

Package ‘pkr’

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Title Pharmacokinetics in R

Description Conduct a noncompartmental analysis as closely as possible to the most widely used commercial software.

Some features are

- 1) CDISC SDTM terms
- 2) Automatic slope selection with the same criterion of WinNonlin(R)
- 3) Supporting both 'linear-up linear-down' and 'linear-up log-down' method
- 4) Interval(partial) AUCs with 'linear' or 'log' interpolation method

* Reference: Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016. (ISBN:9198299107).

Depends R (>= 2.0.0), foreign, binr, forestplot, rtf

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pkr-package

Pharmacokinetics in R

Description

It conducts a noncompartmental analysis(NCA) as closely as possible to the most widely used commercial pharmacokinetic analysis software.

Details

The main functions are

NCA to perform NCA for many subjects.

IndiNCA to perform NCA for one subject.

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

Examples

```
# Theoph and Indometh data: dose in mg, conc in mg/L, time in h
NCA(Theoph, "Subject", "Time", "conc", dose=320, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", uConc="mg/L")

iAUC = data.frame(Name=c("AUC[0-12h]", "AUC[0-24h]"), Start=c(0,0), End=c(12,24)) ; iAUC
NCA(Theoph, "Subject", "Time", "conc", dose=320, iAUC=iAUC, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", iAUC=iAUC, uConc="mg/L")

# writelines(NCA(Theoph, "Subject", "Time", "conc", dose=320, report="Text", uConc="mg/L"),
#             "Theoph_Linear_CoreOutput.txt")
# writelines(NCA(Theoph, "Subject", "Time", "conc", dose=320, fit="Log", report="Text",
#             uConc="mg/L"), "Theoph_Log_CoreOutput.txt")
# writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", report="Text",
#             uConc="mg/L"), "Indometh_Bolus_Linear_CoreOutput.txt")
# writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", fit="Log",
#             report="Text", uConc="mg/L"), "Indometh_Bolus_Log_CoreOutput.txt")
# writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
#             report="Text", uConc="mg/L"), "Indometh_Infusion_Linear_CoreOutput.txt")
# writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
#             fit="Log", report="Text", uConc="mg/L"), "Indometh_Infusion_Log_CoreOutput.txt")

sNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], dose=320, concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
     adm="Bolus", concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
     adm="Infusion", dur=0.25, concUnit="mg/L")

iAUC = data.frame(Name=c("AUC[0-12h]", "AUC[0-24h]"), Start=c(0,0), End=c(12,24)) ; iAUC
sNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], dose=320,
     iAUC=iAUC, concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
     adm="Bolus", iAUC=iAUC, concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
     adm="Infusion", dur=0.25, iAUC=iAUC, concUnit="mg/L")
```

Description

Calculate Area Under the Curve(AUC) and the first Moment Curve(AUMC) in two ways; 'linear trapezoidal method' or 'linear-up and log-down' method. Return a table of cumulative values.

Usage

```
AUC(x, y, down = "Linear")
```

Arguments

x	vector values of independent variable, usually time
y	vector values of dependent variable, usually concentration
down	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC

Details

down="Linear" means linear trapezoidal rule with linear interpolation. down="Log" means linear-up and log-down method.

Value

Table with two columns, AUC and AUMC; the first column values are cumulative AUCs and the second column values cumulative AUMCs.

Author(s)

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References

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. pp687-689. 2011.

See Also

[LinAUC](#), [LogAUC](#)

Examples

```
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], down="Log")
```

BestSlope	<i>Choose best fit slope for the log(y) and x regression by the criteria of adjusted R-square</i>
-----------	---

Description

It sequentially fits ($\log(y) \sim x$) from the last point of x to the previous points with at least 3 points. It chooses a slope the highest adjusted R-square. If the difference is less than $1e-4$, it chooses longer slope.

Usage

```
BestSlope(x, y, adm = "Extravascular", TOL=1e-4)
```

Arguments

x	vector values of x-axis, usually time
y	vector values of y-axis, usually concentration
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
TOL	tolerance. See Phoenix WinNonlin 6.4 User's Guide p33 for the detail.

Details

Choosing the best terminal slope (y in log scale) in pharmacokinetic analysis is somewhat challenging, and it could vary by analysis performer. Phoenix WinNonlin chooses a slope with highest adjusted R-squared and the longest one. Difference of adjusted R-Squared less than TOL considered to be 0. This function uses ordinary least square method (OLS).

Value

R2	R-squared
R2ADJ	adjusted R-squared
LAMZNPT	number of points used for slope
LAMZ	negative of slope, λ_z
b0	intercept of regression line
CORRXY	correlation of $\log(y)$ and x
LAMZLL	earliest x for λ_z
LAMZUL	last x for λ_z
CLSTP	predicted y value at last point, predicted concentration for the last time point

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[Slope](#)

Examples

```
BestSlope(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
BestSlope(Indometh[Indometh$Subject==1, "time"], Indometh[Indometh$Subject==1, "conc"],
          adm="Bolus")
```

combXPT	<i>Combine XPT files</i>
---------	--------------------------

Description

This function combines specified CDISC domain XPT files across the folders.

Usage

```
combXPT(folders, domain)
```

Arguments

- | | |
|---------|---|
| folders | where to find specified CDISC domain XPT files |
| domain | domain XPT files to be comined across the folders |

Details

You need to designate only one CDISC domain name. You may specify one or more folders to find the domain XPT files.

Value

- | | |
|-----|----------------|
| XPT | combined table |
|-----|----------------|

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [readEX](#), [readPC](#)

foreNCA	<i>Forest plot to compare NCA results</i>
---------	---

Description

This function compares NCA results usually from rNCA function

Usage

```
foreNCA(NCAres = "", Pptestcd = "", Pctestcd = "", title = "", ...)
```

Arguments

NCAres	NCA results from rNCA function
Pptestcd	CDISC SDTM PP domain Test Code to compare
Pctestcd	Molecular species to compare specified in Pctestcd of CDISC SDTM PC domain
title	Title of the plot
...	further arguments to pass to the forestplot function

Details

This function calls forestplot in forest package.

