e+04; |(0)| + 1.0000e-15; Error = 9.209e+00
Dataset Nr.: 1; Replication Nr.: 1; Generation = 44; Kao(H) = 1.0000e+01; |(0)| + 1.0000e-15; |(0)| = 8.700e+05; |(0)| + 1.0000e+05; Error = 1.702e+00
```

The screenshot shows a software interface for "Thermosimfit" with a dark theme. The top navigation bar includes tabs for "Optimization", "Sensitivity analysis", and "Batch processing".

Parameter

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d [M] [1/M]	3000000

Advanced options

Boundaries

I(0) value lower boundary [1/M]	0
I(0) value upper boundary [1/M]	1e+00

I(D) value lower boundary [1/M]	0
I(D) value upper boundary [1/M]	1e+00

Batch analysis

How often should each dataset be analyzed (using different seeds)? 3

Start batch analysis Stop optimization Save result of batch analysis

Dataset Nr.: 1; Replication Nr.: 1; Generation = 47; Na^+ [M] = 1.115e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 1.912e+00; $\text{I}(D)$ = 1.729e+00; Error = 1.594e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 47; Na^+ [M] = 5.380e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 0.739e+00; $\text{I}(D)$ = 1.232e+00; Error = 2.099e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 47; Na^+ [M] = 1.115e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 1.912e+00; $\text{I}(D)$ = 1.729e+00; Error = 1.594e+00
Dataset Nr.: 2; Replication Nr.: 1; Generation = 46; Na^+ [M] = 1.115e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 1.912e+00; $\text{I}(D)$ = 1.729e+00; Error = 1.594e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 46; Na^+ [M] = 1.830e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 0.739e+00; $\text{I}(D)$ = 1.232e+00; Error = 2.099e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 46; Na^+ [M] = 1.830e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 0.739e+00; $\text{I}(D)$ = 1.232e+00; Error = 2.099e+00
Dataset Nr.: 3; Replication Nr.: 1; Generation = 46; Na^+ [M] = 1.830e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 0.739e+00; $\text{I}(D)$ = 1.232e+00; Error = 2.099e+00
Dataset Nr.: 3; Replication Nr.: 2; Generation = 46; Na^+ [M] = 1.830e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 0.739e+00; $\text{I}(D)$ = 1.232e+00; Error = 2.099e+00
Dataset Nr.: 3; Replication Nr.: 3; Generation = 46; Na^+ [M] = 1.830e+07; $\text{I}(0)$ = 1.800e-15; $\text{I}(0)$ = 0.739e+00; $\text{I}(D)$ = 1.232e+00; Error = 2.099e+00

Thermosimfit

- Data input
- DSK (const. heat model)
- (DSK const. dye model)
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{d}(H_2O) [1/M]$	3000000
Advanced options	

Boundaries

$k_{d}(H_2O)$ value lower boundary [1/M]	20
$k_{d}(H_2O)$ value upper boundary [1/M]	1e+08
$k_d(H)$ value lower boundary [1/M]	0
$k_d(H)$ value upper boundary [1/M]	1e+08
$k_{dH}(H_2O)$ value lower boundary [1/M]	0
$k_{dH}(H_2O)$ value upper boundary [1/M]	1e+08

Optimization
Sensitivity analysis
Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds):

[Start batch analysis](#) [Stop optimization](#) [Save result of batch analysis](#)

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 49; Kaus(H) = 5.3880e+00; |(0)| + 1.0000e-15; |(0)| = 0.730e+00; |(0)| = 1.232e+00; Error = 2.089e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 49; Kaus(H) = 6.150e+00; |(0)| + 1.0000e-15; |(0)| = 0.834e+00; |(0)| = 1.389e+00; Error = 2.493e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 49; Kaus(H) = 6.150e+00; |(0)| + 1.0000e-15; |(0)| = 0.834e+00; |(0)| = 1.389e+00; Error = 2.493e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 49; Kaus(H) = 6.150e+00; |(0)| + 1.0000e-15; |(0)| = 0.834e+00; |(0)| = 1.389e+00; Error = 2.493e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 49; Kaus(H) = 1.920e+07; |(0)| + 2.400e-01; |(0)| = 7.300e+04; |(0)| = 1.000e-15; Error = 0.209e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 49; Kaus(H) = 1.932e+07; |(0)| + 1.000e-01; |(0)| = 0.730e+00; |(0)| = 1.000e-01; Error = 1.702e+00
```

