Package ‘pkr’

June 4, 2018

Version 0.1.2
Date 2018-06-04
Title Pharmacokinetics in R

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

Depends R (&gt;= 2.0.0), foreign, binr, forestplot, rtf
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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

NCA to perform NCA for many subjects.

IndiNCA to perform NCA for one subject.

Author(s)

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AUC

Calculate Area Under the Curve (AUC) and Area Under the first Moment Curve (AUMC) in a table format

References


Examples

# Theoph and Indometh data: dose in mg, conc in mg/L, time in h
NCA(Theoph, "Subject", "Time", "conc", dose=320, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", uConc="mg/L")

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, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", iAUC=iAUC, uConc="mg/L")

writelines(NCA(Theoph, "Subject", "Time", "conc", dose=320, report="Text", uConc="mg/L"),
"Theoph_Linear_CoreOutput.txt")
writelines(NCA(Theoph, "Subject", "Time", "conc", dose=320, fit="Log", report="Text",
uConc="mg/L"), "Theoph_Log_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", report="Text",
uConc="mg/L"), "Indometh_Bolus_Linear_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", fit="Log",
report="Text", uConc="mg/L"), "Indometh_Bolus_Log_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
report="Text", uConc="mg/L"), "Indometh_Infusion_Linear_CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
fit="Log", report="Text", uConc="mg/L"), "Indometh_Infusion_Log_CoreOutput.txt")

sNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1,"conc"], dose=320, concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1,"conc"], dose=25,
adm="Bolus", concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1,"conc"], dose=25,
adm="Infusion", dur=0.25, concUnit="mg/L")

iAUC = data.frame(Name=c("AUC[0-12h]","AUC[0-24h]"), Start=c(0,0), End=c(12,24)); iAUC
sNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1,"conc"], dose=320,
iAUC=iAUC, concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1,"conc"], dose=25,
adm="Bolus", iAUC=iAUC, concUnit="mg/L")
sNCA(Indometh[Indometh$Subject==1,"time"], Indometh[Indometh$Subject==1,"conc"], dose=25,
adm="Infusion", dur=0.25, iAUC=iAUC, concUnit="mg/L")
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, down = "Linear")

Arguments
x vector values of independent variable, usually time
y vector values of dependent variable, usually concentration
down either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC

Details
down="Linear" means linear trapezoidal rule with linear interpolation. down="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

See Also
LinAUC, LogAUC

Examples
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], down="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) ~ 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, adm = "Extravascular", TOL=1e-4)

Arguments

x vector values of x-axis, usually time
y vector values of y-axis, usually concentration
adm one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
TOL tolerance. See Phoneix WinNonlin 6.4 User’s Guide p33 for the detail.

Details

Choosing the best terminal slope (y in log scale) in pharmacokinetic analysis is somewhat challenging, and it could vary by analysis performer. Pheonix WinNonlin chooses a slope with highest adjusted R-squared and the longest one. Difference of adjusted R-Squared less than TOL considered to be 0. This function uses ordinary least square method (OLS).

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

bestslope(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
bestslope(Indometh[Indometh$Subject==1, "time"], Indometh[Indometh$Subject==1, "conc"],
adm="Bolus")

Description

This function combines specified CDISC domain XPT files across the folders.

Usage

combXPT(folders, domain)

Arguments

folders where to find specified CDISC domain XPT files
domain domain XPT files to be combined across the folders

Details

You need to designate only one CDISC domain name. You may specify one or more folders to find the domain XPT files.

Value

XPT combined table

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

help, readEX, readPC
foreNCA

Forest plot to compare NCA results

Description

This function compares NCA results usually from rNCA function

Usage

foreNCA(NCAres = "", PPTESTCD = "", PCTESTCD = "", title = "", ...)

Arguments

NCAres NCA results from rNCA function
PPTESTCD CDISC SDTM PP domain Test Code to compare
PCTESTCD Molecular species to compare specified in PCTESTCD of CDISC SDTM PC domain
title Title of the plot
... further arguments to pass to the forestplot function

Details

This function calls forestplot in forest package.

Value

Currently, this just plots.

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

help, rNCA
IndiNCA  Noncompartmental Analysis for an Individual

Description

It performs a noncompartmental analysis with one subject data. This will be deprecated. Use snCA() instead.

Usage

IndiNCA(x, y, dose = 0, fit = "Linear", adm = "Extravascular", dur = 0, report = "Table", iAUC = "", uTime = "h", uConc = "ug/L", uDose = "mg")

Arguments

x       vector values of independent variable, usually time
y       vector values of dependent variable, usually concentration
dose    administered dose for the subject
fit     either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC
adm     one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur     infusion duration for constant infusion, otherwise 0
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 intervals for partial (interval) AUC
uTime   unit of time
uConc   unit of concentration
uDose   unit of dose

Details

This performs a noncompartmental analysis for a subject. It returns practically the same result with the most popular commercial software.

