

Package ‘NonCompart’

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Title Noncompartmental Analysis for Pharmacokinetic Data

Description Conduct a noncompartmental analysis as closely as possible to the most widely used commercial software for pharmacokinetic analysis, i.e. 'Phoenix(R) WinNonlin(R)' <<https://www.certara.com/software/pkpd-modeling-and-simulation/phoenix-winnonlin/>>. Some features are

- 1) Use of CDISC SDTM terms
- 2) Automatic slope selection with the same criterion of WinNonlin(R)
- 3) Supporting both 'linear-up linear-down' and 'linear-up log-down' method
- 4) Interval(partial) AUCs with 'linear' or 'log' interpolation method

* Reference: Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016. (ISBN:9198299107).

Depends R (>= 2.0.0)

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R topics documented:

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NonCompart-package *Noncompartmental Analysis for Pharmacokinetic Data*

Description

It conducts a noncompartmental analysis(NCA) as closely as possible to the most widely used commercial pharmacokinetic analysis software.

Details

The main functions are

tblNCA to perform NCA for many subjects.

sNCA to perform NCA for one subject.

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

Examples

```
# Theoph and Indometh data: dose in mg, conc in mg/L, time in h
tblNCA(Theoph, key="Subject", colTime="Time", colConc="conc", dose=320,
      adm="Extravascular", doseUnit="mg", concUnit="mg/L")

tblNCA(Indometh, key="Subject", colTime="time", colConc="conc", dose=25,
      adm="Infusion", dur=0.5, doseUnit="mg", concUnit="mg/L", R2ADJ=0.9)
```

```
# For individual NCA
iAUC = data.frame(Name=c("AUC[0-12h]", "AUC[0-24h]"), Start=c(0,0), End=c(12,24)) ; iAUC

x = Theoph[Theoph$Subject=="1", "Time"]
y = Theoph[Theoph$Subject=="1", "conc"]

sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h", iAUC=iAUC)
sNCA(x, y, dose=320, concUnit="mg/L", iAUC=iAUC)
```

| | |
|-----|--|
| AUC | <i>Calculate Area Under the Curve (AUC) and Area Under the first Moment Curve (AUMC) in a table format</i> |
|-----|--|

Description

Calculate Area Under the Curve(AUC) and the first Moment Curve(AUMC) in two ways; 'linear trapezoidal method' or 'linear-up and log-down' method. Return a table of cumulative values.

Usage

```
AUC(x, y, down = "Linear")
```

Arguments

| | |
|------|---|
| x | vector values of independent variable, usually time |
| y | vector values of dependent variable, usually concentration |
| down | either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC |

Details

down="Linear" means linear trapezoidal rule with linear interpolation. down="Log" means linear-up and log-down method.

Value

Table with two columns, AUC and AUMC; the first column values are cumulative AUCs and the second column values cumulative AUMCs.

Author(s)

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References

Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. pp687-689. 2011.

See Also

[LinAUC](#), [LogAUC](#)

Examples

```
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], down="Log")
```

| | |
|-----------|--|
| BestSlope | <i>Choose the best-fit slope for the log(y) and x regression by the criteria of adjusted R-square.</i> |
|-----------|--|

Description

It sequentially fits $\log(y) \sim x$ from the last point of x to the previous points with at least 3 points. It chooses a slope the highest adjusted R-square. If the difference is less than $1e-4$, it picks longer slope.

Usage

```
BestSlope(x, y, adm = "Extravascular", TOL=1e-4)
```

Arguments

| | |
|-----|--|
| x | vector values of x-axis, usually time |
| y | vector values of y-axis, usually concentration |
| adm | one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode |
| TOL | tolerance. See Phoenix WinNonlin 6.4 User's Guide p33 for the detail. |

Details

Choosing the best terminal slope (y in log scale) in pharmacokinetic analysis is somewhat challenging, and it could vary by analysis performer. Phoenix WinNonlin chooses a slope with highest adjusted R-squared and the longest one. The difference of adjusted R-Squared less than TOL considered to be 0. This function uses ordinary least square method (OLS).

