

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
DA model
Info

Parameter

Host conc. [M]
0.00001

Dye conc. [M]
0.000001

K_d(HG) [1/M]
300000

Advanced options +

Boundaries ⓘ

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

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

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

I(D) 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

Batch analysis

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

Start batch analysis Stop optimization Save result of batch analysis

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

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0.00001

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300000

Advanced options +

Boundaries ⓘ

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

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

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

I(D) 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

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _a (H) _D [L/M]	3000000

Advanced options

Boundaries

K _a (HG) value lower boundary [1/M]	10
K _a (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 2; Ka(HD) = 2.099e+02; I(B) = 2.409e-01; I(HD) = 1.549e-02; I(D) = 9.544e-03; Error = 3.109e-00
Dataset Nr.: 1; Replication Nr.:1; Generation = 2; Ka(HD) = 0.149e+02; I(B) = 1.248e-01; I(HD) = 5.886e-02; I(D) = 3.812e-02; Error = 9.407e-00
Dataset Nr.: 1; Replication Nr.:2; Generation = 2; Ka(HD) = 0.989e+02; I(B) = 1.836e-18; I(HD) = 3.560e+00; I(D) = 1.661e-08; Error = 1.762e+01
Dataset Nr.: 2; Replication Nr.:1; Generation = 2; Ka(HD) = 2.986e+02; I(B) = 2.499e-01; I(HD) = 1.048e+02; I(D) = 9.564e-03; Error = 9.198e-00
Dataset Nr.: 2; Replication Nr.:2; Generation = 2; Ka(HD) = 9.887e+04; I(B) = 2.169e-01; I(HD) = 6.982e-05; I(D) = 8.905e-08; Error = 1.259e+01
Dataset Nr.: 2; Replication Nr.:3; Generation = 2; Ka(HD) = 3.549e+07; I(B) = 2.624e-01; I(HD) = 8.799e-06; I(D) = 1.999e-14; Error = 0.439e+00
```

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

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _a (H0) [L/M]	3000000

Advanced options

Boundaries

K _a (HG) value lower boundary [1/M]	10
K _a (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 4; Ka(H0) = 2.098e+00; I(B) = 2.409e-01; I(HD) = 5.458e-02; I(D) = 2.554e-01; Error = 3.108e-00
Dataset Nr.: 1; Replication Nr.:1; Generation = 4; Ka(H0) = 2.139e+00; I(B) = 1.988e-01; I(HD) = 5.121e-01; I(D) = 2.906e-01; Error = 4.338e-00
Dataset Nr.: 1; Replication Nr.:2; Generation = 4; Ka(H0) = 2.156e+00; I(B) = 1.989e-01; I(HD) = 1.593e+00; I(D) = 9.056e-01; Error = 5.114e-00
Dataset Nr.: 2; Replication Nr.:1; Generation = 4; Ka(H0) = 2.986e+00; I(B) = 2.499e-01; I(HD) = 1.048e+02; I(D) = 9.564e-01; Error = 9.198e-00
Dataset Nr.: 2; Replication Nr.:2; Generation = 4; Ka(H0) = 2.198e+00; I(B) = 9.35e-02; I(HD) = 1.329e+03; I(D) = 1.949e+00; Error = 1.186e+01
Dataset Nr.: 2; Replication Nr.:3; Generation = 4; Ka(H0) = 3.549e+00; I(B) = 2.624e-01; I(HD) = 8.799e-06; I(D) = 1.099e-14; Error = 0.439e+00
```

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

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _a (H) [L/M]	3000000

Advanced options

Boundaries

K _a (HG) value lower boundary [1/M]	10
K _a (HG) value upper boundary [1/M]	1e+00
I(HD) value lower boundary [1/M]	0
I(HD) value upper boundary [1/M]	1e+00
I(D) value lower boundary [1/M]	0
I(D) value upper boundary [1/M]	1e+00

Optimization Sensitivity analysis Batch processing

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 0; Ka(HG) = 0.001e+00; I(B) = 1.000e-15; I(HD) = 5.956e-09; I(D) = 1.000e-15; Error = 8.308e-09
Dataset Nr.: 1; Replication Nr.:1; Generation = 0; Ka(HG) = 1.000e-01; I(B) = 1.000e-15; I(HD) = 9.321e-09; I(D) = 1.000e-15; Error = 8.308e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 0; Ka(HG) = 5.156e-05; I(B) = 1.000e-15; I(HD) = 1.953e-05; I(D) = 9.050e-04; Error = 8.114e-09
Dataset Nr.: 2; Replication Nr.:1; Generation = 6; Ka(HG) = 0.881e+04; I(B) = 1.000e-15; I(HD) = 4.984e-05; I(D) = 1.000e-04; Error = 8.867e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 6; Ka(HG) = 1.000e+01; I(B) = 2.469e-01; I(HD) = 1.000e-15; I(D) = 1.000e-15; Error = 9.235e-09
Dataset Nr.: 2; Replication Nr.:3; Generation = 7; Ka(HG) = 5.049e+07; I(B) = 2.624e-01; I(HD) = 8.799e-06; I(D) = 1.000e-14; Error = 9.439e-09
```

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Data import

DBA (const, host) model

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GDA model

DA model

Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _a (HG) [L/M]	3000000

Advanced options +

Optimization

Sensitivity analysis

Batch processing

Boundaries (Help)

K _a (HG) value lower boundary [1/M]	10
K _a (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

Start batch analysis Stop optimization Save result of batch analysis

