Initialise and verify The COBRA Toolbox

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Reviewers:

MATERIALS - EQUIPMENT SETUP

Please ensure that all the required dependencies of The COBRA Toolbox have been properly installed by following the requirements guide at https://github.com/opencobra/cobratoolbox/blob/gh-pages/docs/requirements.html. In particular, `git` and `curl` must be installed.

PROCEDURE

At the start of each MATLAB session, The COBRA Toolbox must be initialised. Navigate to the directory where you installed The COBRA Toolbox and initialise

```
initCobraToolbox
```

```
                                                    |
      _____   _____   _____   _____      _____      |   COnstraint-Based Reconstruction and Analysis
     /  ___| /  _  \ |  _  \ |  _  \    / ___ \     |   The COBRA Toolbox - 2017
     | |     | | | | | |_| | | |_| |   | |___| |    |
     | |     | | | | |  _  { |  _  /   |  ___  |    |
     | |___  | |_| | | |_| | | | \ \   | |   | |    |   Documentation:
     \_____| \_____/ |_____/ |_|  \_\ |_|   |_|    |   http://opencobra.github.io/cobratoolbox
                                                    |

 > Checking if git is installed ...  Done.
 > Checking if the repository is tracked using git ...  Done.
 > Checking if curl is installed ...  Done.
 > Checking if remote can be reached ...  Done.
 > Initializing and updating submodules ... Done.
 > Adding all the files of The COBRA Toolbox ...  Done.
 > Define CB map output... set to svg.
 > Retrieving models ...   Done.
Warning:  > TranslateSBML is installed but is not working properly.
 > Try running
   >> TranslateSBML('/Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/test/models/Ec_iAF1260_f
   in order to debug.
 > Configuring solver environment variables ...
   - [--*-] ILOG_CPLEX_PATH: ~/Applications/IBM/ILOG/CPLEX_Studio1271/cplex/matlab/x86-64_osx
   - [*---] GUROBI_PATH: /Library/gurobi702/mac64/matlab
   - [----] TOMLAB_PATH :  --> set this path manually after installing the solver ( see instructions )
   - [----] MOSEK_PATH :  --> set this path manually after installing the solver ( see instructions )
   Done.
 > Checking available solvers and solver interfaces ... Done.
 > Setting default solvers ... Done.
 > Saving the MATLAB path ... Done.
   - The MATLAB path was saved in the default location.

 > Summary of available solvers and solver interfaces

   Support     LP   MILP     QP   MIQP    NLP
 ----------------------------------------------------------------------
 cplex_direct  full              0      0      0      0      -
 dqqMinos      full              1      -      -      -      -
 glpk          full              1      1      -      -      -
 gurobi        full              1      1      1      1      -
```

```
ibm_cplex     full              1      1      1      -      -
matlab        full              1      -      -      -      1
mosek         full              0      0      0      -      -
pdco          full              1      -      1      -      -
quadMinos     full              1      -      -      -      1
tomlab_cplex  full              0      0      0      0      -
qpng          experimental      -      -      1      -      -
tomlab_snopt  experimental      -      -      -      -      0
gurobi_mex    legacy            0      0      0      0      -
lindo_old     legacy            0      -      -      -      -
lindo_legacy  legacy            0      -      -      -      -
lp_solve      legacy            1      -      -      -      -
opti          legacy            0      0      0      0      0
----------------------------------------------------------------------
Total         -                 8      3      4      1      2

+ Legend: - = not applicable, 0 = solver not compatible or not installed, 1 = solver installed.


> You can solve LP problems using: 'dqqMinos' - 'glpk' - 'gurobi' - 'ibm_cplex' - 'matlab' - 'pdco' - '
> You can solve MILP problems using: 'glpk' - 'gurobi' - 'ibm_cplex'
> You can solve QP problems using: 'gurobi' - 'ibm_cplex' - 'pdco' - 'qpng'
> You can solve MIQP problems using: 'gurobi'
> You can solve NLP problems using: 'matlab' - 'quadMinos'

> Checking for available updates ...
> There are 438 new commit(s) on <master> and 15 new commit(s) on <develop> [53ffeb @ tutorial_initCobr
> You can update The COBRA Toolbox by running updateCobraToolbox() (from within MATLAB).
```

The user who primarily uses the official openCOBRA repository may automatically initialise The COBRA Toolbox. To do so, edit the MATLAB `startup.m` file and add a line with `initCobraToolbox` so that The COBRA Toolbox is initialised each time that MATLAB is started.

```
if usejava('desktop')  % This line of code is to avoid execution in non gui-environments
    edit startup.m
end
```

ANTICIPATED RESULTS

The initialisation step automatically checks the configuration of all of the required and some of the optional software dependencies. During initialisation, all git submodules are udpated. The solver paths are set when available and compatible. A system-dependent table with the solver status is returned, together with solver suggestions. The user is also presented with options to update The COBRA Toolbox when necessary.

CRITICAL STEP

During initialisation, a check for software dependencies is made and reported to the command window. It is not necessary that all possible dependencies are satisfied before beginning to use the toolbox, e.g., satisfaction of a dependency on a multi-scale linear optimisation solver is not necessary for modelling with a mono-scale metabolic model. However, other software dependencies are essential to be satisfied, e.g., dependency on a linear optimisation solver must be satisfied for any method that uses flux balance analysis.

TROUBLESHOOTING

1. Read the output of the initialisation script in the command window. Any warning or error messages, though often brief, will often point toward the source of the problem during initialisation if read literally.
2. Verify that all software versions are supported and have been correctly installed.
3. Ensure that you are using the latest version of The COBRA Toolbox by typing `updateCobraToolbox`
4. Verify and test The COBRA Toolbox, as described in the "Verify and test The COBRA Toolbox" tutorial.
5. Finally, if nothing else works, consult the COBRA Toolbox forum, as described in the "Engaging with The COBRA Toolbox community" tutorial.

Check available optimisation solvers

At initialisation, one from a set of available optimisation solvers will be selected as the default solver. If `Gurobi` is installed, it is used as the default solver for LP, QP and MILP problems. Otherwise, the `GLPK` solver is selected by for LP and MILP problems. It is important to check if the solvers installed are satisfactory. A table stating the solver compatibility and availability is printed to the user during initialisation.

2| Check the currently selected solvers with `changeCobraSolver`

```
changeCobraSolver
```

```
Defined solvers are:
    CBT_LP_SOLVER: glpk
    CBT_MILP_SOLVER: glpk
    CBT_QP_SOLVER: qpng
    CBT_MIQP_SOLVER: gurobi
    CBT_NLP_SOLVER: matlab
```

ANTICIPATED RESULTS

A list of solvers assigned to solve each class of optimisation solver is returned.

CRITICAL STEP

A dependency on at least one linear optimisation solver must be satisfied for flux balance analysis.

