Package 'pmxTools'

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Type Package

Title Pharmacometric and Pharmacokinetic Toolkit

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Description Pharmacometric tools for common data analytical tasks; closed-form solutions for calculating concentrations at given times after dosing based on compartmental PK models (1-compartment, 2-compartment and 3-compartment, covering infusions, zero- and first-order absorption, and lag times, after single doses and at steady state, per Bertrand & Mentre (2008) <http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf>); parametric simulation from NONMEM-generated parameter estimates and other output; and parsing, tabulating and plotting results generated by Perl-speaks-NONMEM (PsN).

License GPL-2

LazyData TRUE

RoxygenNote 6.1.0

Imports grid, stats, utils, MASS, XML, stringr, ggplot2, magrittr, GGally, plyr, PKNCA

Suggests testthat

NeedsCompilation no

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R topics documented:

`calc_derived_1cpt` *Calculate derived pharmacokinetic parameters for a 1-compartment linear model*

Description

Calculate derived pharmacokinetic parameters for a 1-compartment linear model

Usage

```
calc_derived_1cpt(CL, V, type = "all", sigdig = 5)
```

Arguments

`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`type`	Type of half-life to return (`"Vss"`, `"k10"`, `"thalf"`, `"alpha"`, `"trueA"`, `"fracA"`, `"all"`). Default is `"all"`).
`sigdig`	Number of significant digits to be returned. Default is 5.

Value

Return a list of derived PK parameters for a 2-compartment linear model given provided clearances and volumes.

- `Vss`: V_{ss} (L)
- `k10`: k_{10} (/h)
- `thalf`: $t_{1/2}$ (h)
- `alpha`: α
- `trueA`: true A
- `fracA`: fractional A

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Shafer S. L. CONVERT.XLS

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
params <- calc_derived_1cpt(CL=16, V=25)
```

---

calc_derived_2cpt *Calculate derived pharmacokinetic parameters for a 2-compartment linear model*

Description

Calculate derived pharmacokinetic parameters for a 2-compartment linear model

Usage

```
calc_derived_2cpt(CL, V1, V2, Q, type = "all", sigdig = 5)
```

Arguments

CL	Clearance (L/h)
V1	Central volume of distribution (L)
V2	Peripheral volume of distribution (L)
Q	Intercompartmental clearance (L/h)
type	Type of half-life to return ("Vss", "k10", "k12", "k21", "thalf_alpha", "thalf_beta", "alpha", "beta", "trueA", "trueB", "fracA", "fracB", "all"). Default is "all").
sigdig	Number of significant digits to be returned. Default is 5.

Value

Return a list of derived PK parameters for a 2-compartment linear model given provided clearances and volumes.

- Vss: Volume of distribution at steady state, V_{ss} (L)
- k10: First-order elimination rate, k_{10} (/h)
- k12: First-order rate of transfer from central to peripheral compartment, k_{12} (/h)

- k21: First-order rate of transfer from peripheral to central compartment, k_{21} (/h)
- thalf_alpha: Distributional half-life, $t_{1/2,\alpha}$ (h)
- thalf_beta: Terminal half-life, $t_{1/2,\beta}$ (h)
- alpha: α
- beta: β
- trueA: true A
- trueB: true B
- fracA: fractional A
- fracB: fractional B

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Shafer S. L. CONVERT.XLS

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
params <- calc_derived_2cpt(CL=16, V1=25, V2=50, Q=0.5)
```

---

calc_derived_3cpt *Calculate derived pharmacokinetic parameters for a 3-compartment linear model*

Description

Calculate derived pharmacokinetic parameters for a 3-compartment linear model

Usage

```
calc_derived_3cpt(CL, V1, V2, V3, Q2, Q3, type = "all", sigdig = 5)
```

Arguments

CL	Clearance (L/h)
V1	Central volume of distribution (L)
V2	First peripheral volume of distribution (L)
V3	Second peripheral volume of distribution (L)
Q2	Intercompartmental clearance from central to first peripheral compartment (L/h)

Q3	Intercompartmental clearance from central to second peripheral compartment (L/h)
type	Type of half-life to return ("Vss", "k10", "k12", "k13", "k21", "k31", "thalf_alpha", "thalf_beta", "thalf_gamma", "alpha", "beta", "gamma", "trueA", "trueB", "trueC", "fracA", "fracB", "fracC", "all"). Default is "all").
sigdig	Number of significant digits to be returned. Default is 5.

Value

Return a list of derived PK parameters for a 3-compartment linear model given provided clearances and volumes.

- Vss: Volume of distribution at steady state, V_{ss} (L)
- k10: First-order elimination rate, k_{10} (/h)
- k12: First-order rate of transfer from central to first peripheral compartment, k_{12} (/h)
- k21: First-order rate of transfer from first peripheral to central compartment, k_{21} (/h)
- k13: First-order rate of transfer from central to second peripheral compartment, k_{13} (/h)
- k31: First-order rate of transfer from second peripheral to central compartment,k_{31} (/h)
- thalf_alpha: $t_{1/2,\alpha}$ (h)
- thalf_beta: $t_{1/2,\beta}$ (h)
- thalf_gamma: $t_{1/2,\gamma}$ (h)
- alpha: α
- beta: β
- gamma: β
- trueA: true A
- trueB: true B
- trueC: true C
- fracA: fractional A
- fracB: fractional B
- fracC: fractional C

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Shafer S. L. CONVERT.XLS

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
params <- calc_derived_3cpt(CL=29.4, V1=23.4, V2=114, V3=4614, Q2=270, Q3=73)
```

`calc_sd_1cmt_linear_bolus` *Calculate C(t) for a 1-compartment linear model after a single IV bolus dose*

Description

Calculate C(t) for a 1-compartment linear model after a single IV bolus dose

Usage

