

# Convert a reconstruction into a flux balance analysis model

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Reviewers:

## 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, 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 stoichiometrically 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 analysis, 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/reconXComp
    else
        filename='Recon2.0model.mat';
        if exist('Recon2.0model.mat','file')==2
            model = readCbModel(filename);
        end
    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.mo
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 thought to be involved in mass balanced reactions.

SIntRxnBool n x 1 Boolean of reactions heuristically thought 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 identification as an external reaction. Alternatively, such reactions may be identified by a previous pass through of this tutorial as being of unknown stoichiometric consistency (`model.unknownSConsistencyRxnBool(j)==1`), after the largest stoichiometrically consistent subset of the network has been 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';
        end
    end
end
```

```

        %ATP hydrolysis is not imbalanced like all the other demand reactions so
        %give it a different acronym 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);

```

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%6s\n',nMet0,nRxn0,' totals.')
    fprintf('%6u\t%6u\t%6s\n',nMet0-nMet,nRxn0-nRxn,' duplicates removed.')
    fprintf('%6u\t%6u\t%6s\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,pri

```

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%6s\n',nMet0,nRxn0,' totals.')
    fprintf('%6u\t%6u\t%6s\n',nMet0-nMet,nRxn0-nRxn,' duplicate reactions upto protons removed.')
    fprintf('%6u\t%6u\t%6s\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 thought to be mass balanced, while `model.SIntMetBool` is a boolean of metabolites heuristically thought 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, finding 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,fluxInConsistentRxnBool]=findFluxConsistent(model,param);
    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
    end
    %revise model size
end

```