Verify and test The COBRA Toolbox

TIMING ~ 30 min

3| Optionally test the functionality of The COBRA Toolbox locally, especially if one encounters an error running a function. The test suite runs tailored tests that verify the output and proper execution of core functions on the locally configured system. The full test suite can be invoked by typing:

```
testAll
```

```
The COBRAToolbox testing suite
------------------------------
MoCov and JsonLab are on path, coverage will be computed.


      _____   _____   _____   _____     _____      |
```

```
    /  ___| /   _  \ |   _  \ |   _  \   / ___ \    |   COnstraint-Based Reconstruction and Analysis
    | |     | | | | | |_| | | |_| |  | |___| |   |   The COBRA Toolbox - 2017
    | |     | | | | |   _  { |   _  /  |  ___  |   |
    | |___  | |_| | | |_| | | |  \ \  | |   | |   |   Documentation:
    \_____| \_____/ |_____/ |_|  \_\ |_|   |_|   |   http://opencobra.github.io/cobratoolbox
                                                  |

 > Checking if git is installed ...  Done.
 > Checking if the repository is tracked using git ...  Done.
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Warning:  > TranslateSBML is installed but is not working properly.
 > Try running
   >> TranslateSBML('/Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/test/models/Ec_iAF1260_f
   in order to debug.
 > Configuring solver environment variables ...
   - [--*-] ILOG_CPLEX_PATH: ~/Applications/IBM/ILOG/CPLEX_Studio1271/cplex/matlab/x86-64_osx
   - [*---] GUROBI_PATH: /Library/gurobi702/mac64/matlab
   - [----] TOMLAB_PATH :  --> set this path manually after installing the solver ( see instructions )
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   Done.
 > Checking available solvers and solver interfaces ... Done.
 > Setting default solvers ... Done.
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   - The MATLAB path was saved in the default location.

 > Summary of available solvers and solver interfaces

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 ----------------------------------------------------------------------
 cplex_direct  full              0      0      0      0      -
 dqqMinos      full              1      -      -      -      -
 glpk          full              1      1      -      -      -
 gurobi        full              1      1      1      1      -
 ibm_cplex     full              1      1      1      -      -
 matlab        full              1      -      -      -      1
 mosek         full              0      0      0      -      -
 pdco          full              1      -      1      -      -
 quadMinos     full              1      -      -      -      1
 tomlab_cplex  full              0      0      0      0      -
 qpng          experimental      -      -      1      -      -
 tomlab_snopt  experimental      -      -      -      -      0
 gurobi_mex    legacy            0      0      0      0      -
 lindo_old     legacy            0      -      -      -      -
 lindo_legacy  legacy            0      -      -      -      -
 lp_solve      legacy            1      -      -      -      -
 opti          legacy            0      0      0      0      0
 ----------------------------------------------------------------------
 Total         -                 8      3      4      1      2

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 > You can solve LP problems using: 'dqqMinos' - 'glpk' - 'gurobi' - 'ibm_cplex' - 'matlab' - 'pdco' - '
 > You can solve MILP problems using: 'glpk' - 'gurobi' - 'ibm_cplex'
 > You can solve QP problems using: 'gurobi' - 'ibm_cplex' - 'pdco' - 'qpng'
 > You can solve MIQP problems using: 'gurobi'
 > You can solve NLP problems using: 'matlab' - 'quadMinos'

 > Checking for available updates ...
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 > You can update The COBRA Toolbox by running updateCobraToolbox() (from within MATLAB).
```

```
 -> The code grade is D (10.00%).


   Downloading models to /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/test/models ...
 > Already exists:  AntCore.mat
 > Already exists:  iIT341.xml
 > Already exists:  Abiotrophia_defectiva_ATCC_49176.xml
 > Already exists:  Sc_iND750_flux1.xml
 > Already exists:  ecoli_core_model.mat
 > Already exists:  modelReg.mat
 > Already exists:  iAF1260.mat
 > Already exists:  iJO1366.mat
 > Already exists:  Abiotrophia_defectiva_ATCC_49176.mat
 > Already exists:  Acidaminococcus_fermentans_DSM_20731.mat
 > Already exists:  Acidaminococcus_intestini_RyC_MR95.mat
 > Already exists:  Acidaminococcus_sp_D21.mat
 > Already exists:  Acinetobacter_calcoaceticus_PHEA_2.mat
 > Already exists:  Ec_iAF1260_flux1.xml
 > Already exists:  STM_v1.0.xml
 > Already exists:  ME_matrix_GlcAer_WT.mat
 > Already exists:  Recon2.v04.mat
   Done downloading models.
Running testSparseLP
   Testing sparseLP using gurobi6 ...
   -- testCase 1 with approximation: exp ... Done.
   -- testCase 1 with approximation: cappedL1 ... Done.
   -- testCase 1 with approximation: log ... Done.
   -- testCase 1 with approximation: SCAD ... Done.
   -- testCase 1 with approximation: lp- ... Done.
   -- testCase 1 with approximation: lp+ ... Done.
   -- testCase 2 with approximation: exp ... Done.
   -- testCase 2 with approximation: cappedL1 ... Done.
   -- testCase 2 with approximation: log ... Done.
   -- testCase 2 with approximation: SCAD ... Done.
   -- testCase 2 with approximation: lp- ... Done.
   -- testCase 2 with approximation: lp+ ... Done.
Done.
   Testing sparseLP using glpk ...
   -- testCase 1 with approximation: exp ... Done.
   -- testCase 1 with approximation: cappedL1 ... Done.
   -- testCase 1 with approximation: log ... Done.
   -- testCase 1 with approximation: SCAD ... Done.
   -- testCase 1 with approximation: lp- ... Done.
   -- testCase 1 with approximation: lp+ ... Done.
   -- testCase 2 with approximation: exp ... Done.
   -- testCase 2 with approximation: cappedL1 ... Done.
   -- testCase 2 with approximation: log ... Done.
   -- testCase 2 with approximation: SCAD ... Done.
   -- testCase 2 with approximation: lp- ... Done.
   -- testCase 2 with approximation: lp+ ... Done.
Done.
.
Done testSparseLP

----------

Running testConnectedComponents
Warning: Image Processing Toolbox is not installed or not licensed. Aborting test.

.
Done testConnectedComponents

----------

Running testCorrespondingRowsCols
S =

    -1     0     0     0     0
     2    -3     0     0     0
```

```
     0     4    -5     0     0
     0     0     6    -7     0
     0     0     0     0     8
--- row subset for getCorrespondingRows ----
    -1     0     0
     2    -3     0
     0     4    -5
     0     0     6
     0     0     0
exclusive
    -1     0     0
     2    -3     0
     0     4    -5
inclusive
    -1     0     0
     2    -3     0
     0     4    -5
     0     0     6
partial
     0     0     6
--- col subset for getCorrespondingCols ----
    -1     0     0     0     0
     2    -3     0     0     0
     0     4    -5     0     0
exclusive
    -1     0
     2    -3
     0     4
inclusive
    -1     0     0
     2    -3     0
     0     4    -5
partial
     0
     0
    -5
```

```
.
Done testCorrespondingRowsCols
__________

Running testDeletionStudy
 -- Running testfindBlockedReaction using the solver interface: tomlab_cplex ... Done.
 -- Running testfindBlockedReaction using the solver interface: gurobi6 ...
*** Test basic single gene deletion: ***


*** Deleting gene for ENO: ***

Single gene deletion analysis in progress ...
100%    [....................................]
Single deletion analysis to remove lethal genes
Single gene deletion analysis in progress ...
100%    [....................................]
0 non-lethal genes
Single deletion analysis to remove lethal genes from gene set 2
Single gene deletion analysis in progress ...
100%    [....................................]
1 non-lethal genes
Double gene deletion analysis
Total of 0 pairs to analyze
Double gene deletion analysis in progress ...
Perc complete CPU time
```

```
Starting singleRxnDeletion test:
Single reaction deletion analysis in progress ...

nonZeroInd =

     3
     7
     2
    11

.
Done testFEA
__________

Running testFVA
Starting parallel pool (parpool) using the 'local' profile ... connected to 2 workers.
   Testing flux variability analysis using gurobi ...     Testing flux variability for the following rea
  Columns 1 through 18

    'PGI'    'PFK'    'FBP'    'FBA'    'TPI'    'GAPD'    'PGK'    'PGM'    'ENO'    'PYK'    'PPS'

  Column 19

    'TALA'

12PPDt -10.3706 9.85579 20.2264
    Testing flux variability with printLevel 0:
    Testing flux variability with printLevel 1:
Flux variability analysis in progress ...
    Testing flux variability with test method FBA:
Flux variability analysis in progress ...
    Testing flux variability with test method 0-norm:
Flux variability analysis in progress ...
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.03 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.14 computation time (sec)
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.07 computation time (sec)
---FBA---
  -6.32581 FBA objective.
       327 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
  -6.32581 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
       0.1 computation time (sec)
---FBA---
  -6.32581 FBA objective.
       327 reactions above epsilon = 1e-09
      0.01 computation time (sec)
---Non-convex approximation---
  -6.32581 = Sparse FBA objective.
```

```
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.06 computation time (sec)
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.03 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.14 computation time (sec)
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.06 computation time (sec)
---FBA---
  -10.3706 FBA objective.
       324 reactions above epsilon = 1e-09
      0.01 computation time (sec)
---Non-convex approximation---
  -10.3706 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       324 reactions above epsilon = 1e-09
      0.09 computation time (sec)
---FBA---
  -10.3706 FBA objective.
       324 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
  -10.3706 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       324 reactions above epsilon = 1e-09
      0.07 computation time (sec)
    Testing flux variability with test method 1-norm:
Flux variability analysis in progress ...
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.06 computation time (sec)
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.03 computation time (sec)
---FBA---
  -6.32581 FBA objective.
       327 reactions above epsilon = 1e-09
      0.01 computation time (sec)
---Non-convex approximation---
  -6.32581 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.03 computation time (sec)
```

```
---FBA---
  -6.32581 FBA objective.
       327 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
  -6.32581 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.05 computation time (sec)
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.05 computation time (sec)
---FBA---
         0 FBA objective.
       327 reactions above epsilon = 1e-09
      0.01 computation time (sec)
---Non-convex approximation---
         0 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       327 reactions above epsilon = 1e-09
      0.03 computation time (sec)
---FBA---
  -10.3706 FBA objective.
       324 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
  -10.3706 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       324 reactions above epsilon = 1e-09
      0.04 computation time (sec)
---FBA---
  -10.3706 FBA objective.
       324 reactions above epsilon = 1e-09
      0.02 computation time (sec)
---Non-convex approximation---
  -10.3706 = Sparse FBA objective.
         0 = ||c^T*v - f*||^2.
       324 reactions above epsilon = 1e-09
      0.04 computation time (sec)
    Testing flux variability with test method 2-norm:
Flux variability analysis in progress ...
    Testing flux variability with test method minOrigSol:
Flux variability analysis in progress ...
Done.
.
Done testFVA
__________

Running testFastFVA
 > The CPLEX version has been determined as 1271.

-- Warning:: You may only ouput 4, 7 or 9 variables.

 >> Solving Model.S. (uncoupled)
 >> The number of arguments is: input: 5, output 2.
 >> Size of stoichiometric matrix: (72,95)
 >> Only 2 reactions of 95 are solved (~ 2.11%).
 >> 0 reactions out of 2 are minimized (0.00%).
 >> 0 reactions out of 2 are maximized (0.00%).
 >> 2 reactions out of 2 are minimized and maximized (100.00%).

 -- Starting to loop through the 2 workers. --
```

```
 -- The splitting strategy is 0. --

------------------------------------------------------------------------------
--  Task Launched // TaskID: 1 / 2 (LoopID = 2) <> [2, 2] / [72, 2].
 >> Number of reactions given to the worker: 1
 >> The number of reactions retrieved is 1
 >> Log files will be stored at /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/src/analysis/
 -- Start time:     Mon Jul 10 23:27:24 2017
 >> #Task.ID = 1; logfile: cplexint_logfile_1.log
        -- Minimization (iRound = 0). Number of reactions: 1.
        -- Maximization (iRound = 1). Number of reactions: 1.
 -- End time:     Mon Jul 10 23:27:24 2017
 >> Time spent in FVAc: 0.1 seconds.
------------------------------------------------------------------------------
 ==> 100% done. Analysis completed.

------------------------------------------------------------------------------
--  Task Launched // TaskID: 2 / 2 (LoopID = 1) <> [1, 1] / [72, 2].
 >> Number of reactions given to the worker: 1
 >> The number of reactions retrieved is 1
 >> Log files will be stored at /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/src/analysis/
 -- Start time:     Mon Jul 10 23:27:24 2017
 >> #Task.ID = 2; logfile: cplexint_logfile_2.log
        -- Minimization (iRound = 0). Number of reactions: 1.
        -- Maximization (iRound = 1). Number of reactions: 1.
 -- End time:     Mon Jul 10 23:27:24 2017
 >> Time spent in FVAc: 0.1 seconds.
------------------------------------------------------------------------------
 ==> 100% done. Analysis completed.
 > The CPLEX version has been determined as 1271.

-- Warning:: You may only ouput 4, 7 or 9 variables.

 >> Solving Model.S. (uncoupled)
 >> The number of arguments is: input: 5, output 2.
 >> Size of stoichiometric matrix: (72,95)
 >> Only 2 reactions of 95 are solved (~ 2.11%).
 >> 0 reactions out of 2 are minimized (0.00%).
 >> 0 reactions out of 2 are maximized (0.00%).
 >> 2 reactions out of 2 are minimized and maximized (100.00%).

 -- Starting to loop through the 2 workers. --

 -- The splitting strategy is 0. --

------------------------------------------------------------------------------
--  Task Launched // TaskID: 1 / 2 (LoopID = 2) <> [2, 2] / [72, 2].
 >> Number of reactions given to the worker: 1
 >> The number of reactions retrieved is 1
 >> Log files will be stored at /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/src/analysis/
 -- Start time:     Mon Jul 10 23:27:30 2017
 >> #Task.ID = 1; logfile: cplexint_logfile_1.log
        -- Minimization (iRound = 0). Number of reactions: 1.
        -- Maximization (iRound = 1). Number of reactions: 1.
 -- End time:     Mon Jul 10 23:27:30 2017
 >> Time spent in FVAc: 0.0 seconds.
------------------------------------------------------------------------------
 ==> 100% done. Analysis completed.

------------------------------------------------------------------------------
--  Task Launched // TaskID: 2 / 2 (LoopID = 1) <> [1, 1] / [72, 2].
 >> Number of reactions given to the worker: 1
 >> The number of reactions retrieved is 1
 >> Log files will be stored at /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/src/analysis/
 -- Start time:     Mon Jul 10 23:27:30 2017
 >> #Task.ID = 2; logfile: cplexint_logfile_2.log
        -- Minimization (iRound = 0). Number of reactions: 1.
```

```
        -- Maximization (iRound = 1). Number of reactions: 1.
 -- End time:     Mon Jul 10 23:27:30 2017
 >> Time spent in FVAc: 0.0 seconds.
------------------------------------------------------------------------------
 ==> 100% done. Analysis completed.

Warning: Model already has the same reaction you tried to add: Ex_A[e]
R_AB A[c]  -> B[c]
Warning: Model already has the same reaction you tried to add: At[e]r
    24 Total reactions
    17 Reversible reactions.
     7 Irreversible reactions.
    23 Flux consistent reactions, without flipping.
     1 Flux inconsistent reactions, without flipping.
    24 Flux consistent reactions.
     0 Flux inconsistent reversible reactions left to flip.
fastcc.m: The input model is entirely flux consistent.\n
prepareGapFill finished
Running fastGapFill ...
Variables loaded from .mat file

Run 1 (initial)
|J|=4  |A|=10
|J|=0  |A|=10
Elapsed time is 0.153707 seconds.

Run 2 (hw)
|J|=4  |A|=10
|J|=0  |A|=10
Elapsed time is 0.067852 seconds.

Run 3 (vhw)
|J|=4  |A|=10
|J|=0  |A|=10
Elapsed time is 0.096867 seconds.
Done.
.
Done testFastGapFill
----------

Running testFindBlockedReaction
 -- Running testfindBlockedReaction using the solver interface: tomlab_cplex ... Done.
 -- Running testfindBlockedReaction using the solver interface: gurobi6 ... Done.
 -- Running testfindBlockedReaction using the solver interface: glpk ... Done.
.
Done testFindBlockedReaction
----------

Running testFitC13Data
   Preparing the model using glpk ... We assume that all mass balance constraints are equalities, i.e.,
ommitting reactions due to FVA
ans =
    'EX_lacL'
    'EX_no2'
    'EX_no3'
    'ASNS2'
    'LLACD2'
    'LLACD3'
    'NO3R1'
    'NO3R2'
    'NO2t2r'
    'NO3t7'
    'NTRIR2x'
    'EX_co2_r'

xdir = /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/src/dataIntegration/fluxomics/c13solve
```

```
generating EMU method
generating CUMOMER method
optimizing EMU method
optimizing CUMOMER method
Done.
   Testing fitC13Data using matlab ...
Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

Done.
.
Done testFitC13Data
__________

Running testGDLS
Running testGDLS using gurobi ... Biomass flux:    1.208983
Synthetic flux:  [0.000000, -0.000000]
Iteration 1
-----------
Biomass flux:    0.322736
Synthetic flux:  [17.376573, 17.376573]
Knockout cost:   3
Knockouts:
 ACALD
 CYTBD
 PYK
Biomass_Ecoli_core_w_GAM 0.322736
EX_ac(e) 17.7183
EX_co2(e) -17.9532
EX_for(e) 19.2761
EX_glc(e) -20
EX_h(e) 78.2216
EX_h2o(e) 1.77431
EX_nh4(e) -1.75982
EX_pi(e) -1.18725
EX_succ(e) 17.3766
elapsed_time = 0.9342
Iteration 2
-----------
Biomass flux:    0.145335
Synthetic flux:  [19.169359, 25.376614]
Knockout cost:   4
Knockouts:
 ACALD
 CYTBD
 LDH_D
 PFL
Biomass_Ecoli_core_w_GAM 0.145335
EX_ac(e) 12.4145
EX_co2(e) -12.5203
EX_glc(e) -20
EX_h(e) 66.0832
EX_h2o(e) 13.915
EX_nh4(e) -0.792483
EX_pi(e) -0.534644
EX_succ(e) 25.3766
elapsed_time = 1.7144
Iteration 3
-----------
Biomass flux:    0.127142
```

```
Synthetic flux:  [20.181668, 26.022544]
Knockout cost:   5
Knockouts:
 ACALD
 CYTBD
 LDH_D
 PFL
 THD2
Biomass_Ecoli_core_w_GAM 0.127142
EX_ac(e) 11.6818
EX_co2(e) -12.8643
EX_glc(e) -20
EX_h(e) 66.2773
EX_h2o(e) 14.0844
EX_nh4(e) -0.693281
EX_pi(e) -0.467718
EX_succ(e) 26.0225
elapsed_time = 2.1227
Iteration 4
-----------
Biomass flux:    0.127142
Synthetic flux:  [20.181668, 26.022544]
Knockout cost:   5
Knockouts:
 ACALD
 CYTBD
 LDH_D
 PFL
 THD2
Biomass_Ecoli_core_w_GAM 0.127142
EX_ac(e) 11.6818
EX_co2(e) -12.8643
EX_glc(e) -20
EX_h(e) 66.2773
EX_h2o(e) 14.0844
EX_nh4(e) -0.693281
EX_pi(e) -0.467718
EX_succ(e) 26.0225
elapsed_time = 2.5131
Generating Output
Done.
.
Done testGDLS
----------

Running testConvertOldStyleModel
>> Testing Model conversion and field merging:
Warning: Size of metHMDBID does not fit to mets. Old field metHMDB exists, but cannot be
merged
Warning: Size of metHMDBID does not fit to mets. Old field metHMDB exists, but cannot be
merged

.
Done testConvertOldStyleModel
----------

Running testInchi
.
Done testInchi
----------

Running testMDFBA
Warning: Metabolite A not in model - added to the model
Warning: Metabolite B not in model - added to the model
R1 A  -> B
Warning: Metabolite D not in model - added to the model
```

```
Warning: Metabolite C not in model - added to the model
R2 B + D  -> C
Warning: Metabolite E not in model - added to the model
Warning: Metabolite F not in model - added to the model
R3 C  -> E + F
R4 A  -> D
R5 F  -> D
EX_A A  <=>
EX_E E  <=>
   Testing MDFBA using gurobi6 ...
    Testing MDFBA using glpk ...
    Testing MDFBA using ibm_cplex ...
 .
Done testMDFBA
----------

Running testMOMA
 -- Running testfindBlockedReaction using the solver interface: tomlab_cplex ... MOMA requires a QP solv
 -- Running testfindBlockedReaction using the solver interface: gurobi6 ... Done.
.
Done testMOMA
----------

Running testMPS
 > The interface to 'mps' from solveCobraLP will not be supported anymore.
 -> Use >> writeCbModel(model, 'mps');
 > The interface to 'mps' from solveCobraLP will not be supported anymore.
 -> Use >> writeCbModel(model, 'mps');
 > The interface to 'mps' from solveCobraMILP will not be supported anymore.
 -> Use >> writeCbModel(model, 'mps');
 > The interface to 'mps' from solveCobraLP will not be supported anymore.
 -> Use >> writeCbModel(model, 'mps');
.
Done testMPS
----------

Running testMassChargeBalance
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
```

```
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     4                            R4 -2 H, -2 C, -2 O 3 B[c]  -> D[c]
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
Checked element H
Checking element C
Checking element O
Checking element P
```

```
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
Checked element H
Checking element C
Checking element O
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Checking element N
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Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
```

```
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     4                            R4 -2 H, -2 C, -2 O 3 B[c]  -> D[c]
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
2 B[c] has no formula
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
2 B[c] has no formula
Checked element H
Checking element C
```

```
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
2 B[c] has no formula
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
```

```
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
There are mass imbalanced reactions, see mass_imbalanced_reactions.txt
There are charge imbalanced reactions, see charge_imbalanced_reactions.txt
2 B[c] has no formula
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
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Checking element R
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Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
Checked element H
Checking element C
Checking element O
Checking element P
Checking element S
Checking element N
Checking element Mg
Checking element X
Checking element Fe
Checking element Zn
Checking element Co
Checking element R
Checking element Ca
Checking element Y
Checking element I
Checking element Na
Checking element Cl
Checking element K
Checking element R
Checking element FULLR
     1                          Ex_A -1 H, -1 C, -1 O A[c]  <=>
     6                          Ex_E -2 H, -2 C, -2 O E[c]  ->
Mass balanced, but charged imbalanced reactions:
.
Done testMassChargeBalance

----------
```

```
Running testFluxSplits
 -- Running testFluxSplits using the solver interface: tomlab_cplex ...
Warning: The test testFluxSplits cannot run using the solver interface: tomlab_cplex. The
solver interface is not installed or not configured properly.
 -- Running testFluxSplits using the solver interface: gurobi6 ... Done.
.
Done testFluxSplits
----------

Running testModelBorgifier
modelBorgifier: Loading Ecoli core model.
modelBorgifier: Loading iIT341 model.
The model contains 0 errors and 1 warnings.

modelBorgifier: Testing Cmodel verification... success.
modelBorgifier: Testing Tmodel verification... success.
modelBorgifier: Testing Tmodel building... success.
modelBorgifier: Testing model comparison... success.
modelBorgifier: Loading test matching arrays.
modelBorgifier: Testing model merging and extraction... Matricies are now equal before and after merging
success.
.
Done testModelBorgifier
----------

Running testChangeObjective
Rxn4 not in model
.
Done testChangeObjective
----------

Running testChangeRxnBounds
Warning: Reaction Rxn4 not in model
Warning: Reaction Rxn4 not in model

.
Done testChangeRxnBounds
----------

Running testCheckObjective
summaryT =
    Coefficient    Metabolite    metID            Reaction            RxnID
    -----------    ----------    -----    ------------------------    -----

     -1.496        3pg[c]         3       Biomass_Ecoli_core_w_GAM    13
    -3.7478        accoa[c]      10       Biomass_Ecoli_core_w_GAM    13
      59.81        adp[c]        13       Biomass_Ecoli_core_w_GAM    13
     4.1182        akg[c]        14       Biomass_Ecoli_core_w_GAM    13
     -59.81        atp[c]        17       Biomass_Ecoli_core_w_GAM    13
     3.7478        coa[c]        21       Biomass_Ecoli_core_w_GAM    13
     -0.361        e4p[c]        23       Biomass_Ecoli_core_w_GAM    13
    -0.0709        f6p[c]        26       Biomass_Ecoli_core_w_GAM    13
     -0.129        g3p[c]        33       Biomass_Ecoli_core_w_GAM    13
     -0.205        g6p[c]        34       Biomass_Ecoli_core_w_GAM    13
    -0.2557        gln-L[c]      36       Biomass_Ecoli_core_w_GAM    13
    -4.9414        glu-L[c]      38       Biomass_Ecoli_core_w_GAM    13
     -59.81        h2o[c]        41       Biomass_Ecoli_core_w_GAM    13
      59.81        h[c]          43       Biomass_Ecoli_core_w_GAM    13
     -3.547        nad[c]        50       Biomass_Ecoli_core_w_GAM    13
      3.547        nadh[c]       51       Biomass_Ecoli_core_w_GAM    13
     13.028        nadp[c]       52       Biomass_Ecoli_core_w_GAM    13
    -13.028        nadph[c]      53       Biomass_Ecoli_core_w_GAM    13
    -1.7867        oaa[c]        58       Biomass_Ecoli_core_w_GAM    13
    -0.5191        pep[c]        59       Biomass_Ecoli_core_w_GAM    13
      59.81        pi[c]         60       Biomass_Ecoli_core_w_GAM    13
    -2.8328        pyr[c]        62       Biomass_Ecoli_core_w_GAM    13
```

```
    -0.8977        r5p[c]        66       Biomass_Ecoli_core_w_GAM    13
```

```
summaryT =
    Coefficient    Metabolite    metID            Reaction            RxnID
    ___________    __________    _____    ________________________    _____

         -1        acald[c]       8       ACALD                        1
          1        accoa[c]      10       ACALD                        1
         -1        coa[c]        21       ACALD                        1
          1        h[c]          43       ACALD                        1
         -1        nad[c]        50       ACALD                        1
          1        nadh[c]       51       ACALD                        1
     -1.496        3pg[c]         3       Biomass_Ecoli_core_w_GAM    13
    -3.7478        accoa[c]      10       Biomass_Ecoli_core_w_GAM    13
      59.81        adp[c]        13       Biomass_Ecoli_core_w_GAM    13
     4.1182        akg[c]        14       Biomass_Ecoli_core_w_GAM    13
     -59.81        atp[c]        17       Biomass_Ecoli_core_w_GAM    13
     3.7478        coa[c]        21       Biomass_Ecoli_core_w_GAM    13
     -0.361        e4p[c]        23       Biomass_Ecoli_core_w_GAM    13
    -0.0709        f6p[c]        26       Biomass_Ecoli_core_w_GAM    13
     -0.129        g3p[c]        33       Biomass_Ecoli_core_w_GAM    13
     -0.205        g6p[c]        34       Biomass_Ecoli_core_w_GAM    13
    -0.2557        gln-L[c]      36       Biomass_Ecoli_core_w_GAM    13
    -4.9414        glu-L[c]      38       Biomass_Ecoli_core_w_GAM    13
     -59.81        h2o[c]        41       Biomass_Ecoli_core_w_GAM    13
      59.81        h[c]          43       Biomass_Ecoli_core_w_GAM    13
     -3.547        nad[c]        50       Biomass_Ecoli_core_w_GAM    13
      3.547        nadh[c]       51       Biomass_Ecoli_core_w_GAM    13
     13.028        nadp[c]       52       Biomass_Ecoli_core_w_GAM    13
    -13.028        nadph[c]      53       Biomass_Ecoli_core_w_GAM    13
    -1.7867        oaa[c]        58       Biomass_Ecoli_core_w_GAM    13
    -0.5191        pep[c]        59       Biomass_Ecoli_core_w_GAM    13
      59.81        pi[c]         60       Biomass_Ecoli_core_w_GAM    13
    -2.8328        pyr[c]        62       Biomass_Ecoli_core_w_GAM    13
    -0.8977        r5p[c]        66       Biomass_Ecoli_core_w_GAM    13
```

```
.
Done testCheckObjective

__________

Running testModelManipulation
>> Starting non-empty model tests:
EX_glc glc-D[e]  ->
ABC_def 2 glc-D[e]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction
ABC_def 3 glc-D[e]  <=>
EX_glc-D[e] glc-D[e]  ->
EX_glc-D glc-D  ->
ans =
            S: [12×9 double]
           lb: [9×1 double]
           ub: [9×1 double]
         rxns: {9×1 cell}
         mets: {12×1 cell}
            c: [9×1 double]
    subSystems: {9×1 cell}
Warning: Metabolite A not in model - added to the model
Warning: Metabolite B not in model - added to the model
Warning: Metabolite C not in model - added to the model
newRxn1 A  -> B + 2 C
>> Starting empty model tests:
Warning: Metabolite A not in model - added to the model
Warning: Metabolite B not in model - added to the model
Warning: Metabolite C not in model - added to the model
```

```
newRxn1 A  -> B + 2 C
>> Testing convertToIrreversible (1)
>> Testing convertToReversible
>> Testing convertToIrreversible (2)
>> Testing convertToIrreversible (3)
.
Done testModelManipulation

----------

Running testRemoveDuplicateRxn
Checking for reaction duplicates by stoichiometry (up to orientation) ...
     Keep:  GLCt1 glc-D[e]  -> glc-D
Duplicate:  GLCt1_duplicate_reverse glc-D  <=> glc-D[e]
Checking for reaction duplicates by stoichiometry ...
 no duplicates found.
.
Done testRemoveDuplicateRxn

----------

Running testBuildPairwiseModels
The following fields are missing in several models, they will not be merged:
Abiotrophia_defectiva_ATCC_49176_IEX_adocbl[u]tr Abiotrophia_defectiva_ATCC_49176_adocbl[e]  <=> adocbl
Abiotrophia_defectiva_ATCC_49176_IEX_alaasp[u]tr Abiotrophia_defectiva_ATCC_49176_alaasp[e]  <=> alaasp
Abiotrophia_defectiva_ATCC_49176_IEX_alagln[u]tr Abiotrophia_defectiva_ATCC_49176_alagln[e]  <=> alagln
Abiotrophia_defectiva_ATCC_49176_IEX_alaglu[u]tr Abiotrophia_defectiva_ATCC_49176_alaglu[e]  <=> alaglu
Abiotrophia_defectiva_ATCC_49176_IEX_alagly[u]tr Abiotrophia_defectiva_ATCC_49176_alagly[e]  <=> alagly
