

Package ‘smoke’

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Type Package

Title Small Molecule Octet/BLI Kinetics Experiment

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Description Bio-Layer Interferometry (BLI) is a technology to determine the binding kinetics between biomolecules. BLI signals are small and noisy when small molecules are investigated as ligands (analytes). We develop this package to process and analyze the BLI data acquired on Octet Red96 from Fortebio more accurately.

Sun Q., Li X., et al (2020) <[doi:10.1038/s41467-019-14238-3](https://doi.org/10.1038/s41467-019-14238-3)>.

In this new version, we organize the BLI experiment data and analysis methods into a S4 class with self-explaining structure.

License GPL-2 | GPL-3

Depends R (>= 3.5.0), methods, graphics, grDevices, stats, utils

Imports Rdpack

RdMacros Rdpack

LazyData true

NeedsCompilation no

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smoke-package

*Small Molecule Octet/BLI Kinetics Experiment***Description**

Bio-Layer Interferometry (BLI) is a technology to determine the binding kinetics between biomolecules. BLI signals are small and noisy when small molecules are investigated as ligands (analytes). We develop this package to process and analyze the BLI data acquired on Octet Red96 from Fortebio more accurately. Sun Q., Li X., et al (2020) <doi:10.1038/s41467-019-14238-3>. In this new version, we organize the BLI experiment data and analysis methods into a S4 class with self-explaining structure.

Details

The DESCRIPTION file:

```
Package:      smoke
Type:        Package
Title:       Small Molecule Octet/BLI Kinetics Experiment
Version:     2.0.0
Date:        2020-01-15
Author:      Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer:  Qingan Sun <quinsun@gmail.com>
Description: Bio-Layer Interferometry (BLI) is a technology to determine the binding kinetics between biomolecules. BLI s
License:     GPL-2 | GPL-3
Depends:    R (>= 3.5.0),methods,graphics,grDevices,stats,utils
Imports:    Rdpack
RdMacros:   Rdpack
LazyData:   true
```

Index of help topics:

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```

```

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kinetics       Output kinetics model
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smoke-package  Small Molecule Octet/BLI Kinetics Experiment
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traces-methods  ~~ Methods for Function 'traces' ~~
traces<-       Setter of BLI 'traces'
traces<--methods  ~~ Methods for Function 'traces<-' ~~

```

~~ An overview of how to use the package, including the most important ~~ ~ functions ~~

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
 Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
load("bli.RData")
```

```
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
bli5 <- fitKinetics(bli4)
plotTraces(bli2)
plotKinetics(bli5)
plotResiduals(bli5)
```

alignLoad

Align BLI traces with loading step

Description

Align BLI traces with loading step with the start and end times.

Usage

```
alignLoad(obj, loadStart, loadEnd)
```

Arguments

obj	obj of "Bli" class
loadStart	start time of the loading step
loadEnd	end time of the loading step

Details

This is the optional first step in BLI data processing. The traces in the input "Bli" object is assumed to be paired original dataset. The output "Bli" object contains the traces aligned, and the status of "alignLoad" set to "TRUE".

Value

S4 object of "Bli" class

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
```

alignLoad-methods *~~ Methods for Function alignLoad ~~*

Description

~~ Methods for function alignLoad ~~

Methods

signature(obj = "Bli")

baseline *Align BLI traces with baseline step*

Description

Align BLI traces with the baseline step right before the association step. The start and end times of baseline are input arguments.

Usage

baseline(obj, tStart, tEnd)

Arguments

obj	obj of "Bli" class
tStart	start time of the baseline
tEnd	end time of the baseline

Details

This step follows doubleBlank step. The output "Bli" object contains the traces aligned with baselines, and the status of "baseline" set to "TRUE". Also the traces number will be checked. If it does not equal the number of ligand concentration, a warning will be raised: "ligand concentrations mis-match trace number".

