

Package ‘NonCompart’

January 20, 2017

Version 0.2.7

Date 2017-01-20

Title Noncompartmental Analysis for Pharmacokinetic Data

Description Conduct a noncompartmental analysis as closely as possible to the most widely used commercial software for pharmacokinetic analysis, i.e. 'Phoenix(R) WinNonlin(R)' <<https://www.certara.com/software/pkpd-modeling-and-simulation/phoenix-winnonlin/>>.

Some features include:

- 1) Use CDISC SDTM PP domain terms.
- 2) Automatic slope selection with the same criterion of WinNonlin(R)
- 3) Support both 'linear-up linear-down' and 'linear-up log-down' method
- 4) Calculate partial(interval) AUC with 'linear' or 'log' interpolation method
- 5) Perform a noncompartmental analysis of CDISC standardized pharmacokinetic dataset (.XPT)

For more details on noncompartmental analysis, see the reference: Gabrielson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016. (ISBN:9198299107)

*) Acknowledgement: Author thanks for the careful review and valuable input of Dr. Jee Eun Lee.

Depends R (>= 2.0.0)

Author Kyun-Seop Bae

Maintainer Kyun-Seop Bae <k@acr.kr>

Copyright 2016, Kyun-Seop Bae

License GPL-3

NeedsCompilation no

LazyLoad yes

Repository CRAN

URL <https://cran.r-project.org/package=NonCompart>

Date/Publication 2017-01-01 10:08:58

RoxygenNote 5.0.1

R topics documented:

NonCompart-package	2
AUC	3
BestSlope	4
IndiNCA	5
IntAUC	8

Interpol	9
LinAUC	10
LogAUC	11
NCA	12
Round	15
RptCfg	16
runCDISC	17
Slope	17
Index	19

NonCompart-package	<i>Noncompartmental Analysis for Pharmacokinetic Data</i>
--------------------	---

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.

Acknowledgement

Author thanks for the careful review and valuable input of Dr. Jee Eun Lee.

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.

Examples

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

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)
NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Bolus", iAUC=iAUC)

writeLines(NCA(Theoph, "Subject", "Time", "conc", Dose=320, Report="Text"),
           "Theoph_Linear_CoreOutput.txt")
writeLines(NCA(Theoph, "Subject", "Time", "conc", Dose=320, Method="Log", Report="Text"),
           "Theoph_Log_CoreOutput.txt")
writeLines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Bolus", Report="Text"),
           "Indometh_Bolus_Linear_CoreOutput.txt")
writeLines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Bolus", Method="Log",
               Report="Text"), "Indometh_Bolus_Log_CoreOutput.txt")
writeLines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Infusion", TimeInfusion=0.25,
               Report="Text"), "Indometh_Infusion_Linear_CoreOutput.txt")
writeLines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Infusion", TimeInfusion=0.25,
               Method="Log", Report="Text"), "Indometh_Infusion_Log_CoreOutput.txt")

IndiNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], Dose=320)
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Bolus")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Infusion", TimeInfusion=0.25)

IndiNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], Dose=320,
        Report="Text")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Bolus", Report="Text")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Infusion", TimeInfusion=0.25, Report="Text")

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)
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Bolus", iAUC=iAUC)
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Infusion", TimeInfusion=0.25, iAUC=iAUC)
```

AUC

Calculate Area Under the Curve (AUC) and Area Under the first Moment Curve (AUMC) in a table format

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, Method = "Linear")
```

Arguments

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

Details

Method="Linear" means linear trapezoidal rule with linear interpolation. Method="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)

Kyun-Seop Bae <k@acr.kr>

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"]) # Default is "Linear"
AUC(Theoph[Theoph$Subject==1, "Time"],Theoph[Theoph$Subject==1, "conc"], Method="Log")
```

BestSlope

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

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, AdmMode = "Extravascular")
```

Arguments

x	vector values of x-axis, usually time
y	vector values of y-axis, usually concentration
AdmMode	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode

Details

Choosing the best terminal slope (y in log scale) in pharmacokinetic analysis is somewhat challenging, and it could vary by analysis performer. Currently this function uses ordinary least square method(OLS) only.

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)

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"],
          AdmMode="Bolus")
```

IndiNCA

Noncompartmental Analysis for an Individual

Description

It performs a noncompartmental analysis with one subject data

Usage

```
IndiNCA(x, y, Dose = 0, Method = "Linear", AdmMode = "Extravascular", TimeInfusion = 0,
        RetNames, Report = "Table", iAUC)
```

Arguments

x	vector values of independent variable, usually time
y	vector values of dependent variable, usually concentration
Dose	administered dose for the subject
Method	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
AdmMode	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
TimeInfusion	infusion duration for constant infusion, otherwise 0
RetNames	character vector for the pharmacokinetic parameter names to be returned
Report	either of "Table" or "Text" to specify the type of return value
iAUC	data.frame with three columns, "Name", "Start", "End" to specify the intervals for partial (interval) AUC

Details

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

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)/LAMZ
LAMZ	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
CORRXY	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 _{LST}	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}

AUCIFPD	AUCIFP / Dose
AUCPEO	AUC % extrapolation observed
AUCPEP	AUC % extrapolated for AUCIFP
AUCPBE0	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
VZO	volume of distribution determined by LAMZ and AUCIFO, for intravascular administration
VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZF0	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
CLF0	CLO for extravascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSS0	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

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)
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Bolus")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Infusion", TimeInfusion=0.25)

IndiNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], Dose=320,
        Report="Text")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Bolus", Report="Text")
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Infusion", TimeInfusion=0.25, Report="Text")

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)
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Bolus", iAUC=iAUC)
IndiNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1, "conc"], Dose=25,
        AdmMode="Infusion", TimeInfusion=0.25, iAUC=iAUC)
```