Abiotrophia_defectiva_ATCC_49176_IEX_alahis[u]tr Abiotrophia_defectiva_ATCC_49176_alahis[e]  <=> alahis
Abiotrophia_defectiva_ATCC_49176_IEX_alaleu[u]tr Abiotrophia_defectiva_ATCC_49176_alaleu[e]  <=> alaleu
Abiotrophia_defectiva_ATCC_49176_IEX_alathr[u]tr Abiotrophia_defectiva_ATCC_49176_alathr[e]  <=> alathr
Abiotrophia_defectiva_ATCC_49176_IEX_arab_L[u]tr Abiotrophia_defectiva_ATCC_49176_arab_L[e]  <=> arab_L
Abiotrophia_defectiva_ATCC_49176_IEX_h[u]tr Abiotrophia_defectiva_ATCC_49176_h[e]  <=> h[u]
Abiotrophia_defectiva_ATCC_49176_IEX_arsenb[u]tr Abiotrophia_defectiva_ATCC_49176_arsenb[e]  <=> arsenb
Abiotrophia_defectiva_ATCC_49176_IEX_aso3[u]tr Abiotrophia_defectiva_ATCC_49176_aso3[e]  <=> aso3[u]
Abiotrophia_defectiva_ATCC_49176_IEX_aso4[u]tr Abiotrophia_defectiva_ATCC_49176_aso4[e]  <=> aso4[u]
Abiotrophia_defectiva_ATCC_49176_IEX_btn[u]tr Abiotrophia_defectiva_ATCC_49176_btn[e]  <=> btn[u]
Abiotrophia_defectiva_ATCC_49176_IEX_ca2[u]tr Abiotrophia_defectiva_ATCC_49176_ca2[e]  <=> ca2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_cbl1[u]tr Abiotrophia_defectiva_ATCC_49176_cbl1[e]  <=> cbl1[u]
Abiotrophia_defectiva_ATCC_49176_IEX_cbl2[u]tr Abiotrophia_defectiva_ATCC_49176_cbl2[e]  <=> cbl2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_cd2[u]tr Abiotrophia_defectiva_ATCC_49176_cd2[e]  <=> cd2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_cgly[u]tr Abiotrophia_defectiva_ATCC_49176_cgly[e]  <=> cgly[u]
Abiotrophia_defectiva_ATCC_49176_IEX_co2[u]tr Abiotrophia_defectiva_ATCC_49176_co2[e]  <=> co2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_cobalt2[u]tr Abiotrophia_defectiva_ATCC_49176_cobalt2[e]  <=> cobal
Abiotrophia_defectiva_ATCC_49176_IEX_cu2[u]tr Abiotrophia_defectiva_ATCC_49176_cu2[e]  <=> cu2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_drib[u]tr Abiotrophia_defectiva_ATCC_49176_drib[e]  <=> drib[u]
Abiotrophia_defectiva_ATCC_49176_IEX_4abut[u]tr Abiotrophia_defectiva_ATCC_49176_4abut[e]  <=> 4abut[u]
Abiotrophia_defectiva_ATCC_49176_IEX_arg_L[u]tr Abiotrophia_defectiva_ATCC_49176_arg_L[e]  <=> arg_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_biomass[c]tr Abiotrophia_defectiva_ATCC_49176_biomass[c]  <=> bioma
Abiotrophia_defectiva_ATCC_49176_IEX_cit[u]tr Abiotrophia_defectiva_ATCC_49176_cit[e]  <=> cit[u]
Abiotrophia_defectiva_ATCC_49176_IEX_cl[u]tr Abiotrophia_defectiva_ATCC_49176_cl[e]  <=> cl[u]
Abiotrophia_defectiva_ATCC_49176_IEX_fe2[u]tr Abiotrophia_defectiva_ATCC_49176_fe2[e]  <=> fe2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_fe3[u]tr Abiotrophia_defectiva_ATCC_49176_fe3[e]  <=> fe3[u]
Abiotrophia_defectiva_ATCC_49176_IEX_fol[u]tr Abiotrophia_defectiva_ATCC_49176_fol[e]  <=> fol[u]
Abiotrophia_defectiva_ATCC_49176_IEX_for[u]tr Abiotrophia_defectiva_ATCC_49176_for[e]  <=> for[u]
Abiotrophia_defectiva_ATCC_49176_IEX_gal[u]tr Abiotrophia_defectiva_ATCC_49176_gal[e]  <=> gal[u]
Abiotrophia_defectiva_ATCC_49176_IEX_glc_D[u]tr Abiotrophia_defectiva_ATCC_49176_glc_D[e]  <=> glc_D[u]
Abiotrophia_defectiva_ATCC_49176_IEX_glu_L[u]tr Abiotrophia_defectiva_ATCC_49176_glu_L[e]  <=> glu_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_gly[u]tr Abiotrophia_defectiva_ATCC_49176_gly[e]  <=> gly[u]
Abiotrophia_defectiva_ATCC_49176_IEX_glyasn[u]tr Abiotrophia_defectiva_ATCC_49176_glyasn[e]  <=> glyasn
Abiotrophia_defectiva_ATCC_49176_IEX_glyasp[u]tr Abiotrophia_defectiva_ATCC_49176_glyasp[e]  <=> glyasp
Abiotrophia_defectiva_ATCC_49176_IEX_glyb[u]tr Abiotrophia_defectiva_ATCC_49176_glyb[e]  <=> glyb[u]
Abiotrophia_defectiva_ATCC_49176_IEX_glyc3p[u]tr Abiotrophia_defectiva_ATCC_49176_glyc3p[e]  <=> glyc3p
Abiotrophia_defectiva_ATCC_49176_IEX_glycys[u]tr Abiotrophia_defectiva_ATCC_49176_glycys[e]  <=> glycys
Abiotrophia_defectiva_ATCC_49176_IEX_glygln[u]tr Abiotrophia_defectiva_ATCC_49176_glygln[e]  <=> glygln
Abiotrophia_defectiva_ATCC_49176_IEX_glyglu[u]tr Abiotrophia_defectiva_ATCC_49176_glyglu[e]  <=> glyglu
Abiotrophia_defectiva_ATCC_49176_IEX_glyleu[u]tr Abiotrophia_defectiva_ATCC_49176_glyleu[e]  <=> glyleu
Abiotrophia_defectiva_ATCC_49176_IEX_glymet[u]tr Abiotrophia_defectiva_ATCC_49176_glymet[e]  <=> glymet
Abiotrophia_defectiva_ATCC_49176_IEX_glyphe[u]tr Abiotrophia_defectiva_ATCC_49176_glyphe[e]  <=> glyphe
```

```
Abiotrophia_defectiva_ATCC_49176_IEX_glypro[u]tr Abiotrophia_defectiva_ATCC_49176_glypro[e]  <=> glypro[
Abiotrophia_defectiva_ATCC_49176_IEX_glytyr[u]tr Abiotrophia_defectiva_ATCC_49176_glytyr[e]  <=> glytyr[
Abiotrophia_defectiva_ATCC_49176_IEX_h2o[u]tr Abiotrophia_defectiva_ATCC_49176_h2o[e]  <=> h2o[u]
Abiotrophia_defectiva_ATCC_49176_IEX_hg2[u]tr Abiotrophia_defectiva_ATCC_49176_hg2[e]  <=> hg2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_hxan[u]tr Abiotrophia_defectiva_ATCC_49176_hxan[e]  <=> hxan[u]
Abiotrophia_defectiva_ATCC_49176_IEX_ile_L[u]tr Abiotrophia_defectiva_ATCC_49176_ile_L[e]  <=> ile_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_k[u]tr Abiotrophia_defectiva_ATCC_49176_k[e]  <=> k[u]
Abiotrophia_defectiva_ATCC_49176_IEX_lac_L[u]tr Abiotrophia_defectiva_ATCC_49176_lac_L[e]  <=> lac_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_lcts[u]tr Abiotrophia_defectiva_ATCC_49176_lcts[e]  <=> lcts[u]
Abiotrophia_defectiva_ATCC_49176_IEX_leu_L[u]tr Abiotrophia_defectiva_ATCC_49176_leu_L[e]  <=> leu_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_malt[u]tr Abiotrophia_defectiva_ATCC_49176_malt[e]  <=> malt[u]
Abiotrophia_defectiva_ATCC_49176_IEX_malthx[u]tr Abiotrophia_defectiva_ATCC_49176_malthx[e]  <=> malthx[
Abiotrophia_defectiva_ATCC_49176_IEX_malttr[u]tr Abiotrophia_defectiva_ATCC_49176_malttr[e]  <=> malttr[
Abiotrophia_defectiva_ATCC_49176_IEX_met_D[u]tr Abiotrophia_defectiva_ATCC_49176_met_D[e]  <=> met_D[u]
Abiotrophia_defectiva_ATCC_49176_IEX_met_L[u]tr Abiotrophia_defectiva_ATCC_49176_met_L[e]  <=> met_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_metala[u]tr Abiotrophia_defectiva_ATCC_49176_metala[e]  <=> metala[
Abiotrophia_defectiva_ATCC_49176_IEX_metsox_R_L[u]tr Abiotrophia_defectiva_ATCC_49176_metsox_R_L[e]  <=>
Abiotrophia_defectiva_ATCC_49176_IEX_metsox_S_L[u]tr Abiotrophia_defectiva_ATCC_49176_metsox_S_L[e]  <=>
Abiotrophia_defectiva_ATCC_49176_IEX_mg2[u]tr Abiotrophia_defectiva_ATCC_49176_mg2[e]  <=> mg2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_mn2[u]tr Abiotrophia_defectiva_ATCC_49176_mn2[e]  <=> mn2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_mqn7[u]tr Abiotrophia_defectiva_ATCC_49176_mqn7[e]  <=> mqn7[u]
Abiotrophia_defectiva_ATCC_49176_IEX_na1[u]tr Abiotrophia_defectiva_ATCC_49176_na1[e]  <=> na1[u]
Abiotrophia_defectiva_ATCC_49176_IEX_o2[u]tr Abiotrophia_defectiva_ATCC_49176_o2[e]  <=> o2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_ocdca[u]tr Abiotrophia_defectiva_ATCC_49176_ocdca[e]  <=> ocdca[u]
Abiotrophia_defectiva_ATCC_49176_IEX_orn[u]tr Abiotrophia_defectiva_ATCC_49176_orn[e]  <=> orn[u]
Abiotrophia_defectiva_ATCC_49176_IEX_pb[u]tr Abiotrophia_defectiva_ATCC_49176_pb[e]  <=> pb[u]
Abiotrophia_defectiva_ATCC_49176_IEX_pheme[u]tr Abiotrophia_defectiva_ATCC_49176_pheme[e]  <=> pheme[u]
Abiotrophia_defectiva_ATCC_49176_IEX_pi[u]tr Abiotrophia_defectiva_ATCC_49176_pi[e]  <=> pi[u]
Abiotrophia_defectiva_ATCC_49176_IEX_pro_L[u]tr Abiotrophia_defectiva_ATCC_49176_pro_L[e]  <=> pro_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_rib_D[u]tr Abiotrophia_defectiva_ATCC_49176_rib_D[e]  <=> rib_D[u]
Abiotrophia_defectiva_ATCC_49176_IEX_ribflv[u]tr Abiotrophia_defectiva_ATCC_49176_ribflv[e]  <=> ribflv[
Abiotrophia_defectiva_ATCC_49176_IEX_so4[u]tr Abiotrophia_defectiva_ATCC_49176_so4[e]  <=> so4[u]
Abiotrophia_defectiva_ATCC_49176_IEX_spmd[u]tr Abiotrophia_defectiva_ATCC_49176_spmd[e]  <=> spmd[u]
Abiotrophia_defectiva_ATCC_49176_IEX_taur[u]tr Abiotrophia_defectiva_ATCC_49176_taur[e]  <=> taur[u]
Abiotrophia_defectiva_ATCC_49176_IEX_thm[u]tr Abiotrophia_defectiva_ATCC_49176_thm[e]  <=> thm[u]
Abiotrophia_defectiva_ATCC_49176_IEX_trp_L[u]tr Abiotrophia_defectiva_ATCC_49176_trp_L[e]  <=> trp_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_val_L[u]tr Abiotrophia_defectiva_ATCC_49176_val_L[e]  <=> val_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_xyl_D[u]tr Abiotrophia_defectiva_ATCC_49176_xyl_D[e]  <=> xyl_D[u]
Abiotrophia_defectiva_ATCC_49176_IEX_zn2[u]tr Abiotrophia_defectiva_ATCC_49176_zn2[e]  <=> zn2[u]
Abiotrophia_defectiva_ATCC_49176_IEX_pnto_R[u]tr Abiotrophia_defectiva_ATCC_49176_pnto_R[e]  <=> pnto_R[
Abiotrophia_defectiva_ATCC_49176_IEX_cys_L[u]tr Abiotrophia_defectiva_ATCC_49176_cys_L[e]  <=> cys_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_ala_L[u]tr Abiotrophia_defectiva_ATCC_49176_ala_L[e]  <=> ala_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_asp_L[u]tr Abiotrophia_defectiva_ATCC_49176_asp_L[e]  <=> asp_L[u]
Abiotrophia_defectiva_ATCC_49176_IEX_his_L[u]tr Abiotrophia_defectiva_ATCC_49176_his_L[e]  <=> his_L[u]
```

```
Warning: Metabolite ac[b] not in model - added to the model
Warning: Metabolite h[b] not in model - added to the model

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
EX_ac(e)b ac[b]  ->
Warning: Metabolite acald[b] not in model - added to the model

ACALDtb acald[b]  <=> acald[c]
EX_acald(e)b acald[b]  ->
Warning: Metabolite akg[b] not in model - added to the model

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
EX_akg(e)b akg[b]  ->
Warning: Metabolite co2[b] not in model - added to the model

CO2tb co2[b]  <=> co2[c]
EX_co2(e)b co2[b]  <=>
Warning: Metabolite etoh[b] not in model - added to the model

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_etoh(e)b etoh[b]  ->
Warning: Metabolite for[b] not in model - added to the model

EX_for(e)b for[b]  ->
FORt2b h[b] + for[b]  -> for[c] + h[c]
FORtib for[c]  -> for[b]
```

```
Warning: Metabolite fru[b] not in model - added to the model

EX_fru(e)b fru[b]  ->
FRUpts2b pep[c] + fru[b]  -> f6p[c] + pyr[c]
Warning: Metabolite fum[b] not in model - added to the model

EX_fum(e)b fum[b]  ->
FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Metabolite glc-D[b] not in model - added to the model

EX_glc(e)b glc-D[b]  <=>
GLCptsb pep[c] + glc-D[b]  -> g6p[c] + pyr[c]
Warning: Metabolite gln-L[b] not in model - added to the model

EX_gln_L(e)b gln-L[b]  ->
GLNabcb atp[c] + h2o[c] + gln-L[b]  -> adp[c] + gln-L[c] + h[c] + pi[c]
Warning: Metabolite glu-L[b] not in model - added to the model

EX_glu_L(e)b glu-L[b]  ->
GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite h2o[b] not in model - added to the model

EX_h2o(e)b h2o[b]  <=>
H2Otb h2o[b]  <=> h2o[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
ATPS4rb adp[c] + pi[c] + 4 h[b]  <=> atp[c] + h2o[c] + 3 h[c]
CYTBDb 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + q8[c] + 2 h[b]
Warning: Metabolite lac-D[b] not in model - added to the model

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_h(e)b h[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

FORt2b h[b] + for[b]  -> for[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite mal-L[b] not in model - added to the model

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
NADH16b 4 h[c] + nadh[c] + q8[c]  -> nad[c] + q8h2[c] + 3 h[b]
Warning: Metabolite pi[b] not in model - added to the model

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
Warning: Metabolite pyr[b] not in model - added to the model

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
Warning: Metabolite succ[b] not in model - added to the model

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
THD2b nadh[c] + nadp[c] + 2 h[b]  -> 2 h[c] + nad[c] + nadph[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
EX_lac_D(e)b lac-D[b]  ->
EX_mal_L(e)b mal-L[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
Warning: Metabolite nh4[b] not in model - added to the model

EX_nh4(e)b nh4[b]  <=>
NH4tb nh4[b]  <=> nh4[c]
Warning: Metabolite o2[b] not in model - added to the model

EX_o2(e)b o2[b]  <=>
O2tb o2[b]  <=> o2[c]
```

```
EX_pi(e)b pi[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
EX_pyr(e)b pyr[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
EX_succ(e)b succ[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
Host_IEX_ac[u]tr Host_ac[e]  <=> ac[u]
Host_IEX_acald[u]tr Host_acald[e]  <=> acald[u]
Host_IEX_akg[u]tr Host_akg[e]  <=> akg[u]
Host_IEX_co2[u]tr Host_co2[e]  <=> co2[u]
Host_IEX_etoh[u]tr Host_etoh[e]  <=> etoh[u]
Host_IEX_for[u]tr Host_for[e]  <=> for[u]
Host_IEX_fru[u]tr Host_fru[e]  <=> fru[u]
Host_IEX_fum[u]tr Host_fum[e]  <=> fum[u]
Host_IEX_glc-D[u]tr Host_glc-D[e]  <=> glc-D[u]
Host_IEX_gln-L[u]tr Host_gln-L[e]  <=> gln-L[u]
Host_IEX_glu-L[u]tr Host_glu-L[e]  <=> glu-L[u]
Host_IEX_h2o[u]tr Host_h2o[e]  <=> h2o[u]
Host_IEX_h[u]tr Host_h[e]  <=> h[u]
Host_IEX_lac-D[u]tr Host_lac-D[e]  <=> lac-D[u]
Host_IEX_mal-L[u]tr Host_mal-L[e]  <=> mal-L[u]
Host_IEX_nh4[u]tr Host_nh4[e]  <=> nh4[u]
Host_IEX_o2[u]tr Host_o2[e]  <=> o2[u]
Host_IEX_pi[u]tr Host_pi[e]  <=> pi[u]
Host_IEX_pyr[u]tr Host_pyr[e]  <=> pyr[u]
Host_IEX_succ[u]tr Host_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [.....                                    ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
EX_lac-D[u] lac-D[u]  <=>
```

```
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
   Testing createMultipleSpeciesModel using glpk ... The following fields are missing in several models,
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
model2_IEX_ac[u]tr model2_ac[e]  <=> ac[u]
model2_IEX_acald[u]tr model2_acald[e]  <=> acald[u]
model2_IEX_akg[u]tr model2_akg[e]  <=> akg[u]
model2_IEX_co2[u]tr model2_co2[e]  <=> co2[u]
model2_IEX_etoh[u]tr model2_etoh[e]  <=> etoh[u]
model2_IEX_for[u]tr model2_for[e]  <=> for[u]
model2_IEX_fru[u]tr model2_fru[e]  <=> fru[u]
model2_IEX_fum[u]tr model2_fum[e]  <=> fum[u]
model2_IEX_glc-D[u]tr model2_glc-D[e]  <=> glc-D[u]
model2_IEX_gln-L[u]tr model2_gln-L[e]  <=> gln-L[u]
model2_IEX_glu-L[u]tr model2_glu-L[e]  <=> glu-L[u]
model2_IEX_h2o[u]tr model2_h2o[e]  <=> h2o[u]
model2_IEX_h[u]tr model2_h[e]  <=> h[u]
model2_IEX_lac-D[u]tr model2_lac-D[e]  <=> lac-D[u]
model2_IEX_mal-L[u]tr model2_mal-L[e]  <=> mal-L[u]
model2_IEX_nh4[u]tr model2_nh4[e]  <=> nh4[u]
model2_IEX_o2[u]tr model2_o2[e]  <=> o2[u]
model2_IEX_pi[u]tr model2_pi[e]  <=> pi[u]
model2_IEX_pyr[u]tr model2_pyr[e]  <=> pyr[u]
model2_IEX_succ[u]tr model2_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [.........                                ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
EX_lac-D[u] lac-D[u]  <=>
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
```

```
The following fields are missing in several models, they will not be merged:
Warning: Metabolite ac[b] not in model - added to the model
Warning: Metabolite h[b] not in model - added to the model

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
EX_ac(e)b ac[b]  ->
Warning: Metabolite acald[b] not in model - added to the model

ACALDtb acald[b]  <=> acald[c]
EX_acald(e)b acald[b]  ->
Warning: Metabolite akg[b] not in model - added to the model

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
EX_akg(e)b akg[b]  ->
Warning: Metabolite co2[b] not in model - added to the model

CO2tb co2[b]  <=> co2[c]
EX_co2(e)b co2[b]  <=>
Warning: Metabolite etoh[b] not in model - added to the model

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_etoh(e)b etoh[b]  ->
Warning: Metabolite for[b] not in model - added to the model

EX_for(e)b for[b]  ->
FORt2b h[b] + for[b]  -> for[c] + h[c]
FORtib for[c]  -> for[b]
Warning: Metabolite fru[b] not in model - added to the model

EX_fru(e)b fru[b]  ->
FRUpts2b pep[c] + fru[b]  -> f6p[c] + pyr[c]
Warning: Metabolite fum[b] not in model - added to the model

EX_fum(e)b fum[b]  ->
FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Metabolite glc-D[b] not in model - added to the model

EX_glc(e)b glc-D[b]  <=>
GLCptsb pep[c] + glc-D[b]  -> g6p[c] + pyr[c]
Warning: Metabolite gln-L[b] not in model - added to the model

EX_gln_L(e)b gln-L[b]  ->
GLNabcb atp[c] + h2o[c] + gln-L[b]  -> adp[c] + gln-L[c] + h[c] + pi[c]
Warning: Metabolite glu-L[b] not in model - added to the model

EX_glu_L(e)b glu-L[b]  ->
GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite h2o[b] not in model - added to the model

EX_h2o(e)b h2o[b]  <=>
H2Otb h2o[b]  <=> h2o[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
ATPS4rb adp[c] + pi[c] + 4 h[b]  <=> atp[c] + h2o[c] + 3 h[c]
CYTBDb 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + q8[c] + 2 h[b]
Warning: Metabolite lac-D[b] not in model - added to the model

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_h(e)b h[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

FORt2b h[b] + for[b]  -> for[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite mal-L[b] not in model - added to the model

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
```

```
NADH16b 4 h[c] + nadh[c] + q8[c]  -> nad[c] + q8h2[c] + 3 h[b]
Warning: Metabolite pi[b] not in model - added to the model

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
Warning: Metabolite pyr[b] not in model - added to the model

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
Warning: Metabolite succ[b] not in model - added to the model

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
THD2b nadh[c] + nadp[c] + 2 h[b]  -> 2 h[c] + nad[c] + nadph[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
EX_lac_D(e)b lac-D[b]  ->
EX_mal_L(e)b mal-L[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
Warning: Metabolite nh4[b] not in model - added to the model

EX_nh4(e)b nh4[b]  <=>
NH4tb nh4[b]  <=> nh4[c]
Warning: Metabolite o2[b] not in model - added to the model

EX_o2(e)b o2[b]  <=>
O2tb o2[b]  <=> o2[c]
EX_pi(e)b pi[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
EX_pyr(e)b pyr[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
EX_succ(e)b succ[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
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model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
model2_IEX_ac[u]tr model2_ac[e]  <=> ac[u]
model2_IEX_acald[u]tr model2_acald[e]  <=> acald[u]
model2_IEX_akg[u]tr model2_akg[e]  <=> akg[u]
model2_IEX_co2[u]tr model2_co2[e]  <=> co2[u]
model2_IEX_etoh[u]tr model2_etoh[e]  <=> etoh[u]
model2_IEX_for[u]tr model2_for[e]  <=> for[u]
model2_IEX_fru[u]tr model2_fru[e]  <=> fru[u]
model2_IEX_fum[u]tr model2_fum[e]  <=> fum[u]
model2_IEX_glc-D[u]tr model2_glc-D[e]  <=> glc-D[u]
model2_IEX_gln-L[u]tr model2_gln-L[e]  <=> gln-L[u]
model2_IEX_glu-L[u]tr model2_glu-L[e]  <=> glu-L[u]
model2_IEX_h2o[u]tr model2_h2o[e]  <=> h2o[u]
model2_IEX_h[u]tr model2_h[e]  <=> h[u]
model2_IEX_lac-D[u]tr model2_lac-D[e]  <=> lac-D[u]
model2_IEX_mal-L[u]tr model2_mal-L[e]  <=> mal-L[u]
model2_IEX_nh4[u]tr model2_nh4[e]  <=> nh4[u]
model2_IEX_o2[u]tr model2_o2[e]  <=> o2[u]
model2_IEX_pi[u]tr model2_pi[e]  <=> pi[u]
model2_IEX_pyr[u]tr model2_pyr[e]  <=> pyr[u]
model2_IEX_succ[u]tr model2_succ[e]  <=> succ[u]
Host_IEX_ac[u]tr Host_ac[e]  <=> ac[u]
Host_IEX_acald[u]tr Host_acald[e]  <=> acald[u]
Host_IEX_akg[u]tr Host_akg[e]  <=> akg[u]
Host_IEX_co2[u]tr Host_co2[e]  <=> co2[u]
Host_IEX_etoh[u]tr Host_etoh[e]  <=> etoh[u]
Host_IEX_for[u]tr Host_for[e]  <=> for[u]
Host_IEX_fru[u]tr Host_fru[e]  <=> fru[u]
Host_IEX_fum[u]tr Host_fum[e]  <=> fum[u]
Host_IEX_glc-D[u]tr Host_glc-D[e]  <=> glc-D[u]
Host_IEX_gln-L[u]tr Host_gln-L[e]  <=> gln-L[u]
Host_IEX_glu-L[u]tr Host_glu-L[e]  <=> glu-L[u]
Host_IEX_h2o[u]tr Host_h2o[e]  <=> h2o[u]
Host_IEX_h[u]tr Host_h[e]  <=> h[u]
Host_IEX_lac-D[u]tr Host_lac-D[e]  <=> lac-D[u]
Host_IEX_mal-L[u]tr Host_mal-L[e]  <=> mal-L[u]
Host_IEX_nh4[u]tr Host_nh4[e]  <=> nh4[u]
Host_IEX_o2[u]tr Host_o2[e]  <=> o2[u]
Host_IEX_pi[u]tr Host_pi[e]  <=> pi[u]
Host_IEX_pyr[u]tr Host_pyr[e]  <=> pyr[u]
Host_IEX_succ[u]tr Host_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [.........                                ]Comb
10%     [....                                    ]25%     [.........                                ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
EX_lac-D[u] lac-D[u]  <=>
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
```

```
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
   Testing createMultipleSpeciesModel using glpk ... The following fields are missing in several models,
Warning: Metabolite ac[b] not in model - added to the model
Warning: Metabolite h[b] not in model - added to the model

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
EX_ac(e)b ac[b]  ->
Warning: Metabolite acald[b] not in model - added to the model

ACALDtb acald[b]  <=> acald[c]
EX_acald(e)b acald[b]  ->
Warning: Metabolite akg[b] not in model - added to the model

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
EX_akg(e)b akg[b]  ->
Warning: Metabolite co2[b] not in model - added to the model

CO2tb co2[b]  <=> co2[c]
EX_co2(e)b co2[b]  <=>
Warning: Metabolite etoh[b] not in model - added to the model

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_etoh(e)b etoh[b]  ->
Warning: Metabolite for[b] not in model - added to the model

EX_for(e)b for[b]  ->
FORt2b h[b] + for[b]  -> for[c] + h[c]
FORtib for[c]  -> for[b]
Warning: Metabolite fru[b] not in model - added to the model

EX_fru(e)b fru[b]  ->
FRUpts2b pep[c] + fru[b]  -> f6p[c] + pyr[c]
Warning: Metabolite fum[b] not in model - added to the model

EX_fum(e)b fum[b]  ->
FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Metabolite glc-D[b] not in model - added to the model

EX_glc(e)b glc-D[b]  <=>
GLCptsb pep[c] + glc-D[b]  -> g6p[c] + pyr[c]
Warning: Metabolite gln-L[b] not in model - added to the model

EX_gln_L(e)b gln-L[b]  ->
GLNabcb atp[c] + h2o[c] + gln-L[b]  -> adp[c] + gln-L[c] + h[c] + pi[c]
Warning: Metabolite glu-L[b] not in model - added to the model

EX_glu_L(e)b glu-L[b]  ->
GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite h2o[b] not in model - added to the model

EX_h2o(e)b h2o[b]  <=>
H2Otb h2o[b]  <=> h2o[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
ATPS4rb adp[c] + pi[c] + 4 h[b]  <=> atp[c] + h2o[c] + 3 h[c]
CYTBDb 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + q8[c] + 2 h[b]
Warning: Metabolite lac-D[b] not in model - added to the model

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_h(e)b h[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

FORt2b h[b] + for[b]  -> for[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction
```

```
GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite mal-L[b] not in model - added to the model

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
NADH16b 4 h[c] + nadh[c] + q8[c]  -> nad[c] + q8h2[c] + 3 h[b]
Warning: Metabolite pi[b] not in model - added to the model

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
Warning: Metabolite pyr[b] not in model - added to the model

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
Warning: Metabolite succ[b] not in model - added to the model

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
THD2b nadh[c] + nadp[c] + 2 h[b]  -> 2 h[c] + nad[c] + nadph[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
EX_lac_D(e)b lac-D[b]  ->
EX_mal_L(e)b mal-L[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
Warning: Metabolite nh4[b] not in model - added to the model

EX_nh4(e)b nh4[b]  <=>
NH4tb nh4[b]  <=> nh4[c]
Warning: Metabolite o2[b] not in model - added to the model

EX_o2(e)b o2[b]  <=>
O2tb o2[b]  <=> o2[c]
EX_pi(e)b pi[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
EX_pyr(e)b pyr[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
EX_succ(e)b succ[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
ecoli1_IEX_ac[u]tr ecoli1_ac[e]  <=> ac[u]
ecoli1_IEX_acald[u]tr ecoli1_acald[e]  <=> acald[u]
ecoli1_IEX_akg[u]tr ecoli1_akg[e]  <=> akg[u]
ecoli1_IEX_co2[u]tr ecoli1_co2[e]  <=> co2[u]
ecoli1_IEX_etoh[u]tr ecoli1_etoh[e]  <=> etoh[u]
ecoli1_IEX_for[u]tr ecoli1_for[e]  <=> for[u]
ecoli1_IEX_fru[u]tr ecoli1_fru[e]  <=> fru[u]
ecoli1_IEX_fum[u]tr ecoli1_fum[e]  <=> fum[u]
ecoli1_IEX_glc-D[u]tr ecoli1_glc-D[e]  <=> glc-D[u]
ecoli1_IEX_gln-L[u]tr ecoli1_gln-L[e]  <=> gln-L[u]
ecoli1_IEX_glu-L[u]tr ecoli1_glu-L[e]  <=> glu-L[u]
ecoli1_IEX_h2o[u]tr ecoli1_h2o[e]  <=> h2o[u]
ecoli1_IEX_h[u]tr ecoli1_h[e]  <=> h[u]
ecoli1_IEX_lac-D[u]tr ecoli1_lac-D[e]  <=> lac-D[u]
ecoli1_IEX_mal-L[u]tr ecoli1_mal-L[e]  <=> mal-L[u]
ecoli1_IEX_nh4[u]tr ecoli1_nh4[e]  <=> nh4[u]
ecoli1_IEX_o2[u]tr ecoli1_o2[e]  <=> o2[u]
ecoli1_IEX_pi[u]tr ecoli1_pi[e]  <=> pi[u]
ecoli1_IEX_pyr[u]tr ecoli1_pyr[e]  <=> pyr[u]
ecoli1_IEX_succ[u]tr ecoli1_succ[e]  <=> succ[u]
ecoli1_IEX_ac[u]tr ecoli1_ac[e]  <=> ac[u]
ecoli1_IEX_acald[u]tr ecoli1_acald[e]  <=> acald[u]
ecoli1_IEX_akg[u]tr ecoli1_akg[e]  <=> akg[u]
ecoli1_IEX_co2[u]tr ecoli1_co2[e]  <=> co2[u]
ecoli1_IEX_etoh[u]tr ecoli1_etoh[e]  <=> etoh[u]
ecoli1_IEX_for[u]tr ecoli1_for[e]  <=> for[u]
ecoli1_IEX_fru[u]tr ecoli1_fru[e]  <=> fru[u]
```

```
ecoli1_IEX_fum[u]tr ecoli1_fum[e]  <=> fum[u]
ecoli1_IEX_glc-D[u]tr ecoli1_glc-D[e]  <=> glc-D[u]
ecoli1_IEX_gln-L[u]tr ecoli1_gln-L[e]  <=> gln-L[u]
ecoli1_IEX_glu-L[u]tr ecoli1_glu-L[e]  <=> glu-L[u]
ecoli1_IEX_h2o[u]tr ecoli1_h2o[e]  <=> h2o[u]
ecoli1_IEX_h[u]tr ecoli1_h[e]  <=> h[u]
ecoli1_IEX_lac-D[u]tr ecoli1_lac-D[e]  <=> lac-D[u]
ecoli1_IEX_mal-L[u]tr ecoli1_mal-L[e]  <=> mal-L[u]
ecoli1_IEX_nh4[u]tr ecoli1_nh4[e]  <=> nh4[u]
ecoli1_IEX_o2[u]tr ecoli1_o2[e]  <=> o2[u]
ecoli1_IEX_pi[u]tr ecoli1_pi[e]  <=> pi[u]
ecoli1_IEX_pyr[u]tr ecoli1_pyr[e]  <=> pyr[u]
ecoli1_IEX_succ[u]tr ecoli1_succ[e]  <=> succ[u]
ecoli2_IEX_ac[u]tr ecoli2_ac[e]  <=> ac[u]
ecoli2_IEX_acald[u]tr ecoli2_acald[e]  <=> acald[u]
ecoli2_IEX_akg[u]tr ecoli2_akg[e]  <=> akg[u]
ecoli2_IEX_co2[u]tr ecoli2_co2[e]  <=> co2[u]
ecoli2_IEX_etoh[u]tr ecoli2_etoh[e]  <=> etoh[u]
ecoli2_IEX_for[u]tr ecoli2_for[e]  <=> for[u]
ecoli2_IEX_fru[u]tr ecoli2_fru[e]  <=> fru[u]
ecoli2_IEX_fum[u]tr ecoli2_fum[e]  <=> fum[u]
ecoli2_IEX_glc-D[u]tr ecoli2_glc-D[e]  <=> glc-D[u]
ecoli2_IEX_gln-L[u]tr ecoli2_gln-L[e]  <=> gln-L[u]
ecoli2_IEX_glu-L[u]tr ecoli2_glu-L[e]  <=> glu-L[u]
ecoli2_IEX_h2o[u]tr ecoli2_h2o[e]  <=> h2o[u]
ecoli2_IEX_h[u]tr ecoli2_h[e]  <=> h[u]
ecoli2_IEX_lac-D[u]tr ecoli2_lac-D[e]  <=> lac-D[u]
ecoli2_IEX_mal-L[u]tr ecoli2_mal-L[e]  <=> mal-L[u]
ecoli2_IEX_nh4[u]tr ecoli2_nh4[e]  <=> nh4[u]
ecoli2_IEX_o2[u]tr ecoli2_o2[e]  <=> o2[u]
ecoli2_IEX_pi[u]tr ecoli2_pi[e]  <=> pi[u]
ecoli2_IEX_pyr[u]tr ecoli2_pyr[e]  <=> pyr[u]
ecoli2_IEX_succ[u]tr ecoli2_succ[e]  <=> succ[u]
ecoli3_IEX_ac[u]tr ecoli3_ac[e]  <=> ac[u]
ecoli3_IEX_acald[u]tr ecoli3_acald[e]  <=> acald[u]
ecoli3_IEX_akg[u]tr ecoli3_akg[e]  <=> akg[u]
ecoli3_IEX_co2[u]tr ecoli3_co2[e]  <=> co2[u]
ecoli3_IEX_etoh[u]tr ecoli3_etoh[e]  <=> etoh[u]
ecoli3_IEX_for[u]tr ecoli3_for[e]  <=> for[u]
ecoli3_IEX_fru[u]tr ecoli3_fru[e]  <=> fru[u]
ecoli3_IEX_fum[u]tr ecoli3_fum[e]  <=> fum[u]
ecoli3_IEX_glc-D[u]tr ecoli3_glc-D[e]  <=> glc-D[u]
ecoli3_IEX_gln-L[u]tr ecoli3_gln-L[e]  <=> gln-L[u]
ecoli3_IEX_glu-L[u]tr ecoli3_glu-L[e]  <=> glu-L[u]
ecoli3_IEX_h2o[u]tr ecoli3_h2o[e]  <=> h2o[u]
ecoli3_IEX_h[u]tr ecoli3_h[e]  <=> h[u]
ecoli3_IEX_lac-D[u]tr ecoli3_lac-D[e]  <=> lac-D[u]
ecoli3_IEX_mal-L[u]tr ecoli3_mal-L[e]  <=> mal-L[u]
ecoli3_IEX_nh4[u]tr ecoli3_nh4[e]  <=> nh4[u]
ecoli3_IEX_o2[u]tr ecoli3_o2[e]  <=> o2[u]
ecoli3_IEX_pi[u]tr ecoli3_pi[e]  <=> pi[u]
ecoli3_IEX_pyr[u]tr ecoli3_pyr[e]  <=> pyr[u]
ecoli3_IEX_succ[u]tr ecoli3_succ[e]  <=> succ[u]
modelHost_IEX_ac[u]tr modelHost_ac[e]  <=> ac[u]
modelHost_IEX_acald[u]tr modelHost_acald[e]  <=> acald[u]
modelHost_IEX_akg[u]tr modelHost_akg[e]  <=> akg[u]
modelHost_IEX_co2[u]tr modelHost_co2[e]  <=> co2[u]
modelHost_IEX_etoh[u]tr modelHost_etoh[e]  <=> etoh[u]
modelHost_IEX_for[u]tr modelHost_for[e]  <=> for[u]
modelHost_IEX_fru[u]tr modelHost_fru[e]  <=> fru[u]
modelHost_IEX_fum[u]tr modelHost_fum[e]  <=> fum[u]
modelHost_IEX_glc-D[u]tr modelHost_glc-D[e]  <=> glc-D[u]
modelHost_IEX_gln-L[u]tr modelHost_gln-L[e]  <=> gln-L[u]
modelHost_IEX_glu-L[u]tr modelHost_glu-L[e]  <=> glu-L[u]
modelHost_IEX_h2o[u]tr modelHost_h2o[e]  <=> h2o[u]
modelHost_IEX_h[u]tr modelHost_h[e]  <=> h[u]
modelHost_IEX_lac-D[u]tr modelHost_lac-D[e]  <=> lac-D[u]
modelHost_IEX_mal-L[u]tr modelHost_mal-L[e]  <=> mal-L[u]
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modelHost_IEX_nh4[u]tr modelHost_nh4[e]  <=> nh4[u]
modelHost_IEX_o2[u]tr modelHost_o2[e]  <=> o2[u]
modelHost_IEX_pi[u]tr modelHost_pi[e]  <=> pi[u]
modelHost_IEX_pyr[u]tr modelHost_pyr[e]  <=> pyr[u]
modelHost_IEX_succ[u]tr modelHost_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [.........                                ]Comb
10%     [....                                    ]25%     [.........                                ]Comb
10%     [....                                    ]25%     [.........                                ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
EX_lac-D[u] lac-D[u]  <=>
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
The following fields are missing in several models, they will not be merged:
ecoli1_IEX_ac[u]tr ecoli1_ac[e]  <=> ac[u]
ecoli1_IEX_acald[u]tr ecoli1_acald[e]  <=> acald[u]
ecoli1_IEX_akg[u]tr ecoli1_akg[e]  <=> akg[u]
ecoli1_IEX_co2[u]tr ecoli1_co2[e]  <=> co2[u]
ecoli1_IEX_etoh[u]tr ecoli1_etoh[e]  <=> etoh[u]
ecoli1_IEX_for[u]tr ecoli1_for[e]  <=> for[u]
ecoli1_IEX_fru[u]tr ecoli1_fru[e]  <=> fru[u]
ecoli1_IEX_fum[u]tr ecoli1_fum[e]  <=> fum[u]
ecoli1_IEX_glc-D[u]tr ecoli1_glc-D[e]  <=> glc-D[u]
ecoli1_IEX_gln-L[u]tr ecoli1_gln-L[e]  <=> gln-L[u]
ecoli1_IEX_glu-L[u]tr ecoli1_glu-L[e]  <=> glu-L[u]
ecoli1_IEX_h2o[u]tr ecoli1_h2o[e]  <=> h2o[u]
ecoli1_IEX_h[u]tr ecoli1_h[e]  <=> h[u]
ecoli1_IEX_lac-D[u]tr ecoli1_lac-D[e]  <=> lac-D[u]
ecoli1_IEX_mal-L[u]tr ecoli1_mal-L[e]  <=> mal-L[u]
ecoli1_IEX_nh4[u]tr ecoli1_nh4[e]  <=> nh4[u]
ecoli1_IEX_o2[u]tr ecoli1_o2[e]  <=> o2[u]
ecoli1_IEX_pi[u]tr ecoli1_pi[e]  <=> pi[u]
ecoli1_IEX_pyr[u]tr ecoli1_pyr[e]  <=> pyr[u]
ecoli1_IEX_succ[u]tr ecoli1_succ[e]  <=> succ[u]
ecoli2_IEX_ac[u]tr ecoli2_ac[e]  <=> ac[u]
ecoli2_IEX_acald[u]tr ecoli2_acald[e]  <=> acald[u]
ecoli2_IEX_akg[u]tr ecoli2_akg[e]  <=> akg[u]
ecoli2_IEX_co2[u]tr ecoli2_co2[e]  <=> co2[u]
ecoli2_IEX_etoh[u]tr ecoli2_etoh[e]  <=> etoh[u]
ecoli2_IEX_for[u]tr ecoli2_for[e]  <=> for[u]
ecoli2_IEX_fru[u]tr ecoli2_fru[e]  <=> fru[u]
ecoli2_IEX_fum[u]tr ecoli2_fum[e]  <=> fum[u]
ecoli2_IEX_glc-D[u]tr ecoli2_glc-D[e]  <=> glc-D[u]
ecoli2_IEX_gln-L[u]tr ecoli2_gln-L[e]  <=> gln-L[u]
ecoli2_IEX_glu-L[u]tr ecoli2_glu-L[e]  <=> glu-L[u]
ecoli2_IEX_h2o[u]tr ecoli2_h2o[e]  <=> h2o[u]
ecoli2_IEX_h[u]tr ecoli2_h[e]  <=> h[u]
ecoli2_IEX_lac-D[u]tr ecoli2_lac-D[e]  <=> lac-D[u]
ecoli2_IEX_mal-L[u]tr ecoli2_mal-L[e]  <=> mal-L[u]
ecoli2_IEX_nh4[u]tr ecoli2_nh4[e]  <=> nh4[u]
ecoli2_IEX_o2[u]tr ecoli2_o2[e]  <=> o2[u]
ecoli2_IEX_pi[u]tr ecoli2_pi[e]  <=> pi[u]
ecoli2_IEX_pyr[u]tr ecoli2_pyr[e]  <=> pyr[u]
```

