Package 'PKconverter'

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Type Package

Title The Parameter Converter of the Pharmacokinetic Models

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Description Pharmacokinetics is the study of drug absorption, distribution, metabolism, and excretion. The pharmacokinetics model explains that how the drug concentration change as the drug moves through the different compartments of the body. For pharmacokinetic modeling and analysis, it is essential to understand the basic pharmacokinetic parameters. All parameters are considered, but only some of parameters are used in the model. Therefore, we need to convert the estimated parameters to the other parameters after fitting the specific pharmacokinetic model. This package is developed to help this converting work. For more detailed explanation of pharmacokinetic parameters, see ``Gabrielsson and Weiner" (2007), ``ISBN-10: 9197651001"; ``Benet and Zia-Amirhosseini" (1995) <DOI:10.1177/019262339502300203>; ``Mould and Upton" (2012) <DOI:10.1038/psp.2012.4>; ``Mould and Upton" (2013) <DOI:10.1038/psp.2013.14>.

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Contents

`OneComp_Coefficient_Exponent`
Convert pharmacokinetic parameters for one compartment model

Description

Calculate pharmacokinetic parameters with parameters (A and alpha) in one compartment model "Aexp(-alpha)"

Usage

```
OneComp_Coefficient_Exponent(A,alpha,A.sd=NA,alpha.sd=NA,
          covar=c(Aalpha=NA),...)
```

Arguments

`A`	parameter in one compartment model "Aexp(-alpha)"
`alpha`	parameter in one compartment model "Aexp(-alpha)"
`A.sd`	standard error of A
`alpha.sd`	standard error of alpha
`covar`	covariances among parameters
`...`	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
OneComp_Coefficient_Exponent(A=0.125,alpha=0.5,A.sd=0.002,alpha.sd=0.009)
```

OneComp_Volume_Clearance

Convert pharmacokinetic parameters for one compartment model

Description

Calculate pharmacokinetic parameters with volume of distribution (V1) and clearance (Cl1)

Usage

```
OneComp_Volume_Clearance(V1,Cl1,V1.sd=NA,Cl1.sd=NA,
        covar=c(V1Cl1=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
Cl1	Clearance from compartment 1
V1.sd	standard error of V1
Cl1.sd	standard error of Cl1
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Gabrielsson and Weiner(2006) Pharmacokinetic and Pharmacodynamic Data Analysis: Concepts and Applications, Swedish Academy of Pharmaceutical Sciences.

Examples

```
OneComp_Volume_Clearance(V1=8,Cl1=4,V1.sd=0.01,Cl1.sd=0.01)
```

OneComp_Volume_Clearance_HalfLife

Convert pharmacokinetic parameters for one compartment model

Description

Calculate pharmacokinetic parameters with clearance (Cl1) and half-life (t_alpha)

Usage

```
OneComp_Volume_Clearance_HalfLife(Cl1,t_alpha,
         Cl1.sd=NA,t_alpha.sd=NA,covar=c(Cl1talpha=NA),...)
```

Arguments

Cl1	Clearance from compartment 1
t_alpha	half life of compartment 1
Cl1.sd	standard error of Cl1
t_alpha.sd	standard error of t_alpha
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
OneComp_Volume_Clearance_HalfLife(Cl1=4,t_alpha=0.568,
      Cl1.sd=0.01,t_alpha.sd=0.0003)
```

OneComp_Volume_Exponent

Convert pharmacokinetic parameters for one compartment model

Description

Calculate pharmacokinetic parameters with volume of distribution(V1) and parameter (alpha) in the model "Aexp(-alpha)"

Usage

```
OneComp_Volume_Exponent(V1,alpha,V1.sd=NA,alpha.sd=NA,
         covar=c(V1alpha=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
alpha	parameter in one compartment model "Aexp(-alpha)"
V1.sd	standard error of V1
alpha.sd	standard error of A
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
OneComp_Volume_Exponent(V1=8,alpha=0.5,V1.sd=0.01,alpha.sd=0.001)
```

`OneComp_Volume_RateConstant`
Convert pharmacokinetic parameters for one compartment model

Description

Calculate pharmacokinetic parameters with volume of distribution (V1) and elimination rate constant (k10)

Usage

