‘g2f’ Package

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

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

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]
ASTROCYTE DRAFT GiBBS Lab (2016)

REACTLIST

getReference( )
DOWNLOAD STOICHIOMETRIC REACTIONS FROM THE KEGG DATABASE

REFERENCE

RECON 2.04 Thiele *et al.* (2013)

gapFill( )
FIND AND FILL GAPS

orphanReactants( ) + orphanProducts( )
IDENTIFY INITIAL GAPS

IDENTIFY REACTIONS THAT INCLUDES ORPHANS AS METABOLITES

additionCost( )
CALCULATE ADITION COST

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

IF
ADITION COST ≤ GIVEN LIMIT

ADD REACTION TO REACTIONLIST

orphanReactants( ) + orphanProducts( )
IDENTIFY NEW GAPS

IF n(**INITIAL GAPS** ∈ **NEW GAPS**) ≤ n(**INITIAL GAPS**)

REPEAT UNTIL NO MORE INITIAL GAPS COULD BE FILLED

RETURN REACTIONLIST