Value

| | |
|---------|----------------------------------|
| R2 | R-squared |
| R2ADJ | adjusted R-squared |
| LAMZNPT | number of points used for slope |
| LAMZ | negative of the slope, lambda_z |
| b0 | intercept of the regression line |
| CORRXY | correlation of log(y) and x |

| | |
|--------|--|
| LAMZLL | earliest x for lambda_z |
| LAMZUL | last x for lambda_z |
| CLSTP | predicted y value at the last point, predicted concentration for the last time point |

Author(s)

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See Also

[Slope](#)

Examples

```
BestSlope(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
BestSlope(Indometh[Indometh$Subject==1, "time"], Indometh[Indometh$Subject==1, "conc"],
          adm="Bolus")
```

DetSlope

Determine slope for the log(y) and x regression manually

Description

You choose a slope for terminal half-life.

Usage

```
DetSlope(x, y, sel.1=0, sel.2=0)
```

Arguments

| | |
|-------|--|
| x | vector values of x-axis, usually time |
| y | vector values of y-axis, usually concentration |
| sel.1 | default index of the first element to use |
| sel.2 | default index of the last element to use |

Details

Sometimes BestSlope cannot find terminal slope satisfactorily. Then you can use this function to choose manually. It returns the same format result with BestSlope with an attribute indicating used points.

Value

| | |
|---------|--|
| R2 | R-squared |
| R2ADJ | adjusted R-squared |
| LAMZNPT | number of points used for the slope |
| LAMZ | negative of the slope, lambda_z |
| b0 | intercept of the regression line |
| CORRXY | correlation of log(y) and x |
| LAMZLL | earliest x for lambda_z |
| LAMZUL | last x for lambda_z |
| CLSTP | predicted y value at the last point, predicted concentration for the last time point |

Author(s)

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See Also

[Slope](#)

Examples

```
DetSlope(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
DetSlope(Indometh[Indometh$Subject==2, "time"], Indometh[Indometh$Subject==2, "conc"])
```

IntAUC

Calculate interval AUC

Description

It calculates interval AUC

Usage

```
IntAUC(x, y, t1, t2, Res, down = "Linear")
```

Arguments

| | |
|------|--|
| x | vector values of independent variable, usually time |
| y | vector values of dependent variable, usually concentration |
| t1 | start time for AUC |
| t2 | end time for AUC |
| Res | result from IndiNCA function |
| down | either of "Linear" or "Log" to indicate the way to calculate AUC |

Details

This calculates an interval (partial) AUC (from t1 to t2) with the given series of x and y. If t1 and/or t2 cannot be found within x vector, it interpolates according to the down option.

Value

return interval AUC value (scalar)

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

See Also

[AUC](#), [Interpol](#)

Examples

```
Res = sNCA(Theoph[Theoph$Subject==1,"Time"], Theoph[Theoph$Subject==1, "conc"],
           dose=320, concUnit="mg/L")
IntAUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], t1=0.5, t2=11, Res)
```

Interpol

Interpolate y value

Description

It interpolates y value when a corresponding x value (xnew) does not exist within x vector

Usage

```
Interpol(x, y, xnew, Slope, b0, down = "Linear")
```

Arguments

| | |
|-------|--|
| x | vector values of x-axis, usually time |
| y | vector values of y-axis, usually concentration |
| xnew | new x point to be interpolated, usually new time point |
| Slope | slope of regression $\log(y) \sim x$ |
| b0 | y value of just left point of xnew |
| down | either of "Linear" or "Log" to indicate the way to interpolate |

Details

This function interpolate y value, if xnew is not in x vector. If xnew is in x vector, it just returns the given x and y vector. This function usually is called by IntAUC function Returned vector is sorted in the order of increasing x values.

Value

new x and y vector containing xnew and ynew point

Author(s)

Kyun-Seop Bae <k@acr.kr>

See Also

[IntAUC](#)

Examples

```
x = 10:1 + 0.1
y = -2*x + 40.2
Interpol(x, y, 1.5)
Interpol(x, y, 1.5, down="Log")
```

LinAUC

Area Under the Curve(AUC) and Area Under the first Moment Curve(AUMC) by linear trapezoidal method

Description

It calculates AUC and AUMC using the linear trapezoidal method

Usage

```
LinAUC(x, y)
```


Arguments

| | |
|---|--|
| x | vector values of the independent variable, usually time |
| y | vector values of the dependent variable, usually concentration |

Details

This function returns AUC and AUMC by the linear trapezoidal method.

