

Package ‘PKfit’

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Title A Data Analysis Tool for Pharmacokinetics

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Depends R (>= 2.12.0)

Imports stats4, deSolve, minpack.lm

Description PKfit is a nonlinear regression program which is designed to perform model/curve fitting and model simulations for pharmacokinetics.

License GPL (>= 2)

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<i>aicllsbc</i>	<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).

<i>data.manipulate</i>	<i>Data Manipulation</i>
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Description

Loading data file which was saved as .csv form or .RData form, or key in data in the data editor window.

<i>description_version</i>	<i>Description/logo for PKfit</i>
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Description

Description/logo for PKfit

<i>entertitle</i>	<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.

err_types	<i>To Generate Simulated Values for each PK Parameter Based on Error Types</i>
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Description

Four Error Types are: 1. Normal Error, 2. Uniform Error, 3. Normal Error*True Value, and 4. Uniform Error*True Value

fbolus.mm	<i>Fitting Functions for a One-Compartment, IV-Bolus, Single-Dose, and Michaelis-Menten Elimination 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, single-dose, and Michaelis-Menten elimination model.

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.

fbolus2	<i>Fitting Functions for a three-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 two-compartment, IV-bolus, and single-dose model.

fbolus3	<i>Fitting Functions for a three-Compartment, IV-Bolus, and Single-Dose Model</i>
---------	---

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 three-compartment, IV-bolus, and single-dose model.

fbolus3.mm	<i>Fitting Functions for a three-Compartment, IV-Bolus and Single-Dose Model with Michaelis-Menten Elimination</i>
------------	--

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 three-compartment, IV-bolus, and single-dose model with Michaelis-Menten Elimination.

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.

ffirst.lagm	<i>Fitting Functions for a One-Compartment, Extravascular, Single-Dose, First-Ordered Absorption, and Michaelis-Menten Elimination 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, first-ordered absorption, and Michaelis-Menten elimination with lag time model.

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.

ffirst.nolagm	<i>Fitting Functions for a One-Compartment, Extravascular, Single-Dose, First-Ordered Absorption, and Michaelis-Menten Elimination 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, first-ordered absorption, and Michaelis-Menten elimination without lag time model.

ffirst2	<i>Fitting Functions for a Two-Compartment, Extravascular, 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 two-compartment, extravascular, and first-ordered absorption without lag time model.

finfu.mm	<i>Fitting Functions for a One-Compartment, IV-Infusion, Single-Dose, and Michaelis-Menten Elimination 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-infusion, single-dose, and Michaelis-Menten elimination model.

finfu1	<i>Fitting Functions for a One-Compartment, IV-Infusion, and Single-Dose Model</i>
--------	--

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-infusion, and single-dose model.

finfu2	<i>Fitting Functions for a Two-Compartment, IV-Infusion, 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 two-compartment, IV-infusion, and single-dose model.

fmacro.one	<i>Fitting Functions for a One-Exponential Term Model</i>
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Description

Includes user-supplied functions for model definitions, integration method for solving ordinary differential equations, three kinds of weighting schemes for selection, and fitting algorithms for a one-exponential term model.

fmacro.three	<i>Fitting Functions for a Three-Exponential Term 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 three-exponential term model. terms.

`fmacro.two`*Fitting Functions for a Two-Exponential Term Model*

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 two-exponential term model.

`fzero.nolag`*Fitting Functions for a One-Compartment, Extravascular, Single-Dose, and Zero-Ordered Absorption without Lag Time Model*

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.

`fzero.nolagm`*Fitting Functions for a One-Compartment, Extravascular, Single-Dose, Zero-Ordered Absorption, and Michaelis-Menten Elimination without Lag Time Model*

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, zero-ordered absorption, and Michaelis-Menten elimination without lag time model.

`iv.bolus.demo`*Demo of fitting a set of data obtained from iv bolus*

Description

Demo of fitting a set of data obtained from iv bolus

`iv.route`*Options for Parenteral Models*

Description

Provide the following four PK models for selection: 1. one-compartment, IV-bolus, and single-dose model; 2. one-compartment, IV-bolus, single-dose, and Michaelis-Menten elimination model; 3. one-compartment, IV-infusion, and single dose model; and 4. one-compartment, IV-infusion, single dose, and Michaelis-Menten elimination model.

`macro`*Options for Macroconstant Exponential Models*

Description

Provide the following three PK models for selection: 1. one-exponential term model; 2. two-exponential term model; and 3. three-exponential term model.

`mcsim.demo`*Demo of a Monte-Carlo simulation*

Description

Demo of a Monte-Carlo simulation

`mmpk.demo`*Demo of fitting a Michaelis-Menton model*

Description

Demo of fitting a Michaelis-Menton model

`montecarlo`*Monte carlo simulation*

Description

Monte carlo simulation.

 noniv.route

Options for Extravascular Models

Description

Provide the following six 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; 4. one-compartment, single-dose, first-ordered absorption, and Michaelis-Menten elimination with lag time model; 5. one-compartment, single-dose, first-ordered absorption, and Michaelis-Menten elimination without lag time model; and 6. one-compartment, single-dose, zero-ordered absorption, and Michaelis-Menten elimination without lag time model.

nor.fit

Options for Normal Fitting

Description

Includes data manipulation and models selection.

one.list

Options for One-Compartment Models

Description

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

OutputFilez

OutputFilez

Description

function to automatically setup default output files.