Value

S4 object of "Bli" class

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
```

baseline-methods *~~ Methods for Function baseline ~~*

Description

~~ Methods for function baseline ~~

Methods

```
signature(obj = "Bli")
```

Bli *Constructor of "Bli" class*

Description

Construction of a new "Bli" object with all slots initialized.

Usage

```
Bli(...)
```

Arguments

... .Object in initialize; leave empty

Value

S4 object of "Bli" class

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). “The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD.” *Nature Communications*, **11**(339).

See Also

[Bli-class](#)

Examples

```
bli1 <- Bli()
```

bli

BLI data example

Description

This is an unprocessed BLI data saved in a "BLI" object (Sun et al. 2020).

Usage

```
data("bli")
```

Format

A S4 "Bli" class with 7 slots.

`status` a logical vector indicating this is a raw dataset

`traces` a data.frame with 16 BLI traces at 12290 time points

`ligand` a numeric vector of ligand concentrations

`tExp` a numeric vector of association and dissociation times

`kOn0` a numeric of initial on-rate; empty

`kOff0` a numeric of initial off-rate; empty

`kinetics` a nls object; empty

Source

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). “The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD.” *Nature Communications*, **11**(339).

Examples

```
data(bli)
```


Bli-class

Class "Bli"

Description

Bli is a S4 class to contain the Bli experiment data and analysis result.

Arguments

... .Object in initialize; leave empty

Objects from the Class

Objects can be created by calls of the form Bli(...).

Slots

traces: Object of class "data.frame" of BLI traces; "time" in the 1st column

lig: Object of class "numeric" of ligand concentrations

tExp: Object of class "numeric" of association and dissociation times

status: Object of class "vector" indicator and record of processing

kinetics: Object of class "nls" model of binding kinetics

kOn0: Object of class "numeric" initial value of on-rate

kOff0: Object of class "numeric" initial value of off-rate

Methods

alignLoad signature(obj = "Bli"): Align BLI traces with loading step

baseline signature(obj = "Bli"): Align BLI traces with baseline step

doubleBlank signature(obj = "Bli"): Subtract the double-references

estimate signature(obj = "Bli"): Estimate initial kinetic parameters

fitKinetics signature(obj = "Bli"): Fit binding kinetics

initialize signature(.Object = "Bli"): initializer

kinetics signature(obj = "Bli"): Output kinetics model

kOff0 signature(obj = "Bli"): Getter for "Bli" slot of kOff0

kOff0<- signature(obj = "Bli"): Setter for "Bli" slot of kOff0

kOn0 signature(obj = "Bli"): Getter for "Bli" slot of kOn0

kOn0<- signature(obj = "Bli"): Setter for "Bli" slot of kOn0

ligand signature(obj = "Bli"): Getter for ligand concentration

ligand<- signature(obj = "Bli"): Setter for ligand concentration

plotKinetics signature(obj = "Bli"): Plot kinetics model fitting

plotResiduals signature(obj = "Bli"): Plot residuals from kinetics model fitting

plotTraces signature(obj = "Bli"): Plot BLI traces

show signature(object = "Bli"): show method

status signature(obj = "Bli"): Getter for data processing status

tExp signature(obj = "Bli"): Getter for BLI times tExp

tExp<- signature(obj = "Bli"): Setter for BLI times tExp

traces signature(obj = "Bli"): Getter of BLI traces

traces<- signature(obj = "Bli"): Setter of BLI traces

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini

Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
showClass("Bli")
```

doubleBlank

Substract the double-references

Description

The BLI experiment for small-molecules is designed to have double references: reference biosensor and reference sample, i.e. b

Usage

```
doubleBlank(obj)
```

Arguments

obj obj of "Bli" class

Details

The signal in small-molecule BLI experiment is small in relation to noise. So the experiment design includes double references: reference biosensor and reference sample (no ligand). With subtraction of both, we expect to remove both the background signal and the non-specific binding.

The doubleBlank assumes that traces in the input "Bli" object contains two consecutive sets of columns with the second set as the reference biosensor, and the reference samples as the last column in each set. This means that the traces are "paired" and traces number is even. If not, an error message will be raised: "the double-referenced traces should be paired".

After doubleBlank, the number of traces should be equal to the number of ligand concentration. If not, a warning will be raised: "ligand concentrations mis-match trace number".

