

Thermosimfit

Data import

iBA (const. host) model

iBA (const. dye) model

GDa model

iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

1.7000000

Advanced options

Boundaries

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

10

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

10000000000

i(HG) value lower boundary

0

i(HG) value upper boundary

10000000000

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

0

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

10000000000

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

Thermosimfit

Data import

qBA (const. host) model

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Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

I(HG) value lower boundary

0

I(HG) value upper boundary

10000000000

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

0

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

10000000000

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Dataset = 1; Replicate = 1; Generation = 2; K_a(HG) = 5.850e+03; I(H) = 5.387e-15; I(HD) = 1.583e+09; I(O) = 5.687e-01; Error = 9.231e+08

Dataset = 2; Replicate = 1; Generation = 2; K_a(HG) = 3.134e+02; I(H) = 2.688e-11; I(HD) = 3.369e-05; I(O) = 1.850e+09; Error = 8.041e+08

Dataset = 3; Replicate = 1; Generation = 2; K_a(HG) = 6.820e+09; I(H) = 6.793e+02; I(HD) = 3.282e+01; I(O) = 1.850e+09; Error = 6.325e+08

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Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

I(HG) value lower boundary

0

I(HG) value upper boundary

10000000000

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

0

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

10000000000

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1

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3

Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 8; K_a(HG) = 1.888e+01; I(H) = 1.888e-15; I(HD) = 3.385e+09; I(O) = 8.734e+05; Error = 1.384e+08

Dataset = 2; Replicate = 1; Generation = 7; K_a(HG) = 1.888e+01; I(H) = 1.888e-15; I(HD) = 3.856e+09; I(O) = 1.868e-15; Error = 3.371e+08

Dataset = 3; Replicate = 1; Generation = 8; K_a(HG) = 1.888e+01; I(H) = 3.402e+02; I(HD) = 1.688e+09; I(O) = 6.408e+06; Error = 3.401e+08

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Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

I(HG) value lower boundary

0

I(HG) value upper boundary

10000000000

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

0

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

10000000000

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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 = 17; K_a(HG) = 1.888e+01; I(H) = 1.888e-15; I(HD) = 3.393e+09; I(D) = 6.315e+06; Error = 1.379e+09

Dataset = 2; Replicate = 1; Generation = 15; K_a(HG) = 1.888e+01; I(H) = 2.693e+02; I(HD) = 3.821e+09; I(D) = 1.609e-15; Error = 8.795e-01

Dataset = 3; Replicate = 1; Generation = 15; K_a(HG) = 1.888e+01; I(H) = 1.888e-15; I(HD) = 3.353e+09; I(D) = 2.788e+07; Error = 1.291e+09

[]

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Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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

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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 = 22; K_a(HG) = 1.888e+01; I(H) = 1.888e-15; I(HD) = 3.393e+09; I(D) = 6.315e+06; Error = 1.379e+09

Dataset = 2; Replicate = 1; Generation = 21; K_a(HG) = 1.888e+01; I(H) = 2.693e+02; I(HD) = 3.821e+09; I(D) = 1.688e-15; Error = 8.795e-01

Dataset = 3; Replicate = 1; Generation = 23; K_a(HG) = 1.888e+01; I(H) = 2.151e+02; I(HD) = 3.261e+09; I(D) = 1.988e-15; Error = 9.646e-01

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Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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Start batch analysis

Stop optimization

Save result of batch analysis

Dataset = 1; Replicate = 1; Generation = 29; K_a(HG) = 1.818e+06; I(H) = 1.880e-15; I(HD) = 3.056e+09; I(D) = 1.880e-15; Error = 1.129e+09

Dataset = 2; Replicate = 1; Generation = 27; K_a(HG) = 1.688e+01; I(H) = 2.693e+02; I(HD) = 3.821e+09; I(D) = 1.688e-15; Error = 8.795e-01

Dataset = 3; Replicate = 1; Generation = 29; K_a(HG) = 1.880e+01; I(H) = 2.151e+02; I(HD) = 3.261e+09; I(D) = 1.880e-15; Error = 9.646e-01

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Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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; K_a(HG) = 1.818e+06; I(H) = 1.880e-15; I(HD) = 3.056e+09; I(D) = 1.880e-15; Error = 1.129e+09

Dataset = 2; Replicate = 1; Generation = 35; K_a(HG) = 1.688e+01; I(H) = 2.271e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.838e-01

Dataset = 3; Replicate = 1; Generation = 35; K_a(HG) = 1.688e+01; I(H) = 2.151e+02; I(HD) = 3.201e+09; I(D) = 1.880e-15; Error = 5.646e-01

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Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

