

Thermosimilit

Data import

DLIA (const. host) model

DLIA (const. dye) model

DLIA model

DLA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

boundaries

Help

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

10

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

100000000

HD value lower boundary

0

HD value upper boundary

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

[]

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Data import

DLIA (const. host) model

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Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

boundaries

Help

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

10

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

100000000

HD value lower boundary

0

HD value upper boundary

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

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0.000001

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K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary

0

HD value upper boundary

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 4; K_d (HG) = 4.300e+06; I(H) = 1.900e-01; I(HD) = 1.850e+05; I(O) = 1.340e+04; Error = 8.257e+08

Dataset = 2; Replicate = 1; Generation = 4; K_d (HG) = 2.780e+06; I(H) = 1.140e-02; I(HD) = 1.030e+06; I(O) = 6.300e+01; Error = 4.862e+08

[]

Thermosimilit

Data import

DLBA (const. host) model

DLBA (const. dye) model

DLPA model

DLA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 6; K_d (HG) = 5.768e+06; I(H) = 2.178e-01; I(HD) = 1.618e+05; I(O) = 1.698e+04; Error = 7.382e+08

Dataset = 2; Replicate = 1; Generation = 5; K_d (HG) = 2.785e+06; I(H) = 1.148e-02; I(HD) = 1.638e+06; I(O) = 6.380e+01; Error = 4.862e+08

[]

Thermosimilit

Data import

DLBA (const. host) model

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DLA model

DLA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 8; K_d (HG) = 5.780e+06; I(H) = 2.178e-01; I(HD) = 1.618e+05; I(O) = 1.698e+04; Error = 7.382e+08

Dataset = 2; Replicate = 1; Generation = 8; K_d (HG) = 2.785e+06; I(H) = 1.148e-02; I(HD) = 1.638e+06; I(O) = 6.380e+01; Error = 4.862e+08

[]

Thermosimilit

Data import

DLBA (const. host) model

DLBA (const. dye) model

DLA model

DLA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

3000000

Advanced options

Boundaries

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 10; Ka(HG) = 2.128e+06; I(O) = 1.899e-15; I(HD) = 7.846e+05; I(D) = 5.437e+04; Error = 4.156e+00

Dataset = 2; Replicate = 1; Generation = 10; Ka(HG) = 2.785e+06; I(O) = 1.148e-02; I(HD) = 1.838e+06; I(D) = 6.306e+01; Error = 4.862e+00

[]

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Data import

DISA (const. host) model

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CPA model

QA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

3000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 13; Ka(HG) = 2.128e+06; I(H) = 1.899e-15; I(HD) = 7.846e+05; I(D) = 5.437e+04; Error = 4.156e+00

Dataset = 2; Replicate = 1; Generation = 12; Ka(HG) = 2.785e+06; I(H) = 1.148e-02; I(HD) = 1.838e+06; I(D) = 6.306e+01; Error = 4.862e+00

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

CPA model

QA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

3000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary

0

HD value upper boundary

100000000

HD value lower boundary [1/M]

Help

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 15; Ka(HG) = 2.128e+06; I(O) = 1.899e-15; I(HD) = 7.846e+05; I(D) = 5.437e+04; Error = 4.156e+00

Dataset = 2; Replicate = 1; Generation = 14; Ka(HG) = 2.785e+06; I(O) = 1.148e-02; I(HD) = 1.838e+06; I(D) = 6.306e+01; Error = 4.862e+00

[]

boundaries

@help

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

10

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

1000000000

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

0

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

1000000000

V(U) value lower boundary

0

V(U) value upper boundary

1000000000

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 19; Ka(HG) = 2.128e+08; I(H) = 1.899e-15; I(HD) = 7.846e+05; I(D) = 9.437e+04; Error = 4.155e+08

Dataset = 2; Replicate = 1; Generation = 19; Ka(HG) = 9.688e+08; I(H) = 1.899e-15; I(HD) = 6.615e+05; I(D) = 1.698e+05; Error = 3.771e+08

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 21; Ka(HG) = 2.128e+08; I(0) = 1.099e-15; I(HD) = 7.846e+05; I(D) = 9.437e+04; Error = 4.159e+08

Dataset = 2; Replicate = 1; Generation = 26; Ka(HG) = 9.688e+08; I(0) = 1.099e-15; I(HD) = 6.615e+05; I(D) = 1.698e+05; Error = 3.771e+08

[]

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

 $K_a(\text{HD}) [1/\text{M}]$

3000000

Advanced options

+

Boundaries Help

$K_a(\text{HG})$ value lower boundary [1/M]

10

 $K_a(\text{HG})$ value upper boundary [1/M]

100000000

$l(0)$ value lower boundary

0

$l(0)$ value upper boundary

100000000

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

9

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

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

 Save result of batch analysis

boundaries


help

K_u[HG] value lower boundary [1/M]

10

K_u[HG] value upper boundary [1/M]

1000000000

HHD value lower boundary [1/M]  help

0

HHD value upper boundary [1/M]

1000000000

VU value lower boundary

0

VU value upper boundary

1000000000

VU value lower boundary [1/M]

