‘g2f’ Package

An R Package to Find and Fill Gaps for genome-scale metabolic networks

Kelly Botero, ***Daniel Osorio***, *Janneth Gonzalez and Andres Pinzón-Velasco.*

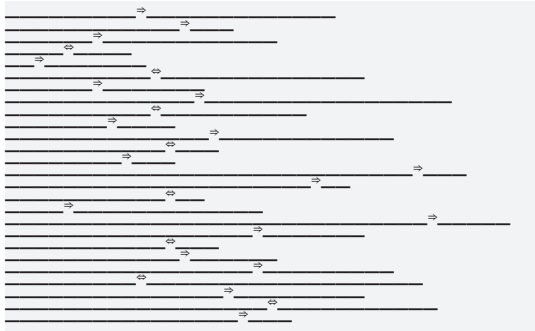
Language: R
Stable: CRAN
Development: gibbslab/g2f
License: GPL-2
Binaries: Windows - Linux - Mac

RXNLIST

h2o[r] + dheas[r] ⇒ h[r] + dhea[r] + so4[r]
uri[e] ⇔ uri[c]
na1[e] + uri[e] ⇒ na1[c] + uri[c]
atp[c] + pi[m] ⇒ pi[c] + atp[m]
na1[e] + gchola[e] ⇒ na1[c] + gchola[c]
...

getReference( )
DOWNLOAD STOICHIOMETRIC REACTIONS FROM THE KEGG DATABASE

REFERENCE



GENOME SCALE METABOLIC NETWORK

additionCost( )
CALCULATE ADITION COST

$$cost = \frac{n(metabolites(newReaction) \notin metabolites(reactionList))}{n(metabolites(newReaction))}$$

gapFill( )
FIND AND FILL GAPS

```
original = n( orphanMetabolites )
do{
    if(orphanMetabolite ∈ metabolites(newReactions)){
        gapFill: | cost ⩽ limit → reaction ∪ newReactions
                 | cost ⩾ limit → reaction
    }
    filled = n(orphans(reaction ∪ newReactions) ∈ orphanMetabolites)
}
while ( original ⩽ filled )
```

blockedReactions( )
IDENTIFY REACTIONS NEVER ACTIVATED