R documentation

of 'armitage_eval2.Rd'

April 27, 2021

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armitage_eval *Evaluate the updated Armitage model*

Description

Evaluate the Armitage model for chemical distributon in vitro. Takes input as data table or vectors of values. Outputs a data table. Updates over the model published in Armitage et al. 2014 include binding to plastic walls and lipid and protein compartments in cells.

Usage

```
armitage_eval(
  casrn.vector = NA_character_,
  nomconc.vector = 1,
  this.well_number = 384,
  this.FBSf = NA_real_,
  tcdata = NA,
  this.sarea = NA_real_,
  this.v_total = NA_real_,
  this.v_working = NA_real_,
  this.cell_yield = NA_real_,
  this.Tsys = 37,
  this.Tref = 298.15,
  this.option.kbsa2 = F,
  this.option.swat2 = F,
  this.pseudooct = 0.01,
  this.memblip = 0.04,
  this.nlom = 0.2,
  this.P_nlom = 0.035,
  this.P_dom = 0.05,
  this.P_cells = 1,
  this.csalt = 0.15,
  this.celldensity = 1,
  this.cellmass = 3,
  this.f_oc = 1
)
```

Arguments

casrn.vector	For vector or single value, CAS number
nomconc.vector	For vector or single value, micromolar nominal concentration (e.g. AC50 value)
this.well_number	For single value, plate format default is 384, used if is.na(tcdata)==T
this.FBSf	Fraction fetal bovine serum, must be entered by user.
tcdata	A data.table with casrn, nomconc, MP, gkow, gkaw, gswat, sarea, v_total, v_working. Otherwise supply single values to this.params.
this.sarea	Surface area per well (m^2)
this.v_total	Total volume per well (m^3)
this.v_working	Working volume per well (m^3)
this.cell_yield	Number of cells per well
this.Tsys	System temperature (degrees C)
this.Tref	Reference temperature (degrees K)
this.option.kbsa2	Use alternative bovine-serum-albumin partitioning model
this.option.swat2	Use alternative water solubility correction
this.pseudooct	Pseudo-octanol cell storage lipid content
this.memblip	Membrane lipid content of cells
this.nlom	Structural protein conent of cells
this.P_nlom	Proportionality constant to octanol structural protein
this.P_dom	Proportionality constant to dissolve organic material
this.P_cells	Proportionality constant to octanol storage lipid
this.csalt	Ionic strength of buffer, mol/L
this.celldensity	Cell density kg/L, g/mL
this.cellmass	Mass per cell, ng/cell
this.f_oc	1, everything assumed to be like proteins

Value

Column	Description	units
casrn	Chemical Abstracts Service Registry Number	
nomconc	Nominal Concentration	mol/L
well_number	Number of wells in plate	unitless
sarea	Surface area of well	m^2
v_total	Total volume of well	m^3
v_working	Filled volume of well	m^3
cell_yield	Number of cells	cells
gkow	log10 octanol-water partition coefficient	log10
logHenry	log10 Henry's law constant '	log10 atm-m3/mol
gswat	log10 Water solubility	log10 mol/L
MP	Melting Point	degrees Celsius

MW	Molecular Weight	g/mol
gkaw	air-water partition coefficient	(mol/m3)/(mol/m3)
dsm		
duow		
duaw		
dumw		
gkmw		
gkcw		
gkbsa		
gkpl		
ksalt		
Tsys		
Tref		
option.kbsa2		
option.swat2		
FBSf		
pseudooct		
memblip		
nlom		
P_nlom		
P_dom	dissolved organic matter b water partition coefficient	Dimesnsionless
P_cells		
csalt		
celldensity		
cellmass		
f_oc		
cellwat		
Tcor		
Vm	Volume of media	L

Author(s)

Greg Honda

References

Armitage, J. M.; Wania, F.; Arnot, J. A. Environ. Sci. Technol. 2014, 48, 9770-9779. https://doi.org/10.1021/es501955g

Honda et al. PloS one 14.5 (2019): e0217564. https://doi.org/10.1371/journal.pone.0217564

Examples

```
library(httk)

# Check to see if we have info on the chemical:
"80-05-7" %in% get_cheminfo()

#We do:
temp <- armitage_eval(casrn.vector = c("80-05-7", "81-81-2"), this.FBSf = 0.1,
this.well_number = 384, nomconc = 10)
```

```
print(temp$cfree.invitro)

# Check to see if we have info on the chemical:
"793-24-8" %in% get_cheminfo()

# Since we don't look up phys-chem from dashboard:
cheminfo <- data.frame(
  Compound="6-PPD",
  CASRN="793-24-8",
  DTXSID="DTXSID9025114",
  logP=4.27,
  logHenry=log10(7.69e-8),
  logWSol=log10(1.58e-4),
  MP= 99.4,
  MW=268.404
  )

# Add the information to HTTK's database:
chem.physical_and_invitro.data <- add_chemtable(
 cheminfo,
 current.table=chem.physical_and_invitro.data,
 data.list=list(
 Compound="Compound",
 CAS="CASRN",
  DTXSID="DTXSID",
  MW="MW",
  logP="logP",
  logHenry="logHenry",
  logWSol="logWSol",
  MP="MP"),
  species="Human",
  reference="CompTox Dashboard 31921")

# Run the Armitage et al. (2014) model:
out <- armitage_eval(
  casrn.vector = "793-24-8",
  this.FBSf = 0.1,
  this.well_number = 384,
  nomconc = 10)

print(out)
```