```

Dataset Nr.: 1; Replication Nr.:1; Generation = 8; Ka(HG) = 1.000e+00; I(B) = 1.000e-15; I(HD) = 4.320e-05; I(D) = 8.000e-05; Error = 8.209e-00
Dataset Nr.: 1; Replication Nr.:1; Generation = 8; Ka(HG) = 3.700e+00; I(B) = 1.000e-15; I(HD) = 3.880e-05; I(D) = 4.440e-05; Error = 4.209e-00
Dataset Nr.: 1; Replication Nr.:2; Generation = 8; Ka(HG) = 5.550e+00; I(B) = 0.500e-05; I(HD) = 4.300e-05; I(D) = 1.000e-05; Error = 6.813e-00
Dataset Nr.: 2; Replication Nr.:1; Generation = 8; Ka(HG) = 5.912e+00; I(B) = 1.000e-15; I(HD) = 4.520e-05; I(D) = 8.000e-03; Error = 8.401e-00
Dataset Nr.: 2; Replication Nr.:2; Generation = 7; Ka(HG) = 1.000e+01; I(B) = 2.460e-01; I(HD) = 1.000e-15; I(D) = 1.000e-15; Error = 9.215e-00
Dataset Nr.: 2; Replication Nr.:3; Generation = 8; Ka(HG) = 5.010e+00; I(B) = 1.000e-15; I(HD) = 1.020e-05; I(D) = 1.000e-15; Error = 6.402e-00

```

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Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (HG) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

Dataset Nr.: 1; Replication Nr.: 1; Generation = 11; K _d (HG) = 0.389e+06; I(B) = 1.088e-15; I(HD) = 7.269e+05; I(D) = 1.009e-15; Error = 5.056e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 11; K _d (HG) = 1.783e+06; I(B) = 1.888e-15; I(HD) = 4.958e+05; I(D) = 1.443e+05; Error = 4.388e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 11; K _d (HG) = 2.559e+06; I(B) = 8.588e-15; I(HD) = 4.382e+05; I(D) = 1.989e+05; Error = 6.813e-09
Dataset Nr.: 2; Replication Nr.: 1; Generation = 11; K _d (HG) = 0.389e+06; I(B) = 1.088e-15; I(HD) = 7.298e+05; I(D) = 1.009e-15; Error = 5.068e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 18; K _d (HG) = 1.887e+07; I(B) = 1.088e-15; I(HD) = 1.482e+06; I(D) = 1.437e+05; Error = 6.914e-09
Dataset Nr.: 2; Replication Nr.: 3; Generation = 11; K _d (HG) = 0.3814e+06; I(B) = 8.359e-15; I(HD) = 8.989e+05; I(D) = 7.774e+04; Error = 4.098e-09

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Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (HG) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
I(HD) value lower boundary [1/M]	0
I(HD) value upper boundary [1/M]	1e+00
I(D) value lower boundary [1/M]	0
I(D) value upper boundary [1/M]	1e+00

Optimization Sensitivity analysis Batch processing

Batch analysis

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

Dataset Nr.: 1; Replication Nr.: 1; Generation = 13; K _d (HG) = 4.339e+06; I(B) = 1.080e-16; I(HD) = 1.000e-05; I(D) = 6.000e-04; Error = 4.346e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 13; K _d (HG) = 4.188e+06; I(B) = 1.080e-16; I(HD) = 7.710e-05; I(D) = 5.800e-04; Error = 4.346e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 13; K _d (HG) = 1.345e+07; I(B) = 6.800e-02; I(HD) = 6.197e-05; I(D) = 1.405e-05; Error = 3.512e-09
Dataset Nr.: 2; Replication Nr.: 1; Generation = 13; K _d (HG) = 4.399e+06; I(B) = 1.080e-15; I(HD) = 1.050e-06; I(D) = 6.055e-04; Error = 4.346e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 12; K _d (HG) = 7.221e+06; I(B) = 1.080e-15; I(HD) = 4.889e-05; I(D) = 2.099e-05; Error = 5.704e-09
Dataset Nr.: 2; Replication Nr.: 3; Generation = 13; K _d (HG) = 8.814e+06; I(B) = 8.000e-02; I(HD) = 8.989e-05; I(D) = 7.774e-04; Error = 4.000e-09

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (HG) [L/M]	3000000

Advanced options +

Boundaries

K _d (HG) value lower boundary [L/M]	10	I(D) value lower boundary [L/M]	0
K _d (HG) value upper boundary [L/M]	1e+00	I(D) value upper boundary	1e+08
I(HD) value lower boundary [L/M]	0	I(D) value lower boundary [L/M]	0
I(HD) value upper boundary [L/M]	1e+00	I(D) value upper boundary [L/M]	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

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

Start batch analysis Stop optimization Save results of batch analysis

Dataset Nr.: 1; Replication Nr.: 1; Generation = 1K; K _d (HG) = 0.000001; I(D) = 1.000e-15; I(HD) = 7.000e-05; I(D) = 1.500e-05; Error = 2.000e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 1K; K _d (HG) = 3.000e-06; I(D) = 1.000e-15; I(HD) = 7.000e-05; I(D) = 1.113e-05; Error = 3.842e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 1K; K _d (HG) = 1.000e-07; I(D) = 6.070e-02; I(HD) = 8.545e-05; I(D) = 1.361e-01; Error = 8.991e-01
Dataset Nr.: 2; Replication Nr.: 1; Generation = 1K; K _d (HG) = 8.923e-06; I(D) = 1.000e-15; I(HD) = 1.047e-06; I(D) = 1.544e-05; Error = 2.568e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 1K; K _d (HG) = 7.221e-06; I(D) = 1.000e-15; I(HD) = 4.889e-05; I(D) = 2.099e-05; Error = 5.704e-09
Dataset Nr.: 2; Replication Nr.: 3; Generation = 1K; K _d (HG) = 3.014e-06; I(D) = 8.000e-02; I(HD) = 8.999e-05; I(D) = 7.774e-04; Error = 4.000e-09

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (HG) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 18; Kd(HG) = 0.000001; I(B) = 1.000e-15; I(HD) = 1.000e-05; I(D) = 1.000e-05; Error = 2.000e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 18; Kd(HG) = 4.000e-06; I(B) = 1.000e-15; I(HD) = 6.870e-05; I(D) = 4.830e-05; Error = 3.000e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 18; Kd(HG) = 1.956e-07; I(B) = 6.670e-02; I(HD) = 8.545e-05; I(D) = 1.361e-05; Error = 8.091e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 18; Kd(HG) = 8.923e-06; I(B) = 1.000e-15; I(HD) = 1.047e-06; I(D) = 1.544e-06; Error = 2.568e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 17; Kd(HG) = 3.591e-06; I(B) = 1.000e-15; I(HD) = 1.052e-06; I(D) = 9.869e-04; Error = 4.021e-09
Dataset Nr.: 2; Replication Nr.:3; Generation = 18; Kd(HG) = 3.814e-06; I(B) = 8.000e-02; I(HD) = 9.989e-05; I(D) = 7.774e-04; Error = 4.000e-09
```