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ecoli2_IEX_succ[u]tr ecoli2_succ[e]  <=> succ[u]
ecoli3_IEX_ac[u]tr ecoli3_ac[e]  <=> ac[u]
ecoli3_IEX_acald[u]tr ecoli3_acald[e]  <=> acald[u]
ecoli3_IEX_akg[u]tr ecoli3_akg[e]  <=> akg[u]
ecoli3_IEX_co2[u]tr ecoli3_co2[e]  <=> co2[u]
ecoli3_IEX_etoh[u]tr ecoli3_etoh[e]  <=> etoh[u]
ecoli3_IEX_for[u]tr ecoli3_for[e]  <=> for[u]
ecoli3_IEX_fru[u]tr ecoli3_fru[e]  <=> fru[u]
ecoli3_IEX_fum[u]tr ecoli3_fum[e]  <=> fum[u]
ecoli3_IEX_glc-D[u]tr ecoli3_glc-D[e]  <=> glc-D[u]
ecoli3_IEX_gln-L[u]tr ecoli3_gln-L[e]  <=> gln-L[u]
ecoli3_IEX_glu-L[u]tr ecoli3_glu-L[e]  <=> glu-L[u]
ecoli3_IEX_h2o[u]tr ecoli3_h2o[e]  <=> h2o[u]
ecoli3_IEX_h[u]tr ecoli3_h[e]  <=> h[u]
ecoli3_IEX_lac-D[u]tr ecoli3_lac-D[e]  <=> lac-D[u]
ecoli3_IEX_mal-L[u]tr ecoli3_mal-L[e]  <=> mal-L[u]
ecoli3_IEX_nh4[u]tr ecoli3_nh4[e]  <=> nh4[u]
ecoli3_IEX_o2[u]tr ecoli3_o2[e]  <=> o2[u]
ecoli3_IEX_pi[u]tr ecoli3_pi[e]  <=> pi[u]
ecoli3_IEX_pyr[u]tr ecoli3_pyr[e]  <=> pyr[u]
ecoli3_IEX_succ[u]tr ecoli3_succ[e]  <=> succ[u]
Combining Genes in Progress ...