Also, after successful doubleBlank, the status of "doubleBlank" will be set to "TRUE". This prevent the user to run doubleBlank twice in accident.

Value

S4 object of "Bli" class

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini

Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
```

doubleBlank-methods *~~ Methods for Function doubleBlank ~~*

Description

~~ Methods for function doubleBlank ~~

Methods

signature(obj = "Bli")

`estimate`*Estimate initial kinetic parameters*

Description

Estimate the initial kinetic parameters, `kOn0` and `kOff0`, and save in the returned "Bli" object. These parameters can serve as the starting value in the next step, `fitKinetics`, to calculate the kinetics binding model of the small-molecule under investigation.

Usage

```
estimate(obj)
```

Arguments

`obj` obj of "Bli" class

Value

S4 object of "Bli" class

Note

`kOn0` and `kOff0` can also be input manually with the setter functions, `kOn0<-` and `kOff0<-`.

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
```

estimate-methods *~~ Methods for Function estimate ~~*

Description

~~ Methods for function estimate ~~

Methods

signature(obj = "Bli")

fitKinetics *Fit binding kinetics*

Description

Fit the BLI traces with a single association-then-dissociation equation.

Usage

fitKinetics(obj)

Arguments

obj obj of "Bli" class

Details

We fit the whole set of BLI traces with a single association-then-dissociation equation (Sun et al. 2020). The fitting model will be stored in the kinetics slot, and the status of "fitKinetics" will be set to "TRUE".

Value

S4 object of "Bli" class

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

See Also

[kinetics](#), [plotKinetics](#), [plotResiduals](#)

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
bli5 <- fitKinetics(bli4)
```

fitKinetics-methods *~~ Methods for Function fitKinetics ~~*

Description

~~ Methods for function fitKinetics ~~

Methods

signature(obj = "Bli")

initialize-methods *~~ Methods for Function initialize ~~*

Description

~~ Methods for function initialize ~~

Methods

signature(.Object = "Bli")

`kinetics`*Output kinetics model*

Description

Output kinetics model with matrix containing KD, rMax, kOn, kOff, and the relevant statistics.

Usage

```
kinetics(obj)
```

Arguments

`obj` obj of "Bli" class

Value

"matrix" with kinetic parameters

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

See Also

[fitKinetics](#)

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
bli5 <- fitKinetics(bli4)
kinetics(bli5)
```

kinetics-methods *~~ Methods for Function kinetics ~~*

Description

~~ Methods for function kinetics ~~

Methods

signature(obj = "Bli")

kOff0 *Getter for "Bli" slot of kOff0*

Description

The getter function for "Bli" slot of kOff0, initial kOff rate.

Usage

```
kOff0(obj)
```

Arguments

obj obj of "Bli" class

Value

numeric of kOff0

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[estimate](#)

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
kOff0(bli4)
```

kOff0-methods *~~ Methods for Function kOff0 ~~*

Description

~~ Methods for function kOff0 ~~

Methods

signature(obj = "Bli")

kOff0<- *Setter for "Bli" slot of kOff0*

Description

The setter function for "Bli" slot of kOff0, initial kOff rate

Usage

```
kOff0(obj) <- value
```

Arguments

obj	obj of "Bli" class
value	initial kOff rate

Value

S4 object of "Bli" class

Note

It is preferred to estimate initial kOff rate.

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
 Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[estimate](#)

Examples

```
bli <- Bli()
kOff0(bli) <- 0.1
```

```
kOff0<--methods      ~~ Methods for Function kOff0<- ~~
```

Description

~~ Methods for function kOff0<- ~~

Methods

```
signature(obj = "Bli")
```

```
kOn0                Getter for "Bli" slot of kOn0
```

Description

The getter function for "Bli" slot of kOn0, initial kOn rate.

Usage

```
kOn0(obj)
```

Arguments

```
obj                obj of "Bli" class
```

Value

numeric of kOn0

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
 Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[estimate](#)

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
kOn0(bli4)
```

kOn0-methods *~~ Methods for Function kOn0 ~~*

Description

~~ Methods for function kOn0 ~~

Methods

signature(obj = "Bli")

kOn0<- *Setter for "Bli" slot of kOn0*

Description

The setter function for "Bli" slot of kOn0, initial kOn rate.