```
calc_sd_1cmt_linear_bolus(t, CL, V, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_1cmt_linear_bolus(t=0:24, CL=6, V=25, dose=600)
```

`calc_sd_1cmt_linear_infusion` *Calculate C(t) for a 1-compartment linear model after a single infusion*

Description

Calculate C(t) for a 1-compartment linear model after a single infusion

Usage

```
calc_sd_1cmt_linear_infusion(t, CL, V, dose, tinf)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`dose`	Dose
`tinf`	Duration of infusion (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_1cmt_linear_infusion(t=0:24, CL=6, V=25, dose=600, tinf=1)
```

`calc_sd_1cmt_linear_oral_0` *Calculate C(t) for a 1-compartment linear model with zero-order absorption after a single oral dose*

Description

Calculate C(t) for a 1-compartment linear model with zero-order absorption after a single oral dose

Usage

```
calc_sd_1cmt_linear_oral_0(t, CL, V, dur, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`dur`	Duration of zero-order absorption (h)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_1cmt_linear_oral_0(t=0:24, CL=6, V=25, dur=1.5, dose=600)
```

`calc_sd_1cmt_linear_oral_0_lag` *Calculate C(t) for a 1-compartment linear model with zero-order absorption after a single oral dose, with lag time*

Description

Calculate C(t) for a 1-compartment linear model with zero-order absorption after a single oral dose, with lag time

Usage

```
calc_sd_1cmt_linear_oral_0_lag(t, CL, V, dur, dose, tlag)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`dur`	Duration of zero-order absorption (h)
`dose`	Dose
`tlag`	Lag time (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_1cmt_linear_oral_0_lag(t=0:24, CL=6, V=25, dur=1.5, dose=600, tlag=1.5)
```

`calc_sd_1cmt_linear_oral_1` *Calculate C(t) for a 1-compartment linear model with first-order absorption after a single oral dose*

Description

Calculate C(t) for a 1-compartment linear model with first-order absorption after a single oral dose

Usage

```
calc_sd_1cmt_linear_oral_1(t, CL, V, ka, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`ka`	First order absorption rate constant (/h)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_1cmt_linear_oral_1(t=0:24, CL=6, V=25, ka=1.1, dose=600)
```

`calc_sd_1cmt_linear_oral_1_lag` *Calculate C(t) for a 1-compartment linear model with first-order absorption after a single oral dose, with lag time*

Description

Calculate C(t) for a 1-compartment linear model with first-order absorption after a single oral dose, with lag time

Usage

```
calc_sd_1cmt_linear_oral_1_lag(t, CL, V, ka, tlag, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`ka`	First order absorption rate constant (/h)
`tlag`	Lag time (h)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_1cmt_linear_oral_1_lag(t=0:24, CL=6, V=25, ka=1.1, dose=600, tlag=2)
```

`calc_sd_2cmt_linear_bolus` *Calculate C(t) for a 2-compartment linear model after a single IV bolus dose*

Description

Calculate C(t) for a 2-compartment linear model after a single IV bolus dose

Usage

```
calc_sd_2cmt_linear_bolus(t, CL, V1, V2, Q, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_2cmt_linear_bolus(t = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 10)
```

`calc_sd_2cmt_linear_infusion` *Calculate C(t) for a 2-compartment linear model after a single infusion*

Description

Calculate C(t) for a 2-compartment linear model after a single infusion

Usage

```
calc_sd_2cmt_linear_infusion(t, CL, V1, V2, Q, dose, tinf)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dose`	Steady state dose
`tinf`	Duration of infusion (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_2cmt_linear_infusion(t = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 10, tinf = 1)
```

`calc_sd_2cmt_linear_oral_0` *Calculate C(t) for a 2-compartment linear model after a single zero-order oral dose*

Description

Calculate C(t) for a 2-compartment linear model after a single zero-order oral dose

Usage

```
calc_sd_2cmt_linear_oral_0(t, CL, V1, V2, Q, dur, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dur`	Duration of zero-order absorption (h)
`dose`	Steady state dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_2cmt_linear_oral_0(t = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, dur = 1)
```

`calc_sd_2cmt_linear_oral_0_lag` *Calculate C(t) for a 2-compartment linear model after a single zero-order oral dose, with lag time*

Description

Calculate C(t) for a 2-compartment linear model after a single zero-order oral dose, with lag time

Usage

```
calc_sd_2cmt_linear_oral_0_lag(t, CL, V1, V2, Q, dur, dose, tlag)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dur`	Duration of zero-order absorption (h)
`dose`	Steady state dose
`tlag`	Lag time (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_2cmt_linear_oral_0_lag(t = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, dur = 1, tlag=2)
```

`calc_sd_2cmt_linear_oral_1` *Calculate C(t) for a 2-compartment linear model after a single first-order oral dose*

Description

Calculate C(t) for a 2-compartment linear model after a single first-order oral dose

Usage

```
calc_sd_2cmt_linear_oral_1(t, CL, V1, V2, Q, ka, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`ka`	First-order absorption rate constant (/h)
`dose`	Steady state dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_2cmt_linear_oral_1(t = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, ka = 1)
```

`calc_sd_2cmt_linear_oral_1_lag` *Calculate C(t) for a 2-compartment linear model after a single first-order oral dose with a lag time*

Description

Calculate C(t) for a 2-compartment linear model after a single first-order oral dose with a lag time

Usage

```
calc_sd_2cmt_linear_oral_1_lag(t, CL, V1, V2, Q, ka, dose, tlag)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`ka`	First-order absorption rate constant (/h)
`dose`	Steady state dose
`tlag`	Lag time (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_2cmt_linear_oral_1_lag(t = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, ka = 1, tlag = 2)
```

`calc_sd_3cmt_linear_bolus` *Calculate C(t) for a 3-compartment linear model after a single IV bolus dose*

Description

Calculate C(t) for a 3-compartment linear model after a single IV bolus dose

Usage

