

# Package ‘ivivc’

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**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

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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).

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

Try again or Leave ivivc package.

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check	<i>Check mechanism</i>
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**Description**

Checking if the initial value for parameter being zero.

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

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

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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.

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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>

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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>

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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>

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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>

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

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

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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.

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InVVTestcsv	<i>choose separator and decimal type</i>
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**Description**

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

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InVVTestdata	<i>Input/Edit In Vivo raw data for extended release formulations with different rates and Edit In Vitro Dissoution 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 Dissoution Data. Loading data file which was saved as .csv form or .RData form, or key in data in the data editor window.

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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;

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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.

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 noniv.route

*Options for Extravascular Models Menu*


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**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;

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 one.list

*Options for One-Compartment Models Menu*


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**Description**

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

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 PK

*PK value from references Menu*


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**Description**

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

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 PKfit

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


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**Description**

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

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 PKvalue

*PK parameter value Menu*


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**Description**

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

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

plot plasma conc.(observed).

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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.

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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..

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

Plot for in vitro dissolution data

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

ivivc Menu

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SelModel

*Model Dependent or Independent Method*

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### **Description**

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

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WagNel

*Wagner-Nelson method*

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### **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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