Convert a reconstruction into a flux balance analysis model

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INTRODUCTION

Even with quality control during the reconstruction process, it is not appropriate to assume that any reconstruction can be converted directly into a model and used to make predictions. A model must satisfy certain assumptions before it can be used to make reliable predictions. Depending on the type of model model, these assumptions will be different. Each assumption should be chemically or biologically motivated and expressed in an unambiguous manner and preferably both intuitively and mathematically. Flux balance analysis is a mathematical method widely used for studying genome-scale biochemical network. Here one aims to predict steady-state reaction fluxes, where there is a balance between production and consumption of each molecular species that is not exchanged across the specified boundary of a system. In this situation, one might obtain erroneous predictions if the system boundary is incorrectly specified. If a reconstruction contains one or more supposedly mass balanced reactions, but which are actually not mass balanced, such reactions in a model can lead to inadvertent leakage of a metabolite from the model, in violation of mass balance. Similarly, when generating a model for flux balance analysis, it is important to ensure that the network is flux consistent, that is, each reaction can carry a non-zero steady state flux.

Given a reconstruction with $\hat{m}$ reactants involved in $\hat{n}$ reactions, this tutorial demonstrates a method to identify and extract the largest subset of the reconstruction whose internal reactions are both stoichoimetrically and flux consistent and whose external reactions are flux consistent. This model is then mathematically consistent with the basic requirements for generation of predictions using flux balance analysis. The identification of the component of the reconstruction that does not satisfy the aforementioned modelling conditions is also useful for targeting reconstruction effort towards resolving stoichiometric inconsistency or resolving flux inconsistency. The example used in this tutorial illustrates the process of extracting a model consistent with flux balance analsis, from a ReconX reconstruction.

PROCEDURE

Select reconstruction to convert into a model and enter parameters

Load the ReconX reconstruction, and save the original reconstruction in the workspace, unless it is already loaded into the workspace.

```
clear model
if ~exist('modelOrig','var')
    %select your own model, or use Recon2.0model instead
    if 0
        filename='Recon3.0model';
        directory='~/work/sbgCloud/programReconstruction/projects/recon2models/data/reconXComparisonModels';
        model = loadIdentifiedModel(filename,directory);
```

```
    else
        filename='Recon2.0model.mat';
        if exist('Recon2.0model.mat','file')==2
            model = readCbModel(filename);
        end
    end
    model.csense(1:size(model.S,1),1)='E';
    modelOrig = model;
else
    model=modelOrig;
end
```

Set the level of printing, zero for silent, higher for more output.

```
printLevel=2;
```

Choose the directory to place the results

```
basePath='~/work/sbgCloud/';
resultsPath=[basePath '/programReconstruction/projects/recon2models/results/
reconXs/' model.modelID];
resultsFileName=[resultsPath filesep model.modelID];
```

Create and enter the folder for the results if it does not already exist

```
if ~exist(resultsPath,'dir')
    mkdir(resultsPath)
end
cd(resultsPath)
```

Optionally create a diary to save the output in case it is very long, this makes it easier to search, especially when debugging the process during the early stages.

```
if 0
    diary([resultsFileName '_diary.txt'])
end
```

Overview some of the key properties of the reconstruction

Noting the initial size of the reconstruction is useful for comparisons later with subsets derived according to mathematical specifications.

```
[nMet,nRxn]=size(model.S);
fprintf('%6s\t%6s\n','#mets','#rxns')
```

```
  #mets     #rxns
```

```
fprintf('%6u\t%6u\t%s\n',nMet,nRxn,' totals.')
```

```
  5063      7335     totals.
```

Make sure the stoichiometric matrix is stored in a sparse format as this accelerates computations with large networks

```
model.S=sparse(model.S);
```

Check in case the reconstruction is a model that is already ready for flux balance analysis

There is no need to run this live script any further if the reconstruction already satisfies the conditions necessary for flux balance analysis. That is if all internal reactants and reactions are stoichiometrically consistent, and all reactions are flux consistent, then the reconstruction satisfies the criteria to designate it a model ready for flux balance analysis.

SIntMetBool	m x 1 Boolean of metabolites heuristically though to be involved in mass balanced reactions.
SIntRxnBool	n x 1 Boolean of reactions heuristically though to be mass balanced.
SConsistentMetBool	m x 1 Boolean vector indicating consistent mets
SConsistentRxnBool	n x 1 Boolean vector indicating consistent rxns
fluxConsistentMetBool	m x 1 Boolean vector indicating flux consistent mets
fluxConsistentRxnBool	n x 1 Boolean vector indicating flux consistent rxns

```
if all(isfield(model,{'SIntMetBool','SIntRxnBool','SConsistentMetBool',...

'SConsistentRxnBool','fluxConsistentMetBool','fluxConsistentRxnBool'}))
    if all(model.SIntMetBool & model.SConsistentMetBool)...
            && nnz(model.SIntRxnBool &
model.SConsistentRxnBool)==nnz(model.SIntRxnBool)...
            && all(model.fluxConsistentMetBool)...
            && all(model.fluxConsistentRxnBool)
        fullyStoichAndFluxConsistent=1;
        fprintf('%s\n','Reconstruction is a model that is already ready for
flux balance analysis')
    end
    return
else
    fullyStoichAndFluxConsistent=0;
    fprintf('%s\n','Reconstruction must be tested to check if it is ready
for flux balance analysis')
end
```

```
Reconstruction must be tested to check if it is ready for flux balance analysis
```

Manually remove certain reactions from the reconstruction

Before attempting to algorithmically remove stoichiometrically or flux inconsistent supposed internal reactions from a reconstruction to generate a model, there is an option to review the content of the reconstruction and manually identify reactions for removal. That is, there are two options:

A. Skip manual review of reconstruction content. Move to the next step.

B. Review the content of the reconstruction and omit any reactions that are assumed to be stoichiometrically or flux inconsistent. With respect to stoichiometric inconsistency, such reactions may be obviously mass imbalanced and not satisfy the heuristic conditions for indentification as an exernal reaction. Alternatively, such reactions may be identified by a previous pass through of this tutorial as being of unknown stoichometric consistent (model.unknownSConsistencyRxnBool(j)==1), after the largest stoichiometrically consistent subset of the network has been is identified. This is an iterative process where multiple rounds of identification of the largest stoichiometrically consistent set and manual curation of the remainder that is of unknown stoichiometric consistency is necessary.

```
if strcmp(filename,'Recon3.0model')
    modelOrig=model;
    if 0
        if 1
            %Rename some of the biomass reactions to make them more
obviously exchange
            %reactions
            model.rxns{strcmp(model.rxns,'biomass_reaction')}=
'EX_biomass_reaction';
            model.rxns{strcmp(model.rxns,'biomass_maintenance')}=
'EX_biomass_maintenance';
            model.rxns{strcmp(model.rxns,'biomass_maintenance_noTrTr')}=
'EX_biomass_maintenance_noTrTr';

            %ATP hydrolysis is not imbalanced like all the other demand
reactions so
            %give it a different accronym ATPM = ATP Maintenance
            bool=strcmp('DM_atp_c_',model.rxns);
            model.rxns{bool}='ATPM';
        end
        [model,removeMetBool,removeRxnBool] =
manuallyAdaptRecon3(model,printLevel);
    else
        [model,removeMetBool,removeRxnBool] =
manuallyAdaptRecon3Ines(model,printLevel);
    end
    [nMet0,nRxn0]=size(modelOrig.S);
    [nMet,nRxn]=size(model.S);
    if nMet0==nMet && nRxn0==nRxn && printLevel>0
        fprintf('%s\n','--- Manually removing rows and columns of the
stoichiometric matrix----')
        fprintf('%6s\t%6s\n','#mets','#rxns')
        fprintf('%6u\t%6u\t%s\n',nMet0,nRxn0,' totals.')
        fprintf('%6u\t%6u\t%s\n',nMet0-nMet,nRxn0-nRxn,' manually removed.')
```

```
            fprintf('%6u\t%6u\t%s\n',nMet,nRxn,' remaining.')
      end
  end
```

Remove any trivial rows and columns of the stoichiometric matrix

Remove any zero rows or columns of the stoichiometric matrix

```
modelOrig=model;
model=removeTrivialStoichiometry(model);
[nMet0,nRxn0]=size(modelOrig.S);
[nMet,nRxn]=size(model.S);
if nMet0==nMet && nRxn0==nRxn && printLevel>0
    fprintf('%s\n','---Checking for Remove any trivial rows and columns of
the stoichiometric matrix----')
    fprintf('%6s\t%6s\n','#mets','#rxns')
    fprintf('%6u\t%6u\t%s\n',nMet0,nRxn0,' totals.')
    fprintf('%6u\t%6u\t%s\n',nMet0-nMet,nRxn0-nRxn,' duplicates removed.')
    fprintf('%6u\t%6u\t%s\n',nMet,nRxn,' remaining.')
end
```

```
  ---Checking for Remove any trivial rows and columns of the stoichiometric matrix----
   #mets      #rxns
    5063       7335      totals.
       0          0      duplicates removed.
    5063       7335      remaining.
```

Check for duplicate columns by detecting the columns of the S matrix that are identical upto scalar multiplication.

```
modelOrig=model;
dupDetectMethod='FR';
dupDetectMethod='S';
removeFlag=0;
[modelOut,removedRxnInd, keptRxnInd] =
checkDuplicateRxn(model,dupDetectMethod,removeFlag,printLevel-2);
```

Remove any duplicate reactions, and uniquely involved reactants, from the stoichiometric matrix.

```
if length(removedRxnInd)>0
    irrevFlag=0;
    metFlag=1;
    %set all reactions reversible that are duplicates
    model.lb(removedRxnInd)=-model.ub(removedRxnInd);
    %remove duplicates
    model = removeRxns(model,model.rxns(removedRxnInd),irrevFlag,metFlag);
end
```

Display the statistics on the duplicate reactions,

```
[nMet0,nRxn0]=size(modelOrig.S);
```

```
[nMet,nRxn]=size(model.S);
if nMet0==nMet && nRxn0==nRxn && printLevel>0
    fprintf('%s\n','---Remove any duplicate reactions----')
    [nMet0,nRxn0]=size(modelOrig.S);
    [nMet,nRxn]=size(model.S);
    fprintf('%6s\t%6s\n','#mets','#rxns')
    fprintf('%6u\t%6u\t%s\n',nMet0,nRxn0,' totals.')
    fprintf('%6u\t%6u\t%s\n',nMet0-nMet,nRxn0-nRxn,' duplicates removed.')
    fprintf('%6u\t%6u\t%s\n',nMet,nRxn,' remaining.')
end
```

```
---Remove any duplicate reactions----
 #mets      #rxns
  5063       7335     totals.
     0          0     duplicates removed.
  5063       7335     remaining.
```

Remove any duplicate reactions upto protons

Remove reactions reactions that differ only in the number of protons involved as substrates or products. Also remove exclusively involved reactants.