```

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

%Recompute
%Heuristically identify exchange reactions and metabolites exclusively involved in exchange
%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)
    34DHPHMT 3,4-Dihydroxyphenylacetate:amet 0-methyltransferase
    3HPCOAHYD 3-hydroxyisobutyryl-Coenzyme A hydrolase
    3HPPD 3-hydroxypropionate dehydrogenase
    3HXKYNDCL 3-Hydroxykynurenamine decarboxy-lyase
    3HXKYNODA 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
    42A12B00X 4-(2-Aminoethyl)-1,2-benzenediol:oxygen oxidoreductase(deaminating)(flavin-containing)
    4MPNTLtr 4-methylpentanal transport (ER)
  5HOXINDACTOXm 5-Hydroxyindoleacetaldehyde:NAD+ oxidoreductase (mito)
  5HOXINOXA 5-Hydroxytryptamine:oxygen oxidoreductase(deaminating)(flavin-containing)
    5HTRPDOX 5-Hydroxy-L-tryptophan:oxygen 2,3-dioxygenase (indole-decyclizing)
    5HXKYNDCL 5-Hydroxykynurenamine decarboxy-lyase
    5HXKYNODA 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)
  AACT8p acetyl-CoA acyltransferase (hexadecanoyl-CoA), peroxisomal
  AACT9p acetyl-CoA acyltransferase (tetracosanoyl-CoA), peroxisomal

```



ACGSm N-acetylglutamate 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 facilitated transport from lysosome  
 ADHAPtx intracellular transport (peroxisome)  
 ADNtl adenosine facilitated 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  
 APRT02 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  
 BAMPPALD0Xm beta-Aminopropion aldehyde:NAD<sup>+</sup> oxidoreductase (m)  
 BBH0X 4-Trimethylammonibutanoate,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)  
 CBL20R NADH:cob(III)amine oxidoreductase  
 CBL2tm Cob(II)amine transport, mitochondrial  
 CBLATm cob(I)amin 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  
 CHSTER0Ltg 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)  
 C02tg CO<sub>2</sub> Golgi transport  
 C02tn CO<sub>2</sub> nuclear transport via diffusion  
 COKECBESr Carboxylesterase (cocaine) (er)  
 CPCTDTX choline-phosphate cytidyltransferase  
 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  
 CY00m2 cytochrome c oxidase, mitochondrial Complex IV  
 CYSLYSL L-Cystine Lysteine-lyase (deaminating)  
 CYSTAm cysteine transaminase (mitochondrial)  
 CYTDtl Cytidine facilitated 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)  
 DOGULN01 2,3-dioxo-L-gulonate:hydrogen peroxide oxireductase  
 DOGULN02 2,3-dioxo-L-gulonate:hydrogen peroxide oxireductase  
 DOPAMT Dopamine:amet O-methyltransferase  
 DORNOp D-ornithine oxidase, perixosomal  
 DPR0Op 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 cytidyltransferase  
 ESTRIOLGLCte glucuronidated compound transport  
 ESTRIOLGLCtr glucuronidated compound transport  
 ESTRIOLtr estriol intracellular transport

EX\_2425dhvitd2(e) 24R,25-Dihydroxyvitamin D2 exchange  
 EX\_25hvitd2(e) 25-Hydroxyvitamin D2 exchange  
 EX\_ahandrostanglc(e) Etiocholan-3 $\alpha$ -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<sup>+</sup> 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  
   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 glm6masnB1 endoplasmic reticulum to Golgi transport  
 G1M7MASNBterg glm7masnC endoplasmic reticulum to Golgi transport  
 G1M7MASNCterg glm7masnC endoplasmic reticulum to Golgi transport  
 G1M8MASNterg glm8masn transport from endoplasmic reticulum to Golgi apparatus  
   G1PTT glucose-1-phosphate thymidyltransferase  
 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, Golgi  
   GALNACT3g uridine diphosphoacetylgalactosamine-chondroitin acetylgalactosaminyltransferase II, Golgi  
   GALNACT4g uridine diphosphoacetylgalactosamine-chondroitin acetylgalactosaminyltransferase II, Golgi  
   GALNACT5g uridine diphosphoacetylgalactosamine-chondroitin acetylgalactosaminyltransferase II, Golgi  
     GALOR D-Galactose:NADP<sup>+</sup> 1-oxidoreductase  
     GALT2g UDP-D-galactose:galactosylxylose galactosyltransferase, Golgi apparatus  
     GALTg UDP-D-galactose:D-xylose galactosyltransferase, Golgi apparatus  
     GA01 Ganglioside O-acetylation  
     GA02 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  
GLAC0 D-Glucuronolactone:NAD+ oxidoreductase  
GLAC0m 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  
GLY0Xm hydroxyacylglutathione hydrolase, mitochondrial  
GLYt2rL glycine reversible transport via proton symport (lysosome)  
GPAMm\_hs glycerol-3-phosphate acyltransferase  
GSNKm guanosine kinase (mitochondrial)  
GSNtl guanosine facilitated transport from lysosome  
GSNtm guanosine facilitated transport in mitochondria  
GTPCI GTP cyclohydrolase I  
GTPCIn GTP cyclohydrolase I, nuclear  
GTPtn GTP diffusion in nucleus  
H2C03Dm 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 facilitated transport from lysosome  
IMACTD Imidazole acetaldehyde dehydrogenase  
IMACTD\_m Imidazole acetaldehyde dehydrogenase (mito)  
INSKm inosine kinase, mitochondrial  
INSTl inosine facilitated transport from lysosome  
INSTm inosine facilitated 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)  
 LIP0ti 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\_6Bler mannosidase I, endoplasmic reticulum (glm6masnB1-producing)  
 MAN1\_7Ber mannosidase I, endoplasmic reticulum (glm7masnB-producing)  
 MAN2\_6Bler mannosidase II, endoplasmic reticulum (glm6masnB1-producing)  
 MAN2\_7Cer mannosidase II, endoplasmic reticulum (glm7masnC-producing)  
 MAOLNOR monoamine oxidase (L-Normetanephine)  
 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 Mesoconyl-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  
 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  
 NABTN0 N4-Acetylaminobutanal:NAD+ oxidoreductase  
 NABTN0m 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)  
 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)  
 PPIIt 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)  
 PR0tm L-proline transport, mitochondrial  
 PRPNCOAHDx 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<sup>+</sup> oxidoreductase  
 PYLALDOXm Perillyl aldehyde:NAD<sup>+</sup> 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-acyltransferase  
 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  
 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 adenyltransferase  
 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  
 SRTN230X 5-Hydroxytryptamine:oxygen 2,3-dioxygenase (indole-decylizing)  
 SRTNACT Acetyl-CoA:aralkylamine N-acetyltransferase  
 SRTNMTX S-Adenosyl-L-methionine:amine N-methyltransferase (srtn)  
 STS1r Steryl-sulfatase  
 STS2r Steryl-sulfatase  
 T2M26DCOAHM trans-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA hydro-lyase (m)  
 T2M26DCOAHX 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 facilitated 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)  
  Uritl uridine facilitated transport from lysosome  
  Uritm uridine facilitated 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-aminopropionitrile  
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 and  
  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:1.1.1.1  
  r0220 Propinol adenylate:CoA ligase (AMP-forming) Propanoate metabolism EC:6.2.1.17 EC:6.2.1.17  
  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 biosynthesis  
 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 groups  
 r0466 alpha-Aminobutyryl histidine hydrolase Urea cycle and metabolism of amino groups EC:3.4.13.1  
 r0510 steroyl-CoA,hydrogen-donor:oxygen oxidoreductase Polyunsaturated fatty acid biosynthesis  
 r0511 steroyl-CoA,hydrogen-donor:oxygen oxidoreductase Polyunsaturated fatty acid biosynthesis  
 r0537 Sphinganine-1-phosphate palmitaldehyde-lyase Sphingolipid metabolism EC:4.1.2.27  
 r0546 Phenylacetaldehyde:NAD+ oxidoreductase Phenylalanine metabolism / Styrene degradation EC:1.1.1.15  
 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 metabolism  
 r0626 5beta-Cholestane-3alpha,7alpha,12alpha,26-tetraol:NAD+ 26-oxidoreductase Bile acid biosynthesis  
