Package ‘pmb’

March 5, 2018

Title  Protein Binding Models
Version 1.1.0
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 (>= 3.4.0)
License  MIT + file LICENSE
Encoding  UTF-8

URL  https://github.com/jonathanrd/pbm
BugReports  https://github.com/jonathanrd/pbm/issues
LazyData  true
RoxygenNote  6.0.1.9000
Suggests  testthat, knitr, rmarkdown
VignetteBuilder  knitr
NeedsCompilation  no
Author  Jonathan Davies [aut, cre] (<https://orcid.org/0000-0002-4986-8594>)
Maintainer  Jonathan Davies <jd769@bath.ac.uk>
Repository  CRAN
Date/Publication  2018-03-05 20:00:04 UTC

R topics documented:

- binding1to1 ................................................................. 2
- binding2to1 ................................................................. 2

Index  4
binding1to1  
*Generate a 1:1 Binding Curve*

**Description**

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

**Usage**

```r
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**

```r
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**

```r
binding2to1(t, t0, conc, kon_1, koff_1, rmax_1, kon_2, koff_2, rmax_2, drift = 0, offset = 0, doffset = 0)
```

**Examples**

```r
time <- seq(1,2000)
curve <- binding2to1(time,1000,6e-9,1000,0.01,0.6)
plot(curve)
```
**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**

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

*Topic binding1to1
  binding1to1, 2
*Topic binding2to1
  binding2to1, 2

binding1to1, 2
binding2to1, 2