Save a temporary model for testing, before making any changes.

```
modelH=model;
```

Find the proton indicies in different compartments. A proton, with index i, is asumed to be represented by an abbreviation within model.mets{i} like h[*], where * denotes the compartment symbol.

```
nMetChars=zeros(length(modelH.mets),1);
for m=1:length(modelH.mets)
    nMetChars(m,1)=length(modelH.mets{m});
end
protonMetBool=strncmp(modelH.mets,'h',1) & nMetChars==length('h[*]');
if printLevel>2
    disp(modelH.mets(protonMetBool))
end
```

Zero out the proton stoichiometric coefficients from the temporary model for testing

```
modelH.S(protonMetBool,:)=0;
```

Check for duplicate columns, upto protons, by detecting the columns of the S matrix that are identical upto scalar multiplication.

```
dupDetectMethod='FR';
removeFlag=0;
[modelOut,removedRxnInd, keptRxnInd] =
checkDuplicateRxn(modelH,dupDetectMethod,removeFlag,printLevel-1);
```

```
Checking for reaction duplicates by stoichiometry (up to orientation) ...
      Keep:      BTNt2      btn[e]        <=>       btn[c]
 Duplicate:      BTNt4i     btn[e]         ->       btn[c]
 Warning: EX_h(e) has more than one replicate
      Keep:      EX_h(e)            <=>
 Duplicate:      Htr               <=>
      Keep:      GLCt1r     glc_D[e]       <=>     glc_D[c]
 Duplicate:      GLCt2_2     glc_D[e]       <=>      glc_D[c]
      Keep:      NACUP    nac[e]      ->     nac[c]
 Duplicate:      NACDe    nac[c]      ->     nac[e]
      Keep:      ORNt4m     orn[m] + citr_L[c]       <=>      orn[c] + citr_L[m]
 Duplicate:      r0947     orn[m] + citr_L[c]        ->     orn[c] + citr_L[m]
```

Remove any duplicate reactions from the stoichiometric matrix, but do not remove the protons.

```
if length(removedRxnInd)>0
    irrevFlag=0;
    metFlag=0;%dont remove the protons
    model = removeRxns(model,model.rxns(removedRxnInd),irrevFlag,metFlag);
end
```

Display statistics of the removed reactions

```
if printLevel>0
    [nMet0,nRxn0]=size(modelOrig.S);
    [nMet,nRxn]=size(model.S);
    fprintf('%6s\t%6s\n','#mets','#rxns')
    fprintf('%6u\t%6u\t%s\n',nMet0,nRxn0,' totals.')
    fprintf('%6u\t%6u\t%s\n',nMet0-nMet,nRxn0-nRxn,' duplicate reactions
upto protons removed.')
    fprintf('%6u\t%6u\t%s\n',nMet,nRxn,' remaining.')
end
```

```
 #mets     #rxns
  5063      7335     totals.
     0         5     duplicate reactions upto protons removed.
  5063      7330     remaining.
```

```
%model size
[nMet,nRxn]=size(model.S);
```

Heuristically identify exchange reactions and metabolites exclusively involved in exchange reactions

An external reaction is one that is heuristically identified by a single stoichiometric coefficient in the corresponding column of S, or an (abbreviated) reaction name matching a pattern (e.g. prefix EX_) or an external subsystem assignment. Any remaining reaction is assumed to be an internal reaction. If a reaction is not external then it is denoted an internal reaction. External reactants are exclusively involved in exchange reactions, and internal reactants otherwise. The findSExRxnInd function finds the external reactions in the model which export or import mass from or to the model, e.g. Exchange reactions, Demand reactions, Sink reactions.

```
if ~isfield(model,'SIntMetBool')  ||  ~isfield(model,'SIntRxnBool')
```

```
        model = findSExRxnInd(model,[],printLevel-1);
end
```

EXPECTED RESULTS

In the returned model, model.SIntRxnBool, is a boolean of reactions heuristically though to be mass balanced, while model.SIntMetBool is a boolean of metabolites heuristically though to be involved in mass balanced reactions.

CAUTION

The aforementioned assignments of external and internal reactions and reactants is the result of a heuristic and might result in one or more errors, either due to misspecification or because the names of external reactions and external subsystems often vary between laboratories.

