

# Package ‘caffsim’

July 17, 2018

**Title** Simulation of Plasma Caffeine Concentrations by Using Population Pharmacokinetic Model

**Version** 0.2.4

**Date** 2018-07-16

**Description** Simulate plasma caffeine concentrations using population pharmacokinetic model described in Lee, Kim, Perera, McLachlan and Bae (2015) <doi:10.1007/s00431-015-2581-x> and the package was published <doi:10.12793/tcp.2017.25.3.141>.

**Depends** R (>= 3.3.2)

**Encoding** UTF-8

**License** GPL-3 | file LICENSE

**LazyData** true

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**Imports** mgcv, dplyr, tidyr, tibble, ggplot2, shiny, markdown

**NeedsCompilation** no

**URL** <https://github.com/asancpt/caffsim>

**BugReports** <https://github.com/asancpt/caffsim/issues>

**RoxygenNote** 6.0.1

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caffConcTime	Create a concentration-time dataset of single oral dosing of caffeine
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**Description**

caffConcTime will create a dataset of the concentration-time curve.

**Usage**

```
caffConcTime(Weight, Dose, N = 20)
```

**Arguments**

Weight	Body weight (kg)
Dose	Dose of single caffeine (mg)
N	The number of simulated subjects

**Value**

The dataset of concentration and time of simulated subjects

**See Also**

<https://asancpt.github.io/caffsim>

**Examples**

```
caffConcTime(Weight = 20, Dose = 200, N = 20)
caffConcTime(20, 200)
```

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caffConcTimeMulti	Create a concentration-time dataset of multiple oral dosing of caffeine
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**Description**

caffConcTimeMulti will create a dataset of the concentration-time curve of multiple oral administration of caffeine.

**Usage**

```
caffConcTimeMulti(Weight, Dose, N = 20, Tau = 8, Repeat = 4)
```

**Arguments**

Weight	Body weight (kg)
Dose	Dose of single caffeine (mg)
N	The number of simulated subjects
Tau	The interval of multiple dosing (hour)
Repeat	The number of dosing

**Value**

The dataset of concentration and time of simulated subjects of multiple dosing

**See Also**

<https://asancpt.github.io/caffsim>

**Examples**

```
caffConcTimeMulti(Weight = 20, Dose = 200, N = 20, Tau = 8, Repeat = 4)
caffConcTimeMulti(20, 200)
```

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caffDescstat	<i>Calculate descriptive statistics of simulated pharmacokinetic parameters</i>
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**Description**

caffDescstat will calculate descriptive statistics of simulated PK parameters

**Usage**

```
caffDescstat(caffPkparamData)
```

**Arguments**

caffPkparamData  
data frame generated by caffPkparam function

**Value**

The descriptive statistics of pharmacokinetic parameters

**See Also**

<https://asancpt.github.io/caffsim>

**Examples**

```
caffDescstat(caffPkparam(20,500))
caffDescstat(caffPkparamMulti(20,500))
caffDescExample <- cbind(caffDescstat(caffPkparam(20,500)),
                        caffDescstat(caffPkparam(50,500))[,2])
colnames(caffDescExample)[2:3] <- c('20 kg', '50 kg')
caffDescExample
```

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caffOverdose	<i>Calculate a duration of toxic concentration over specified levels (40 mg/L or 80 mg/L)</i>
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### Description

caffOverdose calculates a time duration of plasma caffeine concentration over specified toxic limits (40 mg/L or 80 mg/L)

### Usage

```
caffOverdose(caffConcTimeData)
```

### Arguments

caffConcTimeData  
data frame containing concentration-time data

### Value

descriptive statistics of duration of toxic concentrations

### See Also

<https://asan.shinyapps.io/caff/>

### Examples

```
caffOverdose(caffConcTime(Weight = 20, Dose = 200, N = 20))
caffOverdose(caffConcTimeMulti(Weight = 20, Dose = 200, N = 20, Tau = 8, Repeat = 4))
```

---

caffPkparam	<i>Create a dataset of pharmacokinetic parameters of single oral dosing of caffeine</i>
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### Description

caffPkparam will create a dataset for simulation of single dose of caffeine

### Usage

```
caffPkparam(Weight, Dose, N = 20)
```

### Arguments

Weight	Body weight (kg)
Dose	Dose of single caffeine (mg)
N	The number of simulated subjects

**Value**

The dataset of pharmacokinetic parameters of subjects after single caffeine dose following multivariate normal

**See Also**

<https://asancpt.github.io/caffsim>

**Examples**

```
caffPkparam(Weight = 20, Dose = 200, N = 20)
caffPkparam(20, 500)
```

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caffPkparamMulti	<i>Create a dataset of pharmacokinetic parameters of multiple oral dosing of caffeine</i>
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**Description**

caffPkparamMulti will create a dataset for simulation of multiple dose of caffeine.

**Usage**

```
caffPkparamMulti(Weight, Dose, N = 20, Tau = 8)
```

**Arguments**

Weight	Body weight (kg)
Dose	Dose of multiple caffeine (mg)
N	The number of simulated subjects
Tau	The interval of multiple dosing (hour)

**Value**

The dataset of pharmacokinetic parameters of subjects after multiple caffeine dose following multivariate normal

**See Also**

<https://asancpt.github.io/caffsim>

**Examples**

```
caffPkparamMulti(Weight = 20, Dose = 200, N = 20, Tau = 8)
caffPkparamMulti(20, 500)
```

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caffPlot	<i>Plot plasma concentration-time curves of single oral dosing of caffeine</i>
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**Description**

caffPlot will create concentration-time curve after single dose of caffeine

**Usage**

```
caffPlot(caffConcTimeData, log = FALSE)
```

**Arguments**

caffConcTimeData	data frame of concentration-time dataset having column names Subject, Time, and Conc (case-sensitive)
log	y axis log

**Value**

The concentration-time curve

**See Also**

<https://asancpt.github.io/caffsim>

**Examples**

```
caffPlot(caffConcTime(Weight = 20, Dose = 200, N = 20))
```

---

caffPlotMulti	<i>Plot plasma concentration-time curves of multiple oral dosing of caffeine</i>
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**Description**

caffPlotMulti will create concentration-time curve after multiple doses of caffeine

**Usage**

```
caffPlotMulti(caffConcTimeMultiData, log = FALSE)
```

**Arguments**

caffConcTimeMultiData	data frame of concentration-time dataset having column names Subject, Time, and Conc (case-sensitive)
log	y axis log

**Value**

The concentration-time curve

**See Also**

<https://asancpt.github.io/caffsim>

**Examples**

```
caffPlotMulti(caffConcTimeMulti(Weight = 20, Dose = 200, N = 20, Tau = 8, Repeat = 4))
```

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caffShiny

*Run Shiny app to interactively simulate single and multiple dosing for plasma caffeine concentration*

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**Description**

caffShiny runs an internal shiny app Caffeine Concentration Predictor in order to interactively simulate plasma caffeine concentration.

**Usage**

```
caffShiny()
```

**See Also**

<https://asan.shinyapps.io/caff/>

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UnitTable

*Unit data of PK parameters*

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**Description**

A dataset containing information regarding unit data of pharmacokinetic parameters

**Usage**

```
UnitTable
```

**Format**

A data frame with 16 rows and 2 variables:

**Parameters** Abbreviated pharmacokinetic parameters

**Parameter** Pharmacokinetic parameters in full name

**See Also**

<https://asancpt.github.io/caffsim>

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