Thermosimfit

- Data input
- DSK (const. heat model)
- (DSK (const. dye) model)
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

$k_{dH} \text{ value lower boundary } [1/\text{M}]$	20	$k_{dH} \text{ value upper boundary }$	0
$k_{dH} \text{ value upper boundary } [1/\text{M}]$	1e+08	$k_{dH} \text{ value lower boundary }$	1e+08
$\text{[DH] value lower boundary } [1/\text{M}]$		$\text{[DH] value upper boundary } [1/\text{M}]$	$\text{[DH] value lower boundary } [1/\text{M}]$
0		0	1e+08
$\text{[DH] value upper boundary } [1/\text{M}]$		$\text{[DH] value lower boundary } [1/\text{M}]$	
1e+08		1e+08	

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```

Dataset Nr.: 1; Replication Nr.: 1; Generation = 53; Kain(H) = 5.3880e+00; |(0)| + 1.0000e-15; |(0)| = 8.798e+05; |(0)| + 1.232e+05; Error = 2.089e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 53; Kain(H) = 6.1500e+00; |(0)| + 1.0000e-15; |(0)| = 9.894e+05; |(0)| + 1.389e+05; Error = 2.493e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 53; Kain(H) = 6.9120e+00; |(0)| + 1.0000e-15; |(0)| = 1.094e+06; |(0)| + 1.446e+05; Error = 2.897e+00
Dataset Nr.: 2; Replication Nr.: 1; Generation = 52; Kain(H) = 1.920e+07; |(0)| + 2.400e-01; |(0)| = 7.408e+04; |(0)| + 1.000e-15; Error = 9.209e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 52; Kain(H) = 1.932e+07; |(0)| + 1.000e-01; |(0)| = 8.720e+04; |(0)| + 1.000e-08; Error = 1.702e+00

```

Thermosimfit

- Data input
- DSK (const. heat model)
- (DSK (const. dye) model)
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

$k_{dH} \text{ value lower boundary } [1/\text{M}]$	20	$k_{dH} \text{ value upper boundary }$	0
$k_{dH} \text{ value upper boundary } [1/\text{M}]$	1e+08	$k_{dH} \text{ value lower boundary }$	1e+08
$\text{[DH] value lower boundary } [1/\text{M}]$		$\text{[DH] value upper boundary }$	0
$\text{[DH] value upper boundary } [1/\text{M}]$		$\text{[DH] value lower boundary }$	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```

Dataset Nr.: 1; Replication Nr.: 1; Generation = 96; Kaus(H) = 5.3880e+00; |(0)| + 1.0000e-15; |(0)| = 0.739e+05; |(0)| + 1.233e+05; Error = 2.089e+00
Dataset Nr.: 1; Replication Nr.: 2; Generation = 96; Kaus(H) = 6.150e+00; |(0)| + 1.0000e-15; |(0)| = 0.834e+05; |(0)| + 1.389e+05; Error = 2.493e+00
Dataset Nr.: 1; Replication Nr.: 3; Generation = 96; Kaus(H) = 6.912e+00; |(0)| + 1.0000e-15; |(0)| = 0.934e+05; |(0)| + 1.545e+05; Error = 2.897e+00
Dataset Nr.: 2; Replication Nr.: 1; Generation = 96; Kaus(H) = 1.920e+07; |(0)| + 2.400e-01; |(0)| = 7.308e+04; |(0)| + 1.000e-15; Error = 9.209e+00
Dataset Nr.: 2; Replication Nr.: 2; Generation = 96; Kaus(H) = 1.923e+07; |(0)| + 2.400e-01; |(0)| = 7.309e+04; |(0)| + 1.000e-15; Error = 9.209e+00
Dataset Nr.: 2; Replication Nr.: 3; Generation = 96; Kaus(H) = 1.923e+07; |(0)| + 2.400e-01; |(0)| = 7.309e+04; |(0)| + 1.000e-15; Error = 9.209e+00