Find the reactions that are flux inconsistent

Ultimately we seek to identify the set of stoichiometrically consistent reactions that are also flux consistent, with no bounds on reaction rates. However, finiding the stoichiometrically consistent subset can be demanding for large models so first we identify the subset of reactions that are flux consistent and focus on them.

```
modelOrig=model;
model.lb(~model.SIntRxnBool)=-1000;
model.ub(~model.SIntRxnBool)= 1000;
if 1
    if ~isfield(model,'fluxConsistentMetBool') ||
~isfield(model,'fluxConsistentRxnBool')
        param.epsilon=1e-4;
        param.modeFlag=0;
        param.method='null_fastcc';
        %param.method='fastcc';

[fluxConsistentMetBool,fluxConsistentRxnBool,fluxInConsistentMetBool,fluxInCo
nsistentRxnBool,model] = findFluxConsistentSubset(model,param,printLevel-1);
    end
    % Remove reactions that are flux inconsistent
    if any(fluxInConsistentRxnBool)
        irrevFlag=0;
        metFlag=1;
        model =
removeRxns(model,model.rxns(fluxInConsistentRxnBool),irrevFlag,metFlag);
        [nMet0,nRxn0]=size(modelOrig.S);
        [nMet,nRxn]=size(model.S);

        if printLevel>0
            fprintf('%s\n','-------')
            fprintf('%6s\t%6s\n','#mets','#rxns')
            fprintf('%6u\t%6u\t%s\n',nMet0,nRxn0,' totals.')
            fprintf('%6u\t%6u\t%s\n',nMet0-nMet,nRxn0-nRxn,' flux
inconsistent reactions removed.')
```

```
            fprintf('%6u\t%6u\t%s\n',nMet,nRxn,' remaining.')
            fprintf('%s\n','-------')
            if printLevel>1
                for n=1:nRxn0
                    if fluxInConsistentRxnBool(n)

fprintf('%15s\t%-100s\n',modelOrig.rxns{n},modelOrig.rxnNames{n})
                    end
                end
            end
        end
        %revise model size
        [nMet,nRxn]=size(model.S);

        %Recompute
        %Heuristically identify exchange reactions and metabolites
exclusively involved in exchange reactions
        %finds the reactions in the model which export/import from the model
        %boundary i.e. mass unbalanced reactions
        %e.g. Exchange reactions
        %      Demand reactions
        %      Sink reactions

        model = findSExRxnInd(model,[],0);
        if printLevel>0
            fprintf('%s\n','------end------')
        end
    end
end
```

```
-------
 #mets     #rxns
  5063      7330     totals.
  2123      2140     flux inconsistent reactions removed.
  2940      5190     remaining.
-------
1a_24_25VITD2Hm    1-alpha-Vitamin D-24,25-hydroxylase (D2)
1a_24_25VITD3Hm    1-alpha-Vitamin D-24,25-hydroxylase (D3)
   1a_25VITD2Hm    1-alpha,24R,25-Vitamin D-hydroxylase (D2)
   1a_25VITD3Hm    1-alpha,24R,25-Vitamin D-hydroxylase (D3)
   24_25DHVITD2t   24,25-Dihydroxyvitamin D2 transport from cytoplasm
  24_25DHVITD2tm   24,25-Dihydroxyvitamin D2 transport from mitochondria
   24_25VITD2Hm    24R-Vitamin D-25-hydroxylase (D2)
       25HVITD2t   25-hydroxyvitamin D2 transport from cytoplasm
  25HVITD2tin_m    25-hydroxyvitamin D2 transport in mitochondria
      25VITD2Hm    1-alpha-Vitamin D-25-hydroxylase (D2)
      25VITD3Hm    1-alpha-Vitamin D-25-hydroxylase (D3)
      34DHPHAMT    3,4-Dihydroxyphenylacetate:amet O-methyltransferase
      3HPCOAHYD    3-hydroxyisobutyryl-Coenzyme A hydrolase
         3HPPD     3-hydroxypropionate dehydrogenase
      3HXKYNDCL    3-Hydroxykynurenamine decarboxy-lyase
     3HXKYNOXDA    3-Hydroxykynurenamine:oxygen oxidoreductase(deaminating)(flavin-containing)
      3M4HDXPAC    3-Methoxy-4-hydroxyphenylacetaldehyde:NAD+ oxidoreductase
      3MOXTYROX    3-Methoxytyramine:oxygen oxidoreductase (deaminating)
        3NTD7l     3'-nucleotidase (AMP), lysosome
      42A12BOOX    4-(2-Aminoethyl)-1,2-benzenediol:oxygen oxidoreductase(deaminating)(flavin-containing)
```

```
4MPTNLtr          4-methylpentanal transport (ER)
5HOXINDACTOXm     5-Hydroxyindoleacetaldehyde:NAD+ oxidoreductase (mito)
5HOXINOXDA        5-Hydroxytryptamine:oxygen oxidoreductase(deaminating)(flavin-containing)
5HTRPDOX          5-Hydroxy-L-tryptophan:oxygen 2,3-dioxygenase (indole-decyclizing)
5HXKYNDCL         5-Hydroxykynurenamine decarboxy-lyase
5HXKYNOXDA        5-Hydroxykynurenamine:oxygen oxidoreductase(deaminating)(flavin-containing)
A_MANASE          alpha-mannosidase
A4GALTc           Lactosylceramide 4-alpha-galactosyltransferase
A4GNT1g           alpha 1,4-N-acetylglucosaminyltransferase, Golgi apparatus
ABUTt2rL          4-aminobutyrate reversible transport in via proton symport (lysosome)
ACACT8p           acetyl-CoA acyltransferase (hexadecanoyl-CoA), peroxisomal
ACACT9p           acetyl-CoA acyltransferase (tetracosanoyl-CoA), peroxisomal
ACGSm             N-acteylglutamate synthase, mitochondrial
ACOATA            Acetyl-CoA ACP transacylase
ACODA             acetylornithine deacetylase
ACSOMT            S-Adenosyl-L-methionine:N-acetylserotonin O-methyltransferase
ACSRTNMT          S-Adenosyl-L-homocysteine:N-acetylserotonin O-methyltransferase
ACtg              acetate transport, Golgi apparatus
ADEtl             adenine facilated transport from lysosome
ADHAPtx           intracellular transport (peroxisome)
ADNtl             adenosine facilated transport from lysosome
ADPGLC            ADPglucose diphosphatase
ADPMAN            ADPmannose diphosphatase
ADPRDPm           ADPribose diphosphatase (mitochondrial)
ADSELK            adenylyl-selenate kinase
AGLPC             alkyl acylglycerol phosphocholine transferase
AGLPED            alkyl acyl glycerophosphoethanolamine desaturase
AGLPET            alkyl acylglycerol phosphoethanolamine transferase
AGLPH             alkyl glycerol phosphate hydrolase
AGLPR             alkyl glycerol phosphate reductase
AGLPT             alkyl glycerol phosphate acyltransferase
AGPex             alkyl glycerol phosphate transport
AGPRim            N-acetyl-g-glutamyl-phosphate reductase, irreversible, mitochondrial
AGPSx             alkylglycerone phosphate synthase
AHANDROSTANGLCte   glucuronidated compound transport
AHANDROSTANGLCtr   glucuronidated compound transport
AHCYStn           S-adenosyl-L-homocysteine nuclear transport
ALAt2rL           L-alanine reversible transport via proton symport (lysosome)
ALDD20x           aldehyde dehydrogenase (indole-3-acetaldehyde, NAD)
ALDD20xm          aldehyde dehydrogenase (indole-3-acetaldehyde, NAD), mitochondrial
ALKP              alkaline phosphatase
ALOX12            Arachidonate 12-lipoxygenase
ALOX12R           Arachidonate 12-lipoxygenase R
ALOX15            Arachidonate 15-lipoxygenase
AMACR2r           alpha-methylacyl-CoA racemase (reductase)
AMACRr            alpha-methylacyl-CoA racemase
AMETtn            S-adenosyl-L-methionine nuclear transport
AMPtr             AMP transporter, endoplasmic reticulum
AP4AH1            Ap4A hydrolase, asymmetrically
APRTO2            N-acetylputrescine: oxygen oxireductase (deaminating)
AQCOBALt          Aquacob(III)alamin uptake
ARTFR11           R group artificial flux
ARTFR12           R group artificial flux (C16:1)
ARTFR13           R group artificial flux
ARTFR202          R group artificial flux (C18:3, n-3)
ARTFR203          R group artificial flux
ARTFR204          R group artificial flux
ARTFR205          R group artificial flux
ARTFR206          R group artificial flux
ARTFR207          R group artificial flux
ARTFR208          R group artificial flux
ARTFR209          R group artificial flux
ARTFR210          R group artificial flux
ARTFR211          R group artificial flux
```

```
   ARTFR212     R group artificial flux
   ARTFR213     R group artificial flux
    ARTFR31     R group artificial flux
    ARTFR32     R group artificial flux
    ARTFR33     R group artificial flux
    ARTFR34     R group artificial flux
    ARTFR41     R group artificial flux
    ARTFR42     R group artificial flux
    ARTFR43     R group artificial flux
    ARTFR44     R group artificial flux
    ARTFR45     R group artificial flux
    ARTFR46     R group artificial flux
    ARTFR51     R group artificial flux
    ARTFR52     R group artificial flux
    ARTFR53     R group artificial flux
    ARTFR54     R group artificial flux
    ARTFR55     R group artificial flux
    ARTFR56     R group artificial flux
    ARTFR57     R group artificial flux
    ARTFR61     R group artificial flux
    ARTPLM1     R group to palmitate conversion
   ARTPLM1m     R group to palmitate conversion
    ARTPLM2     R group to palmitate conversion
   ARTPLM2m     R group to palmitate conversion
    ARTPLM3     R group to palmitate conversion
   ARTPLM3m     R group to palmitate conversion
BAMPPALDOXm     beta-Aminopropion aldehyde:NAD+ oxidoreductase (m)
      BBHOX     4-Trimethylammoniobutanoate,2-oxoglutarate:oxygen oxidoreductase (3-hydroxylating)
   BDG2HCGHD    beta-D-Glucosyl-2-coumarinate glucohydrolase
     BTNt2m     Biotin reversible transport via proton symport, mitochondria
        BZt     benzoate transport (diffusion)
       BZtr     Benzene transporter, endoplasmic reticulum
C2M26DCOAHLm    cis-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA hydro-lyase (m)
C2M26DCOAHLx    cis-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA hydro-lyase (x)
      CBL2OR    NADH:cob(III)alamine oxidoreductase
      CBL2tm    Cob(II)alamine transport, mitochondrial
     CBLATm     cob(I)alamin adenosyltransferase, mitochondrial
     CBPPer     Carbamoyl phosphate phosphotransferase, endoplasmic reticulum
     CBPter     carbamoyl phosphate transport, endoplasmic reticulum
       CBR1     Carbonyl reductase [NADPH] 1
     CCA_D3t    Calcitroic acid transport from cytosol
    CCA_D3tm    Calcitroic acid transport from mitochondria
  CHSTEROLtg    cholesterol efflux (ATP depedent), golgi
     CHTNASE    chitinase
   CITMCOAHm    L-Citramalyl-CoA hydro-lyase, mitochondrial
   CITMCOALm    L-Citramalyl-CoA pyruvate-lyase
   CLPNDCPT1    carnitine O-palmitoyltransferase
   CLPNDCPT2    carnitine transferase
   CLPNDCRNt    transport into the mitochondria (carnitine)
      CO2tg     CO2 Golgi transport
      CO2tn     CO2 nuclear transport via diffusion
   COKECBESr    Carboxylesterase (cocaine) (er)
    CPCTDTX     choline-phosphate cytidylyltransferase
    CRTNsyn     Creatinine synthase
    CRTSLtr     cortisol intracellular transport
   CRTSTRNtr    corticosterone intracellular transport
    CSPG_At     chondroitin sulfate A transport, golgi to extracellular
    CSPG_Bt     chondroitin sulfate B transport, golgi to extracellular
    CSPG_Ct     chondroitin sulfate C transport, golgi to extracellular
    CSPG_Dt     chondroitin sulfate D transport, golgi to extracellular
    CSPG_Et     chondroitin sulfate E transport, golgi to extracellular
     CYOOm2     cytochrome c oxidase, mitochondrial Complex IV
    CYSLYSL     L-Cystine Lyseine-lyase (deaminating)
     CYSTAm     cysteine transaminase (mitochondrial)
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      CYTDtl     Cytidine facilated transport from lysosome
    DALAt2rL     D-alanine transport via proton symport (lysosome)
      DARGOp     D-arginine oxidase, perixosomal
      DASCBH     L-Dehydroascorbate lactonohydrolase
        DCIm     dodecenoyl-Coenzyme A delta isomerase
       DCK1m     Deoxycytidine kinase, mitochondrial (ATP)
   DEDOLP1_L     dehydrodolichol diphosphate phosphatase (liver)
   DEDOLP1_U     dehydrodolichol diphosphate phosphatase (uterus)
   DEDOLP2_L     dehydrodolichol phosphate phosphatase (liver)
   DEDOLP2_U     dehydrodolichol phosphate phosphatase (uterus)
    DEDOLR_L     dehydrodolichol reductase (liver)
    DEDOLR_U     dehydrodolichol reductase (uterus)
       DHAPA     dihydroxyacetone phosphate acyltransferase
      DHAPAx     dihydroxyacetone phosphate acyltransferase
      DHEAStr     dheas intracellular transport
     D_LACtm     D-lactate transport, mitochondrial
DM_m_em_3gacpail_prot_hs_r_    DM m(em)3gacpail prot hs(r)
  DMHPTCRNCPT1    carnitine fatty-acyl transferase
      DNAMTn     DNA (cytosine-5-)-methyltransferase, nucleus
     DNAMTSEn    DNA (cytosine-5-)-methyltransferase, nucleus
     DOGULND1    2,3-dioxo-L-gulonate decarboxylase (L-lyxonate-forming)
     DOGULND2    2,3-dioxo-L-gulonate decarboxylase (L-xylonate-forming)
     DOGULNO1    2,3-dioxo-L-gulonate:hydrogen peroxide oxireductase
     DOGULNO2    2,3-dioxo-L-gulonate:hydrogen peroxide oxireductase
      DOPAMT     Dopamine:amet O-methyltransferase
      DORNOp     D-ornithine oxidase, perixosomal
      DPROOp     D-proline oxidase, perixosomal
      ECGISOr    Ecgonine isomerase (ER)
      ECOAH1x    3-hydroxyacyl-CoA dehydratase (3-hydroxybutanoyl-CoA) (perioxisome)
      EGMESTr    ecgonine methyl esterase (ER)
       EHGLAT    L-erythro-4-Hydroxyglutamate:2-oxoglutarate aminotransferase
       ENGASE    endo-beta-N-acetylglucosaminidase
      ENGASE2    endo-beta-N-acetylglucosaminidase
      ENMAN1g    Endomannosidase (glc1man-producing), Golgi apparatus
      ENMAN2g    Endomannosidase (glc2man-producing), Golgi apparatus
      ENMAN3g    Endomannosidase (glc3man-producing), Golgi apparatus
      ENMAN4g    Endomannosidase (m6masnC-producing), Golgi apparatus
      ENMAN5g    Endomannosidase (m6masnB2-producing), Golgi apparatus
      ENMAN6g    Endomannosidase (m5masnB1-producing), Golgi apparatus
       EPCTX     ethanolamine-phosphate cytidylyltransferase
  ESTRIOLGLCte   glucuronidated compound transport
  ESTRIOLGLCtr   glucuronidated compound transport
     ESTRIOLtr   estriol intracellular transport
EX_2425dhvitd2(e)    24R,25-Dihyoxyvitamin D2 exchange
 EX_25hvitd2(e)    25-Hydroxyvitamin D2 exchange
EX_ahandrostanglc(e)    Etiocholan-3alpha-ol-17-one 3-glucuronide exchange
  EX_aqcobal(e)    Aquacob(III)alamin exchange
       EX_bz(e)    Benzoate exchange
      EX_ca2(e)    Calcium exchange
   EX_cca_d3(e)    Calcitroic acid (D3) exchange
EX_estriolglc(e)    16-Glucuronide-estriol exchange
    EX_hom_L(e)    L-Homoserine exchange
        EX_k(e)    K+ exchange
  EX_lipoate(e)    Lipoate exchange
      EX_na1(e)    exchange reaction for Sodium
EX_nifedipine(e)     nifedipine exchange
   EX_peplys(e)    Peptidyl-L-lysine exchange
     EX_phyQ(e)    Phylloquinone exchange
    EX_pro_D(e)    D-Proline exchange
      EX_sel(e)    Selenate exchange
    EX_ser_D(e)    D-Serine exchange
    EX_vitd2(e)    Vitamin D2 exchange
EX_whtststerone(e)    w hydroxy testosterone exchange
EX_xolest_hs(e)    cholesterol ester exchange
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      FA120ACPH    fatty-acyl-ACP hydrolase
      FA140ACPH    fatty-acyl-ACP hydrolase
      FA141ACPH    fatty-acyl-ACP hydrolase
      FA160ACPH    fatty-acyl-ACP hydrolase
      FA161ACPH    fatty-acyl-ACP hydrolase
      FA180ACPH    fatty-acyl-ACP hydrolase
      FA181ACPH    fatty-acyl-ACP hydrolase
     FA1821ACPH    fatty-acyl-ACP hydrolase
     FA1822ACPH    fatty-acyl-ACP hydrolase
      FA182ACPH    fatty-acyl-ACP hydrolase
         FORtrn    Formate transport, nuclear
           FRTT    farnesyltranstransferase
             FT    farnesyltranstransferase (trans,trans,cis-geranylgeranyl diphosphate-generating)
 G1M6MASNB1terg    g1m6masnB1 endoplasmic reticulum to Golgi transport
  G1M7MASNBterg    g1m7masnC endoplasmic reticulum to Golgi transport
  G1M7MASNCterg    g1m7masnC endoplasmic reticulum to Golgi transport
   G1M8MASNterg    g1m8masn transport from endoplasmic reticulum to Golgi apparatus
          G1PTT    glucose-1-phosphate thymidylyltransferase
   G2M8MASNterg    g2m8masn transport from endoplasmic reticulum to Golgi apparatus
   G3M8MASNterg    g3m8masn transport from endoplasmic reticulum to Golgi apparatus
     GALNACT1g     UDPGal-chondroitin acetylgalactosaminyltransferase I, Golgi
     GALNACT2g     uridine diphosphoacetylgalactosamine-chondroitin acetylgalactosaminyltransferase II, Go
     GALNACT3g     uridine diphosphoacetylgalactosamine-chondroitin acetylgalactosaminyltransferase II, Go
     GALNACT4g     uridine diphosphoacetylgalactosamine-chondroitin acetylgalactosaminyltransferase II, Go
     GALNACT5g     uridine diphosphoacetylgalactosamine-chondroitin acetylgalactosaminyltransferase II, Go
          GALOR    D-Galactose:NADP+ 1-oxidoreductase
         GALT2g    UDP-D-galactose:galactosylxylose galactosyltransferase, Golgi apparatus
          GALTg    UDP-D-galactose:D-xylose galactosyltransferase, Golgi apparatus
           GAO1    Ganglioside O-acetylation
           GAO2    Ganglioside O-acetylation
        GCALDDm    Glycolaldehyde dehydrogenase, mitochondrial
          GGT_L    geranylgeranyltransferase (liver)
          GGT_U    geranylgeranyltransferase (uterus)
          GHMT3    glycine hydroxymethyltransferase
         GHMT3m    glycine hydroxymethyltransferase, mitochondrial
           GK1m    guanylate kinase (GMP:ATP), mitochondrial
          GLACO    D-Glucuronolactone:NAD+ oxidoreductase
         GLACOm    D-Glucuronolactone:NAD+ oxidoreductase, mitochondrial
        GLCAE1g    chondroitin-glucuronate 5-epimerase
        GLCAE2g    heparosan-N-sulfate-glucuronate 5-epimerase
        GLCAT2g    chondroitin glucuronyltransferase II, Golgi apparatus
        GLCAT3g    chondroitin glucuronyltransferase II, Golgi apparatus
        GLCAT4g    chondroitin glucuronyltransferase II, Golgi apparatus
        GLCAT5g    chondroitin glucuronyltransferase II, Golgi apparatus
        GLCAT6g    heparan glucuronyltransferase II
        GLCAT7g    heparan glucuronyltransferase II
        GLCAT8g    heparan glucuronyltransferase II
        GLCAT9g    heparan glucuronyltransferase II
         GLCATg    UDP-D-glucuronate:galactosylgalactosylxylose glucuronosyltransferase, Golgi apparatus
     GLCNACDASg    GlcNAc N-deacetylase / N-sulfotransferase