Value

Currently, this just plots.

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [rNCA](#)

IndiNCA

*Noncompartmental Analysis for an Individual***Description**

It performs a noncompartmental analysis with one subject data. This will be deprecated. Use `sNCA()` instead.

Usage

```
IndiNCA(x, y, dose = 0, fit = "Linear", adm = "Extravascular", dur = 0,
        report = "Table", iAUC = "", uTime = "h", uConc = "ug/L", uDose = "mg")
```

Arguments

<code>x</code>	vector values of independent variable, usually time
<code>y</code>	vector values of dependent variable, usually concentration
<code>dose</code>	administered dose for the subject
<code>fit</code>	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
<code>adm</code>	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
<code>dur</code>	infusion duration for constant infusion, otherwise 0
<code>report</code>	either of "Table" or "Text" to specify the type of return value
<code>iAUC</code>	data.frame with three columns, "Name", "Start", "End" to specify the intervals for partial (interval) AUC
<code>uTime</code>	unit of time
<code>uConc</code>	unit of concentration
<code>uDose</code>	unit of dose

Details

This performs a noncompartmental analysis for a subject. It returns practically the same result with the most popular commercial software.

Value

<code>C_{MAX}</code>	maximum concentration, C_{max}
<code>C_{MAXD}</code>	dose normalized C_{max} , C_{MAX} / Dose , C_{max} / Dose
<code>T_{MAX}</code>	time of maximum concentration, T_{max}
<code>T_{LAG}</code>	time to observe the first non-zero concentration, for extravascular administration only
<code>CL_{ST}</code>	last positive concentration observed, C_{last}
<code>CL_{STP}</code>	last positive concentration predicted, C_{last_pred}

TLST	time of last positive concentration, Tlast
LAMZHL	half-life by lambda z, $\ln(2)/\text{LAMZ}$
LAMZ	lambda_z negative of best fit terminal slope
LAMZLL	earliest time for LAMZ
LAMZUL	last time for LAMZ
LAMZNPT	number of points for LAMZ
CORRXY	correlation of log(concentration) and time
R2	R-squared
R2ADJ	R-squared adjusted
C0	back extrapolated concentration at time 0, for bolus intravascular administration only
AUCLST	AUC from 0 to TLST
AUCALL	AUC using all the given points, including trailing zero concentrations
AUCIFO	AUC infinity observed
AUCIFOD	AUCIFO / Dose
AUCIFP	AUC infinity predicted using CLSTP instead of CLST
AUCIFPD	AUCIFP / Dose
AUCPEO	AUC % extrapolation observed
AUCPEP	AUC % extrapolated for AUCIFP
AUCPBEO	AUC % back extrapolation observed, for bolus IV administration only
AUCPBEP	AUC % back extrapolation predicted with AUCIFP, for bolus IV administration only
AUMCLST	AUMC to the TLST
AUMCIFO	AUMC infinity observed using CLST
AUMCIFP	AUMC infinity determined by CLSTP
AUMCPEO	AUMC % extrapolated observed
AUMCPEP	AUMC % extrapolated predicted
MRTIVLST	mean residence time (MRT) to TLST, for intravascular administration
MRTIVIFO	mean residence time (MRT) infinity using CLST, for intravascular administration
MRTIVIFP	mean residence time (MRT) infinity using CLSTP, for intravascular administration
MRTEVLST	mean residence time (MRT) to TLST, for extravascular administration
MRTEVIFO	mean residence time (MRT) infinity using CLST, for extravascular administration
MRTEVIFP	mean residence time (MRT) infinity using CLSTP, for extravascular administration
VZ0	volume of distribution determined by LAMZ and AUCIFO, for intravascular administration

VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZFO	VZO for extravascular administration, VZO/F, F is bioavailability
VZFP	VZP for extravascular administration, VZP/F, F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLFO	CLO for extravascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSSO	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at steady state using CLSTP, for intravascular administration only

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

See Also

[AUC](#), [BestSlope](#)

Examples

```
IndiNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], dose=320, uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
  adm="Bolus", uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
  adm="Infusion", dur=0.25, uConc="mg/L")

IndiNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], dose=320,
  report="Text", uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
  adm="Bolus", report="Text", uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
  adm="Infusion", dur=0.25, report="Text", uConc="mg/L")

iAUC = data.frame(Name=c("AUC[0-12h]", "AUC[0-24h]"), Start=c(0,0), End=c(12,24)) ; iAUC
IndiNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], dose=320,
```

```

      iAUC=iAUC, uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
      adm="Bolus", iAUC=iAUC, uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], dose=25,
      adm="Infusion", dur=0.25, iAUC=iAUC, uConc="mg/L")

```

IntAUC

*Calculate interval AUC***Description**

It calculates interval AUC

Usage

```
IntAUC(x, y, t1, t2, Res, down = "Linear")
```

Arguments

x	vector values of independent variable, usually time
y	vector values of dependent variable, usually concentration
t1	start time for AUC
t2	end time for AUC
Res	result from IndiNCA function
down	either of "Linear" or "Log" to indicate the way to calculate AUC

Details

This calculates an interval (partial) AUC (from t1 to t2) with the given series of x and y. If t1 and/or t2 cannot be found within x vector, it interpolates according to the down option.

Value

return interval AUC value (scalar)

Author(s)

Kyun-Seop Bae <k@acr.kr>

References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

See Also

[AUC](#), [Interpol](#)

Examples

```
Res = sNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"],
           dose=320, concUnit="mg/L")
IntAUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], t1=0.5, t2=11, Res)
```

Interpol	<i>Interpolate y value</i>
----------	----------------------------

Description

It interpolates y value when a corresponding x value (xnew) does not exist within x vector

Usage

```
Interpol(x, y, xnew, Slope, b0, down = "Linear")
```

Arguments

- x vector values of x-axis, usually time
- y vector values of y-axis, usually concentration
- xnew new x point to be interpolated, usually new time point
- Slope slope of regression $\log(y) \sim x$
- b0 y value of just left point of xnew
- down either of "Linear" or "Log" to indicate the way to interpolate

Details

This function interpolate y value, if xnew is not in x vector. If xnew is in x vector, it just returns the given x and y vector. This function usually is called by IntAUC function Returned vector is sorted in the order of increasing x values.

