

### Convert a reconstruction into a flux balance analysis model

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**Citizenship:**

## INTRODUCTION

model with quality control during the reconstruction process, this is not appropriate to assume that any reconstruction can be converted directly to 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 networks. 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  $M$  reactants involved in  $N$  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 Recon3D reconstruction.

## PROCEDURE

Select reconstruction to convert into a model and enter parameters

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

```
clear model
if ~exists('modelDir'),'mkdir')
    %Specify your own model, or use Recon2-Model instead
    if 0
        T1filename='Recon2_Model';
        directory='~/work/figCloud/projects/Recon2/figCloud/projects/reconModel/data/recon2-comparisonModels';
        model = loadIdentifiedModel(T1filename,directory);
    else
        T1filename='Recon2_Model.mat';
        if exists('Recon2_Model.mat'),'T1'==2
            model = readCIModel(T1filename);
        end
    end
    model.L_cenSize(T1size(model.L_N,1),2)='R';
    model.DIRg = model.L;
else
    model=load(DIRg);
end
```

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

or 181149403

Choose the direction to place the results

```
basePath = "/work/30g/1000/"
resultPaths = basePath + "programReconstruction/projects/reconModels/results/recon/" + model.modelID
resultFileName = resultPaths + fileName + model.modelID
```

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

```
17 result(resultPath, "dir")
    mkdir(resultPath)
end
cat(resultPath)
```

*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.*

```
17 0
    diary([resultsCPU letname '_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.

```

@getT_n@K@ = size(model.S)
fprintf('Nb of %s : %d\n', RootS, #Roots)

Roots = zeros(1, #Roots)

fprintf('Nb of %s : %d\n', @get_n@K@, size(S, 1))

```

1994.02 21079 9a4a74.

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

model: the source model,  $n$  is



```

    fprintf('NulTNuTNuN',dMet,dMet,' remaining.')
```

```

end

---Checking for Remove any trivial rows and columns of the stoichiometric matrix---
dMet=dMet
NulN TNU Totals.
0 0 duplicates removed.
NulN TNU remaining.
```

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

```

mode l2 r g=mode l;
dupDetectMethod='FR';
dupDetectMethod='S';
reverseFlag=0;
[mode lOut,reverseIndex, keyTran lnd]= checkDuplicateOn (mode l,dupDetectMethod,reverseFlag,prntLevel-2);
```

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

```

l7 length(reverseIndex);
l=rev l g=0;
set l g=1;
%not all reactions reversible that are duplicates
mode l, l= (reverseIndex)~=mode l, l, reverseIndex);
%remove duplicates
mode l = reverseIndex(mode l,mode l,reverseIndex), l, reverseFlag, set l g=1;
end
```

Display the statistics on the duplicate reactions.

```

[dMetR,dMetC]=size(mode lOut,3);
[dMetR,dMetC]=size(mode l,3);
l7 dMetR==dMetC && dMetR==dMetC && prntLevel=0
fprintf('NulN',---Remove any duplicate reactions---')
[dMetR,dMetC]=size(mode lOut,3);
[dMetR,dMetC]=size(mode l,3);
fprintf('NulTNuTNuN',dMetR,dMetC,' Totals.')
```

```

end

---Remove any duplicate reactions---
dMet=dMet
NulN TNU Totals.
0 0 duplicates removed.
NulN TNU 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.

```

mode l=mode l;
```

Find the proton indices in different compartments. A proton, with index *i*, is assumed to be represented by an abbreviation within model.mets() like *H<sub>i</sub><sup>+</sup>*, where *i* denotes the compartment symbol.

```

dMetChar=rev l g=length(mode l,3);
for d=1:length(mode l,3)
    dMetChar(d,1)=length(mode l,3);
end
prntLevel=1-2;
disp(mode l,3);
end
```

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

```

mode l,3 (prntLevel,1)=0;
```