I(HG) value lower boundary

0

I(HG) value upper boundary

10000000000

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

0

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

10000000000

Optimization

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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; K_a(HG) = 1.818e+06; I(H) = 1.880e-15; I(HD) = 3.056e+09; I(D) = 1.880e-15; Error = 1.129e+09

Dataset = 2; Replicate = 1; Generation = 49; K_a(HG) = 1.688e+01; I(H) = 2.271e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.838e-01

Dataset = 3; Replicate = 1; Generation = 42; K_a(HG) = 1.489e+01; I(H) = 2.151e+02; I(HD) = 3.201e+09; I(D) = 1.880e-15; Error = 5.646e-01

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Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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; K_a(HG) = 1.168e+06; I(H) = 1.889e-15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.126e+09

Dataset = 2; Replicate = 1; Generation = 46; K_a(HG) = 1.688e+01; I(H) = 2.271e+02; I(HD) = 3.818e+09; I(D) = 6.48e+07; Error = 3.838e-01

Dataset = 3; Replicate = 1; Generation = 49; K_a(HG) = 1.489e+01; I(H) = 2.151e+02; I(HD) = 3.201e+09; I(D) = 5.989e-15; Error = 5.646e-01

[]

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Data import

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Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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; K_a(HG) = 1.168e+06; I(H) = 1.889e-15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.126e+09

Dataset = 2; Replicate = 1; Generation = 52; K_a(HG) = 1.688e+01; I(H) = 2.271e+52; I(HD) = 3.818e+09; I(D) = 6.489e+07; Error = 3.838e-01

Dataset = 3; Replicate = 1; Generation = 55; K_a(HG) = 1.489e+01; I(H) = 2.151e+52; I(HD) = 1.201e+09; I(D) = 1.889e-15; Error = 5.646e-01

[]

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Data import

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Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 61; K_a(HG) = 1.168e+06; I(H) = 1.889e-15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.126e+09

Dataset = 2; Replicate = 1; Generation = 58; K_a(HG) = 1.688e+01; I(H) = 2.271e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.833e-01

Dataset = 3; Replicate = 1; Generation = 62; K_a(HG) = 1.489e+01; I(H) = 2.151e+02; I(HD) = 1.201e+09; I(D) = 1.989e-15; Error = 5.646e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 67; K_a(HG) = 1.168e+06; I(H) = 1.889e-15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.126e+09

Dataset = 2; Replicate = 1; Generation = 66; K_a(HG) = 1.688e+01; I(H) = 2.271e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.833e-01

Dataset = 3; Replicate = 1; Generation = 69; K_a(HG) = 1.489e+01; I(H) = 2.151e+02; I(HD) = 1.201e+09; I(D) = 1.989e-15; Error = 5.646e-01

[]

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Data import

qDA (const. host) model

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qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

Optimization

Sensitivity analysis

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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 = 75; K_a(HG) = 1.108e+06; I(H) = 1.880e-15; I(HD) = 3.489e+09; I(D) = 7.880e+06; Error = 1.120e+09

Dataset = 2; Replicate = 1; Generation = 75; K_a(HG) = 1.688e+01; I(H) = 2.271e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.833e-01

Dataset = 3; Replicate = 1; Generation = 75; K_a(HG) = 1.489e+01; I(H) = 2.151e+02; I(HD) = 1.201e+09; I(D) = 1.980e-15; Error = 5.646e-01

[]

Thermosimfit

Data import

iBA (const. host) model

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iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

I(H) value lower boundary

0

I(H) value upper boundary

10000000000

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

0

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

10000000000

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 = 81; K_a(HG) = 1.108e+06; I(H) = 1.880e-15; I(HD) = 3.489e+09; I(D) = 7.880e+06; Error = 1.120e+09

Dataset = 2; Replicate = 1; Generation = 79; K_a(HG) = 1.688e+01; I(H) = 2.171e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.838e-01

Dataset = 3; Replicate = 1; Generation = 82; K_a(HG) = 1.489e+01; I(H) = 2.361e+02; I(HD) = 1.230e+09; I(D) = 1.080e-15; Error = 5.446e-01

[]

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Data import

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Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 88; K_a(HG) = 1.168e+06; I(H) = 1.889e-15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.126e+09

Dataset = 2; Replicate = 1; Generation = 86; K_a(HG) = 1.688e+01; I(H) = 2.171e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.838e-01

Dataset = 3; Replicate = 1; Generation = 89; K_a(HG) = 1.489e+01; I(H) = 2.361e+02; I(HD) = 1.230e+09; I(D) = 1.989e-15; Error = 5.448e-01

[]

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Data import

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iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

I(HD) value lower boundary [1M]

0

I(HD) value upper boundary [1M]

10000000000

I(HD) value lower boundary [1M]

0

I(HD) value upper boundary [1M]

10000000000

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 = 95; K_a(HG) = 1.168e+06; I(H) = 1.889e-15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.126e+09