Value

new x and y vector containing xnew and ynew point

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[IntAUC](#)

Examples

```
x = 10:1 + 0.1
y = -2*x + 40.2
Interpol(x, y, 1.5)
Interpol(x, y, 1.5, down="Log")
```

LinAUC	<i>Area Under the Curve(AUC) and Area Under the first Moment Curve(AUMC) by linear trapezoidal method</i>
--------	---

Description

It calculates AUC and AUMC using linear trapezoidal method

Usage

```
LinAUC(x, y)
```

Arguments

x	vector values of independent variable, usually time
y	vector values of dependent variable, usually concentration

Details

This function returns AUC and AUMC by linear trapezoidal method.

Value

AUC	area under the curve
AUMC	area under the first moment curve

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

See Also

[LogAUC](#), [AUC](#)

Examples

```
LinAUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"]) # compare the last line
```

loadEXPC	<i>Load EX and PC domain files in folders</i>
----------	---

Description

This loads and returns EX and PC domain files in the specified folders

Usage

```
loadEXPC(folders)
```

Arguments

folders folders where to find EX and PC domain files

Details

This reads EX and PC domain files in the specified folder. This calls readEX and readPC functions.

Value

EX	combined EX domain data
PC	combined PC doamin data

Author(s)

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See Also

[help](#), [readEX](#), [readPC](#)

LogAUC	<i>Area Under the Curve(AUC) and Area Under the first Moment Curve(AUMC) by linear-up log-down method</i>
--------	---

Description

It calculates AUC and AUMC using linear-up log-down method

Usage

```
LogAUC(x, y)
```

Arguments

x	vector values of independent variable, usually time
y	vector values of dependent variable, usually concentration

Details

This function returns AUC and AUMC by linear-up log-down method.

Value

AUC	area under the curve
AUMC	area under the first moment curve

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

See Also

[LinAUC,AUC](#)

Examples

```
LogAUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
# Compare the last line with the above
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], down="Log")
```

Description

conduct noncompartmental analysis for many subjects in a data table

Usage

```
NCA(concData, id, Time, conc, trt="", fit = "Linear", dose = 0,
    adm = "Extravascular", dur = 0, report = "Table", iAUC = "",
    uTime = "h", uConc = "ug/L", uDose = "mg")
```

Arguments

concData	name of data table containing time-concentration data of multiple subjects
id	column name for subject ID
Time	column name for the time
conc	column name for the concentration
trt	column name for the treatment code. This is useful for crossover study like bioequivalence trial.
fit	one of "Linear" or "Log" to indicate the way to calculate AUC
dose	administered dose. One should be careful for the unit. This can be a vector containing dose for each subject in order.
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	infusion duration for constant infusion, otherwise 0. This can be a vector containing values for each subject in order.
report	either of "Table" or "Text" to specify the type of return value
iAUC	data.frame with three columns, "Name", "Start", "End" to specify partial interval AUC
uTime	unit of time
uConc	unit of concentration
uDose	unit of dose

Details

This function calls IndiNCA repeatedly to do NCA for each subject. If you specify Report="Text", this function returns in free text format to be used in a report file.

Value

C _{MAX}	maximum concentration, C _{max}
C _{MAXD}	dose normalized C _{max} , C _{MAX} / Dose, C _{max} / Dose
T _{MAX}	time of maximum concentration, T _{max}
T _{LAG}	time to observe the first non-zero concentration, for extravascular administration only
CL _{ST}	last positive concentration observed, C _{last}
CL _{STP}	last positive concentration predicted, C _{last_pred}
T _{LAST}	time of last positive concentration, T _{last}
LAM _{ZHL}	half-life by lambda z, ln(2)/LAM _Z
LAM _Z	lambda _z negative of best fit terminal slope
LAM _{ZLL}	earliest time for LAM _Z
LAM _{ZUL}	last time for LAM _Z
LAM _{ZNPT}	number of points for LAM _Z
COR _{RXY}	correlation of log(concentration) and time
R ²	R-squared
R ² _{ADJ}	R-squared adjusted
C ₀	back extrapolated concentration at time 0, for bolus intravascular administration only
AUC _{CLST}	AUC from 0 to T _{LAST}
AUC _{ALL}	AUC using all the given points, including trailing zero concentrations
AUC _{IFO}	AUC infinity observed
AUC _{IFOD}	AUC _{IFO} / Dose
AUC _{IFP}	AUC infinity predicted using CL _{STP} instead of CL _{ST}
AUC _{IFPD}	AUC _{IFP} / Dose
AUC _{PEO}	AUC % extrapolation observed
AUC _{PEP}	AUC % extrapolated for AUC _{IFP}
AUC _{PBEO}	AUC % back extrapolation observed, for bolus IV administration only
AUC _{PBEP}	AUC % back extrapolation predicted with AUC _{IFP} , for bolus IV administration only
AUM _{CLST}	AUMC to the T _{LAST}
AUM _{CIFO}	AUMC infinity observed using CL _{ST}
AUM _{CIFP}	AUMC infinity determined by CL _{STP}
AUM _{CPEO}	AUMC % extrapolated observed
AUM _{CPEP}	AUMC % extrapolated predicted
MRT _{IVLST}	mean residence time (MRT) to T _{LAST} , for intravascular administration
MRT _{IVIFO}	mean residence time (MRT) infinity using CL _{ST} , for intravascular administration

