Package 'equil2'

July 22, 2025

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)

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Encoding UTF-8

RoxygenNote 7.2.2

Config/testthat/edition 3

URL https://billdenney.github.io/equil2/

VignetteBuilder knitr

Language en-US

NeedsCompilation no

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Repository CRAN

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add_units *Add units to support unit conversion for calculations*

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

equil2 *Calculate urine saturation with the EQUIL-2 algorithm*

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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