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (HG) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 21; Kd(HG) = 0.000001; I(0) = 1.000e-15; I(HD) = 1.000e-05; I(D) = 1.000e-05; Error = 2.000e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 21; Kd(HG) = 4.000e-06; I(0) = 1.000e-15; I(HD) = 4.000e-05; I(D) = 4.000e-05; Error = 3.000e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 21; Kd(HG) = 7.000e-07; I(0) = 7.000e-02; I(HD) = 9.543e-05; I(D) = 1.259e-01; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 21; Kd(HG) = 8.023e-06; I(0) = 1.000e-15; I(HD) = 1.047e-06; I(D) = 1.544e-06; Error = 2.568e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 28; Kd(HG) = 3.591e-06; I(0) = 1.000e-15; I(HD) = 1.052e-06; I(D) = 9.869e-04; Error = 4.021e-08
Dataset Nr.: 2; Replication Nr.:3; Generation = 28; Kd(HG) = 3.814e-06; I(0) = 8.000e-02; I(HD) = 9.989e-05; I(D) = 7.774e-04; Error = 4.000e-09
```

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.00001
K _d (HG) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 23; Kd(HG) = 0.024e+06; I(B) = 1.080e-15; I(HD) = 7.450e-05; I(D) = 1.544e-05; Error = 2.056e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 23; Kd(HG) = 8.924e+06; I(B) = 1.080e-15; I(HD) = 7.450e-05; I(D) = 1.544e-05; Error = 2.056e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 23; Kd(HG) = 2.979e+07; I(B) = 7.340e-02; I(HD) = 9.543e+05; I(D) = 1.259e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 23; Kd(HG) = 8.923e+06; I(B) = 1.080e-15; I(HD) = 1.047e-06; I(D) = 1.544e-06; Error = 2.568e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 22; Kd(HG) = 3.591e+06; I(B) = 1.080e-15; I(HD) = 1.052e+06; I(D) = 9.869e-04; Error = 4.021e-09
Dataset Nr.: 2; Replication Nr.:3; Generation = 22; Kd(HG) = 3.814e+06; I(B) = 8.305e-02; I(HD) = 9.989e+05; I(D) = 7.774e-04; Error = 4.009e-09
```