MRTIVIFP	mean residence time (MRT) infinity using CLSTP, for intravascular administration
MRTEVLST	mean residence time (MRT) to TLST, for extravascular administration
MRTEVIFO	mean residence time (MRT) infinity using CLST, for extravascular administration
MRTEVIFP	mean residence time (MRT) infinity using CLSTP, for extravascular administration
VZO	volume of distribution determined by LAMZ and AUCIFO, for intravascular administration
VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZFO	VZO for extravascular administration, VZO/F , F is bioavailability
VZFP	VZP for extravascular administration, VZP/F , F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLFO	CLO for extravascular administration, CLO/F , F is bioavailability
CLFP	CLP for extravascular administration, CLP/F , F is bioavailability
VSSO	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at steady state using CLSTP, for intravascular administration only

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
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See Also

[SNCA](#)

Examples

```
# Theoph and Indometh data: dose in mg, conc in mg/L, time in h
NCA(Theoph, "Subject", "Time", "conc", dose=320, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", uConc="mg/L")

iAUC = data.frame(Name=c("AUC[0-12h]", "AUC[0-24h]"), Start=c(0,0), End=c(12,24)) ; iAUC
NCA(Theoph, "Subject", "Time", "conc", dose=320, iAUC=iAUC, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", iAUC=iAUC, uConc="mg/L")

# writeLines(NCA(Theoph, "Subject", "Time", "conc", dose=320, report="Text", uConc="mg/L"),
#             "Theoph_Linear_CoreOutput.txt")
# writeLines(NCA(Theoph, "Subject", "Time", "conc", dose=320, fit="Log", report="Text",
#             uConc="mg/L"), "Theoph_Log_CoreOutput.txt")
# writeLines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", report="Text",
#             uConc="mg/L"), "Indometh_Bolus_Linear_CoreOutput.txt")
# writeLines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", fit="Log",
#             report="Text", uConc="mg/L"), "Indometh_Bolus_Log_CoreOutput.txt")
# writeLines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
#             report="Text", uConc="mg/L"), "Indometh_Infusion_Linear_CoreOutput.txt")
# writeLines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
#             fit="Log", report="Text", uConc="mg/L"), "Indometh_Infusion_Log_CoreOutput.txt")
```

NCA0

NCA of SDTM data for single subject

Description

This performs Noncompartmental Analysis(NCA) for only one subject from the CDISC EX and PC domain.

Usage

```
NCA0(EX0, PC0, fit="Linear")
```

Arguments

EX0	Data of one subject from EX domain
PC0	Data of one subject from PC domain
fit	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC

Details

This calls IndiNCA function. This is called by rNCA function.

Value

This returns NCA results vector.

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [rNCA](#), [sNCA](#)

pdfNCA

NCA output to pdf file

Description

This output NCA result in a pdf file.

Usage

```
pdfNCA(fileName = "Temp-NCA.pdf", concData, colSubj = "Subject", colTime = "Time",  
        colConc = "conc", dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg",  
        timeUnit = "h", concUnit = "ug/L", down="Linear", MW = 0)
```

Arguments

fileName	file name to save
concData	concentration data table
colSubj	column name for subject ID
colTime	column name for time
colConc	column name for concentration
dose	administered dose
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion
doseUnit	unit of dose
timeUnit	unit of time
concUnit	unit of concentration
down	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
MW	molecular weight of drug

Value

C _{MAX}	maximum concentration, C _{max}
C _{MAXD}	dose normalized C _{max} , C _{MAX} / Dose, C _{max} / Dose
T _{MAX}	time of maximum concentration, T _{max}
T _{LAG}	time to observe the first non-zero concentration, for extravascular administration only
CL _{ST}	last positive concentration observed, C _{last}
CL _{STP}	last positive concentration predicted, C _{last_pred}
T _{LAST}	time of last positive concentration, T _{last}
LAM _{ZHL}	half-life by lambda z, ln(2)/LAM _Z
LAM _Z	lambda_z negative of best fit terminal slope
LAM _{ZLL}	earliest time for LAM _Z
LAM _{ZUL}	last time for LAM _Z
LAM _{ZNPT}	number of points for LAM _Z
COR _{RXY}	correlation of log(concentration) and time
R ²	R-squared
R ² _{ADJ}	R-squared adjusted
C ₀	back extrapolated concentration at time 0, for bolus intravascular administration only
AUC _{CLST}	AUC from 0 to T _{LAST}
AUC _{ALL}	AUC using all the given points, including trailing zero concentrations
AUC _{IFO}	AUC infinity observed
AUC _{IFOD}	AUC _{IFO} / Dose
AUC _{IFP}	AUC infinity predicted using CL _{STP} instead of CL _{ST}
AUC _{IFPD}	AUC _{IFP} / Dose
AUC _{PEO}	AUC % extrapolation observed
AUC _{PEP}	AUC % extrapolated for AUC _{IFP}
AUC _{PBEO}	AUC % back extrapolation observed, for bolus IV administration only
AUC _{PBEP}	AUC % back extrapolation predicted with AUC _{IFP} , for bolus IV administration only
AUM _{CLST}	AUMC to the T _{LAST}
AUM _{CIFO}	AUMC infinity observed using CL _{ST}
AUM _{CIFP}	AUMC infinity determined by CL _{STP}
AUM _{CPEO}	AUMC % extrapolated observed
AUM _{CPEP}	AUMC % extrapolated predicted
MRT _{IVLST}	mean residence time (MRT) to T _{LAST} , for intravascular administration
MRT _{IVIFO}	mean residence time (MRT) infinity using CL _{ST} , for intravascular administration

MRTIVIFP	mean residence time (MRT) infinity using CLSTP, for intravascular administration
MRTEVLST	mean residence time (MRT) to TLST, for extravascular administration
MRTEVIFO	mean residence time (MRT) infinity using CLST, for extravascular administration
MRTEVIFP	mean residence time (MRT) infinity using CLSTP, for extravascular administration
VZO	volume of distribution determined by LAMZ and AUCIFO, for intravascular administration
VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZFO	VZO for extravascular administration, VZO/F, F is bioavailability
VZFP	VZP for extravascular administration, VZP/F, F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLFO	CLO for extravascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSSO	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at steady state using CLSTP, for intravascular administration only

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [txtNCA](#), [rtfNCA](#)

Examples

```
#pdfNCA(fileName="NCA-Theoph.pdf", Theoph, colSubj="Subject", colTime="Time",
#      colConc="conc", dose=320, doseUnit="mg", timeUnit="h", concUnit="mg/L")
#pdfNCA(fileName="NCA-Indometh.pdf", Indometh, colSubj="Subject", colTime="time",
#      colConc="conc", adm="Infusion", dur=0.5, dose=25, doseUnit="mg",
#      timeUnit="h", concUnit="mg/L")
```

plotFit	<i>Plot best fit slope</i>
---------	----------------------------

Description

Automatically select best fit slope for the given x(usually time) and log(y)(usually concentration) values.