 r0648 (5-Glutamyl)-peptide:amino-acid 5-glutamyltransferase Cyanoamino acid metabolism EC:2.3.1.21  
 r0649 (5-Glutamyl)-peptide:amino-acid 5-glutamyltransferase Cyanoamino acid metabolism EC:2.3.1.21  
 r0673 6-Lactoyl-5,6,7,8-tetrahydropterin:NADP+ 2-oxidoreductase Folate biosynthesis EC:1.1.1.2  
 r0678 Acyl-[acyl-carrier-protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating)  
 r0681 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.21  
 r0682 Butyryl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-acylating)  
 r0691 (3R)-3-Hydroxybutanoyl-[acyl-carrier protein]:NADP+ oxidoreductase Fatty acid biosynthesis  
 r0692 (3R)-3-Hydroxydecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis  
 r0693 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.21  
 r0694 (3R)-3-Hydroxyoctanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis  
 r0695 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase; (3R)-3-Hydroxyoctanoyl-[acyl-carrier-protein]  
 r0696 (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis  
 r0697 (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.21  
 r0701 (3R)-3-Hydroxytetradecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis  
 r0702 (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.21  
 r0708 2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl) dihydropteridine triphosphate 7,8-diphosphate  
 r0709 r0709  
 r0712 Dodecanoyl-[acyl-carrier protein]: malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-acylating)  
 r0713 dodecanoyl-[acyl-carrier-protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating)  
 r0737 3-Ketolactose galactohydrolase Galactose metabolism EC:3.2.1.23  
 r0760 butyryl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating)  
 r0761 (3R)-3-Hydroxyhexanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis  
 r0762 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.21  
 r0763 Hexanoyl-[acyl-carrier protein]:oxoacyl- and enoyl-reducing and thioester-hydrolysing) Fatty acid biosynthesis  
 r0764 hexanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating)  
 r0765 Octanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-acylating)  
 r0766 Octanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating)

r0767 Decanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-  
 r0768 Decanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarb  
 r0769 (3R)-3-Hydroxydodecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynth  
 r0770 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3  
 r0771 Tetradecanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoa  
 r0772 Tetradecanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (o  
 r0773 Hexadecanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacy  
 r0775 Formamidopyrimidine nucleoside triphosphate 7,8-8,9-dihydrolase Folate biosynthesis EC:3  
 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  
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 r1056 Vesicular transport  
 r1057 Vesicular transport  
 r1059 Major Facilitator(MFS) TCDB:2.A.18.6.7  
 r1061 Vesicular transport  
 r1062 Vesicular transport  
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 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 Protein assembly  
r1094 serpin peptidase inhibitor, clade A (alpha-1 antiproteinase, antitrypsin), member 1 Protein assembly  
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:1.1.1.170  
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  
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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  
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:2.3.1.85  
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  
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r1333 Protein degradation  
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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  
r1403 Protein degradation  
r1411 D-Galactosyl-N-acetyl-D-galactosaminyl-(N-acetylneuraminy)-D- galactosyl-D-glucosylcera  
r1430 [Acyl-carrier-protein] 4-pantetheine-phosphohydrolase Pantothenate and CoA biosynthesis  
r1431 2-Deoxyuridine 5-diphosphate:oxidized-thioredoxin 2-oxidoreductase Pyrimidine metabolism  
r1432 2-Deoxyuridine 5-diphosphate:oxidized-thioredoxin 2-oxidoreductase Pyrimidine metabolism  
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 (Zn<sup>2+</sup>)-Iron (Fe<sup>2+</sup>) 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

[illegible]



[illegible]

r2276 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2277 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2278 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2279 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2280 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2281 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2282 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2283 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2284 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2285 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2286 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2287 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
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 r2290 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 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  
 r2295 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2296 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2297 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2298 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2299 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2300 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2301 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2302 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2303 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 r2304 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.5  
 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  
 r2495 Resistance-Nodulation-Cell Division (RND) TCDB:2.A.60.1.14  
 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

EX\_so3(e) Sulfite exchange

RE0066C RE0066

RE0066M RE0066  
RE0066R RE0066  
RE0124C RE0124  
RE0344M RE0344  
RE0344X RE0344  
RE0452N RE0452  
RE0456M RE0456  
RE0456N RE0456  
RE0512C RE0512  
RE0512X RE0512  
RE0549C RE0549  
RE0569C RE0569  
RE0570C RE0570  
RE0571C RE0571  
RE0572N RE0572  
RE0573N RE0573  
RE0574C RE0574  
RE0575C RE0575  
RE0576C RE0576  
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RE0690X RE0690  
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RE0702N RE0702  
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RE0827X RE0827  
RE0828C RE0828  
RE0828X RE0828  
RE0864C RE0864  
RE0875C RE0875  
RE0908G RE0908  
RE0908R RE0908  
RE0915C RE0915  
RE0916C RE0916

RE0916G RE0916  
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RE1100L RE1100  
RE1100R RE1100  
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RE1135G RE1135

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RE1235C RE1235  
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RE1587C RE1587  
RE1587L RE1587

RE1587R RE1587  
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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) Lepidimoid 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) tauroolithocholate exchange
EX_HC02193(e) glycolithocholate exchange
EX_HC02195(e) tauroursodeoxycholate exchange
EX_HC02196(e) glycoursoodeoxycholate 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-triiodothyronine 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
FA0XC11BRC9BRx fatty acid beta oxidation(C11br-->C9br)x
FA0XC13BRC11BRx fatty acid beta oxidation(C13br-->C11br)x
FA0XC15BRC13BRx fatty acid beta oxidation(C15br-->C13br)x
FA0XC9BRC7BRm 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_ohl(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**