      GLCNACT1g    alpha-N-acetylglucosaminyltransferase I, Golgi apparatus
      GLCNACT2g    alpha-N-acetylglucosaminyltransferase II
      GLCNACT3g    alpha-N-acetylglucosaminyltransferase II
      GLCNACT4g    alpha-N-acetylglucosaminyltransferase II
      GLCNACT5g    alpha-N-acetylglucosaminyltransferase II
       GLYCLTDym    Glycolate dehydrogenase (NADP), mitochondrial
         GLYOXm    hydroxyacylglutathione hydrolase, mitochondrial
        GLYt2rL    glycine reversible transport via proton symport (lysosome)
       GPAMm_hs    glycerol-3-phosphate acyltransferase
         GSNKm     guanosine kinase (mitochondrial)
          GSNtl    guanosine facilated transport from lysosome
          GSNtm    guanosine facilated transport in mitochondria
          GTPCI    GTP cyclohydrolase I
         GTPCIn    GTP cyclohydrolase I, nuclear
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     GTPtn       GTP diffusion in nucleus
    H2CO3Dm      carboxylic acid dissociation
   H8MTer_L      H8 mannosyltransferase, endoplasmic reticulum
   H8MTer_U      H8 mannosyltransferase, endoplasmic reticulum
     HACD1x      3-hydroxyacyl-CoA dehydrogenase (acetoacetyl-CoA) (peroxisome)
   HEXCCPT1      carnitine O-palmitoyltransferase
   HEXCCPT2      carnitine transferase
   HEXCCRNt      transport into the mitochondria (carnitine)
    HISTASE      Histaminase
   HMGCOARr      Hydroxymethylglutaryl CoA reductase (ir)
   HPYRDCm       hydroxypyruvate decarboxylase, mitochondria
   HSD3B13       3 beta-hydroxysteroid dehydrogenase/delta 5-->4-isomerase type I
     HSPGt       heparan sulfate transport, golgi to extracellular
    HXANtl       hypoxanthine facilated transport from lysosome
    IMACTD       Imidazole acetaldeyde dehydrogenase
   IMACTD_m      Imidazole acetaldeyde dehydrogenase (mito)
     INSKm       insosine kinase, mitochondrial
     INStl       inosine facilated transport from lysosome
     INStm       inosine facilated transport in mitochondria
     IPDPtr      Isopentenyl diphosphate transport (ER)
      Kt3g       potassium transport  via proton antiport
    LACZly       b-galactosidase,lysosomal
   LCADi_Dm      lactaldehyde dehydrogenase, mitochondrial
    LCADim       lactaldehyde dehydrogenase, mitochondrial
    LCTStl       lactose transport from cytosol to lysosome (via autophagocytosis)
   LCYSTATm      L-Cysteate:2-oxoglutarate aminotransferase, mitochondrial
    LDH_Lm       L-lactate dehydrogenase
  LEUKTRB4tr     leukotriene intracellular transport
   LGNCCPT1      carnitine O-palmitoyltransferase
   LGNCCPT2      transport into the mitochondria (carnitine)
   LGNCCRNt      transport into the mitochondria (carnitine)
    LIPOti       Lipoate transport via sodium symport
   L_LACtcm      L-lactate transport via diffusion (cytosol to mitochondria)
   LNS14DM       cytochrome P450 lanosterol 14-alpha-demethylase (NADP)
       LS3       Lumisterol 3 formation
     LTDCL       L-Tryptophan decarboxy-lyase
   LYSMTF1n      histone-lysine N-methyltransferase, nuclear
   LYSMTF2n      histone-lysine N-methyltransferase, nuclear
   LYSMTF3n      histone-lysine N-methyltransferase, nuclear
   M4ATAer       M4A transamidase, endoplasmic reticulum
   M4BET2er      M4B phosphoethanolaminyl transferase, endoplasmic reticulum
    MALTly       alpha-glucosidase, lysosomal
  MAN1_6B1er     mannosidase I, endoplasmic reticulum (g1m6masnB1-producing)
   MAN1_7Ber     mannosidase I, endoplasmic reticulum (g1m7masnB-producing)
  MAN2_6B1er     mannosidase II, endoplasmic reticulum (g1m6masnB1-producing)
   MAN2_7Cer     mannosidase II, endoplasmic reticulum (g1m7masnC-producing)
    MAOLNOR      monoamine oxidase (L-Normetanephrine)
      MCDp       Malonyl-CoA Decarboxylase peroxisomal
     MCOATA      Malonyl-CoA-ACP transacylase
     MCOATAm     Malonyl-CoA-ACP transacylase, mitochondrial
 MELATN23DOX     Melatonin:oxygen 2,3-dioxygenase (indole-decyclizing)
     MEOHtr      Methanol transporter, endoplasmic reticulum
   MESCOALm      Mesaconyl-CoA pyruvate-lyase
    MGACONm      methylglutaconase, mitochondrial
   MI13456PK     inositol-1,3,4,5,6-pentakisphosphate 2-kinase
  MI13456Ptn     inositol 1,3,4,5,6-pentakisphosphate nuclear transport (diffusion)
   MI1345PKn     inositol-1,3,4,5-triphosphate 6-kinase, nucleus
   MI1346PKn     inositol-1,3,4,6-tetrakisphosphate 5-kinase, nucleus
   MI1346Ptn     1D-myo-Inositol 1,3,4,6-tetrakisphosphate nuclear transport (diffusion)
    MI134PK      inositol-1,3,4-trisphosphate 6-kinase
   MI1456PKn     inositol-1,4,5,6- tetrakisphosphate 3-kinase, nucleus
   MI145P6Kn     inositol-1,4,5-triphosphate 6-kinase, nucleus
   MI145PKn      inositol-1,4,5-trisphosphate 3-kinase, nucleus
   MI3456PK      inositol-3,4,5,6-tetrakisphosphate 1-kinase
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     MICITDr      2-methylisocitrate dehydratase
    MINOHPtn      inositol hexakisphosphate nuclear transport (diffusion)
      MLTG1       Maltodextrin glucosidase (maltotriose)
     MLTG1ly      Maltodextrin glucosidase (maltotriose), lysosome
       MMCD       Methylmalonyl-CoA decarboxylase
      MMCDp       Methylmalonyl-CoA decarboxylase, peroxisomal
      NABTNO      N4-Acetylaminobutanal:NAD+ oxidoreductase
     NABTNOm      N4-Acetylaminobutanal:NAD+ oxidoreductase (m)
       NADK       NAD kinase
      NADPN       NADP nucleosidase
     NAt3_1g      sodium proton antiporter (H:NA is 1:1)
    NDPK10m       nucleoside-diphosphate kinase (ATP:dIDP), mitochondrial
     NDPK2m       nucleoside-diphosphate kinase (ATP:UDP), mitochondrial
     NDPK9m       nucleoside-diphosphate kinase (ATP:IDP), mitochondrial
  NIFEDIPINEte    xenobiotic transport
     NMNATm       nicotinamide-nucleotide adenylyltransferase, mitochondrial
    NMPTRCOX      N-Methylputrescine:oxygen oxidoreductase (deaminating)
      NNATm       nicotinate-nucleotide adenylyltransferase, mitochondrial
    NRVNCCPT1     carnitine O-palmitoyltransferase
    NRVNCCPT2     carnitine transferase
    NRVNCCRNt     transport into the mitochondria (carnitine)
      NTD12       5'-nucleotidase (dIMP)
      NTD2l       5'-nucleotidase (UMP), lysosome
      NTD2m       5'-nucleotidase (UMP), mitochondrial
      NTD3l       5'-nucleotidase (dCMP), lysosomal
      NTD4l       5'-nucleotidase (CMP), lysosome
      NTD5l       5'-nucleotidase (dTMP), lysosomal
      NTD6l       5'-nucleotidase (dAMP), lysosome
      NTD7l       5'-nucleotidase (AMP), lysosome
      NTD8l       5'-nucleotidase (dGMP), lysosomal
      NTD9l       5'-nucleotidase (GMP), lysosome
   NTMELYStner    protein trimethyl lysine transport (nucleus to ER)
     NTPP10       Nucleoside triphosphate pyrophosphorylase (ditp)
     NTPP11       Nucleoside triphosphate pyrophosphorylase (xtp)
      NTPP9       Nucleoside triphosphate pyrophosphorylase (itp)
     P4503A4      cytochrome P450 3A4
    P4503A43r     cytochrome p450 P450 3A43
     P4504B1r     cytochrome P450 4B1
   P4504F121r     cytochrome p450 4F12/4F2
   P4504F122r     cytochrome p450 4F12/4F2
    P4504F81r     cytochrome p450 4F8
    P450LTB4r     cytochrome p450 leukotriene B4
     PCLYSOX      Procollagen-lysine 1, 2-oxoglutarate 5-dioxygenase
      PDE1g       3',5'-cyclic-nucleotide phosphodiesterase,Golgi
      PDE4g       3',5'-cyclic-nucleotide phosphodiesterase, Golgi
     PE_HStg      phosphatidylethanolamine scramblase
   PECGONCOATr    Pseudoecgonine CoA transferase (ER)
     PEPLYStn     peptide (lysine) nuclear transport via diffusion
      PGDIr       Prostaglandin-H2 D-isomerase [Precursor]
      PGESr       Prostaglandin E synthase
     PGLYCP       Phosphoglycolate phosphatase
     PHETA1       phenylalanine transaminase
     PHETA1m      phenylalanine transaminase (m)
    PI45PLCn      phosphatidylinositol 4,5-bisphosphate phospholipase C, nucleus
     PI4P3Ker     phosphatidylinositol 4-phosphate 3-kinase, endoplasmic reticulum
     PI5P3Ker     phosphatidylinositol-5-phosphate 3-kinase, endoplasmic reticulum
      PIt2m       phosphate transporter, mitochondrial
       PLA2       phospholipase A2
     PLYSPSer     protein lysine peptidase (endoplasmic reticulum)
   PMI12346PH     5-diphosphoinositol-1,2,3,4,6-pentakisphosphate diphosphohydrolase
   PMI12346PHn    5-diphosphoinositol-1,2,3,4,6-pentakisphosphate diphosphohydrolase, nuclear
    PMI1346PH     diphosphoinositol-1,3,4,6-tetrakisphosphate diphosphohydrolase
    PMI1346PHn    diphosphoinositol-1,3,4,6-tetrakisphosphate diphosphohydrolase, nucleus
      PNTKm       pantothenate kinase (mitochondrial)
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          PPA2    inorganic triphosphatase
         PPA2m    inorganic triphosphatase, mitochondrial
   PPMI12346Ptn    5-diphosphatidylinositol pentakisphosphate nuclear transport (diffusion)
    PPMI1346Ptn    diphosphatidylinositol tetrakisphosphate nuclear transport (diffusion)
          PPOR    Phenylpyruvate:oxygen oxidoreductase (hydroxylating,decarboxylating)
        PPPItn    Inorganic triphosphate transport through nuclear pore
    PROAKGOX1r    L-Proline,2-oxoglutarate:oxygen oxidoreductase (4-hydroxylating) (ER)
       PRODt2r    D-proline reversible transport via proton symport
      PRODt2rL    D-proline reversible transport via proton symport (lysosome)
       PROt2rL    L-proline reversible transport via proton symport (lysosome)
         PROtm    L-proline transport, mitochondrial
   PRPNCOAHYDx    Propenoyl-CoA hydrolase (x)
       PS_HSter    phosphatidylserine scramblase
       PS_HStg    phosphatidylserine scramblase
         PTE2x    peroxisomal acyl-CoA thioesterase
         PTE5x    peroxisomal acyl-CoA thioesterase
         PTHPS    6-pyruvoyltetrahydropterin synthase
        PTHPSn    6-pyruvoyltetrahydropterin synthase, nuclear
       PTRCAT1    Putrescine acetyltransferase
      PYAM5Ptm    Pyridoxamine 5'-phosphate transport via diffusion, mitochondrial
      PYDX5Ptm    Pyridoxal 5'-phosphate transport via diffusion, mitochondrial
      PYLALDOX    Perillyl aldehyde:NAD+ oxidoreductase
     PYLALDOXm    Perillyl aldehyde:NAD+ oxidoreductase (m)
       QUILSYN    Quinolinate Synthase (Eukaryotic)
          RAtn    Retinoate transport, nuclear
         RBK_D    D-ribulokinase
        RETNCOA    Retinoyl CoA formation
        RTOT_2    R total flux 2 position
        RTOT_3    R total flux 3 position
         RTOT1    R total flux
         RTOT2    R total flux
         RTOT3    R total flux
         RTOT4    R total flux
         RTOT5    R total flux
         RTOT6    R total flux
 RTOTAL2CRNCPT1    carnitine fatty-acyl transferase
 RTOTAL2CRNCPT2    R group transport into the mitochondria
    RTOTAL2CRNt    R group transport into the mitochondria
 RTOTAL3CRNCPT1    carnitine fatty-acyl transferase
 RTOTAL3CRNCPT2    R group transport into the mitochondria
    RTOTAL3CRNt    R group transport into the mitochondria
  RTOTALCRNCPT1    carnitine fatty-acyl transferase
  RTOTALCRNCPT2    R group transport into the mitochondria
     RTOTALCRNt    R group transport into the mitochondria
      Rtotaltp    fatty acid intracellular transport
         S2T1g    chondroitin 2-sulfotransferase, Golgi
         S2T2g    chondroitin 2-sulfotransferase, Golgi
         S2T3g    uronyl 2-sulfotransferase, Golgi
         S2T4g    uronyl 2-sulfotransferase, Golgi
         S3T1g    heparin-glucosamine 3-O-sulfotransferase
         S3T2g    heparin-glucosamine 3-O-sulfotransferase
         S3T3g    heparin-glucosamine 3-O-sulfotransferase
         S4T1g    chondroitin 4-sulfotransferase, Golgi apparatus
         S4T2g    chondroitin 4-sulfotransferase, Golgi apparatus
         S4T3g    chondroitin 4-sulfotransferase, Golgi apparatus
         S4T4g    chondroitin 4-sulfotransferase, Golgi apparatus
         S4T5g    chondroitin 4-sulfotransferase, Golgi apparatus
         S4T6g    chondroitin 4-sulfotransferase, Golgi apparatus
        S6T19g    chondroitin 6-sulfotransferase, Golgi apparatus
        S6T20g    chondroitin 6-sulfotransferase, Golgi apparatus
        S6T21g    chondroitin 6-sulfotransferase, Golgi apparatus
        S6T22g    chondroitin 6-sulfotransferase, Golgi apparatus
        S6T23g    chondroitin 6-sulfotransferase, Golgi apparatus
        S6T24g    chondroitin 6-sulfotransferase, Golgi apparatus
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      S6T25g     heparan sulfate 6-sulfotransferase, Golgi apparatus
     SALMCOM     S-Adenosyl-L-methionine:catechol O-methyltransferase
     SARCOXp     sarcosine oxidase, peroxisomal
     SARCStp     Sarcosine transport (peroxisomal)
   SEAHCYSHYD    Se-Adenosylselenohomocysteine hydrolase
    SEAHCYStn    Se-adenosyl-seleno-L-homocysteine nuclear transport
    SEASMETtn    Se-adenosyl-seleno-L-methionine nuclear transport
      SELADT     selenate adenylyltransferase
     SELCYSLY    selenocysteine lyase
    SELCYSLY2    selenocysteine lyase
    SELCYSTGL    selanocystathionine g-lyase
     SELCYSTS    selanocystathionine beta-synthase
     SELMETAT    selenomethionine adenosyltransferase
      SELNPS     Selenophosphate synthase
     SELt4_3     selenate transport via sodium symport
     SGPL11r     Sphingosine-1-phosphate lyase 1
      SIAASE     sialidase
       SLDxm     L-sulfolactate dehydrogenase (NAD+), mitochondrial
      SOAT11     sterol O-acyltransferase (acyl-Coenzyme A: cholesterol acyltransferase) 1
     SOAT11r     sterol O-acyltransferase (acyl-Coenzyme A: cholesterol acyltransferase) 1
      SOAT12     sterol O-acyltransferase (acyl-Coenzyme A: cholesterol acyltransferase) 1
     SOAT12r     sterol O-acyltransferase (acyl-Coenzyme A: cholesterol acyltransferase) 1
         SPR     sepiapterin reductase
        SPRn     sepiapterin reductase, nuclear
    SRTN23OX     5-Hydroxytryptamine:oxygen 2,3-dioxygenase (indole-decyclizing)
     SRTNACT     Acetyl-CoA:aralkylamine N-acetyltransferase
     SRTNMTX     S-Adenosyl-L-methionine:amine N-methyltransferase (srtn)
       STS1r     Steryl-sulfatase
       STS2r     Steryl-sulfatase
 T2M26DCOAHLm    trans-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA hydro-lyase (m)
 T2M26DCOAHLx    trans-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA hydro-lyase (x)
    T4HCINNOX    4-Coumarate:oxygen oxidoreductase
       TDPDRE    dTDP-4-dehydrorhamnose 3,5-epimerase
       TDPDRR    dTDP-4-dehydrorhamnose reductase
       TDPGDH    dTDPglucose 4,6-dehydratase
  TETPENT3CPT1   carnitine O-palmitoyltransferase
  TETPENT3CPT2   carnitine transferase
  TETPENT3CRNt   transport into the mitochondria (carnitine)
  TETPENT6CPT1   carnitine O-palmitoyltransferase
  TETPENT6CPT2   carnitine transferase
  TETPENT6CRNt   transport into the mitochondria (carnitine)
   TETTET6CPT1   carnitine O-palmitoyltransferase
   TETTET6CPT2   carnitine transferase
   TETTET6CRNt   transport into the mitochondria (carnitine)
       THMt2m    Thiamine transport in via proton symport, mitochondrial
        THRS     threonine synthase
      THYMDtl    thymidine facilated transport from lysosome
      TMABADH    4-trimethylaminobutyraldehyde dehydrogenase
      TMLYSOX    trimethyllysine dioxygenase
      TMLYSter   trimethyl-L-lysine transport (ER to cytosol)
        TRDRm    thioredoxin reductase (NADPH)
        TREH     alpha,alpha-trehalase
     TRYPTAOX    Tryptamine:oxygen oxidoreductase(deaminating)(flavin-containing)
         TS3     Tachysterol 3 formation
     UDPGALt2g   UDPgalactose transport (Golgi)
     UDPGLCAtg   UDPGlcA Golgi transport via UMP antiport
      UDPGLCtg   UDP-Glc Golgi transport via CMP antiport
      UDPGLDCg   UDP-D-glucuronate decarboxylase, Golgi apparatus
     UDPXYLter   UDP-Xyl endoplasmic reticular transport via CMP antiport
      UDPXYLtg   UDP-Xyl Golgi transport via CMP antiport
    UGALNACter   UDP-GalNAc endoplasmic reticulum transport via CMP antiport
      UGT1A7r    UDP-glucuronosyltransferase 1-10 precursor, microsomal
      UGT1A8r    UDP-glucuronosyltransferase 1-10 precursor, microsomal
        UMPKm    UMP kinase (mitochondrial, ATP)
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          Uritl   uridine facilated transport from lysosome
          Uritm   uridine facilated transport in mitochondria
          UTPtn   UTP diffusion in nucleus
       VITD2Hm    Vitamin D-25-hydroxylase (D2)
        VITD2t    Vitamin D2 release
       VITD2tm    Vitamin D2 transport from mitochondria
       VITD3Hm    Vitamin D-25-hydroxylase (D3)
       VITD3tm    Vitamin D3 transport from mitochondria
 WHTSTSTERONEte   omega hydroxy testosterone transport
     XOL7AH2tr    lipid, flip-flop intracellular transport
  XOLDIOLONEtm    lipid, flip-flop intracellular transport
      XOLESTte    cholesterol ester transporter
    XOLTRIOLtr    lipid, flip-flop intracellular transport
       XSERtg     Xyl-L-Ser (protein) transport from endoplasmic reticulum to Golgi apparatus
        XYLTer    UDP-xylose:protein xylosyltransferase, endoplasmic reticulum
  EX_HC01440(e)   Exchange of 3-Keto-beta-D-galactose
  EX_HC01441(e)   Exchange of Lactose-6P
  EX_HC01446(e)   Exchange of 3-Ketolactose
  EX_HC01577(e)   Exchange of gamma-Glutamyl-beta-cyanoalanine
  EX_HC01700(e)   Exchange of gamma-Glutamyl-3-aminopropiononitrile
  EX_HC02160(e)   Exchange of GM2-pool
  EX_HC02161(e)   Exchange of GM1-pool
          r0001   Virtual reaction/potential definition
          r0023   NADH:ferricytochrome-b5 oxidoreductase Aminosugars metabolism EC:1.6.2.2
          r0024   N-(omega)-Hydroxyarginine,NADPH:oxygen oxidoreductase (nitric-oxide-forming) Arginine a
          r0120   GTP 7,8-8,9-dihydrolase Folate biosynthesis EC:3.5.4.16
          r0121   r0121
          r0205   sn-Glycerol-3-phosphate:(acceptor) 2-oxidoreductase Glycerophospholipid metabolism EC:1