Usage

```
plotFit(concData, id, Time, conc, mol = "", adm = "Extravascular", ID = "", Mol = "")
```

Arguments

concData	name of data table containing time-concentration data of multiple subjects
id	column name for subject ID
Time	column name for the time
conc	column name for the concentration
mol	column name for molecular species
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
ID	Subject ID for this plot
Mol	the name of molecular species to see

Details

Find the best fit slope then plot it. Currently this function uses ordinary least square method(OLS) only. This function calls BestSlope function.

Value

R2	R-squared
R2ADJ	adjusted R-squared
LAMZNPT	number of points used for slope
LAMZ	negative of slope, lambda_z
b0	intercept of regression line
CORRXY	correlation of log(y) and x
LAMZLL	earliest x for lambda_z
LAMZUL	last x for lambda_z
CLSTP	predicted y value at last point, predicted concentration for the last time point

Author(s)

Jee Eun Lee <JeeEun.Lee@fda.hhs.gov>

See Also[BestSlope](#)**Examples**

```
plotFit(Theoph, "Subject", "Time", "conc", ID="1")
plotFit(Indometh, "Subject", "time", "conc", adm="Bolus", ID="1")
```

plotPK

*Plot concentration vs. time curve for individuals and collectively.***Description**

Generates individual and superposed concentration vs. time curve and save it in pdf files.

Usage

```
plotPK(concData, id, Time, conc, unitTime = "hr", unitConc = "ng/mL", trt = "",
       fit = "Linear", dose = 0, adm = "Extravascular", dur = 0, outdir = "Output")
```

Arguments

concData	name of data table containing time-concentration data of multiple subjects
id	column name for subject ID
Time	column name for the time
conc	column name for the concentration
unitTime	unit for the time
unitConc	unit for the concentration
trt	column name for the treatment code. This is useful for crossover study like bioequivalence trial.
fit	one of "Linear" or "Log" to indicate the way to calculate AUC
dose	administered dose. One should be careful for the unit. This can be a vector containing dose for each subject in order.
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	infusion duration for constant infusion, otherwise 0. This can be a vector containing values for each subject in order.
outdir	name of the folder to be used for the output files

Details

This function generates plots for individual and summary concentration vs. time curve. This function calls `NCA()`.

Value

This function saves pdf files and tiff files in the outdir folder.

Author(s)

Jee Eun Lee <JeeEun.Lee@fda.hhs.gov>

See Also

[NCA](#)

Examples

```
# plotPK(Theoph, "Subject", "Time", "conc", unitTime="hr", unitConc="mg/L", dose=320)
# plotPK(Indometh, "Subject", "time", "conc", unitTime="hr", unitConc="mg/L", adm="Bolus", dose=25)
```

readEX

Read EX domain files

Description

This reads EX domain files from the specified folders.

Usage

```
readEX(folders)
```

Arguments

folders folders where to find EX domain files

Details

This calls combXPT function. This is called by loadEXPC function.

Value

This returns combined table of EX domain.

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [combXPT](#), [loadEXPC](#)

readPC	<i>Read PC domain files</i>
--------	-----------------------------

Description

This reads PC domain files from the specified folders.

Usage

```
readPC(folders)
```

Arguments

folders folders where to find PC domain files

Details

This calls combXPT function. This is called by loadEXPC function.

Value

This returns combined table of PC domain.

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [combXPT](#), [loadEXPC](#)

rNCA	<i>Do NCA for review</i>
------	--------------------------

Description

This performs NCA from the CDISC EX and PC datasets.

Usage

```
rNCA(ex, pc, study = "", trt = "", id = "", analyte = "",
      codeBQL = c("< 0", "<0", "NQ", "BLQ", "BQL", "BQoL", "<LOQ"),
      fit="Linear", MinPoints = 5)
```

Arguments

ex	EX domain data, usually from the loadEXPC
pc	PC domain data, usually from the loadEXPC
study	vector of study names in EX and PC domain to do NCA
trt	vector of treatment names in EXTRT to do NCA
id	vector of subject IDs in USUBJID to do NCA
analyte	vector of molecular species in PCTESTCD to do NCA
codeBQL	symbols of below the quantitation limit
fit	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
MinPoints	minimum number of sampling points for NCA

Details

This calls NCA0. Results of this can be further processed by foreNCA to plot and compare between studies and dose groups.

Value

This returns a table of NCA results

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [NCA0](#), [loadEXPC](#), [foreNCA](#)

Round

Round Half Away from Zero

Description

This is an ordinary rounding function, so called round half away from zero

Usage

```
Round(x, n = 0)
```

Arguments

x	numeric to be rounded
n	indicating decimal digits

Details

The function round in R base rounds to the even number, i.e. round(0.5) is 0 not 1. If you want rounding 0.5 be 1, you can use this Round function. This function is for the consistency with other software like MS-Excel, SAS.

Value

ordinarily rounded value

Author(s)

Kyun-Seop Bae <k@acr.kr>

References

See wikipedia subject "Rounding"

Examples

```
(x = 1:10 - 0.5)
Round(x)
round(x) # compare with the above
```

RptCfg

NCA Report Configuration Table

Description

Contains the names and order of column of return table/text by IndiNCA and NCA functions

Usage

RptCfg

Format

A data frame with 48 observations on the following 10 variables.

