# Package 'NonCompart'

January 20, 2017

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<b>Date</b> 2017-01-20
Title Noncompartmental Analysis for Pharmacokinetic Data
<ul> <li>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)' <a href="https://www.certara.com/software/pkpd-modeling-and-simulation/phoenix-winnonlin/">https://www.certara.com/software/pkpd-modeling-and-simulation/phoenix-winnonlin/</a>&gt;. Some features include: <ol> <li>Use CDISC SDTM PP domain terms.</li> <li>Automatic slope selection with the same criterion of WinNonlin(R)</li> <li>Support both 'linear-up linear-down' and 'linear-up log-down' method</li> <li>Calculate partial(interval) AUC with 'linear' or 'log' interpolation method</li> <li>Perform a noncompartmental analysis of CDISC standardized pharmacokinetic dataset (.XPT) For more details on noncompartmental analysis, see the reference: Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016. (ISBN:9198299107)</li> <li>Acknowledgement: Author thanks for the careful review and valuable input of Dr. Jee Eun Lee</li> </ol> </li> </ul>
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NonCompart-package

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NonCompart-package

Noncompartmental Analysis for Pharmacokinetic Data

#### **Description**

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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.

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#### **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")
```

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#### Arguments

			1. 1 .	11
X	vector values	of independent	variable.	usualiv 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 then 1e-4, it chooses longer slope.

## Usage

```
BestSlope(x, y, AdmMode = "Extravascular")
```

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#### 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 adminis-

tration 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**

IndiNCA

Noncompartmental Analysis for an Individual

## **Description**

It performs a noncompartmental analysis with one subject data

## Usage

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#### **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 adminis-

tration 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 invervals

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

CMAX maximum concentration, Cmax

CMAXD dose normalized Cmax, CMAX / Dose, Cmax / Dose

TMAX time of maximum concentration, Tmax

TLAG time to observe the first non-zero concentration, for extravascular administration

only

CLST last positive concentration observed, Clast

CLSTP last positive concentration predicted, Clast\_pred

TLST time of last positive concentration, Tlast

LAMZHL half-life by lambda z, ln(2)/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

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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
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
VSS0	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at stead 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.

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#### 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$Subject==1, "Time"], Theoph[Theoph$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

Calculate interval AUC

## **Description**

It calculates interval AUC

## Usage

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

#### **Arguments**

Х	vector values of independent variable, usually time
у	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.

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#### 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) \\ IntAUC(Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], Theoph[Theoph$Subject==1, "conc"], Theoph[Theoph$Subject==1, "t1=0.5, t2=11, Res], Theoph[Theoph$Subject==1, "t1=0.5
```

Interpol

Interpolate y value

#### **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
У	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.

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#### 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

Area Under the Curve(AUC) and Area Under the first Moment Curve(AUMC) by linear trapezoidal method

## **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>

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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
```

LogAUC

Area Under the Curve(AUC) and Area Under the first Moment Curve(AUMC) by linear-up log-down method

## **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>

NCA NCA

#### 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

## 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 $\parbox{\ensuremath{\square}}$
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 $\ensuremath{AUC}$

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## **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

nuc	
CMAX	maximum concentration, Cmax
CMAXD	dose normalized Cmax, CMAX / Dose, Cmax / Dose
TMAX	time of maximum concentration, Tmax
TLAG	time to observe the first non-zero concentration, for extravascular administration only
CLST	last positive concentration observed, Clast
CLSTP	last positive concentration predicted, Clast_pred
TLST	time of last positive concentration, Tlast
LAMZHL	half-life by lambda z, ln(2)/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
AUCPE0	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 administra-

tion

NCA NCA

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 $% \left( \frac{1}{2}\right) =\frac{1}{2}\left( \frac{1}{$
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
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 stead 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)
```

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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 roundedn 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
```

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RptCfg

NCA Report Configuation Table

## **Description**

Contains the names and order of colum 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 peferred 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 17

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**

```
    vector values of independent variable, usually time
    vector values of dependent variable, usually concentration
```

Slope

#### **Details**

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

## Value

R2	R-squared
114	it squareu

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

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#### See Also

BestSlope

## **Examples**

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

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