```

The screenshot shows the Thermosimfit software interface. The left sidebar contains a tree view of project files: 'Thermosimfit' (selected), 'Data import', 'DCA (constant heat) model', 'DCA (constant dye) model', 'DCA model', and 'DO model'. Below the tree is a status bar showing '0 ms'.

The main workspace is divided into two panes. The left pane is titled 'Parameter' and contains input fields for 'Host conc. [M]' (0.000001), 'Dye conc. [M]' (0.000001), and 'K_d[M] value [M]' (300000). It also includes an 'Advanced options' section. The right pane is titled 'Boundaries' and contains input fields for 'I(D) value lower boundary 1[M]' (0), 'I(D) value upper boundary 1[M]' (1e+00), 'I(D) value lower boundary 1[M]' (0), and 'I(D) value upper boundary 1[M]' (1e+00).

Below these panes are tabs for 'Optimization', 'Sensitivity analysis', and 'Batch processing'. The 'Batch processing' tab is active, showing a 'Batch analysis' section. It asks 'How often should each dataset be analyzed (using different seeds)?' with a dropdown set to '3'. There are buttons for 'Start batch analysis' and 'Stop optimization' (with a progress bar), and a link to 'Save result of batch analysis'. A large text area displays the results of the batch analysis for three datasets (Nr. 1 and Nr. 2, each with 3 replicates). Each dataset shows a series of equations for variables I(0) and I(D) across 15 generations, with error values ranging from 1.594e+00 to 1.792e+00.

Thermosimfit

- Data input
- DSK (const. heat model)
- (bla) const. dye model
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dye}^{(H2O)}[1/M]$	3000000
Advanced options	

Boundaries

$k_{dye}^{(H2O)}$ value lower boundary [1/M]	20
$k_{dye}^{(H2O)}$ value upper boundary [1/M]	1e+08
$k_{dye}^{(H2O)}$ value lower boundary [1/M]	0
$k_{dye}^{(H2O)}$ value upper boundary [1/M]	1e+08
$k_{dye}^{(H2O)}$ value lower boundary [1/M]	0
$k_{dye}^{(H2O)}$ value upper boundary [1/M]	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```

