Package 'ncar'

July 16, 2021

Version 0.4.4	
Date 2021-07-16 KST	
Title Noncompartmental Analysis for Pharmacokinetic Report	
Description Conduct a noncompartmental analysis with industrial strength. Some features are 1) CDISC SDTM terms 2) Automatic or manual slope selection 3) Supporting both 'linear-up linear-down' and 'linear-up log-down' method 4) Interval(partial) AUCs with 'linear' or 'log' interpolation method 5) Produce pdf, rtf, text report files. * Reference: Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016. (ISBN:9198299107).	
Depends rtf, NonCompart ($\xi = 0.4.9$)	
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NeedsCompilation no	
LazyLoad yes	
Repository CRAN	
URL https://cran.r-project.org/package=ncar R topics documented:	
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Noncompartmental Analysis for Pharmacokinetic Report

Description

It can report a noncompartmental analysis (NCA) with industrial strength.

Details

```
pdfNCA to produce PDF file format NCA. rtfNCA to produce rtf file format NCA.
```

Author(s)

Kyun-Seop Bae ¡k@acr.kr;

The main functions are

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
# Output to PDF file
#pdfNCA(fileName="NCA-Theoph.pdf", Theoph, key="Subject", colTime="Time",
                        colConc="conc", dose=320, doseUnit="mg", timeUnit="h", concUnit="mg/L")
\verb| \#pdfNCA(fileName="NCA-Theoph.pdf", Theoph, key=c("Subject", "Wt"), colTime="Time", line of the color of 
                        #pdfNCA(fileName="NCA-Indometh.pdf", Indometh, key="Subject", colTime="time",
                        colConc="conc", adm="Infusion", dur=0.5, dose=25, doseUnit="mg",
                        timeUnit="h", concUnit="mg/L")
# Output to RTF file
#rtfNCA(fileName="NCA-Theoph.rtf", Theoph, key="Subject", colTime="Time",
                        colConc="conc", dose=320, doseUnit="mg", timeUnit="h", concUnit="mg/L")
#rtfNCA(fileName="NCA-Theoph.rtf", Theoph, key=c("Subject", "Wt"), colTime="Time",
# colConc="conc", dose=320, doseUnit="mg", timeUnit="h", concUnit="mg/L")
#rtfNCA(fileName="NCA-Indometh.rtf", Indometh, key="Subject", colTime="time",
                        colConc="conc", adm="Infusion", dur=0.5, dose=25, doseUnit="mg",
                        timeUnit="h", concUnit="mg/L")
```

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pdfNCA	NCA output to pdf file	

Description

This output NCA result in a pdf file.

Usage

```
pdfNCA(fileName = "Temp-NCA.pdf", concData, key = "Subject", colTime = "Time",
    colConc = "conc", dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg",
    timeUnit = "h", concUnit = "ug/L", down="Linear", R2ADJ = 0, MW = 0,
    iAUC = "", excludeDelta = 1)
```

Arguments

fileName file name to save

concData concentration data table

key column names of concData to be shown in 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 ad-

ministration 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

R2ADJ Minimum adjusted R-square value to determine terminal slope automat-

ically

MW molecular weight of drug

iAUC interval AUC information in a dataframe with "Name", "Start", and

"End" columns

excludeDelta Improvement of R2ADJ larger than this value could exclude the last point.

Default value 1 is for the compatibility with other software. Author rec-

ommends to use excludeDelta option with about 0.3.

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 admin-

istration only

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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

 $\begin{array}{ll} \mathsf{LAMZLL} & \text{earliest time for LAMZ} \\ \mathsf{LAMZUL} & \text{last time for LAMZ} \end{array}$

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 admin-

istration 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 admin-

istration 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 admin-

istration

MRTIVIFP mean residence time (MRT) infinity using CLSTP, for intravascular ad-

ministration

MRTEVLST mean residence time (MRT) to TLST, for extravascular administration mean residence time (MRT) infinity using CLST, for extravascular ad-

ministration

MRTEVIFP mean residence time (MRT) infinity using CLSTP, for extravascular ad-

ministration

VZO volume of distribution determined by LAMZ and AUCIFO, for intravas-

cular administration

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VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration $$
VZFO	VZO for extravascular administration, VZO/F, F is bioavailability
VZFP	VZP for extravascular administration, VZP/F, F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLFO	CLO for extra vascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSS0	volume of distribution at steady state using CLST, for intravascular administration only $$
VSSP	volume of distribution at stead state using CLSTP, for intravascular administration only

Author(s)

Kyun-Seop Bae ¡k@acr.kr;

See Also