```
OneComp_Volume_RateConstant(V1,k10,
             V1.sd=NA,k10.sd=NA,covar=c(V1k10=0),...)
```

Arguments

`V1`	The volume of distribution of compartment 1
`k10`	elimination rate constant
`V1.sd`	standard error of V1
`k10.sd`	standard error of k10
`covar`	covariances among parameters
`...`	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
OneComp_Volume_RateConstant(V1=8,k10=0.5,V1.sd=0.01,k10.sd=0.002)
```

PKconverterApp *Shiny App for converting the pharmacokinetic parameters*

Description

Pharmacokinetics is the study of drug absorption, distribution, metabolism, and excretion. The pharmacokinetics model explains that how the drug concentration change as the drug moves through the different compartments of the body. For pharmacokinetic modeling and analysis, it is essential to understand the basic pharmacokinetic parameters. All parameters are considered, but only some of parameters are used in the model. Therefore,we need to convert the estimated parameters to the other parameters after fitting the specific pharmacokinetic model.

Usage

```
PKconverterApp()
```

Examples

```
#PKconverterApp()
```

ThreeComp_Coefficient_Exponent
Convert pharmacokinetic parameters for three compartment model

Description

Calculate pharmacokinetic parameters with parameters (A, B, C, alpha, beta, and gamma) in two compartment model "Aexp(-alpha)+Bexp(-beta)+Cexp(-gamma)"

Usage

```
ThreeComp_Coefficient_Exponent(A,B,C,alpha,beta,gamma,A.sd=NA,
   B.sd=NA,C.sd=NA,alpha.sd=NA,beta.sd=NA,gamma.sd=NA,
   covar=c(AB=NA,AC=NA,Aalpha=NA,Abeta=NA,Agamma=NA,BC=NA,Balpha=NA,
   Bbeta=NA,Bgamma=NA,Calpha=NA,Cbeta=NA,Cgamma=NA,alphabeta=NA,
   alphagamma=NA,betagamma=NA),...)
```

Arguments

A	parameter in one compartment model "Aexp(-alpha)"
B	parameter in two compartment model "Aexp(-alpha)+Bexp(-beta)"
C	parameter in three compartment model "Aexp(-alpha)+Bexp(-beta)+Cexp(-gamma)"
alpha	parameter in one compartment model "Aexp(-alpha)"
beta	parameter in two compartment model "Aexp(-alpha)+Bexp(-beta)"

gamma	parameter in three compartment model "Aexp(-alpha)+Bexp(-beta)+Cexp(-gamma)"
A.sd	standard error of A
B.sd	standard error of B
C.sd	standard error of C
alpha.sd	standard error of alpha
beta.sd	standard error of beta
gamma.sd	standard error of gamma
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
ThreeComp_Coefficient_Exponent(A=12.2,B=3.76,C=1.44,
alpha=0.870,beta=0.12,gamma=0.013, A.sd=0.2,B.sd=0.005,C.sd=0.0005,
alpha.sd=0.009,beta.sd=0.006,gamma.sd=0.00005)
```

ThreeComp_Volume_Clearance

Convert pharmacokinetic parameters for three compartment model

---

Description

Calculate pharmacokinetic parameters with volume of distributions (V1, V2 and V3) and clearances (Cl1, Cl2, and Cl3)

Usage

```
ThreeComp_Volume_Clearance(V1,V2,V3,Cl1,Cl2,Cl3,
 V1.sd=NA,V2.sd=NA,V3.sd=NA, Cl1.sd=NA,Cl2.sd=NA,Cl3.sd=NA,
 covar=c(V1V2=NA,V1V3=NA,V1Cl1=NA,
   V1Cl2=NA,V1Cl3=NA,V2V3=NA,V2Cl1=NA,V2Cl2=NA,V2Cl3=NA,
   V3Cl1=NA,V3Cl2=NA,V3Cl3=NA,Cl1Cl2=NA,Cl1Cl3=NA,Cl2Cl3=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
V2	The volume of distribution of compartment 2
V3	The volume of distribution of compartment 3
Cl1	Clearance from compartment 1
Cl2	Clearance from compartment 2