Usage

```
kOn0(obj) <- value
```

Arguments

obj	obj of "Bli" class
value	initial kOn rate

Value

S4 object of "Bli" class

Note

It is preferred to estimate initial kOn rate.

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
 Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[estimate](#)

Examples

```
bli <- Bli()
kOn0(bli) <- 0.1
```

```
kOn0<--methods      ~~ Methods for Function kOn0<- ~~
```

Description

~~ Methods for function kOn0<- ~~

Methods

```
signature(obj = "Bli")
```

```
ligand              Getter for "Bli" slot of ligand concentration
```

Description

The getter function for "Bli" slot of ligand concentration. If the slot is empty, there will be an error message: "please input ligand concentration".

Usage

```
ligand(obj)
```

Arguments

```
obj              obj of "Bli" class
```

Value

a numeric vector for the ligand concentration in BLI experiment

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[ligand<-](#)

Examples

```
load("bli.RData")  
conc <- ligand(bli)
```

ligand-methods *~~ Methods for Function ligand ~~*

Description

~~ Methods for function ligand ~~

Methods

signature(obj = "Bli")

ligand<- *Setter for "Bli" slot of ligand concentration*

Description

The setter function for "Bli" slot of ligand concentration in BLI experiment.

Usage

```
ligand(obj) <- value
```

Arguments

obj	obj of "Bli" class
value	value numeric vector of ligand concentrations

Value

S4 object of "Bli" class

Note

The ligand concentrations do not include the blank control (0).

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[ligand](#)

Examples

```
bli1 <- Bli()  
ligand(bli1) <- 16/2^(0:6)
```

```
ligand<--methods      ~~ Methods for Function ligand<- ~~
```

Description

```
~~ Methods for function ligand<- ~~
```

Methods

```
signature(obj = "Bli")
```

```
nls-class            Class nls
```

Description

Registration of S3 nls into S4 class.

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
 Maintainer: Qingan Sun <quinsun@gmail.com>

```
plotKinetics        Plot kinetics model fitting
```

Description

Plot the BLI traces with the kinetics-model fitting.

Usage

```
plotKinetics(obj, ...)
```

Arguments

```
obj          obj of "Bli" class
...          Arguments to be passed to methods, such as graphical parameters
```

Note

This method only works after fitKinetics.

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). “The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD.” *Nature Communications*, **11**(339).

See Also

[fitKinetics](#), [plotResiduals](#)

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
bli5 <- fitKinetics(bli4)
plotKinetics(bli5)
```

plotKinetics-methods *~~ Methods for Function plotKinetics ~~*

Description

~~ Methods for function plotKinetics ~~

Methods

```
signature(obj = "Bli")
```

plotResiduals *Plot residuals from kinetics model fitting*

Description

Plot the residuals from the kinetics-model fitting

Usage

```
plotResiduals(obj, ...)
```

Arguments

obj obj of "Bli" class
... Arguments to be passed to methods, such as graphical parameters

Note

This method only works after fitKinetics.

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

See Also

[fitKinetics](#), [plotKinetics](#)

Examples

```
load("bli.RData")
bli1 <- alignLoad(bli, 180, 780)
bli2 <- doubleBlank(bli1)
bli3 <- baseline(bli2, 1080, 1260)
bli4 <- estimate(bli3)
bli5 <- fitKinetics(bli4)
plotResiduals(bli5)
```

plotResiduals-methods ~~ *Methods for Function plotResiduals* ~~

Description

~~ Methods for function plotResiduals ~~

Methods

signature(obj = "Bli")

`plotTraces`*Plot BLI traces*

Description

Plot the BLI traces in the "Bli" object.

Usage

```
plotTraces(obj, ...)
```

Arguments

<code>obj</code>	obj of "Bli" class
<code>...</code>	Arguments to be passed to methods, such as graphical parameters

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[plotKinetics](#), [plotResiduals](#)

Examples