Dataset = 2; Replicate = 1; Generation = 95; K_a(HG) = 1.688e+01; I(H) = 2.171e+02; I(HD) = 3.818e+09; I(D) = 6.403e+07; Error = 3.838e-01

Dataset = 3; Replicate = 1; Generation = 95; K_a(HG) = 1.489e+01; I(H) = 2.361e+02; I(HD) = 3.230e+09; I(D) = 5.989e-15; Error = 5.448e-01

[]

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Data import

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Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 191; Ka(HG) = 1.169e+06; I(H) = 1.899e+15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.120e+00

Dataset = 2; Replicate = 1; Generation = 99; Ka(HG) = 1.888e+01; I(H) = 2.271e+02; I(HD) = 3.919e+09; I(D) = 6.489e+07; Error = 3.639e-01

Dataset = 3; Replicate = 1; Generation = 100; Ka(HG) = 1.899e+01; I(H) = 2.313e+02; I(HD) = 5.179e+09; I(D) = 4.582e+06; Error = 5.183e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

I(HG) value lower boundary

0

I(H) value upper boundary

10000000000

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

0

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

10000000000

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 = 190; Ka(HG) = 1.169e+06; I(H) = 1.099e+15; I(HD) = 3.489e+09; I(D) = 7.089e+06; Error = 1.120e+00

Dataset = 2; Replicate = 1; Generation = 197; Ka(HG) = 1.089e+01; I(H) = 2.271e+02; I(HD) = 3.010e+00; I(D) = 6.409e+07; Error = 3.030e-01

Dataset = 3; Replicate = 1; Generation = 190; Ka(HG) = 1.089e+01; I(H) = 2.313e+02; I(HD) = 3.170e+00; I(D) = 4.502e+06; Error = 5.103e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 115; Ka(HG) = 1.169e+06; I(H) = 1.899e+15; I(HD) = 3.489e+09; I(D) = 7.889e+06; Error = 1.120e+00

Dataset = 2; Replicate = 1; Generation = 113; Ka(HG) = 1.899e+01; I(H) = 2.271e+02; I(HD) = 3.619e+00; I(D) = 6.489e+07; Error = 3.639e-01

Dataset = 3; Replicate = 1; Generation = 116; Ka(HG) = 1.899e+01; I(H) = 2.313e+02; I(HD) = 3.179e+00; I(D) = 4.582e+06; Error = 5.183e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 122; Ka(HG) = 1.516e+06; I(H) = 1.898e-15; I(HD) = 3.513e+09; I(D) = 1.888e-15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 120; Ka(HG) = 1.888e+01; I(H) = 2.271e+02; I(HD) = 3.618e+00; I(D) = 6.489e+07; Error = 3.638e-01

Dataset = 3; Replicate = 1; Generation = 122; Ka(HG) = 1.888e+01; I(H) = 2.313e+02; I(HD) = 3.178e+00; I(D) = 4.582e+06; Error = 5.183e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 120; Ka(HG) = 1.516e+06; I(H) = 1.898e-15; I(HD) = 3.513e+09; I(D) = 1.888e-15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 120; Ka(HG) = 1.888e+01; I(H) = 2.315e+02; I(HD) = 3.616e+00; I(D) = 9.133e+07; Error = 2.795e-01

Dataset = 3; Replicate = 1; Generation = 120; Ka(HG) = 1.888e+01; I(H) = 2.315e+02; I(HD) = 3.178e+00; I(D) = 4.582e+06; Error = 3.183e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 130; Ka(HG) = 1.516e+06; I(H) = 1.898e-15; I(HD) = 3.513e+09; I(D) = 1.888e-15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 134; Ka(HG) = 1.888e+01; I(H) = 2.335e+02; I(HD) = 3.616e+00; I(D) = 9.131e+07; Error = 2.795e-01

Dataset = 3; Replicate = 1; Generation = 130; Ka(HG) = 1.888e+01; I(H) = 1.703e+02; I(HD) = 3.500e+00; I(D) = 1.133e+08; Error = 3.475e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 144; Ka(HG) = 1.516e+06; I(H) = 1.898e+15; I(HD) = 3.513e+09; I(D) = 1.888e+15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 142; Ka(HG) = 1.888e+01; I(H) = 2.335e+02; I(HD) = 3.616e+00; I(D) = 9.131e+07; Error = 2.795e+01

Dataset = 3; Replicate = 1; Generation = 144; Ka(HG) = 1.888e+01; I(H) = 2.220e+02; I(HD) = 3.220e+00; I(D) = 1.620e+07; Error = 3.462e+01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 151; Ka(HG) = 1.516e+06; I(H) = 1.898e+15; I(HD) = 3.513e+09; I(D) = 1.888e+15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 149; Ka(HG) = 1.888e+01; I(H) = 2.335e+02; I(HD) = 3.616e+00; I(D) = 9.131e+07; Error = 2.795e+01

