Package 'pbm'

October 14, 2022

Title Protein Binding Models

Version 1.2.1

Description Binding models which are useful when analysing protein-ligand interactions by techniques such as Biolayer Interferometry (BLI) or Surface Plasmon Resonance (SPR). Naman B. Shah, Thomas M. Duncan (2014) <doi:10.3791/51383>. Hoang H. Nguyen et al. (2015) <doi:10.3390/s150510481>. After initial binding parameters are known, binding curves can be simulated and parameters can be varied. The models within this package may also be used to fit a curve to measured binding data using non-linear regression.

Depends R (>= 3.4.4)

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Encoding UTF-8

URL https://github.com/jonathanrd/pbm

BugReports https://github.com/jonathanrd/pbm/issues

RoxygenNote 7.1.1

Suggests testthat, knitr, rmarkdown, ggplot2, gridExtra

VignetteBuilder knitr

NeedsCompilation no

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Repository CRAN

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R topics documented:

binding1to1 *Generate a 1:1 Binding Curve*

Description

Returns a response value for given parameters at time, t.

Usage

```
binding1to1(t, t0, conc, kon, koff, rmax, drift = 0, offset = 0, doffset = 0)
```

Arguments

t	Time.
t0	Time of dissociation.
conc	Analyte concentration.
kon	Kon binding constant.
koff	Koff binding constant.
rmax	Maximum response, Rmax.
drift	Optional. Parameter to add a linear baseline drift.
offset	Optional. Applies a global offset to the response value.
doffset	Optional. Applies an offset at the start of dissociation.

Examples

```
time <- seq(1,2000)
curve <- binding1to1(time,1000,6e-9,1000,0.01,0.6)
plot(curve)
```

binding2to1 *Generate a 2:1 Binding Curve*

Description

Returns a response value for given parameters at time, t.

Usage

```
binding2to1(
  t,
  t0,
  conc,
  kon1,
  koff1,
  rmax1,
  kon2,
  koff2,
  rmax2,
  drift = 0,
  offset = 0,
  doffset = 0
)
```

Arguments

t	Time.
t0	Time of dissociation.
conc	Analyte concentration.
kon1	Kon binding constant for first component.
koff1	Koff binding constant for first component.
rmax1	Maximum response, Rmax, for first component.
kon2	Kon binding constant for second component.
koff2	Koff binding constant for second component.
rmax2	Maximum response, Rmax, for second component.
drift	Optional. Parameter to add a linear baseline drift.
offset	Optional. Applies a global offset to the response value.
doffset	Optional. Applies an offset at the start of dissociation.

Examples

```
time <- seq(1,2000)
curve <- binding2to1(time,1000,900e-9,10000,0.01,0.4,2000,0.0003,0.5)
plot(curve)
```

req *Response at equilibrium*

Description

Returns the response value at equilibrium from concentration, Rmax and KD.

Usage

```
req(conc, rmax, kd)
```

Arguments

conc	Analyte concentration.
rmax	Maximum response.
kd	Equilibrium dissociation constant.

Examples

```
req(6e-7,1.2,6e-7)
```

tteq *Time to Equilibrium*

Description

Returns the time taken to reach 95% equilibrium.

Usage

```
tteq(conc, kon, koff, theta = 0.95)
```

Arguments

conc	Analyte concentration.
kon	Kon binding constant.
koff	Koff binding constant.
theta	Default 0.95.

Examples

```
tteq(6e-7,20000,0.01)
```

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