

# Package ‘PKfit’

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**Title** A Data Analysis Tool for Pharmacokinetics

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**Depends** R (>= 2.8.0), stats4, odesolve, rgenoud

**Description** PKfit is a nonlinear regression (including a genetic algorithm) program which was 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).

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<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>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.

---

<i>fbolus.mm</i>	<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>
---------	---

---

**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 Two-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 two-compartment, IV-bolus, and single-dose model.

---

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

---

**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>
--------------	---

---

**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>
---------------	---

---

**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>
---------	--

---

**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>
----------	--

---

**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>
--------	--

---

**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>
------------	---

---

**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>
--------------	---

---

**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.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	<i>Options for Macroconstant Exponential Models</i>
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---

**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.

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montecarlo	<i>Monte carlo simulation</i>
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**Description**

Monte carlo simulation.

---

noniv.route	<i>Options for Extravascular Models</i>
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---

**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	<i>Options for Normal Fitting</i>
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---

**Description**

Includes data manipulation and models selection.

---

one.list	<i>Options for One-Compartment Models</i>
----------	---

---

**Description**

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

---

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                      *Options for Simulation Functions*

---

**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.

---

PKmenu                      *Main Menu for the PKfit Package*

---

**Description**

PKmenu presents a simple menu-based interface in the PKfit package

**Usage**

PKmenu()

---

plotting.lin                      *Plot for Linear Model*

---

**Description**

Plot for linear pharmacokinetic model.

---

plotting.non                      *Plot for Nonlinear Model*

---

**Description**

Plot for nonlinear pharmacokinetic model.

---

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

**Description**

Plot for simulation model.

---

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>
-----------	--

---

**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.

---

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

---

**Description**

Display simulation output for a one-compartment, IV-bolus, single-dose, and Michaelis-Menten elimination model and plots.

---

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.

---

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

---

**Description**

Display simulation output for one-compartment, IV-bolus, and single-dose model and plots.

---

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.

---

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

---

**Description**

Display simulation output for a two-compartment, IV-bolus, and single-dose model and plots.

---

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

---

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

---

sfirst.mm.out	<i>Simulation Output for a One-Compartment, Extravascular, First-Ordered Absorption, and Michaelis-Menten Elimination Model</i>
---------------	---

---

**Description**

Display simulation output for a one-compartment, extravascular, first-ordered absorption, and Michaelis-Menten elimination model and plots.

---

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>
---------------	--

---

**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.

---

sfirst1.out	<i>Simulation Output for a One-Compartment, Extravascular, Single-Dose, and First-Ordered Absorption Model</i>
-------------	--

---

**Description**

Display simulation output for a one-compartment, extravascular, single-dose, and first-ordered absorption model and plots.

---

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.

---

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

---

**Description**

Display simulation output for a two-compartment, extravascular, single-dose, and first-ordered absorption without lag time model and plots.

---

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

---

**Description**

Display simulation output for a one-compartment, IV-infusion, single-dose and Michaelis-Menten elimination model and plots.

---

sinfu1	<i>Simulation Functions for a One-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.

---

sinfu1.out	<i>Simulation Output for a One-Compartment, IV-infusion, and Single-Dose Model</i>
------------	--

---

**Description**

Display simulation output for a one-compartment, IV-infusion, and single-dose model and plots.

---

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.

---

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

---

**Description**

Display simulation output for a two-compartment model, IV-infusion, and single-dose model and plots.

---

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

---

**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`*Simulation Functions for a One-Exponential Term Model*

---

**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`*Simulation Output for a One-Exponential Term Model*

---

**Description**

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

---

`smacro.three`*Simulation Functions for a Three-Exponential Term Model*

---

**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`*Simulation Output for a Three-Exponential Term Model*

---

**Description**

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

---

`smacro.two`*Simulation Functions for a Two-Exponential Term Model*

---

**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	<i>Options for One-Compartment, and IV-Dosing PK Models Simulation</i>
---------------	--

---

**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.

---

sone.noniv.route	<i>Option for One-Compartment, and Extravascular PK Models Simulation</i>
------------------	---

---

**Description**

Provide the following six PK models for selection: 1. single-dose, and first-ordered absorption with lag time model; 2. single-dose, and first-ordered absorption without lag time model; 3. single-dose, and zero-ordered absorption without lag time model; 4. single-dose, first-ordered absorption, and Michaelis-Menten elimination with lag time model; 5. single-dose, first-ordered absorption, and Michaelis-Menten elimination without lag time model; and 6. single-dose, zero-ordered absorption, and Michaelis-Menten elimination without lag time model.

---

stwo.all	<i>Options for Two-Compartment PK Models Simulation</i>
----------	---

---

**Description**

Provides the following three 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.

---

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

---

**Description**

Display simulation output for a one-compartment, extravascular, single-dose, zero-ordered absorption, and Michaelis-Menten elimination without lag time model and plots.

---

szero.nolag	<i>Simulation Functions for a One-Compartment, Extravascular, Single-Dose, and Zero-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.

---

szero.nolagm	<i>Simulation Functions for a One-Compartment, Extravascular, Single-Dose, Zero-Ordered Absorption, and Michaelis-Menten Elimination 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.

---

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

---

**Description**

Display simulation output for a one-compartment, extravascular, single-dose, and zero-ordered absorption without lag time model and plots.

---

`two.list`*Options for Two-Compartment Models*

---

**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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