# 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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**License** GPL-3

**NeedsCompilation** no

**LazyLoad** yes

**Repository** CRAN

**URL** https://cran.r-project.org/package=NonCompart

## R topics documented:

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NonCompart-package *Noncompartmental Analysis for Pharmacokinetic Data*

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## 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)

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.

## 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 *Calculate Area Under the Curve (AUC) and Area Under the first Moment Curve (AUMC) in a table format*

## 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)

Kyun-Seop Bae <k@acr.kr>

## 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` *Choose the best-fit slope for the log(y) and x regression by the criteria of adjusted R-square.*

## Description

It sequentially fits (log(y) ~ 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 then 1e-4, it pickes 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 Phoneix 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. Pheonix 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)

Kyun-Seop Bae <k@acr.kr>

## 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)

Kyun-Seop Bae <k@acr.kr>

## 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)

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

`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) ~ 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 *Area Under the Curve(AUC) and Area Under the first Moment Curve(AUMC) by linear-up log-down method*

## 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)

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

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) ~ x*

## Description

It calculates the slope with linear regression of log(y) ~ 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(concentration) ~ 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, 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

`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

| | |
|---|---|
| CMAX | maximum concentration, Cmax |
| CMAXD | dose normalized Cmax, CMAX / Dose, Cmax / Dose |
| TMAX | time of maximum concentration, Tmax |
| TLAG | time to observe the first non-zero concentration, for extravascular administration only |
| CLST | last positive concentration observed, Clast |
| CLSTP | last positive concentration predicted, Clast_pred |
| TLST | time of last positive concentration, Tlast |
| LAMZHL | half-life by lambda z, ln(2)/LAMZ |
| LAMZ | lambda_z negative of the best-fit terminal slope |

| | |
|---|---|
| LAMZLL | earliest time for LAMZ |
| LAMZUL | last time for LAMZ |
| LAMZNPT | number of points for LAMZ |
| CORRXY | correlation of log(concentration) and time |
| R2 | R-squared |
| R2ADJ | R-squared adjusted |
| C0 | 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)

Kyun-Seop Bae <k@acr.kr>

## 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)

Kyun-Seop Bae <k@acr.kr>

## 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 PPTESTCD |
| `timeUnit` | unit of time |
| `concUnit` | unit of concentration |
| `doseUnit` | unit of dose |
| `MW` | molecular weight of drug |

## Value

| | |
|---|---|
| `row names` | PPTESTCD |
| `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` *Retuns a conversion factor for the amount calculation from urine concentration and volume*

## Description

You can get a conversion factor for the multiplication: conc * vol * factor = 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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