Value

| | |
|------|-----------------------------------|
| AUC | area under the curve |
| AUMC | area under the first moment curve |

Author(s)

Kyun-Seop Bae <k@acr.kr>

References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

See Also

[LogAUC](#), [AUC](#)

Examples

```
LinAUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"]) # compare the last line
```

| | |
|--------|---|
| LogAUC | <i>Area Under the Curve(AUC) and Area Under the first Moment Curve(AUMC) by linear-up log-down method</i> |
|--------|---|

Description

It calculates AUC and AUMC using the linear-up log-down method

Usage

```
LogAUC(x, y)
```

Arguments

| | |
|---|--|
| x | vector values of the independent variable, usually time |
| y | vector values of the dependent variable, usually concentration |

Details

This function returns AUC and AUMC by the linear-up log-down method.

Value

| | |
|------|-----------------------------------|
| AUC | area under the curve |
| AUMC | area under the first moment curve |

Author(s)

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References

1. Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.
2. Shargel L, Yu A. Applied Biopharmaceutics and Pharmacokinetics. 7th ed. 2015.
3. Rowland M, Tozer TN. Clinical Pharmacokinetics and Pharmacodynamics - Concepts and Applications. 4th ed. 2011.
4. Gibaldi M, Perrier D. Pharmacokinetics. 2nd ed. revised and expanded. 1982.

See Also

[LinAUC,AUC](#)

Examples

```
LogAUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"])
# Compare the last line with the above
AUC(Theoph[Theoph$Subject==1, "Time"], Theoph[Theoph$Subject==1, "conc"], down="Log")
```

Slope

Get the Slope of regression $\log(y) \sim x$

Description

It calculates the slope with linear regression of $\log(y) \sim x$

Usage

Slope(x, y)

Arguments

| | |
|---|--|
| x | vector values of the independent variable, usually time |
| y | vector values of the dependent variable, usually concentration |

Details

With time-concentration curve, you frequently need to estimate slope in $\log(\text{concentration}) \sim \text{time}$. This function is usually called by `BestSlope` function, and you seldom need to call this function directly.

Value

| | |
|---------|--|
| R2 | R-squared |
| R2ADJ | adjusted R-squared |
| LAMZNPT | number of points used for slope |
| LAMZ | negative of the slope, λ_z |
| b0 | intercept of the regression line |
| CORRXY | correlation of $\log(y)$ and x |
| LAMZLL | earliest x for λ_z |
| LAMZUL | last x for λ_z |
| CLSTP | predicted y value at the last point, predicted concentration for the last time point |

Author(s)

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See Also

[BestSlope](#)

Examples

```
Slope(Indometh[Indometh$Subject==1, "time"], Indometh[Indometh$Subject==1, "conc"])
```

sNCA

Simplest NCA

Description

This is the work-horse function for NCA.

Usage

```
sNCA(x, y, dose = 0, adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h",
      concUnit = "ug/L", iAUC = "", down = "Linear", R2ADJ = 0.9, MW = 0, returnNA = FALSE)
```

Arguments

| | |
|----------|--|
| x | usually time |
| y | usually concentration |
| dose | given amount |
| adm | one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode |
| dur | duration of infusion |
| doseUnit | unit of dose |
| timeUnit | unit of time |
| concUnit | unit of concentration |
| iAUC | interval AUCs to calculate |
| down | either of "Linear" or "Log" to indicate the way to calculate AUC and AUMC |
| R2ADJ | Minimum adjusted R-square value to determine terminal slope automatically |
| MW | molecular weight of the drug |
| returnNA | deprecated, just for backward compatibility |

Details

This will replace IndiNCA.

Value

| | |
|---------------------|---|
| C _{MAX} | maximum concentration, C _{max} |
| C _{MAXD} | dose normalized C _{max} , C _{MAX} / Dose, C _{max} / Dose |
| T _{MAX} | time of maximum concentration, T _{max} |
| T _{LAG} | time to observe the first non-zero concentration, for extravascular administration only |
| CL _{ST} | last positive concentration observed, C _{last} |
| CL _{STP} | last positive concentration predicted, C _{last_pred} |
| T _{LST} | time of last positive concentration, T _{last} |
| LAM _{ZHL} | half-life by lambda z, ln(2)/LAMZ |
| LAM _Z | lambda_z negative of the best-fit terminal slope |
| LAM _{ZLL} | earliest time for LAMZ |
| LAM _{ZUL} | last time for LAMZ |
| LAM _{ZNPT} | number of points for LAMZ |
| CORR _{XY} | correlation of log(concentration) and time |
| R ₂ | R-squared |
| R _{2ADJ} | R-squared adjusted |
| C ₀ | back extrapolated concentration at time 0, for intravascular bolus administration only |

