

MINVAL - MINimal VALidation for Stoichiometric Reactions

Daniel Osorio, Janneth Gonzalez and Andres Pinzon-Velasco

2016-09-29

Introduction to MINVAL

The **MINVAL** package was designed as a tool to identify orphan metabolites and evaluate the mass and charge balance of stoichiometric reactions. MINVAL also includes functions to write models in TSV and SBML formats, extract all reactants, products, metabolite names and compartments from a metabolic reconstruction.

Getting started

```
library(minval)
library(sybilSBML)

glycolysis <- read.csv2(system.file("extdata", "glycolysisKEGG.csv", package = "minval"))
dim(glycolysis)

## [1] 23 7

colnames(glycolysis)

## [1] "ID" "DESCRIPTION" "REACTION" "GPR" "LOWER.BOUND"
## [6] "UPPER.BOUND" "OBJECTIVE"

head(glycolysis$REACTION)

## [1] NADH[c] <=> NADH[b]
## [2] H+[c] <=> H+[b]
## [3] Pyruvate[c] <=> Pyruvate[b]
## [4] alpha-D-Glucose[c] <=> alpha-D-Glucose[b]
## [5] NAD+[c] <=> NAD+[b]
## [6] Orthophosphate[c] <=> Orthophosphate[b]
## 23 Levels: 2 2 beta-D-Fructose 1,6-bisphosphate[c] <=> Glycerone phosphate[c] + D-Glyceraldehyde 3-phosphate[c]

valid <- isValidSyntax(glycolysis$REACTION)

## Warning: Reaction 12: Invalid coefficients. Metabolites should have just
## one coefficient.

## Warning: Reaction 11: Invalid directionality symbols. Please use <=> or =>
## instead of <-> or -> or -->.

valid

## [1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE FALSE
## [12] FALSE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
## [23] TRUE

glycolysisValidated <- mapReactions(reactionList = valid,
                                   referenceData = glycolysis,
```

```

by = "bool",
inverse = FALSE)

dim(glycolysisValidated)

## [1] 21 7

convert2sbml(glycolysisValidated,"glycolysisValidated.xml")
glycoModel <- readSBMLmod("glycolysisValidated.xml")
glycoModel

## model name:          model
## number of compartments 2
##                      c
##                      b
## number of reactions:  21
## number of metabolites: 18
## number of unique genes: 26
## objective function:    +1 R00200

optimizeProb(glycoModel)

## solver:              glpkAPI
## method:              simplex
## algorithm:           fba
## number of variables: 21
## number of constraints: 18
## return value of solver: solution process was successful
## solution status:     solution is optimal
## value of objective function (fba): 502.000000
## value of objective function (model): 502.000000

chemicalData <- read.csv2(system.file("extdata", "chemData.csv", package = "minval"))
head(chemicalData)

##           NAME      FORMULA    MASS CHARGE
## 1           H2O          H2O  18.0106      0
## 2            H+           H   1.0078      1
## 3           ATP C10H16N5O13P3 506.9957      0
## 4          NAD+ C21H28N7O14P2 664.1169      1
## 5 3-Phospho-D-glyceroyl phosphate C3H8O10P2 265.9593      0
## 6 beta-D-Fructose 6-phosphate C6H13O9P 260.0297      0

balanced <- isBalanced(reactionList = glycolysisValidated$REACTION,
                      referenceData = chemicalData,
                      ids = "NAME",
                      mFormula = "FORMULA")

balanced

## [1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE FALSE FALSE
## [12] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE

glycolysisBalanced <- mapReactions(reactionList = balanced,
                                   referenceData = glycolysisValidated,
                                   by = "bool",
                                   inverse = FALSE)

dim(glycolysisBalanced)

## [1] 19 7

```

```
convert2sbml(glycolysisBalanced,"glycolysisBalanced.xml")
glycoModel <- readSBMLmod("glycolysisBalanced.xml")
glycoModel
```

```
## model name:          model
## number of compartments 2
##                      c
##                      b
## number of reactions:  19
## number of metabolites: 18
## number of unique genes: 26
## objective function:   +1 R00200
```

```
optimizeProb(glycoModel)
```

```
## solver:              glpkAPI
## method:              simplex
## algorithm:           fba
## number of variables:  19
## number of constraints: 18
## return value of solver: solution process was successful
## solution status:      solution is optimal
## value of objective function (fba): 2.000000
## value of objective function (model): 2.000000
```