```
calc_sd_3cmt_linear_bolus(t, CL, V1, V2, V3, Q2, Q3, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_3cmt_linear_bolus(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, dose = 100)
```

`calc_sd_3cmt_linear_infusion` *Calculate C(t) for a 3-compartment linear model after a single IV infusion*

Description

Calculate C(t) for a 3-compartment linear model after a single IV infusion

Usage

```
calc_sd_3cmt_linear_infusion(t, CL, V1, V2, V3, Q2, Q3, dose, tinf)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`dose`	Dose
`tinf`	Duration of infusion (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_3cmt_linear_infusion(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, dose = 100, tinf=1)
```

`calc_sd_3cmt_linear_oral_0` *Calculate C(t) for a 3-compartment linear model after a single dose, with zero-order absorption*

Description

Calculate C(t) for a 3-compartment linear model after a single dose, with zero-order absorption

Usage

```
calc_sd_3cmt_linear_oral_0(t, CL, V1, V2, V3, Q2, Q3, dur, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`dur`	Duration of zero-order absorption (h)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_3cmt_linear_oral_0(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, dur = 1, dose = 100)
```

`calc_sd_3cmt_linear_oral_0_lag` *Calculate C(t) for a 3-compartment linear model after a single dose, with zero-order absorption and a lag time*

Description

Calculate C(t) for a 3-compartment linear model after a single dose, with zero-order absorption and a lag time

Usage

```
calc_sd_3cmt_linear_oral_0_lag(t, CL, V1, V2, V3, Q2, Q3, dur, dose, tlag)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`dur`	Duration of zero-order absorption (h)
`dose`	Dose
`tlag`	Lag time (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_3cmt_linear_oral_0_lag(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, dur = 1, dose = 100, tlag=1.5)
```

`calc_sd_3cmt_linear_oral_1` *Calculate C(t) for a 3-compartment linear model after a single oral dose*

Description

Calculate C(t) for a 3-compartment linear model after a single oral dose

Usage

```
calc_sd_3cmt_linear_oral_1(t, CL, V1, V2, V3, Q2, Q3, ka, dose)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`ka`	First-order absorption rate constant (/h)
`dose`	Dose

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_3cmt_linear_oral_1(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, ka = 1, dose = 100)
```

`calc_sd_3cmt_linear_oral_1_lag` *Calculate C(t) for a 3-compartment linear model after a single oral dose*

Description

Calculate C(t) for a 3-compartment linear model after a single oral dose

Usage

```
calc_sd_3cmt_linear_oral_1_lag(t, CL, V1, V2, V3, Q2, Q3, ka, dose, tlag)
```

Arguments

`t`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`ka`	First-order absorption rate constant (/h)
`dose`	Dose
`tlag`	Lag time (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_sd_3cmt_linear_oral_1_lag(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, ka = 1, dose = 100, tlag = 1.5)
```

---

calc_ss_1cmt_linear_bolus

Calculate C(t) for a 1-compartment linear model with IV bolus dosing at steady state

---

Description

Calculate C(t) for a 1-compartment linear model with IV bolus dosing at steady state

Usage

```
calc_ss_1cmt_linear_bolus(tad, CL, V, dose, tau)
```

Arguments

tad	Time after dose (h)
CL	Clearance (L/h)
V	Central volume of distribution (L)
dose	Steady state dose
tau	Dosing interval (h)

Value

Concentration of drug at requested time (tad) after dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_1cmt_linear_bolus(t=0:24, CL=6, V=25, dose=600, tau=24)
```

`calc_ss_1cmt_linear_infusion` *Calculate C(t) for a 1-compartment linear model with infusion at steady state*

Description

Calculate C(t) for a 1-compartment linear model with infusion at steady state

Usage

```
calc_ss_1cmt_linear_infusion(tad, CL, V, dose, tinf, tau)
```

Arguments

`tad`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`dose`	Steady state dose
`tinf`	Duration of infusion (h)
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time (`tad`) after dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_1cmt_linear_infusion(tad=0:36, CL=2, V=25, dose=600, tinf=1, tau=24)
```

`calc_ss_1cmt_linear_oral_0` *Calculate C(t) for a 1-compartment linear model with zero-order oral absorption at steady state*

Description

Calculate C(t) for a 1-compartment linear model with zero-order oral absorption at steady state

Usage

```
calc_ss_1cmt_linear_oral_0(tad, CL, V, dur, dose, tau)
```

Arguments

`tad`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`dur`	Duration of zero-order absorption (h)
`dose`	Steady state dose
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time (`tad`) after dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_1cmt_linear_oral_0(tad=0:36, CL=2, V=25, dose=600, dur=1, tau=24)
```

`calc_ss_1cmt_linear_oral_0_lag` *Calculate C(t) for a 1-compartment linear model with zero-order oral absorption at steady state, with lag time*

Description

Calculate C(t) for a 1-compartment linear model with zero-order oral absorption at steady state, with lag time

Usage

```
calc_ss_1cmt_linear_oral_0_lag(tad, CL, V, dur, dose, tau, tlag)
```

Arguments

`tad`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`dur`	Duration of zero-order absorption (h)
`dose`	Steady state dose
`tau`	Dosing interval (h)
`tlag`	Lag time (h)

Value

Concentration of drug at requested time (`tad`) after dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_1cmt_linear_oral_0_lag(tad=0:36, CL=2, V=25, dose=600, dur=1, tau=24, tlag=1.5)
```

`calc_ss_1cmt_linear_oral_1` *Calculate C(t) for a 1-compartment linear model with first-order oral absorption at steady state*

Description

Calculate C(t) for a 1-compartment linear model with first-order oral absorption at steady state

