

Package ‘ivivc’

January 2, 2012

Version 0.1.5

Date 2009-10-10

Title A data analysis tool for in vitro-in vivo correlation (IVIVC)

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Depends R (>= 2.9.2), stats4, rgenoud, odesolve, reshape, sciplot

Description a menu-driven package for IVIVC model buidling and model validation

License GPL (>= 2)

URL <http://pkpd.kmu.edu.tw/ivivc>

Repository CRAN

Date/Publication 2009-10-12 12:39:13

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aicllsbc	<i>Evaluation of model fit</i>
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Description

Three methods for evaluating model fitting: 1. AIC (Akaike's information criterion), 2. Log likelihood, and 3. BIC (Bayesian information criterion, also known as Schwarz's Bayesian criterion).

bye	<i>The final step Menu</i>
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Description

Try again or Leave ivivc package.

check	<i>Check mechanism</i>
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Description

Checking if the initial value for parameter being zero.

DepModel	<i>Model Dependent Method Menu</i>
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Description

Provide the following one method for selection: 1. Model Dependent Method

entertitle	<i>Enter the title for plots</i>
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Description

If users want to use their own name for x-axis and y-axis, allow them to enter it.

fbolus1	<i>Fitting Functions for a One-Compartment, IV-Bolus, and Single-Dose Model</i>
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Description

Includes user-supplied functions for model definition, integration method for solving ordinary differential equations, three kinds of weighting schemes for selection, and fitting algorithms for a one-compartment, IV-bolus, and single-dose model.

References

C. Y. Lee and Y. J. Lee. PKfit: A Data Analysis Tool for Pharmacokinetics. <http://ce.kmu.edu.tw/index.htm>

ffirst.lag	<i>Fitting Functions for a One-Compartment, Extravascular, Single-Dose, and First-Ordered Absorption with Lag Time Model</i>
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Description

Includes user-supplied functions for model definition, integration method for solving ordinary differential equations, three kinds of weighting schemes for selection, and fitting algorithms for a one-compartment, extravascular, single-dose, and first-ordered absorption with lag time model.

References

C. Y. Lee and Y. J. Lee. PKfit: A Data Analysis Tool for Pharmacokinetics. <http://ce.kmu.edu.tw/index.htm>

ffirst.nolag	<i>Fitting Functions for a One-Compartment, Extravascular, Single-Dose, and First-Ordered Absorption without Lag Time Model</i>
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Description

Includes user-supplied functions for model definition, integration method for solving ordinary differential equations, three kinds of weighting schemes for selection, and fitting algorithms for a one-compartment, extravascular, single-dose, and first-ordered absorption without lag time model.

References

C. Y. Lee and Y. J. Lee. PKfit: A Data Analysis Tool for Pharmacokinetics. <http://ce.kmu.edu.tw/index.htm>

fzero.nolag	<i>Fitting Functions for a One-Compartment, Extravascular, Single-Dose, and Zero-Ordered Absorption without Lag Time Model</i>
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Description

Includes user-supplied functions for model definition, integration method for solving ordinary differential equations, three kinds of weighting schemes for selection, and fitting algorithms for a one-compartment, extravascular, and zero-ordered absorption without lag time model.

References

C. Y. Lee and Y. J. Lee. PKfit: A Data Analysis Tool for Pharmacokinetics. <http://ce.kmu.edu.tw/index.htm>

InVVRefcsv	<i>choose separator and decimal type</i>
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Description

Separator : comma, semicolon ,white space. Decimal: comma, point.

InVVRefdata	<i>Input/Edit In Vivo raw data for IV, oral solution or IR drugs</i>
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Description

Users input/edit In Vivo raw data for IV, oral solution or IR drugs. Loading data file which was saved as .csv form or .RData form, or key in data in the data editor window.

InVVTtestcsv	<i>choose separator and decimal type</i>
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Description

Separator : comma, semicolon ,white space. Decimal: comma, point.

InVVTtestdata	<i>Input/Edit In Vivo raw data for extended release formulations with different rates and Edit In Vitro Dissolution Data</i>
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Description

Users input/edit edit In Vivo raw data for extended release formulations with different rates and In Vitro Dissolution Data. Loading data file which was saved as .csv form or .RData form, or key in data in the data editor window.

iv.route	<i>Options for Parenteral Models Menu</i>
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Description

Provide the following one PK models for selection: 1. one-compartment, IV-bolus, and single-dose model;

ivivc_demo	<i>ivivc Demo</i>
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Description

1.iv data: Dose=200 mg Vd=35 L Ke=0.0863 h-1 2.in vitro dissolution (FRD) and in vivo observed plasma conc.(conc.obs) Time=c(0,1,2,3,4,5,6,7,8) FRD=c(0,18.7,45.3,62.4,77.3,84.9,91.5,92.7,95.8) conc.obs=c(0,0.891,1.997,2.616,3.411,3.33,3.868,3.371,3.433)

References

C. J. Shishoo, S. S. Savale, S. A. Shah, , I. S. Rathod, and P. K. Mukherjee, Indian J.Pharm. Sci., 2002, 64, 222.

 noniv.route

Options for Extravascular Models Menu

Description

Provide the following three PK models for selection: 1. one-compartment, single-dose, and first-ordered absorption with lag time model; 2. one-compartment, single-dose, and first-ordered absorption without lag time model; 3. one-compartment, single-dose, and zero-ordered absorption without lag time model;

 one.list

Options for One-Compartment Models Menu

Description

Provide the following two PK models for selection: 1. IV (bolus or infusion) model; and 2. non IV route model.

 PK

PK value from references Menu

Description

Users can use an existed PK Data Files or Enter PK value from references

 PKfit

PK fitting for IV, IR, oral solution data: PK fitting Menu

Description

Provide the following one method for selection: 1. 1-Compartment PK Model

 PKvalue

PK parameter value Menu

Description

User can get PK parameters from curve fitting (PKfit), or enter PK parameters from Literatures.

plotting.cp	<i>plot plasma conc.</i>
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Description

plot plasma conc.(observed).

plotting.lin	<i>Plot for Linear Model</i>
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Description

Plot for linear pharmacokinetic model for IV, oral solution or IR drug.

plotting.non	<i>Plot for Nonlinear Model</i>
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Description

Plot for nonlinear pharmacokinetic model for IV, oral solution or IR drug..

plotting.vitro	<i>plot in vitro dissolution</i>
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Description

Plot for in vitro dissolution data

run	<i>List of ivivc Menu</i>
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Description

ivivc Menu

SelModel

Model Dependent or Independent Method

Description

Provide the following one method for selection: 1. Model Dependent Method

WagNel

Wagner-Nelson method

Description

Nine functions in Wagner-Nelson method: 1.calculate AUC(0~t) 2.calculate Fab (3.perform a Linear Regression 4.calculate FABpred(5.calculate conc.pred (predicted concentration) 6.PEC-max(Average absolute prediction error of Cmax) 7.PEAUC (Average absolute prediction error of AUC) 8.Plot In vivo Absorption : Fraction of Absorption(9.In vivo plasma concentration (Predicted): Plasma conc. vs. time

References

Dr.Mukesh Gohel * , R. R. Delvadia, D. C. Parikh, M. M. Zinzuwadia, C. D. Soni, K. G. Sarvaiya R. Joshi and A. S. Dabhi. Simplified Mathematical Approach for Back Calculation in Wagner-Nelson Method. <http://www.pharmainfo.net/reviews/simplified-mathematical-approach-back-calculation-wagner-nelson-method>

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