| | |
|----------|---|
| AUCLST | AUC from 0 to TLST |
| AUCALL | AUC using all the given points, including trailing zero concentrations |
| AUCIFO | AUC infinity observed |
| AUCIFOD | AUCIFO / Dose |
| AUCIFP | AUC infinity predicted using CLSTP instead of CLST |
| AUCIFPD | AUCIFP / Dose |
| AUCPEO | AUC % extrapolation observed |
| AUCPEP | AUC % extrapolated for AUCIFP |
| AUCPBEO | AUC % back extrapolation observed, for bolus IV administration only |
| AUCPBEP | AUC % back extrapolation predicted with AUCIFP, for bolus IV administration only |
| AUMCLST | AUMC to the TLST |
| AUMCIFO | AUMC infinity observed using CLST |
| AUMCIFP | AUMC infinity determined by CLSTP |
| AUMCPEO | AUMC % extrapolated observed |
| AUMCPEP | AUMC % extrapolated predicted |
| MRTIVLST | mean residence time (MRT) to TLST, for intravascular administration |
| MRTIVIFO | mean residence time (MRT) infinity using CLST, for intravascular administration |
| MRTIVIFP | mean residence time (MRT) infinity using CLSTP, for intravascular administration |
| MRTEVLST | mean residence time (MRT) to TLST, for extravascular administration |
| MRTEVIFO | mean residence time (MRT) infinity using CLST, for extravascular administration |
| MRTEVIFP | mean residence time (MRT) infinity using CLSTP, for extravascular administration |
| VZO | volume of distribution determined by LAMZ and AUCIFO, for intravascular administration |
| VZP | volume of distribution determined by LAMZ and AUCIFP, for intravascular administration |
| VZFO | VZO for extravascular administration, VZO/F, F is bioavailability |
| VZFP | VZP for extravascular administration, VZP/F, F is bioavailability |
| CLO | clearance using AUCIFO, for intravascular administration |
| CLP | clearance using AUCIFP, for intravascular administration |
| CLFO | CLO for extravascular administration, CLO/F, F is bioavailability |
| CLFP | CLP for extravascular administration, CLP/F, F is bioavailability |
| VSSO | volume of distribution at steady state using CLST, for intravascular administration only |
| VSSP | volume of distribution at steady state using CLSTP, for intravascular administration only |

Author(s)

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References

Gabrielsson J, Weiner D. Pharmacokinetic and Pharmacodynamic Data Analysis - Concepts and Applications. 5th ed. 2016.

See Also

[help, tblNCA](#)

Examples

```
# For one subject
x = Theoph[Theoph$Subject=="1", "Time"]
y = Theoph[Theoph$Subject=="1", "conc"]

sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h")
sNCA(x, y, dose=320, concUnit="mg/L")

iAUC = data.frame(Name=c("AUC[0-12h]", "AUC[0-24h]"), Start=c(0,0), End=c(12,24))
sNCA(x, y, dose=320, doseUnit="mg", concUnit="mg/L", timeUnit="h", iAUC=iAUC)

MW = 180.164 # Molecular weight of theophylline

sNCA(x, y/MW, dose=320, doseUnit="mg", concUnit="mmol/L", timeUnit="h")
sNCA(x, y/MW, dose=320, doseUnit="mg", concUnit="mmol/L", timeUnit="h", MW=MW)
sNCA(x, y, dose=320/MW, doseUnit="mmol", concUnit="mg/L", timeUnit="h", MW=MW)
sNCA(x, y/MW, dose=320/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW)

sNCA(x, y/MW, dose=320/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW)
sNCA(x, y/MW, doseUnit="mmol", concUnit="mmol/L", timeUnit="h", MW=MW)
sNCA(x, y/MW, dose=as.numeric(NA), doseUnit="mmol", concUnit="mmol/L", timeUnit="h",
      MW=MW)

sNCA(x, y, dose=320, concUnit="mg/L", timeUnit="hr")
sNCA(x*60, y, dose=320, concUnit="mg/L", timeUnit="min")
```

tblNCA

Table output NCA

Description

Do multiple NCA and returns a result table.