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Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (HG) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

Start batch analysis Stop optimization Save results of batch analysis

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 25; Ke(HG) = 0.024e+06; I(B) = 1.080e-15; I(HD) = 7.450e-05; I(D) = 1.544e-05; Error = 2.050e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 25; Ke(HG) = 8.924e+06; I(B) = 1.080e-15; I(HD) = 7.450e-05; I(D) = 1.544e-05; Error = 2.050e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 25; Ke(HG) = 2.979e+07; I(B) = 7.340e-02; I(HD) = 9.543e+05; I(D) = 1.259e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 25; Ke(HG) = 8.923e+06; I(B) = 1.080e-15; I(HD) = 1.047e-06; I(D) = 1.544e-05; Error = 2.568e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 24; Ke(HG) = 3.591e+06; I(B) = 1.080e-15; I(HD) = 1.052e+06; I(D) = 3.868e-04; Error = 4.021e-08
Dataset Nr.: 2; Replication Nr.:3; Generation = 25; Ke(HG) = 4.202e+06; I(B) = 1.080e-15; I(HD) = 8.047e-05; I(D) = 3.041e-06; Error = 3.316e-09
```

Thermosimfit

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

Parameters

Host conc. [M]:
0.000001

Dye conc. [M]:
0.000001

K_d(H) [L/M]:
3000000

Advanced options

Boundaries

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

K_d(HG) value upper boundary [1/M]:
1e+00

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

I(HD) value upper boundary [1/M]:
1e+00

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

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

Optimization Sensitivity analysis Batch processing

Batch analysis

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

Dataset Nr.: 1; Replication Nr.: 1; Generation = 27; K _d (HG) = 0.027e+06; I(H) = 1.080e-15; I(HD) = 1.947e+05; I(D) = 1.544e+05; Error = 2.056e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 27; K _d (HG) = 0.028e+06; I(H) = 1.080e-15; I(HD) = 1.947e+05; I(D) = 1.544e+05; Error = 2.056e-09
Dataset Nr.: 1; Replication Nr.: 2; Generation = 28; K _d (HG) = 2.979e+07; I(H) = 7.340e-02; I(HD) = 9.540e+05; I(D) = 1.759e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.: 1; Generation = 27; K _d (HG) = 8.923e+06; I(H) = 1.080e-15; I(HD) = 1.047e+06; I(D) = 1.544e+05; Error = 2.568e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 26; K _d (HG) = 2.531e+07; I(H) = 1.080e-15; I(HD) = 9.798e+05; I(D) = 2.216e+05; Error = 1.979e-09
Dataset Nr.: 2; Replication Nr.: 3; Generation = 27; K _d (HG) = 1.200e+07; I(H) = 1.080e-15; I(HD) = 8.409e+05; I(D) = 1.812e+05; Error = 3.077e-09

Thermosimfit

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

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 29; Kd(HG) = 0.000001; I(B) = 1.000e-15; I(HD) = 1.000e-05; I(D) = 1.000e-05; Error = 2.000e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 29; Kd(HG) = 8.988e-06; I(B) = 1.000e-15; I(HD) = 8.988e-05; I(D) = 1.374e-05; Error = 6.818e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 38; Kd(HG) = 7.979e-07; I(B) = 7.340e-02; I(HD) = 8.540e-05; I(D) = 1.759e-05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 38; Kd(HG) = 8.923e-06; I(B) = 1.000e-15; I(HD) = 1.047e-06; I(D) = 1.544e-06; Error = 2.568e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 28; Kd(HG) = 2.531e-07; I(B) = 1.000e-15; I(HD) = 9.798e-05; I(D) = 2.216e-05; Error = 1.579e-09
Dataset Nr.: 2; Replication Nr.:3; Generation = 29; Kd(HG) = 1.200e-07; I(B) = 1.000e-15; I(HD) = 8.409e-05; I(D) = 1.832e-05; Error = 3.077e-09
```

