

# Package: equil2 (via r-universe)

August 13, 2024

**Title** Calculate Urinary Saturation with the EQUIL2 Algorithm

**Version** 1.0.0

**Description** Saturation of ionic substances in urine is calculated based on sodium, potassium, calcium, magnesium, ammonia, chloride, phosphate, sulfate, oxalate, citrate, ph, and urate. This program is intended for research use, only. The code within is translated from EQUIL2 Visual Basic code based on Werness, et al (1985) ``EQUIL2: a BASIC computer program for the calculation of urinary saturation" <doi:10.1016/s0022-5347(17)47703-2> to R. The Visual Basic code was kindly provided by Dr. John Lieske of the Mayo Clinic.

**Imports** units

**Suggests** covr, knitr, rmarkdown, spelling, testthat (>= 3.0.0)

**License** MIT + file LICENSE

**Encoding** UTF-8

**Roxygen** list(markdown = TRUE)

**RoxygenNote** 7.2.2

**Config/testthat/edition** 3

**URL** <https://billdenney.github.io/equil2/>

**VignetteBuilder** knitr

**Language** en-US

**Repository** <https://billdenney.r-universe.dev>

**RemoteUrl** <https://github.com/billdenney/equil2>

**RemoteRef** HEAD

**RemoteSha** 5a102a9df6bd40f75e99135309efd12c042622a0

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add_units	<i>Add units to support unit conversion for calculations</i>
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**Description**

Units are added to support molecular weight and mEq/L conversions. Units are named with the unit, an underscore, and the chemical species in lower case. Examples are "g\_ammonia", "mol\_ammonia", and "Eq\_ammonia". Species with units are all species inputs for the equil2() function.

**Usage**

```
add_units()
```

**Value**

NULL, the function is used for its side-effects

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equil2	<i>Calculate urine saturation with the EQUIL-2 algorithm</i>
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**Description**

Calculate urine saturation with the EQUIL-2 algorithm

**Usage**

```
equil2(  
  sodium_mEq_L,  
  potassium_mEq_L,  
  calcium_mg_dL,  
  magnesium_mg_dL,  
  ammonia_mEq_L,  
  chloride_mEq_L,  
  phosphate_mg_dL,  
  sulfate_mg_dL,  
  oxalate_mg_dL,  
  citrate_mg_dL,  
  pH,  
  urate_mg_dL  
)
```

**Arguments**

sodium_mEq_L, potassium_mEq_L, ammonia_mEq_L, chloride_mEq_L	Concentration of the given species in mEq/L (or a unit value that can be converted to mEq/L)
calcium_mg_dL, magnesium_mg_dL, phosphate_mg_dL, sulfate_mg_dL, oxalate_mg_dL, citrate_mg_dL, urate_mg_dL	Concentration of the given species in mg/dL (or a unit value that can be converted to mg/dL)
pH	The urine pH

**Details**

This program is intended for research use, only. The code within is translated from Visual Basic code based on Werness, et al 1985 to R. The Visual Basic code was kindly provided by Dr. John Lieske of the Mayo Clinic.

**Value**

A data.frame with three columns:

- "species" indicating the chemical species
- "super\_saturation" is the supersaturation ratio. This is SS as defined in Werness 1985.
- "neg\_delta\_Gibbs" which is the negative of the change in Gibbs free energy of transfer from a supersaturated to a saturated solution (the value is negative for under-saturated solutions, zero for solutions at the solubility product, and positive for supersaturated solutions). This is DG as defined in Werness 1985.

**References**

Werness PG, Brown CM, Smith LH, Finlayson B. Equil2: A Basic Computer Program for the Calculation of Urinary Saturation. *Journal of Urology*. 1985;134(6):1242-1244. doi:10.1016/S0022-5347(17)47703-2

**Examples**

```
# Example values from https://files.labcorp.com/testmenu-d8/sample_reports/306266.pdf
equil2(
  sodium_mEq_L=units::set_units(45, "mmol_sodium/L"),
  potassium_mEq_L=units::set_units(55, "mmol_potassium/L"),
  calcium_mg_dL=units::set_units(15, "mg_calcium/dL"),
  magnesium_mg_dL=units::set_units(15, "mg_magnesium/dL"),
  ammonia_mEq_L=units::set_units(10, "ug_ammonia/dL"),
  chloride_mEq_L=units::set_units(75, "mmol_chloride/L"),
  phosphate_mg_dL=units::set_units(100, "mg_phosphate/dL"),
  sulfate_mg_dL=units::set_units(20, "mEq_sulfate/L"),
  oxalate_mg_dL=units::set_units(10, "mg_oxalate/L"),
  citrate_mg_dL=units::set_units(400, "mg_citrate/L"),
  pH=5.5,
  urate_mg_dL=units::set_units(50, "mg_urate/dL")
)
```

)

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