Usage

```
calc_ss_1cmt_linear_oral_1(tad, CL, V, ka, dose, tau)
```

Arguments

`tad`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`ka`	First order absorption rate constant (/h)
`dose`	Steady state dose
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time (`tad`) after dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_1cmt_linear_oral_1(tad=0:36, CL=2, V=25, dose=600, ka=0.25, tau=24)
```

`calc_ss_1cmt_linear_oral_1_lag` *Calculate C(t) for a 1-compartment linear model with first-order oral absorption at steady state, with lag time*

Description

Calculate C(t) for a 1-compartment linear model with first-order oral absorption at steady state, with lag time

Usage

```
calc_ss_1cmt_linear_oral_1_lag(tad, CL, V, ka, dose, tlag, tau)
```

Arguments

`tad`	Time after dose (h)
`CL`	Clearance (L/h)
`V`	Central volume of distribution (L)
`ka`	First order absorption rate constant (/h)
`dose`	Steady state dose
`tlag`	Lag time (h)
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time (`tad`) after dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_1cmt_linear_oral_1_lag(tad=0:36, CL=2, V=25, dose=600,
    ka=0.25, tlag=0.75, tau=24)
```

`calc_ss_2cmt_linear_bolus` *Calculate C(t) for a 2-compartment linear model with IV bolus dosing at steady-state*

Description

Calculate C(t) for a 2-compartment linear model with IV bolus dosing at steady-state

Usage

```
calc_ss_2cmt_linear_bolus(tad, CL, V1, V2, Q, dose, tau)
```

Arguments

`tad`	Time after last dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dose`	Steady state dose
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time after last dose (`tad`) at steady state, given regular IV bolus dosing and provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_2cmt_linear_bolus(tad = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 10, tau=24)
```

`calc_ss_2cmt_linear_infusion` *Calculate C(t) for a 2-compartment linear model with infusion at steady state*

Description

Calculate C(t) for a 2-compartment linear model with infusion at steady state

Usage

```
calc_ss_2cmt_linear_infusion(tad, CL, V1, V2, Q, dose, tinf, tau)
```

Arguments

`tad`	Time after last dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dose`	Steady state dose
`tinf`	Duration of infusion (h)
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time after last dose (`tad`), given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_2cmt_linear_infusion(tad = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 10, tinf = 1, tau = 12)
```

`calc_ss_2cmt_linear_oral_0` *Calculate C(t) for a 2-compartment linear model at steady-state with zero-order oral dosing*

Description

Calculate C(t) for a 2-compartment linear model at steady-state with zero-order oral dosing

Usage

```
calc_ss_2cmt_linear_oral_0(tad, CL, V1, V2, Q, dur, dose, tau)
```

Arguments

`tad`	Time after last dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dur`	Duration of zero-order absorption (h)
`dose`	Steady state dose
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time (`tad`) at steady-state, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_2cmt_linear_oral_0(tad = 23, CL = 2.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, dur = 1, tau = 24)
```

`calc_ss_2cmt_linear_oral_0_lag` *Calculate C(t) for a 2-compartment linear model at steady-state with zero-order oral dosing and a lag time*

Description

Calculate C(t) for a 2-compartment linear model at steady-state with zero-order oral dosing and a lag time

Usage

```
calc_ss_2cmt_linear_oral_0_lag(tad, CL, V1, V2, Q, dur, dose, tau, tlag)
```

Arguments

`tad`	Time after last dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`dur`	Duration of zero-order absorption (h)
`dose`	Steady state dose
`tau`	Dosing interval (h)
`tlag`	Lag time (h)

Value

Concentration of drug at requested time (`tad`) at steady-state, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_2cmt_linear_oral_0_lag(tad = 23, CL = 2.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, dur = 1, tau = 24, tlag=2)
```

`calc_ss_2cmt_linear_oral_1`

Calculate C(t) for a 2-compartment linear model at steady-state with first-order oral dosing

---

Description

Calculate C(t) for a 2-compartment linear model at steady-state with first-order oral dosing

Usage

```
calc_ss_2cmt_linear_oral_1(tad, CL, V1, V2, Q, ka, dose, tau)
```

Arguments

`tad`	Time after last dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`ka`	First-order absorption rate constant (/h)
`dose`	Steady state dose
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time after last dose (`tad`) at steady-state, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_2cmt_linear_oral_1(tad = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, ka = 1, tau=24)
```

`calc_ss_2cmt_linear_oral_1_lag` *Calculate C(t) for a 2-compartment linear model at steady-state with first-order oral dosing*

Description

Calculate C(t) for a 2-compartment linear model at steady-state with first-order oral dosing

Usage

```
calc_ss_2cmt_linear_oral_1_lag(tad, CL, V1, V2, Q, ka, dose, tau, tlag)
```

Arguments

`tad`	Time after last dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	Peripheral volume of distribution (L)
`Q`	Intercompartmental clearance (L/h)
`ka`	First-order absorption rate constant (/h)
`dose`	Steady state dose
`tau`	Dosing interval (h)
`tlag`	Lag time (h)

Value

Concentration of drug at requested time after last dose (`tad`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_2cmt_linear_oral_1_lag(tad = 11.75, CL = 7.5, V1 = 20, V2 = 30, Q = 0.5,
    dose = 1000, ka = 1, tau=24, tlag=2)
```

`calc_ss_3cmt_linear_bolus` *Calculate C(t) for a 3-compartment linear model at steady state with IV bolus dosing*

Description

Calculate C(t) for a 3-compartment linear model at steady state with IV bolus dosing

Usage

```
calc_ss_3cmt_linear_bolus(tad, CL, V1, V2, V3, Q2, Q3, dose, tau)
```

Arguments

`tad`	Time after last dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`dose`	Dose
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time (`tad`) at steady state, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_3cmt_linear_bolus(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, dose = 100, tau=24)
```

`calc_ss_3cmt_linear_infusion` *Calculate C(t) for a 3-compartment linear model at steady state with IV infusions*

Description

Calculate C(t) for a 3-compartment linear model at steady state with IV infusions

Usage

