Package ‘pbm’

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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). Na- man B. Shah, Thomas M. Dun- can (2014) <doi:10.3791/51383>. Hoang H. Nguyen et al. (2015) <doi:10.3390/s150510481>. Af- ter initial binding parameters are known, binding curves can be simulated and parame- ters can be varied. The models within this package may also be used to fit a curve to mea- sured binding data using non-linear regression.
Depends R (>= 3.4.4)
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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

\[\text{binding2to1}(t, t0, \text{conc}, \text{kon1}, \text{koff1}, \text{rmax1}, \text{kon2}, \text{koff2}, \text{rmax2}, \text{drift} = 0, \text{offset} = 0, \text{doffset} = 0)\]

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

```r
  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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