PK.fit

Options for PK Models

Description

Provide the following four PK models for selection: 1. one-compartment model; 2. two-compartment model; and 3. macroconstant exponential functions.

PK.sim	<i>Options for Simulation Functions</i>
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Description

Provide the following four PK models for selection: 1. one-compartment, and IV (bolus or infusion) model; 2. one-compartment, and non IV route model; 3. two-compartment model; and 4. macroconstant exponential functions.

PK.sim.MD	<i>Menu for Simulation Functions with Multiple-Dose</i>
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Description

Menu for Simulation Functions with Multiple-Dose

PK.sim.SD	<i>Menu for Simulation Functions with Single-Dose</i>
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Description

Menu for Simulation Functions with Single-Dose

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

Plot for linear pharmacokinetic model.

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

Plot for nonlinear pharmacokinetic model.

plotting.sim	<i>Plot for Simulation Model for single-dosing</i>
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Description

Plot for simulation model for single-dosing.

run	<i>Main Menu for the PKfit Package</i>
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Description

a simple menu-based interface in the PKfit package

Usage

run()

savefile	<i>Enter the name for file</i>
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Description

If users want to save file, allow them to enter the name for file.

sbolus.mm	<i>Simulation Functions for a One-Compartment, IV-Bolus, Single-Dose, and Michaelis-Menten Elimination Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

sbolus1	<i>Simulation functions for a One-Compartment, IV-Bolus, and Single-Dose Model</i>
---------	--

Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

sbolus2	<i>Simulation Functions for a Two-Compartment, IV-Bolus, and Single-Dose Model</i>
---------	--

Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

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

Includes entering initial values Of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

sfirst.lagm	<i>Simulation Functions for a One-Compartment, Extravascular, Single-Dose, First-Ordered Absorption, and Michaelis-Menten Elimination with Lag Time Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

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

Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, uniform error*true value.

sfirst.nolagm	<i>Simulation Functions for a One-Compartment, Extravascular, Single-Dose, First-Ordered Absorption, and Michaelis-Menten Elimination without Lag Time Model</i>
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Description

Consisting of entering the parameter initial value and five error types for selection: no error, normal error, uniform error, normal error*true value, uniform error*true value.

sfirst2	<i>Simulation Functions for a Two-Compartment, Extravascular, Single-Dose, and First-Ordered Absorption without Lag Time Model</i>
---------	--

Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

sinfu.mm	<i>Simulation Functions for a One-Compartment, IV-Infusion, and Michaelis-Menten Elimination Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

sinful	<i>Simulation Functions for a One-Compartment, IV-Infusion, and Single-Dose Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

sinfu2	<i>Simulation Functions for a Two-Compartment, IV-Infusion, and Single-Dose Model</i>
--------	---

Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

smacro	<i>Options for Macroconstant Exponential Models Simulation</i>
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Description

Provides the following three models for selection: 1. one-exponential term model; 2. two-exponential term model; and 3. three-exponential term model.

smacro.one	<i>Simulation Functions for a One-Exponential Term Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

smacro.one.out	<i>Simulation Output for a One-Exponential Term Model</i>
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Description

Display simulation output for one-exponential term model and plots.

smacro.three	<i>Simulation Functions for a Three-Exponential Term Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

smacro.three.out	<i>Simulation Output for a Three-Exponential Term Model</i>
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Description

Display simulation output for a three-exponential term model and plots.

smacro.two	<i>Simulation Functions for a Two-Exponential Term Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

smacro.two.out	<i>Simulation Output for a Two-Exponential Term Model</i>
----------------	---

Description

Display simulation output for a two-exponential term model and plots.

sone.iv.route.MD	<i>Menu for One-Compartment, and IV-Dosing PK Models Simulation for Multiple-Dose</i>
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Description

Menu for One-Compartment, and IV-Dosing PK Models Simulation for Multiple-Dose

sone.iv.route.SD	<i>Menu for One-Compartment, and IV-Dosing PK Models Simulation for Single-Dose</i>
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Description

Menu for One-Compartment, and IV-Dosing PK Models Simulation for Single-Dose

sone.noniv.route.MD	<i>Menu for One-Compartment, and Extravascular PK Models Simulation of Multiple-Dose</i>
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Description

Menu for One-Compartment, and Extravascular PK Models Simulation of Multiple-Dose

sone.noniv.route.SD	<i>Menu for One-Compartment, and Extravascular PK Models Simulation of Single-Dose</i>
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Description

Menu for One-Compartment, and Extravascular PK Models Simulation of Single-Dose

stwo.MD.all	<i>Menu for Two-Compartment PK Models Simulation of Multiple-Dose</i>
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Description

Menu for Two-Compartment PK Models Simulation of Multiple-Dose

stwo.SD.all	<i>Menu for Two-Compartment PK Models Simulation of Single-Dose</i>
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Description

Menu for Two-Compartment PK Models Simulation of Single-Dose

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

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, uniform error*true value.

szero.nolagm	<i>Simulation Functions for a One-Compartment, Extravascular, Single-Dose, Zero-Ordered Absorption, and Michaelis-Menten Elimination without Lag Time Model</i>
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Description

Includes entering initial values of PK parameters and five error types for selection: no error, normal error, uniform error, normal error*true value, and uniform error*true value.

two.list	<i>Options for Two-Compartment Models</i>
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Description

Provide the following three PK models for selection: 1. two-compartment, IV-bolus, and single-dose model; 2. two-compartment, IV-infusion, and single-dose model; and 3. two-compartment, extravascular, single-dose, and first-ordered absorption without lag time model.

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