```
calc_ss_3cmt_linear_infusion(tad, CL, V1, V2, V3, Q2, Q3, dose, tinf, tau)
```

Arguments

`tad`	Time after dose (h)
`CL`	Clearance (L/h)
`V1`	Central volume of distribution (L)
`V2`	First peripheral volume of distribution (L)
`V3`	Second peripheral volume of distribution (L)
`Q2`	Intercompartmental clearance between V1 and V2 (L/h)
`Q3`	Intercompartmental clearance between V2 and V3 (L/h)
`dose`	Dose
`tinf`	Duration of infusion (h)
`tau`	Dosing interval (h)

Value

Concentration of drug at requested time (`t`) after a single dose, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_3cmt_linear_infusion(tad = 11.75, CL = 2.5, V1 = 20, V2 = 50,
    V3 = 100, Q2 = 0.5, Q3 = 0.05, dose = 1000, tinf=1, tau=24)
```

---

calc_ss_3cmt_linear_oral_0

Calculate C(t) for a 3-compartment linear model at steady state, with zero-order absorption

---

Description

Calculate C(t) for a 3-compartment linear model at steady state, with zero-order absorption

Usage

```
calc_ss_3cmt_linear_oral_0(tad, CL, V1, V2, V3, Q2, Q3, dur, dose, tau)
```

Arguments

tad	Time after dose (h)
CL	Clearance (L/h)
V1	Central volume of distribution (L)
V2	First peripheral volume of distribution (L)
V3	Second peripheral volume of distribution (L)
Q2	Intercompartmental clearance between V1 and V2 (L/h)
Q3	Intercompartmental clearance between V2 and V3 (L/h)
dur	Duration of zero-order absorption (h)
dose	Dose
tau	Dosing interval (h)

Value

Concentration of drug at requested time after dose (tad) at steady state, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_3cmt_linear_oral_0(tad = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, dur = 1, dose = 100, tau = 24)
```

---

calc_ss_3cmt_linear_oral_0_lag

Calculate C(t) for a 3-compartment linear model at steady state, with zero-order absorption and lag time

---

Description

Calculate C(t) for a 3-compartment linear model at steady state, with zero-order absorption and lag time

Usage

```
calc_ss_3cmt_linear_oral_0_lag(tad, CL, V1, V2, V3, Q2, Q3, dur, dose, tau,
  tlag)
```

Arguments

tad	Time after dose (h)
CL	Clearance (L/h)
V1	Central volume of distribution (L)
V2	First peripheral volume of distribution (L)
V3	Second peripheral volume of distribution (L)
Q2	Intercompartmental clearance between V1 and V2 (L/h)
Q3	Intercompartmental clearance between V2 and V3 (L/h)
dur	Duration of zero-order absorption (h)
dose	Dose
tau	Dosing interval (h)
tlag	Lag time (h)

Value

Concentration of drug at requested time after dose (tad) at steady state, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_3cmt_linear_oral_0_lag(tad = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, dur = 1, dose = 100, tau = 24, tlag = 1.5)
```

---

calc_ss_3cmt_linear_oral_1

Calculate C(t) for a 3-compartment linear model at steady-state with first-order oral dosing

---

Description

Calculate C(t) for a 3-compartment linear model at steady-state with first-order oral dosing

Usage

```
calc_ss_3cmt_linear_oral_1(tad, CL, V1, V2, V3, Q2, Q3, ka, dose, tau)
```

Arguments

tad	Time after dose (h)
CL	Clearance (L/h)
V1	Central volume of distribution (L)
V2	First peripheral volume of distribution (L)
V3	Second peripheral volume of distribution (L)
Q2	Intercompartmental clearance between V1 and V2 (L/h)
Q3	Intercompartmental clearance between V2 and V3 (L/h)
ka	First-order absorption rate constant (/h)
dose	Dose
tau	Dosing interval (h)

Value

Concentration of drug at requested time (t) at steady state, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_3cmt_linear_oral_1(tad = 11.75, CL = 3.5, V1 = 20,
    V2 = 500, V3 = 200, Q2 = 0.5, Q3 = 0.05, ka = 1, dose = 100, tau = 24)
```

---

calc_ss_3cmt_linear_oral_1_lag

Calculate C(t) for a 3-compartment linear model at steady-state with first-order oral dosing with a lag time

---

Description

Calculate C(t) for a 3-compartment linear model at steady-state with first-order oral dosing with a lag time

Usage

```
calc_ss_3cmt_linear_oral_1_lag(tad, CL, V1, V2, V3, Q2, Q3, ka, dose, tau,
  tlag)
```

Arguments

tad	Time after dose (h)
CL	Clearance (L/h)
V1	Central volume of distribution (L)
V2	First peripheral volume of distribution (L)
V3	Second peripheral volume of distribution (L)
Q2	Intercompartmental clearance between V1 and V2 (L/h)

Q3	Intercompartmental clearance between V2 and V3 (L/h)
ka	First-order absorption rate constant (/h)
dose	Dose
tau	Dosing interval (h)
tlag	Lag time (h)

Value

Concentration of drug at requested time (t) at steady state after oral dosing, given provided set of parameters and variables.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

References

Bertrand J & Mentre F (2008). Mathematical Expressions of the Pharmacokinetic and Pharmacodynamic Models implemented in the Monolix software. http://lixoft.com/wp-content/uploads/2016/03/PKPDlibrary.pdf

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications (4th). Lippincott Williams & Wilkins, Philadelphia, 2010.

Examples

```
Ctrough <- calc_ss_3cmt_linear_oral_1_lag(t = 11.75, CL = 3.5, V1 = 20, V2 = 500,
    V3 = 200, Q2 = 0.5, Q3 = 0.05, ka = 1, dose = 100, tau=24, tlag = 1.5)
```

---

get_auc

Calculate the area under the curve (AUC) for each subject over the time interval for dependent variables (dv) using the trapezoidal rule.

Description

Calculate the area under the curve (AUC) for each subject over the time interval for dependent variables (dv) using the trapezoidal rule.

Usage