Dataset = 3; Replicate = 1; Generation = 151; Ka(HG) = 1.888e+01; I(H) = 2.220e+02; I(HD) = 3.220e+00; I(D) = 1.620e+07; Error = 3.462e+01

[]

Thermosimfit

Data import

IBA (const. host) model

IBA (const. dye) model

IDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 150; Ka(HG) = 1.516e+06; I(H) = 1.898e+15; I(HD) = 3.513e+09; I(D) = 1.888e+15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 150; Ka(HG) = 1.888e+01; I(H) = 2.335e+02; I(HD) = 3.616e+00; I(D) = 9.131e+07; Error = 2.795e+01

Dataset = 3; Replicate = 1; Generation = 150; Ka(HG) = 1.888e+01; I(H) = 2.220e+02; I(HD) = 3.220e+00; I(D) = 1.620e+07; Error = 3.462e+01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 100; Ka(HG) = 1.516e+06; I(H) = 1.898e-15; I(HD) = 3.513e+09; I(D) = 1.888e-15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 102; Ka(HG) = 1.888e+01; I(H) = 2.274e+02; I(HD) = 2.986e+00; I(D) = 9.322e+07; Error = 2.772e-01

Dataset = 3; Replicate = 1; Generation = 104; Ka(HG) = 1.888e+01; I(H) = 2.220e+02; I(HD) = 3.220e+00; I(D) = 1.420e+07; Error = 3.462e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

iDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 172; Ka(HG) = 1.516e+06; I(H) = 1.898e+15; I(HD) = 3.513e+09; I(D) = 1.888e+15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 169; Ka(HG) = 1.888e+01; I(H) = 1.274e+02; I(HD) = 2.985e+00; I(D) = 9.322e+07; Error = 2.772e+01

Dataset = 3; Replicate = 1; Generation = 171; Ka(HG) = 1.888e+01; I(H) = 1.888e+02; I(HD) = 3.075e+00; I(D) = 1.888e+00; Error = 3.250e+01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 180; Ka(HG) = 1.516e+06; I(H) = 1.898e+15; I(HD) = 3.513e+09; I(D) = 1.888e+15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 170; Ka(HG) = 1.888e+01; I(H) = 1.274e+02; I(HD) = 2.685e+00; I(D) = 9.322e+07; Error = 2.772e+01

Dataset = 3; Replicate = 1; Generation = 170; Ka(HG) = 1.888e+01; I(H) = 1.888e+02; I(HD) = 3.075e+00; I(D) = 1.888e+00; Error = 3.250e+01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 187; Ka(HG) = 1.516e+06; I(H) = 1.898e-15; I(HD) = 3.513e+09; I(D) = 1.888e-15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 185; Ka(HG) = 1.888e+01; I(H) = 1.274e+02; I(HD) = 2.985e+00; I(D) = 9.322e+07; Error = 2.772e-01

Dataset = 3; Replicate = 1; Generation = 187; Ka(HG) = 1.888e+01; I(H) = 1.888e+02; I(HD) = 3.975e+00; I(D) = 1.888e+00; Error = 3.250e-01

[]

Thermosimfit

Data import

qBA (const. host) model

qBA (const. dye) model

qDA model

IDA model

Info

Parameter

Host conc. [M]

0.00000105

Guest conc. [M]

0.00000132

K_a(HD) [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

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

0

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

10000000000

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

0

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

10000000000

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 = 190; Ka(HG) = 1.516e+06; I(H) = 1.898e-15; I(HD) = 3.513e+09; I(D) = 1.888e-15; Error = 1.884e+00

Dataset = 2; Replicate = 1; Generation = 193; Ka(HG) = 1.888e+01; I(H) = 1.274e+02; I(HD) = 2.685e+00; I(D) = 9.322e+07; Error = 2.772e-01

Dataset = 3; Replicate = 1; Generation = 190; Ka(HG) = 1.888e+01; I(H) = 1.888e+02; I(HD) = 3.075e+00; I(D) = 1.888e+00; Error = 3.259e-01

[]

Parameter

Host conc. [M]

0.00000165

Guest conc. [M]

0.00000132

$K_d(\text{Hb})$ [1/M]

17000000

Advanced options

Boundaries

Help

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

10

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

10000000000

$\text{I}(\text{Hb})$ value lower boundary [1/M]

0

$\text{I}(\text{Hb})$ value upper boundary [1/M]

10000000000

$\text{I}(\text{I})$ value lower boundary

0

$\text{I}(\text{I})$ value upper boundary

10000000000

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

0

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

10000000000

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