Value

CMA    maximum concentration, Cmax
CMAXD  dose normalized Cmax, CMAX / Dose, Cmax / Dose
TMA    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

AUCIF0  
AUC infinity observed

AUCIFO  
AUCIFO / Dose

AUCIFPD  
AUC infinity predicted using CLSTP instead of CLST

AUCIFPD  
AUCIFPD / Dose

AUCPEO  
AUC % extrapolation observed

AUCPEP  
AUC % extrapolated for AUCIFP

AUCPBE0  
AUC % back extrapolation observed, for bolus IV administration only

AUCPBE0  
AUCPBE0 / Dose

AUCPBE0  
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, VZOF/F, F is bioavailability
VZFP  VZP for extravascular administration, VZPF/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>

References


See Also

AUC, BestSlope

Examples

IndiNCA(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], dose=320, uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1, "Time"], Indometh[Indometh$Subject==1, "conc"], dose=25, adm="Bolus", uConc="mg/L")
IndiNCA(Indometh[Indometh$Subject==1, "time"], Indometh[Indometh$Subject==1, "conc"], dose=25, adm="Infusion", dur=0.25, uConc="mg/L")

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,
Calculate interval AUC

Description
It calculates interval AUC

Usage
InAUC(x, y, t1, t2, Res, down = "Linear")

Arguments
x vector values of independent variable, usually time
y vector values of dependent variable, usually concentration
t1 start time for AUC
t2 end time for AUC
Res result from Indinca function
down 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 down option.

Value
return interval AUC value (scalar)

Author(s)
Kyun-Seop Bae <k@acr.kr>

References
Interpol

See Also

AUC, Interpol

Examples

Res = sNCA(Theoph$Subject==1,"Time", Theoph$Subject==1, "conc", dose=320, concUnit="mg/L")
IntAUC(Theoph$Subject==1, "Time", Theoph$Subject==1, "conc", t1=0.5, t2=11, Res)

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, down = "Linear")

Arguments

x vector values of x-axis, usually time
y vector values of y-axis, usually concentration
xnew new x point to be interpolated, usually new time point
Slope slope of regression log(y) ~ x
b0 y value of just left point of xnew
down 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.

Value

new x and y vector containing xnew and ynew point

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

IntAUC
**LinAUC**

**Examples**

\[
\begin{align*}
  x &= 10 + 0.1 \\
  y &= -2x + 40.2 \\
  &\text{Interpol}(x, y, 1.5) \\
  &\text{Interpol}(x, y, 1.5, \text{down="Log"})
\end{align*}
\]

---

**Description**

It calculates AUC and AUMC using linear trapezoidal method.

**Usage**

\[
\text{LinAUC}(x, y)
\]

**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>

**References**

loadEXPC

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"])

loadEXPC folders

Load EX and PC domain files in folders

Description

This loads and returns EX and PC domain files in the specified folders

Usage

loadEXPC(folders)

Arguments

folders folders where to find EX and PC domain files

Details

This reads EX and PC domain files in the specified folder. This calls readEX and readPC functions.

Value

EX combined EX domain data
PC combined PC domain data

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

help, readEX, readPC
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>

**References**


**See Also**

LinAUC, AUC

**Examples**

```r
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"], down="Log")
```
Noncompartmental analysis for a dataset with multiple subjects

Description

conduct noncompartmental analysis for many subjects in a data table

Usage

NCA(concData, id, Time, conc, trt="", fit = "Linear", dose = 0,
adm = "Extravascular", dur = 0, report = "Table", iAUC = "",
uti = "h", uConc = "ug/L", uDose = "mg")

Arguments

concData name of data table containing time-concentration data of multiple subjects
id column name for subject ID
Time column name for the time
conc column name for the concentration
trt column name for the treatment code. This is useful for crossover study like bioequivalence trial.
fit 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.
adm one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur 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 AUC
uti unit of time
uConc unit of concentration
uDose unit of dose