PPTESTCD a character vector of CDISC SDTM PPTESTCD

SYNONYM a character vector of CDISC SDTM PPTESTCD Synonym

NCI a character vector of NCI preferred terms

WNL a character vector of WinNonlin(R) software variables

ExtravascularDefault a numeric vector of ordering in report for extravascular administration, Zero means exclusion in the report.

ExtravascularWNL a numeric vector of WinNonlin(R) style ordering in report for extravascular administration, Zero means exclusion in the report.

BolusDefault a numeric vector of ordering in report for extravascular administration, Zero means exclusion in the report.

BolusWNL a numeric vector of WinNonlin(R) style ordering in report for extravascular administration, Zero means exclusion in the report.

InfusionDefault a numeric vector of ordering in report for extravascular administration, Zero means exclusion in the report.

InfusionWNL a numeric vector of WinNonlin(R) style ordering in report for extravascular administration, Zero means exclusion in the report.

Details

This table should exist in pkr package. User can edit this table for shaping the report in one's own style.

rtfNCA	<i>NCA output to rtf file</i>
--------	-------------------------------

Description

This output NCA result in a rtf file.

Usage

```
rtfNCA(fileName = "Temp-NCA.rtf", concData, colSubj = "Subject", colTime = "Time",
  colConc = "conc", dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg",
  timeUnit = "h", concUnit = "ug/L", down="Linear", MW = 0)
```

Arguments

fileName	file name to save
concData	concentration data table
colSubj	column name for subject ID
colTime	column name for time
colConc	column name for concentration
dose	administered dose
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion
doseUnit	unit of dose
timeUnit	unit of time
concUnit	unit of concentration
down	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
MW	molecular weight of drug

Value

C _{MAX}	maximum concentration, C _{max}
C _{MAXD}	dose normalized C _{max} , C _{MAX} / Dose, C _{max} / Dose
T _{MAX}	time of maximum concentration, T _{max}
T _{LAG}	time to observe the first non-zero concentration, for extravascular administration only
CL _{ST}	last positive concentration observed, C _{last}
CL _{STP}	last positive concentration predicted, C _{last_pred}
T _{LST}	time of last positive concentration, T _{last}
LAM _{ZHL}	half-life by lambda z, $\ln(2)/\text{LAMZ}$
LAM _Z	lambda_z negative of best fit terminal slope
LAM _{ZLL}	earliest time for LAMZ
LAM _{ZUL}	last time for LAMZ
LAM _{ZNPT}	number of points for LAMZ
COR _{RXY}	correlation of log(concentration) and time
R ₂	R-squared
R _{2ADJ}	R-squared adjusted
C ₀	back extrapolated concentration at time 0, for bolus intravascular administration only
AU _{CLST}	AUC from 0 to T _{LST}
AU _{CALL}	AUC using all the given points, including trailing zero concentrations
AU _{CIFO}	AUC infinity observed
AU _{CIFOD}	AU _{CIFO} / Dose
AU _{CIFP}	AUC infinity predicted using CL _{STP} instead of CL _{ST}
AU _{CIFPD}	AU _{CIFP} / Dose
AU _{CPEO}	AUC % extrapolation observed
AU _{CPEP}	AUC % extrapolated for AU _{CIFP}
AU _{CPBEO}	AUC % back extrapolation observed, for bolus IV administration only
AU _{CPBEP}	AUC % back extrapolation predicted with AU _{CIFP} , for bolus IV administration only
AU _{MCLST}	AUMC to the T _{LST}
AU _{MCIFO}	AUMC infinity observed using CL _{ST}
AU _{MCIFP}	AUMC infinity determined by CL _{STP}
AU _{MCPEO}	AUMC % extrapolated observed
AU _{MCPEP}	AUMC % extrapolated predicted
MRT _{IVLST}	mean residence time (MRT) to T _{LST} , for intravascular administration
MRT _{IVIFO}	mean residence time (MRT) infinity using CL _{ST} , for intravascular administration

MRTIVIFP	mean residence time (MRT) infinity using CLSTP, for intravascular administration
MRTEVLST	mean residence time (MRT) to TLST, for extravascular administration
MRTEVIFO	mean residence time (MRT) infinity using CLST, for extravascular administration
MRTEVIFP	mean residence time (MRT) infinity using CLSTP, for extravascular administration
VZO	volume of distribution determined by LAMZ and AUCIFO, for intravascular administration
VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZFO	VZO for extravascular administration, VZO/F, F is bioavailability
VZFP	VZP for extravascular administration, VZP/F, F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLFO	CLO for extravascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSSO	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at steady state using CLSTP, for intravascular administration only

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[help](#), [txtNCA](#), [pdfNCA](#)

Examples

```
#rtfNCA(fileName="NCA-Theoph.rtf", Theoph, colSubj="Subject", colTime="Time",
#      colConc="conc", dose=320, doseUnit="mg", timeUnit="h", concUnit="mg/L")
#rtfNCA(fileName="NCA-Indometh.rtf", Indometh, colSubj="Subject", colTime="time",
#      colConc="conc", adm="Infusion", dur=0.5, dose=25, doseUnit="mg",
#      timeUnit="h", concUnit="mg/L")
```

Slope

Get the Slope of regression $\log(y) \sim x$ **Description**

It calculates the slope with linear regression of $\log(y) \sim x$

Usage

```
Slope(x, y)
```

Arguments

x	vector values of independent variable, usually time
y	vector values of dependent variable, usually concentration

Details

With time-concentration curve, you frequently need to estimate slope in $\log(\text{concentration}) \sim \text{time}$. This function is usually called by BestSlope function and you seldom need to call this function directly.

Value

R2	R-squared
R2ADJ	adjusted R-squared
LAMZNPT	number of points used for slope
LAMZ	negative of slope, λ_z
b0	intercept of regression line
CORRXY	correlation of $\log(y)$ and x
LAMZLL	earliest x for λ_z
LAMZUL	last x for λ_z
CLSTP	predicted y value at last point, predicted concentration for the last time point

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[BestSlope](#)

Examples

```
Slope(Indometh[Indometh$Subject==1, "time"], Indometh[Indometh$Subject==1, "conc"])
```

sNCA	<i>Simplest NCA</i>
------	---------------------

Description

This is the work-horse function for NCA.