```
get_auc(data, time = "TIME", id = "ID", dv = "DV")
```

Arguments

data	A data frame.
time	A string containing the name of the chronologically ordered time variable in data.
id	A string containing the name of the ID column (defining subject level data) in data.
dv	A string containing the name of the dependent variable column in data.

Value

A data frame containing one AUC value for every subject as defined by id.

Based on the AUC function originally written by Leonid Gibiansky in package MIfuns 5.1, from Metrum Institute.

Author(s)

Leonid Gibiansky, <lgibiansky@quantpharm.com>

References

https://code.google.com/archive/p/mifuns/

Examples

```
## Not run:
 AUCs <- get_auc(myAUCdata)

## End(Not run)
```

---

get_est_table *Create a table of model parameter estimates from a NONMEM output object.*

Description

Create a table of model parameter estimates from a NONMEM output object.

Usage

```
get_est_table(x, thetaLabels = c(), omegaLabels = c(),
  sigmaLabels = c(), sigdig = 3)
```

Arguments

x	A NONMEM output object generated using read_nm.
thetaLabels	A vector containing labels for THETA parameters.
omegaLabels	A vector containing labels for OMEGA parameters.
sigmaLabels	A vector containing labels for SIGMA parameters.
sigdig	The desired number of significant digits to display.

Value

A named vector of NONMEM model parameter estimates.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 nmOutput <- read_nm("run315.xml")
 estTab   <- get_est_table(nmOutput)

## End(Not run)
```

---

get_omega *Extract variability parameter estimates from a NONMEM output object.*

Description

Extract variability parameter estimates from a NONMEM output object.

Usage

```
get_omega(x, output = "est", sigdig = 6, sep = "-")
```

Arguments

x	A NONMEM output object generated using read_nm.
output	A flag specifying the matrix or matrices to be output. Valid flag values are est (the default), se, rse, cor, cse, 95ci, or all.
sigdig	Specifies the number of significant digits to be provided (default=6).
sep	Specifies the separator character to use for 95% confidence intervals (default="-").

Value

A symmetrical matrix, or a list of symmetrical matrices if `all` is specified.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

`est` returns the estimated OMEGA variance-covariance matrix. `se` returns the standard errors for the estimated OMEGA variance-covariance matrix. `rse` returns the relative standard errors for the estimated OMEGA variance-covariance matrix (se/est*100). `cor` returns the correlation matrix matrix. `cse` returns the standard errors for the correlation matrix. `95ci` returns the asymptotic 95% confidence intervals for the elements of the OMEGA variance-covariance matrix (est +/- 1.96*se). `all` returns all available OMEGA matrices.

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 nmOutput  <- read_nm("run315.xml")
 omegas    <- get_omega(nmOutput)
 omegaRSEs <- get_omega(nmOutput, "rse")

## End(Not run)
```

---

get_shrinkage *Extract shrinkage estimates from a NONMEM output object.*

Description

Extract shrinkage estimates from a NONMEM output object.

Usage

```
get_shrinkage(x, output = "eta", sigdig = 3)
```

Arguments

`x`	A NONMEM output object generated using `read_nm`.
`output`	A flag specifying the shrinkage estimates to be output. Valid flag values are `eta` (the default), `epsilon`, or `all`.
`sigdig`	Specifies the number of significant digits to be provided (default=3).

Value

A named vector of NONMEM shrinkage estimates, or in the case of `all`, a list of named vectors.

`eta` returns a vector of ETA shrinkages, as reported by NONMEM. `epsilon` returns EPSILON shrinkage, as reported by NONMEM. `all` returns both ETA and EPSILON shrinkage estimates as a list of vectors.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 nmOutput <- read_nm("run315.xml")
 shr <- get_shrinkage(nmOutput, output="all")

## End(Not run)
```

---

get_sigma *Extract residual variability parameter estimates from a NONMEM output object.*

Description

Extract residual variability parameter estimates from a NONMEM output object.

Usage

```
get_sigma(x, output = "est", sigdig = 6, sep = "-")
```

Arguments

`x`	A NONMEM output object generated using `read_nm`.
`output`	A flag specifying the matrix or matrices to be output. Valid flag values are `est` (the default), `se`, `rse`, `cor`, `cse`, `95ci`, or `all`.
`sigdig`	Specifies the number of significant digits to be provided (default=6).
`sep`	Specifies the separator character to use for 95% confidence intervals (default="-").

Value

A symmetrical matrix, or a list of symmetrical matrices if `all` is specified.

`est` returns the estimated SIGMA variance-covariance matrix. `se` returns the standard errors for the estimated SIGMA variance-covariance matrix. `rse` returns the relative standard errors for the estimated SIGMA variance-covariance matrix (se/est*100). `cor` returns the correlation matrix matrix. `cse` returns the standard errors for the correlation matrix. `95ci` returns the asymptotic 95% confidence intervals for the elements of the SIGMA variance-covariance matrix (est +/- 1.96*se). `all` returns all available SIGMA matrices.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 nmOutput <- read_nm("run315.xml")
 sigmas   <- get_sigma(nmOutput)
 sigmaRSEs <- get_sigma(nmOutput, "rse")

## End(Not run)
```

`get_theta` *Extract structural model parameter estimates and associated information from a NONMEM output object.*

Description

Extract structural model parameter estimates and associated information from a NONMEM output object.

Usage

```
get_theta(x, output = "est", sigdig = 6, sep = "-")
```

Arguments

`x`	A NONMEM output object generated using `read_nm`.
`output`	A flag specifying the matrix or matrices to be output. Valid flag values are `est` (the default), `se`, `rse`, `95ci`, or `all`.
`sigdig`	Specifies the number of significant digits to be provided (default=6).
`sep`	Specifies the separator character to use for 95% confidence intervals (default="-").

Value

A named vector of NONMEM model parameter estimates, or in the case of `all`, a list of named vectors.

`est` returns a vector of THETA values. `se` returns a vector of THETA standard errors. `rse` returns a vector of THETA relative standard errors (se/est*100). `95ci` returns a vector of the asymptotic 95% confidence intervals for the elements of THETA (est +/- 1.96*se). `all` returns all available THETA information as a list of named vectors.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 nmOutput <- read_nm("run315.xml")
 thetas <- get_theta(nmOutput)

## End(Not run)
```

---

gm *Calculate geometric mean*

Description

Calculate geometric mean

Usage

```
gm(x)
```

Arguments

x	Numeric vector.