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.
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMAX</td>
<td>maximum concentration, Cmax</td>
</tr>
<tr>
<td>CMAXD</td>
<td>dose normalized Cmax, CMAX / Dose, Cmax / Dose</td>
</tr>
<tr>
<td>TMAX</td>
<td>time of maximum concentration, Tmax</td>
</tr>
<tr>
<td>TLAG</td>
<td>time to observe the first non-zero concentration, for extravascular only</td>
</tr>
<tr>
<td>CLST</td>
<td>last positive concentration observed, Clast</td>
</tr>
<tr>
<td>CLSTP</td>
<td>last positive concentration predicted, Clast_pred</td>
</tr>
<tr>
<td>TLST</td>
<td>time of last positive concentration, Tlast</td>
</tr>
<tr>
<td>LAMZHL</td>
<td>half-life by lambda z, ln(2)/LAMZ</td>
</tr>
<tr>
<td>LAMZ</td>
<td>lambda_z negative of best fit terminal slope</td>
</tr>
<tr>
<td>LAMZLL</td>
<td>earliest time for LAMZ</td>
</tr>
<tr>
<td>LAMZUL</td>
<td>last time for LAMZ</td>
</tr>
<tr>
<td>LAMZNPT</td>
<td>number of points for LAMZ</td>
</tr>
<tr>
<td>CORRXY</td>
<td>correlation of log(concentration) and time</td>
</tr>
<tr>
<td>R2</td>
<td>R-squared</td>
</tr>
<tr>
<td>R2ADJ</td>
<td>R-squared adjusted</td>
</tr>
<tr>
<td>C0</td>
<td>back extrapolated concentration at time 0, for bolus intravascular only</td>
</tr>
<tr>
<td>AUCLST</td>
<td>AUC from 0 to TLST</td>
</tr>
<tr>
<td>AUCALL</td>
<td>AUC using all the given points, including trailing zero concentrations</td>
</tr>
<tr>
<td>AUCIFO</td>
<td>AUC infinity observed</td>
</tr>
<tr>
<td>AUCIFOD</td>
<td>AUCIFO / Dose</td>
</tr>
<tr>
<td>AUCIFP</td>
<td>AUC infinity predicted using CLSTP instead of CLST</td>
</tr>
<tr>
<td>AUCIFPD</td>
<td>AUCIFP / Dose</td>
</tr>
<tr>
<td>AUCPE0</td>
<td>AUC % extrapolation observed</td>
</tr>
<tr>
<td>AUCPEP</td>
<td>AUC % extrapolated for AUCIFP</td>
</tr>
<tr>
<td>AUCPBE0</td>
<td>AUC % back extrapolation observed, for bolus IV administration only</td>
</tr>
<tr>
<td>AUCPBEP</td>
<td>AUC % back extrapolation predicted with AUCIFP, for bolus IV administration only</td>
</tr>
<tr>
<td>AUMCLST</td>
<td>AUMC to the TLST</td>
</tr>
<tr>
<td>AUMCIFO</td>
<td>AUMC infinity observed using CLST</td>
</tr>
<tr>
<td>AUMCIFP</td>
<td>AUMC infinity determined by CLSTTP</td>
</tr>
<tr>
<td>AUMCPE0</td>
<td>AUMC % extrapolated observed</td>
</tr>
<tr>
<td>AUMCPEP</td>
<td>AUMC % extrapolated predicted</td>
</tr>
<tr>
<td>MRTIVLST</td>
<td>mean residence time (MRT) to TLST, for intravascular administration</td>
</tr>
<tr>
<td>MRTIVIFO</td>
<td>mean residence time (MRT) infinity using CLST, for intravascular administration</td>
</tr>
<tr>
<td>Term</td>
<td>Description</td>
</tr>
<tr>
<td>-----------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>MRTIVIFP</td>
<td>mean residence time (MRT) infinity using CLSTP, for intravascular administra-</td>
</tr>
<tr>
<td>MRTEVLST</td>
<td>mean residence time (MRT) to TLST, for extravascular administration</td>
</tr>
<tr>
<td>MRTEVIFO</td>
<td>mean residence time (MRT) infinity using CLST, for extravascular administra-</td>
</tr>
<tr>
<td>MRTEVIFP</td>
<td>mean residence time (MRT) infinity using CLSTP, for extravascular administra-</td>
</tr>
<tr>
<td>VZ0</td>
<td>volume of distribution determined by LAMZ and AUCIFO, for intravascular adm-</td>
</tr>
<tr>
<td>VZP</td>
<td>volume of distribution determined by LAMZ and AUCIFP, for intravascular adm-</td>
</tr>
<tr>
<td>VZFO</td>
<td>VZO for extravascular administration, VZO/F, F is bioavailability</td>
</tr>
<tr>
<td>VZFP</td>
<td>VZP for extravascular administration, VZP/F, F is bioavailability</td>
</tr>
<tr>
<td>CLO</td>
<td>clearance using AUCIFO, for intravascular administration</td>
</tr>
<tr>
<td>CLP</td>
<td>clearance using AUCIFP, for intravascular administration</td>
</tr>
<tr>
<td>CLFO</td>
<td>CLO for extravascular administration, CLO/F, F is bioavailability</td>
</tr>
<tr>
<td>CLFP</td>
<td>CLP for extravascular administration, CLP/F, F is bioavailability</td>
</tr>
<tr>
<td>VSS0</td>
<td>volume of distribution at steady state using CLST, for intravascular administra-</td>
</tr>
<tr>
<td>VSSP</td>
<td>volume of distribution at steady state using CLSTP, for intravascular administra-</td>
</tr>
</tbody>
</table>