Warning: Metabolite ac[b] not in model - added to the model
Warning: Metabolite h[b] not in model - added to the model

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
EX_ac(e)b ac[b]  ->
Warning: Metabolite acald[b] not in model - added to the model

ACALDtb acald[b]  <=> acald[c]
EX_acald(e)b acald[b]  ->
Warning: Metabolite akg[b] not in model - added to the model

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
EX_akg(e)b akg[b]  ->
Warning: Metabolite co2[b] not in model - added to the model

CO2tb co2[b]  <=> co2[c]
EX_co2(e)b co2[b]  <=>
Warning: Metabolite etoh[b] not in model - added to the model

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_etoh(e)b etoh[b]  ->
Warning: Metabolite for[b] not in model - added to the model

EX_for(e)b for[b]  ->
FORt2b h[b] + for[b]  -> for[c] + h[c]
FORtib for[c]  -> for[b]
Warning: Metabolite fru[b] not in model - added to the model

EX_fru(e)b fru[b]  ->
FRUpts2b pep[c] + fru[b]  -> f6p[c] + pyr[c]
Warning: Metabolite fum[b] not in model - added to the model

EX_fum(e)b fum[b]  ->
FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Metabolite glc-D[b] not in model - added to the model

EX_glc(e)b glc-D[b]  <=>
GLCptsb pep[c] + glc-D[b]  -> g6p[c] + pyr[c]
Warning: Metabolite gln-L[b] not in model - added to the model

EX_gln_L(e)b gln-L[b]  ->
GLNabcb atp[c] + h2o[c] + gln-L[b]  -> adp[c] + gln-L[c] + h[c] + pi[c]
Warning: Metabolite glu-L[b] not in model - added to the model

EX_glu_L(e)b glu-L[b]  ->
GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite h2o[b] not in model - added to the model

EX_h2o(e)b h2o[b]  <=>
H2Otb h2o[b]  <=> h2o[c]
Warning: Reaction with the same name already exists in the model, updating the reaction
```

```
ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
ATPS4rb adp[c] + pi[c] + 4 h[b]  <=> atp[c] + h2o[c] + 3 h[c]
CYTBDb 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + q8[c] + 2 h[b]
Warning: Metabolite lac-D[b] not in model - added to the model

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_h(e)b h[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

FORt2b h[b] + for[b]  -> for[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite mal-L[b] not in model - added to the model

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
NADH16b 4 h[c] + nadh[c] + q8[c]  -> nad[c] + q8h2[c] + 3 h[b]
Warning: Metabolite pi[b] not in model - added to the model

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
Warning: Metabolite pyr[b] not in model - added to the model

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
Warning: Metabolite succ[b] not in model - added to the model

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
THD2b nadh[c] + nadp[c] + 2 h[b]  -> 2 h[c] + nad[c] + nadph[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
EX_lac_D(e)b lac-D[b]  ->
EX_mal_L(e)b mal-L[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
Warning: Metabolite nh4[b] not in model - added to the model

EX_nh4(e)b nh4[b]  <=>
NH4tb nh4[b]  <=> nh4[c]
Warning: Metabolite o2[b] not in model - added to the model

EX_o2(e)b o2[b]  <=>
O2tb o2[b]  <=> o2[c]
EX_pi(e)b pi[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
EX_pyr(e)b pyr[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
EX_succ(e)b succ[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
```

```
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
Host_IEX_ac[u]tr Host_ac[e]  <=> ac[u]
Host_IEX_acald[u]tr Host_acald[e]  <=> acald[u]
Host_IEX_akg[u]tr Host_akg[e]  <=> akg[u]
Host_IEX_co2[u]tr Host_co2[e]  <=> co2[u]
Host_IEX_etoh[u]tr Host_etoh[e]  <=> etoh[u]
Host_IEX_for[u]tr Host_for[e]  <=> for[u]
Host_IEX_fru[u]tr Host_fru[e]  <=> fru[u]
Host_IEX_fum[u]tr Host_fum[e]  <=> fum[u]
Host_IEX_glc-D[u]tr Host_glc-D[e]  <=> glc-D[u]
Host_IEX_gln-L[u]tr Host_gln-L[e]  <=> gln-L[u]
Host_IEX_glu-L[u]tr Host_glu-L[e]  <=> glu-L[u]
Host_IEX_h2o[u]tr Host_h2o[e]  <=> h2o[u]
Host_IEX_h[u]tr Host_h[e]  <=> h[u]
Host_IEX_lac-D[u]tr Host_lac-D[e]  <=> lac-D[u]
Host_IEX_mal-L[u]tr Host_mal-L[e]  <=> mal-L[u]
Host_IEX_nh4[u]tr Host_nh4[e]  <=> nh4[u]
Host_IEX_o2[u]tr Host_o2[e]  <=> o2[u]
Host_IEX_pi[u]tr Host_pi[e]  <=> pi[u]
Host_IEX_pyr[u]tr Host_pyr[e]  <=> pyr[u]
Host_IEX_succ[u]tr Host_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [.........                                ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
EX_lac-D[u] lac-D[u]  <=>
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
   Testing createMultipleSpeciesModel using gurobi6 ... The following fields are missing in several mode
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
```

```
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
model2_IEX_ac[u]tr model2_ac[e]  <=> ac[u]
model2_IEX_acald[u]tr model2_acald[e]  <=> acald[u]
model2_IEX_akg[u]tr model2_akg[e]  <=> akg[u]
model2_IEX_co2[u]tr model2_co2[e]  <=> co2[u]
model2_IEX_etoh[u]tr model2_etoh[e]  <=> etoh[u]
model2_IEX_for[u]tr model2_for[e]  <=> for[u]
model2_IEX_fru[u]tr model2_fru[e]  <=> fru[u]
model2_IEX_fum[u]tr model2_fum[e]  <=> fum[u]
model2_IEX_glc-D[u]tr model2_glc-D[e]  <=> glc-D[u]
model2_IEX_gln-L[u]tr model2_gln-L[e]  <=> gln-L[u]
model2_IEX_glu-L[u]tr model2_glu-L[e]  <=> glu-L[u]
model2_IEX_h2o[u]tr model2_h2o[e]  <=> h2o[u]
model2_IEX_h[u]tr model2_h[e]  <=> h[u]
model2_IEX_lac-D[u]tr model2_lac-D[e]  <=> lac-D[u]
model2_IEX_mal-L[u]tr model2_mal-L[e]  <=> mal-L[u]
model2_IEX_nh4[u]tr model2_nh4[e]  <=> nh4[u]
model2_IEX_o2[u]tr model2_o2[e]  <=> o2[u]
model2_IEX_pi[u]tr model2_pi[e]  <=> pi[u]
model2_IEX_pyr[u]tr model2_pyr[e]  <=> pyr[u]
model2_IEX_succ[u]tr model2_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [.........                                ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
EX_lac-D[u] lac-D[u]  <=>
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
The following fields are missing in several models, they will not be merged:
Warning: Metabolite ac[b] not in model - added to the model
Warning: Metabolite h[b] not in model - added to the model

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
EX_ac(e)b ac[b]  ->
Warning: Metabolite acald[b] not in model - added to the model

ACALDtb acald[b]  <=> acald[c]
EX_acald(e)b acald[b]  ->
Warning: Metabolite akg[b] not in model - added to the model

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
EX_akg(e)b akg[b]  ->
Warning: Metabolite co2[b] not in model - added to the model

CO2tb co2[b]  <=> co2[c]
EX_co2(e)b co2[b]  <=>
Warning: Metabolite etoh[b] not in model - added to the model

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_etoh(e)b etoh[b]  ->
Warning: Metabolite for[b] not in model - added to the model

EX_for(e)b for[b]  ->
```

```
FORt2b h[b] + for[b]  -> for[c] + h[c]
FORtib for[c]  -> for[b]
Warning: Metabolite fru[b] not in model - added to the model

EX_fru(e)b fru[b]  ->
FRUpts2b pep[c] + fru[b]  -> f6p[c] + pyr[c]
Warning: Metabolite fum[b] not in model - added to the model

EX_fum(e)b fum[b]  ->
FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Metabolite glc-D[b] not in model - added to the model

EX_glc(e)b glc-D[b]  <=>
GLCptsb pep[c] + glc-D[b]  -> g6p[c] + pyr[c]
Warning: Metabolite gln-L[b] not in model - added to the model

EX_gln_L(e)b gln-L[b]  ->
GLNabcb atp[c] + h2o[c] + gln-L[b]  -> adp[c] + gln-L[c] + h[c] + pi[c]
Warning: Metabolite glu-L[b] not in model - added to the model

EX_glu_L(e)b glu-L[b]  ->
GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite h2o[b] not in model - added to the model

EX_h2o(e)b h2o[b]  <=>
H2Otb h2o[b]  <=> h2o[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
ATPS4rb adp[c] + pi[c] + 4 h[b]  <=> atp[c] + h2o[c] + 3 h[c]
CYTBDb 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + q8[c] + 2 h[b]
Warning: Metabolite lac-D[b] not in model - added to the model

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_h(e)b h[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

FORt2b h[b] + for[b]  -> for[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite mal-L[b] not in model - added to the model

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
NADH16b 4 h[c] + nadh[c] + q8[c]  -> nad[c] + q8h2[c] + 3 h[b]
Warning: Metabolite pi[b] not in model - added to the model

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
Warning: Metabolite pyr[b] not in model - added to the model

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
Warning: Metabolite succ[b] not in model - added to the model

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
THD2b nadh[c] + nadp[c] + 2 h[b]  -> 2 h[c] + nad[c] + nadph[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
EX_lac_D(e)b lac-D[b]  ->
EX_mal_L(e)b mal-L[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
Warning: Metabolite nh4[b] not in model - added to the model

EX_nh4(e)b nh4[b]  <=>
NH4tb nh4[b]  <=> nh4[c]
Warning: Metabolite o2[b] not in model - added to the model
```

```
EX_o2(e)b o2[b]  <=>
O2tb o2[b]  <=> o2[c]
EX_pi(e)b pi[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
EX_pyr(e)b pyr[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
EX_succ(e)b succ[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
model1_IEX_ac[u]tr model1_ac[e]  <=> ac[u]
model1_IEX_acald[u]tr model1_acald[e]  <=> acald[u]
model1_IEX_akg[u]tr model1_akg[e]  <=> akg[u]
model1_IEX_co2[u]tr model1_co2[e]  <=> co2[u]
model1_IEX_etoh[u]tr model1_etoh[e]  <=> etoh[u]
model1_IEX_for[u]tr model1_for[e]  <=> for[u]
model1_IEX_fru[u]tr model1_fru[e]  <=> fru[u]
model1_IEX_fum[u]tr model1_fum[e]  <=> fum[u]
model1_IEX_glc-D[u]tr model1_glc-D[e]  <=> glc-D[u]
model1_IEX_gln-L[u]tr model1_gln-L[e]  <=> gln-L[u]
model1_IEX_glu-L[u]tr model1_glu-L[e]  <=> glu-L[u]
model1_IEX_h2o[u]tr model1_h2o[e]  <=> h2o[u]
model1_IEX_h[u]tr model1_h[e]  <=> h[u]
model1_IEX_lac-D[u]tr model1_lac-D[e]  <=> lac-D[u]
model1_IEX_mal-L[u]tr model1_mal-L[e]  <=> mal-L[u]
model1_IEX_nh4[u]tr model1_nh4[e]  <=> nh4[u]
model1_IEX_o2[u]tr model1_o2[e]  <=> o2[u]
model1_IEX_pi[u]tr model1_pi[e]  <=> pi[u]
model1_IEX_pyr[u]tr model1_pyr[e]  <=> pyr[u]
model1_IEX_succ[u]tr model1_succ[e]  <=> succ[u]
model2_IEX_ac[u]tr model2_ac[e]  <=> ac[u]
model2_IEX_acald[u]tr model2_acald[e]  <=> acald[u]
model2_IEX_akg[u]tr model2_akg[e]  <=> akg[u]
model2_IEX_co2[u]tr model2_co2[e]  <=> co2[u]
model2_IEX_etoh[u]tr model2_etoh[e]  <=> etoh[u]
model2_IEX_for[u]tr model2_for[e]  <=> for[u]
model2_IEX_fru[u]tr model2_fru[e]  <=> fru[u]
model2_IEX_fum[u]tr model2_fum[e]  <=> fum[u]
model2_IEX_glc-D[u]tr model2_glc-D[e]  <=> glc-D[u]
model2_IEX_gln-L[u]tr model2_gln-L[e]  <=> gln-L[u]
model2_IEX_glu-L[u]tr model2_glu-L[e]  <=> glu-L[u]
model2_IEX_h2o[u]tr model2_h2o[e]  <=> h2o[u]
```

```
model2_IEX_h[u]tr model2_h[e]  <=> h[u]
model2_IEX_lac-D[u]tr model2_lac-D[e]  <=> lac-D[u]
model2_IEX_mal-L[u]tr model2_mal-L[e]  <=> mal-L[u]
model2_IEX_nh4[u]tr model2_nh4[e]  <=> nh4[u]
model2_IEX_o2[u]tr model2_o2[e]  <=> o2[u]
model2_IEX_pi[u]tr model2_pi[e]  <=> pi[u]
model2_IEX_pyr[u]tr model2_pyr[e]  <=> pyr[u]
model2_IEX_succ[u]tr model2_succ[e]  <=> succ[u]
Host_IEX_ac[u]tr Host_ac[e]  <=> ac[u]
Host_IEX_acald[u]tr Host_acald[e]  <=> acald[u]
Host_IEX_akg[u]tr Host_akg[e]  <=> akg[u]
Host_IEX_co2[u]tr Host_co2[e]  <=> co2[u]
Host_IEX_etoh[u]tr Host_etoh[e]  <=> etoh[u]
Host_IEX_for[u]tr Host_for[e]  <=> for[u]
Host_IEX_fru[u]tr Host_fru[e]  <=> fru[u]
Host_IEX_fum[u]tr Host_fum[e]  <=> fum[u]
Host_IEX_glc-D[u]tr Host_glc-D[e]  <=> glc-D[u]
Host_IEX_gln-L[u]tr Host_gln-L[e]  <=> gln-L[u]
Host_IEX_glu-L[u]tr Host_glu-L[e]  <=> glu-L[u]
Host_IEX_h2o[u]tr Host_h2o[e]  <=> h2o[u]
Host_IEX_h[u]tr Host_h[e]  <=> h[u]
Host_IEX_lac-D[u]tr Host_lac-D[e]  <=> lac-D[u]
Host_IEX_mal-L[u]tr Host_mal-L[e]  <=> mal-L[u]
Host_IEX_nh4[u]tr Host_nh4[e]  <=> nh4[u]
Host_IEX_o2[u]tr Host_o2[e]  <=> o2[u]
Host_IEX_pi[u]tr Host_pi[e]  <=> pi[u]
Host_IEX_pyr[u]tr Host_pyr[e]  <=> pyr[u]
Host_IEX_succ[u]tr Host_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [..........                                ]Comb
10%     [....                                    ]25%     [..........                                ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
EX_lac-D[u] lac-D[u]  <=>
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
   Testing createMultipleSpeciesModel using gurobi6 ... The following fields are missing in several mode
Warning: Metabolite ac[b] not in model - added to the model
Warning: Metabolite h[b] not in model - added to the model

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
EX_ac(e)b ac[b]  ->
Warning: Metabolite acald[b] not in model - added to the model

ACALDtb acald[b]  <=> acald[c]
EX_acald(e)b acald[b]  ->
Warning: Metabolite akg[b] not in model - added to the model

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
EX_akg(e)b akg[b]  ->
Warning: Metabolite co2[b] not in model - added to the model

CO2tb co2[b]  <=> co2[c]
EX_co2(e)b co2[b]  <=>
Warning: Metabolite etoh[b] not in model - added to the model
```

```
ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_etoh(e)b etoh[b]  ->
Warning: Metabolite for[b] not in model - added to the model

EX_for(e)b for[b]  ->
FORt2b h[b] + for[b]  -> for[c] + h[c]
FORtib for[c]  -> for[b]
Warning: Metabolite fru[b] not in model - added to the model

EX_fru(e)b fru[b]  ->
FRUpts2b pep[c] + fru[b]  -> f6p[c] + pyr[c]
Warning: Metabolite fum[b] not in model - added to the model

EX_fum(e)b fum[b]  ->
FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Metabolite glc-D[b] not in model - added to the model

EX_glc(e)b glc-D[b]  <=>
GLCptsb pep[c] + glc-D[b]  -> g6p[c] + pyr[c]
Warning: Metabolite gln-L[b] not in model - added to the model

EX_gln_L(e)b gln-L[b]  ->
GLNabcb atp[c] + h2o[c] + gln-L[b]  -> adp[c] + gln-L[c] + h[c] + pi[c]
Warning: Metabolite glu-L[b] not in model - added to the model

EX_glu_L(e)b glu-L[b]  ->
GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite h2o[b] not in model - added to the model

EX_h2o(e)b h2o[b]  <=>
H2Otb h2o[b]  <=> h2o[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ACt2rb ac[b] + h[b]  <=> ac[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

AKGt2rb h[b] + akg[b]  <=> akg[c] + h[c]
ATPS4rb adp[c] + pi[c] + 4 h[b]  <=> atp[c] + h2o[c] + 3 h[c]
CYTBDb 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + q8[c] + 2 h[b]
Warning: Metabolite lac-D[b] not in model - added to the model

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

ETOHt2rb h[b] + etoh[b]  <=> etoh[c] + h[c]
EX_h(e)b h[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

FORt2b h[b] + for[b]  -> for[c] + h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

FUMt2_2b 2 h[b] + fum[b]  -> fum[c] + 2 h[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

GLUt2rb h[b] + glu-L[b]  <=> glu-L[c] + h[c]
Warning: Metabolite mal-L[b] not in model - added to the model

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
NADH16b 4 h[c] + nadh[c] + q8[c]  -> nad[c] + q8h2[c] + 3 h[b]
Warning: Metabolite pi[b] not in model - added to the model

PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
Warning: Metabolite pyr[b] not in model - added to the model

PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
Warning: Metabolite succ[b] not in model - added to the model

SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
THD2b nadh[c] + nadp[c] + 2 h[b]  -> 2 h[c] + nad[c] + nadph[c]
Warning: Reaction with the same name already exists in the model, updating the reaction

D_LACt2b h[b] + lac-D[b]  <=> h[c] + lac-D[c]
EX_lac_D(e)b lac-D[b]  ->
EX_mal_L(e)b mal-L[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction

MALt2_2b 2 h[b] + mal-L[b]  -> 2 h[c] + mal-L[c]
```

```
Warning: Metabolite nh4[b] not in model - added to the model
EX_nh4(e)b nh4[b]  <=>
NH4tb nh4[b]  <=> nh4[c]
Warning: Metabolite o2[b] not in model - added to the model
EX_o2(e)b o2[b]  <=>
O2tb o2[b]  <=> o2[c]
EX_pi(e)b pi[b]  <=>
Warning: Reaction with the same name already exists in the model, updating the reaction
PIt2rb h[b] + pi[b]  <=> h[c] + pi[c]
EX_pyr(e)b pyr[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction
PYRt2rb h[b] + pyr[b]  <=> h[c] + pyr[c]
EX_succ(e)b succ[b]  ->
Warning: Reaction with the same name already exists in the model, updating the reaction
SUCCt2_2b 2 h[b] + succ[b]  -> 2 h[c] + succ[c]
Warning: Reaction with the same name already exists in the model, updating the reaction
SUCCt3b succ[c] + h[b]  -> h[c] + succ[b]
ecoli1_IEX_ac[u]tr ecoli1_ac[e]  <=> ac[u]
ecoli1_IEX_acald[u]tr ecoli1_acald[e]  <=> acald[u]
ecoli1_IEX_akg[u]tr ecoli1_akg[e]  <=> akg[u]
ecoli1_IEX_co2[u]tr ecoli1_co2[e]  <=> co2[u]
ecoli1_IEX_etoh[u]tr ecoli1_etoh[e]  <=> etoh[u]
ecoli1_IEX_for[u]tr ecoli1_for[e]  <=> for[u]
ecoli1_IEX_fru[u]tr ecoli1_fru[e]  <=> fru[u]
ecoli1_IEX_fum[u]tr ecoli1_fum[e]  <=> fum[u]
ecoli1_IEX_glc-D[u]tr ecoli1_glc-D[e]  <=> glc-D[u]
ecoli1_IEX_gln-L[u]tr ecoli1_gln-L[e]  <=> gln-L[u]
ecoli1_IEX_glu-L[u]tr ecoli1_glu-L[e]  <=> glu-L[u]
ecoli1_IEX_h2o[u]tr ecoli1_h2o[e]  <=> h2o[u]
ecoli1_IEX_h[u]tr ecoli1_h[e]  <=> h[u]
ecoli1_IEX_lac-D[u]tr ecoli1_lac-D[e]  <=> lac-D[u]
ecoli1_IEX_mal-L[u]tr ecoli1_mal-L[e]  <=> mal-L[u]
ecoli1_IEX_nh4[u]tr ecoli1_nh4[e]  <=> nh4[u]
ecoli1_IEX_o2[u]tr ecoli1_o2[e]  <=> o2[u]
ecoli1_IEX_pi[u]tr ecoli1_pi[e]  <=> pi[u]
ecoli1_IEX_pyr[u]tr ecoli1_pyr[e]  <=> pyr[u]
ecoli1_IEX_succ[u]tr ecoli1_succ[e]  <=> succ[u]
ecoli1_IEX_ac[u]tr ecoli1_ac[e]  <=> ac[u]
ecoli1_IEX_acald[u]tr ecoli1_acald[e]  <=> acald[u]
ecoli1_IEX_akg[u]tr ecoli1_akg[e]  <=> akg[u]
ecoli1_IEX_co2[u]tr ecoli1_co2[e]  <=> co2[u]
ecoli1_IEX_etoh[u]tr ecoli1_etoh[e]  <=> etoh[u]
ecoli1_IEX_for[u]tr ecoli1_for[e]  <=> for[u]
ecoli1_IEX_fru[u]tr ecoli1_fru[e]  <=> fru[u]
ecoli1_IEX_fum[u]tr ecoli1_fum[e]  <=> fum[u]
ecoli1_IEX_glc-D[u]tr ecoli1_glc-D[e]  <=> glc-D[u]
ecoli1_IEX_gln-L[u]tr ecoli1_gln-L[e]  <=> gln-L[u]
ecoli1_IEX_glu-L[u]tr ecoli1_glu-L[e]  <=> glu-L[u]
ecoli1_IEX_h2o[u]tr ecoli1_h2o[e]  <=> h2o[u]
ecoli1_IEX_h[u]tr ecoli1_h[e]  <=> h[u]
ecoli1_IEX_lac-D[u]tr ecoli1_lac-D[e]  <=> lac-D[u]
ecoli1_IEX_mal-L[u]tr ecoli1_mal-L[e]  <=> mal-L[u]
ecoli1_IEX_nh4[u]tr ecoli1_nh4[e]  <=> nh4[u]
ecoli1_IEX_o2[u]tr ecoli1_o2[e]  <=> o2[u]
ecoli1_IEX_pi[u]tr ecoli1_pi[e]  <=> pi[u]
ecoli1_IEX_pyr[u]tr ecoli1_pyr[e]  <=> pyr[u]
ecoli1_IEX_succ[u]tr ecoli1_succ[e]  <=> succ[u]
ecoli2_IEX_ac[u]tr ecoli2_ac[e]  <=> ac[u]
ecoli2_IEX_acald[u]tr ecoli2_acald[e]  <=> acald[u]
ecoli2_IEX_akg[u]tr ecoli2_akg[e]  <=> akg[u]
ecoli2_IEX_co2[u]tr ecoli2_co2[e]  <=> co2[u]
ecoli2_IEX_etoh[u]tr ecoli2_etoh[e]  <=> etoh[u]
ecoli2_IEX_for[u]tr ecoli2_for[e]  <=> for[u]
ecoli2_IEX_fru[u]tr ecoli2_fru[e]  <=> fru[u]
ecoli2_IEX_fum[u]tr ecoli2_fum[e]  <=> fum[u]
```

```
ecoli2_IEX_glc-D[u]tr ecoli2_glc-D[e]  <=> glc-D[u]
ecoli2_IEX_gln-L[u]tr ecoli2_gln-L[e]  <=> gln-L[u]
ecoli2_IEX_glu-L[u]tr ecoli2_glu-L[e]  <=> glu-L[u]
ecoli2_IEX_h2o[u]tr ecoli2_h2o[e]  <=> h2o[u]
ecoli2_IEX_h[u]tr ecoli2_h[e]  <=> h[u]
ecoli2_IEX_lac-D[u]tr ecoli2_lac-D[e]  <=> lac-D[u]
ecoli2_IEX_mal-L[u]tr ecoli2_mal-L[e]  <=> mal-L[u]
ecoli2_IEX_nh4[u]tr ecoli2_nh4[e]  <=> nh4[u]
ecoli2_IEX_o2[u]tr ecoli2_o2[e]  <=> o2[u]
ecoli2_IEX_pi[u]tr ecoli2_pi[e]  <=> pi[u]
ecoli2_IEX_pyr[u]tr ecoli2_pyr[e]  <=> pyr[u]
ecoli2_IEX_succ[u]tr ecoli2_succ[e]  <=> succ[u]
ecoli3_IEX_ac[u]tr ecoli3_ac[e]  <=> ac[u]
ecoli3_IEX_acald[u]tr ecoli3_acald[e]  <=> acald[u]
ecoli3_IEX_akg[u]tr ecoli3_akg[e]  <=> akg[u]
ecoli3_IEX_co2[u]tr ecoli3_co2[e]  <=> co2[u]
ecoli3_IEX_etoh[u]tr ecoli3_etoh[e]  <=> etoh[u]
ecoli3_IEX_for[u]tr ecoli3_for[e]  <=> for[u]
ecoli3_IEX_fru[u]tr ecoli3_fru[e]  <=> fru[u]
ecoli3_IEX_fum[u]tr ecoli3_fum[e]  <=> fum[u]
ecoli3_IEX_glc-D[u]tr ecoli3_glc-D[e]  <=> glc-D[u]
ecoli3_IEX_gln-L[u]tr ecoli3_gln-L[e]  <=> gln-L[u]
ecoli3_IEX_glu-L[u]tr ecoli3_glu-L[e]  <=> glu-L[u]
ecoli3_IEX_h2o[u]tr ecoli3_h2o[e]  <=> h2o[u]
ecoli3_IEX_h[u]tr ecoli3_h[e]  <=> h[u]
ecoli3_IEX_lac-D[u]tr ecoli3_lac-D[e]  <=> lac-D[u]
ecoli3_IEX_mal-L[u]tr ecoli3_mal-L[e]  <=> mal-L[u]
ecoli3_IEX_nh4[u]tr ecoli3_nh4[e]  <=> nh4[u]
ecoli3_IEX_o2[u]tr ecoli3_o2[e]  <=> o2[u]
ecoli3_IEX_pi[u]tr ecoli3_pi[e]  <=> pi[u]
ecoli3_IEX_pyr[u]tr ecoli3_pyr[e]  <=> pyr[u]
ecoli3_IEX_succ[u]tr ecoli3_succ[e]  <=> succ[u]
modelHost_IEX_ac[u]tr modelHost_ac[e]  <=> ac[u]
modelHost_IEX_acald[u]tr modelHost_acald[e]  <=> acald[u]
modelHost_IEX_akg[u]tr modelHost_akg[e]  <=> akg[u]
modelHost_IEX_co2[u]tr modelHost_co2[e]  <=> co2[u]
modelHost_IEX_etoh[u]tr modelHost_etoh[e]  <=> etoh[u]
modelHost_IEX_for[u]tr modelHost_for[e]  <=> for[u]
modelHost_IEX_fru[u]tr modelHost_fru[e]  <=> fru[u]
modelHost_IEX_fum[u]tr modelHost_fum[e]  <=> fum[u]
modelHost_IEX_glc-D[u]tr modelHost_glc-D[e]  <=> glc-D[u]
modelHost_IEX_gln-L[u]tr modelHost_gln-L[e]  <=> gln-L[u]
modelHost_IEX_glu-L[u]tr modelHost_glu-L[e]  <=> glu-L[u]
modelHost_IEX_h2o[u]tr modelHost_h2o[e]  <=> h2o[u]
modelHost_IEX_h[u]tr modelHost_h[e]  <=> h[u]
modelHost_IEX_lac-D[u]tr modelHost_lac-D[e]  <=> lac-D[u]
modelHost_IEX_mal-L[u]tr modelHost_mal-L[e]  <=> mal-L[u]
modelHost_IEX_nh4[u]tr modelHost_nh4[e]  <=> nh4[u]
modelHost_IEX_o2[u]tr modelHost_o2[e]  <=> o2[u]
modelHost_IEX_pi[u]tr modelHost_pi[e]  <=> pi[u]
modelHost_IEX_pyr[u]tr modelHost_pyr[e]  <=> pyr[u]
modelHost_IEX_succ[u]tr modelHost_succ[e]  <=> succ[u]
Combining Genes in Progress ...
10%     [....                                    ]25%     [.........                                ]Comb
10%     [....                                    ]25%     [.........                                ]Comb
10%     [....                                    ]25%     [.........                                ]Comb
EX_acald[u] acald[u]  <=>
EX_akg[u] akg[u]  <=>
EX_co2[u] co2[u]  <=>
EX_etoh[u] etoh[u]  <=>
EX_for[u] for[u]  <=>
EX_fru[u] fru[u]  <=>
EX_fum[u] fum[u]  <=>
EX_glc-D[u] glc-D[u]  <=>
EX_gln-L[u] gln-L[u]  <=>
EX_glu-L[u] glu-L[u]  <=>
EX_h2o[u] h2o[u]  <=>
EX_h[u] h[u]  <=>
```