IntAUC	<i>Calculate interval AUC</i>
--------	-------------------------------

Description

It calculates interval AUC

Usage

```
IntAUC(x, y, t1, t2, Res, Method = "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
Method	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 Method.

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 = IndiNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"], Dose=320)
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, Method = "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
Method	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, Method="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)

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

[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
```

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)

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

[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"], Method="Log")
```

NCA

Noncompartmental analysis for a dataset with multiple subjects

Description

conduct noncompartmental analysis for many subjects in a data table

Usage

```
NCA(Data, colSubj, colTime, colConc, colTrt, Method = "Linear", Dose = 0,
     AdmMode = "Extravascular", TimeInfusion = 0, Report = "Table", iAUC)
```

Arguments

Data	name of data table containing time-concentration data of multiple subjects
colSubj	column name for subject ID
colTime	column name for the time
colConc	column name for the concentration
colTrt	column name for the treatment code. This is useful for crossover study like bioequivalence trial.
Method	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.
AdmMode	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
TimeInfusion	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

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 _{LST}	time of last positive concentration, T _{last}
LAM _{ZHL}	half-life by lambda z, ln(2)/LAMZ
LAMZ	lambda_z negative of best fit terminal slope
LAMZ _{LL}	earliest time for LAMZ
LAMZ _{UL}	last time for LAMZ
LAMZ _{NPT}	number of points for LAMZ
CORRXY	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 _{LST}	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 _{LST}	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

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

[IndiNCA](#)

Examples

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

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)
NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Bolus", iAUC=iAUC)
```

```
writelines(NCA(Theoph, "Subject", "Time", "conc", Dose=320, Report="Text"),
            "Theoph_Linear_CoreOutput.txt")
writelines(NCA(Theoph, "Subject", "Time", "conc", Dose=320, Method="Log", Report="Text"),
            "Theoph_Log_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Bolus", Report="Text"),
            "Indometh_Bolus_Linear_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Bolus", Method="Log",
            Report="Text"), "Indometh_Bolus_Log_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Infusion", TimeInfusion=0.25,
            Report="Text"), "Indometh_Infusion_Linear_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", Dose=25, AdmMode="Infusion", TimeInfusion=0.25,
            Method="Log", Report="Text"), "Indometh_Infusion_Log_CoreOutput.txt")
```

Round	<i>Round Half Away from Zero</i>
-------	----------------------------------

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	<i>NCA Report Configuration Table</i>
--------	---------------------------------------

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 NonCompart package. User can edit this table for shaping the report in one's own style.

runCDISC

*Conduct a noncompartmental analysis with CDISC dataset***Description**

runCDISC uses NonCompart package to perform a noncompartmental analysis of CDISC standardized pharmacokinetic dataset.

Usage

```
runCDISC(wd = getwd(), filenameDM = "DM", filenameEX = "EX",
         filenamePC = "PC", extension = ".xpt", incl_arm = NULL)
```

Arguments

wd	Working directory of CDISC dataset, containing DM, EX and PC
filenameDM	A filename of DM domain. Usually DM or dm
filenameEX	A filename of EX domain. Usually EX or ex
filenamePC	A filename of PC domain. Usually PC or pc
extension	file extension, currently supporting only .xpt
incl_arm	Vector of study arms of interest

Value

List of output data of noncompartmental analysis

Examples

```
#Currently there is no publicly open CDISC dataset for presenting an example.
```

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"])
```

Index

- *Topic **AUC**
 - AUC, [3](#)
 - IntAUC, [8](#)
 - LinAUC, [10](#)
 - LogAUC, [11](#)
 - *Topic **AUMC**
 - AUC, [3](#)
 - *Topic **NCA**
 - IndiNCA, [5](#)
 - NCA, [12](#)
 - NonCompart-package, [2](#)
 - *Topic **Slope**
 - BestSlope, [4](#)
 - *Topic **best fit slope**
 - BestSlope, [4](#)
 - *Topic **datasets**
 - RptCfg, [16](#)
 - *Topic **interpolation**
 - Interpol, [9](#)
 - *Topic **interval AUC**
 - IntAUC, [8](#)
 - Interpol, [9](#)
 - *Topic **noncompartmenal analysis**
 - IndiNCA, [5](#)
 - *Topic **package**
 - NonCompart-package, [2](#)
 - *Topic **partial AUC**
 - IntAUC, [8](#)
 - Interpol, [9](#)
 - *Topic **rounding**
 - Round, [15](#)
 - *Topic **round**
 - Round, [15](#)
 - *Topic **slope**
 - Slope, [17](#)
- AUC, [3](#), [8](#), [9](#), [11](#), [12](#)
- BestSlope, [4](#), [8](#), [18](#)
- IndiNCA, [5](#), [14](#)
- IntAUC, [8](#), [10](#)
- Interpol, [9](#), [9](#)
- LinAUC, [4](#), [10](#), [12](#)
- LogAUC, [4](#), [11](#), [11](#)
- NCA, [12](#)
- NonCompart (NonCompart-package), [2](#)
- NonCompart-package, [2](#)
- Round, [15](#)
- RptCfg, [16](#)
- runCDISC, [17](#)
- Slope, [5](#), [17](#)