**Author(s)**

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**References**


**See Also**

sNCA
Examples

# Theoph and Indometh data: dose in mg, conc in mg/L, time in h
NCA(Theoph, "Subject", "Time", "conc", dose=320, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", uConc="mg/L")

iAUC = data.frame(Names=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, uConc="mg/L")
NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", iAUC=iAUC, uConc="mg/L")

writelines(NCA(Theoph, "Subject", "Time", "conc", dose=320, report="Text", uConc="mg/L"),
           "Theoph Linear CoreOutput.txt")
writelines(NCA(Theoph, "Subject", "Time", "conc", dose=320, fit="Log", report="Text",
               uConc="mg/L"), "Theoph Log CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", report="Text",
               uConc="mg/L"), "Indometh Bolus Linear CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus", fit="Log",
               report="Text", uConc="mg/L"), "Indometh Bolus Log CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
               report="Text", uConc="mg/L"), "Indometh Infusion Linear CoreOutput.txt")
writelines(NCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion", dur=0.25,
               fit="Log", report="Text", uConc="mg/L"), "Indometh Infusion Log CoreOutput.txt")

Description

This performs Noncompartmental Analysis (NCA) for only one subject from the CDISC EX and PC domain.

Usage

NCA0(EX0, PC0, fit="Linear")

Arguments

EX0  Data of one subject from EX domain
PC0  Data of one subject from PC domain
fit  either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC

Details

This calls IndiNCA function. This is called by rNCA function.

Value

This returns NCA results vector.
Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

help, rNCA, sNCA

pdfNCA  NCA output to pdf file

Description

This output NCA result in a pdf file.

Usage

pdfNCA(filename = "Temp-NCA.pdf", concData, colSubj = "Subject", colTime = "Time", 
colConc = "conc", dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg", 
timeUnit = "h", concUnit = "ug/L", down="Linear", MW = 0)

Arguments

fileName  file name to save
concData  concentration data table
colSubj  column name for subject ID
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
MW  molecular weight of drug
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMAX</td>
<td>maximum concentration, Cmax</td>
</tr>
<tr>
<td>CMAXD</td>
<td>dose normalized Cmax, CMAX / Dose, Cmax / Dose</td>
</tr>
<tr>
<td>TMAX</td>
<td>time of maximum concentration, Tmax</td>
</tr>
<tr>
<td>TLAG</td>
<td>time to observe the first non-zero concentration, for extravascular administration only</td>
</tr>
<tr>
<td>CLST</td>
<td>last positive concentration observed, Clast</td>
</tr>
<tr>
<td>CLSTP</td>
<td>last positive concentration predicted, Clast_pred</td>
</tr>
<tr>
<td>TLST</td>
<td>time of last positive concentration, Tlast</td>
</tr>
<tr>
<td>LAMZHL</td>
<td>half-life by lambda z, ln(2)/LAMZ</td>
</tr>
<tr>
<td>LAMZ</td>
<td>lambda_z negative of best fit terminal slope</td>
</tr>
<tr>
<td>LAMZLL</td>
<td>earliest time for LAMZ</td>
</tr>
<tr>
<td>LAMZUL</td>
<td>last time for LAMZ</td>
</tr>
<tr>
<td>LAMZNPT</td>
<td>number of points for LAMZ</td>
</tr>
<tr>
<td>CORRXY</td>
<td>correlation of log(concentration) and time</td>
</tr>
<tr>
<td>R2</td>
<td>R-squared</td>
</tr>
<tr>
<td>R2ADJ</td>
<td>R-squared adjusted</td>
</tr>
<tr>
<td>C0</td>
<td>back extrapolated concentration at time 0, for bolus intravascular administration only</td>
</tr>
<tr>
<td>AUCLST</td>
<td>AUC from 0 to TLST</td>
</tr>
<tr>
<td>AUCALL</td>
<td>AUC using all the given points, including trailing zero concentrations</td>
</tr>
<tr>
<td>AUCIFO</td>
<td>AUC infinity observed</td>
</tr>
<tr>
<td>AUCIFOD</td>
<td>AUCIFO / Dose</td>
</tr>
<tr>
<td>AUCIFP</td>
<td>AUC infinity predicted using CLSTP instead of CLST</td>
</tr>
<tr>
<td>AUCIFPD</td>
<td>AUCIFP / Dose</td>
</tr>
<tr>
<td>AUCPE0</td>
<td>AUC % extrapolation observed</td>
</tr>
<tr>
<td>AUCPEP</td>
<td>AUC % extrapolated for AUCIFP</td>
</tr>
<tr>
<td>AUCPBE0</td>
<td>AUC % back extrapolation observed, for bolus IV administration only</td>
</tr>
<tr>
<td>AUCPBEP</td>
<td>AUC % back extrapolation predicted with AUCIFP, for bolus IV administration only</td>
</tr>
<tr>
<td>AUMCLST</td>
<td>AUMC to the TLST</td>
</tr>
<tr>
<td>AUMCIFO</td>
<td>AUMC infinity observed using CLST</td>
</tr>
<tr>
<td>AUMCIFP</td>
<td>AUMC infinity determined by CLSTP</td>
</tr>
<tr>
<td>AUMCPE0</td>
<td>AUMC % extrapolated observed</td>
</tr>
<tr>
<td>AUMCPEP</td>
<td>AUMC % extrapolated predicted</td>
</tr>
<tr>
<td>MRTIVLST</td>
<td>mean residence time (MRT) to TLST, for intravascular administration</td>
</tr>
<tr>
<td>MRTIVIFO</td>
<td>mean residence time (MRT) infinity using CLST, for intravascular administration</td>
</tr>
</tbody>
</table>
MRTIVIFP mean residence time (MRT) infinity using CLSTP, for intravascular administration

