

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Initializing...

2000px × 1000px

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Initializing...

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(0) value lower boundary

0

I(0) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 0; Ka(HG) = 4.173e+05; I(0) = 1.000e-15; I(HD) = 3.724e+06; I(D) = 3.680e+07; Error = 2.692e+00

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 15; Ka(HG) = 1.888e+61; I(O) = 3.444e+62; I(HD) = 1.888e-15; I(D) = 3.798e+67; Error = 1.529e+68

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 22; Ka(HG) = 5.221e+05; I(O) = 3.566e+02; I(HD) = 4.560e+07; I(D) = 3.802e+07; Error = 1.529e+09

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 29; Ka(HG) = 5.975e+06; I(O) = 3.540e+02; I(HD) = 2.737e+07; I(D) = 3.744e+07; Error = 1.511e+00

Registered S3 method overwritten by 'sensitivity': method from print.src dplyr

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

Help

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Sensitivity analysis

Batch processing

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 36;  $K_a(\text{HG}) = 5.975\text{e}+06$ ;  $I(\text{O}) = 3.540\text{e}+02$ ;  $I(\text{HD}) = 2.737\text{e}+07$ ;  $I(\text{D}) = 3.744\text{e}+07$ ; Error = 1.511e+09

Thermosimfit

Data import

DBA (const. host) model

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IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 43;  $K_a(\text{HG}) = 7.605\text{e}+05$ ;  $I(\text{O}) = 3.533\text{e}+02$ ;  $I(\text{HD}) = 2.538\text{e}+07$ ;  $I(\text{D}) = 3.699\text{e}+07$ ; Error = 1.580\text{e}+09

2000px × 1000px



Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 49; Ka(HG) = 7.685e+05; I(O) = 3.533e+02; I(HD) = 2.538e+07; I(D) = 3.699e+07; Error = 1.588e+09

2000px × 1000px

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 59; Ka(HG) = 7.605e+05; I(O) = 3.533e+02; I(HD) = 2.538e+07; I(D) = 3.699e+07; Error = 1.580e+09

2000px × 1000px

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 65; Ka(HG) = 7.685e+05; I(O) = 3.533e+02; I(HD) = 2.538e+07; I(D) = 3.699e+07; Error = 1.580e+09

Thermosimfit

Data import

DBA (const. host) model

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GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 72;  $K_a(\text{HG}) = 7.605\text{e}+05$ ;  $I(\text{O}) = 3.530\text{e}+02$ ;  $I(\text{HD}) = 2.530\text{e}+07$ ;  $I(\text{D}) = 3.609\text{e}+07$ ; Error = 1.500\text{e}+00

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = T8;  $K_a(\text{HG}) = 7.605\text{e}+05$ ;  $I(\text{O}) = 3.530\text{e}+02$ ;  $I(\text{HD}) = 2.530\text{e}+07$ ;  $I(\text{D}) = 3.609\text{e}+07$ ; Error = 1.500\text{e}+00

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 07; Ka(HG) = 7.605e+05; I(O) = 3.530e+02; I(HD) = 2.530e+07; I(D) = 3.609e+07; Error = 1.500e+00

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 91; Ka(HG) = 7.695e+05; I(O) = 3.533e+02; I(HD) = 2.538e+07; I(D) = 3.699e+07; Error = 1.580e+09

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 181;  $K_a(\text{HG}) = 7.685\text{e}+05$ ;  $I(\text{O}) = 3.533\text{e}+02$ ;  $I(\text{HD}) = 2.538\text{e}+07$ ;  $I(\text{D}) = 3.699\text{e}+07$ ; Error = 1.500\text{e}+00



Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 188;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HG}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 115;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 121;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+00

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 129;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 134;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+00

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 142;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 158;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 155;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+00



Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 183;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 188;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 175;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+00

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 184;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

K<sub>a</sub>(HD) [1/M]

181

Advanced options

Boundaries

K<sub>a</sub>(HG) value lower boundary [1/M]

10

K<sub>a</sub>(HG) value upper boundary [1/M]

100000000

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

0

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

100000000

I(O) value lower boundary

0

I(O) value upper boundary

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 189; Ka(HG) = 6.588e+05; I(θ) = 3.521e+02; I(HD) = 5.395e+07; I(D) = 3.703e+07; Error = 1.497e+08

Thermosimfit

Data import

DBA (const. host) model

DBA (const. dya) model

GDA model

IDA model

Info

Parameter

Host conc. [M]

0.000103

Guest conc. [M]

0.00105

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

181

Advanced options

Boundaries

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

10

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

100000000

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

0

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

100000000

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

0

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

1000

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

0

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

100000000

Optimization

Start optimization

Stop optimization

Save result of optimization

Choose file type:

Excel

Generation = 198;  $K_a(\text{HG}) = 6.588\text{e}+05$ ;  $I(\text{O}) = 3.521\text{e}+02$ ;  $I(\text{HD}) = 5.395\text{e}+07$ ;  $I(\text{D}) = 3.703\text{e}+07$ ; Error = 1.497\text{e}+08