Thermosimfit

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

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 33; Kd(HG) = 7.819e+06; I(B) = 1.000e-15; I(HD) = 8.990e-05; I(D) = 1.001e-05; Error = 1.000e-06
Dataset Nr.: 1; Replication Nr.:2; Generation = 33; Kd(HG) = 8.385e+06; I(B) = 1.000e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.518e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 33; Kd(HG) = 7.879e+07; I(B) = 7.340e-02; I(HD) = 8.543e+05; I(D) = 1.759e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 33; Kd(HG) = 7.819e+06; I(B) = 1.000e-15; I(HD) = 8.990e-05; I(D) = 1.031e-05; Error = 1.959e-06
Dataset Nr.: 2; Replication Nr.:2; Generation = 31; Kd(HG) = 2.531e+07; I(B) = 1.000e-15; I(HD) = 9.798e-05; I(D) = 2.216e-05; Error = 1.579e-08
Dataset Nr.: 2; Replication Nr.:3; Generation = 32; Kd(HG) = 8.049e+06; I(B) = 1.000e-15; I(HD) = 8.057e-05; I(D) = 1.623e-05; Error = 2.291e-09
```

Thermosimfit

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

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 34; Kd(HG) = 7.819e+06; I(B) = 1.000e-15; I(HD) = 8.990e-05; I(D) = 1.001e-05; Error = 1.000e-06
Dataset Nr.: 1; Replication Nr.: 1; Generation = 34; Kd(HG) = 8.385e+06; I(B) = 1.000e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.518e-09
Dataset Nr.: 1; Replication Nr.: 2; Generation = 35; Kd(HG) = 7.879e+07; I(B) = 7.340e-02; I(HD) = 8.543e+05; I(D) = 1.759e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.: 1; Generation = 34; Kd(HG) = 7.819e+06; I(B) = 1.000e-15; I(HD) = 8.990e-05; I(D) = 1.031e-05; Error = 1.959e-06
Dataset Nr.: 2; Replication Nr.: 2; Generation = 34; Kd(HG) = 2.531e+07; I(B) = 1.000e-15; I(HD) = 9.798e-05; I(D) = 2.216e-05; Error = 1.579e-08
Dataset Nr.: 2; Replication Nr.: 3; Generation = 34; Kd(HG) = 8.049e+06; I(B) = 1.000e-15; I(HD) = 8.057e-05; I(D) = 1.623e-05; Error = 2.291e-09
```

Thermosimfit

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

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
I(HD) value lower boundary [1/M]	0
I(HD) value upper boundary [1/M]	1e+00
I(D) value lower boundary [1/M]	0
I(D) value upper boundary [1/M]	1e+00