Value

The geometric mean. NA is returned if there are any non-positive elements in x.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

Examples

```
gm(c(0.5, 7, 8, 5))
```

---

pcv *Calculate percentage coefficient of variation*

Description

Calculate percentage coefficient of variation

Usage

```
pcv(x, na.rm = FALSE)
```

Arguments

x	Numeric vector.
na.rm	A logical value indicating whether NA values should be stripped before the computation proceeds.

Value

The percentage coefficient of variation.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

Examples

```
pcv(rnorm(50, 5, 7.56))
```

---

pk_curve *Provide concentration-time curves.*

Description

Provide concentration-time curves.

Usage

```
pk_curve(t, model = "1cmt_oral", params = list(ka = 2.77, CL = 2.5, V =
  25), dose = 600, ii = 24, addl = 0, ss = F)
```

Arguments

t	Observation time in h, specified as a vector.
model	The model to use. Must be one of "1cmt_bolus", "1cmt_infusion", "1cmt_oral", "2cmt_bolus", "2cmt_infusion", "2cmt_oral", "3cmt_bolus", "3cmt_infusion", "3cmt_oral". The default is "1cmt_oral".
params	A named list containing parameter values for the selected model type.
dose	Dose amount.
ii	Interdose interval (or tau), in hours (default 24).
addl	Number of additional doses (default 0).
ss	Assume steady state concentration (default FALSE).

Value

A data frame containing times (t) and concentrations (cp).

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

Examples

```
plot(pk_curve(t=seq(0,72,by=0.1), model="3cmt_oral", ii=12, addl=5,
  params=list(CL=2.5, V1=25, V2=2, V3=5, Q2=0.5, Q3=0.25, ka=1)), type="l")
```

---

plot_nmprogress *Plot NONMEM parameter estimation by iteration.*

Description

plot_nmprogress returns a plot or set of plots showing the evolution of parameter estimates by iteration.

Usage

```
plot_nmprogress(fileName, fileExt = ".lst", metric = "perc",
  lineCol = "#902C10", idlineCol = "black")
```

Arguments

fileName	A NONMEM output file prefix, without extension (e.g. 'run315').
fileExt	The file extension for NONMEM output, set to '.lst' by default.
metric	What to show in the plot. Allowed options are 'est' (the actual estimate) or 'perc' (the percentage change in the estimated or OFV since estimation began). Default is 'perc'.
lineCol	Line color. Default is '#902C10'.
idlineCol	Identity line color (only used if 'perc' metric is selected). Default is black.

Value

A set of plots.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
plot_nmprogress("run315")
plot_nmprogress("run315", ".nmlst")

## End(Not run)
```

---

read_nm *Read NONMEM 7.2+ output into a list of lists.*

Description

Read NONMEM 7.2+ output into a list of lists.

Usage

```
read_nm(fileName)
```

Arguments

fileName	A NONMEM XML output file (e.g. "run315.xml").

Value

A list of lists corresponding to a NONMEM output object.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
nmOutput <- read_nm("run315.xml")

## End(Not run)
```

`read_nmcov` *Read in the NONMEM variance-covariance matrix.*

Description

Read in the NONMEM variance-covariance matrix.

Usage

```
read_nmcov(fileName)
```

Arguments

`fileName`	Root filename for the NONMEM run (e.g. "run315"). This function reads the ".cov" NONMEM output table, and will return an error if this is missing.

Value

A symmetrical variance-covariance matrix covering all model parameters.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
nmVcov <- read_nmcov("run315")

## End(Not run)
```

`read_nmext` *Read NONMEM output into a list.*

Description

`read_nmext` returns a summary of a given NONMEM run, including termination messages, parameter estimates, and precision estimates. Minimally, the NONMEM output and '.ext' files must be available.

Usage

```
read_nmext(fileName, fileExt = ".lst")
```

Arguments

`fileName`	A NONMEM output file prefix, without extension (e.g. "run315").
`fileExt`	The file extension for NONMEM output, set to ".lst" by default.

Value

A list of lists, containing 'Termination' (summary of NONMEM's termination output, including shrinkages and ETABAR estimates), 'OFV' (the objective function value), 'Thetas' (a vector of structural parameter estimates, or THETAs), 'Omega', a list of lists containing the OMEGA matrix, 'Sigma', a list of lists containing the SIGMA matrix, 'seThetas', a vector of standard errors for THETAs, 'seOmega', a list of lists containing standard errors for the OMEGA matrix, and 'seSigma', a list of lists containing standard errors for the SIGMA matrix.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
read_nmext("run315")
read_nmext("run315", ".nmlst")

## End(Not run)
```

`read_nmtables` *Reads NONMEM output tables.*

Description

Reads NONMEM output tables.

Usage

```
read_nmtables(tableFiles = NULL, runNo = NULL, tabSuffix = "",
  tableNames = c("sdtab", "mutab", "patab", "catab", "cotab", "mytab",
  "extra", "xptab"), quiet = FALSE, ...)
```

Arguments

`tableFiles`	NONMEM table files to be read.
`runNo`	Run number.
`tabSuffix`	Table file suffix.
`tableNames`	List of root table names, using the Xpose naming convention as the default.
`quiet`	Flag for displaying intermediate output (defaults to `FALSE`).
`...`	Additional arguments.