Cl3	Clearance from compartment 3
V1.sd	standard error of V1
V2.sd	standard error of V2
V3.sd	standard error of V3
Cl1.sd	standard error of Cl1
Cl2.sd	standard error of Cl2
Cl3.sd	standard error of Cl3
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
ThreeComp_Volume_Clearance(V1=10,V2=100,V3=1000,Cl1=3,Cl2=2,Cl3=1,
  V1.sd=0.01,V2.sd=0.1,V3.sd=1,Cl1.sd=0.01,Cl2.sd=0.01,Cl3.sd=0.01)
```

ThreeComp_Volume_Clearance_HalfLife

Convert pharmacokinetic parameters for three compartment model

---

Description

Calculate pharmacokinetic parameters with volume of distributions (Vd and V1), clearance (Cl1) and half-lives (t_alpha, t_beta, and t_gamma)

Usage

```
ThreeComp_Volume_Clearance_HalfLife(V1,Vd,Cl1,t_alpha,t_beta,t_gamma,
 V1.sd=NA,Vd.sd=NA,Cl1.sd=NA,t_alpha.sd=NA,t_beta.sd=NA,t_gamma.sd=NA,
 covar=c(V1Vd=NA,V1Cl1=NA,V1talpha=NA,V1tbeta=NA,V1tgamma=NA,VdCl1=NA,
   Vdtalpha=NA,Vdtbeta=NA,Vdtgamma=NA,Cl1talpha=NA,Cl1tbeta=NA,
   Cl1tgamma=NA,talphatbeta=NA,talphatgamma=NA,tbetatgamma=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
Vd	Total volume of distributions
Cl1	Clearance from compartment 1
t_alpha	half life of compartment 1
t_beta	half life of compartment 2

t_gamma	half life of compartment 3
V1.sd	standard error of V1
Vd.sd	standard error of Vd
Cl1.sd	standard error of Cl1
t_alpha.sd	standard error of t_alpha
t_beta.sd	standard error of t_beta
t_gamma.sd	standard error of t_gamma
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
ThreeComp_Volume_Clearance_HalfLife(V1=5,Vd=1110,Cl1=3,
t_alpha=1.142,t_beta=52.2,t_gamma=931, V1.sd=0.01,Vd.sd=20,Cl1.sd=0.01,
t_alpha.sd=0.002,t_beta.sd=0.5,t_gamma.sd=5.6)
```

ThreeComp_Volume_Exponent

Convert pharmacokinetic parameters for three compartment model

---

Description

Calculate pharmacokinetic parameters with volume of distribution(V1), transfer rate constant (k12 and k31), and parameters (alpha, beta and gamma) in the model "Aexp(-alpha)+Bexp(-beta)+Cexp(-gamma)"

Usage

```
ThreeComp_Volume_Exponent(V1,alpha,beta,gamma,k21,k31,
 V1.sd=NA,alpha.sd=NA,beta.sd=NA,gamma.sd=NA,k21.sd=NA,k31.sd=NA,
 covar=c(V1alpha=NA,V1beta=NA,V1gamma=NA,V1k21=NA,V1k31=NA,
   alphabeta=NA,alphagamma=NA,alphak21=NA,alphak31=NA,
   betagamma=NA,betak21=NA,betak31=NA,gammak21=NA,gammak31=NA,
   k21k31=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
alpha	parameter in one compartment model "Aexp(-alpha)"
beta	parameter in two compartment model "Aexp(-alpha)+Bexp(-beta)"
gamma	parameter in three compartment model "Aexp(-alpha)+Bexp(-beta)+Cexp(-gamma)"
k21	transfer rate constants from compartment 2 to compartment 1
k31	transfer rate constants from compartment 3 to compartment 1
V1.sd	standard error of V1
alpha.sd	standard error of alpha
beta.sd	standard error of beta
gamma.sd	standard error of gamma
k21.sd	standard error of k21
k31.sd	standard error of k31
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
ThreeComp_Volume_Exponent(V1=10,alpha=0.6, beta=0.013, gamma=0.00074,
   k21=0.02, k31=0.001, V1.sd=0.01,alpha.sd=0.01,beta.sd=0.00005,
   gamma.sd=0.000002, k21.sd=0.0006,k31.sd=0.0000005)
```

ThreeComp_Volume_RateConstant

Convert pharmacokinetic parameters for three compartment model

---

Description

Calculate pharmacokinetic parameters with volume of distribution (V1), elimination rate constant (k10), and transter rate constants (k12, k13, k21, and k31)

Usage