Usage

```
sNCA(x, y, dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h",
     concUnit = "ug/L", iAUC = "", down = "Linear", MW = 0, returnNA = TRUE)
```

Arguments

x	usually time
y	usually concentration
dose	given amount
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion
doseUnit	unit of dose
timeUnit	unit of time
concUnit	unit of concentration
iAUC	interval AUCs to calculate
down	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
MW	molecular weight of the drug
returnNA	if returnNA is TRUE, it returns NA values also.

Details

This will replace IndiNCA.

Value

C _{MAX}	maximum concentration, C _{max}
C _{MAXD}	dose normalized C _{max} , C _{MAX} / Dose, C _{max} / Dose
T _{MAX}	time of maximum concentration, T _{max}
T _{LAG}	time to observe the first non-zero concentration, for extravascular administration only
C _{LST}	last positive concentration observed, C _{last}
C _{LSTP}	last positive concentration predicted, C _{last_pred}
T _{LST}	time of last positive concentration, T _{last}

LAMZHL	half-life by lambda z, $\ln(2)/\text{LAMZ}$
LAMZ	lambda_z negative of best fit terminal slope
LAMZLL	earliest time for LAMZ
LAMZUL	last time for LAMZ
LAMZNPT	number of points for LAMZ
CORRXY	correlation of log(concentration) and time
R2	R-squared
R2ADJ	R-squared adjusted
C0	back extrapolated concentration at time 0, for bolus intravascular administration only
AUCLST	AUC from 0 to TLST
AUCALL	AUC using all the given points, including trailing zero concentrations
AUCIFO	AUC infinity observed
AUCIFOD	AUCIFO / Dose
AUCIFP	AUC infinity predicted using CLSTP instead of CLST
AUCIFPD	AUCIFP / Dose
AUCPEO	AUC % extrapolation observed
AUCPEP	AUC % extrapolated for AUCIFP
AUCPBEO	AUC % back extrapolation observed, for bolus IV administration only
AUCPBEP	AUC % back extrapolation predicted with AUCIFP, for bolus IV administration only
AUMCLST	AUMC to the TLST
AUMCIFO	AUMC infinity observed using CLST
AUMCIFP	AUMC infinity determined by CLSTP
AUMCPEO	AUMC % extrapolated observed
AUMCPEP	AUMC % extrapolated predicted
MRTIVLST	mean residence time (MRT) to TLST, for intravascular administration
MRTIVIFO	mean residence time (MRT) infinity using CLST, for intravascular administration
MRTIVIFP	mean residence time (MRT) infinity using CLSTP, for intravascular administration
MRTEVLST	mean residence time (MRT) to TLST, for extravascular administration
MRTEVIFO	mean residence time (MRT) infinity using CLST, for extravascular administration
MRTEVIFP	mean residence time (MRT) infinity using CLSTP, for extravascular administration
VZ0	volume of distribution determined by LAMZ and AUCIFO, for intravascular administration

VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZFO	VZO for extravascular administration, VZO/F, F is bioavailability
VZFP	VZP for extravascular administration, VZP/F, F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLFO	CLO for extravascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSSO	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at steady state using CLSTP, for intravascular administration only

Author(s)

Kyun-Seop Bae <k@acr.kr>

References

Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.

See Also

[help](#), [tblNCA](#)

Examples

```
# For one subject
x = Theoph[Theoph$Subject=="1", "Time"]
y = Theoph[Theoph$Subject=="1", "conc"]

sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h")
sNCA(x, y, dose=320, concUnit="mg/L", returnNA=FALSE)

iAUC = data.frame(Name=c("AUC[0-12h]", "AUC[0-24h]"), Start=c(0,0), End=c(12,24))
sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h", iAUC=iAUC)

MW = 180.164 # Molecular weight of theophylline

sNCA(x, y/MW, dose=320, doseUnit="mg", concUnit="mmol/L", timeUnit="h")
sNCA(x, y/MW, dose=320, doseUnit="mg", concUnit="mmol/L", timeUnit="h", MW=MW)
sNCA(x, y, dose=320/MW, doseUnit="mmol", concUnit="mg/L", timeUnit="h", MW=MW)
sNCA(x, y/MW, dose=320/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW)

sNCA(x, y/MW, dose=320/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW,
      returnNA=FALSE)
sNCA(x, y/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW, returnNA=FALSE)
sNCA(x, y/MW, dose=as.numeric(NA), doseUnit="mmol", concUnit="mmol/L", timeUnit="h",
```

```

MW=MW, returnNA=FALSE)

sNCA(x, y, dose=320, concUnit="mg/L", timeUnit="hr")
sNCA(x*60, y, dose=320, concUnit="mg/L", timeUnit="min")

```

tblNCA

Table output NCA

Description

do multiple NCA and returns a result table.

Usage

```
tblNCA(concData, key = "Subject", colTime = "Time", colConc = "conc", dose = 0,
      adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h",
      concUnit = "ug/L", down = "Linear", MW = 0, returnNA = FALSE)
```

Arguments

concData	concentration data table
key	column names of concData to be shown at the output table
colTime	column name for time
colConc	column name for concentration
dose	administered dose
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion
doseUnit	unit of dose
timeUnit	unit of time
concUnit	unit of concentration
down	method to calculate AUC, "Linear" or "Log"
MW	molecular weight of drug
returnNA	if returnNA is TRUE, it returns NA values also.

Value

Basically same with [sNCA](#)

Author(s)

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See Also[help](#), [sNCA](#)**Examples**

```
tblNCA(Theoph, key="Subject", dose=320, concUnit="mg/L")
tblNCA(Indometh, key="Subject", colTime="time", colConc="conc", dose=25,
      adm="Infusion", dur=0.5, concUnit="mg/L")
```

txtNCA	<i>Text output of NCA for one subject</i>
--------	---

Description

This is the text form output.