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

```

dupDetectMethod='FR';
reverseFlag=0;
[mode lOut,reverseIndex, keyTran lnd]= checkDuplicateOn (mode l,dupDetectMethod,reverseFlag,prntLevel-1);
```

```

Checking for reaction duplicates by stoichiometry (up to orientation) ...
Keep: B2NG lbn[s] -> lbn[s]
Duplicate: B2NGL lbn[s] -> lbn[s]
Warning: EX_h[s] has more than one replicate
Keep: EX_h[s] ->
Duplicate: HIR ->
Keep: GLC1R glc_B[s] -> glc_B[s]
Duplicate: GLC1_2 glc_B[s] -> glc_B[s]
Keep: NACDP aac[s] -> aac[s]
Duplicate: NACDP aac[s] -> aac[s]
Keep: OPR1a aro[s] + c1lr_b[s] -> aro[s] + c1lr_b[s]
Duplicate: OPR1T aro[s] + c1lr_b[s] -> aro[s] + c1lr_b[s]

```

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

```

17 length(removeDuplicates)
17 revFlag=0
setFlag=0
model = removeReactions(model, model, rownames(removeDuplicates), 1, revFlag, setFlag)
end

```

Display statistics of the removed reactions

```

17 printLevel0
[0PrT,0Ran]=size(modelPrT,0)
[0PrT,0Ran]=size(model,0)
fprintf("NbrPrT/NbrRan", "0PrT", "0Ran")
fprintf("NbrPrT/NbrT/NbrA", 0PrT,0Ran, " NbrA")
fprintf("NbrPrT/NbrT/NbrA", 0PrT-0PrT,0Ran-0Ran, " duplicate reactions upto proteins removed.")
fprintf("NbrPrT/NbrT/NbrA", 0PrT,0Ran, " remaining.")
end

```

```

NbrT NbrR NbrA
0 0 0 duplicate reactions upto proteins removed.
0 0 0 remaining.

```

```

%model_size
[0PrT,0Ran]=size(model,0)

```

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 reactions are exclusively involved in exchange reactions, and internal reactions otherwise. The first `findReactions` 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.

```

17 ~isTolEx(model, "EXOTR|TR|EX") || ~isTolEx(model, "EXOTR|TR|EX")
model = findReactions(model, [], 0, 0, 0, 0)
end

```

## EXPECTED RESULTS

In the returned model, `model.findReactions`, is a boolean of reactions heuristically thought to be mass balanced, while `model.findReactions` 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 misclassification 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.

```

model_size=0
model_size=(model_size+1)-1000
model_size=(model_size+1)-1000
17 1
17 ~isTolEx(model, "EXOTR|TR|EX") || ~isTolEx(model, "EXOTR|TR|EX")
getFlag=0
setFlag=0
getFlag=0
setFlag=0
[FluxConsistentReactions, FluxConsistentReactions, FluxConsistentReactions, FluxConsistentReactions, model] = findFluxConsistentSubset(model)
end
% Remove reactions that are flux inconsistent
17 any(FluxConsistentReactions)
17 revFlag=0
setFlag=0
model = removeReactions(model, model, rownames(FluxConsistentReactions), 1, revFlag, setFlag)
[0PrT,0Ran]=size(modelPrT,0)
[0PrT,0Ran]=size(model,0)
17 printLevel0
fprintf("NbrPrT", "0PrT")
fprintf("NbrPrT/NbrRan", "0PrT", "0Ran")
fprintf("NbrPrT/NbrT/NbrA", 0PrT,0Ran, " NbrA")
fprintf("NbrPrT/NbrT/NbrA", 0PrT-0PrT,0Ran-0Ran, " Flux inconsistent reactions removed.")