Dataset Nr.: 1; Replication Nr.: 2; Generation = 62; Kaus(H) = 1.0000e+07; |(0)| + 1.0000e-15; |(0)| = 7.914e-05; |(0)| + 1.0000e-05; Error = 1.643e-08
Dataset Nr.: 1; Replication Nr.: 1; Generation = 59; Kaus(H) = 6.150e+06; |(0)| + 1.0000e-15; |(0)| = 9.834e-05; |(0)| + 1.0000e-05; Error = 2.493e-08
Dataset Nr.: 1; Replication Nr.: 3; Generation = 61; Kaus(H) = 1.0000e+07; |(0)| + 1.0000e-15; |(0)| = 7.914e-05; |(0)| + 1.0000e-05; Error = 1.643e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 61; Kaus(H) = 1.920e+07; |(0)| + 2.400e-01; |(0)| = 7.308e-04; |(0)| + 1.0000e-15; Error = 8.209e-08
Dataset Nr.: 2; Replication Nr.: 3; Generation = 61; Kaus(H) = 1.323e+07; |(0)| + 1.0000e-15; |(0)| = 8.702e-05; |(0)| + 1.0000e-05; Error = 1.509e-08

```

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	0
k_{dH} value lower boundary [1/M]	1e+08
k_{dH} value upper boundary [1/M]	2e+08
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds):

[Start batch analysis](#) [Stop optimization](#) [Save result of batch analysis](#)

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 65; Kaus(H) = 1.0000e+07; (1|0) + 1.0000e-15; (2|0) = 7.914e-05; (1|0) + 1.0000e-05; Error = 1.643e-09
Dataset Nr.: 1; Replication Nr.: 3; Generation = 63; Kaus(H) = 6.150e-06; (1|0) + 1.0000e-15; (2|0) = 9.834e-05; (1|0) + 1.0000e-05; Error = 2.493e-09
Dataset Nr.: 1; Replication Nr.: 4; Generation = 64; Kaus(H) = 5.935e-06; (1|0) + 1.0000e-15; (2|0) = 6.138e-05; (1|0) + 1.0000e-05; Error = 2.493e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 65; Kaus(H) = 5.935e-06; (1|0) + 1.0000e-15; (2|0) = 6.138e-05; (1|0) + 1.0000e-05; Error = 5.239e-09
Dataset Nr.: 2; Replication Nr.: 3; Generation = 64; Kaus(H) = 1.032e-07; (1|0) + 1.0000e-15; (2|0) = 1.702e-06; (1|0) + 1.0000e-05; Error = 3.569e-09
```

Thermosimfit

- Data import
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	0
k_{dH} value lower boundary [1/M]	1e+08
k_{dH} value upper boundary [1/M]	2e+08
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+08

Optimization
Sensitivity analysis
Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds):

[Start batch analysis](#) [Stop optimization](#) [Save result of batch analysis](#)

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 68; Kaus(H) = 1.0000e+07; (1|0) + 1.0000e-15; (2|0) = 7.914e-05; (1|0) + 1.0000e-05; Error = 1.643e-09
Dataset Nr.: 1; Replication Nr.: 2; Generation = 69; Kaus(H) = 6.150e-06; (1|0) + 1.0000e-15; (2|0) = 9.834e-05; (1|0) + 1.0000e-05; Error = 2.493e-09
Dataset Nr.: 1; Replication Nr.: 2; Generation = 70; Kaus(H) = 3.875e-06; (1|0) + 1.0000e-15; (2|0) = 1.571e-04; (1|0) + 1.0000e-05; Error = 3.982e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 68; Kaus(H) = 5.935e-06; (1|0) + 1.0000e-15; (2|0) = 6.138e-05; (1|0) + 1.0000e-05; Error = 5.239e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 69; Kaus(H) = 1.032e-05; (1|0) + 1.0000e-15; (2|0) = 8.702e-06; (1|0) + 1.0000e-05; Error = 1.509e-08
```

Thermosimfit

- Data import
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

$k_{dH} \text{ value lower boundary } [1/\text{M}]$	20	$k_{dH} \text{ value upper boundary }$	0
$k_{dH} \text{ value upper boundary } [1/\text{M}]$	1e+08	$k_{dH} \text{ value lower boundary }$	1e+08
$(\text{Dy}) \text{ value lower boundary } [1/\text{M}]$		$(\text{Dy}) \text{ value upper boundary }$	0
$(\text{Dy}) \text{ value upper boundary } [1/\text{M}]$		$(\text{Dy}) \text{ value lower boundary }$	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```

Dataset Nr.: 1; Replication Nr.: 2; Generation = 72; Kain(H) = 1.0000e+07; (1)(0) + 1.0000e-15; (2)(0) = 7.914e-05; (1)(0) + 1.0000e-05; Error = 1.643e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 72; Kain(H) = 1.0000e+07; (1)(0) + 1.0000e-15; (2)(0) = 7.914e-05; (1)(0) + 1.0000e-05; Error = 1.643e-08
Dataset Nr.: 1; Replication Nr.: 1; Generation = 49; Kain(H) = 6.150e-06; (1)(0) + 1.0000e-15; (2)(0) = 9.834e-05; (1)(0) + 1.0000e-05; Error = 2.493e-08
Dataset Nr.: 1; Replication Nr.: 1; Generation = 49; Kain(H) = 6.150e-06; (1)(0) + 1.0000e-15; (2)(0) = 9.834e-05; (1)(0) + 1.0000e-05; Error = 2.493e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 71; Kain(H) = 5.935e-05; (1)(0) + 1.0000e-15; (2)(0) = 6.138e-05; (1)(0) + 1.0000e-05; Error = 5.239e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 78; Kain(H) = 1.032e-07; (1)(0) + 1.0000e-15; (2)(0) = 1.702e-08; (1)(0) + 1.0000e-05; Error = 3.569e-08