MRTEVLIST 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, colSubj="Subject", colTime="Time",
# colConc="conc", dose=320, doseUnit="mg", timeUnit="h", concUnit="mg/L")
#pdfNCA(fileName="NCA-Indometh.pdf", Indometh, colSubj="Subject", colTime="time",
# colConc="conc", adm="Infusion", dur=0.5, dose=25, doseUnit="mg",
# timeUnit="h", concUnit="mg/L")
**Description**

Automatically select best fit slope for the given x (usually time) and log(y) (usually concentration) values.

**Usage**

```r
plotFit(concData, id, Time, conc, mol = "", adm = "Extravascular", ID = "", Mol = "")
```

**Arguments**

- `concData` name of data table containing time-concentration data of multiple subjects
- `id` column name for subject ID
- `Time` column name for the time
- `conc` column name for the concentration
- `mol` column name for molecular species
- `adm` one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
- `ID` Subject ID for this plot
- `Mol` the name of molecular species to see

**Details**

Find the best fit slope then plot it. Currently this function uses ordinary least square method (OLS) only. This function calls BestSlope function.

**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)**

Jee Eun Lee <JeeEun.Lee@fda.hhs.gov>
plotpk

Plot concentration vs. time curve for individuals and collectively.

Description

Generates individual and superposed concentration vs. time curve and save it in pdf files.

Usage

plotpk(concData, id, Time, conc, unitTime = "hr", unitConc = "ng/mL", trt = ",", fit = "Linear", dose = 0, adm = "Extravascular", dur = 0, outdir = "Output")

Arguments

concData name of data table containing time-concentration data of multiple subjects
id column name for subject ID
Time column name for the time
conc column name for the concentration
unitTime unit for the time
unitConc unit for the concentration
trt column name for the treatment code. This is useful for crossover study like bioequivalence trial.
fit 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.
adm one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode
dur infusion duration for constant infusion, otherwise 0. This can be a vector containing values for each subject in order.
outdir name of the folder to be used for the output files

details

This function generates plots for individual and summary concentration vs. time curve. This function calles NCA().
Value

This function saves pdf files and tiff files in the outdir folder.

Author(s)

Jee Eun Lee <JeeEun.Lee@fda.hhs.gov>

See Also

NCA

Examples

plotPK(Theoph, "Subject", "Time", "conc", unitTime="hr", unitConc="mg/L", dose=320)
plotPK(Indometh, "Subject", "time", "conc", unitTime="hr", unitConc="mg/L", adm="Bolus", dose=25)

readEX                Read EX domain files

Description

This reads EX domain files from the specified folders.

Usage

readEX(folders)

Arguments

folders       folders where to find EX doamin files

Details

This calls combXPT function. This is called by loadEXPC function.

Value

This returns combined table of EX doamin.

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

help, combXPT, loadEXPC
readPC  
*Read PC domain files*

**Description**
This reads PC domain files from the specified folders.

**Usage**
```
readPC(folders)
```

**Arguments**
- `folders` folders where to find PC doamin files

**Details**
This calls `combxpt` function. This is called by `loadEXPC` function.

**Value**
This returns combined table of PC doamin.

**Author(s)**
Kyun-Seop Bae <k@acr.kr>

**See Also**
- `help`, `combxpt`, `loadEXPC`

---

rNCA  
*Do NCA for review*

**Description**
This performs NCA from the CDISC EX and PC datasets.

**Usage**
```
rNCA(ex, pc, study = "", trt = "", id = "", analyte = "",
codeBQL = c("< θ", "<θ", "NQ", "BLQ", "BQL", "BQoL", "<LOQ"),
fit="Linear", MinPoints = 5)
```
Round

Arguments

- **ex**: EX domain data, usually from the `loadEXPC`.
- **pc**: PC domain data, usually from the `loadEXPC`.
- **study**: vector of study names in EX and PC domain to do NCA.
- **trt**: vector of treatment names in EXTRT to do NCA.
- **id**: vector of subject IDs in USUBJID to do NCA.
- **analyte**: vector of molecular species in PCTESTCD to do NCA.
- **codeBQL**: symbols of below the quantitation limit.
- **fit**: either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC.
- **MinPoints**: minimum number of sampling points for NCA.

