

Package ‘ncar’

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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 R (>= 3.5.0)

Imports NonCompart (>= 0.8.0), R.oo, R.methodsS3

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Schaffer (vendored from the 'rtf' package, GPL (>= 2))

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ncar-package	<i>Noncompartmental Analysis for Pharmacokinetic Report</i>
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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
#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")
```

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, SS = FALSE, iAUC = "", excludeDelta = 1, UsePoints = NULL)
```

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, a scalar or a vector
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion, a scalar or a vector
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
SS	if steady-state, this should be TRUE. AUCLST (AUClast) is used instead of AUCIFO (AUCinf) for the calculation of Vz (VZFO, VZO), CL (CLFO, CLO), and Vdss (VSSO).

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 recommends to use excludeDelta option with about 0.3.
UsePoints	A list of length equal to the number of subjects/NCAs. Each element is a vector of indices of points to calculate terminal slope for the corresponding subject. Values of use points should not be zero. Use only when automatic determination is not satisfactory. If this is used, R2ADJ option is ignored.

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
LAM _Z	lambda_z negative of best fit terminal slope
LAM _{ZLL}	earliest time for LAMZ
LAM _{ZUL}	last time for LAMZ
LAM _{ZNPT}	number of points for LAMZ
COR _{RXY}	correlation of log(concentration) and time
R ²	R-squared
R _{2ADJ}	R-squared adjusted
C ₀	back extrapolated concentration at time 0, for bolus intravascular administration only
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 _{I_FO_D}	AUC _{IFO} / Dose
AUC _{I_FP}	AUC infinity predicted using CL _{STP} instead of CL _{ST}
AUC _{I_FP_D}	AUC _{I_FP} / Dose
AUC _{PEO}	AUC % extrapolation observed
AUC _{PEP}	AUC % extrapolated for AUC _{I_FP}
AUC _{P_BE_O}	AUC % back extrapolation observed, for bolus IV administration only
AUC _{P_BE_P}	AUC % back extrapolation predicted with AUC _{I_FP} , 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
VSSO	volume of distribution at steady state using CLST, for intravascular administration only
VSSP	volume of distribution at steady state using CLSTP, for intravascular administration only

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

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

Examples

```
#pdfNCA(fileName="NCA-Theoph.pdf", Theoph, 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, a vector
y	usually concentration, a vector
dose	given amount, a scalar
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion, a scalar
doseUnit	unit of dose
down	either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC

Value

Text form output from the conversion of table form output

Author(s)

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See Also

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

Examples

```
x = Theoph[Theoph$Subject=="1","Time"]
y = Theoph[Theoph$Subject=="1","conc"]
z = NonCompartment::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 rounded
n	indicating decimal digits

Details

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

Value

ordinarily rounded value

Author(s)

Kyun-Seop Bae <k@acr.kr>

References

See wikipedia subject "Rounding"

Examples

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

RptCfg

NCA Report Configuration Table

Description

Contains the names and order of column of return table/text in outputs

Usage

RptCfg

Format

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

PPTTESTCD a character vector of CDISC SDTM PPTTESTCD

SYNONYM a character vector of CDISC SDTM PPTTESTCD 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 this package.

rtfNCA	<i>NCA output to rtf file</i>
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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, SS = FALSE, iAUC = "", excludeDelta = 1, UsePoints = NULL)
```

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, a scalar or a vector
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion, a scalar or a vector
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
SS	if steady-state, this should be TRUE. AUCLST (AUClast) is used instead of AUCIFO (AUCinf) for the calculation of Vz (VZFO, VZO), CL (CLFO, CLO), and Vdss (VSSO).
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 recommends to use excludeDelta option with about 0.3.
UsePoints	A list of length equal to the number of subjects/NCAs. Each element is a vector of indices of points to calculate terminal slope for the corresponding subject. Values of use points should not be zero. Use only when automatic determination is not satisfactory. If this is used, R2ADJ option is ignored.

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

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

Author(s)

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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

```
txtNCA(x, y, dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg",
       timeUnit = "h", concUnit = "ug/L", iAUC = "", down="Linear", R2ADJ=0,
       MW = 0, SS = FALSE, excludeDelta = 1, UsePoints = NULL)
```

Arguments

x	usually time
y	usually concentration
dose	given amount, a scalar
adm	one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur	duration of infusion, a scalar
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
SS	if steady-state, this should be TRUE. AUCLST (AUClast) is used instead of AUCIFO (AUCinf) for the calculation of Vz (VZFO, VZO), CL (CLFO, CLO), and Vdss (VSSO).
excludeDelta	Improvement of R2ADJ larger than this value could exclude the last point. Default value 1 is for the compatibility with other software. Author recommends to use excludeDelta option with about 0.3.
UsePoints	Indices of points to calculate terminal slope. Values of use points should not be zero. Use only when automatic determination is not satisfactory. If this is used, R2ADJ option is ignored.

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
LAM _Z	lambda_z negative of best fit terminal slope
LAM _{ZLL}	earliest time for LAMZ
LAM _{ZUL}	last time for LAMZ
LAM _{ZNPT}	number of points for LAMZ
COR _{RXY}	correlation of log(concentration) and time
R ₂	R-squared
R _{2ADJ}	R-squared adjusted
C ₀	back extrapolated concentration at time 0, for bolus intravascular administration only
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 _{IFO} D	AUC _{IFO} / Dose
AUC _I FP	AUC infinity predicted using CL _{STP} instead of CL _{ST}
AUC _I FPD	AUC _I FP / Dose
AUC _{PEO}	AUC % extrapolation observed
AUC _{PEP}	AUC % extrapolated for AUC _I FP
AUC _P BEO	AUC % back extrapolation observed, for bolus IV administration only
AUC _P BEP	AUC % back extrapolation predicted with AUC _I FP, for bolus IV administration only
AUM _{CLST}	AUMC to the T _{LST}
AUM _C IFO	AUMC infinity observed using CL _{ST}
AUM _C IFP	AUMC infinity determined by CL _{STP}
AUM _C PEO	AUMC % extrapolated observed
AUM _C PEP	AUMC % extrapolated predicted
MRT _I VLST	mean residence time (MRT) to T _{LST} , for intravascular administration
MRT _I VIFO	mean residence time (MRT) infinity using CL _{ST} , for intravascular administration

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

Author(s)

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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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