0

VU value upper boundary [1/M]

1000000000

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

CPA model

QA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 28; Ka(HG) = 2.128e+06; I(H) = 1.099e-15; I(HD) = 7.846e+05; I(D) = 9.437e+04; Error = 4.156e+00

Dataset = 2; Replicate = 1; Generation = 27; Ka(HG) = 1.914e+07; I(H) = 1.099e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 38; Ka(HG) = 2.128e+06; I(H) = 1.099e-15; I(HD) = 7.846e+05; I(D) = 9.437e+04; Error = 4.156e+00

Dataset = 2; Replicate = 1; Generation = 29; Ka(HG) = 1.914e+07; I(H) = 1.099e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DBA (const. host) model

DBA (const. dye) model

DBA model

DBA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 32; Ka(HG) = 2.128e+06; I(0) = 1.000e-15; I(HD) = 7.846e+05; I(D) = 9.437e+04; Error = 4.156e+00

Dataset = 2; Replicate = 1; Generation = 32; Ka(HG) = 1.914e+07; I(0) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DBA (const. host) model

DBA (const. dye) model

DBA model

DBA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 34; Ka(HG) = 2.128e+06; I(H) = 1.099e-15; I(HD) = 7.846e+05; I(D) = 9.437e+04; Error = 4.156e+00

Dataset = 2; Replicate = 1; Generation = 34; Ka(HG) = 1.914e+07; I(H) = 1.099e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DiSA (const. host) model

DiSA (const. dye) model

DiSA model

DiA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 36; Ka(HG) = 1.051e+07; I(0) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.906e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 36; Ka(HG) = 1.916e+07; I(0) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 38; Ka(HG) = 1.051e+07; I(O) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.906e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 38; Ka(HG) = 1.916e+07; I(O) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DiSA (const. host) model

DiSA (const. dye) model

DiSA model

DiA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 41; Ka(HG) = 1.051e+07; I(H) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.906e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 48; Ka(HG) = 1.916e+07; I(H) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 44; Ka(HG) = 1.051e+07; I(H) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.906e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 43; Ka(HG) = 1.916e+07; I(H) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 45; Ka(HG) = 1.051e+07; I(H) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.956e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 45; Ka(HG) = 1.916e+07; I(H) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DBA (const. host) model

DBA (const. dye) model

DBA model

DBA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 47; Ka(HG) = 1.051e+07; I(O) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.906e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 47; Ka(HG) = 1.916e+07; I(O) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimult

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 48; Ka(HG) = 1.051e+07; I(H) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.905e+05; Error = 5.387e+00

Dataset = 2; Replicate = 1; Generation = 48; Ka(HG) = 1.914e+07; I(H) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DiSA (const. host) model

DiSA (const. dye) model

DiSA model

DiA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

I(H) value lower boundary

0

I(H) value upper boundary

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 51; Ka(HG) = 1.051e+07; I(H) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.906e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 51; Ka(HG) = 1.916e+07; I(H) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

HD value lower boundary

0

HD value upper boundary

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 54; Ka(HG) = 1.051e+07; I(O) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.956e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 54; Ka(HG) = 1.916e+07; I(O) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

IDA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

$K_a(\text{HD})$ [1/M]

3000000

Advanced options

+

Boundaries Help

K₂(HG) value lower boundary [1/M]

10

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

100000000

$l(0)$ value lower boundary

0

t(0) value upper boundary

100000000

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

☐

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

100000000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

 Save result of batch analysis

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary

0

HD value upper boundary

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 58; Ka(HG) = 1.051e+07; I(0) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.906e+05; Error = 5.397e+00

Dataset = 2; Replicate = 1; Generation = 58; Ka(HG) = 1.916e+07; I(0) = 1.000e-15; I(HD) = 9.448e+05; I(D) = 2.041e+05; Error = 7.229e-01

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

+

Boundaries

Help

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 62; Ka(HG) = 1.051e+07; I(0) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.956e+05; Error = 5.387e+00

Dataset = 2; Replicate = 1; Generation = 62; Ka(HG) = 1.741e+07; I(0) = 1.000e-15; I(HD) = 9.568e+05; I(D) = 1.956e+05; Error = 6.369e-01

[]

Thermosimilit

Data import

DISA (const. host) model

DISA (const. dye) model

DISA model

DISA model

Info

Parameter

Host conc. [M]

0.000001

Dye conc. [M]

0.000001

K_d (HD) [1/M]

1000000

Advanced options

Boundaries

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

10

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

100000000

HD value lower boundary [1/M]

0

HD value upper boundary [1/M]

100000000

Optimization

Sensitivity analysis

Batch processing

Batch analysis

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

1

How many cores should be used for the batch analysis?

3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 64; Ka(HG) = 1.051e+07; I(H) = 1.000e-15; I(HD) = 7.889e+05; I(D) = 1.956e+05; Error = 5.387e+00

Dataset = 2; Replicate = 1; Generation = 64; Ka(HG) = 1.741e+07; I(H) = 1.000e-15; I(HD) = 9.568e+05; I(D) = 1.956e+05; Error = 6.369e-01

[]