Usage

```
txtNCA(x, y, dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h",
      concUnit = "ug/L", iAUC = "", down="Linear", MW = 0, returnNA = FALSE)
```

Arguments

x	usually time
y	usually concentration
dose	given amount
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion
doseUnit	unit of dose
timeUnit	unit of time
concUnit	unit of concentration
iAUC	interval AUCs to calculate
down	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
MW	molecular weight of the drug
returnNA	if returnNA is TRUE, it returns NA values also.

Value

C _{MAX}	maximum concentration, C _{max}
C _{MAXD}	dose normalized C _{max} , C _{MAX} / Dose, C _{max} / Dose
T _{MAX}	time of maximum concentration, T _{max}
T _{LAG}	time to observe the first non-zero concentration, for extravascular administration only
CL _{ST}	last positive concentration observed, C _{last}
CL _{STP}	last positive concentration predicted, C _{last_pred}
T _{LST}	time of last positive concentration, T _{last}
LAM _{ZHL}	half-life by lambda z, ln(2)/LAM _Z
LAM _Z	lambda_z negative of best fit terminal slope
LAM _{ZLL}	earliest time for LAM _Z
LAM _{ZUL}	last time for LAM _Z
LAM _{ZNPT}	number of points for LAM _Z
COR _{RXY}	correlation of log(concentration) and time
R ²	R-squared
R ² _{ADJ}	R-squared adjusted
C ₀	back extrapolated concentration at time 0, for bolus intravascular administration only
AUC _{CLST}	AUC from 0 to T _{LST}
AUC _{ALL}	AUC using all the given points, including trailing zero concentrations
AUC _{IFO}	AUC infinity observed
AUC _{IFOD}	AUC _{IFO} / Dose
AUC _{IFP}	AUC infinity predicted using CL _{STP} instead of CL _{ST}
AUC _{IFPD}	AUC _{IFP} / Dose
AUC _{PEO}	AUC % extrapolation observed
AUC _{PEP}	AUC % extrapolated for AUC _{IFP}
AUC _{PBEO}	AUC % back extrapolation observed, for bolus IV administration only
AUC _{PBEP}	AUC % back extrapolation predicted with AUC _{IFP} , for bolus IV administration only
AUM _{CLST}	AUMC to the T _{LST}
AUM _{CIFO}	AUMC infinity observed using CL _{ST}
AUM _{CIFP}	AUMC infinity determined by CL _{STP}
AUM _{CPEO}	AUMC % extrapolated observed
AUM _{CPEP}	AUMC % extrapolated predicted
MRT _{IVLST}	mean residence time (MRT) to T _{LST} , for intravascular administration
MRT _{IVIFO}	mean residence time (MRT) infinity using CL _{ST} , for intravascular administration

MRTIVIFP	mean residence time (MRT) infinity using CLSTP, for intravascular administration
MRTEVLST	mean residence time (MRT) to TLST, for extravascular administration
MRTEVIFO	mean residence time (MRT) infinity using CLST, for extravascular administration
MRTEVIFP	mean residence time (MRT) infinity using CLSTP, for extravascular administration
VZO	volume of distribution determined by LAMZ and AUCIFO, for intravascular administration
VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZFO	VZO for extravascular administration, VZO/F, F is bioavailability
VZFP	VZP for extravascular administration, VZP/F, F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLFO	CLO for extravascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSSO	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at steady state using CLSTP, for intravascular administration only

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See Also

[help](#), [pdfNCA](#), [rtfNCA](#)

Examples

```
# For one subject
txtNCA(Theoph[Theoph$Subject=="1", "Time"], Theoph[Theoph$Subject=="1", "conc"],
       dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h")

# or equivalently
x = Theoph[Theoph$Subject=="1", "Time"]
y = Theoph[Theoph$Subject=="1", "conc"]
txtNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h")

# For all subjects
IDs = sort(as.numeric(unique(Theoph[, "Subject"])))
nID = length(IDs)
Res = vector()
for (i in 1:nID) {
```

```

tRes = txtNCA(Theoph[Theoph[, "Subject"]==IDs[i], "Time"],
              Theoph[Theoph[, "Subject"]==IDs[i], "conc"],
              dose=320, concUnit="mg/L", returnNA=FALSE)
tRes = c(paste("ID =", IDs[i]), tRes, "")
Res = c(Res, tRes)
}
Res

```

Unit

*Disply CDISC standard units and multiplied factor of NCA results***Description**

It displays CDISC PP output units and multiplication factor for them.

Usage

```
Unit(code = "", timeUnit = "h", concUnit = "ng/mL", doseUnit = "mg", MW = 0)
```

Arguments

code	vector of PPTESTCD
timeUnit	unit of time
concUnit	unit of concentration
doseUnit	unit of dose
MW	molecular weight of drug

Value

row names	PPTESTCD
Unit	unit
Factor	internal mulitpilcation factor

Author(s)

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Examples

```

Unit(concUnit="ug/L", doseUnit="mg")
Unit(concUnit="ng/L", doseUnit="mg")

Unit(concUnit="umol/L", doseUnit="mmol")
Unit(concUnit="nmol/L", doseUnit="mmol")

Unit(concUnit="mmol/L", doseUnit="mg", MW=500)
Unit(concUnit="umol/L", doseUnit="mg", MW=500)

```



```
Unit(concUnit="nmol/L", doseUnit="mg", MW=500)  
Unit(concUnit="nmol/mL", doseUnit="mg", MW=500)
```

```
Unit(concUnit="ug/L", doseUnit="mmol", MW=500)  
Unit(concUnit="ug/L", doseUnit="mol", MW=500)  
Unit(concUnit="ng/L", doseUnit="mmol", MW=500)  
Unit(concUnit="ng/mL", doseUnit="mmol", MW=500)
```

```
Unit(concUnit="nmol/L", doseUnit="mg")  
Unit(concUnit="ug/L", doseUnit="mmol")
```

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