Optimization Sensitivity analysis Batch processing

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 36; Kd(HG) = 7.819e+06; I(B) = 1.000e-15; I(HD) = 8.990e-05; I(D) = 1.001e-05; Error = 1.000e-06
Dataset Nr.: 1; Replication Nr.:2; Generation = 36; Kd(HG) = 8.385e+06; I(B) = 1.000e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.518e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 37; Kd(HG) = 7.879e+07; I(B) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.759e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 36; Kd(HG) = 7.819e+06; I(B) = 1.000e-15; I(HD) = 8.990e-05; I(D) = 1.031e-05; Error = 1.959e-06
Dataset Nr.: 2; Replication Nr.:2; Generation = 35; Kd(HG) = 2.531e+07; I(B) = 1.000e-15; I(HD) = 9.789e-05; I(D) = 2.216e-05; Error = 1.579e-00
Dataset Nr.: 2; Replication Nr.:3; Generation = 36; Kd(HG) = 8.049e+06; I(B) = 1.000e-15; I(HD) = 8.057e-05; I(D) = 1.623e-05; Error = 2.291e-00
```

Thermosimfit

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

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 39; Ke(HG) = 7.834e+06; I(B) = 1.080e-15; I(HD) = 8.960e-05; I(D) = 1.031e-05; Error = 1.030e-06
Dataset Nr.: 1; Replication Nr.:2; Generation = 39; Ke(HG) = 8.385e+06; I(B) = 1.080e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.513e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 39; Ke(HG) = 7.879e+07; I(B) = 7.340e-02; I(HD) = 8.543e-05; I(D) = 1.759e-05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 39; Ke(HG) = 7.819e+06; I(B) = 1.080e-15; I(HD) = 8.950e-05; I(D) = 1.031e-05; Error = 1.959e-00
Dataset Nr.: 2; Replication Nr.:2; Generation = 38; Ke(HG) = 2.531e+07; I(B) = 1.080e-15; I(HD) = 9.780e-05; I(D) = 2.216e-05; Error = 1.579e-00
Dataset Nr.: 2; Replication Nr.:3; Generation = 39; Ke(HG) = 8.049e+06; I(B) = 1.080e-15; I(HD) = 8.057e-05; I(D) = 1.623e-05; Error = 2.291e-00
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 42; Kd(HG) = 1.134e+07; I(B) = 1.088e-16; I(HD) = 1.925e+06; I(D) = 1.728e+05; Error = 1.594e-06
Dataset Nr.: 1; Replication Nr.:1; Generation = 42; Kd(HG) = 0.388e+06; I(B) = 1.088e-15; I(HD) = 8.343e+05; I(D) = 1.374e+05; Error = 2.538e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 42; Kd(HG) = 7.979e+07; I(B) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 42; Kd(HG) = 1.116e+07; I(B) = 1.088e-15; I(HD) = 1.012e+06; I(D) = 1.728e+05; Error = 1.594e-06
Dataset Nr.: 2; Replication Nr.:2; Generation = 48; Kd(HG) = 2.531e+07; I(B) = 1.088e-15; I(HD) = 9.788e+05; I(D) = 2.216e+05; Error = 1.579e-08
Dataset Nr.: 2; Replication Nr.:3; Generation = 41; Kd(HG) = 8.049e+06; I(B) = 1.088e-15; I(HD) = 8.057e+05; I(D) = 1.623e+05; Error = 2.201e-09
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.: 1; Generation = 44; Kd(HG) = 1.134e+07; I(H) = 1.000e-15; I(HD) = 1.000e-05; I(D) = 1.738e-05; Error = 1.594e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 44; Kd(HG) = 0.385e+06; I(H) = 1.000e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.538e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 44; Kd(HG) = 7.979e+07; I(H) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.: 1; Generation = 45; Kd(HG) = 1.116e+07; I(H) = 1.000e-15; I(HD) = 1.012e-06; I(D) = 1.728e-05; Error = 1.594e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 43; Kd(HG) = 2.531e+07; I(H) = 1.000e-15; I(HD) = 9.788e-05; I(D) = 2.216e-05; Error = 1.579e-09
Dataset Nr.: 2; Replication Nr.: 3; Generation = 44; Kd(HG) = 8.049e+06; I(H) = 1.000e-15; I(HD) = 8.057e-05; I(D) = 1.623e-05; Error = 2.201e-09
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 47; Kd(HG) = 1.134e+07; I(H) = 1.000e-16; I(HD) = 1.000e-06; I(D) = 1.728e-05; Error = 1.594e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 47; Kd(HG) = 0.388e+06; I(H) = 1.000e-16; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.518e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 47; Kd(HG) = 2.979e+07; I(H) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 47; Kd(HG) = 1.116e+07; I(H) = 1.000e-15; I(HD) = 1.012e-06; I(D) = 1.728e-05; Error = 1.594e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 45; Kd(HG) = 1.766e+07; I(H) = 1.000e-15; I(HD) = 9.176e-05; I(D) = 2.045e-05; Error = 1.094e-09
Dataset Nr.: 2; Replication Nr.:3; Generation = 46; Kd(HG) = 8.269e+06; I(H) = 1.000e-15; I(HD) = 8.187e-05; I(D) = 1.623e-05; Error = 2.291e-09