```

Thermosimfit

- Data input
- DSA (const. heat model)
- DSA (const. dye model)
- DSA model
- DSA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

k_{dH} value lower boundary [1/M]	22
k_{dH} value upper boundary [1/M]	0
k_{dH} value lower boundary [1/M]	1e+08
k_{dH} value upper boundary [1/M]	2e+08
k_{dH} value lower boundary [1/M]	0
k_{dH} value upper boundary [1/M]	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds):

[Start batch analysis](#) [Stop optimization](#) [Save result of batch analysis](#)

```
Dataset Nr.: 1; Replication Nr.: 2; Generation = 75; Kais(H) = 1.0000e+07; |(0)| = 1.0000e-15; |(0)| = 7.914e-05; |(0)| = 1.0000e-05; Error = 1.043e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 72; Kais(H) = 6.150e+06; |(0)| = 1.0000e-15; |(0)| = 9.834e-05; |(0)| = 1.0000e-05; Error = 2.493e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 75; Kais(H) = 5.932e+06; |(0)| = 1.0000e-15; |(0)| = 6.138e-05; |(0)| = 1.0000e-05; Error = 1.043e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 75; Kais(H) = 5.932e+06; |(0)| = 1.0000e-15; |(0)| = 6.138e-05; |(0)| = 1.0000e-05; Error = 5.239e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 74; Kais(H) = 1.032e+07; |(0)| = 1.0000e-15; |(0)| = 8.709e-05; |(0)| = 1.0000e-05; Error = 1.509e-08
```

Thermosimlit

- Data input
- DSK (const. heat model)
- (DSK (const. dye) model)
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{d}(H_2O)[1/M]$	3000000
3000000	

Advanced options

Boundaries

$k_{d}(H_2O)$ value lower boundary [1/M]	20
$k_{d}(H_2O)$ value upper boundary [1/M]	1e+00
$k_{d}(H_2O)$ value lower boundary [1/M]	0
$k_{d}(H_2O)$ value upper boundary [1/M]	1e+00
$k_{d}(H_2O)$ value lower boundary [1/M]	0
$k_{d}(H_2O)$ value upper boundary [1/M]	1e+00

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization Save result of batch analysis

```

Dataset Nr.: 1; Replication Nr.: 2; Generation = 77; Kast(H) = 1.0000e+07; |(0)| = 1.0000e-15; |(0)| = 7.914e-05; |(0)| = 1.0000e-05; Error = 1.634e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 77; Kast(H) = 6.150e+06; |(0)| = 1.0000e-15; |(0)| = 9.834e-05; |(0)| = 1.0000e-05; Error = 2.493e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 77; Kast(H) = 5.935e+06; |(0)| = 1.0000e-15; |(0)| = 6.138e-05; |(0)| = 1.0000e-05; Error = 1.569e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 77; Kast(H) = 5.935e+06; |(0)| = 1.0000e-15; |(0)| = 6.138e-05; |(0)| = 1.0000e-05; Error = 5.239e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 78; Kast(H) = 1.032e+07; |(0)| = 1.0000e-15; |(0)| = 8.709e-05; |(0)| = 1.0000e-05; Error = 3.569e-08