Usage

```
tblNCA(concData, key = "Subject", colTime = "Time", colConc = "conc", dose = 0,
       adm = "Extravascular", dur = 0, doseUnit = "mg", timeUnit = "h",
       concUnit = "ug/L", down = "Linear", R2ADJ = 0.9, MW = 0)
```

Arguments

| | |
|----------|--|
| concData | concentration data table |
| key | column names of concData to be shown in the output table |
| colTime | column name for time |
| colConc | column name for concentration |
| dose | administered dose |
| adm | one of "Bolus" or "Infusion" or "Extravascular" to indicate drug administration mode |
| dur | duration of infusion |
| doseUnit | unit of dose |
| timeUnit | unit of time |
| concUnit | unit of concentration |
| down | method to calculate AUC, "Linear" or "Log" |
| R2ADJ | Lowest threshold of adjusted R-square value to do manual slope determination |
| MW | molecular weight of drug |

Value

Basically same with [sNCA](#)

Author(s)

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See Also

[help](#), [sNCA](#)

Examples

```
tblNCA(Theoph, key="Subject", dose=320, concUnit="mg/L")
tblNCA(Indometh, key="Subject", colTime="time", colConc="conc", dose=25,
      adm="Infusion", dur=0.5, concUnit="mg/L")
```

Unit

*Display CDISC standard units and multiplied factor of NCA results***Description**

It displays CDISC PP output units and multiplication factor for them.

Usage

```
Unit(code = "", timeUnit = "h", concUnit = "ng/mL", doseUnit = "mg", MW = 0)
```

Arguments

| | |
|----------|--------------------------|
| code | vector of PPTTESTCD |
| timeUnit | unit of time |
| concUnit | unit of concentration |
| doseUnit | unit of dose |
| MW | molecular weight of drug |

Value

| | |
|-----------|--------------------------------|
| row names | PPTTESTCD |
| Unit | unit |
| Factor | internal mulitplication factor |

Author(s)

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Examples

```
Unit(concUnit="ug/L", doseUnit="mg")
Unit(concUnit="ng/L", doseUnit="mg")

Unit(concUnit="umol/L", doseUnit="mmol")
Unit(concUnit="nmol/L", doseUnit="mmol")

Unit(concUnit="mmol/L", doseUnit="mg", MW=500)
Unit(concUnit="umol/L", doseUnit="mg", MW=500)
Unit(concUnit="nmol/L", doseUnit="mg", MW=500)
Unit(concUnit="nmol/mL", doseUnit="mg", MW=500)

Unit(concUnit="ug/L", doseUnit="mmol", MW=500)
Unit(concUnit="ug/L", doseUnit="mol", MW=500)
Unit(concUnit="ng/L", doseUnit="mmol", MW=500)
Unit(concUnit="ng/mL", doseUnit="mmol", MW=500)
```



```
Unit(concUnit="nmol/L", doseUnit="mg")
Unit(concUnit="ug/L", doseUnit="mmol")
```

| | |
|-----------|---|
| UnitUrine | <i>Returns a conversion factor for the amount calculation from urine concentration and volume</i> |
|-----------|---|

Description

You can get a conversion factor for the multiplication: $\text{conc} * \text{vol} * \text{factor} = \text{amount}$ in the given unit.

Usage

```
UnitUrine(conU = "ng/mL", volU = "mL", amtU = "mg", MW = 0)
```

Arguments

| | |
|------|--------------------|
| conU | concentration unit |
| volU | volume unit |
| amtU | amount unit |
| MW | molecular weight |

Value

| | |
|--------|--|
| Factor | conversion factor for multiplication with the unit in name |
|--------|--|

Author(s)

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Examples

```
UnitUrine()
UnitUrine("ng/mL", "mL", "mg")
UnitUrine("ug/L", "mL", "mg")
UnitUrine("ug/L", "L", "mg")

UnitUrine("ng/mL", "mL", "g")

UnitUrine("ng/mL", "mL", "mol", MW=500)
UnitUrine("ng/mL", "mL", "mmol", MW=500)
UnitUrine("ng/mL", "mL", "umol", MW=500)
```

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