

Package ‘PKfit’

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Title Data Analysis Tool for Pharmacokinetics

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Depends R (>= 2.12.0)

Imports optimx, 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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R topics documented:

aicllsbc	3
data.manipulate	3
description_version	3
entertitle	3
err_types	4
fbolus.mm	4
fbolus1	4
fbolus2	4
fbolus3	5
fbolus3.mm	5
ffirst.lag	5
ffirst.lagm	5

ffirst.nolag	6
ffirst.nolagm	6
ffirst2	6
finfu.mm	6
finfu1	7
finfu2	7
fmacro.one	7
fmacro.three	7
fmacro.two	8
fzero.nolag	8
fzero.nolagm	8
iv.bolus.demo	8
iv.route	9
macro	9
mcsim.demo	9
mmpk.demo	9
montecarlo	9
noniv.route	10
nor.fit	10
one.list	10
OutputFilez	10
PK.fit	10
PK.sim	11
PK.sim.MD	11
PK.sim.SD	11
plotting.lin	11
plotting.non	11
plotting.sim	12
run	12
savefile	12
sbolus.mm	12
sbolus1	12
sbolus2	13
sfirst.lag	13
sfirst.lagm	13
sfirst.nolag	13
sfirst.nolagm	14
sfirst2	14
sinfu.mm	14
sinfu1	14
sinfu2	15
smacro	15
smacro.one	15
smacro.one.out	15
smacro.three	15
smacro.three.out	16
smacro.two	16
smacro.two.out	16

<i>aicllsbc</i>	3
sone.iv.route.MD	16
sone.iv.route.SD	16
sone.noniv.route.MD	17
sone.noniv.route.SD	17
stwo.MD.all	17
stwo.SD.all	17
szero.nolag	17
szero.nolagm	18
two.list	18
Index	19

<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>
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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, 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	<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>
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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.

OutputFilez	<i>OutputFilez</i>
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Description

function to automatically setup default output files.

PK.fit	<i>Options for PK Models</i>
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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>
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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.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>
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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.

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>
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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.

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

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.

Index

*Topic **misc**

- aicllsbc, 3
- data.manipulate, 3
- description_version, 3
- entertitle, 3
- err_types, 4
- fbolus.mm, 4
- fbolus1, 4
- fbolus2, 4
- fbolus3, 5
- fbolus3.mm, 5
- ffirst.lag, 5
- ffirst.lagm, 5
- ffirst.nolag, 6
- ffirst.nolagm, 6
- ffirst2, 6
- finfu.mm, 6
- finfu1, 7
- finfu2, 7
- fmacro.one, 7
- fmacro.three, 7
- fmacro.two, 8
- fzero.nolag, 8
- fzero.nolagm, 8
- iv.bolus.demo, 8
- iv.route, 9
- macro, 9
- mcsim.demo, 9
- mmpk.demo, 9
- montecarlo, 9
- noniv.route, 10
- nor.fit, 10
- one.list, 10
- OutputFilez, 10
- PK.fit, 10
- PK.sim, 11
- PK.sim.MD, 11
- PK.sim.SD, 11
- plotting.lin, 11

- plotting.non, 11
- plotting.sim, 12
- run, 12
- savefile, 12
- sbolus.mm, 12
- sbolus1, 12
- sbolus2, 13
- sfirst.lag, 13
- sfirst.lagm, 13
- sfirst.nolag, 13
- sfirst.nolagm, 14
- sfirst2, 14
- sinfu.mm, 14
- sinfu1, 14
- sinfu2, 15
- smacro, 15
- smacro.one, 15
- smacro.one.out, 15
- smacro.three, 15
- smacro.three.out, 16
- smacro.two, 16
- smacro.two.out, 16
- sone.iv.route.MD, 16
- sone.iv.route.SD, 16
- sone.noniv.route.MD, 17
- sone.noniv.route.SD, 17
- stwo.MD.all, 17
- stwo.SD.all, 17
- szero.nolag, 17
- szero.nolagm, 18
- two.list, 18

- aicllsbc, 3
- data.manipulate, 3
- description_version, 3
- entertitle, 3
- err_types, 4
- fbolus.mm, 4

fbolus1, 4
fbolus2, 4
fbolus3, 5
fbolus3.mm, 5
ffirst.lag, 5
ffirst.lagm, 5
ffirst.nolag, 6
ffirst.nolagm, 6
ffirst2, 6
finfu.mm, 6
finfu1, 7
finfu2, 7
fmacro.one, 7
fmacro.three, 7
fmacro.two, 8
fzero.nolag, 8
fzero.nolagm, 8

iv.bolus.demo, 8
iv.route, 9

macro, 9
mcsim.demo, 9
mmpk.demo, 9
montecarlo, 9

noniv.route, 10
nor.fit, 10

one.list, 10
OutputFilez, 10

PK.fit, 10
PK.sim, 11
PK.sim.MD, 11
PK.sim.SD, 11
plotting.lin, 11
plotting.non, 11
plotting.sim, 12

run, 12

savefile, 12
sbolus.mm, 12
sbolus1, 12
sbolus2, 13
sfirst.lag, 13
sfirst.lagm, 13
sfirst.nolag, 13
sfirst.nolagm, 14

sfirst2, 14
sinfu.mm, 14
sinfu1, 14
sinfu2, 15
smacro, 15
smacro.one, 15
smacro.one.out, 15
smacro.three, 15
smacro.three.out, 16
smacro.two, 16
smacro.two.out, 16
sone.iv.route.MD, 16
sone.iv.route.SD, 16
sone.noniv.route.MD, 17
sone.noniv.route.SD, 17
stwo.MD.all, 17
stwo.SD.all, 17
szero.nolag, 17
szero.nolagm, 18

two.list, 18