

# Package ‘popPK’

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**Title** Summary of Population Pharmacokinetic Analysis

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**Depends** R (>= 2.12.2), Hmisc, lattice, grid, xpose4

**Suggests** R2wd

**Description** This package uses xpose4 to create standard graphs and tables for NONMEM runs.

**License** GPL (>= 2)

**LazyLoad** Yes

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Covariates	<i>Covariates function for popPK</i>
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**Description**

Creates individual parameter-covariate graphs, quantile summary graphs, and forest plot of covariate effects. Population predicted relationships specified in `info$cov.rel` are superimposed on the parameter-covariate graphs.

**Usage**

```
Covariates(info)
```

**Arguments**

`info` See [popPK](#)

**Value**

Creates individual parameter-covariate (`parm.vs.cov`) and quantile summary (`parm.vs.cov.quantile`) graphs. Graphs with population predicted relationships specified in `info$cov.rel` are superimposed on the parameter-covariate graphs (`plotCov`). Forest plot with covariate effects (`ForestPlot`)

**Note**

For examples see [popPK](#).

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CreateInfo	<i>Create info list function for popPK</i>
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**Description**

Creates info list for popPK data.

**Usage**

```
CreateInfo(info)
```

**Arguments**

`info` See [popPK](#)

**Value**

Creates info list with all required arguments.

**Note**

For examples see [popPK](#).

**Author(s)**

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Demographics

*Demographics function for popPK*

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**Description**

Creates summary demographic tables and graphs.

**Usage**

Demographics(info)

**Arguments**

info            See [popPK](#)

**Value**

Creates tables (CatCovariates and ConCovariates), histograms (CovHist, CatHist), and scatter plot matrices of continuous covariates (CovSplom).

**Note**

For examples see [popPK](#).

**Author(s)**

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Diagnostics

*Diagnostic function for popPK*

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**Description**

Creates concentration-time profiles and goodness-of-fit graphs for popPK.

**Usage**

```
Diagnostics(info)
```

**Arguments**

info            See [popPK](#)

**Value**

Creates concentration-time profile graphs (conc.vs.time and ind.plots) and goodness-of-fit graphs (dv.vs.pred, dv.vs.ipred, wres.vs.time, iwres.vs.time, wres.vs.pred, iwres.vs.ipred, qqnorm.wres, qqnorm.iwres, histogram.wres, histogram.iwres), and histograms (CovHist, CatHist).

**Note**

For examples see [popPK](#).

**Author(s)**

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Estimates

*Estimates function for popPK*

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**Description**

Creates tables of NONMEM parameter estimates.

**Usage**

```
Estimates(info)
```

**Arguments**

info            See [popPK](#)

**Value**

Creates data.frame with parameter estimates (ThetaEstimates) for Covariates function, tables of NONMEM parameter estimates (NMestimates), summary of individual parameter estimates (ParameterSummary), scatter plot matrices of individual and random-effects parameters (ParmSplom and RanSplom), and histograms of individual and random-effects parameters (ParmHist and RanHist).

**Note**

For examples see [popPK](#).

**Author(s)**

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popPK

*Summary of Population Pharmacokinetic Analysis*

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**Description**

This package creates graphs and tables for NONMEM runs

**Usage**

```
popPK(info)
```

**Arguments**

info	A list including the following elements:
path	The path where the NONMEM control stream, output, data, and tables are located (Required).
run.no	The NONMEM run number (e.g. 1 for run1.mod/ctl) (Required).
alpha	Alpha level for parameter mean in quantile plot (default is 0.05).
bins	Cut-off points to group specified covariates by. The minimum and maximum value of the covariate will automatically be added and values outside the range of the covariate will be removed (default is to use quantiles).
cat.level	Substitute categorical covariates values with text string (e.g. SEX=list(Male='0', Female='1')).
cex	Size of symbols (default is 1, 1, 1, 1, 1, 1, 1, 1).
col	Colors for symbols (default is 'black', 'red', 'grey', 'blue', 'orange', 'green', 'yellow', 'brown').
cov.rel	List of identified parameter-covariate equations to plot (maximum of 1 continuous and 1 categorical covariate per equation).
covs	List of labels for covariates (default is covariate name in patab/catab).
device	Graphical device to print to (options: "wmf", "bmp", "jpg", "pdf", "png", or "tiff") (default is "pdf").