Details

This calls NCA0. Results of this can be further processed by foreNCA to plot and compare between studies and dose groups.

Value

This returns a table of NCA results.

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

`help`, `NCA0`, `loadEXPC`, `foreNCA`

---

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

---

<table>
<thead>
<tr>
<th>RptCfg</th>
<th>NCA Report Configuration Table</th>
</tr>
</thead>
</table>

**Description**

Contains the names and order of columns 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 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 pkr package. User can edit this table for shaping the report in one’s own style.

---

**rtfNCA NCA output to rtf file**

---

**Description**

This output NCA result in a rtf file.

**Usage**

```r
tfnca(fileName = "Temp-NCA.rtf", concData, colSubj = "Subject", colTime = "Time", colConc = "conc", dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h", concUnit = "ug/L", down="Linear", MW = 0)
```

**Arguments**

- `fileName` file name to save
- `concData` concentration data table
- `colSubj` column name for subject ID
- `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
- `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

- **Clstpred**  
  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

- **Aucifd**  
  AUCIFO / Dose

- **Aucifp**  
  AUC infinity predicted using CLSTP instead of CLST

- **Aucifpd**  
  AUCIFP / Dose

- **Aucpeo**  
  AUC % extrapolation observed

- **Aucpep**  
  AUC % extrapolated for AUCIFP

- **Aucpeo**  
  AUC % back extrapolation observed, for bolus IV administration only

- **Aucpep**  
  AUC % back extrapolation predicted with AUCIFP, for bolus IV administration only

- **Auclst**  
  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

CL0      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, pdfNCA

Examples

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

*Get the Slope of regression* $\log(y) \sim x$

**Description**

It calculates the slope with linear regression of $\log(y) \sim x$

**Usage**

```r
Slope(x, y)
```

**Arguments**

- `x`: vector values of independent variable, usually time
- `y`: vector values of dependent variable, usually concentration

**Details**

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

**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**

`BestSlope`

**Examples**

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

This is the work-horse function for NCA.

**Usage**

```r
sNCA(x, y, dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h", concUnit = "ug/L", iAUC = "", down = "Linear", MW = 0, returnNA = TRUE)
```

**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
- `MW` molecular weight of the drug
- `returnNA` if `returnNA` is TRUE, it returns NA values also.

**Details**

This will replace IndiNCA.

**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
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAMZHL</td>
<td>half-life by lambda z, ln(2)/LAMZ</td>
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<tr>
<td>LAMZ</td>
<td>lambda_z negative of best fit terminal slope</td>
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<tr>
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<td>LAMZUL</td>
<td>last time for LAMZ</td>
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<tr>
<td>CORRXY</td>
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</tr>
<tr>
<td>R2</td>
<td>R-squared</td>
</tr>
<tr>
<td>R2ADJ</td>
<td>R-squared adjusted</td>
</tr>
</tbody>
</table>
| C0            | back extrapolated concentration at time 0, for bolus intravascular administra-
|               | tion 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                                                |
| AUCPBE0       | AUC % back extrapolation observed, for bolus IV administration only          |
| AUCPBEP       | AUC % back extrapolation predicted with AUCIFP, for bolus IV administra-
|               | tion 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           |
| MRTEVIFO      | mean residence time (MRT) infinity using CLST, for extravascular administra-
|               | tion                                                                       |
| MRTEVIFP      | mean residence time (MRT) infinity using CLSTP, for extravascular administra-
|               | tion                                                                       |
| V20           | volume of distribution determined by LAMZ and AUCIFO, for intravascular admini-
|               | stration                                                                   |
sNCA

VZP  volume of distribution determined by LAMZ and AUCIFP, for intravascular administration
VZFO  VZO for extravascular administration, VZO/F, F is bioavailability
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VSS0  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>

References


See Also

help, tblNCA

Examples

# For one subject
x = Theoph[Theoph$Subject=="1","Time"]
y = Theoph[Theoph$Subject=="1","conc"]
sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h")
sNCA(x, y, dose=320, concUnit="mg/L", returnNA=FALSE)

iAUC = data.frame(Name=c("AUC[0-12h]","AUC[0-24h]"): Start=c(0,0), End=c(12,24))
sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h", iAUC=iAUC)

