

# Package ‘ncar’

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**Title** Noncompartmental Analysis for Pharmacokinetic Report

**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 are

- 1) CDISC SDTM terms
- 2) Automatic slope selection with the same criterion of WinNonlin(R)
- 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 (>= 2.0.0), rtf, NonCompart (>= 0.3.3)

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

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)
```

**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

**Value**

C <sub>MAX</sub>	maximum concentration, C <sub>max</sub>
C <sub>MAXD</sub>	dose normalized C <sub>max</sub> , C <sub>MAX</sub> / Dose, C <sub>max</sub> / Dose
T <sub>MAX</sub>	time of maximum concentration, T <sub>max</sub>
T <sub>LAG</sub>	time to observe the first non-zero concentration, for extravascular administration only
CL <sub>ST</sub>	last positive concentration observed, C <sub>last</sub>
CL <sub>STP</sub>	last positive concentration predicted, C <sub>last_pred</sub>
TL <sub>ST</sub>	time of last positive concentration, T <sub>last</sub>
LAM <sub>ZHL</sub>	half-life by lambda z, ln(2)/LAMZ
LAM <sub>Z</sub>	lambda_z negative of best fit terminal slope
LAM <sub>ZLL</sub>	earliest time for LAMZ
LAM <sub>ZUL</sub>	last time for LAMZ
LAM <sub>ZNPT</sub>	number of points for LAMZ
COR <sub>RXY</sub>	correlation of log(concentration) and time
R <sub>2</sub>	R-squared
R <sub>2ADJ</sub>	R-squared adjusted
C <sub>0</sub>	back extrapolated concentration at time 0, for bolus intravascular administration only
AUC <sub>CLST</sub>	AUC from 0 to TL <sub>ST</sub>
AUC <sub>ALL</sub>	AUC using all the given points, including trailing zero concentrations
AUC <sub>IFO</sub>	AUC infinity observed
AUC <sub>IFO</sub> D	AUC <sub>IFO</sub> / Dose
AUC <sub>I</sub> FP	AUC infinity predicted using CL <sub>STP</sub> instead of CL <sub>ST</sub>
AUC <sub>I</sub> FPD	AUC <sub>I</sub> FP / Dose
AUC <sub>PEO</sub>	AUC % extrapolation observed
AUC <sub>PEP</sub>	AUC % extrapolated for AUC <sub>I</sub> FP
AUC <sub>P</sub> BEO	AUC % back extrapolation observed, for bolus IV administration only
AUC <sub>P</sub> BEP	AUC % back extrapolation predicted with AUC <sub>I</sub> FP, for bolus IV administration only
AUM <sub>CLST</sub>	AUMC to the TL <sub>ST</sub>
AUM <sub>C</sub> IFO	AUMC infinity observed using CL <sub>ST</sub>
AUM <sub>C</sub> IFP	AUMC infinity determined by CL <sub>STP</sub>
AUM <sub>C</sub> PEO	AUMC % extrapolated observed
AUM <sub>C</sub> PEP	AUMC % extrapolated predicted
MRT <sub>I</sub> VLST	mean residence time (MRT) to TL <sub>ST</sub> , for intravascular administration
MRT <sub>I</sub> VIFO	mean residence time (MRT) infinity using CL <sub>ST</sub> , 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](#), [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
 

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---

*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
y	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 AUMC

**Value**

Text form output from the conversion 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 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.



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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)
```

### 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

### 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, $\ln(2)/\text{LAMZ}$
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 $\log(\text{concentration})$ 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 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
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)
```

**Arguments**

x	usually time
y	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

**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 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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