          r0220   Propinol adenylate:CoA ligase (AMP-forming) Propanoate metabolism EC:6.2.1.17 EC:6.2.1.
          r0221   Propinol adenylate:CoA ligase (AMP-forming) Propanoate metabolism EC:6.2.1.17
          r0318   Propanoate:CoA ligase (AMP-forming) Propanoate metabolism EC:6.2.1.1 EC:6.2.1.17
          r0319   Propanoate:CoA ligase (AMP-forming) Propanoate metabolism EC:6.2.1.1 EC:6.2.1.17
          r0366   [Acyl-carrier-protein] 4-pantetheine-phosphohydrolase Pantothenate and CoA biosynthesis
          r0368   CoA:apo-[acyl-carrier-protein] pantetheinephosphotransferase Pantothenate and CoA biosy
          r0380   Lactose 6-phosphate galactohydrolase Galactose metabolism EC:3.2.1.23
          r0402   Tetrahydrobiopterin:NADP+ oxidoreductase Folate biosynthesis EC:1.1.1.153
          r0430   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0431   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0432   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0433   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0438   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0439   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0440   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0444   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0445   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0446   Palmitoyl-CoA:L-carnitine O-palmitoyltransferase Fatty acid metabolism EC:2.3.1.21
          r0465   L-Histidine:4-aminobutanoate ligase (AMP-forming) Urea cycle and metabolism of amino gr
          r0466   alpha-Aminobutyryl histidine hydrolase Urea cycle and metabolism of amino groups EC:3.4
          r0510   steroyl-CoA,hydrogen-donor:oxygen oxidoreductase Polyunsaturated fatty acid biosynthesi
          r0511   steroyl-CoA,hydrogen-donor:oxygen oxidoreductase Polyunsaturated fatty acid biosynthesi
          r0537   Sphinganine-1-phosphate pamlmitaldehyde-lyase Sphingolipid metabolism EC:4.1.2.27
          r0546   Phenylacetaldehyde:NAD+ oxidoreductase Phenylalanine metabolism / Styrene degradation E
          r0548   Aldehyde:NADP+ oxidoreductase Phenylalanine metabolism EC:1.2.1.5
          r0598   L-Fucose ketol-isomerase Fructose and mannose metabolism EC:5.3.1.25
          r0625   3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-al:NAD+ 26-oxidoreductase Bile acid
          r0626   5beta-Cholestane-3alpha,7alpha,12alpha,26-tetraol:NAD+ 26-oxidoreductase Bile acid bios
          r0648   (5-Glutamyl)-peptide:amino-acid 5-glutamyltransferase Cyanoamino acid metabolism EC:2.3
          r0649   (5-Glutamyl)-peptide:amino-acid 5-glutamyltransferase Cyanoamino acid metabolism EC:2.3
          r0673   6-Lactoyl-5,6,7,8-tetrahydropterin:NADP+ 2-oxidoreductase Folate biosynthesis EC:1.1.1.
          r0678   Acyl-[acyl-carrier-protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxy
          r0681   (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.
          r0682   Butyryl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
          r0691   (3R)-3-Hydroxybutanoyl-[acyl-carrier protein]:NADP+ oxidoreductase Fatty acid biosynthe
          r0692   (3R)-3-Hydroxydecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthe
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r0693    (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.
r0694    (3R)-3-Hydroxyoctanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthe
r0695    (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase; (3R)-3-Hydroxyoctanoyl-[acyl
r0696    (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynth
r0697    (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2
r0701    (3R)-3-Hydroxytetradecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid bios
r0702    (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2
r0708    2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl) dihydropteridine triphosphate 7,8-
r0709    r0709
r0712    Dodecanoyl-[acyl-carrier protein]: malonyl-CoA C-acyltransferase(decarboxylating, oxoac
r0713    dodecanoyl-[acyl-carrier-protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (dec
r0737    3-Ketolactose galactohydrolase Galactose metabolism EC:3.2.1.23
r0760    butyryl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarb
r0761    (3R)-3-Hydroxyhexanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthe
r0762    (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.
r0763    Hexanoyl-[acyl-carrier protein]:oxoacyl- and enoyl-reducing and thioester-hydrolysing)
r0764    hexanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decar
r0765    Octanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
r0766    Octanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decar
r0767    Decanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
r0768    Decanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decar
r0769    (3R)-3-Hydroxydodecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynt
r0770    (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.
r0771    Tetradecanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxo
r0772    Tetradecanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (
r0773    Hexadecanoyl-[acyl-carrier protein:malonyl-CoA C-acyltransferase(decarboxylating, oxoac
r0775    Formamidopyrimidine nucleoside triphosphate 7,8-8,9-dihydrolase Folate biosynthesis EC:
r0776    r0776
r0777    GTP 7,8-8,9-dihydrolase Folate biosynthesis EC:3.5.4.16
r0778    r0778
r0786    sphinganine-1-phosphate palmitaldehyde-lyase Sphingolipid metabolism EC:4.1.2.27
r0800    Virtual reaction/potential definition
r0802    Vesicular transport
r0803    Vesicular transport
r0804    Vesicular transport
r0805    Vesicular transport
r0806    Vesicular transport
r0807    Vesicular transport
r0808    Vesicular transport
r0825    Vesicular transport
r0826    Transport reaction
r0859    Postulated transport reaction
r0886    Postulated transport reaction
r0925    Vesicular transport
r0927    Free diffusion
r0988    Postulated transport reaction
r0992    Na(+)/bile acid cotransporter Active transport
r1000    Facilitated diffusion
r1001    Facilitated diffusion
r1002    Facilitated diffusion
r1003    Facilitated diffusion
r1004    Facilitated diffusion
r1005    Facilitated diffusion
r1006    Facilitated diffusion
r1021    Postulated transport reaction
r1027    Active transport
r1033    Vesicular transport
r1034    Vesicular transport
r1048    Vesicular transport
r1049    Vesicular transport
r1054    Vesicular transport
r1055    Vesicular transport
r1056    Vesicular transport
r1057    Vesicular transport
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r1059    Major Facilitator(MFS) TCDB:2.A.18.6.7
r1061    Vesicular transport
r1062    Vesicular transport
r1063    Vesicular transport
r1064    Postulated transport reaction
r1067    Vesicular transport
r1068    Vesicular transport
r1071    Transport reaction
r1073    Transport reaction
r1074    Vesicular transport
r1076    Postulated transport reaction
r1077    Vesicular transport
r1080    Vesicular transport
r1081    Vesicular transport
r1082    Vesicular transport
r1092    albumin  Protein assembly
r1093    serpin peptidase inhibitor, clade A (alpha-1 antiproteinase, antitrypsin), member 3  Pr
r1094    serpin peptidase inhibitor, clade A (alpha-1 antiproteinase, antitrypsin), member 1  Pr
r1095    apolipoprotein B  Protein assembly
r1096    NADH dehydrogenase (ubiquinone) 1, alpha/beta subcomplex, 1  Protein assembly
r1097    ACP Protein assembly
r1098    Apo-CIB Protein assembly
r1099    Apo-CII Protein assembly
r1100    Apo-CIII Protein assembly
r1101    Fibrinogen alpha chain Protein assembly
r1102    Haptoglobin Protein assembly
r1103    Plasminogen Protein assembly
r1104    Prothrombin Protein assembly
r1105    T9 Protein assembly
r1112    Apo-E Protein assembly
r1113    Apo-AI Protein assembly
r1127    Transport reaction
r1128    Transport reaction
r1129    Transport reaction
r1130    Transport reaction
r1131    Transport reaction
r1132    Transport reaction
r1133    Transport reaction
r1134    methylsterol monooxygenase Biosynthesis of steroids EC:1.14.13.72
r1135    hydroxysteroid (17-beta) dehydrogenase 7  Biosynthesis of steroids EC:1.1.1.270
r1136    sterol-4alpha-carboxylate 3-dehydrogenase (decarboxylating) Biosynthesis of steroids EC
r1137    NAD(P) dependent steroid dehydrogenase-like  EC:1.1.1.170
r1140    Vesicular transport
r1146    Biosynthesis of steroids Enzyme catalyzed
r1159    Vesicular transport
r1165    EC:2.3.1.26
r1166    EC:2.3.1.26
r1169    EC:2.3.1.26
r1170    EC:2.3.1.26
r1171    EC:2.3.1.26
r1173    EC:3.1.1.13
r1174    EC:3.1.1.13
r1175    EC:3.1.1.13
r1176    EC:3.1.1.13
r1178    EC:3.1.1.13
r1180    EC:3.1.1.13
r1181    EC:3.1.1.13
r1182    EC:3.1.1.13
r1183    EC:3.1.1.13
r1184    EC:3.1.1.13
r1185    EC:2.3.1.15
r1186    EC:2.3.1.15
r1187    EC:2.3.1.15
r1188    EC:2.3.1.15
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r1189    EC:2.3.1.15
r1190    EC:2.3.1.15
r1251    EC:6.2.1.3
r1253    EC:6.2.1.3
r1290    Postulated transport reaction
r1293    ADF Protein assembly
r1294    MTRX Protein assembly
r1313    3-oxoacyl-ACP synthase, mitochondrial  Polyunsaturated fatty acid biosynthesis EC:2.3.1
r1314    fatty acid synthase   Polyunsaturated fatty acid biosynthesis EC:2.3.1.85
r1315    fatty acid synthase   Polyunsaturated fatty acid biosynthesis EC:2.3.1.85
r1316    fatty acid synthase   Polyunsaturated fatty acid biosynthesis EC:2.3.1.85
r1317    oleoyl-ACP hydrolase   EC:2.3.1.85
r1319    Virtual reaction/potential definition
r1320    Virtual reaction/potential definition
r1321    Virtual reaction/potential definition
r1322    Virtual reaction/potential definition
r1323    Virtual reaction/potential definition
r1324    Virtual reaction/potential definition
r1325    Virtual reaction/potential definition
r1326    Virtual reaction/potential definition
r1327    Virtual reaction/potential definition
r1328    Virtual reaction/potential definition
r1329    Virtual reaction/potential definition
r1330    Virtual reaction/potential definition
r1331    Virtual reaction/potential definition
r1332    Virtual reaction/potential definition
r1333    Protein degradation
r1334    Protein degradation
r1335    Protein degradation
r1336    Protein degradation
r1337    Protein degradation
r1338    Protein degradation
r1339    Protein degradation
r1340    Protein degradation
r1341    Protein degradation
r1342    Protein degradation
r1343    Protein degradation
r1344    Protein degradation
r1345    Protein degradation
r1346    Protein degradation
r1347    Protein degradation
r1348    Protein degradation
r1349    Protein degradation
r1350    Protein degradation
r1351    Protein degradation
r1352    Protein degradation
r1353    Protein degradation
r1354    Protein degradation
r1355    Protein degradation
r1356    Protein degradation
r1357    Protein degradation
r1358    Protein degradation
r1359    Protein degradation
r1382    folylpolyglutamyl synthetase  EC:6.3.2.17
r1383    gamma-glutamyl hydrolase  EC:3.4.19.9
r1386    Virtual reaction/potential definition
r1391    amylo-1,6-glucosidase, 4-alpha-glucanotransferase   EC:2.4.1.25
r1392    amylo-1,6-glucosidase, 4-alpha-glucanotransferase   EC:3.2.1.33
r1393    EC:2.4.1.1
r1394    EC:2.3.1.21
r1395    carnitine acetyltransferase  EC:2.3.1.7
r1398    EC:2.3.1.21
r1399    carnitine acetyltransferase  EC:2.3.1.7
r1402    glycogenin  Protein assembly
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r1403    Protein degradation
r1411    D-Galactosyl-N-acetyl-D-galactosaminyl-(N-acetylneuraminyl)-D- galactosyl-D-glucosylcer
r1430    [Acyl-carrier-protein] 4-pantetheine-phosphohydrolase Pantothenate and CoA biosynthesis
r1431    2-Deoxyuridine 5-diphosphate:oxidized-thioredoxin 2-oxidoreductase Pyrimidine metabolis
r1432    2-Deoxyuridine 5-diphosphate:oxidized-thioredoxin 2-oxidoreductase Pyrimidine metabolis
r1436    Transport reaction
r1437    Transport reaction
r1440    Transport reaction
r1441    Active transport
r1455    Transport reaction
r1457    hexadecanal:NADP+ delta2-oxidoreductase EC:1.3.1.27
r1468    Postulated transport reaction
r1472    long-chain-acyl-CoA dehydrogenase EC:1.3.99.13
r1474    EC:4.2.1.17
r1477    EC:1.1.1.35
r1479    EC:2.3.1.16
r1481    EC:2.3.1.16
r1501    Glycoside-Pentoside-Hexuronide (GPH):Cation Symporter TCDB:2.A.28.1.1
r1502    Glycoside-Pentoside-Hexuronide (GPH):Cation Symporter TCDB:2.A.28.1.1
r1503    Glycoside-Pentoside-Hexuronide (GPH):Cation Symporter TCDB:2.A.28.1.1
r1526    ATP-binding Cassette (ABC) TCDB:3.A.1.211.1
r1531    ATP-binding Cassette (ABC) TCDB:3.A.1.208.15
r1532    ATP-binding Cassette (ABC) TCDB:3.A.1.208.15
r1533    ATP-binding Cassette (ABC) TCDB:3.A.1.208.15
r2073    Zinc (Zn2+)-Iron (Fe2+) Permease (ZIP), TCDB:2.A.55.2.3
r2143    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2146    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2147    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2148    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2149    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2151    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2152    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2153    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2154    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2155    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2156    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2157    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2158    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2159    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2160    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2161    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2162    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2163    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2164    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2165    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2166    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2167    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2168    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2169    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2170    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2171    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2172    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2173    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2174    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2175    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2176    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2177    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2178    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2179    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2180    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2181    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2182    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2183    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2184    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
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r2185    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2186    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2187    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2188    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2189    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2190    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2191    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2192    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2203    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2204    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2205    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2206    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2207    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2208    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2209    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2210    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2211    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2212    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2213    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2214    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2215    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2216    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2217    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2218    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2219    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2220    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2221    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2222    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2223    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2224    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2225    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2226    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2227    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2228    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2229    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2230    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2231    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2232    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2233    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2234    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2235    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2236    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2237    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2238    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2239    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2240    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2241    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2242    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2243    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2244    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2245    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2246    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2247    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2248    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2249    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2250    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2251    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2252    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2253    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2254    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2255    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2256    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2257    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2258    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
