Package 'anabel'

May 11, 2023

Title Analysis of Binding Events + 1

Version 3.0.1

Description A free software for a fast and easy analysis of 1:1 molecular interaction studies.
This package is suitable for a high-throughput data analysis.
Both the online app and the package are completely open source.
You provide a table of sensogram, tell 'anabel' which method to use,
and it takes care of all fitting details.
The first two releases of 'anabel' were created and implemented as in
(<doi:10.1177/1177932218821383>, <doi:10.1093/database/baz101>).

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Encoding UTF-8

RoxygenNote 7.2.3

VignetteBuilder knitr

LazyData true

Imports cli (>= 3.4), dplyr (>= 1.0), ggplot2 (>= 3.3), kableExtra (>= 1.3), minpack.lm (>= 1.2), openxlsx (>= 4.2), progress (>= 1.2), purrr (>= 0.3), qpdf, reshape2 (>= 1.4), rlang (>= 1.0), stats (>= 4.0), tidyr (>= 1.2), utils (>= 4.0)

Depends R (>= 4.0)

Suggests htmltools (>= 0.5), knitr (>= 1.36), rmarkdown (>= 2.17), testthat (>= 3.0.0), withr

Config/testthat/edition 3

NeedsCompilation no

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R topics documented:

`convert_toMolar` *Convert a unit to molar*

Description

convert the value into molar.

Usage

```
convert_toMolar(val, unit)
```

Arguments

`val`	numeric value of the analyte concentration
`unit`	character string indicating the unit from which, the analyte concentration will be converted into molar.

Details

supported units are: millimolar, micromolar, nanomolar and picomolar. The name of the unit could be written, or its abbreviation such as: nanomolar (nm), micromolar (mim), picomolar (pm), or millimolar (mm). The unite in either form is case insensitive.

Value

The value of analyte concentration in molar

Examples

```
convert_toMolar(120, "nanomolar")
convert_toMolar(120, "nm")
convert_toMolar(120, "millimolar")
convert_toMolar(120, "mm")
convert_toMolar(120, "micromolar")
convert_toMolar(120, "mim")
convert_toMolar(120, "picomolar")
```

```
convert_toMolar(120, "pm")
```

`MCK_dataset` *Simulated data of binding curve for MCK.*

Description

A dataset containing 5 different binding curves of different analyte concentrations. Ka = 1e+7nM, Kd = 1e-2

Usage

```
data(MCK_dataset)
```

Format

A data frame with 403 rows and 6 variables:

Time time points of the binding interaction from start to end

Conc..50.nM. binding curve generated with analyte concentration = 50nM

Conc..16.7.nM. binding curve generated with analyte concentration = 16.7nM

Conc..5.56.nM. binding curve generated with analyte concentration = 5.56nM

Conc..1.85.nM. binding curve generated with analyte concentration = 1.85nM

Conc..6.17e.1.nM. binding curve generated with analyte concentration = 0.617nM

Source

https://apps.cytivalifesciences.com/spr/

`MCK_dataset_drift` *Simulated data of binding curve for MCK with linear drift.*

Description

A dataset containing 5 different binding curves of different analyte concentrations with induced baseline drift = -0.01. Ka = 1e+7nM, Kd = 1e-2

Usage

```
data(MCK_dataset)
```

Format

A data frame with 403 rows and 6 variables:

Time time points of the binding interaction from start to end

Conc..50.nM. binding curve generated with analyte concentration = 50nM

Conc..16.7.nM. binding curve generated with analyte concentration = 16.7nM

Conc..5.56.nM. binding curve generated with analyte concentration = 5.56nM

Conc..1.85.nM. binding curve generated with analyte concentration = 1.85nM

Conc..6.17e.1.nM. binding curve generated with analyte concentration = 0.617nM

Source

https://apps.cytivalifesciences.com/spr/

`run_anabel` *Analysis for 1:1 Biomolecular Interactions*

Description

Analysis for 1:1 biomolecular interactions, using one of single-curve analysis (SCA), single-cycle kinetics (SCK) or multi-cycle kinetics (MCK)

Usage

```
run_anabel(
  input = NA,
  samples_names_file = NULL,
  tstart = NA,
  tend = NA,
  tass = NA,
  tdiss = NA,
  conc = NA,
  drift = FALSE,
  decay = FALSE,
  quiet = TRUE,
  method = "SCA",
  outdir = NA,
  generate_output = "none",
  generate_Report = FALSE,
  generate_Plots = FALSE,
  generate_Tables = FALSE,
  save_tables_as = "xlsx",
  debug_mode = FALSE
)
```