Value

A data frame.

Note

Adapted from Xpose 4 (https://CRAN.R-project.org/package=xpose4).

Author(s)

Justin Wilkins, Niclas Jonsson, Andrew Hooker

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Jonsson EN, Karlsson MO. Xpose–an S-PLUS based population pharmacokinetic/pharmacodynamic model building aid for NONMEM. Comput Methods Programs Biomed. 1999 Jan;58(1):51-64

Examples

```
## Not run:
tables <- read_nmtables(315)

## End(Not run)
```

read_scm *Read PsN SCM output into a format suitable for further use.*

Description

read_scm returns a summary of a Perl-speaks-NONMEM (PsN, https://uupharmacometrics.github.io/PsN/) SCM (stepwise covariate modeling) procedure. It depends on the presence of an scmlog.txt file in the specified directory.

Usage

```
read_scm(dir, startPhase = "forward")
```

Arguments

dir	A PsN SCM folder (containing scmlog.txt).
startPhase	Where to start collating the output; can be "forward" (the default) or "backward".

Value

A list of data frames, containing

forward	all models evaluated during the forward inclusion step of covariate model building
forwardSummary	the covariate relationships selected at each forward step
backward	all models evaluated during the backward elimination step of covariate model building
backwardSummary	the covariate relationships eliminated at each backward step

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Lindbom L, Ribbing J & Jonsson EN (2004). Perl-speaks-NONMEM (PsN) - A Perl module for NONMEM related programming. Computer Methods and Programs in Biomedicine, 75(2), 85-94. https://doi.org/10.1016/j.cmpb.2003.11.003

Lindbom L, Pihlgren P & Jonsson N (2005). PsN-Toolkit - A collection of computer intensive statistical methods for non-linear mixed effect modeling using NONMEM. Computer Methods and Programs in Biomedicine, 79(3), 241-257. https://doi.org/10.1016/j.cmpb.2005.04.005

Examples

```
## Not run:
scm <- readSCM("E:/DrugX/ModelDevelopment/scm310")

## End(Not run)
```

`sample_omega` *Sample from the multivariate normal distribution using the OMEGA variance-covariance matrix to generate new sets of simulated ETAs from NONMEM output.*

Description

Sample from the multivariate normal distribution using the OMEGA variance-covariance matrix to generate new sets of simulated ETAs from NONMEM output.

Usage

```
sample_omega(nmRun, n, seed)
```

Arguments

`nmRun`	Root filename for the NONMEM run (e.g. "run315").
`n`	Number of samples required.
`seed`	Random seed.

Value

A data frame containing `n` samples from the multivariate normal distribution, using the estimated NONMEM OMEGA variance-covariance matrix. This provides `n` sets of ETA estimates suitable for simulation of new patients.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 omDist <- sample_omega("run315", 5000, seed=740727)

## End(Not run)
```

`sample_sigma` *Sample from the multivariate normal distribution using the SIGMA variance-covariance matrix to generate new sets of simulated EPSILONs from NONMEM output.*

Description

Sample from the multivariate normal distribution using the SIGMA variance-covariance matrix to generate new sets of simulated EPSILONs from NONMEM output.

Usage

```
sample_sigma(nmRun, n, seed)
```

Arguments

`nmRun`	Root filename for the NONMEM run (e.g. "run315").
`n`	Number of samples required.
`seed`	Random seed.

Value

A data frame containing `n` samples from the multivariate normal distribution, using the estimated NONMEM SIGMA variance-covariance matrix. This provides `n` sets of EPSILON estimates suitable for simulation of new datasets.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 sigDist <- sample_sigma("run315", 5000, seed=740727)

## End(Not run)
```

`sample_uncert` *Sample from the multivariate normal distribution to generate new sets of parameters from NONMEM output.*

Description

Sample from the multivariate normal distribution to generate new sets of parameters from NONMEM output.

Usage

```
sample_uncert(nmRun, n, seed)
```

Arguments

`nmRun`	Root filename for the NONMEM run (e.g. "run315").
`n`	Number of samples required.
`seed`	Random seed.

Value

A data frame containing `n` samples from the multivariate normal distribution, using NONMEM typical parameter estimates the NONMEM variance-covariance matrix (from the *.cov file). This provides `n` sets of parameter estimates sampled from the uncertainty distribution, suitable for simulation under model uncertainty.

Author(s)

Justin Wilkins, <justin.wilkins@occams.com>

See Also

NONMEM (http://www.iconplc.com/innovation/nonmem/)

Examples

```
## Not run:
 nmMatrix <- sample_uncert("run315", 5000, seed=740727)

## End(Not run)
```

table_rtf *Read NONMEM output into a list.*

Description

table_rtf generates an RTF table from a data frame.

Usage

```
table_rtf(df, outFile = NULL, rtfFile = TRUE, boldHeader = TRUE,
  rowNames = FALSE, ...)
```

Arguments

df	A data frame.
outFile	A filename for writing the table to. If NULL, writes to console.
rtfFile	If TRUE (the default), then add RTF tabs to generate a fully formatted RTF file.
boldHeader	If TRUE, make the header bold.
rowNames	If TRUE, include row names in the table. Default is FALSE.
...	Other formatting options for the table body.

Value

An RTF table based on the data frame provided.

Author(s)

John Johnson, <johndjohnson@gmail.com>

References

http://www.r-bloggers.com/another-solution-to-the-r-to-word-table-problem/

Examples

```
## Not run:
scm <- read_scm("E:/DrugX/ModelDevelopment/scm310")
myRTF <- table_rtf(scm$forwardSummary)

## End(Not run)
```

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