

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, 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/recon2models';
        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/'];
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 identification as an external reaction. Alternatively, such reactions may be identified by a previous pass through of this tutorial as being of unknown stoichiometric consistent (`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_noTrTr';

            %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
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
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);
```

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);

```

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 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,fluxInConsistentRxnBool]=findFluxConsistent(model,param);
    end
    % Remove reactions that are flux inconsistent
    if any(fluxInConsistentRxnBool)
        irrevFlag=0;
```

```

metFlag=1;
model = removeRxnns(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
%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
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 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)
3NTD71	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-decycling)
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-acetylglutamate synthase, mitochondrial
ACOATA	Acetyl-CoA ACP transacylase
ACODA	acetylornithine deacetylase
ACSOMT	S-Adenosyl-L-methionine:N-acetylserotonin O-methyltransferase
ACSRNTMT	S-Adenosyl-L-homocysteine:N-acetylserotonin O-methyltransferase
ACTg	acetate transport, Golgi apparatus
ADEt1	adenine facilitated transport from lysosome
ADHAPtx	intracellular transport (peroxisome)
ADNt1	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
APRTO2	N-acetylputrescine: oxygen oxidoreductase (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-Trimethylammonio-butanoate,2-oxoglutarate:oxygen oxidoreductase (3-hydroxylating)
BDG2HCGHD	beta-D-Glucosyl-2-coumarinate glucosylhydrolase
BTnt2m	Biotin reversible transport via proton symport, mitochondria
BZt	benzoate transport (diffusion)
BZtr	Benzene transporter, endoplasmic reticulum
C2M26DCOAHm	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 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
CYOOm2	cytochrome c oxidase, mitochondrial Complex IV
CYSLYSL	L-Cystine Lysteine-lyase (deaminating)
CYSTAm	cysteine transaminase (mitochondrial)
CYTDt1	Cytidine faciliated 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)
DMHPTCRNCT1	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 cytidyltransferase
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_nal(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	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 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+ 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 facilitated transport from lysosome
GSNtm	guanosine facilitated transport in mitochondria
GTPCI	GTP cyclohydrolase I
GTPCIn	GTP cyclohydrolase I, nuclear
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)
HEXCCT1	carnitine O-palmitoyltransferase
HEXCCT2	carnitine transferase
HEXCCTn	transport into the mitochondria (carnitine)
HISTASE	Histaminase
HMGCOAr	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)
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_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	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)
MI13456Pkn	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
NABTNO	N4-Acetylaminobutanal:NAD ⁺ oxidoreductase
NABTNom	N4-Acetylaminobutanal:NAD ⁺ oxidoreductase (m)
NADK	NAD kinase
NADPN	NADP nucleosidase
NAt3_lg	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 adenyllyltransferase, mitochondrial
NMPTRCOX	N-Methylputrescine:oxygen oxidoreductase (deaminating)
NNATm	nicotinate-nucleotide adenyllyltransferase, mitochondrial
NRVNCCPT1	carnitine O-palmitoyltransferase
NRVNCCPT2	carnitine transferase
NRVNCCRnt	transport into the mitochondria (carnitine)
NTD12	5'-nucleotidase (dIMP)
NTD21	5'-nucleotidase (UMP), lysosome
NTD2m	5'-nucleotidase (UMP), mitochondrial
NTD31	5'-nucleotidase (dCMP), lysosomal
NTD41	5'-nucleotidase (CMP), lysosome
NTD51	5'-nucleotidase (dTMP), lysosomal
NTD61	5'-nucleotidase (dAMP), lysosome
NTD71	5'-nucleotidase (AMP), lysosome
NTD81	5'-nucleotidase (dGMP), lysosomal
NTD91	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)
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	Quinolate 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
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 adenyllyltransferase
SELCYSLY	selenocysteine lyase
SELCYSLY2	selenocysteine lyase
SELCYSTGL	selenocystathionine g-lyase
SELCYSTS	selenocystathionine 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 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

UDPGLCDG	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
XOLDIOLONEm	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 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:2.3.1.16
 r0673 6-Lactoyl-5,6,7,8-tetrahydropterin:NADP+ 2-oxidoreductase Folate biosynthesis EC:1.1.1.16
 r0678 Acyl-[acyl-carrier-protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating, oxoacyl-
 r0681 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.16
 r0682 Butyryl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
 r0691 (3R)-3-Hydroxybutanoyl-[acyl-carrier protein]:NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.16
 r0692 (3R)-3-Hydroxydecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.16
 r0693 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.16
 r0694 (3R)-3-Hydroxyoctanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.16
 r0695 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase; (3R)-3-Hydroxyoctanoyl-[acyl-
 r0696 (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.16
 r0697 (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.16
 r0701 (3R)-3-Hydroxytetradecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.16
 r0702 (3R)-3-Hydroxypalmitoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.16
 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, oxoacyl-
 r0713 dodecanoyl-[acyl-carrier-protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating, oxoacyl-
 r0737 3-Ketolactose galactohydrolase Galactose metabolism EC:3.2.1.23
 r0760 butyryl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating, oxoacyl-
 r0761 (3R)-3-Hydroxyhexanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.16
 r0762 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.16
 r0763 Hexanoyl-[acyl-carrier protein]:oxoacyl- and enoyl-reducing and thioester-hydrolysing
 r0764 hexanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating, oxoacyl-
 r0765 Octanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
 r0766 Octanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating, oxoacyl-
 r0767 Decanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
 r0768 Decanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating, oxoacyl-
 r0769 (3R)-3-Hydroxydodecanoyl-[acyl-carrier-protein]:NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.16
 r0770 (3R)-3-Hydroxybutanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.16
 r0771 Tetradecanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
 r0772 Tetradecanoyl-[acyl-carrier protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating, oxoacyl-
 r0773 Hexadecanoyl-[acyl-carrier protein]:malonyl-CoA C-acyltransferase(decarboxylating, oxoacyl-
 r0775 Formamidopyrimidine nucleoside triphosphate 7,8-8,9-dihydrolase Folate biosynthesis EC:1.1.1.16
 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
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
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
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
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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
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