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 49; Kd(HG) = 1.134e+07; I(B) = 1.088e-16; I(HD) = 1.925e+06; I(D) = 1.728e+05; Error = 1.594e-06
Dataset Nr.: 1; Replication Nr.:1; Generation = 50; Kd(HG) = 0.388e+06; I(B) = 1.088e-15; I(HD) = 8.343e+05; I(D) = 1.374e+05; Error = 2.538e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 58; Kd(HG) = 2.979e+07; I(B) = 7.340e-02; I(HD) = 8.542e+05; Error = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 49; Kd(HG) = 1.116e+07; I(B) = 1.088e-15; I(HD) = 1.012e+06; I(D) = 1.728e+05; Error = 1.594e-06
Dataset Nr.: 2; Replication Nr.:2; Generation = 47; Kd(HG) = 1.946e+07; I(B) = 1.088e-15; I(HD) = 1.088e+06; I(D) = 1.938e+05; Error = 6.410e-01
Dataset Nr.: 2; Replication Nr.:3; Generation = 48; Kd(HG) = 8.269e+06; I(B) = 1.088e-15; I(HD) = 8.197e+05; I(D) = 8.623e+05; Error = 2.291e-09
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]:
0.000001

Dye conc. [M]:
0.000001

K_d(H) [L/M]:
3000000

Advanced options

Boundaries

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

K_d(HG) value upper boundary [1/M]:
1e+00

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

I(HD) value upper boundary [1/M]:
1e+00

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

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

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

Dataset Nr.: 1; Replication Nr.: 1; Generation = 51; K _d (HG) = 1.134e+07; I(H) = 1.000e-16; I(HD) = 1.000e-06; I(D) = 1.734e-06; Error = 1.594e-06
Dataset Nr.: 1; Replication Nr.: 1; Generation = 52; K _d (HG) = 0.388e+06; I(H) = 1.000e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.533e-09
Dataset Nr.: 1; Replication Nr.: 2; Generation = 51; K _d (HG) = 2.979e+07; I(H) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.758e-05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.: 1; Generation = 51; K _d (HG) = 1.116e+07; I(H) = 1.000e-15; I(HD) = 1.012e-06; I(D) = 1.728e-05; Error = 1.594e-06
Dataset Nr.: 2; Replication Nr.: 2; Generation = 48; K _d (HG) = 1.946e+07; I(H) = 1.000e-15; I(HD) = 1.088e-06; I(D) = 1.938e-05; Error = 6.410e-01
Dataset Nr.: 2; Replication Nr.: 3; Generation = 56; K _d (HG) = 8.269e+06; I(H) = 1.000e-15; I(HD) = 8.197e-05; I(D) = 1.621e-05; Error = 2.201e-09

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 54; Kd(HG) = 1.134e+07; I(B) = 1.088e-15; I(HD) = 1.925e+06; I(D) = 1.728e+05; Error = 1.594e-09
Dataset Nr.: 1; Replication Nr.:1; Generation = 54; Kd(HG) = 0.388e+06; I(B) = 1.088e-15; I(HD) = 8.343e+05; I(D) = 1.374e+05; Error = 2.538e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 54; Kd(HG) = 2.879e+07; I(B) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 54; Kd(HG) = 1.116e+07; I(B) = 1.088e-15; I(HD) = 1.012e+06; I(D) = 1.728e+05; Error = 1.594e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 52; Kd(HG) = 1.946e+07; I(B) = 1.088e-15; I(HD) = 1.088e+06; I(D) = 1.938e+05; Error = 6.419e-01
Dataset Nr.: 2; Replication Nr.:3; Generation = 53; Kd(HG) = 8.269e+06; I(B) = 1.088e-15; I(HD) = 8.1979e+05; I(D) = 3.623e+05; Error = 2.291e-09
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]:
0.000001

Dye conc. [M]:
0.000001

K_d(HG) [L/M]:
3000000

Advanced options

Boundaries

K_d(HG) value lower boundary [L/M]:
10

K_d(HG) value upper boundary [L/M]:
1e+00

I(HD) value lower boundary [L/M]:
0

I(HD) value upper boundary [L/M]:
1e+00

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

I(D) value upper boundary [L/M]:
1e+00

Optimization
Sensitivity analysis
Batch processing

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 57; Kd(HG) = 1.134e+07; I(B) = 1.080e-16; I(HD) = 1.920e-06; I(D) = 1.728e-06; Error = 1.594e-06
Dataset Nr.: 1; Replication Nr.:1; Generation = 56; Kd(HG) = 0.388e+06; I(B) = 1.080e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.533e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 56; Kd(HG) = 2.979e+07; I(B) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 57; Kd(HG) = 1.116e+07; I(B) = 1.080e-15; I(HD) = 1.012e-06; I(D) = 1.728e-06; Error = 1.594e-06
Dataset Nr.: 2; Replication Nr.:2; Generation = 54; Kd(HG) = 1.946e+07; I(B) = 1.080e-15; I(HD) = 1.080e-06; I(D) = 1.938e-05; Error = 6.410e-01
Dataset Nr.: 2; Replication Nr.:3; Generation = 56; Kd(HG) = 8.269e+06; I(B) = 1.080e-15; I(HD) = 8.197e-05; I(D) = 1.623e-05; Error = 2.291e-09
```