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r2259    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2260    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2261    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2262    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2263    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2264    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2265    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2266    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2267    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2268    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2269    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2270    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2271    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2272    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
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r2288    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2289    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
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r2291    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2292    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2293    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2294    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
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r2296    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2297    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
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r2301    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
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r2305    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2306    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2307    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5
r2436    Mitochondrial Carrier (MC) TCDB:2.A.29.8.3
r2438    Mitochondrial Carrier (MC) TCDB:2.A.29.8.3
r2482    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2483    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2484    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2485    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2486    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2487    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2488    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2489    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2490    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2491    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2492    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2493    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
r2494    Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
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      r2496      Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14
      r2498      ATP-binding Cassette (ABC) TCDB:3.A.1.203.3
      r2502      ATP-binding Cassette (ABC) TCDB:3.A.1.203.3
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   RE0570C       RE0570
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   RE0572N       RE0572
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   RE0918C       RE0918
   RE0918G       RE0918
   RE0918R       RE0918
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RE3010X    RE3010
RE3011M    RE3011
RE3012C    RE3012
RE3012M    RE3012
RE3013C    RE3013
RE3013R    RE3013
RE3014C    RE3014
RE3015C    RE3015
RE3018C    RE3018
RE3018R    RE3018
RE3019C    RE3019
RE3019R    RE3019
RE3020C    RE3020
RE3020R    RE3020
RE3021C    RE3021
RE3022C    RE3022
RE3033C    RE3033
RE3033N    RE3033
RE3033R    RE3033
RE3036C    RE3036
```

```
RE3036N    RE3036
RE3038C    RE3038
RE3038N    RE3038
RE3038R    RE3038
RE3038X    RE3038
RE3039C    RE3039
RE3040C    RE3040
RE3040R    RE3040
RE3040X    RE3040
RE3041C    RE3041
RE3041N    RE3041
RE3044C    RE3044
RE3044N    RE3044
RE3045C    RE3045
RE3051C    RE3051
RE3052C    RE3052
RE3053C    RE3053
RE3066X    RE3066
RE3072X    RE3072
RE3073X    RE3073
RE3075C    RE3075
RE3075X    RE3075
RE3076X    RE3076
RE3079C    RE3079
RE3081X    RE3081
RE3082X    RE3082
RE3083X    RE3083
RE3084X    RE3084
RE3086X    RE3086
RE3087X    RE3087
RE3088X    RE3088
RE3089X    RE3089
RE3090X    RE3090
RE3092X    RE3092
RE3093X    RE3093
RE3095C    RE3095
RE3095L    RE3095
RE3095X    RE3095
RE3097X    RE3097
RE3103C    RE3103
RE3103R    RE3103
RE3104C    RE3104
RE3104R    RE3104
RE3106C    RE3106
RE3106R    RE3106
RE3108C    RE3108
RE3110C    RE3110
RE3110R    RE3110
RE3111C    RE3111
RE3111M    RE3111
RE3111R    RE3111
RE3112C    RE3112
RE3112R    RE3112
RE3113C    RE3113
RE3113R    RE3113
RE3114R    RE3114
RE3119C    RE3119
RE3119R    RE3119
RE3120C    RE3120
RE3120R    RE3120
RE3121C    RE3121
RE3121R    RE3121
RE3122C    RE3122
RE3122R    RE3122
```

```
RE3123C    RE3123
RE3123R    RE3123
RE3124C    RE3124
RE3124R    RE3124
RE3125C    RE3125
RE3125R    RE3125
RE3126C    RE3126
RE3126R    RE3126
RE3129N    RE3129
RE3132C    RE3132
RE3132R    RE3132
RE3134C    RE3134
RE3134R    RE3134
RE3136C    RE3136
RE3139X    RE3139
RE3140X    RE3140
RE3141X    RE3141
RE3144C    RE3144
RE3144M    RE3144
RE3145X    RE3145
RE3146C    RE3146
RE3146R    RE3146
RE3147C    RE3147
RE3147R    RE3147
RE3148C    RE3148
RE3148R    RE3148
RE3150C    RE3150
RE3150R    RE3150
RE3151C    RE3151
RE3151R    RE3151
RE3152C    RE3152
RE3152R    RE3152
RE3153C    RE3153
RE3153R    RE3153
RE3154C    RE3154
RE3154R    RE3154
RE3155C    RE3155
RE3155R    RE3155
RE3156X    RE3156
RE3157X    RE3157
RE3158X    RE3158
RE3159X    RE3159
RE3160C    RE3160
RE3160R    RE3160
RE3161C    RE3161
RE3161R    RE3161
RE3162C    RE3162
RE3162R    RE3162
RE3163C    RE3163
RE3163R    RE3163
RE3164C    RE3164
RE3164R    RE3164
RE3165C    RE3165
RE3165R    RE3165
RE3166C    RE3166
RE3166R    RE3166
RE3167C    RE3167
RE3167R    RE3167
RE3168C    RE3168
RE3168R    RE3168
RE3169C    RE3169
RE3169R    RE3169
RE3170C    RE3170
RE3170R    RE3170
```

```
RE3171C    RE3171
RE3171R    RE3171
RE3172C    RE3172
RE3172R    RE3172
RE3173C    RE3173
RE3173R    RE3173
RE3174C    RE3174
RE3174R    RE3174
RE3175C    RE3175
RE3175R    RE3175
RE3176C    RE3176
RE3176R    RE3176
RE3177M    RE3177
RE3178M    RE3178
RE3179M    RE3179
RE3180C    RE3180
RE3181C    RE3181
RE3184M    RE3184
RE3185M    RE3185
RE3186M    RE3186
RE3189M    RE3189
RE3190M    RE3190
RE3191M    RE3191
RE3192M    RE3192
RE3193M    RE3193
RE3194M    RE3194
RE3195M    RE3195
RE3201C    RE3201
RE3218L    RE3218
RE3218R    RE3218
RE3220C    RE3220
RE3220L    RE3220
RE3220R    RE3220
RE3224C    RE3224
RE3224R    RE3224
RE3225C    RE3225
RE3225R    RE3225
RE3226C    RE3226
RE3226R    RE3226
RE3227C    RE3227
RE3227R    RE3227
RE3228C    RE3228
RE3228R    RE3228
RE3229C    RE3229
RE3229R    RE3229
RE3230C    RE3230
RE3230R    RE3230
RE3231C    RE3231
RE3231R    RE3231
RE3232C    RE3232
RE3232R    RE3232
RE3233C    RE3233
RE3233G    RE3233
RE3233L    RE3233
RE3234C    RE3234
RE3234R    RE3234
RE3235C    RE3235
RE3235R    RE3235
RE3236C    RE3236
RE3236R    RE3236
RE3237C    RE3237
RE3238C    RE3238
RE3239C    RE3239
RE3247M    RE3247
```

```
RE3247X      RE3247
RE3248M      RE3248
RE3248X      RE3248
RE3250C      RE3250
RE3250M      RE3250
RE3250X      RE3250
RE3251M      RE3251
RE3258C      RE3258
RE3258R      RE3258
RE3259C      RE3259
RE3259R      RE3259
RE3260C      RE3260
RE3260R      RE3260
RE3261C      RE3261
RE3261R      RE3261
RE3263C      RE3263
RE3264C      RE3264
RE3264R      RE3264
RE3265C      RE3265
RE3265R      RE3265
RE3267E      RE3267
RE3267G      RE3267
RE3267M      RE3267
RE3267N      RE3267
RE3267R      RE3267
RE3268C      RE3268
RE3273G      RE3273
RE3273R      RE3273
RE3286C      RE3286
RE3286R      RE3286
RE3287C      RE3287
RE3287R      RE3287
RE3288C      RE3288
RE3288R      RE3288
RE3289C      RE3289
RE3289R      RE3289
RE3295C      RE3295
RE3301G      RE3301
RE3301R      RE3301
RE3307C      RE3307
RE3307M      RE3307
RE3307X      RE3307
RE3308C      RE3308
RE3308M      RE3308
RE3308R      RE3308
RE3308X      RE3308
RE3310C      RE3310
RE3310R      RE3310
RE3334M      RE3334
RE3334X      RE3334
RE3335C      RE3335
RE3335M      RE3335
RE3335R      RE3335
RE3335X      RE3335
RE3336M      RE3336
RE3336X      RE3336
RE3337M      RE3337
RE3337X      RE3337
RE3338C      RE3338
RE3338M      RE3338
RE3338X      RE3338
RE3339C      RE3339
RE3339M      RE3339
RE3339X      RE3339
```

```
RE3340C     RE3340
RE3340M     RE3340
RE3340X     RE3340
RE3341M     RE3341
RE3341X     RE3341
RE3342M     RE3342
RE3342X     RE3342
RE3343C     RE3343
RE3343M     RE3343
RE3343X     RE3343
RE3344M     RE3344
RE3344X     RE3344
RE3345C     RE3345
RE3345M     RE3345
RE3345R     RE3345
RE3345X     RE3345
RE3346R     RE3346
RE3352C     RE3352
RE3367C     RE3367
RE3367X     RE3367
RE3370C     RE3370
RE3370R     RE3370
RE3372C     RE3372
RE3378C     RE3378
RE3381L     RE3381
RE3383M     RE3383
RE3384M     RE3384
RE3385M     RE3385
RE3386M     RE3386
RE3387M     RE3387
RE3388M     RE3388
RE3389M     RE3389
RE3390M     RE3390
RE3391M     RE3391
RE3392M     RE3392
RE3393M     RE3393
RE3394M     RE3394
RE3395M     RE3395
RE3396M     RE3396
RE3397M     RE3397
RE3398M     RE3398
RE3399M     RE3399
RE3400M     RE3400
RE3401M     RE3401
RE3402M     RE3402
RE3403M     RE3403
RE3404M     RE3404
RE3407C     RE3407
RE3408C     RE3408
RE3409C     RE3409
RE3410C     RE3410
RE3411C     RE3411
RE3412C     RE3412
RE3413C     RE3413
RE3414C     RE3414
RE3415C     RE3415
RE3417C     RE3417
RE3420C     RE3420
RE3421M     RE3421
RE3422C     RE3422
RE3423C     RE3423
RE3430C     RE3430
RE3430M     RE3430
RE3430X     RE3430
```

```
RE3431C    RE3431
RE3432C    RE3432
RE3432M    RE3432
RE3432X    RE3432
RE3434C    RE3434
RE3434R    RE3434
RE3435C    RE3435
RE3435R    RE3435
RE3436C    RE3436
RE3436R    RE3436
RE3437C    RE3437
RE3440C    RE3440
RE3440R    RE3440
RE3443M    RE3443
RE3443X    RE3443
RE3444C    RE3444
RE3444M    RE3444
RE3444X    RE3444
RE3445M    RE3445
RE3445X    RE3445
RE3446C    RE3446
RE3446M    RE3446
RE3446R    RE3446
RE3446X    RE3446
RE3447M    RE3447
RE3447X    RE3447
RE3448C    RE3448
RE3448M    RE3448
RE3448X    RE3448
RE3449C    RE3449
RE3450C    RE3450
RE3451C    RE3451
RE3452C    RE3452
RE3453C    RE3453
RE3454C    RE3454
RE3455C    RE3455
RE3456C    RE3456
RE3457C    RE3457
RE3458C    RE3458
RE3459C    RE3459
RE3460C    RE3460
RE3464C    RE3464
RE3464R    RE3464
RE3469C    RE3469
RE3470C    RE3470
RE3470M    RE3470
RE3470X    RE3470
RE3474C    RE3474
RE3474R    RE3474
RE3475C    RE3475
RE3475N    RE3475
RE3476C    RE3476
RE3476M    RE3476
RE3476X    RE3476
RE3477C    RE3477
RE3485C    RE3485
RE3485N    RE3485
RE3486C    RE3486
RE3488C    RE3488
RE3488N    RE3488
RE3488R    RE3488
RE3488X    RE3488
RE3490C    RE3490
RE3491C    RE3491
```

```
RE3492C     RE3492
RE3493C     RE3493
RE3494C     RE3494
RE3495C     RE3495
RE3496C     RE3496
RE3496N     RE3496
RE3498N     RE3498
RE3498R     RE3498
RE3499C     RE3499
RE3500C     RE3500
RE3500R     RE3500
RE3500X     RE3500
RE3501C     RE3501
RE3501R     RE3501
RE3501X     RE3501
RE3502C     RE3502
RE3502X     RE3502
RE3503C     RE3503
RE3503N     RE3503
RE3506C     RE3506
RE3506R     RE3506
RE3511C     RE3511
RE3511M     RE3511
RE3511R     RE3511
RE3513C     RE3513
RE3513N     RE3513
RE3513R     RE3513
RE3514C     RE3514
RE3514R     RE3514
RE3515C     RE3515
RE3518C     RE3518
RE3518R     RE3518
RE3519C     RE3519
RE3519R     RE3519
RE3519X     RE3519
RE3520C     RE3520
RE3520M     RE3520
RE3520N     RE3520
RE3521C     RE3521
RE3521M     RE3521
RE3521R     RE3521
RE3521X     RE3521
RE3522C     RE3522
RE3522R     RE3522
RE3525C     RE3525
RE3525M     RE3525
RE3525N     RE3525
RE3525R     RE3525
RE3525X     RE3525
RE3526C     RE3526
RE3526M     RE3526
RE3526X     RE3526
RE3532C     RE3532
RE3532M     RE3532
RE3532R     RE3532
RE3533C     RE3533
RE3533M     RE3533
RE3533R     RE3533
RE3534C     RE3534
RE3534M     RE3534
RE3534R     RE3534
RE3535R     RE3535
RE3536C     RE3536
RE3537C     RE3537
```

```
RE3550X      RE3550
RE3551X      RE3551
RE3552X      RE3552
RE3554C      RE3554
RE3554M      RE3554
RE3554R      RE3554
RE3557C      RE3557
RE3557M      RE3557
RE3557R      RE3557
RE3559M      RE3559
RE3559X      RE3559
RE3560C      RE3560
RE3560M      RE3560
RE3560X      RE3560
RE3561M      RE3561
RE3561X      RE3561
RE3562C      RE3562
RE3562M      RE3562
RE3562R      RE3562
RE3562X      RE3562
RE3563M      RE3563
RE3563X      RE3563
RE3564C      RE3564
RE3564M      RE3564
RE3564X      RE3564
RE3570C      RE3570
RE3571C      RE3571
RE3571R      RE3571
RE3572X      RE3572
RE3573X      RE3573
RE3574X      RE3574
RE3575X      RE3575
RE3576X      RE3576
RE3577X      RE3577
RE3578X      RE3578
RE3580X      RE3580
RE3581X      RE3581
RE3582X      RE3582
RE3583X      RE3583
RE3586X      RE3586
RE3587C      RE3587
RE3587N      RE3587
RE3596C      RE3596
RE3596M      RE3596
RE3596X      RE3596
RE3597C      RE3597
RE3597M      RE3597
RE3597X      RE3597
RE3624X      RE3624
RE3627C      RE3627
RE3627X      RE3627
RE3631C      RE3631
RE3633C      RE3633
RE3636C      RE3636
RE3637C      RE3637
RN0001C      RN0001
RN0001R      RN0001
RN0002N      RN0002
RN0002R      RN0002
RN0013C      RN0013
RN0014R      RN0014
RN0020C      RN0020
RN0020R      RN0020
RN0021C      RN0021
```

```
RN0021R      RN0021
RN0021X      RN0021
RN0022C      RN0022
RN0022R      RN0022
RN0022X      RN0022
RN0023C      RN0023
RN0023R      RN0023
RN0023X      RN0023
RN0027C      RN0027
RN0027R      RN0027
RN0028C      RN0028
RN0028R      RN0028
RN0028X      RN0028
RN0029C      RN0029
RN0029R      RN0029
RN0030C      RN0030
RN0030R      RN0030
RN0031C      RN0031
RN0031R      RN0031
RN0031X      RN0031
RN0032C      RN0032
RN0032R      RN0032
EX_HC00955(e)    L-3-Cyanoalanine exchange
EX_HC00001(e)    Albumin exchange
EX_HC00002(e)    Antichymotrypsin exchange
EX_HC00003(e)    Antitrypsin exchange
EX_HC00004(e)    ApoA1 exchange
EX_HC01787(e)    Lepidimoide exchange
EX_HC01852(e)    Fibrinogen exchange
EX_HC01939(e)    Haptoglobin exchange
EX_HC01942(e)    Plasminogen exchange
EX_HC01943(e)    Prothrombin exchange
EX_HC01944(e)    ApoTransferin exchange
EX_HC02192(e)    taurolithocholate exchange
EX_HC02193(e)    glycolithocholate exchange
EX_HC02195(e)    tauroursodeoxycholate exchange
EX_HC02196(e)    glycoursodeoxycholate exchange
EX_HC02220(e)    sulfochenodeoxycholate exchange
EX_HC02154(e)    GM4-pool exchange
EX_HC02175(e)    caprate exchange
EX_HC02199(e)    glutathionyl-leuc4 exchange
EX_HC02200(e)    S-glutathionyl-2-4-dinitrobenzene exchange
EX_HC02201(e)    S-glutathionyl-ethacrynic-acid exchange
EX_HC02172(e)    Zinc exchange
EX_HC02191(e)    lithocholate exchange
EX_HC02194(e)    ursodeoxycholate exchange
EX_HC02197(e)    sulfoglycolithocholate(2-) exchange
EX_HC02198(e)    2-[(4R)-4-[(1S,2S,5R,7R,10R,11S,14R,15R)-2,15-dimethyl-5-(sulfonatooxy)tetracyclo[8.7.0
EX_HC02187(e)    reverse-triiodthyronine exchange
EX_HC02180(e)    thromboxane-b2 exchange
EX_HC02179(e)    20-hydroxy-arachidonate exchange
EX_HC02208(e)    prostaglandin-d1 exchange
EX_HC02210(e)    prostaglandin-d3 exchange
EX_HC02213(e)    prostaglandin-e3 exchange
EX_HC02214(e)    prostaglandin-f1alpha exchange
EX_HC02216(e)    prostaglandin-f2beta exchange
EX_HC02217(e)    prostaglandin-g2 exchange
EX_CE1950(e)     cyanosulfurous acid anion exchange
EX_cynt(e)       Cyanate exchange
EX_cdpea(e)      CDP-ethanolamine(1-) exchange
EX_12dgr120(e)   1,2-Diacyl-sn-glycerol (didodecanoyl, n-C12:0) exchange
FAOXC11BRC9BRx   fatty acid beta oxidation(C11br-->C9br)x
FAOXC13BRC11BRx  fatty acid beta oxidation(C13br-->C11br)x
FAOXC15BRC13BRx  fatty acid beta oxidation(C15br-->C13br)x
```

```
    FAOXC9BRC7BRm      fatty acid beta oxidation(C9br-->C7br)m
       CARhPTtc        Transport of L-Carnosine by hPT3 or hPT4 peptide transporter.
         CBLTDe        release of B12 by simple diffusion
      BIDGLCURr        bilirubin di-glucuronide production
   EX_adpcbl(e)        exchange reaction for Adenosylcobalamin
      EX_oh1(e)        exchange reaction for hydroxide ion
          FADtm        Transport of fad into mitochondria
          NADtm        transport of NAD into mitochondria
------end------
```