```
EX_lac-D[u] lac-D[u]  <=>
EX_mal-L[u] mal-L[u]  <=>
EX_nh4[u] nh4[u]  <=>
EX_o2[u] o2[u]  <=>
EX_pi[u] pi[u]  <=>
EX_pyr[u] pyr[u]  <=>
EX_succ[u] succ[u]  <=>
The following fields are missing in several models, they will not be merged:
ecoli1_IEX_ac[u]tr ecoli1_ac[e]  <=> ac[u]
ecoli1_IEX_acald[u]tr ecoli1_acald[e]  <=> acald[u]
ecoli1_IEX_akg[u]tr ecoli1_akg[e]  <=> akg[u]
ecoli1_IEX_co2[u]tr ecoli1_co2[e]  <=> co2[u]
ecoli1_IEX_etoh[u]tr ecoli1_etoh[e]  <=> etoh[u]
ecoli1_IEX_for[u]tr ecoli1_for[e]  <=> for[u]
ecoli1_IEX_fru[u]tr ecoli1_fru[e]  <=> fru[u]
ecoli1_IEX_fum[u]tr ecoli1_fum[e]  <=> fum[u]
ecoli1_IEX_glc-D[u]tr ecoli1_glc-D[e]  <=> glc-D[u]
ecoli1_IEX_gln-L[u]tr ecoli1_gln-L[e]  <=> gln-L[u]
ecoli1_IEX_glu-L[u]tr ecoli1_glu-L[e]  <=> glu-L[u]
ecoli1_IEX_h2o[u]tr ecoli1_h2o[e]  <=> h2o[u]
ecoli1_IEX_h[u]tr ecoli1_h[e]  <=> h[u]
ecoli1_IEX_lac-D[u]tr ecoli1_lac-D[e]  <=> lac-D[u]
ecoli1_IEX_mal-L[u]tr ecoli1_mal-L[e]  <=> mal-L[u]
ecoli1_IEX_nh4[u]tr ecoli1_nh4[e]  <=> nh4[u]
ecoli1_IEX_o2[u]tr ecoli1_o2[e]  <=> o2[u]
ecoli1_IEX_pi[u]tr ecoli1_pi[e]  <=> pi[u]
ecoli1_IEX_pyr[u]tr ecoli1_pyr[e]  <=> pyr[u]
ecoli1_IEX_succ[u]tr ecoli1_succ[e]  <=> succ[u]
ecoli2_IEX_ac[u]tr ecoli2_ac[e]  <=> ac[u]
ecoli2_IEX_acald[u]tr ecoli2_acald[e]  <=> acald[u]
ecoli2_IEX_akg[u]tr ecoli2_akg[e]  <=> akg[u]
ecoli2_IEX_co2[u]tr ecoli2_co2[e]  <=> co2[u]
ecoli2_IEX_etoh[u]tr ecoli2_etoh[e]  <=> etoh[u]
ecoli2_IEX_for[u]tr ecoli2_for[e]  <=> for[u]
ecoli2_IEX_fru[u]tr ecoli2_fru[e]  <=> fru[u]
ecoli2_IEX_fum[u]tr ecoli2_fum[e]  <=> fum[u]
ecoli2_IEX_glc-D[u]tr ecoli2_glc-D[e]  <=> glc-D[u]
ecoli2_IEX_gln-L[u]tr ecoli2_gln-L[e]  <=> gln-L[u]
ecoli2_IEX_glu-L[u]tr ecoli2_glu-L[e]  <=> glu-L[u]
ecoli2_IEX_h2o[u]tr ecoli2_h2o[e]  <=> h2o[u]
ecoli2_IEX_h[u]tr ecoli2_h[e]  <=> h[u]
ecoli2_IEX_lac-D[u]tr ecoli2_lac-D[e]  <=> lac-D[u]
ecoli2_IEX_mal-L[u]tr ecoli2_mal-L[e]  <=> mal-L[u]
ecoli2_IEX_nh4[u]tr ecoli2_nh4[e]  <=> nh4[u]
ecoli2_IEX_o2[u]tr ecoli2_o2[e]  <=> o2[u]
ecoli2_IEX_pi[u]tr ecoli2_pi[e]  <=> pi[u]
ecoli2_IEX_pyr[u]tr ecoli2_pyr[e]  <=> pyr[u]
ecoli2_IEX_succ[u]tr ecoli2_succ[e]  <=> succ[u]
ecoli3_IEX_ac[u]tr ecoli3_ac[e]  <=> ac[u]
ecoli3_IEX_acald[u]tr ecoli3_acald[e]  <=> acald[u]
ecoli3_IEX_akg[u]tr ecoli3_akg[e]  <=> akg[u]
ecoli3_IEX_co2[u]tr ecoli3_co2[e]  <=> co2[u]
ecoli3_IEX_etoh[u]tr ecoli3_etoh[e]  <=> etoh[u]
ecoli3_IEX_for[u]tr ecoli3_for[e]  <=> for[u]
ecoli3_IEX_fru[u]tr ecoli3_fru[e]  <=> fru[u]
ecoli3_IEX_fum[u]tr ecoli3_fum[e]  <=> fum[u]
ecoli3_IEX_glc-D[u]tr ecoli3_glc-D[e]  <=> glc-D[u]
ecoli3_IEX_gln-L[u]tr ecoli3_gln-L[e]  <=> gln-L[u]
ecoli3_IEX_glu-L[u]tr ecoli3_glu-L[e]  <=> glu-L[u]
ecoli3_IEX_h2o[u]tr ecoli3_h2o[e]  <=> h2o[u]
ecoli3_IEX_h[u]tr ecoli3_h[e]  <=> h[u]
ecoli3_IEX_lac-D[u]tr ecoli3_lac-D[e]  <=> lac-D[u]
ecoli3_IEX_mal-L[u]tr ecoli3_mal-L[e]  <=> mal-L[u]
ecoli3_IEX_nh4[u]tr ecoli3_nh4[e]  <=> nh4[u]
ecoli3_IEX_o2[u]tr ecoli3_o2[e]  <=> o2[u]
ecoli3_IEX_pi[u]tr ecoli3_pi[e]  <=> pi[u]
ecoli3_IEX_pyr[u]tr ecoli3_pyr[e]  <=> pyr[u]
ecoli3_IEX_succ[u]tr ecoli3_succ[e]  <=> succ[u]
```

```
Combining Genes in Progress ...
```

```
Warning: Reaction EX_fuc_L[u] not in model
Warning: Reaction EX_glcn[u] not in model
Warning: Reaction EX_rmn[u] not in model
Warning: Reaction EX_oxa[u] not in model
Warning: Reaction EX_melib[u] not in model
Warning: Reaction EX_cellb[u] not in model
Warning: Reaction EX_strch1[u] not in model
Warning: Reaction EX_amylopect900[u] not in model
Warning: Reaction EX_amylose300[u] not in model
Warning: Reaction EX_arabinan101[u] not in model
Warning: Reaction EX_arabinogal[u] not in model
Warning: Reaction EX_arabinoxyl[u] not in model
Warning: Reaction EX_bglc[u] not in model
Warning: Reaction EX_cellul[u] not in model
Warning: Reaction EX_dextran40[u] not in model
Warning: Reaction EX_galmannan[u] not in model
Warning: Reaction EX_glcmannan[u] not in model
Warning: Reaction EX_homogal[u] not in model
Warning: Reaction EX_inulin[u] not in model
Warning: Reaction EX_kestopt[u] not in model
Warning: Reaction EX_levan1000[u] not in model
Warning: Reaction EX_lmn30[u] not in model
Warning: Reaction EX_lichn[u] not in model
Warning: Reaction EX_pect[u] not in model
Warning: Reaction EX_raffin[u] not in model
Warning: Reaction EX_rhamnogalurI[u] not in model
Warning: Reaction EX_rhamnogalurII[u] not in model
Warning: Reaction EX_starch1200[u] not in model
Warning: Reaction EX_xylan[u] not in model
Warning: Reaction EX_xyluglc[u] not in model
Warning: Reaction EX_arachd[u] not in model
Warning: Reaction EX_chsterol[u] not in model
Warning: Reaction EX_hdca[u] not in model
Warning: Reaction EX_hdcea[u] not in model
Warning: Reaction EX_lnlc[u] not in model
Warning: Reaction EX_lnlnca[u] not in model
Warning: Reaction EX_lnlncg[u] not in model
Warning: Reaction EX_ocdcea[u] not in model
Warning: Reaction EX_octa[u] not in model
Warning: Reaction EX_12dgr180[u] not in model
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Warning: Reaction EX_acmana[u] not in model
Warning: Reaction EX_acnam[u] not in model
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Warning: Reaction EX_ala_D[u] not in model
Warning: Reaction EX_amet[u] not in model
Warning: Reaction EX_amp[u] not in model
Warning: Reaction EX_anth[u] not in model
Warning: Reaction EX_arab_D[u] not in model
Warning: Reaction EX_avite1[u] not in model
Warning: Reaction EX_chol[u] not in model
Warning: Reaction EX_chor[u] not in model
Warning: Reaction EX_ddca[u] not in model
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Warning: Reaction EX_fe3dcit[u] not in model
Warning: Reaction EX_glu_D[u] not in model
Warning: Reaction EX_gsn[u] not in model
Warning: Reaction EX_gthox[u] not in model
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Warning: Reaction EX_indole[u] not in model
Warning: Reaction EX_lanost[u] not in model
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Warning: Reaction EX_chsterol[u] not in model
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Warning: Reaction EX_sel[u] not in model
Warning: Reaction EX_thf[u] not in model
Warning: Reaction EX_vitd3[u] not in model
Warning: Reaction EX_meoh[u] not in model
Warning: Reaction EX_fuc_L[u] not in model
Warning: Reaction EX_glcn[u] not in model
Warning: Reaction EX_rmn[u] not in model
Warning: Reaction EX_oxa[u] not in model
Warning: Reaction EX_melib[u] not in model
Warning: Reaction EX_cellb[u] not in model
Warning: Reaction EX_strch1[u] not in model
Warning: Reaction EX_amylopect900[u] not in model
```

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Warning: Reaction EX_amylose300[u] not in model
Warning: Reaction EX_arabinan101[u] not in model
Warning: Reaction EX_arabinogal[u] not in model
Warning: Reaction EX_arabinoxyl[u] not in model
Warning: Reaction EX_bglc[u] not in model
Warning: Reaction EX_cellul[u] not in model
Warning: Reaction EX_dextran40[u] not in model
Warning: Reaction EX_galmannan[u] not in model
Warning: Reaction EX_glcmannan[u] not in model
Warning: Reaction EX_homogal[u] not in model
Warning: Reaction EX_inulin[u] not in model
Warning: Reaction EX_kestopt[u] not in model
Warning: Reaction EX_levan1000[u] not in model
Warning: Reaction EX_lmn30[u] not in model
Warning: Reaction EX_lichn[u] not in model
Warning: Reaction EX_pect[u] not in model
Warning: Reaction EX_raffin[u] not in model
Warning: Reaction EX_rhamnogalurI[u] not in model
Warning: Reaction EX_rhamnogalurII[u] not in model
Warning: Reaction EX_starch1200[u] not in model
Warning: Reaction EX_xylan[u] not in model
Warning: Reaction EX_xyluglc[u] not in model
Warning: Reaction EX_arachd[u] not in model
Warning: Reaction EX_chsterol[u] not in model
Warning: Reaction EX_hdca[u] not in model
Warning: Reaction EX_hdcea[u] not in model
Warning: Reaction EX_lnlc[u] not in model
Warning: Reaction EX_lnlnca[u] not in model
Warning: Reaction EX_lnlncg[u] not in model
Warning: Reaction EX_ocdcea[u] not in model
Warning: Reaction EX_octa[u] not in model
Warning: Reaction EX_12dgr180[u] not in model
Warning: Reaction EX_4abz[u] not in model
Warning: Reaction EX_4hbz[u] not in model
Warning: Reaction EX_5aop[u] not in model
Warning: Reaction EX_acmana[u] not in model
Warning: Reaction EX_acnam[u] not in model
Warning: Reaction EX_adn[u] not in model
Warning: Reaction EX_ala_D[u] not in model
Warning: Reaction EX_amet[u] not in model
Warning: Reaction EX_amp[u] not in model
Warning: Reaction EX_anth[u] not in model
Warning: Reaction EX_arab_D[u] not in model
Warning: Reaction EX_avite1[u] not in model
Warning: Reaction EX_chol[u] not in model
Warning: Reaction EX_chor[u] not in model
Warning: Reaction EX_ddca[u] not in model
Warning: Reaction EX_fald[u] not in model
Warning: Reaction EX_fe3dcit[u] not in model
Warning: Reaction EX_glu_D[u] not in model
Warning: Reaction EX_gsn[u] not in model
Warning: Reaction EX_gthox[u] not in model
Warning: Reaction EX_gthrd[u] not in model
Warning: Reaction EX_h2s[u] not in model
Warning: Reaction EX_hom_L[u] not in model
Warning: Reaction EX_indole[u] not in model
Warning: Reaction EX_lanost[u] not in model
```

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Warning: Reaction EX_mobd[u] not in model
Warning: Reaction EX_ncam[u] not in model
Warning: Reaction EX_nmn[u] not in model
Warning: Reaction EX_no2[u] not in model
Warning: Reaction EX_no2[u] not in model
Warning: Reaction EX_no3[u] not in model
Warning: Reaction EX_phyQ[u] not in model
Warning: Reaction EX_pime[u] not in model
Warning: Reaction EX_ptrc[u] not in model
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Warning: Reaction EX_hdcea[u] not in model
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Warning: Reaction EX_octa[u] not in model
Warning: Reaction EX_12dgr180[u] not in model
Warning: Reaction EX_4abz[u] not in model
Warning: Reaction EX_4hbz[u] not in model
```

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Warning: Reaction EX_5aop[u] not in model
Warning: Reaction EX_acmana[u] not in model
Warning: Reaction EX_acnam[u] not in model
Warning: Reaction EX_adn[u] not in model
Warning: Reaction EX_ala_D[u] not in model
Warning: Reaction EX_amet[u] not in model
Warning: Reaction EX_amp[u] not in model
Warning: Reaction EX_anth[u] not in model
Warning: Reaction EX_arab_D[u] not in model
Warning: Reaction EX_avite1[u] not in model
Warning: Reaction EX_chol[u] not in model
Warning: Reaction EX_chor[u] not in model
Warning: Reaction EX_ddca[u] not in model
Warning: Reaction EX_fald[u] not in model
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Warning: Reaction EX_lanost[u] not in model
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Warning: Reaction EX_ncam[u] not in model
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Warning: Reaction EX_pime[u] not in model
Warning: Reaction EX_ptrc[u] not in model
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Warning: Reaction EX_sel[u] not in model
Warning: Reaction EX_thf[u] not in model
Warning: Reaction EX_vitd3[u] not in model
Warning: Reaction EX_meoh[u] not in model
Done.
   Testing simulation pairwise interactions using glpk ...
Warning: Reaction EX_fuc_L[u] not in model
Warning: Reaction EX_glcn[u] not in model
Warning: Reaction EX_rmn[u] not in model
Warning: Reaction EX_oxa[u] not in model
Warning: Reaction EX_melib[u] not in model
Warning: Reaction EX_cellb[u] not in model
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Warning: Reaction EX_dextran40[u] not in model
Warning: Reaction EX_galmannan[u] not in model
Warning: Reaction EX_glcmannan[u] not in model
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Warning: Reaction EX_inulin[u] not in model
Warning: Reaction EX_kestopt[u] not in model
Warning: Reaction EX_levan1000[u] not in model
Warning: Reaction EX_lmn30[u] not in model
Warning: Reaction EX_lichn[u] not in model
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Warning: Reaction EX_no3[u] not in model
Warning: Reaction EX_phyQ[u] not in model
Warning: Reaction EX_pime[u] not in model
Warning: Reaction EX_ptrc[u] not in model
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Warning: Reaction EX_retinol[u] not in model
Warning: Reaction EX_sel[u] not in model
Warning: Reaction EX_thf[u] not in model
Warning: Reaction EX_vitd3[u] not in model
Warning: Reaction EX_meoh[u] not in model
Warning: Reaction EX_fuc_L[u] not in model
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Warning: Reaction EX_amet[u] not in model
Warning: Reaction EX_amp[u] not in model
Warning: Reaction EX_anth[u] not in model
Warning: Reaction EX_arab_D[u] not in model
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Warning: Reaction EX_avite1[u] not in model
Warning: Reaction EX_chol[u] not in model
Warning: Reaction EX_chor[u] not in model
Warning: Reaction EX_ddca[u] not in model
Warning: Reaction EX_fald[u] not in model
Warning: Reaction EX_fe3dcit[u] not in model
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Warning: Reaction EX_rhamnogalurII[u] not in model
Warning: Reaction EX_starch1200[u] not in model
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Warning: Reaction EX_gthox[u] not in model
Warning: Reaction EX_gthrd[u] not in model
Warning: Reaction EX_h2s[u] not in model
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Warning: Reaction EX_hom_L[u] not in model
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Warning: Reaction EX_starch1200[u] not in model
Warning: Reaction EX_xylan[u] not in model
Warning: Reaction EX_xyluglc[u] not in model
Warning: Reaction EX_arachd[u] not in model
Warning: Reaction EX_chsterol[u] not in model
Warning: Reaction EX_hdca[u] not in model
Warning: Reaction EX_hdcea[u] not in model
Warning: Reaction EX_lnlc[u] not in model
Warning: Reaction EX_lnlnca[u] not in model
Warning: Reaction EX_lnlncg[u] not in model
Warning: Reaction EX_ocdcea[u] not in model
Warning: Reaction EX_octa[u] not in model
```

```
Warning: Reaction EX_12dgr180[u] not in model
Warning: Reaction EX_4abz[u] not in model
Warning: Reaction EX_4hbz[u] not in model
Warning: Reaction EX_5aop[u] not in model
Warning: Reaction EX_acmana[u] not in model
Warning: Reaction EX_acnam[u] not in model
Warning: Reaction EX_adn[u] not in model
Warning: Reaction EX_ala_D[u] not in model
Warning: Reaction EX_amet[u] not in model
Warning: Reaction EX_amp[u] not in model
Warning: Reaction EX_anth[u] not in model
Warning: Reaction EX_arab_D[u] not in model
Warning: Reaction EX_avite1[u] not in model
Warning: Reaction EX_chol[u] not in model
Warning: Reaction EX_chor[u] not in model
Warning: Reaction EX_ddca[u] not in model
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Warning: Reaction EX_fe3dcit[u] not in model
Warning: Reaction EX_glu_D[u] not in model
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Warning: Reaction EX_ncam[u] not in model
Warning: Reaction EX_nmn[u] not in model
Warning: Reaction EX_no2[u] not in model
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Warning: Reaction EX_no3[u] not in model
Warning: Reaction EX_phyQ[u] not in model
Warning: Reaction EX_pime[u] not in model
Warning: Reaction EX_ptrc[u] not in model
Warning: Reaction EX_pydx5p[u] not in model
Warning: Reaction EX_retinol[u] not in model
Warning: Reaction EX_sel[u] not in model
Warning: Reaction EX_thf[u] not in model
Warning: Reaction EX_vitd3[u] not in model
Warning: Reaction EX_meoh[u] not in model
Warning: Reaction EX_fuc_L[u] not in model
Warning: Reaction EX_glcn[u] not in model
Warning: Reaction EX_rmn[u] not in model
Warning: Reaction EX_oxa[u] not in model
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Warning: Reaction EX_cellb[u] not in model
Warning: Reaction EX_strch1[u] not in model
Warning: Reaction EX_amylopect900[u] not in model
Warning: Reaction EX_amylose300[u] not in model
Warning: Reaction EX_arabinan101[u] not in model
Warning: Reaction EX_arabinogal[u] not in model
Warning: Reaction EX_arabinoxyl[u] not in model
Warning: Reaction EX_bglc[u] not in model
Warning: Reaction EX_cellul[u] not in model
Warning: Reaction EX_dextran40[u] not in model
Warning: Reaction EX_galmannan[u] not in model
```

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Warning: Reaction EX_glcmannan[u] not in model
Warning: Reaction EX_homogal[u] not in model
Warning: Reaction EX_inulin[u] not in model
Warning: Reaction EX_kestopt[u] not in model
Warning: Reaction EX_levan1000[u] not in model
Warning: Reaction EX_lmn30[u] not in model
Warning: Reaction EX_lichn[u] not in model
Warning: Reaction EX_pect[u] not in model
Warning: Reaction EX_raffin[u] not in model
Warning: Reaction EX_rhamnogalurI[u] not in model
Warning: Reaction EX_rhamnogalurII[u] not in model
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Warning: Reaction EX_no2[u] not in model
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Warning: Reaction EX_no3[u] not in model
Warning: Reaction EX_phyQ[u] not in model
Warning: Reaction EX_pime[u] not in model
```

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Warning: Reaction EX_ptrc[u] not in model
Warning: Reaction EX_pydx5p[u] not in model
Warning: Reaction EX_retinol[u] not in model
Warning: Reaction EX_sel[u] not in model
Warning: Reaction EX_thf[u] not in model
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Warning: Reaction EX_arab_D[u] not in model
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Warning: Reaction EX_starch1200[u] not in model
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```

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```

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Warning: Reaction EX_h2s[u] not in model
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Warning: Reaction EX_sel[u] not in model
Warning: Reaction EX_thf[u] not in model
Warning: Reaction EX_vitd3[u] not in model
Warning: Reaction EX_meoh[u] not in model
Done.
.
Done testSimulationPairwiseInteractions
----------

Running testNullspace
testNullspace passed: norm(S*Z,inf) = 1.6e-10, while tolerance is =  1.0e-09
.
Done testNullspace
----------

Running testOptKnock
   Testing optKnock using gurobi6 ...

Substrate = EX_glc(e)
Target reaction= EX_succ(e)
Optknock solution is: 26.057230
ans =
    'ACALD'
    'GLUDy'
    'LDH_D'
    'PFL'
    'THD2'

Done.
.
Done testOptKnock
----------

Running testOptimizeCbModel
   Testing optimizeCbModel using solver glpk ... Done.
.
Done testOptimizeCbModel
----------

Running testOutputNetworkCytoscape
.
Done testOutputNetworkCytoscape
----------

Running testPaint4Net
Running Paint4Net using solver glpk ...
Start_time = 2017_7_10_23_36_1.1077
```

```
End_time = 2017_7_10_23_36_2.266
Total_time = 0_0_0_0_0_1.1584
Start_time = 2017_7_10_23_36_2.2793
End_time = 2017_7_10_23_36_2.4793
Total_time = 0_0_0_0_0_0.20013
Start_time = 2017_7_10_23_36_2.4889
Biograph object with 9 nodes and 8 edges.
End_time = 2017_7_10_23_36_5.4624
Total_time = 0_0_0_0_0_2.9735
Start_time = 2017_7_10_23_36_5.5034
End_time = 2017_7_10_23_36_5.7112
Total_time = 0_0_0_0_0_0.20775
Start_time = 2017_7_10_23_36_5.722
Biograph object with 7 nodes and 6 edges.
End_time = 2017_7_10_23_36_6.5564
Total_time = 0_0_0_0_0_0.83445
Start_time = 2017_7_10_23_36_6.5971
Biograph object with 76 nodes and 145 edges.
End_time = 2017_7_10_23_36_9.1183
Total_time = 0_0_0_0_0_2.5212
Start_time = 2017_7_10_23_36_9.1824
Biograph object with 129 nodes and 249 edges.
End_time = 2017_7_10_23_36_13.5262
Total_time = 0_0_0_0_0_4.3438
Start_time = 2017_7_10_23_36_13.8507
Biograph object with 18 nodes and 27 edges.
End_time = 2017_7_10_23_36_14.845
Total_time = 0_0_0_0_0_0.9943
Start_time = 2017_7_10_23_36_14.8962
Biograph object with 5 nodes and 4 edges.
End_time = 2017_7_10_23_36_15.5513
Total_time = 0_0_0_0_0_0.65534
Start_time = 2017_7_10_23_36_15.5804
Biograph object with 5 nodes and 4 edges.
End_time = 2017_7_10_23_36_16.1934
Total_time = 0_0_0_0_0_0.61297
Start_time = 2017_7_10_23_36_16.2176
Biograph object with 10 nodes and 12 edges.
End_time = 2017_7_10_23_36_16.9031
Total_time = 0_0_0_0_0_0.68552
Start_time = 2017_7_10_23_36_16.9315
Biograph object with 6 nodes and 5 edges.
End_time = 2017_7_10_23_36_17.5296
Total_time = 0_0_0_0_0_0.59814
Start_time = 2017_7_10_23_36_17.5431
Biograph object with 5 nodes and 4 edges.
End_time = 2017_7_10_23_36_18.2998
Total_time = 0_0_0_0_0_0.7569
Start_time = 2017_7_10_23_36_18.3054
Biograph object with 4 nodes and 3 edges.
End_time = 2017_7_10_23_36_19.0108
Total_time = 0_0_0_0_0_0.70543
Start_time = 2017_7_10_23_36_19.0158
```

```
Biograph object with 3 nodes and 2 edges.
End_time = 2017_7_10_23_36_19.6573
Total_time = 0_0_0_0_0_0.64159
Start_time = 2017_7_10_23_36_19.7348
Biograph object with 10 nodes and 12 edges.
End_time = 2017_7_10_23_36_20.5906
Total_time = 0_0_0_0_0_0.85594
Start_time = 2017_7_10_23_36_20.5988
Biograph object with 14 nodes and 17 edges.
End_time = 2017_7_10_23_36_21.6016
Total_time = 0_0_0_0_0_1.0029
Start_time = 2017_7_10_23_36_21.6054
Biograph object with 17 nodes and 22 edges.
End_time = 2017_7_10_23_36_22.5523
Total_time = 0_0_0_0_0_0.94689
Start_time = 2017_7_10_23_36_22.5572
Biograph object with 20 nodes and 26 edges.
End_time = 2017_7_10_23_36_23.5322
Total_time = 0_0_0_0_0_0.97501
Start_time = 2017_7_10_23_36_23.6603
Biograph object with 10 nodes and 12 edges.
End_time = 2017_7_10_23_36_24.4139
Total_time = 0_0_0_0_0_0.75358
Start_time = 2017_7_10_23_36_24.4426
End_time = 2017_7_10_23_36_24.6454
Total_time = 0_0_0_0_0_0.20275
Start_time = 2017_7_10_23_36_24.6494
Biograph object with 20 nodes and 26 edges.
End_time = 2017_7_10_23_36_25.6183
Total_time = 0_0_0_0_0_0.96896
Start_time = 2017_7_10_23_36_25.6568
Biograph object with 11 nodes and 14 edges.
End_time = 2017_7_10_23_36_26.4577
Total_time = 0_0_0_0_0_0.801
Start_time = 2017_7_10_23_36_26.4901
Biograph object with 11 nodes and 14 edges.
End_time = 2017_7_10_23_36_27.4937
Total_time = 0_0_0_0_0_1.0038
Start_time = 2017_7_10_23_36_27.5198
Biograph object with 16 nodes and 21 edges.
End_time = 2017_7_10_23_36_28.3162
Total_time = 0_0_0_0_0_0.79635
Start_time = 2017_7_10_23_36_28.3497
Biograph object with 21 nodes and 26 edges.
End_time = 2017_7_10_23_36_29.2832
Total_time = 0_0_0_0_0_0.93348
Start_time = 2017_7_10_23_36_29.324
Biograph object with 20 nodes and 26 edges.
End_time = 2017_7_10_23_36_30.1993
Total_time = 0_0_0_0_0_0.8753
Start_time = 2017_7_10_23_36_30.2388
Biograph object with 20 nodes and 26 edges.
End_time = 2017_7_10_23_36_31.1069
```

```
Total_time = 0_0_0_0_0_0.86806
Start_time = 2017_7_10_23_36_31.1465
Biograph object with 10 nodes and 12 edges.
End_time = 2017_7_10_23_36_31.8173
Total_time = 0_0_0_0_0_0.67075
Start_time = 2017_7_10_23_36_31.8453
Biograph object with 9 nodes and 10 edges.
End_time = 2017_7_10_23_36_32.4951
Total_time = 0_0_0_0_0_0.64981
Start_time = 2017_7_10_23_36_32.5208
Biograph object with 9 nodes and 11 edges.
End_time = 2017_7_10_23_36_33.1838
Total_time = 0_0_0_0_0_0.66297
Start_time = 2017_7_10_23_36_33.2141
Biograph object with 10 nodes and 12 edges.
End_time = 2017_7_10_23_36_33.9482
Total_time = 0_0_0_0_0_0.73411
Done.
.
Done testPaint4Net
----------

Running testPrintConstraints
Warning: File 'printConstraints.txt' not found.
MinConstraints:
ACALD -1000
ACALDt -1000
ACKr -1000
ACONTa -1000
ACONTb -1000
ACt2r -1000
ADK1 -1000
AKGt2r -1000
ALCD2x -1000
ATPM 8.39
ATPS4r -1000
CO2t -1000
D_LACt2 -1000
ENO -1000
ETOHt2r -1000
EX_co2(e) -1000
EX_glc(e) -10
EX_h(e) -1000
EX_h2o(e) -1000
EX_nh4(e) -1000
EX_o2(e) -1000
EX_pi(e) -1000
FBA -1000
FUM -1000
G6PDH2r -1000
GAPD -1000
GLUDy -1000
GLUt2r -1000
H2Ot -1000
ICDHyr -1000
LDH_D -1000
MDH -1000
NH4t -1000
O2t -1000
PGI -1000
PGK -1000
PGM -1000
```