MW = 180.164 # Molecular weight of theophylline
sNCA(x, y/MW, dose=320, doseUnit="mg", concUnit="mmol/L", timeUnit="h")
sNCA(x, y/MW, dose=320, doseUnit="mg", concUnit="mmol/L", timeUnit="h", MW=MW)
sNCA(x, y/MW, dose=320/MW, doseUnit="mmol", concUnit="mg/L", timeUnit="h", MW=MW)
sNCA(x, y/MW, dose=320/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW)
sNCA(x, y/MW, dose=320/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW, returnNA=FALSE)
sNCA(x, y/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW, returnNA=FALSE)
sNCA(x, y/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW, returnNA=FALSE)
sNCA(x, y/MW, dose=as.numeric(NA), doseUnit="mmol", concUnit="mmol/L", timeUnit="h",
```r
sNCA(x, y, dose=320, concUnit="mg/L", timeUnit="hr")
sNCA(x*60, y, dose=320, concUnit="mg/L", timeUnit="min")
```

### Description

Do multiple NCA and returns a result table.

### Usage

```r
tblNCA(concData, key = "Subject", colTime = "Time", colConc = "conc", dose = 0,
       adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h",
       concUnit = "ug/L", down = "Linear", MW = 0, returnNA = FALSE)
```

### Arguments

- `concData`: concentration data table
- `key`: column names of concData to be shown at 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`: method to calculate AUC, "Linear" or "Log"
- `MW`: molecular weight of drug
- `returnNA`: if returnNA is TRUE, it returns NA values also.

### Value

Basically same with `sNCA`

### Author(s)

Kyun-Seop Bae <k@acr.kr>
See Also

help, snca

Examples

tblnca(Theoph, key="Subject", dose=320, concUnit="mg/L")
tblnca(Indometh, key="Subject", colTime="time", colConc="conc", dose=25,
    adm="Infusion", dur=0.5, concUnit="mg/L")

txtNCA

<table>
<thead>
<tr>
<th>Text output of NCA for one subject</th>
</tr>
</thead>
</table>