Find mass leaks or siphons within the heuristically internal part, without using the bounds given by the model

```matlab
if 1
    modelBoundsFlag=0;
    leakParams.epsilon=1e-4;
    leakParams.method='dc';
    leakParams.theta=0.5;

[leakMetBool,leakRxnBool,siphonMetBool,siphonRxnBool,leakY,siphonY,statp,stat
n] =...
        findMassLeaksAndSiphons(model,model.SIntMetBool,model.SIntRxnBool,...
        modelBoundsFlag,leakParams,printLevel);
end
```

```
   2940       4559      subset tested for leakage (dc method, with infinite flux bounds)...
      0          0      semipositive leaking metabolites (and exclusive reactions).
      0          0      seminegative siphon metabolites (and exclusive reactions).
```

Find the maximal set of reactions that are stoichiometrically consistent

```matlab
if ~isfield(model,'SConsistentMetBool') ||
~isfield(model,'SConsistentRxnBool')
    if strcmp(model.modelID,'HMRdatabase2_00')
        massBalanceCheck=0;
    else
        massBalanceCheck=1;
    end
    if 1

[SConsistentMetBool,SConsistentRxnBool,SInConsistentMetBool,SInConsistentRxnB
ool,unknownSConsistencyMetBool,unknownSConsistencyRxnBool,model]...
            =findStoichConsistentSubset(model,massBalanceCheck,printLevel);
    else
        %print out problematic reactions to file
        resultsFileName=[resultsPath filesep model.modelID];

[SConsistentMetBool,SConsistentRxnBool,SInConsistentMetBool,SInConsistentRxnB
ool,unknownSConsistencyMetBool,unknownSConsistencyRxnBool,model]...

=findStoichConsistentSubset(model,massBalanceCheck,printLevel,resultsFileName
);
```

```
        end
end
```

```
-------
  #mets     #rxns
   2940      5190      totals.
-------
      0       631      heuristically exchange.
   2940      4559      heuristically non-exchange.
   2203      4534      seemingly elementally balanced.
   2203      4534      seemingly elementally balanced and stoichiometrically consistent.
    737       656      seemingly elementally imbalanced.
-------
   2203      4534      heuristically non-exchange and seemingly elementally balanced.
   2203      4534      seemingly elementally balanced and stoichiometrically consistent.
    737        25      heuristically non-exchange and seemingly elementally imbalanced.
-------
Iteration #1 minimum cardinality of conservation relaxation vector.
   2940      4559      unknown consistency.
   2940      4559      being tested.
   2940      4559      ... of which are stoichiometrically consistent by min cardinality of stoich consisten
   2940      4559     Confirmed stoichiometrically consistent by leak/siphon testing.
      0         0      ... of which are of unknown consistency.
--- Summary of stoichiometric consistency ----
   2940      5190      totals.
      0       631      heuristically exchange.
   2940      4559      heuristically non-exchange:
   2940      4559      ... of which are stoichiometrically consistent.
      0         0      ... of which are stoichiometrically inconsistent.
      0         0      ... of which are of unknown consistency.
---
      0         0      heuristically non-exchange and stoichiometrically inconsistent or unknown consistency
      0         0      ... of which are elementally imbalanced (inclusively involved metabolite).
      0         0      ... of which are elementally imbalanced (exclusively involved metabolite).
   2940      4559     Confirmed stoichiometrically consistent by leak/siphon testing.
--- END ----
```

```matlab
rxnBool=model.SInConsistentRxnBool & model.SIntRxnBool;
if any(rxnBool)
    if printLevel>0
        fprintf('%s\n','Stoichiometrically inconsistent heuristically non-
exchange reactions:')
    end
    for n=1:nRxn
        if rxnBool(n)

fprintf('%20s\t%50s\t%s\n',model.rxns{n},model.rxnNames{n},model.subSystems{n
})
        end
    end
    if printLevel>0
        fprintf('%s\n','--------------')
    end
end

rxnBool=model.unknownSConsistencyRxnBool & model.SIntRxnBool;
if any(rxnBool)
```

```matlab
    if printLevel>0
        fprintf('%s\n','Unknown consistency heuristically non-exchange
reactions:')
    end
    for n=1:nRxn
        if rxnBool(n)

fprintf('%20s\t%50s\t%s\n',model.rxns{n},model.rxnNames{n},model.subSystems{n
})
        end
    end
    if printLevel>0
        fprintf('%s\n','--------------')
    end
end
```