```

if 1
  modelBoundsFlag=0;
  leakParams.epsilon=1e-4;
  leakParams.method='dc';
  leakParams.theta=0.5;
  [leakMetBool,leakRxnBool,siphonMetBool,siphonRxnBool,leakY,siphonY,statp,statn] =...

```



```

end
    findMassLeaksAndSiphons(model,model.SIntMetBool,model.SIntRxnBool,...
    modelBoundsFlag,leakParams,printLevel);

```

```

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

```

if ~isfield(model,'SConsistentMetBool') || ~isfield(model,'SConsistentRxnBool')
    if strcmp(model.modelID,'HMRdatabase2_00')
        massBalanceCheck=0;
    else
        massBalanceCheck=1;
    end
    if 1
        [SConsistentMetBool,SConsistentRxnBool,SInConsistentMetBool,SInConsistentRxnBool,unknown]
            =findStoichConsistentSubset(model,massBalanceCheck,printLevel);
    else
        %print out problematic reactions to file
        resultsFileName=[resultsPath filesep model.modelID];
        [SConsistentMetBool,SConsistentRxnBool,SInConsistentMetBool,SInConsistentRxnBool,unknown]
            =findStoichConsistentSubset(model,massBalanceCheck,printLevel,resultsFileName);
    end
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 consistency
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 ---

```

```

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)
    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
end

```

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

```

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),' heurist
    end

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

    %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.SConsistentRxnB

```

```

        checksPassed=checksPassed+1;
        if printLevel>1
            fprintf('%6u\t%6u\t%s\n',nnz(model.SIntMetBool),nnz(model.SIntRxnBool),' All i
        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,statn]...
        =findMassLeaksAndSiphons(model,model.SConsistentMetBool,model.SConsistentRxnBool,m

    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),'
        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
    maxCardinalityConsParams.method = 'quasiConcave';%seems to work the best, but sometime
    maxCardinalityConsParams.theta = 0.5;
    maxCardinalityConsParams.eta=getCobraSolverParams('LP', 'feasTol')*100;
    [maxConservationMetBool,maxConservationRxnBool,solution]=maxCardinalityConservationVec

    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(maxConservationRxnBool),'
        end
    end

    %Check that each of the reactions in the model (with open external reactions) is flux
    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,fluxInConsistentRxnBool]...

    if nnz(fluxConsistentMetBool)==size(model.S,1) && nnz(fluxConsistentRxnBool)==size(model.SIntRxnBool)
        checksPassed=checksPassed+1;
        if printLevel>1
            fprintf('%6u\t%6u\t%s\n',nnz(fluxConsistentMetBool),nnz(fluxConsistentRxnBool),'
        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 consist
        end
    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.

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