PIt2r -1000
PTAr -1000
PYRt2r -1000
RPE -1000
RPI -1000
SUCOAS -1000
TALA -1000
TKT1 -1000
TKT2 -1000
TPI -1000
maxConstraints:
ACALD 1000
ACALDt 1000
ACKr 1000
ACONTa 1000
ACONTb 1000
ACt2r 1000
ADK1 1000
AKGDH 1000
AKGt2r 1000
ALCD2x 1000
ATPM 1000
ATPS4r 1000
Biomass_Ecoli_core_w_GAM 1000
CO2t 1000
CS 1000
CYTBD 1000
D_LACt2 1000
ENO 1000
ETOHt2r 1000
EX_ac(e) 1000
EX_acald(e) 1000
EX_akg(e) 1000
EX_co2(e) 1000
EX_etoh(e) 1000
EX_for(e) 1000
EX_fru(e) 1000
EX_fum(e) 1000
EX_glc(e) 1000
EX_gln_L(e) 1000
EX_glu_L(e) 1000
EX_h(e) 1000
EX_h2o(e) 1000
EX_lac_D(e) 1000
EX_mal_L(e) 1000
EX_nh4(e) 1000
EX_o2(e) 1000
EX_pi(e) 1000
EX_pyr(e) 1000
EX_succ(e) 1000
FBA 1000
FBP 1000
FORt2 1000
FORti 1000
FRD7 1000
FRUpts2 1000
FUM 1000
FUMt2_2 1000
G6PDH2r 1000
GAPD 1000
GLCpts 1000
GLNS 1000
GLNabc 1000
GLUDy 1000
GLUN 1000
GLUSy 1000
GLUt2r 1000
GND 1000

```
H2Ot 1000
ICDHyr 1000
ICL 1000
LDH_D 1000
MALS 1000
MALt2_2 1000
MDH 1000
ME1 1000
ME2 1000
NADH16 1000
NADTRHD 1000
NH4t 1000
O2t 1000
PDH 1000
PFK 1000
PFL 1000
PGI 1000
PGK 1000
PGL 1000
PGM 1000
PIt2r 1000
PPC 1000
PPCK 1000
PPS 1000
PTAr 1000
PYK 1000
PYRt2r 1000
RPE 1000
RPI 1000
SUCCt2_2 1000
SUCCt3 1000
SUCDi 1000
SUCOAS 1000
TALA 1000
THD2 1000
TKT1 1000
TKT2 1000
TPI 1000

================================================================================
Error occurred in testPrintConstraints/testPrintConstraints and it did not run to completion.

    ---------
    Error ID:
    ---------
    'MATLAB:REGEXP:invalidInputs'

    --------------
    Error Details:
    --------------
    Error using regexp
    The 'STRING' input must be either a char row vector, a cell array of char row vectors, or a string a

    Error in splitString>splitOneString (line 43)
    [startIndex, endIndex] = regexp(string, delimiter);

    Error in splitString (line 34)
        fields = splitOneString(string, delimiter);

    Error in readMixedData (line 39)
    tmp = splitString(line, delimiter);

    Error in testPrintConstraints (line 31)
    text2 = readMixedData('printConstraints.txt');
================================================================================
.
Done testPrintConstraints
__________
```

```
Running testPrintFluxVector
Warning: File 'printFluxVector.txt' not found.
ACALD 0.537667
ACALDt 1.83389
ACKr -2.25885
ACONTa 0.862173
ACONTb 0.318765
ACt2r -1.30769
ADK1 -0.433592
AKGDH 0.342624
AKGt2r 3.5784
ALCD2x 2.76944
ATPM -1.34989
ATPS4r 3.03492
Biomass_Ecoli_core_w_GAM 0.725404
CO2t -0.0630549
CS 0.714743
CYTBD -0.204966
D_LACt2 -0.124144
ENO 1.4897
ETOHt2r 1.40903
EX_ac(e) 1.41719
EX_acald(e) 0.671497
EX_akg(e) -1.20749
EX_co2(e) 0.717239
EX_etoh(e) 1.63024
EX_for(e) 0.488894
EX_fru(e) 1.03469
EX_fum(e) 0.726885
EX_glc(e) -0.303441
EX_gln_L(e) 0.293871
EX_glu_L(e) -0.787283
EX_h(e) 0.888396
EX_h2o(e) -1.14707
EX_lac_D(e) -1.06887
EX_mal_L(e) -0.809499
EX_nh4(e) -2.94428
EX_o2(e) 1.43838
EX_pi(e) 0.325191
EX_pyr(e) -0.754928
EX_succ(e) 1.3703
FBA -1.71152
FBP -0.102242
FORt2 -0.241447
FORti 0.319207
FRD7 0.312859
FRUpts2 -0.86488
FUM -0.0300513
FUMt2_2 -0.164879
G6PDH2r 0.627707
GAPD 1.09327
GLCpts 1.10927
GLNS -0.863653
GLNabc 0.0773591
GLUDy -1.21412
GLUN -1.1135
GLUSy -0.00684933
GLUt2r 1.53263
GND -0.769666
H2Ot 0.371379
ICDHyr -0.225584
ICL 1.11736
LDH_D -1.08906
MALS 0.0325575
MALt2_2 0.552527
MDH 1.10061
```

```
ME1 1.54421
ME2 0.0859311
NADH16 -1.49159
NADTRHD -0.742302
NH4t -1.06158
O2t 2.35046
PDH -0.615602
PFK 0.748077
PFL -0.192419
PGI 0.88861
PGK -0.764849
PGL -1.40227
PGM -1.42238
PIt2r 0.488194
PPC -0.177375
PPCK -0.196053
PPS 1.41931
PTAr 0.291584
PYK 0.197811
PYRt2r 1.5877
RPE -0.804466
RPI 0.696624
SUCCt2_2 0.835088
SUCCt3 -0.243715
SUCDi 0.21567
SUCOAS -1.16584
TALA -1.14795
THD2 0.104875
TKT1 0.722254
TKT2 2.58549
TPI -0.666891

================================================================================
Error occurred in testPrintFluxVector/testPrintFluxVector and it did not run to completion.

    ---------
    Error ID:
    ---------
    'MATLAB:assertion:failed'

    --------------
    Error Details:
    --------------
    Error using testPrintFluxVector (line 38)
    Assertion failed.
================================================================================
.
Done testPrintFluxVector

__________

Running testPrintRxnFormula
Warning: File 'printRxnFormula.txt' not found.

ACALD acald[c] + coa[c] + nad[c]  <=> accoa[c] + h[c] + nadh[c]
ACALDt acald[e]  <=> acald[c]
ACKr ac[c] + atp[c]  <=> actp[c] + adp[c]
ACONTa cit[c]  <=> acon-C[c] + h2o[c]
ACONTb acon-C[c] + h2o[c]  <=> icit[c]
ACt2r ac[e] + h[e]  <=> ac[c] + h[c]
ADK1 amp[c] + atp[c]  <=> 2 adp[c]
AKGDH akg[c] + coa[c] + nad[c]  -> co2[c] + nadh[c] + succoa[c]
AKGt2r akg[e] + h[e]  <=> akg[c] + h[c]
ALCD2x etoh[c] + nad[c]  <=> acald[c] + h[c] + nadh[c]
ATPM atp[c] + h2o[c]  -> adp[c] + h[c] + pi[c]
ATPS4r adp[c] + 4 h[e] + pi[c]  <=> atp[c] + h2o[c] + 3 h[c]
Biomass_Ecoli_core_w_GAM 1.496 3pg[c] + 3.7478 accoa[c] + 59.81 atp[c] + 0.361 e4p[c] + 0.0709 f6p[c] +
CO2t co2[e]  <=> co2[c]
CS accoa[c] + h2o[c] + oaa[c]  -> cit[c] + coa[c] + h[c]
```

```
CYTBD 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + 2 h[e] + q8[c]
D_LACt2 h[e] + lac-D[e]  <=> h[c] + lac-D[c]
ENO 2pg[c]  <=> h2o[c] + pep[c]
ETOHt2r etoh[e] + h[e]  <=> etoh[c] + h[c]
EX_ac(e) ac[e]  ->
EX_acald(e) acald[e]  ->
EX_akg(e) akg[e]  ->
EX_co2(e) co2[e]  <=>
EX_etoh(e) etoh[e]  ->
EX_for(e) for[e]  ->
EX_fru(e) fru[e]  ->
EX_fum(e) fum[e]  ->
EX_glc(e) glc-D[e]  <=>
EX_gln_L(e) gln-L[e]  ->
EX_glu_L(e) glu-L[e]  ->
EX_h(e) h[e]  <=>
EX_h2o(e) h2o[e]  <=>
EX_lac_D(e) lac-D[e]  ->
EX_mal_L(e) mal-L[e]  ->
EX_nh4(e) nh4[e]  <=>
EX_o2(e) o2[e]  <=>
EX_pi(e) pi[e]  <=>
EX_pyr(e) pyr[e]  ->
EX_succ(e) succ[e]  ->
FBA fdp[c]  <=> dhap[c] + g3p[c]
FBP fdp[c] + h2o[c]  -> f6p[c] + pi[c]
FORt2 for[e] + h[e]  -> for[c] + h[c]
FORti for[c]  -> for[e]
FRD7 fum[c] + q8h2[c]  -> q8[c] + succ[c]
FRUpts2 fru[e] + pep[c]  -> f6p[c] + pyr[c]
FUM fum[c] + h2o[c]  <=> mal-L[c]
FUMt2_2 fum[e] + 2 h[e]  -> fum[c] + 2 h[c]
G6PDH2r g6p[c] + nadp[c]  <=> 6pgl[c] + h[c] + nadph[c]
GAPD g3p[c] + nad[c] + pi[c]  <=> 13dpg[c] + h[c] + nadh[c]
GLCpts glc-D[e] + pep[c]  -> g6p[c] + pyr[c]
GLNS atp[c] + glu-L[c] + nh4[c]  -> adp[c] + gln-L[c] + h[c] + pi[c]
GLNabc atp[c] + gln-L[e] + h2o[c]  -> adp[c] + gln-L[c] + h[c] + pi[c]
GLUDy glu-L[c] + h2o[c] + nadp[c]  <=> akg[c] + h[c] + nadph[c] + nh4[c]
GLUN gln-L[c] + h2o[c]  -> glu-L[c] + nh4[c]
GLUSy akg[c] + gln-L[c] + h[c] + nadph[c]  -> 2 glu-L[c] + nadp[c]
GLUt2r glu-L[e] + h[e]  <=> glu-L[c] + h[c]
GND 6pgc[c] + nadp[c]  -> co2[c] + nadph[c] + ru5p-D[c]
H2Ot h2o[e]  <=> h2o[c]
ICDHyr icit[c] + nadp[c]  <=> akg[c] + co2[c] + nadph[c]
ICL icit[c]  -> glx[c] + succ[c]
LDH_D lac-D[c] + nad[c]  <=> h[c] + nadh[c] + pyr[c]
MALS accoa[c] + glx[c] + h2o[c]  -> coa[c] + h[c] + mal-L[c]
MALt2_2 2 h[e] + mal-L[e]  -> 2 h[c] + mal-L[c]
MDH mal-L[c] + nad[c]  <=> h[c] + nadh[c] + oaa[c]
ME1 mal-L[c] + nad[c]  -> co2[c] + nadh[c] + pyr[c]
ME2 mal-L[c] + nadp[c]  -> co2[c] + nadph[c] + pyr[c]
NADH16 4 h[c] + nadh[c] + q8[c]  -> 3 h[e] + nad[c] + q8h2[c]
NADTRHD nad[c] + nadph[c]  -> nadh[c] + nadp[c]
NH4t nh4[e]  <=> nh4[c]
O2t o2[e]  <=> o2[c]
PDH coa[c] + nad[c] + pyr[c]  -> accoa[c] + co2[c] + nadh[c]
PFK atp[c] + f6p[c]  -> adp[c] + fdp[c] + h[c]
PFL coa[c] + pyr[c]  -> accoa[c] + for[c]
PGI g6p[c]  <=> f6p[c]
PGK 3pg[c] + atp[c]  <=> 13dpg[c] + adp[c]
PGL 6pgl[c] + h2o[c]  -> 6pgc[c] + h[c]
PGM 2pg[c]  <=> 3pg[c]
PIt2r h[e] + pi[e]  <=> h[c] + pi[c]
PPC co2[c] + h2o[c] + pep[c]  -> h[c] + oaa[c] + pi[c]
PPCK atp[c] + oaa[c]  -> adp[c] + co2[c] + pep[c]
PPS atp[c] + h2o[c] + pyr[c]  -> amp[c] + 2 h[c] + pep[c] + pi[c]
PTAr accoa[c] + pi[c]  <=> actp[c] + coa[c]
PYK adp[c] + h[c] + pep[c]  -> atp[c] + pyr[c]
```

```
PYRt2r h[e] + pyr[e]  <=> h[c] + pyr[c]
RPE ru5p-D[c]  <=> xu5p-D[c]
RPI r5p[c]  <=> ru5p-D[c]
SUCCt2_2 2 h[e] + succ[e]  -> 2 h[c] + succ[c]
SUCCt3 h[e] + succ[c]  -> h[c] + succ[e]
SUCDi q8[c] + succ[c]  -> fum[c] + q8h2[c]
SUCOAS atp[c] + coa[c] + succ[c]  <=> adp[c] + pi[c] + succoa[c]
TALA g3p[c] + s7p[c]  <=> e4p[c] + f6p[c]
THD2 2 h[e] + nadh[c] + nadp[c]  -> 2 h[c] + nad[c] + nadph[c]
TKT1 r5p[c] + xu5p-D[c]  <=> g3p[c] + s7p[c]
TKT2 e4p[c] + xu5p-D[c]  <=> f6p[c] + g3p[c]
TPI dhap[c]  <=> g3p[c]

================================================================================
Error occurred in testPrintRxnFormula/testPrintRxnFormula and it did not run to completion.

    ---------
    Error ID:
    ---------
    'MATLAB:assertion:failed'

    --------------
    Error Details:
    --------------
    Error using testPrintRxnFormula (line 34)
    Assertion failed.
================================================================================
.
Done testPrintRxnFormula
__________

Running testPrintUptakeBound
Warning: File 'printUptakeBound.txt' not found.

EX_co2(e) -1000
EX_glc(e) -10
EX_h(e) -1000
EX_h2o(e) -1000
EX_nh4(e) -1000
EX_o2(e) -1000
EX_pi(e) -1000

================================================================================
Error occurred in testPrintUptakeBound/testPrintUptakeBound and it did not run to completion.

    ---------
    Error ID:
    ---------
    'MATLAB:assertion:failed'

    --------------
    Error Details:
    --------------
    Error using testPrintUptakeBound (line 33)
    Assertion failed.
================================================================================
.
Done testPrintUptakeBound
__________

Running testSurfNet
Warning: File 'surfNet.txt' not found.

Met #1  13dpg[c], 3-Phospho-D-glyceroyl-phosphate, C3H4O10P2
Consuming reactions: none
Producing reactions:
  #49  GAPD, Bd: -1000 / 1000, glyceraldehyde-3-phosphate dehydrogenase
  g3p[c] + nad[c] + pi[c] <=> 13dpg[c] + h[c] + nadh[c]
```

```
  #75  PGK, Bd: -1000 / 1000, phosphoglycerate kinase
  3pg[c] + atp[c] <=> 13dpg[c] + adp[c]

Show previous steps...

================================================================================
Error occurred in testSurfNet/testSurfNet and it did not run to completion.

    ---------
    Error ID:
    ---------
    'MATLAB:assertion:failed'

    --------------
    Error Details:
    --------------
    Error using testSurfNet (line 32)
    Assertion failed.
================================================================================
.
Done testSurfNet
__________

Running testGPR2Genes
.
Done testGPR2Genes
__________

Running testGetGeneList
.
Done testGetGeneList
__________

Running testLegalRxnFormula
ACALD acald[c] + coa[c] + nad[c]  <=> accoa[c] + h[c] + nadh[c]
.
Done testLegalRxnFormula
__________

Running testLoadReaction
.
Done testLoadReaction
__________

Running testMets2str
.
Done testMets2str
__________

Running testModel2data
Warning: Metabolite acald[c] not in model - added to the model
Warning: Metabolite coa[c] not in model - added to the model
Warning: Metabolite nad[c] not in model - added to the model
Warning: Metabolite accoa[c] not in model - added to the model
Warning: Metabolite h[c] not in model - added to the model
Warning: Metabolite nadh[c] not in model - added to the model

New gene b0351 added to model
New gene b1241 added to model
ACALD acald[c] + coa[c] + nad[c]  <=> accoa[c] + h[c] + nadh[c]
Warning: Metabolite acald[e] not in model - added to the model

New gene s0001 added to model
ACALDt acald[e]  <=> acald[c]
Warning: Metabolite ac[c] not in model - added to the model
Warning: Metabolite atp[c] not in model - added to the model
Warning: Metabolite actp[c] not in model - added to the model
```

```
Warning: Metabolite adp[c] not in model - added to the model

New gene b3115 added to model
New gene b2296 added to model
New gene b1849 added to model
ACKr ac[c] + atp[c]  <=> actp[c] + adp[c]
Warning: Metabolite cit[c] not in model - added to the model
Warning: Metabolite acon-C[c] not in model - added to the model
Warning: Metabolite h2o[c] not in model - added to the model

New gene b0118 added to model
New gene b1276 added to model
ACONTa cit[c]  <=> acon-C[c] + h2o[c]
Warning: Metabolite icit[c] not in model - added to the model

ACONTb acon-C[c] + h2o[c]  <=> icit[c]
Warning: Metabolite ac[e] not in model - added to the model
Warning: Metabolite h[e] not in model - added to the model

ACt2r ac[e] + h[e]  <=> h[c] + ac[c]
Warning: Metabolite amp[c] not in model - added to the model

New gene b0474 added to model
ADK1 atp[c] + amp[c]  <=> 2 adp[c]
Warning: Metabolite akg[c] not in model - added to the model
Warning: Metabolite co2[c] not in model - added to the model
Warning: Metabolite succoa[c] not in model - added to the model

New gene b0116 added to model
New gene b0726 added to model
New gene b0727 added to model
AKGDH coa[c] + nad[c] + akg[c]  -> nadh[c] + co2[c] + succoa[c]
Warning: Metabolite akg[e] not in model - added to the model

New gene b2587 added to model
AKGt2r h[e] + akg[e]  <=> h[c] + akg[c]
Warning: Metabolite etoh[c] not in model - added to the model

New gene b0356 added to model
New gene b1478 added to model
ALCD2x nad[c] + etoh[c]  <=> acald[c] + h[c] + nadh[c]
Warning: Metabolite pi[c] not in model - added to the model

ATPM atp[c] + h2o[c]  -> h[c] + adp[c] + pi[c]
New gene b3736 added to model
New gene b3737 added to model
New gene b3738 added to model
New gene b3731 added to model
New gene b3732 added to model
New gene b3733 added to model
New gene b3734 added to model
New gene b3735 added to model
New gene b3739 added to model
ATPS4r adp[c] + 4 h[e] + pi[c]  <=> 3 h[c] + atp[c] + h2o[c]
Warning: Metabolite 3pg[c] not in model - added to the model
Warning: Metabolite e4p[c] not in model - added to the model
Warning: Metabolite f6p[c] not in model - added to the model
Warning: Metabolite g3p[c] not in model - added to the model
Warning: Metabolite g6p[c] not in model - added to the model
Warning: Metabolite gln-L[c] not in model - added to the model
Warning: Metabolite glu-L[c] not in model - added to the model
Warning: Metabolite nadph[c] not in model - added to the model
Warning: Metabolite oaa[c] not in model - added to the model
Warning: Metabolite pep[c] not in model - added to the model
Warning: Metabolite pyr[c] not in model - added to the model
Warning: Metabolite r5p[c] not in model - added to the model
Warning: Metabolite nadp[c] not in model - added to the model

Biomass_Ecoli_core_w_GAM 3.547 nad[c] + 3.7478 accoa[c] + 59.81 atp[c] + 59.81 h2o[c] + 1.496 3pg[c] + 0
Warning: Metabolite co2[e] not in model - added to the model
```

```
CO2t co2[e]  <=> co2[c]
New gene b0720 added to model
CS accoa[c] + h2o[c] + oaa[c]  -> coa[c] + h[c] + cit[c]
Warning: Metabolite o2[c] not in model - added to the model
Warning: Metabolite q8h2[c] not in model - added to the model
Warning: Metabolite q8[c] not in model - added to the model
New gene b0978 added to model
New gene b0979 added to model
New gene b0733 added to model
New gene b0734 added to model
CYTBD 2 h[c] + 0.5 o2[c] + q8h2[c]  -> h2o[c] + 2 h[e] + q8[c]
Warning: Metabolite lac-D[e] not in model - added to the model
Warning: Metabolite lac-D[c] not in model - added to the model
New gene b2975 added to model
New gene b3603 added to model
D_LACt2 h[e] + lac-D[e]  <=> h[c] + lac-D[c]
Warning: Metabolite 2pg[c] not in model - added to the model
New gene b2779 added to model
ENO 2pg[c]  <=> h2o[c] + pep[c]
Warning: Metabolite etoh[e] not in model - added to the model
ETOHt2r h[e] + etoh[e]  <=> h[c] + etoh[c]
EX_ac(e) ac[e]  ->
EX_acald(e) acald[e]  ->
EX_akg(e) akg[e]  ->
EX_co2(e) co2[e]  <=>
EX_etoh(e) etoh[e]  ->
Warning: Metabolite for[e] not in model - added to the model
EX_for(e) for[e]  ->
Warning: Metabolite fru[e] not in model - added to the model
EX_fru(e) fru[e]  ->
Warning: Metabolite fum[e] not in model - added to the model
EX_fum(e) fum[e]  ->
Warning: Metabolite glc-D[e] not in model - added to the model
EX_glc(e) glc-D[e]  <=>
Warning: Metabolite gln-L[e] not in model - added to the model
EX_gln_L(e) gln-L[e]  ->
Warning: Metabolite glu-L[e] not in model - added to the model
EX_glu_L(e) glu-L[e]  ->
EX_h(e) h[e]  <=>
Warning: Metabolite h2o[e] not in model - added to the model
EX_h2o(e) h2o[e]  <=>
EX_lac_D(e) lac-D[e]  ->
Warning: Metabolite mal-L[e] not in model - added to the model
EX_mal_L(e) mal-L[e]  ->
Warning: Metabolite nh4[e] not in model - added to the model
EX_nh4(e) nh4[e]  <=>
Warning: Metabolite o2[e] not in model - added to the model
EX_o2(e) o2[e]  <=>
Warning: Metabolite pi[e] not in model - added to the model
EX_pi(e) pi[e]  <=>
Warning: Metabolite pyr[e] not in model - added to the model
EX_pyr(e) pyr[e]  ->
Warning: Metabolite succ[e] not in model - added to the model
EX_succ(e) succ[e]  ->
Warning: Metabolite fdp[c] not in model - added to the model
Warning: Metabolite dhap[c] not in model - added to the model
New gene b2097 added to model
New gene b1773 added to model
```

```
New gene b2925 added to model
FBA fdp[c]  <=> g3p[c] + dhap[c]
New gene b3925 added to model
New gene b4232 added to model
FBP h2o[c] + fdp[c]  -> pi[c] + f6p[c]
Warning: Metabolite for[c] not in model - added to the model

New gene b0904 added to model
New gene b2492 added to model
FORt2 h[e] + for[e]  -> h[c] + for[c]
FORti for[c]  -> for[e]
Warning: Metabolite fum[c] not in model - added to the model
Warning: Metabolite succ[c] not in model - added to the model

New gene b4151 added to model
New gene b4152 added to model
New gene b4153 added to model
New gene b4154 added to model
FRD7 q8h2[c] + fum[c]  -> q8[c] + succ[c]
New gene b1817 added to model
New gene b1818 added to model
New gene b1819 added to model
New gene b2415 added to model
New gene b2416 added to model
FRUpts2 pep[c] + fru[e]  -> f6p[c] + pyr[c]
Warning: Metabolite mal-L[c] not in model - added to the model

New gene b1612 added to model
New gene b4122 added to model
New gene b1611 added to model
FUM h2o[c] + fum[c]  <=> mal-L[c]
New gene b3528 added to model
FUMt2_2 2 h[e] + fum[e]  -> 2 h[c] + fum[c]
Warning: Metabolite 6pgl[c] not in model - added to the model

New gene b1852 added to model
G6PDH2r g6p[c] + nadp[c]  <=> h[c] + nadph[c] + 6pgl[c]
Warning: Metabolite 13dpg[c] not in model - added to the model

New gene b1779 added to model
GAPD nad[c] + pi[c] + g3p[c]  <=> h[c] + nadh[c] + 13dpg[c]
New gene b2417 added to model
New gene b1101 added to model
New gene b1621 added to model
GLCpts pep[c] + glc-D[e]  -> g6p[c] + pyr[c]
Warning: Metabolite nh4[c] not in model - added to the model

New gene b3870 added to model
New gene b1297 added to model
GLNS atp[c] + glu-L[c] + nh4[c]  -> h[c] + adp[c] + pi[c] + gln-L[c]
New gene b0811 added to model
New gene b0810 added to model
New gene b0809 added to model
GLNabc atp[c] + h2o[c] + gln-L[e]  -> h[c] + adp[c] + pi[c] + gln-L[c]
New gene b1761 added to model
GLUDy h2o[c] + glu-L[c] + nadp[c]  <=> h[c] + akg[c] + nadph[c] + nh4[c]
New gene b1812 added to model
New gene b0485 added to model
New gene b1524 added to model
GLUN h2o[c] + gln-L[c]  -> glu-L[c] + nh4[c]
New gene b3212 added to model
New gene b3213 added to model
GLUSy h[c] + akg[c] + gln-L[c] + nadph[c]  -> 2 glu-L[c] + nadp[c]
New gene b4077 added to model
GLUt2r h[e] + glu-L[e]  <=> h[c] + glu-L[c]
Warning: Metabolite 6pgc[c] not in model - added to the model
Warning: Metabolite ru5p-D[c] not in model - added to the model

New gene b2029 added to model
GND nadp[c] + 6pgc[c]  -> co2[c] + nadph[c] + ru5p-D[c]
New gene b0875 added to model
```

```
H2Ot h2o[e]  <=> h2o[c]
New gene b1136 added to model
ICDHyr icit[c] + nadp[c]  <=> akg[c] + co2[c] + nadph[c]
Warning: Metabolite glx[c] not in model - added to the model
New gene b4015 added to model
ICL icit[c]  -> succ[c] + glx[c]
New gene b2133 added to model
New gene b1380 added to model
LDH_D nad[c] + lac-D[c]  <=> h[c] + nadh[c] + pyr[c]
New gene b4014 added to model
New gene b2976 added to model
MALS accoa[c] + h2o[c] + glx[c]  -> coa[c] + h[c] + mal-L[c]
MALt2_2 2 h[e] + mal-L[e]  -> 2 h[c] + mal-L[c]
New gene b3236 added to model
MDH nad[c] + mal-L[c]  <=> h[c] + nadh[c] + oaa[c]
New gene b1479 added to model
ME1 nad[c] + mal-L[c]  -> nadh[c] + co2[c] + pyr[c]
New gene b2463 added to model
ME2 nadp[c] + mal-L[c]  -> co2[c] + nadph[c] + pyr[c]
New gene b2276 added to model
New gene b2277 added to model
New gene b2278 added to model
New gene b2279 added to model
New gene b2280 added to model
New gene b2281 added to model
New gene b2282 added to model
New gene b2283 added to model
New gene b2284 added to model
New gene b2285 added to model
New gene b2286 added to model
New gene b2287 added to model
New gene b2288 added to model
NADH16 4 h[c] + nadh[c] + q8[c]  -> nad[c] + 3 h[e] + q8h2[c]
New gene b3962 added to model
New gene b1602 added to model
New gene b1603 added to model
NADTRHD nad[c] + nadph[c]  -> nadh[c] + nadp[c]
New gene b0451 added to model
NH4t nh4[e]  <=> nh4[c]
O2t o2[e]  <=> o2[c]
New gene b0114 added to model
New gene b0115 added to model
PDH coa[c] + nad[c] + pyr[c]  -> accoa[c] + nadh[c] + co2[c]
New gene b3916 added to model
New gene b1723 added to model
PFK atp[c] + f6p[c]  -> h[c] + adp[c] + fdp[c]
New gene b0902 added to model
New gene b0903 added to model
New gene b2579 added to model
New gene b3114 added to model
New gene b3951 added to model
New gene b3952 added to model
PFL coa[c] + pyr[c]  -> accoa[c] + for[c]
New gene b4025 added to model
PGI g6p[c]  <=> f6p[c]
New gene b2926 added to model
PGK atp[c] + 3pg[c]  <=> adp[c] + 13dpg[c]
New gene b0767 added to model
PGL h2o[c] + 6pgl[c]  -> h[c] + 6pgc[c]
New gene b3612 added to model
New gene b4395 added to model
New gene b0755 added to model
PGM 2pg[c]  <=> 3pg[c]
New gene b2987 added to model
New gene b3493 added to model
PIt2r h[e] + pi[e]  <=> h[c] + pi[c]
New gene b3956 added to model
```

```
PPC h2o[c] + co2[c] + pep[c]  -> h[c] + pi[c] + oaa[c]
New gene b3403 added to model
PPCK atp[c] + oaa[c]  -> adp[c] + co2[c] + pep[c]
New gene b1702 added to model
PPS atp[c] + h2o[c] + pyr[c]  -> 2 h[c] + amp[c] + pi[c] + pep[c]
New gene b2297 added to model
New gene b2458 added to model
PTAr accoa[c] + pi[c]  <=> coa[c] + actp[c]
New gene b1854 added to model
New gene b1676 added to model
PYK h[c] + adp[c] + pep[c]  -> atp[c] + pyr[c]
PYRt2r h[e] + pyr[e]  <=> h[c] + pyr[c]
Warning: Metabolite xu5p-D[c] not in model - added to the model
New gene b3386 added to model
New gene b4301 added to model
RPE ru5p-D[c]  <=> xu5p-D[c]
New gene b2914 added to model
New gene b4090 added to model
RPI r5p[c]  <=> ru5p-D[c]
SUCCt2_2 2 h[e] + succ[e]  -> 2 h[c] + succ[c]
SUCCt3 h[e] + succ[c]  -> h[c] + succ[e]
New gene b0721 added to model
New gene b0722 added to model
New gene b0723 added to model
New gene b0724 added to model
SUCDi q8[c] + succ[c]  -> q8h2[c] + fum[c]
New gene b0728 added to model
New gene b0729 added to model
SUCOAS coa[c] + atp[c] + succ[c]  <=> adp[c] + succoa[c] + pi[c]
Warning: Metabolite s7p[c] not in model - added to the model
New gene b2464 added to model
New gene b0008 added to model
TALA g3p[c] + s7p[c]  <=> e4p[c] + f6p[c]
THD2 nadh[c] + 2 h[e] + nadp[c]  -> nad[c] + 2 h[c] + nadph[c]
New gene b2935 added to model
New gene b2465 added to model
TKT1 r5p[c] + xu5p-D[c]  <=> g3p[c] + s7p[c]
TKT2 e4p[c] + xu5p-D[c]  <=> f6p[c] + g3p[c]
New gene b3919 added to model
TPI dhap[c]  <=> g3p[c]
.
Done testModel2data
----------

Running testNeighborRxn2data
ACALDt acald[e]  <=> acald[c]
AKGDH akg[c] + coa[c] + nad[c]  -> co2[c] + nadh[c] + succoa[c]
ALCD2x etoh[c] + nad[c]  <=> acald[c] + h[c] + nadh[c]
Biomass_Ecoli_core_w_GAM 1.496 3pg[c] + 3.7478 accoa[c] + 59.81 atp[c] + 0.361 e4p[c] + 0.0709 f6p[c] +
CS accoa[c] + h2o[c] + oaa[c]  -> cit[c] + coa[c] + h[c]
GAPD g3p[c] + nad[c] + pi[c]  <=> 13dpg[c] + h[c] + nadh[c]
LDH_D lac-D[c] + nad[c]  <=> h[c] + nadh[c] + pyr[c]
MALS accoa[c] + glx[c] + h2o[c]  -> coa[c] + h[c] + mal-L[c]
MDH mal-L[c] + nad[c]  <=> h[c] + nadh[c] + oaa[c]
ME1 mal-L[c] + nad[c]  -> co2[c] + nadh[c] + pyr[c]
NADH16 4 h[c] + nadh[c] + q8[c]  -> 3 h[e] + nad[c] + q8h2[c]
NADTRHD nad[c] + nadph[c]  -> nadh[c] + nadp[c]
PDH coa[c] + nad[c] + pyr[c]  -> accoa[c] + co2[c] + nadh[c]
PFL coa[c] + pyr[c]  -> accoa[c] + for[c]
PTAr accoa[c] + pi[c]  <=> actp[c] + coa[c]
SUCOAS atp[c] + coa[c] + succ[c]  <=> adp[c] + pi[c] + succoa[c]
THD2 2 h[e] + nadh[c] + nadp[c]  -> 2 h[c] + nad[c] + nadph[c]
.
Done testNeighborRxn2data
----------
```

```
Running testRBioNetSaveLoad
```

```
compartments =
    'Acidocalcisome (a)'
    'Chloroplast (h)'
    'Cytoplasm  (c)'
    'Endoplasmatic reticulum (r)'
    'Extracellular space (e)'
    'Flagellum (f)'
    'Glycosome (y)'
    'Glyoxysome (o)'
    'Golgi apparatus (g)'
    'Lysosome (l)'
    'Mitochondrion (m)'
    'Nucleus (n)'
    'Periplasm (p)'
    'Peroxisom (x)'
    'Stebbis (s)'
    'Vacuole (v)'
```

```
metab =
    '13dpg'        '3-Phospho-D-glyceroyl phosphate'                    'C3H8O10P2'        'C3H4O10P
    '2pg'          'D-Glycerate 2-phosphate'                            'C3H7O7P'          'C3H4O7P'
    '3pg'          '3-Phospho-D-glycerate'                              'C3H7O7P'          'C3H4O7P'
    'L2aadp'       'L-2-Aminoadipate'                                   ''                 'C6H10NO4
    'L2aadp6sa'    'L-allysine'                                         'C6H11NO3'         'C6H11NO3
    'acald'        'Acetaldehyde'                                       ''                 'C2H4O'
    'adp'          'ADP'                                                'C10H15N5O10P2'    'C10H12N5
    'amp'          'AMP'                                                'C10H14N5O7P'      'C10H12N5
    'arg-L'        'L-Arginine'                                         'C6H14N4O2'        'C6H15N4O
    'argsuc'       'N(omega)-(L-Arginino)succinate'                     'C10H18N4O6'       'C10H17N4
    'asp-L'        'L-Aspartate'                                        'C4H7NO4'          'C4H6NO4'
    'atp'          'ATP(4-)'                                            'C10H16N5O13P3'    'C10H12N5
    'cbp'          'Carbamoyl phosphate'                                'CH4NO5P'          'CH2NO5P'
    'citr-L'       'L-Citrulline'                                       'C6H13N3O3'        'C6H13N3O
    'dhap'         'Dihydroxyacetone phosphate'                         'C3H7O6P'          'C3H5O6P'
    'etoh'         'Ethanol'                                            ''                 'C2H6O'
    'f6p'          'D-Fructose 6-phosphate'                             'C6H13O9P'         'C6H11O9P
    'fdp'          'D-Fructose 1,6-bisphosphate'                        'C6H14O12P2'       'C6H10O12
    'fum'          'Fumarate'                                           'C4H4O4'           'C4H2O4'
    'g3p'          'Glyceraldehyde 3-phosphate'                         'C3H7O6P'          'C3H5O6P'
    'g6p'          'D-Glucose 6-phosphate'                              'C6H13O9P'         'C6H11O9P
    'glc-D'        'gluko'                                              ''                 'C3H4O1'
    'glc-L'        'gluko'                                              ''                 'C3H4O1'
```

```
rxn =
    'ARGN'                      'arginase'
    'ARGSL'                     'argininosuccinate lyase'
    'ARGSS'                     'argininosuccinate synthase'
    'CBPSam'                    'carbamoyl-phosphate synthase (ammonia) (mitochondria)'
    'ENO'                       'enolase'
    'Ex_glc-L(e)'               'Ex_glc-L(e)'
    'FBA'                       'fructose-bisphosphate aldolase'
    'GAPD'                      'glyceraldehyde-3-phosphate dehydrogenase'
    'Glc-Dt'                    'Glc-Dt'
    'HEX1'                      'hexokinase (D-glucose:ATP)'
    'OCBTm'                     'ornithine carbamoyltransferase, irreversible'
    'PFK'                       'phosphofructokinase'
    'PGI'                       'glucose-6-phosphate isomerase'
```

```
ans = 0
ans = 0
ans = 0
```

```
.
Done testRBioNetSaveLoad

__________
```

```
Running testReactionEq
.
Done testReactionEq
----------

Running testSimilarity
.
Done testSimilarity
----------

Running testRank
getRankLUSOL: U appears to be singular, as judged by lu6chk.
.
Done testRank
----------

Running testReconMap
.
Done testReconMap
----------

Running testRobustnessAnalysis
Robustness analysis in progress ...
5%      [..                                      ]10%     [....                                    ]15%
Double robustness analysis in progress ...
4%      [.                                       ]8%      [...                                     ]12%
.
Done testRobustnessAnalysis
----------

Running testReadSBML
   Testing Abiotrophia_defectiva_ATCC_49176.xml ...
   Testing with solver gurobi6 ...
 Done.
   Testing with solver glpk ...
 Done.
   Testing STM_v1.0.xml ...
   Testing with solver gurobi6 ...
 Done.
   Testing with solver glpk ...
 Done.
   Testing iIT341.xml ...
The model contains 0 errors and 1 warnings.

   Testing with solver gurobi6 ...
 Done.
   Testing with solver glpk ...
 Done.
   Testing readSBML for models with symbols in objective reactions ...
Warning: Metabolite a[e] not in model - added to the model
EX_a(e) a[e]  <=>
Warning: Metabolite b[e] not in model - added to the model
EX_b(e) b[e]  <=>
Document written
 Done.

   Testing readSBML for models with >1 objective reactions ...
Warning: Metabolite a[e] not in model - added to the model
EX_a a[e]  <=>
Warning: Metabolite b[e] not in model - added to the model
EX_b b[e]  <=>
Document written
 Done.

.
```

```
Done testReadSBML
----------

Running testWriteSBML
Document written
.
Done testWriteSBML
----------

Running testGpSampler
   Testing readSBML using gurobi6 ...
A set to S
Warning:  csense not set.  Defaulting to all Equality constraints
Generating warmup points
Warning: Need a minimum of 190 warmup points
Creating warmup points ...
1%      [                                       ]2%      [                                                  ]3%
Sampling
         1 s 50 steps
         2 s 100 steps
A set to S
Warning:  csense not set.  Defaulting to all Equality constraints
Generating warmup points
Creating warmup points ...
1%      [                                       ]2%      [                                                  ]3%
Sampling
         1 s 50 steps
         1 s 100 steps
         2 s 150 steps
         3 s 200 steps
 Done.
   Testing readSBML using glpk ...
A set to S
Warning:  csense not set.  Defaulting to all Equality constraints
Generating warmup points
Warning: Need a minimum of 190 warmup points
Creating warmup points ...
1%      [                                       ]2%      [                                                  ]3%
Sampling
         0 s 50 steps
         1 s 100 steps
         1 s 150 steps
         2 s 200 steps
         2 s 250 steps
A set to S
Warning:  csense not set.  Defaulting to all Equality constraints
Generating warmup points
Creating warmup points ...
1%      [                                       ]2%      [                                                  ]3%
Sampling
         0 s 50 steps
         1 s 100 steps
         1 s 150 steps
         2 s 200 steps
         2 s 250 steps
 Done.
.
Done testGpSampler
----------

Running testSampleCbModel
   Testing sampleCbModel using gurobi6 ...
```

```
Testing the artificial centering hit-and-run (ACHR) sampler
.Prepare model for sampling
Original model: 95 rxns 72 metabolites
Reduce model
Model reduction in progress ...
```

```
Sample files generated
```

```
Testing the coordinate hit-and-run with rounding (CHRR) sampler
.Checking for width 0 facets...
 > The CPLEX version has been determined as 1271.

-- Warning:: You may only ouput 4, 7 or 9 variables.

 >> Solving Model.S. (uncoupled)
 >> The number of arguments is: input: 2, output 2.
 >> Size of stoichiometric matrix: (72,95)
 >> All reactions are solved (95 reactions - 100%).
 >> 0 reactions out of 95 are minimized (0.00%).
 >> 0 reactions out of 95 are maximized (0.00%).
 >> 95 reactions out of 95 are minimized and maximized (100.00%).

 -- Starting to loop through the 2 workers. --

 -- The splitting strategy is 0. --

--------------------------------------------------------------------------------
--  Task Launched // TaskID: 2 / 2 (LoopID = 1) <> [1, 48] / [72, 95].
 >> Number of reactions given to the worker: 48
 >> The number of reactions retrieved is 48
 >> Log files will be stored at /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/src/analysis/
 -- Start time:     Mon Jul 10 23:41:20 2017
 >> #Task.ID = 2; logfile: cplexint_logfile_2.log

 -- Warning:: The optPercentage is higher than 90. The solution process might take longer than you expec

        -- Minimization (iRound = 0). Number of reactions: 48.
        -- Maximization (iRound = 1). Number of reactions: 48.
 -- End time:     Mon Jul 10 23:41:20 2017
 >> Time spent in FVAc: 0.0 seconds.
--------------------------------------------------------------------------------
 ==> 100% done. Analysis completed.

--------------------------------------------------------------------------------
--  Task Launched // TaskID: 1 / 2 (LoopID = 2) <> [49, 95] / [72, 95].
 >> Number of reactions given to the worker: 47
 >> The number of reactions retrieved is 47
 >> Log files will be stored at /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/src/analysis/
 -- Start time:     Mon Jul 10 23:41:20 2017
 >> #Task.ID = 1; logfile: cplexint_logfile_1.log

 -- Warning:: The optPercentage is higher than 90. The solution process might take longer than you expec

        -- Minimization (iRound = 0). Number of reactions: 47.
        -- Maximization (iRound = 1). Number of reactions: 47.
 -- End time:     Mon Jul 10 23:41:20 2017
 >> Time spent in FVAc: 0.0 seconds.
--------------------------------------------------------------------------------
 ==> 100% done. Analysis completed.
Currently (P.A, P.b) are in 95 dimensions
Warning: Rank deficient, rank = 72, tol =  1.058366e-10.
```

```
Now in 23 dimensions after restricting
Removed 168 zero rows
Rounding...
Iteration 1: reg=1.0e-04, ellipsoid vol=1.8e+44, longest axis=4.0e+02, shortest axis=5.6e+00, x0 dist to
Iteration 2: reg=1.0e-05, ellipsoid vol=1.6e+06, longest axis=7.0e+01, shortest axis=4.2e-01, x0 dist to
Iteration 3: reg=1.0e-06, ellipsoid vol=8.2e+01, longest axis=3.9e+00, shortest axis=1.0e+00, x0 dist to
```

```
  Converged!
Iteration 4: reg=1.0e-07, ellipsoid vol=1.0e+00, longest axis=1.0e+00, shortest axis=1.0e+00, x0 dist to
Maximum volume ellipsoid found, and the origin is inside the transformed polytope.
Generating samples...
 Done.
   Testing sampleCbModel using tomlab_cplex ...
.
Done testSampleCbModel
__________

Running testChangeCobraSolver

 > Gurobi interface added to MATLAB path.
 > Solver for LP problems has been set to pdco.
 > Solver for QP problems has been set to pdco.
 > Solver pdco not supported for problems of type MILP. Currently used: gurobi
 > Solver pdco not supported for problems of type MIQP. Currently used: gurobi
 > Solver pdco not supported for problems of type NLP. Currently used: matlab
 > The interface to 'mps' from 'changeCobraSolver()' is no longer supported.
Defined solvers are:
    CBT_LP_SOLVER: matlab
    CBT_MILP_SOLVER: gurobi
    CBT_QP_SOLVER: pdco
    CBT_MIQP_SOLVER: gurobi
    CBT_NLP_SOLVER: matlab
.
Done testChangeCobraSolver
__________

Running testOptimizeCbModelNLP

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

1 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

2 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

3 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>
```

```
4 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

5 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

6 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

7 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than
the default value of the step size tolerance and constraints are
satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

8 0.222222

Local minimum possible. Constraints satisfied.

fmincon stopped because the size of the current step is less than

Warning: Your current settings will run a different algorithm ('dual-simplex') in a future
release.

Optimization terminated.
Done.
   Testing testDifferentLPSolvers using mosek ... Done.
   Testing testDifferentLPSolvers using pdco ... Done.
   Testing testDifferentLPSolvers using quadMinos ... Done.
   Testing testDifferentLPSolvers using tomlab_cplex ... Done.
   Testing testDifferentLPSolvers using mosek_linprog ... Done.
   Testing testDifferentLPSolvers using dqqMinos ... Done.

 Summary:
              time           obj        y(rand)        w(rand)              solver
  1       0.007258       0.873922       0.113308       0.091665                glpk
  2       0.015219       0.873922       0.113308       0.091665              gurobi                prim
  3       0.016387       0.873922       0.113308       0.091665              gurobi                  du
  4       0.006096       0.873922       0.113308       0.091665              gurobi
  5       0.003458       0.873922       0.113308       0.091665              gurobi
  6       1.118791       0.873922      -0.113308       0.091665           ibm_cplex
  7       0.283916       0.873922       0.113308       0.091665           ibm_cplex
```

```
  8       0.084194       0.873922       0.113308       0.091665           ibm_cplex                 Prim
  9       0.077555       0.873922       0.113308       0.091665           ibm_cplex                   Du
 10       0.118015       0.873922       0.113308       0.091665           ibm_cplex Barrier (Interior po
 11       0.091582       0.873922       0.113308       0.091665           ibm_cplex
 12       0.044317       0.873922       0.113308       0.091665           ibm_cplex Concurrent Dual, Bar
 13       1.163474       0.873922      -0.113308      47.449667              matlab
 14       0.578750       0.873922       0.113047       0.235520                pdco
 15       0.722514       0.873922       0.113308       0.091665           quadMinos
 16       1.116479       0.873922       0.082753       0.091665            dqqMinos

Testing model with linear constraint matrix that has 2 rows and 2 columns...
   Testing testDifferentLPSolvers using cplex_direct ... Done.
   Testing testDifferentLPSolvers using glpk ... Done.
   Testing testDifferentLPSolvers using gurobi ... Done.
   Testing testDifferentLPSolvers using ibm_cplex ... Done.
   Testing testDifferentLPSolvers using matlab ...
Warning: Your current settings will run a different algorithm ('dual-simplex') in a future
release.

Optimization terminated.
Done.
   Testing testDifferentLPSolvers using mosek ... Done.
   Testing testDifferentLPSolvers using pdco ...
Step lengths too smallDone.
   Testing testDifferentLPSolvers using quadMinos ... Done.
   Testing testDifferentLPSolvers using tomlab_cplex ... Done.
   Testing testDifferentLPSolvers using mosek_linprog ... Done.
   Testing testDifferentLPSolvers using dqqMinos ... Done.

 Summary:
             time            obj        y(rand)        w(rand)              solver
 1       0.039485     600.000000      -0.000000    -200.000000                glpk
 2       0.030732     600.000000      -0.000000    -200.000000              gurobi                 prim
 3       0.003360     600.000000      -0.000000    -200.000000              gurobi                   du
 4       0.003711     600.000000      -0.000000    -200.000000              gurobi
 5       0.003578     600.000000      -0.000000    -200.000000              gurobi
 6       0.468829     600.000000            NaN    -200.000000           ibm_cplex
 7       0.128601     600.000000       0.000000    -200.000000           ibm_cplex
 8       0.042051     600.000000       0.000000    -200.000000           ibm_cplex                 Prim
 9       0.055734     600.000000       0.000000    -200.000000           ibm_cplex                   Du
10       0.058161     600.000000       0.000000    -200.000000           ibm_cplex Barrier (Interior po
11       0.043785     600.000000       0.000000    -200.000000           ibm_cplex
12       0.041826     600.000000       0.000000    -200.000000           ibm_cplex Concurrent Dual, Bar
13       0.276404     600.000000            NaN    -200.000000              matlab
14       0.153336     600.000000       0.000000    -200.000000                pdco
15       0.409377     600.000000       0.000000    -200.000000           quadMinos
16       0.521503     600.000000      -1.000000    -200.000000            dqqMinos

Testing model with linear constraint matrix that has 1 rows and 1 columns...
   Testing testDifferentLPSolvers using cplex_direct ... Done.
   Testing testDifferentLPSolvers using glpk ... Done.
   Testing testDifferentLPSolvers using gurobi ... Done.
   Testing testDifferentLPSolvers using ibm_cplex ... Done.
   Testing testDifferentLPSolvers using matlab ...
Warning: Your current settings will run a different algorithm ('dual-simplex') in a future
release.

Optimization terminated.
Done.
   Testing testDifferentLPSolvers using mosek ... Done.
   Testing testDifferentLPSolvers using pdco ... Done.
   Testing testDifferentLPSolvers using quadMinos ... Done.
   Testing testDifferentLPSolvers using tomlab_cplex ... Done.
   Testing testDifferentLPSolvers using mosek_linprog ... Done.
   Testing testDifferentLPSolvers using dqqMinos ... Done.

 Summary:
             time            obj        y(rand)        w(rand)              solver
```

```
  1       0.034351       1.000000       1.000000      -0.000000               glpk
  2       0.044266       1.000000       1.000000      -0.000000             gurobi                  prim
  3       0.006474       1.000000       1.000000      -0.000000             gurobi                    du
  4       0.002831       1.000000       1.000000      -0.000000             gurobi
  5       0.002151       1.000000       1.000000      -0.000000             gurobi
  6       0.718281       1.000000            NaN       0.000000          ibm_cplex
  7       0.252342       1.000000       1.000000       0.000000          ibm_cplex
  8       0.065038       1.000000       1.000000       0.000000          ibm_cplex                  Prim
  9       0.111645       1.000000       1.000000       0.000000          ibm_cplex                    Du
 10       0.087616       1.000000       1.000000       0.000000          ibm_cplex Barrier (Interior po
 11       0.046074       1.000000       1.000000       0.000000          ibm_cplex
 12       0.081628       1.000000       1.000000       0.000000          ibm_cplex Concurrent Dual, Bar
 13       0.484464       1.000000            NaN       0.000000             matlab
 14       0.204483       1.000000       1.000000       0.000000               pdco
 15       0.478640       1.000000       1.000000      -0.000000          quadMinos
 16       0.378096       1.000000      -1.000000      -0.000000           dqqMinos
.
Done testSolveCobraLP
----------

Running testSolveCobraLPCPLEX
TOMLAB CPLEX is not installed.

 IBM ILOG CPLEX - ILOGsimple - is incompatible with this version of MATLAB, please downgrade or change s

 IBM ILOG CPLEX - ILOGcomplex - is incompatible with this version of MATLAB, please downgrade or change
.
Done testSolveCobraLPCPLEX
----------

Running testSolveCobraMILP
   Running solveCobraLPCPLEX using cplex_direct ... Done.
   Running solveCobraLPCPLEX using ibm_cplex ... Done.
   Running solveCobraLPCPLEX using tomlab_cplex ... Done.
   Running solveCobraLPCPLEX using gurobi6 ... Done.
   Running solveCobraLPCPLEX using glpk ... Done.
.
Done testSolveCobraMILP
----------

Running testSolveCobraMIQP
   Running testSolveCobraQP using gurobi ... Done.
.
Done testSolveCobraMIQP
----------

Running testSolveCobraNLP
   Testing solveCobraNLP using matlab ...
Local minimum found that satisfies the constraints.

Optimization completed because the objective function is non-decreasing in
feasible directions, to within the default value of the optimality tolerance,
and constraints are satisfied to within the default value of the constraint tolerance.

<stopping criteria details>

Done.
.
Done testSolveCobraNLP
----------

Running testSolveCobraQP
   Running testSolveCobraQP using ibm_cplex ... CPXPARAM_QPMethod                                 1
CPXPARAM_Read_APIEncoding                        "*"
CPXPARAM_Output_CloneLog                         1
Number of nonzeros in lower triangle of Q = 1
Using Approximate Minimum Degree ordering
Total time for automatic ordering = 0.01 sec. (0.00 ticks)
```

```
Summary statistics for factor of Q:
  Rows in Factor            = 2
  Integer space required    = 2
  Total non-zeros in factor = 3
  Total FP ops to factor    = 5
Tried aggregator 1 time.
No QP presolve or aggregator reductions.
Presolve time = 0.04 sec. (0.00 ticks)

Using LP solver to compute a starting basis.
Using devex.

Iteration log . . .
Iteration:     1    Objective     =            -0.027778
Done.
   Running testSolveCobraQP using gurobi ... Done.
   Running testSolveCobraQP using qpng ... Done.
.
Done testSolveCobraQP
__________

Running testMinSpan

 > Gurobi interface added to MATLAB path.
 > Solver for LP problems has been set to gurobi.

 > Gurobi interface added to MATLAB path.
 > Solver for MILP problems has been set to gurobi.

 > Gurobi interface added to MATLAB path.
 > Solver for QP problems has been set to gurobi.

 > Gurobi interface added to MATLAB path.
 > Solver for MIQP problems has been set to gurobi.
 > Solver gurobi not supported for problems of type NLP. Currently used: matlab

 > Gurobi interface added to MATLAB path.
.
Done testMinSpan
__________

Running testSubspaces
Calculating the Moore-Penrose Pseudoinverse... finished. toc = 0.0059991
Calculating the Moore-Penrose Pseudoinverse... finished. toc = 0.0021184
Calculating the Moore-Penrose Pseudoinverse... finished. toc = 0.001039
Calculating the Moore-Penrose Pseudoinverse... finished. toc = 0.0010853
Calculating the Moore-Penrose Pseudoinverse... finished. toc = 0.0012903

 ----------------------- Scaling summary report -----------------------

 Name of model:                                 Ecoli_core_model
 Estimation level:                              fine (scltol = 1.00)
 Name of matrix:                                S
 Size of matrix:
        * metabolites:                          72
        * reactions:                            95
 Stoichiometric coefficients:
        * Minimum (absolute non-zero value):    7.09e-02
        * Maximum (absolute non-zero value):    5.98e+01
 Lower bound coefficients:
        * Minimum (absolute non-zero value):    8.39e+00
        * Maximum (absolute non-zero value):    1.00e+03
 Upper bound coefficients:
        * Minimum (absolute non-zero value):    1.00e+03
        * Maximum (absolute non-zero value):    1.00e+03
 Row scaling coefficients:
        * Minimum:                              2.66e-01 (row #: 26)
        * Maximum:                              7.73e+00 (row #: 13)
```

```
Column scaling coefficients:
       * Minimum:                            1.29e-01 (column #: 11)
       * Maximum:                            7.73e+00 (column #: 13)

--------------------------------- Ratios --------------------------------

Ratio of stoichiometric coefficients:         8.44e+02
Order of magnitude diff. (stoich. coeff.):    2

Ratio of lower bounds:                        1.19e+02
Order of magnitude diff. (lower bounds):      2

Ratio of upper bounds:                        1.00e+00
Order of magnitude diff. (upper bounds):      0

Ratio of row scaling coefficients:            2.90e+01
Order of magnitude diff. (row scaling):       1

Ratio of column scaling coefficients:         5.98e+01
Order of magnitude diff. (column scaling):    1

-------------------------------------------------------------------------

-> The model is well scaled. Double precision is recommended.


----------------------- Scaling summary report ------------------------

Name of model:                                Ecoli_core_model
Estimation level:                             fine (scltol = 1.00)
Name of matrix:                               S
Size of matrix:
       * metabolites:                         72
       * reactions:                           95
Stoichiometric coefficients:
       * Minimum (absolute non-zero value):   7.09e-02
       * Maximum (absolute non-zero value):   5.98e+01
Lower bound coefficients:
       * Minimum (absolute non-zero value):   8.39e+00
       * Maximum (absolute non-zero value):   1.00e+03
Upper bound coefficients:
       * Minimum (absolute non-zero value):   1.00e+03
       * Maximum (absolute non-zero value):   1.00e+03
Row scaling coefficients:
       * Minimum:                             2.66e-01 (row #: 26)
       * Maximum:                             7.73e+00 (row #: 13)
Column scaling coefficients:
       * Minimum:                             1.29e-01 (column #: 11)
       * Maximum:                             7.73e+00 (column #: 13)

--------------------------------- Ratios --------------------------------

Ratio of stoichiometric coefficients:         8.44e+02
Order of magnitude diff. (stoich. coeff.):    2

Ratio of lower bounds:                        1.19e+02
Order of magnitude diff. (lower bounds):      2

Ratio of upper bounds:                        1.00e+00
Order of magnitude diff. (upper bounds):      0

Ratio of row scaling coefficients:            2.90e+01
Order of magnitude diff. (row scaling):       1

Ratio of column scaling coefficients:         5.98e+01
Order of magnitude diff. (column scaling):    1

-------------------------------------------------------------------------
```

```
 -> The model is well scaled. Double precision is recommended.


 ------------------------ Scaling summary report ------------------------
```