Sanity check of stoichiometric and flux consistency of model with open external reactions

```matlab
    if  all(model.SIntMetBool & model.SConsistentMetBool)...
            && nnz(model.SIntRxnBool &
model.SConsistentRxnBool)==nnz(model.SIntRxnBool)...
            && all(model.fluxConsistentMetBool)...
            && all(model.fluxConsistentRxnBool)

        [nMet,nRxn]=size(model.S);
        if printLevel>1
            fprintf('%6s\t%6s\n','#mets','#rxns')
            fprintf('%6u\t%6u\t%s\n',nMet,nRxn,' totals.')

fprintf('%6u\t%6u\t%s\n',nnz(~model.SIntMetBool),nnz(~model.SIntRxnBool),'
heuristically exchange.')
        end

        checksPassed=0;
        %Check that all heuristically non-exchange reactions are also
stoichiometrically consistent

        %exchange reactions
        model.EXRxnBool=strncmp('EX_', model.rxns, 3)==1;
        %demand reactions going out of model
        model.DMRxnBool=strncmp('DM_', model.rxns, 3)==1;
        %sink reactions going into or out of model
        model.SinkRxnBool=strncmp('sink_', model.rxns, 5)==1;
        %all heuristic non-exchanges, i.e., supposedly all external reactions
        bool=~(model.EXRxnBool | model.DMRxnBool | model.SinkRxnBool);
        if nnz(bool & model.SIntRxnBool &
model.SConsistentRxnBool)==nnz(model.SConsistentRxnBool)
            checksPassed=checksPassed+1;
            if printLevel>1
```

```matlab
                fprintf('%6u\t%6u\t%s\n',nnz(model.SIntMetBool),nnz(model.SIntRxnBool),' All
internally stoichiometrically consistent. (Check 1: minimum cardinality of
conservation relaxation vector.)');
            end
        end

        %Check for mass leaks or siphons in the stoichiometrically
consistent part
        %There should be no leaks or siphons in the stiochiometrically
consistent part
        modelBoundsFlag=0;
        leakParams.epsilon=1e-4;
        leakParams.eta = getCobraSolverParams('LP', 'feasTol')*100;
        leakParams.method='dc';

[leakMetBool,leakRxnBool,siphonMetBool,siphonRxnBool,leakY,siphonY,statp,stat
n]...

=findMassLeaksAndSiphons(model,model.SConsistentMetBool,model.SConsistentRxnB
ool,modelBoundsFlag,leakParams,printLevel);

        if nnz(leakMetBool)==0 && nnz(leakRxnBool)==0 &&
nnz(siphonMetBool)==0 && nnz(siphonRxnBool)==0
            checksPassed=checksPassed+1;
            if printLevel>1
                fprintf('%6u\t%6u\t%s\n',nnz(leakMetBool |
siphonMetBool),nnz(leakRxnBool | siphonRxnBool),' No internal leaks or
siphons. (Check 2: leak/siphon tests.)');
            end
        end

        %Check that the maximal conservation vector is nonzero for each the
        %internal stoichiometric matrix
        maxCardinalityConsParams.epsilon=1e-4;%1/epsilon is the largest mass
considered, needed for numerical stability
        maxCardinalityConsParams.method = 'quasiConcave';%seems to work the
best, but sometimes infeasible
        maxCardinalityConsParams.theta = 0.5;
        maxCardinalityConsParams.eta=getCobraSolverParams('LP',
'feasTol')*100;

[maxConservationMetBool,maxConservationRxnBool,solution]=maxCardinalityConser
vationVector(model.S(model.SConsistentMetBool,model.SConsistentRxnBool),
maxCardinalityConsParams);

        if nnz(maxConservationMetBool)==size(model.S,1) &&
nnz(maxConservationRxnBool)==nnz(model.SIntRxnBool)
            checksPassed=checksPassed+1;
            if printLevel>1
```

```
fprintf('%6u\t%6u\t%s\n',nnz(maxConservationMetBool),nnz(maxConservationRxnBo
ol),' All internally stoichiometrically consistent. (Check 3: maximim
cardinality conservation vector.)');
            end
        end

        %Check that each of the reactions in the model (with open external
reactions) is flux consistent
        modelOpen=model;
        modelOpen.lb(~model.SIntRxnBool)=-1000;
        modelOpen.ub(~model.SIntRxnBool)= 1000;
        param.epsilon=1e-4;
        param.modeFlag=0;
        param.method='null_fastcc';

[fluxConsistentMetBool,fluxConsistentRxnBool,fluxInConsistentMetBool,fluxInCo
nsistentRxnBool,modelOpen] =
findFluxConsistentSubset(modelOpen,param,printLevel-2);

        if nnz(fluxConsistentMetBool)==size(model.S,1) &&
nnz(fluxConsistentRxnBool)==size(model.S,2)
            checksPassed=checksPassed+1;
            if printLevel>1

fprintf('%6u\t%6u\t%s\n',nnz(fluxConsistentMetBool),nnz(fluxConsistentRxnBool
),' All flux consistent. (Check 4: maximim cardinality constrained right
nullspace.)');
            end
        end

        if checksPassed==4
            %save the model with open exchanges as the default generic
            %model
            model=modelOpen;
            if printLevel>0
                fprintf('%s\n','Open external reactions is
stoichiometrically and flux consistent. A flux balance model generated from
a reconstruction. GREAT!!!!');
            end
        end
        save([resultsFileName '_consistent.mat'],'model')
    end
```

REFERENCES

Gevorgyan, A., Poolman, M. G., Fell D., Detection of stoichiometric inconsistencies in biomolecular models. Bioinformatics, 24(19):2245–51, 2008.

Fleming, R.M.T., et al., Cardinality optimisation in constraint-based modelling: Application to Recon 3D (submitted), 2017.

Brunk, E. et al. Recon 3D: A resource enabling a three-dimensional view of gene variation in human metabolism. (submitted) 2017.