```
ThreeComp_Volume_RateConstant(V1,k10,k12,k13,k21,k31,
 V1.sd=NA,k10.sd=NA,k12.sd=NA,
 k13.sd=NA,k21.sd=NA,k31.sd=NA,covar=c(V1k10=NA,V1k12=NA,V1k13=NA,
   V1k21=NA,V1k31=NA,k10k12=NA,k10k13=NA,k10k21=NA,k10k31=NA,
   k12k13=NA,k12k21=NA,k12k31=NA,k13k21=NA,k13k31=NA,k21k31=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
k10	elimination rate constant
k12	transfer rate constants from compartment 1 to compartment 2
k13	transfer rate constants from compartment 1 to compartment 3
k21	transfer rate constants from compartment 2 to compartment 1
k31	transfer rate constants from compartment 3 to compartment 1
V1.sd	standard error of V1
k10.sd	standard error of k10
k12.sd	standard error of k12
k13.sd	standard error of k13
k21.sd	standard error of k21
k31.sd	standard error of k31
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
ThreeComp_Volume_RateConstant(V1=10,k10=0.3,k12=0.2,k13=0.1,k21=0.02,
        k31=0.001,V1.sd=0.1,k10.sd=0.002,k12.sd=0.001,
        k13.sd=0.0005,k21.sd=0.0005,k31.sd=0.000005)
```

TwoComp_Coefficient_Exponent

Convert pharmacokinetic parameters for two compartment model

Description

Calculate pharmacokinetic parameters with parameters (A, B, alpha and beta) in two compartment model "Aexp(-alpha)+Bexp(-beta)"

Usage

```
TwoComp_Coefficient_Exponent(A,B,alpha,beta,
 A.sd=NA,B.sd=NA,alpha.sd=NA,beta.sd=NA,
 covar=c(AB=NA,Aalpha=NA,Abeta=NA,Balpha=NA,Bbeta=NA,alphabeta=NA),...)
```

Arguments

A	parameter in one compartment model "Aexp(-alpha)"
B	parameter in two compartment model "Aexp(-alpha)+Bexp(-beta)"
alpha	parameter in one compartment model "Aexp(-alpha)"
beta	parameter in two compartment model "Aexp(-alpha)+Bexp(-beta)"
A.sd	standard error of A
B.sd	standard error of B
alpha.sd	standard error of alpha
beta.sd	standard error of beta
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
TwoComp_Coefficient_Exponent(A=0.196,B=0.0036,alpha=1.221,beta=0.0287,
A.sd=0.002,B.sd=0.00005,alpha.sd=0.09,beta.sd=0.0006)
```

TwoComp_Volume_Clearance

Convert pharmacokinetic parameters for two compartment model

Description

Calculate pharmacokinetic parameters with volume of distributions (V1 and V2) and clearances (Cl1 and Cl2)

Usage

```
TwoComp_Volume_Clearance(V1,V2,Cl1,Cl2,
                  V1.sd=NA,V2.sd=NA,Cl1.sd=NA,Cl2.sd=NA,
                  covar=c(V1V2=0,V1Cl1=0,V1Cl2=0,
                    V2Cl1=0,V2Cl2=0,Cl1Cl2=0),...)
```

Arguments

V1	The volume of distribution of compartment 1
V2	The volume of distribution of compartment 2
Cl1	Clearance from compartment 1
Cl2	Clearance from compartment 2