Warning: > TranslateSBML is installed but is not working properly.

```
 > Try running
   >> TranslateSBML('/Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox/test/models/Ec_iAF1260_f
   in order to debug.
 > Configuring solver environment variables ...
   - [--*-] ILOG_CPLEX_PATH: ~/Applications/IBM/ILOG/CPLEX_Studio1271/cplex/matlab/x86-64_osx
   - [*---] GUROBI_PATH: /Library/gurobi702/mac64/matlab
   - [----] TOMLAB_PATH :  --> set this path manually after installing the solver ( see instructions )
   - [----] MOSEK_PATH :  --> set this path manually after installing the solver ( see instructions )
   Done.
 > Checking available solvers and solver interfaces ... Done.
 > Setting default solvers ... Done.
 > Saving the MATLAB path ... Done.
   - The MATLAB path was saved in the default location.

 > Summary of available solvers and solver interfaces

   Support     LP   MILP     QP   MIQP    NLP
 ----------------------------------------------------------------------
 cplex_direct  full               0      0      0      0      -
 dqqMinos      full               1      -      -      -      -
 glpk          full               1      1      -      -      -
 gurobi        full               1      1      1      1      -
 ibm_cplex     full               1      1      1      -      -
 matlab        full               1      -      -      -      1
 mosek         full               0      0      0      -      -
 pdco          full               1      -      1      -      -
 quadMinos     full               1      -      -      -      1
 tomlab_cplex  full               0      0      0      0      -
 qpng          experimental       -      -      1      -      -
 tomlab_snopt  experimental       -      -      -      -      0
 gurobi_mex    legacy             0      0      0      0      -
 lindo_old     legacy             0      -      -      -      -
 lindo_legacy  legacy             0      -      -      -      -
 lp_solve      legacy             1      -      -      -      -
 opti          legacy             0      0      0      0      0
 ----------------------------------------------------------------------
 Total         -                  8      3      4      1      2

 + Legend: - = not applicable, 0 = solver not compatible or not installed, 1 = solver installed.


 > You can solve LP problems using: 'dqqMinos' - 'glpk' - 'gurobi' - 'ibm_cplex' - 'matlab' - 'pdco' - '
 > You can solve MILP problems using: 'glpk' - 'gurobi' - 'ibm_cplex'
 > You can solve QP problems using: 'gurobi' - 'ibm_cplex' - 'pdco' - 'qpng'
 > You can solve MIQP problems using: 'gurobi'
 > You can solve NLP problems using: 'matlab' - 'quadMinos'

 > Checking for available updates ...
 > There are 438 new commit(s) on <master> and 15 new commit(s) on <develop> [b263ce @ fix_init]
 > You can update The COBRA Toolbox by running updateCobraToolbox() (from within MATLAB).
Elapsed time is 36.024427 seconds.

--------------------------------------------------------------------------------------------------------
MATLAB Version: 9.1.0.441655 (R2016b)
MATLAB License Number: 886910
Operating System: Mac OS X  Version: 10.12.5 Build: 16F73
Java Version: Java 1.7.0_75-b13 with Oracle Corporation Java HotSpot(TM) 64-Bit Server VM mixed mode
--------------------------------------------------------------------------------------------------------
MATLAB                                                Version 9.1         (R2016b)
Simulink                                              Version 8.8         (R2016b)
```

```
Aerospace Blockset                                    Version 3.18        (R2016b)
Aerospace Toolbox                                     Version 2.18        (R2016b)
Antenna Toolbox                                       Version 2.1         (R2016b)
Bioinformatics Toolbox                                Version 4.7         (R2016b)
Communications System Toolbox                         Version 6.3         (R2016b)
Computer Vision System Toolbox                        Version 7.2         (R2016b)
Control System Toolbox                                Version 10.1        (R2016b)
Curve Fitting Toolbox                                 Version 3.5.4       (R2016b)
DSP System Toolbox                                    Version 9.3         (R2016b)
Database Toolbox                                      Version 7.0         (R2016b)
Datafeed Toolbox                                      Version 5.4         (R2016b)
Econometrics Toolbox                                  Version 3.5         (R2016b)
Embedded Coder                                        Version 6.11        (R2016b)
Filter Design HDL Coder                               Version 3.1         (R2016b)
Financial Instruments Toolbox                         Version 2.4         (R2016b)
Financial Toolbox                                     Version 5.8         (R2016b)
Fixed-Point Designer                                  Version 5.3         (R2016b)
Fuzzy Logic Toolbox                                   Version 2.2.24      (R2016b)
Global Optimization Toolbox                           Version 3.4.1       (R2016b)
HDL Coder                                             Version 3.9         (R2016b)
Image Acquisition Toolbox                             Version 5.1         (R2016b)
Image Processing Toolbox                              Version 9.5         (R2016b)
Instrument Control Toolbox                            Version 3.10        (R2016b)
LTE System Toolbox                                    Version 2.3         (R2016b)
MATLAB Coder                                          Version 3.2         (R2016b)
MATLAB Compiler                                       Version 6.3         (R2016b)
MATLAB Compiler SDK                                   Version 6.3         (R2016b)
MATLAB Report Generator                               Version 5.1         (R2016b)
Mapping Toolbox                                       Version 4.4         (R2016b)
Model Predictive Control Toolbox                      Version 5.2.1       (R2016b)
Neural Network Toolbox                                Version 9.1         (R2016b)
Optimization Toolbox                                  Version 7.5         (R2016b)
Parallel Computing Toolbox                            Version 6.9         (R2016b)
Partial Differential Equation Toolbox                 Version 2.3         (R2016b)
Phased Array System Toolbox                           Version 3.3         (R2016b)
RF Toolbox                                            Version 3.1         (R2016b)
Robotics System Toolbox                               Version 1.3         (R2016b)
Robust Control Toolbox                                Version 6.2         (R2016b)
Signal Processing Toolbox                             Version 7.3         (R2016b)
SimBiology                                            Version 5.5         (R2016b)
SimEvents                                             Version 5.1         (R2016b)
SimRF                                                 Version 5.1         (R2016b)
Simscape                                              Version 4.1         (R2016b)
Simscape Driveline                                    Version 2.11        (R2016b)
Simscape Electronics                                  Version 2.10        (R2016b)
Simscape Fluids                                       Version 2.1         (R2016b)
Simscape Multibody                                    Version 4.9         (R2016b)
Simscape Power Systems                                Version 6.6         (R2016b)
Simulink 3D Animation                                 Version 7.6         (R2016b)
Simulink Coder                                        Version 8.11        (R2016b)
Simulink Control Design                               Version 4.4         (R2016b)
Simulink Design Optimization                          Version 3.1         (R2016b)
Simulink Design Verifier                              Version 3.2         (R2016b)
Simulink Desktop Real-Time                            Version 5.3         (R2016b)
Simulink Report Generator                             Version 5.1         (R2016b)
Simulink Test                                         Version 2.1         (R2016b)
Simulink Verification and Validation                  Version 3.12        (R2016b)
Stateflow                                             Version 8.8         (R2016b)
Statistics and Machine Learning Toolbox               Version 11.0        (R2016b)
Symbolic Math Toolbox                                 Version 7.1         (R2016b)
System Identification Toolbox                         Version 9.5         (R2016b)
Trading Toolbox                                       Version 3.1         (R2016b)
Wavelet Toolbox                                       Version 4.17        (R2016b)

 > Default shell       :        /bin/bash
 > Version of shell    :        GNU bash, version 3.2.57(1)-release (x86_64-apple-darwin16)
Copyright (C) 2007 Free Software Foundation, Inc.
 > Architecture        :        MACI64
```

```
 > MATLAB folder       :        /Applications/MATLAB_R2016b.app
 > COBRA Toolbox root  :        /Users/syarra/Dropbox/uni.lu/github/opencobra/cobratoolbox
 > git version         :        git version 2.11.0 (Apple Git-81)
 > curl version        :        curl 7.51.0 (x86_64-apple-darwin16.0)
 > CBT_LP_SOLVER       :        gurobi
 > CBT_MILP_SOLVER     :        gurobi
 > CBT_QP_SOLVER       :        gurobi
 > CBT_MIQP_SOLVER     :        gurobi
 > CBT_NLP_SOLVER      :        matlab
 > GUROBI_PATH         :        /Library/gurobi702/mac64/matlab
 > ILOG_CPLEX_PATH     :        /Users/syarra/Applications/IBM/ILOG/CPLEX_Studio1271/cplex/matlab/x86-64
 > TOMLAB_PATH         :
 > MOSEK_PATH          :

 > --------------------------------- END OF CONFIGURATION REPORT --------------------------------

 >  Please send the report located in
```

```
.
Done testParseBoolean
----------

Running testPrintLabeledData
row1 1 1 1
row2 1 1 1
row3 1 1 1
.
Done testPrintLabeledData
----------

Running testPrintMatrix
0.0000 1.0000 2.0000
2.0000 3.0000 4.0000
4.0000 5.0000 6.0000
7.0000 8.0000 9.0000
0.3518 0.5180 0.2740 0.3828 0.5846 0.0135 0.6654 0.3807 0.8404 0.1602
0.3353 0.2109 0.5995 0.1802 0.7478 0.4814 0.9108 0.8939 0.7814 0.2258
0.0161 0.4768 0.5732 0.3383 0.1188 0.5120 0.0100 0.4329 0.1976 0.3269
0.6866 0.4644 0.8208 0.1708 0.5475 0.1923 0.5274 0.7410 0.6297 0.3118
0.5508 0.4822 0.7254 0.4326 0.5294 0.8981 0.6695 0.8076 0.3909 0.2427
0.4776 0.2129 0.6360 0.5817 0.2610 0.0065 0.2427 0.5685 0.6685 0.5975
0.4511 0.0616 0.0689 0.0090 0.3183 0.1818 0.8479 0.8831 0.7795 0.4761
0.7668 0.9701 0.2949 0.8403 0.7569 0.8081 0.8456 0.6858 0.4574 0.0602
0.6098 0.4628 0.9605 0.9961 0.7630 0.8579 0.3325 0.8421 0.0828 0.7457
0.7837 0.5344 0.9651 0.2406 0.2720 0.8729 0.7323 0.5837 0.6193 0.5776
0.35 0.52 0.27 0.38 0.58 0.01 0.67 0.38 0.84 0.16
0.34 0.21 0.60 0.18 0.75 0.48 0.91 0.89 0.78 0.23
0.02 0.48 0.57 0.34 0.12 0.51 0.01 0.43 0.20 0.33
0.69 0.46 0.82 0.17 0.55 0.19 0.53 0.74 0.63 0.31
0.55 0.48 0.73 0.43 0.53 0.90 0.67 0.81 0.39 0.24
0.48 0.21 0.64 0.58 0.26 0.01 0.24 0.57 0.67 0.60
0.45 0.06 0.07 0.01 0.32 0.18 0.85 0.88 0.78 0.48
0.77 0.97 0.29 0.84 0.76 0.81 0.85 0.69 0.46 0.06
0.61 0.46 0.96 1.00 0.76 0.86 0.33 0.84 0.08 0.75
0.78 0.53 0.97 0.24 0.27 0.87 0.73 0.58 0.62 0.58
data1 =

    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
data2 =

    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
```

```
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
    6.6600    6.6600    6.6600    6.6600    6.6600    6.6600
```

```
.
Done testPrintMatrix
__________

Running testReadMixedData
[id1,id2,id3] = textread('testData_readMixedData.txt', ' %s %s %s', 'delimiter', ',','headerlines',1);
data = [];
[,d1,d2,d3] = textread('testData_readMixedData.txt', ' %f %f %f', 'delimiter', ',','headerlines',1);
data = [d1 d2 d3 ];
.
Done testReadMixedData
__________

Running testReporterMets
.
Done testReporterMets
__________

Running testSelMatrix
.
Done testSelMatrix
__________

Running testShowprogress
Testing show progress, mode = 0:
Testing show progress, mode = 1:
Testing showprogress ...
10%     [....                                  ]20%     [........                                  ]30%
Testing showprogress ...
5%      [..                                    ]10%     [....                                      ]15%
Testing showprogress ...
3%      [.                                     ]6%      [..                                        ]10%

Testing show progress, mode = 2:

Testing showprogress ...
.
Done testShowprogress
__________

Running testSplitString
.
Done testSplitString
__________

Running testTranslateList
.
Done testTranslateList
__________

Running testUnionCell
No match:  1 String1
No match:  1 String2
.
Done testUnionCell
__________

Running testExtremePathways
```

```
P =
   All zero sparse: 4×10

We assume that equalities are present.
```

```
P =
   All zero sparse: 4×10

P =
   (2,1)        1
   (3,1)       -1
   (5,1)        1
   (2,2)        1
   (3,2)       -1
   (4,2)       -1
   (6,2)        1
   (1,3)        2
   (3,3)        1
   (4,3)        1
   (7,3)        2
   (8,3)        1
   (9,3)        1

V =
   All zero sparse: 9×1
```

```
.
Done testExtremePathways
----------

Running testFindExtremePathway
   Testing findExtremePathway using gurobi ... Done
   Testing findExtremePathway using glpk ... Done
.
Done testFindExtremePathway
----------

Running testLrsInputHalfspace
We assume that equalities are present.
We assume that equalities are present.
We assume that equalities are present.
We assume that equalities are present.
.
Done testLrsInputHalfspace
----------

Running testMatrixCoherence
.
Done testMatrixCoherence
----------

Running testMoieties

Atom mappings found for 4 model reactions.
Generating atom transition network for reactions with atom mappings.

 -- Running testMoieties using the solver interface: gurobi6 ... Done
.
Done testMoieties
----------

Running testConvertHypergraph2BipartiteGraph

B1
    -1     0     0     0     1     0
     0     1    -1     0     0     0
     0     0     0     1     0    -1
     1    -1     0     0     0     0
     0     0     1    -1     0     0
     0     0     0     0    -1     1
```

```
A
     6     0     0     1     0     1
     0     0     0     1     1     0
     0     0     0     0     1     1
     1     1     0     0     0     0
     0     1     1     0     0     0
     1     0     1     0     0     0
Warning: NARGCHK will be removed in a future release. Use NARGINCHK or NARGOUTCHK instead.
B1
    -1     0     0
     0     1     0
     0     0     1
     0     0     0
     1    -1    -1


A
     5     0     0     0     1
     0     0     0     0     1
     0     0     0     0     1
     0     0     0     0     0
     1     1     1     0     0
Warning: NARGCHK will be removed in a future release. Use NARGINCHK or NARGOUTCHK instead.
Elapsed time is 0.000240 seconds.
Elapsed time is 0.005143 seconds.
.
Done testConvertHypergraph2BipartiteGraph
----------

Running testXls2Model
New gene Gene1 added to model
New gene Gene2 added to model
New gene Gene3 added to model
BIOMASS_REACTION pyr[c] + 20 atp[c]  ->
pyr_lac pyr[c]  -> lac[c]
EX_lac lac[c]  ->
EX_glc glc[c]  ->
glycolysis glc[c]  -> 2 pyr[c] + 2 atp[c]
oxphos pyr[c]  -> 18 atp[c] + co2[c]
EX_co2 co2[c]  ->
ATPM atp[c]  ->
New gene Gene1 added to model
New gene Gene2 added to model
New gene Gene3 added to model
BIOMASS_REACTION pyr[c] + 20 atp[c]  ->
pyr_lac pyr[c]  -> lac[c]
EX_lac lac[c]  ->
EX_glc glc[c]  ->
glycolysis glc[c]  -> 2 pyr[c] + 2 atp[c]
oxphos pyr[c]  -> 18 atp[c] + co2[c]
EX_co2 co2[c]  ->
ATPM atp[c]  ->
BIOMASS_REACTION pyr[c] + 20 atp[c]  ->
pyr_lac pyr[c]  -> lac[c]
EX_lac lac[c]  ->
EX_glc glc[c]  ->
glycolysis glc[c]  -> 2 pyr[c] + 2 atp[c]
oxphos pyr[c]  -> 18 atp[c] + co2[c]
EX_co2 co2[c]  ->
ATPM atp[c]  ->
BIOMASS_REACTION pyr[c] + 20 atp[c]  ->
pyr_lac pyr[c]  -> lac[c]
EX_lac lac[c]  ->
```

```
EX_glc glc[c]  ->
glycolysis glc[c]  -> 2 pyr[c] + 2 atp[c]
oxphos pyr[c]  -> 18 atp[c] + co2[c]
EX_co2 co2[c]  ->
ATPM atp[c]  ->
.
Done testXls2Model
__________

Running testpFBA
 -- Running testfindBlockedReaction using the solver interface: tomlab_cplex ...  -- Running testfindBlo
*** Test basic pFBA calculations ***


** Optimal solution - minimize flux not associated with gene: glucose
Single gene deletion analysis in progress ...

ans =
                                        Name                                                 Passed    Failed    I
    ____________________________________________________________________________________    ______    ______    _

    'testSparseLP/testSparseLP'                                                              true      false     t
    'testConnectedComponents/TheModelCreatedLooksAsFollows_'                                 true      false     t
    'testCorrespondingRowsCols/testCorrespondingRowsCols'                                    true      false     t
    'testDeletionStudy/testDeletionStudy'                                                    true      false     t
    'testDetectDeadEnds/testDetectDeadEnds'                                                  true      false     t
    'testDynamicFBA/testDynamicFBA'                                                          true      false     t
    'testElementalBalance/testElementalBalance'                                              true      false     t
    'testFBA/testFBA'                                                                        true      false     t
    'testFEA/testFEA'                                                                        true      false     t
    'testFVA/testFVA'                                                                        true      false     t
    'testFastFVA/testFastFVA'                                                                true      false     t
    'testFastGapFill/testFastGapFill'                                                        true      false     t
    'testFindBlockedReaction/testFindBlockedReaction'                                        true      false     t
    'testFitC13Data/testFitC13Data'                                                          true      false     t
    'testGDLS/testGDLS'                                                                      true      false     t
    'testConvertOldStyleModel/testConvertOldStyleModel'                                      true      false     t
    'testInchi/testInchi'                                                                    true      false     t
    'testMDFBA/testMDFBA'                                                                    true      false     t
    'testMOMA/testMOMA'                                                                      true      false     t
    'testMPS/testMPS'                                                                        true      false     t
    'testMassChargeBalance/testMassChargeBalance'                                            true      false     t
    'testFluxSplits/testFluxSplits'                                                          true      false     t
    'testModelBorgifier/testModelBorgifier'                                                  true      false     t
    'testChangeObjective/testChangeObjective'                                                true      false     t
    'testChangeRxnBounds/testChangeRxnBounds'                                                true      false     t
    'testCheckObjective/testCheckObjective'                                                  true      false     t
    'testModelManipulation/testModelManipulation'                                            true      false     t
    'testRemoveDuplicateRxn/testRemoveDuplicateRxn'                                          true      false     t
    'testBuildPairwiseModels/testBuildPairwiseModels'                                        true      false     t
    'testCoupleRxnList2Rxn/testCoupleRxnList2Rxn'                                            true      false     t
    'testCreateMultipleSpeciesModel/testCreateMultipleSpeciesModel'                          true      false     t
    'testSimulationPairwiseInteractions/testSimulationPairwiseInteractions'                  true      false     t
    'testNullspace/testNullspace'                                                            true      false     t
    'testOptKnock/testOptKnock'                                                              true      false     t
    'testOptimizeCbModel/testOptimizeCbModel'                                                true      false     t
    'testOutputNetworkCytoscape/testOutputNetworkCytoscape'                                  true      false     t
    'testPaint4Net/testPaint4Net'                                                            true      false     t
    'testPrintConstraints/testPrintConstraints'                                              false     true      t
    'testPrintFluxVector/testPrintFluxVector'                                                false     true      t
    'testPrintRxnFormula/testPrintRxnFormula'                                                false     true      t
    'testPrintUptakeBound/testPrintUptakeBound'                                              false     true      t
    'testSurfNet/testSurfNet'                                                                false     true      t
    'testGPR2Genes/testGPR2Genes'                                                            true      false     t
    'testGetGeneList/testGetGeneList'                                                        true      false     t
    'testLegalRxnFormula/testLegalRxnFormula'                                                true      false     t
    'testLoadReaction/testLoadReaction'                                                      true      false     t
```

```
    'testMets2str/testMets2str'                                                           true      false     t
    'testModel2data/testModel2data'                                                       true      false     t
    'testNeighborRxn2data/testNeighborRxn2data'                                           true      false     t
    'testRBioNetSaveLoad/testRBioNetSaveLoad'                                             true      false     t
    'testReactionEq/testReactionEq'                                                       true      false     t
    'testSimilarity/testSimilarity'                                                       true      false     t
    'testRank/testRank'                                                                   true      false     t
    'testReconMap/testReconMap'                                                           true      false     t
    'testRobustnessAnalysis/testRobustnessAnalysis'                                       true      false     t
    'testReadSBML/testReadSBML'                                                           true      false     t
    'testWriteSBML/testWriteSBML'                                                         true      false     t
    'testGpSampler/testGpSampler'                                                         true      false     t
    'testSampleCbModel/testSampleCbModel'                                                 true      false     t
    'testChangeCobraSolver/testChangeCobraSolver'                                         true      false     t
    'testOptimizeCbModelNLP/testOptimizeCbModelNLP'                                       true      false     t
    'testSolveCobraLP/testSolveCobraLP'                                                   true      false     t
    'testSolveCobraLPCPLEX/testSolveCobraLPCPLEX'                                         true      false     t
    'testSolveCobraMILP/testSolveCobraMILP'                                               true      false     t
    'testSolveCobraMIQP/testSolveCobraMIQP'                                               true      false     t
    'testSolveCobraNLP/testSolveCobraNLP'                                                 true      false     t
```

```
Warning: Name is nonexistent or not a directory: /Users/syarra/Dropbox/uni.lu/github/
opencobra/cobratoolbox/tutorials/engagingWithTheCommunity
Warning: A value of class "com.mathworks.mde.cmdwin.XCmdWndView" was indexed with no
subscripts specified. Currently the result of this operation is the indexed value itself,
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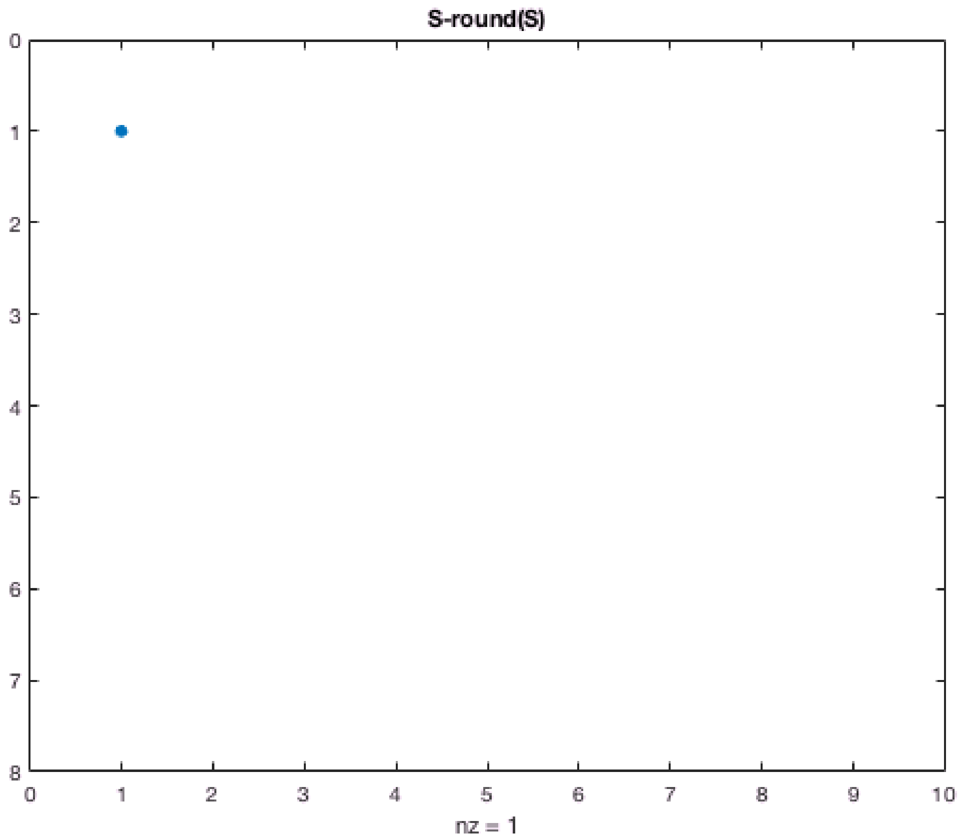

ANTICIPATED RESULTS

The test suite starts by initialising The COBRA Toolbox and thereafter, all of the tests are run. At the end of the test run, a comprehensive summary table is presented in which the respective tests and their test outcome is shown. On a properly configured system that is compatible with the most recent version of The COBRA Toolbox, all tests should pass.

TROUBLESHOOTING

If some third party dependencies are not properly installed, some tests may fail. The test suite, despite some tests failing, is not interrupted. The tests that fail are listed with a false status in the column Passed. The specific test can then be run individually to determine the exact cause of the error. If the error can be fixed, follow the tutorial on how to contribute to The COBRA Toolbox and contribute a fix.