[illegible]

[illegible]

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
RE0577M	RE0577
RE0577X	RE0577
RE0578C	RE0578
RE0578M	RE0578
RE0578X	RE0578
RE0579C	RE0579
RE0579M	RE0579
RE0579X	RE0579
RE0580L	RE0580
RE0580R	RE0580
RE0581C	RE0581
RE0581R	RE0581
RE0582N	RE0582
RE0583N	RE0583
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RE0702M	RE0702
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
RE0916R	RE0916
RE0918C	RE0918
RE0918G	RE0918
RE0918R	RE0918
RE0919C	RE0919
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RE0920R	RE0920
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RE0925R	RE0925
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RE0927C	RE0927
RE0927R	RE0927
RE0928C	RE0928
RE0928R	RE0928
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RE0937C	RE0937
RE0938C	RE0938
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RE1050L	RE1050
RE1050N	RE1050
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RE1077C	RE1077
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RE1096M	RE1096
RE1096R	RE1096
RE1099C	RE1099
RE1099G	RE1099
RE1099L	RE1099
RE1099R	RE1099
RE1100G	RE1100
RE1100L	RE1100
RE1100R	RE1100
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RE1135R	RE1135
RE1233M	RE1233
RE1234C	RE1234
RE1235C	RE1235
RE1236C	RE1236
RE1238X	RE1238
RE1240C	RE1240
RE1266C	RE1266

RE1308C	RE1308
RE1308M	RE1308
RE1309C	RE1309
RE1309M	RE1309
RE1310C	RE1310
RE1310M	RE1310
RE1311C	RE1311
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RE1317C	RE1317
RE1441G	RE1441
RE1473C	RE1473
RE1508C	RE1508
RE1514M	RE1514
RE1514X	RE1514
RE1516X	RE1516
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RE1518X	RE1518
RE1519X	RE1519
RE1520X	RE1520
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RE1534X	RE1534
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RE1538X	RE1538
RE1539C	RE1539
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RE1573X	RE1573
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RE1582R	RE1582
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RE1630R	RE1630
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RE1632C	RE1632
RE1632R	RE1632
RE1635C	RE1635
RE1635M	RE1635
RE1635R	RE1635
RE1635X	RE1635
RE1651C	RE1651
RE1653C	RE1653
RE1699C	RE1699
RE1700C	RE1700
RE1701C	RE1701
RE1702C	RE1702
RE1711C	RE1711

RE1711M	RE1711
RE1796C	RE1796
RE1803C	RE1803
RE1806C	RE1806
RE1806R	RE1806
RE1808R	RE1808
RE1809C	RE1809
RE1809R	RE1809
RE1811C	RE1811
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RE1812C	RE1812
RE1812R	RE1812
RE1815C	RE1815
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RE1835M	RE1835
RE1835X	RE1835
RE1836C	RE1836
RE1836M	RE1836
RE1846C	RE1846
RE1846X	RE1846
RE1860C	RE1860
RE1899C	RE1899
RE1904C	RE1904
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RE1905C	RE1905
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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)	tauroolithocholate 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-flalpha 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_adpcb1(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

```

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

```

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] = findStoichConsistentSubset(model,massBalanceCheck,printLevel);
    else
        %print out problematic reactions to file
        resultsFileName=[resultsPath filesep model.modelID];
        [SConsistentMetBool,SConsistentRxnBool,SInConsistentMetBool,SInConsistentRxnBool] = 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 consistent
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
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),' ')
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
        fprintf('%6u\t%6u\t%s\n',nnz(model.SIntMetBool),nnz(model.SIntRxnBool),' ')
    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);

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

if nnz(maxConservationMetBool)==size(model.S,1) && nnz(maxConservationRxnBool)=
    checksPassed=checksPassed+1;
    if printLevel>1
        fprintf('%6u\t%6u\t%s\n',nnz(maxConservationMetBool),nnz(maxConservatio
    end
end

%Check that each of the reactions in the model (with open external reactions) i
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,fluxInCons

if nnz(fluxConsistentMetBool)==size(model.S,1) && nnz(fluxConsistentRxnBool)==s
    checksPassed=checksPassed+1;
    if printLevel>1
        fprintf('%6u\t%6u\t%s\n',nnz(fluxConsistentMetBool),nnz(fluxConsistentR
    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
    end
end
save([resultsFileName '_consistent.mat'],'model')
end

```

REFERENCES

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