```
load("bli.RData")  
plotTraces(bli)
```

`plotTraces-methods`*~~ Methods for Function plotTraces ~~*

Description

~~ Methods for function plotTraces ~~

Methods

```
signature(obj = "Bli")
```

show-methods *~~ Methods for Function show ~~*

Description

~~ Methods for function show ~~

Methods

signature(object = "Bli")

status *Getter for data processing status*

Description

The getter function for the data processing status.

Usage

status(obj)

Arguments

obj obj of "Bli" class

Value

"logical" vector as the indicator of the status of data analysis

Note

There is no Setter for status by design.

Because status is modified automatically during data processing, there is no need for the user to change the status manually.

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini

Maintainer: Qingan Sun <quinsun@gmail.com>

See Also

[alignLoad](#), [doubleBlank](#), [baseline](#), [estimate](#), [fitKinetics](#)

Examples

```
bli <- Bli()
status(bli)
```

status-methods *~~ Methods for Function status ~~*

Description

~~ Methods for function status ~~

Methods

```
signature(obj = "Bli")
```

tExp *Getter for BLI times tExp*

Description

The getter function for BLI times tExp, the start time of association and dissociation steps.

Usage

```
tExp(obj)
```

Arguments

obj obj of "Bli" class

Value

"numeric" vector for the start time of association and dissociation steps

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
load("bli.RData")
tExp(bli)
```

tExp-methods *~~ Methods for Function tExp ~~*

Description

~~ Methods for function tExp ~~

Methods

signature(obj = "Bli")

tExp<- *Setter for BLI times tExp*

Description

The setter function for BLI times tExp, the start time of association and dissociation steps.

Usage

```
tExp(obj) <- value
```

Arguments

obj obj of "Bli" class
value "numeric" vector for the start time of association and dissociation steps

Value

S4 object of "Bli" class

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). "The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD." *Nature Communications*, **11**(339).

Examples

```
bli <- Bli()  
tExp(bli) <- c(1260,1860)
```

tExp<--methods	<i>~~ Methods for Function tExp<- ~~</i>
----------------	---

Description

~~ Methods for function tExp<- ~~

Methods

signature(obj = "Bli")

traces	<i>Getter of BLI traces</i>
--------	-----------------------------

Description

The getter function of BLI traces. The first column of this data.frame is the time in second; the following columns are the BLI traces.

Usage

traces(obj)

Arguments

obj obj of "Bli" class

Value

"data.frame" of BLI traces

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
 Maintainer: Qingan Sun <quinsun@gmail.com>

Examples

```
load("bli.RData")
traces(bli)
```

```
traces-methods      ~~ Methods for Function traces ~~
```

Description

~~ Methods for function traces ~~

Methods

```
signature(obj = "Bli")
```

```
traces<-           Setter of BLI traces
```

Description

The setter function of BLI traces. The input "data.frame" contains the times in the first column and the BLI traces in the following columns.

Usage

```
traces(obj) <- value
```

Arguments

```
obj           obj of "Bli" class
value        "data.frame" of BLI traces
```

Details

There may be two kinds of input "data.frame":

The "original" data with times in the first column, and two consecutive sets of BLI traces in the remaining columns. The second set are the traces from the reference biosensor. In both sets, the last trace is from the reference sample (no ligand).

The user may input the traces of which the double references have been subtracted. In this case, the first column is still the time. The rest of the columns contain the traces with the exact number of the length of ligand concentration.

Value

S4 object of "Bli" class

Author(s)

Qingan Sun, Xiaojun Li, James C Sacchettini
 Maintainer: Qingan Sun <quinsun@gmail.com>

References

Sun Q, Li X, Perez LM, Shi W, Zhang Y, Sacchettini JC (2020). “The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD.” *Nature Communications*, **11**(339).

See Also

[doubleBlank](#)

Examples

```
bli <- Bli()  
# traces(bli) <- read.csv("traces.csv")
```

traces<--methods *~~ Methods for Function traces<- ~~*

Description

~~ Methods for function traces<- ~~

Methods

signature(obj = "Bli")

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