Arguments

input	Data.frame, an excel, or a csv file (full path) - required
samples_names_file	An optional data.frame, an excel, or a csv file (full path) containing the samples names. If provided, it must have two columns, Name and ID. ID: names of columns in the input file; Name: sample's names.
tstart	Numeric value of time's starting point (default: minimum time point in the input)
tend	Numeric value of time's ending point (default: maximum time point in the input)
tass	Numeric value of association time - required
tdiss	Numeric value of dissociation time - required
conc	Numeric value, the used concentration of the analyte; should be in molar (see convert_toMolar) - required
drift	Boolean value, to apply drift correction (default: FALSE)
decay	Boolean value, to apply surface decay correction (default: FALSE)
quiet	Boolean value, to suppress notifications, messages and warnings (default: TRUE)
method	a character string indicating which fitting method to be used. One of "SCA", "SCK", or "MCK", case insensitive (default: SCA).
outdir	Path and name of the output directory in which the results will be saved (default: NA)
generate_output	a character string indicating what kind of output will be generated. One of "none", "all", or "customized", case insensitive (default: none). If "all" or "customized" were given, outdir is required. If "customized" was given, at least one of generate_Plots, generate_Tables, or/and generate_Report must be set to TRUE
generate_Report	Boolean value, should anabel generate a summary report of the experiment? (default: FALSE)
generate_Plots	Boolean value, should anabel generate plots? (default: FALSE). generate_output must be set to "customized"
generate_Tables	Boolean value, should anabel generate tables? (default: FALSE)
save_tables_as	a character string indicating data format to save the tables with; could be "xlsx", "csv", "txt" or "rds", case insensitive, (default: xlsx)
debug_mode	Boolean value, anabel will return additional fitting details for each curve and the estimated response (default: FALSE)

Value

default returned value is a list of two data frames, the kinetics table and the fit value of each time point (fit_raw). If dev_mode was set to TRUE a third data frame will be returned containing the initial value of the parameters and the fitting function.

References

Determination of rate and equilibrium binding constants for macromolecular interactions by surface plasmon resonance. D J O'Shannessy, M Brigham-Burke, K K Soneson, P Hensley, I Brooks Analytical biochemistry *212*, 457-468 (1993)

Analyzing a kinetic titration series using affinity biosensors. Robert Karlsson, Phinikoula S Katsamba, Helena Nordin, Ewa Pol, David G Myszka Analytical Biochemistry *349*, 136–147 (2006)

Anabel: an online tool for the real-time kinetic analysis of binding events. Stefan D Krämer, Johannes Wöhrle , Christin Rath, Günter Roth Bioinformatics and Biology Insights *13*, 1-10 (2019)

See Also

convert_toMolar

Examples

```
# To analyse data using MCK method:
run_anabel(
  input = MCK_dataset, tstart = 1, tass = 21, tdiss = 140,
  conc = c(3.9E-9, 1.6E-8, 6.2E-8, 2.5E-7, 1.0e-6), method = "MCK"
)
```

SCA_dataset *Simulated data for SCA method.*

Description

A simulated data containing interaction information of three binding curves all generated with concentration 5e-08,

Usage

```
data(SCA_dataset)
```

Format

A data frame with 453 rows and four variables:

Time time points of the binding interaction from start till the experiment's end

Sample.A sample one with Ka = 1e+7nM, Kd = 1e-2

Sample.B sample two with Ka = 1e+6nM, Kd = 5e-2

Sample.C sample four with Ka = 1e+6nM, Kd = 1e-3

Source

https://apps.cytivalifesciences.com/spr/

SCA_dataset_drift *Simulated data for SCA method with linear drift.*

Description

A simulated data containing interaction information of three binding curves all generated with concentration 5e-08, baseline drift = -0.019

Usage

```
data(SCA_dataset)
```

Format

A data frame with 453 rows and four variables:

Time time points of the binding interaction from start till the experiment's end

Sample.A sample one with Ka = 1e+7nM, Kd = 1e-2

Sample.B sample two with Ka = 1e+6nM, Kd = 5e-2

Sample.C sample four with Ka = 1e+6nM, Kd = 1e-3

Source

https://apps.cytivalifesciences.com/spr/

SCK_dataset *Simulated data of different binding curves for SCK method.*

Description

A dataset contains one binding curve with 5 titrations-series (5 injection-series), as follows: tass: 50, 220, 390, 560, 730; tdiss: 150, 320, 490, 660, 830; conc: 6.17e-10 1.85e-09 5.56e-09 1.67e-08 5.00e-08 M

Usage

```
data(SCK_dataset)
```

Format

A data frame with 1091 rows and 6 variables:

Time time points of the binding interaction from start to end

Sample.A sample containing 5 titerations with Ka = 1e+6nM, Kd = 1e-2

Source

https://apps.cytivalifesciences.com/spr/

SCK_dataset_decay *Simulated data of different binding curves for SCK method with exponential decay.*

Description

A dataset contains one binding curve with 5 titrations-series (5 injection-series), as follows: tass: 50, 220, 390, 560, 730; tdiss: 150, 320, 490, 660, 830; conc: 6.17e-10 1.85e-09 5.56e-09 1.67e-08 5.00e-08 M

Usage

```
data(SCK_dataset)
```

Format

A data frame with 1091 rows and 6 variables:

Time time points of the binding interaction from start to end

Sample.A sample containing 5 titerations with Ka = 1e+6nM, Kd = 1e-2

Source

https://apps.cytivalifesciences.com/spr/

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