Thermosimfit

Data import

DBA (const, host) model

DBA (const, dye) model

GDA model

DA model

Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
I(HD) value lower boundary [1/M]	0
I(HD) value upper boundary [1/M]	1e+00

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

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

Start batch analysis Stop optimization Save results of batch analysis

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 99; Kd(HG) = 1.134e+07; I(B) = 1.000e-16; I(HD) = 1.000e-06; I(D) = 1.738e-06; Error = 1.594e-06
Dataset Nr.: 1; Replication Nr.:2; Generation = 99; Kd(HG) = 0.388e+06; I(B) = 1.000e-15; I(HD) = 8.343e-05; I(D) = 1.374e-05; Error = 2.538e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 99; Kd(HG) = 2.979e+07; I(B) = 7.340e-02; I(HD) = 8.542e+05; I(D) = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 99; Kd(HG) = 1.116e+07; I(B) = 1.000e-15; I(HD) = 1.012e-06; I(D) = 1.728e-06; Error = 1.594e-06
Dataset Nr.: 2; Replication Nr.:2; Generation = 96; Kd(HG) = 1.946e+07; I(B) = 1.000e-15; I(HD) = 1.088e-06; I(D) = 1.938e-06; Error = 6.410e-01
Dataset Nr.: 2; Replication Nr.:3; Generation = 98; Kd(HG) = 8.269e+06; I(B) = 1.000e-15; I(HD) = 8.197e-05; I(D) = 1.621e-05; Error = 2.291e-09
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 62; Kd(HG) = 1.134e+07; I(H) = 1.000e-15; I(HD) = 1.000e-05; I(D) = 1.793e-09; Error = 1.064e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 62; Kd(HG) = 8.984e+06; I(H) = 1.000e-15; I(HD) = 7.933e-05; I(D) = 1.793e-09; Error = 1.064e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 62; Kd(HG) = 7.979e+07; I(H) = 7.340e-02; I(HD) = 9.542e-05; I(D) = 1.793e-05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 61; Kd(HG) = 1.116e+07; I(H) = 1.000e-15; I(HD) = 1.012e-06; I(D) = 1.728e-05; Error = 1.594e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 59; Kd(HG) = 1.946e+07; I(H) = 1.000e-15; I(HD) = 1.000e-06; I(D) = 1.938e-05; Error = 6.410e-01
Dataset Nr.: 2; Replication Nr.:3; Generation = 60; Kd(HG) = 8.269e+06; I(H) = 1.000e-15; I(HD) = 8.197e-05; I(D) = 1.621e-05; Error = 2.291e-09
```

Thermosimfit

- Data import
- DBA (const, host) model
- DBA (const, dye) model
- GDA model
- DA model
- Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options +

Boundaries

K _d (HG) value lower boundary [1/M]	10	I(D) value lower boundary [1/M]	0
K _d (HG) value upper boundary [1/M]	1e+03	I(D) value upper boundary	1e+08
I(HD) value lower boundary [1/M]	0	I(D) value lower boundary [1/M]	0
I(HD) value upper boundary [1/M]	1e+03	I(D) value upper boundary [1/M]	1e+08

Optimization Sensitivity analysis Batch processing

Batch analysis

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

Start batch analysis Stop optimization Save results of batch analysis

Dataset Nr.: 1; Replication Nr.: 1; Generation = 63; K _d (HG) = 1.134e+07; I(B) = 1.088e-15; I(HD) = 1.932e+05; I(D) = 1.728e+05; Error = 1.984e-09
Dataset Nr.: 1; Replication Nr.: 1; Generation = 63; K _d (HG) = 8.984e+06; I(B) = 1.888e-15; I(HD) = 7.932e+05; I(D) = 1.788e+05; Error = 1.984e-09
Dataset Nr.: 1; Replication Nr.: 2; Generation = 63; K _d (HG) = 7.979e+07; I(B) = 7.340e-02; I(HD) = 9.542e+05; I(D) = 1.759e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.: 1; Generation = 63; K _d (HG) = 1.116e+07; I(B) = 1.088e-15; I(HD) = 1.012e+06; I(D) = 1.728e+05; Error = 1.594e-09
Dataset Nr.: 2; Replication Nr.: 2; Generation = 66; K _d (HG) = 1.946e+07; I(B) = 1.088e-15; I(HD) = 1.088e+06; I(D) = 1.938e+05; Error = 6.419e-01
Dataset Nr.: 2; Replication Nr.: 3; Generation = 62; K _d (HG) = 8.269e+06; I(B) = 1.088e-15; I(HD) = 8.1979e+05; I(D) = 1.621e+05; Error = 2.291e-09

Thermosimfit

Data import

DBA (const, host) model

DBA (const, dye) model

GDA model

DA model

Info

Parameters

Host conc. [M]	0.000001
Dye conc. [M]	0.000001
K _d (H) [L/M]	3000000

Advanced options

Boundaries

K _d (HG) value lower boundary [1/M]	10
K _d (HG) value upper boundary [1/M]	1e+00
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

Batch analysis

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

```
Dataset Nr.: 1; Replication Nr.:1; Generation = 60; Kd(HG) = 1.1346e+07; I(B) = 1.088e-15; I(HD) = 1.932e+05; I(D) = 1.728e+05; Error = 1.984e-09
Dataset Nr.: 1; Replication Nr.:2; Generation = 80; Kd(HG) = 8.984e+06; I(B) = 1.88e-15; I(HD) = 7.932e+05; I(D) = 1.788e+05; Error = 1.984e-09
Dataset Nr.: 1; Replication Nr.:3; Generation = 66; Kd(HG) = 2.979e+07; I(B) = 7.348e-02; I(HD) = 9.542e+05; I(D) = 1.758e+05; Error = 2.937e-01
Dataset Nr.: 2; Replication Nr.:1; Generation = 65; Kd(HG) = 1.116e+07; I(B) = 1.088e-15; I(HD) = 1.012e+06; I(D) = 1.728e+05; Error = 1.594e-09
Dataset Nr.: 2; Replication Nr.:2; Generation = 63; Kd(HG) = 1.946e+07; I(B) = 1.088e-15; I(HD) = 1.088e+06; I(D) = 1.938e+05; Error = 6.419e-01
Dataset Nr.: 2; Replication Nr.:3; Generation = 64; Kd(HG) = 8.269e+06; I(B) = 1.088e-15; I(HD) = 8.1979e+05; I(D) = 1.621e+05; Error = 2.291e-09
```