```
help, txtNCA, rtfNCA
```

Examples

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

Res2Txt

Convert sNCA output table to text form

Description

This converts the table output of sNCA to text form output.

Usage

6 Round

Arguments

ResNCA	Output table from sNCA
x	usually time
У	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
down	either of "Linear" or "Log" to indicate the way to calculate AUC and

Value

Text form output from the coversion of table form output

AUMC

Author(s)

```
Kyun-Seop Bae ¡k@acr.kr¿
```

See Also

```
txtNCA, pdfNCA, rtfNCA
```

Examples

```
x = Theoph[Theoph$Subject=="1","Time"]
y = Theoph[Theoph$Subject=="1","conc"]
z = sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h")
Res2Txt(z, x, y)
```

Round

 $Round\ Half\ Away\ from\ Zero$

${\bf Description}$

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

Usage

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

Arguments

```
{\sf x} numeric to be rounded {\sf n} indicating decimal digits
```

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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 Configuation Table

Description

Contains the names and order of colum of return table/text in ouputs

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.

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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 this package.

rtfNCA

NCA output to rtf file

Description

This output NCA result in a rtf file.

Usage

```
rtfNCA(fileName = "Temp-NCA.rtf", concData, key = "Subject", colTime = "Time",
    colConc = "conc", dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg",
    timeUnit = "h", concUnit = "ug/L", down="Linear", R2ADJ = 0, MW = 0,
    iAUC = "", excludeDelta = 1)
```

Arguments

fileName file name to save

concData concentration data table

key column names of concData to be shown in the output

colTime column name for time

colConc column name for concentration

dose administered dose

adm one of "Bolus" or "Infusion" or "Extravascular" to indicate drug ad-

ministration 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

R2ADJ Minimum adjusted R-square value to determine terminal slope automat-

ically

MW molecular weight of drug

iAUC interval AUC information in a dataframe with "Name", "Start", and

"End" columns

excludeDelta Improvement of R2ADJ larger than this value could exclude the last point.

Default value 1 is for the compatibility with other software. Author rec-

ommends to use excludeDelta option with about 0.3.

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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 admin-

istration 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

LAMZUL earliest time for LAMZ

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 admin-

istration 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 admin-

istration 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 admin-

istration

MRTIVIFP mean residence time (MRT) infinity using CLSTP, for intravascular ad-

ministration

MRTEVLST mean residence time (MRT) to TLST, for extravascular administration

MRTEVIFO	mean residence time (MRT) infinity using CLST, for extravascular administration $% \left(1\right) =\left(1\right) \left(1\right) \left$
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 $$
VZFO	VZO for extravascular administration, VZO/F, F is bioavailability
VZFP	VZP for extravascular administration, VZP/F , F is bioavailability
CLO	clearance using AUCIFO, for intravascular administration
CLP	clearance using AUCIFP, for intravascular administration
CLF0	CLO for extravascular administration, CLO/F, F is bioavailability
CLFP	CLP for extravascular administration, CLP/F, F is bioavailability
VSS0	volume of distribution at steady state using CLST, for intravascular administration only $$
VSSP	volume of distribution at stead state using CLSTP, for intravascular administration only

Author(s)

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See Also

```
help, txtNCA, pdfNCA
```

Examples

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

txtNCA

Text output of NCA for one subject

Description

This is the text form output.

Usage

Arguments

x usually time

y usually concentration

dose given amount

adm one of "Bolus" or "Infusion" or "Extravascular" to indicate drug ad-

ministration 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

R2ADJ Minimum adjusted R-square value to determine terminal slope automat-

ically

MW molecular weight of the drug

excludeDelta Improvement of R2ADJ larger than this value could exclude the last point.

Default value 1 is for the compatibility with other software. Author rec-

ommends to use excludeDelta option with about 0.3.

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 admin-

istration 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

 $\begin{array}{ll} \mbox{LAMZLL} & \mbox{earliest time for LAMZ} \\ \mbox{LAMZUL} & \mbox{last time for LAMZ} \\ \end{array}$

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 admin-

istration 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	$\mathrm{AUC}~\%$ 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 $$
VZP	volume of distribution determined by LAMZ and AUCIFP, for intravascular administration $$
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 stead state using CLSTP, for intravascular administration only $$

Author(s)

Kyun-Seop Bae ¡k@acr.kr¿

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")
  tRes = c(paste("ID =", IDs[i]), tRes, "")
 Res = c(Res, tRes)
}
Res
```

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