Package 'ncar'

June 11, 2021

Version 0.4.3

Date 2021-06-11 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 (>= 0.3.3)
Author Kyun-Seop Bae [aut]
Maintainer Kyun-Seop Bae <k@acr.kr></k@acr.kr>
Copyright 2016-, Kyun-Seop Bae
License GPL-3
NeedsCompilation no
LazyLoad yes
Repository CRAN
<pre>URL https://cran.r-project.org/package=ncar</pre>
R topics documented:
ncar-package 2 pdfNCA 3 Res2Txt 4 Round 6 RptCfg 7 rtfNCA 3 txtNCA 10 Index 1
index 1.

2 ncar-package

ncar-package

Noncompartmental Analysis for Pharmacokinetic Report

Description

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

Details

The main functions are

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

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
# 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")
#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")
# Output to RTF file
\verb| #rtfNCA(fileName="NCA-Theoph.rtf", Theoph, key="Subject", colTime="Time", theoph, the colTime is a subject of the colTime is a subject of
                         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")
```

pdfNCA 3

pdfNCA	NCA output to pdf file

Description

This output NCA result in a pdf file.

Usage

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 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
R2ADJ	Minimum adjusted R-square value to determine terminal slope automatically
MW	molecular weight of drug
iAUC	interval AUC information in a dataframe with "Name", "Start", and "End" columns

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

4 pdfNCA

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

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

AUMCPEP

AUMCIFO AUMC infinity observed using CLST

AUMCIFP AUMC infinity determined by CLSTP

AUMCPEO AUMC % extrapolated observed

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

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

tion

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

MRTEVIFO mean residence time (MRT) infinity using CLST, for extravascular administra-

tion

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

tion

VZO volume of distribution determined by LAMZ and AUCIFO, for intravascular

administration

VZP volume of distribution determined by LAMZ and AUCIFP, for intravascular ad-

ministration

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

Res2Txt 5

CLFC)	CLO for extravascular administration, CLO/F, F is bioavailability
CLFF	•	CLP for extravascular administration, CLP/F, F is bioavailability
VSSO)	volume of distribution at steady state using CLST, for intravascular administration only $% \left(1\right) =\left(1\right) \left(1\right)$
VSSF	o	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

```
Res2Txt(ResNCA, x, y, dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg", down = "Linear")
```

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 $% \left(1\right) =\left(1\right) \left($
dur	duration of infusion
doseUnit	unit of dose
down	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC

6 Round

Value

Text form output from the coversion of table form output

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

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"

RptCfg 7

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.

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

Description

This output NCA result in a rtf file.

Usage

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 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
R2ADJ	Minimum adjusted R-square value to determine terminal slope automatically
MW	molecular weight of drug
iAUC	interval AUC information in a dataframe with "Name", "Start", and "End" columns

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

rtfNCA 9

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

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

AUMCPEP

AUMCIFO AUMC infinity observed using CLST

AUMCIFP AUMC infinity determined by CLSTP

AUMCPEO AUMC % extrapolated observed

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

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

tion

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

MRTEVIFO mean residence time (MRT) infinity using CLST, for extravascular administra-

tion

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

tion

VZO volume of distribution determined by LAMZ and AUCIFO, for intravascular

administration

VZP volume of distribution determined by LAMZ and AUCIFP, for intravascular ad-

ministration

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

10 txtNCA

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, 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

х	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
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 automatically
MW	molecular weight of the drug

txtNCA 11

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

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 administra-

tion

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

tion

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

12 txtNCA

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
```

Index

```
* NCA
    ncar-package, 2
* Output Form
    pdfNCA, 3
    Res2Txt, 5
    rtfNCA, 8
    txtNCA, 10
* datasets
    RptCfg, 7
*\ package
    ncar-package, 2
* rounding
    Round, 6
help, 5, 10, 12
ncar (ncar-package), 2
ncar-package, 2
pdfNCA, 3, 6, 10, 12
Res2Txt, 5
Round, 6
RptCfg, 7
rtfNCA, 5, 6, 8, 12
txtNCA, 5, 6, 10, 10
```