**digits** Number of significant digits to be used in tables.  
**drug.name** Drug name.  
**etas** List of labels for inter-individual variability parameters (default is omega name in control stream specified by ";").  
**group.by** Variable to group symbols in graphs by.  
**ind.plots** Plot individual concentration-time profiles (default is FALSE).  
**line.col** Line colors for parameter-covariate relationships (default is 'black', 'red', 'grey', 'blue', 'orange', 'green', 'yellow', 'brown').  
**lloq** Insert lower limit of quantification in goodness-of-fit graphs.  
**log.covs** Log transform covariates in Covariates function (default is FALSE).  
**log.obs** Log transform observations in Diagnostics function (default is FALSE).  
**log.parms** Log transform parameters in Covariates function (default is FALSE).  
**log.pred** Log transform predictions in Diagnostics function (default is FALSE).  
**lty** Line types for parameter-covariate equations (default is 1 (solid)).  
**lwd** Line width (default is 1).  
**mean** Parameter mean for quantile plots (default is "geometric", otherwise "arithmetic").  
**output** Output folder for graphs and tables (default is NA which will print to the screen).  
**pch** Symbols (default is 20 (closed circle), 1 (open circle), 15 (solid square), 22 (open square), 17 (solid triangle), 2 (open triangle), 215 (x), 3 (+)).  
**prefix** Prefix of your NONMEM control stream (default is run).  
**quantiles** Number of bins to group the covariates in (default is 4).  
**report** Create summary report in Word. This feature only works on Windows and requires R2wd package is installed along with statconnDCOM) (default is FALSE).  
**scale** Scale which the parameters were estimated in NONMEM (options='normal' or 'log').  
**smooth** Insert smooth (default is FALSE).  
**strat.by** Variable to stratify panels by in graphs.  
**suffix** NONMEM output table suffix (default is no suffix or .csv).  
**thetas** List of labels for fixed-effects parameters (default is theta name in control stream specified by ";").  
**units** Units for time and concentration.

### Value

The popPK function creates standard graphs and tables to summarize population pharmacokinetic analysis using NONMEM.

### Note

**DISCLAIMER:** This R package does not reflect the official policy of the FDA. No official endorsement by the FDA is intended or should be inferred. Use of the popPK package is at your own risk.

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**See Also**

[xposeData](#), [Demographics](#), [Diagnostics](#), [Estimates](#), and [Covariates](#)

**Examples**

```
#Restrictions
#No time-varying covariates
#One $THETA, $OMEGA, and $SIGMA for each parameter in the NONMEM control stream
#Only 1 continuous covariate pr equation in info$cov.rel
#Only bivariate categorical covariates in info$cov.rel coded as THETA(X)**CAT

info <-list(
  path=paste(R.home(), "/library/popPK/extdata",sep=""),
  run.no=1,
  output=NA,
  thetas=list(CL="Clearance (L/hr)",V="Volume of distribution (L)",
  KA="Absorption rate constant (1/hr)"),
  etas= list(ETA1="CL",ETA2="V",ETA3="KA"),
  covs = list(BW="Weight (kg)",AGE="Age (years)",ISM="Sex",RACE="Race"),
  cat.level=list(ISM = list(Male=1,Female=0),
  RACE = list(White=1,Black=2,Asian=3,Other=4)),
  group.by = "ISM",
  units = list(time="hr",conc="ng/mL"),
  drug.name = "Drug X",
  quantiles=4,
  log.pred=TRUE,log.obs=TRUE,
  bins=list(AGE=c(25,41)),
  cov.rel=list(CL~THETA(1)*1.01^ISM*(BW/70)^THETA(4),
  "Estimated exponent"=V~THETA(2)*(BW/70)^THETA(5),
  "Allometric"=V~THETA(2)*(BW/70)^1),
  report=TRUE
)

## Not run:
xposeData(info)
Demographics(info)
Diagnostics(info)
Estimates(info)
Covariates(info)
## End(Not run)
```

**Description**

Creates info list for popPK data.

**Usage**

```
printGraph(name,device,height,width)
```

**Arguments**

name	File name of graph.
device	Graphical device to print to (options: "wmf", "bmp", "jpg", "pdf", "png", or "tiff") (default is "pdf").
height	Height of graph.
width	Width of graph.

**Note**

For examples see [popPK](#).

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xpdb

*xpose data object created by xposeData*

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**Description**

xpose data object.

**Author(s)**

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xposeData

*Import data for popPK*

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### **Description**

Import NONMEM run using xpose.data function in xpose4 for popPK.

### **Usage**

```
xposeData(info)
```

### **Arguments**

info            See [popPK](#)

### **Value**

xpdb            xposeData returns the xpose.data object xpdb.

### **Note**

For examples see [popPK](#).

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