V1.sd	standard error of V1
V2.sd	standard error of V2
Cl1.sd	standard error of Cl1
Cl2.sd	standard error of Cl2
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
TwoComp_Volume_Clearance(V1=5,V2=50,Cl1=3.5,Cl2=2.5,
        V1.sd=0.01,V2.sd=0.1,Cl1.sd=0.01,Cl2.sd=0.01)
```

TwoComp_Volume_Clearance_HalfLife

Convert pharmacokinetic parameters for two compartment model

Description

Calculate pharmacokinetic parameters with volume of distribution(V1), clearance (Cl1) and half-lives (t_alpha and t_beta)

Usage

```
TwoComp_Volume_Clearance_HalfLife(V1,Cl1,t_alpha,t_beta,
 V1.sd=NA,Cl1.sd=NA,t_alpha.sd=NA,
 t_beta.sd=NA,covar=c(V1Cl1=NA,V1talpha=NA,V1tbeta=NA,Cl1talpha=NA,
   Cl1tbeta=NA,talphatbeta=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
Cl1	Clearance from compartment 1
t_alpha	half life of compartment 1
t_beta	half life of compartment 2
V1.sd	standard error of V1
Cl1.sd	standard error of Cl1
t_alpha.sd	standard error of t_alpha
t_beta.sd	standard error of t_beta
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
TwoComp_Volume_Clearance_HalfLife(V1=5,Cl1=3.5,t_alpha=0.568,t_beta=24.2,
V1.sd=0.01,Cl1.sd=0.01,t_alpha.sd=0.002,t_beta.sd=0.5)
```

TwoComp_Volume_Exponent

Convert pharmacokinetic parameters for two compartment model

Description

Calculate pharmacokinetic parameters with volume of distribution(V1), transfer rate constant (k12), and parameters (alpha and beta) in the model "Aexp(-alpha)+Bexp(-beta)"

Usage

```
TwoComp_Volume_Exponent(V1,alpha,beta,k21,V1.sd=NA,
 alpha.sd=NA,beta.sd=NA,k21.sd=NA,
 covar=c(V1alpha=NA,V1beta=NA,V1k21=NA,alphabeta=NA,
 alphak21=NA,betak21=NA),...)
```

Arguments

V1	The volume of distribution of compartment 1
alpha	parameter in one compartment model "Aexp(-alpha)"
beta	parameter in two compartment model "Aexp(-alpha)+Bexp(-beta)"
k21	transfer rate constants from compartment 2 to compartment 1
V1.sd	standard error of V1
alpha.sd	standard error of alpha
beta.sd	standard error of beta
k21.sd	standard error of k21
covar	covariances among parameters
...	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
TwoComp_Volume_Exponent(V1=5,alpha=1.221, beta=0.029, k21=0.05,
V1.sd=0.01,alpha.sd=0.01,beta.sd=0.00005,k21.sd=0.0006)
```

`TwoComp_Volume_RateConstant` *Convert pharmacokinetic parameters for two compartment model*

Description

Calculate pharmacokinetic parameters with volume of distribution (V1), elimination rate constant (k10), and transter rate constants (k12, k21)

Usage

```
TwoComp_Volume_RateConstant(V1,k10,k12,k21,
              V1.sd=NA,k10.sd=NA,k12.sd=NA,k21.sd=NA,
              covar=c(V1k10=NA,V1k12=NA,V1k21=NA,
              k10k12=NA,k10k21=NA,k12k21=NA),...)
```

Arguments

`V1`	The volume of distribution of compartment 1
`k10`	elimination rate constant
`k12`	transfer rate constants from compartment 1 to compartment 2
`k21`	transfer rate constants from compartment 2 to compartment 1
`V1.sd`	standard error of V1
`k10.sd`	standard error of k10
`k12.sd`	standard error of k12
`k21.sd`	standard error of k21
`covar`	covariances among parameters
`...`	arguments to be passed to methods

References

http://www.nonmemcourse.com/convert.xls

Examples

```
TwoComp_Volume_RateConstant(V1=5,k10=0.7,k12=0.5,k21=0.05,
        V1.sd=0.01,k10.sd=0.002,k12.sd=0.001,k21.sd=0.0005)
```

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