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", MW = 0, returnNA = FALSE)
```

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
- **MW**: molecular weight of the drug
- **returnNA**: if returnNA is TRUE, it returns NA values also.
## Value

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
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<tr>
<td>CMAX</td>
<td>maximum concentration, Cmax</td>
</tr>
<tr>
<td>CMAXD</td>
<td>dose normalized Cmax, CMAX / Dose, Cmax / Dose</td>
</tr>
<tr>
<td>TMAX</td>
<td>time of maximum concentration, Tmax</td>
</tr>
<tr>
<td>TLAG</td>
<td>time to observe the first non-zero concentration, for extravascular administration only</td>
</tr>
<tr>
<td>CLST</td>
<td>last positive concentration observed, Clast</td>
</tr>
<tr>
<td>CLSTP</td>
<td>last positive concentration predicted, Clast_pred</td>
</tr>
<tr>
<td>TLST</td>
<td>time of last positive concentration, Tlast</td>
</tr>
<tr>
<td>LAMZHL</td>
<td>half-life by lambda z, ln(2)/LAMZ</td>
</tr>
<tr>
<td>LAMZ</td>
<td>lambda_z negative of best fit terminal slope</td>
</tr>
<tr>
<td>LAMZLL</td>
<td>earliest time for LAMZ</td>
</tr>
<tr>
<td>LAMZUL</td>
<td>last time for LAMZ</td>
</tr>
<tr>
<td>LAMZNPT</td>
<td>number of points for LAMZ</td>
</tr>
<tr>
<td>CORRXY</td>
<td>correlation of log(concentration) and time</td>
</tr>
<tr>
<td>R2</td>
<td>R-squared</td>
</tr>
<tr>
<td>R2ADJ</td>
<td>R-squared adjusted</td>
</tr>
<tr>
<td>C0</td>
<td>back extrapolated concentration at time 0, for bolus intravascular administration only</td>
</tr>
<tr>
<td>AUCLST</td>
<td>AUC from 0 to TLST</td>
</tr>
<tr>
<td>AUCALL</td>
<td>AUC using all the given points, including trailing zero concentrations</td>
</tr>
<tr>
<td>AUCIFO</td>
<td>AUC infinity observed</td>
</tr>
<tr>
<td>AUCIF0D</td>
<td>AUCIFO / Dose</td>
</tr>
<tr>
<td>AUCIFP</td>
<td>AUC infinity predicted using CLSTP instead of CLST</td>
</tr>
<tr>
<td>AUCIFPD</td>
<td>AUCIFP / Dose</td>
</tr>
<tr>
<td>AUCPE0</td>
<td>AUC % extrapolation observed</td>
</tr>
<tr>
<td>AUCPEP</td>
<td>AUC % extrapolated for AUCIFP</td>
</tr>
<tr>
<td>AUCPBE0</td>
<td>AUC % back extrapolation observed, for bolus IV administration only</td>
</tr>
<tr>
<td>AUCPBEP</td>
<td>AUC % back extrapolation predicted with AUCIFP, for bolus IV administration only</td>
</tr>
<tr>
<td>AUMCLST</td>
<td>AUMC to the TLST</td>
</tr>
<tr>
<td>AUMCIFO</td>
<td>AUMC infinity observed using CLST</td>
</tr>
<tr>
<td>AUMCIFP</td>
<td>AUMC infinity determined by CLSTP</td>
</tr>
<tr>
<td>AUMCPE0</td>
<td>AUMC % extrapolated observed</td>
</tr>
<tr>
<td>AUMCPEP</td>
<td>AUMC % extrapolated predicted</td>
</tr>
<tr>
<td>MRTIVLST</td>
<td>mean residence time (MRT) to TLST, for intravascular administration</td>
</tr>
<tr>
<td>MRTIVIFO</td>
<td>mean residence time (MRT) infinity using CLST, for intravascular administration</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>MRTIVFP</td>
<td>mean residence time (MRT) infinity using CLSTP, for intravascular administration</td>
</tr>
<tr>
<td>MRTEVLST</td>
<td>mean residence time (MRT) to TLST, for extravascular administration</td>
</tr>
<tr>
<td>MRTEVIFO</td>
<td>mean residence time (MRT) infinity using CLST, for extravascular administration</td>
</tr>
<tr>
<td>MRTEVIFP</td>
<td>mean residence time (MRT) infinity using CLSTP, for extravascular administration</td>
</tr>
<tr>
<td>VZ0</td>
<td>volume of distribution determined by LAMZ and AUCIFO, for intravascular administration</td>
</tr>
<tr>
<td>VZP</td>
<td>volume of distribution determined by LAMZ and AUCIFP, for intravascular administration</td>
</tr>
<tr>
<td>VZFO</td>
<td>VZO for extravascular administration, VZO/F, F is bioavailability</td>
</tr>
<tr>
<td>VZFP</td>
<td>VZP for extravascular administration, VZP/F, F is bioavailability</td>
</tr>
<tr>
<td>CL0</td>
<td>clearance using AUCIFO, for intravascular administration</td>
</tr>
<tr>
<td>CLP</td>
<td>clearance using AUCIFP, for intravascular administration</td>
</tr>
<tr>
<td>CL0F</td>
<td>CLO for extravascular administration, CLO/F, F is bioavailability</td>
</tr>
<tr>
<td>CLFP</td>
<td>CLP for extravascular administration, CLP/F, F is bioavailability</td>
</tr>
<tr>
<td>VSS0</td>
<td>volume of distribution at steady state using CLST, for intravascular administration only</td>
</tr>
<tr>
<td>VSSP</td>
<td>volume of distribution at steady state using CLSTP, for intravascular administration only</td>
</tr>
</tbody>
</table>

**Author(s)**

Kyun-Seop Bae <k@acr.kr>

**See Also**

help, pdfNCA, rtfNCA

**Examples**

```r
# 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) {
```
Unit

Display CDISC standard units and multiplied factor of NCA results

Description

It displays CDISC PP output units and multiplication factor for them.

Usage

Unit(code = "", timeUnit = "h", concUnit = "ng/mL", doseUnit = "mg", MW = 0)

Arguments

code vector of PPTESTCD
timeUnit unit of time
concUnit unit of concentration
doseUnit unit of dose
MW molecular weight of drug

Value

row names PPTESTCD
Unit unit
Factor internal multiplication factor

Author(s)

Kyun-Seop Bae <k@acr.kr>

Examples

Unit(concUnit="ug/L", doseUnit="mg")
Unit(concUnit="ng/L", doseUnit="mg")
Unit(concUnit="umol/L", doseUnit="mmol")
Unit(concUnit="mmol/L", doseUnit="mmol")
Unit(concUnit="mmol/L", doseUnit="mg", MW=500)
Unit(concUnit="umol/L", doseUnit="mg", MW=500)
Unit

Unit(concUnit="nmol/L", doseUnit="mg", MW=500)
Unit(concUnit="nmol/mL", doseUnit="mg", MW=500)

Unit(concUnit="ug/L", doseUnit="mmol", MW=500)
Unit(concUnit="ug/L", doseUnit="mol", MW=500)
Unit(concUnit="ng/L", doseUnit="mmol", MW=500)
Unit(concUnit="ng/mL", doseUnit="mmol", MW=500)

Unit(concUnit="nmol/L", doseUnit="mg")
Unit(concUnit="ug/L", doseUnit="mmol")
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