```

Thermosimlit

- Data input
- DSK (const. heat model)
- (DSK (const. dye) model)
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]: 0.000001
Dye conc. [M]: 0.000001
 $k_{dH} \text{[M]}^{-1}$: 3000000

Advanced options

Boundaries

k_{dH} value lower boundary [1/M]: 20
 k_{dH} value upper boundary [1/M]: 1e+08

H_2O value lower boundary [1/M]: 0
 H_2O value upper boundary [1/M]: 1e+08

H_2O value lower boundary [1/M]: 0
 H_2O value upper boundary [1/M]: 1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```

Dataset Nr.: 1; Replication Nr.: 2; Generation = 89; Kao(H) = 1.0000e+07; |(0)| = 1.0000e-15; |(0)| = 7.914e-05; |(0)| = 1.0000e-05; Error = 1.634e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 89; Kao(H) = 6.150e+06; |(0)| = 1.0000e-15; |(0)| = 9.834e-05; |(0)| = 1.0000e-05; Error = 2.493e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 89; Kao(H) = 5.932e+06; |(0)| = 1.0000e-15; |(0)| = 1.0000e-05; Error = 1.5000e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 81; Kao(H) = 5.932e+06; |(0)| = 1.0000e-15; |(0)| = 6.138e-05; |(0)| = 1.0000e-05; Error = 5.239e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 89; Kao(H) = 1.0000e-15; |(0)| = 1.0000e-15; |(0)| = 8.702e-05; |(0)| = 1.5000e-08

```

Thermosimlit

- Data input
- DSK (const. heat model)
- (DSK (const. dye) model)
- DSK model
- DSK model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
$k_{dH} \text{[M]}^{-1}$	3000000
Advanced options	

Boundaries

$k_{dH} \text{ value lower boundary } [1/\text{M}]$	20	$k_{dH} \text{ value upper boundary }$	0
$k_{dH} \text{ value upper boundary } [1/\text{M}]$	1e+08	$k_{dH} \text{ value lower boundary }$	1e+08
$\text{[DH] value lower boundary } [1/\text{M}]$		$\text{[DH] value upper boundary } [1/\text{M}]$	$\text{[DH] value lower boundary } [1/\text{M}]$
0		0	1e+08
$\text{[DH] value upper boundary } [1/\text{M}]$		$\text{[DH] value lower boundary } [1/\text{M}]$	
1e+08		1e+08	

Optimization Sensitivity analysis Batch processing

Batch analysis

How often should each dataset be analyzed (using different seeds): 3

Start batch analysis Stop optimization

```

Dataset Nr.: 1; Replication Nr.: 2; Generation = 81; Kaus(H) = 1.0000e+07; (1)(0) + 1.0000e-15; (1)(0) = 7.914e-05; (1)(0) + 1.0000e-05; Error = 1.634e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 81; Kaus(H) = 6.150e-06; (1)(0) + 1.0000e-15; (1)(0) = 9.834e-05; (1)(0) + 1.0000e-05; Error = 2.493e-08
Dataset Nr.: 1; Replication Nr.: 2; Generation = 81; Kaus(H) = 5.935e-06; (1)(0) + 1.0000e-15; (1)(0) = 6.138e-05; (1)(0) + 1.0000e-05; Error = 1.509e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 84; Kaus(H) = 5.935e-06; (1)(0) + 1.0000e-15; (1)(0) = 6.138e-05; (1)(0) + 1.0000e-05; Error = 5.239e-08
Dataset Nr.: 2; Replication Nr.: 2; Generation = 85; Kaus(H) = 1.0000e-05; (1)(0) + 1.0000e-15; (1)(0) = 1.702e-05; (1)(0) + 1.0000e-05; Error = 3.509e-08

```