```



ADPGK1 adenylyl glycerol phosphate reductase  
ADPGP1 adenylyl glycerol phosphate acyltransferase  
ADPGL1 adenylyl glycerol phosphate transferase  
ADPGL1B N-acetyl-L-glutaryl-L-glutamate reductase, irreversible, mitochondrial  
ADPGL1C adenylylglutamate phosphate synthase  
ADPGL1TADPGL1C1C2C3C4C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100C101C102C103C104C105C106C107C108C109C110C111C112C113C114C115C116C117C118C119C120C121C122C123C124C125C126C127C128C129C130C131C132C133C134C135C136C137C138C139C140C141C142C143C144C145C146C147C148C149C150C151C152C153C154C155C156C157C158C159C160C161C162C163C164C165C166C167C168C169C170C171C172C173C174C175C176C177C178C179C180C181C182C183C184C185C186C187C188C189C190C191C192C193C194C195C196C197C198C199C200C201C202C203C204C205C206C207C208C209C210C211C212C213C214C215C216C217C218C219C220C221C222C223C224C225C226C227C228C229C230C231C232C233C234C235C236C237C238C239C240C241C242C243C244C245C246C247C248C249C250C251C252C253C254C255C256C257C258C259C260C261C262C263C264C265C266C267C268C269C270C271C272C273C274C275C276C277C278C279C280C281C282C283C284C285C286C287C288C289C290C291C292C293C294C295C296C297C298C299C300C301C302C303C304C305C306C307C308C309C310C311C312C313C314C315C316C317C318C319C320C321C322C323C324C325C326C327C328C329C330C331C332C333C334C335C336C337C338C339C340C341C342C343C344C345C346C347C348C349C350C351C352C353C354C355C356C357C358C359C360C361C362C363C364C365C366C367C368C369C370C371C372C373C374C375C376C377C378C379C380C381C382C383C384C385C386C387C388C389C390C391C392C393C394C395C396C397C398C399C400C401C402C403C404C405C406C407C408C409C410C411C412C413C414C415C416C417C418C419C420C421C422C423C424C425C426C427C428C429C430C431C432C433C434C435C436C437C438C439C440C441C442C443C444C445C446C447C448C449C450C451C452C453C454C455C456C457C458C459C460C461C462C463C464C465C466C467C468C469C470C471C472C473C474C475C476C477C478C479C480C481C482C483C484C485C486C487C488C489C490C491C492C493C494C495C496C497C498C499C500C501C502C503C504C505C506C507C508C509C510C511C512C513C514C515C516C517C518C519C520C521C522C523C524C525C526C527C528C529C530C531C532C533C534C535C536C537C538C539C540C541C542C543C544C545C546C547C548C549C550C551C552C553C554C555C556C557C558C559C560C561C562C563C564C565C566C567C568C569C570C571C572C573C574C575C576C577C578C579C580C581C582C583C584C585C586C587C588C589C590C591C592C593C594C595C596C597C598C599C600C601C602C603C604C605C606C607C608C609C610C611C612C613C614C615C616C617C618C619C620C621C622C623C624C625C626C627C628C629C630C631C632C633C634C635C636C637C638C639C640C641C642C643C644C645C646C647C648C649C650C651C652C653C654C655C656C657C658C659C660C661C662C663C664C665C666C667C668C669C670C671C672C673C674C675C676C677C678C679C680C681C682C683C684C685C686C687C688C689C690C691C692C693C694C695C696C697C698C699C700C701C702C703C704C705C706C707C708C709C710C711C712C713C714C715C716C717C718C719C720C721C722C723C724C725C726C727C728C729C730C731C732C733C734C735C736C737C738C739C740C741C742C743C744C745C746C747C748C749C750C751C752C753C754C755C756C757C758C759C760C761C762C763C764C765C766C767C768C769C770C771C772C773C774C775C776C777C778C779C780C781C782C783C784C785C786C787C788C789C790C791C792C793C794C795C796C797C798C799C800C801C802C803C804C805C806C807C808C809C810C811C812C813C814C815C816C817C818C819C820C821C822C823C824C825C826C827C828C829C830C831C832C833C834C835C836C837C838C839C840C841C842C843C844C845C846C847C848C849C850C851C852C853C854C855C856C857C858C859C860C861C862C863C864C865C866C867C868C869C870C871C872C873C874C875C876C877C878C879C880C881C882C883C884C885C886C887C888C889C890C891C892C893C894C895C896C897C898C899C900C901C902C903C904C905C906C907C908C909C910C911C912C913C914C915C916C917C918C919C920C921C922C923C924C925C926C927C928C929C930C931C932C933C934C935C936C937C938C939C940C941C942C943C944C945C946C947C948C949C950C951C952C953C954C955C956C957C958C959C960C961C962C963C964C965C966C967C968C969C970C971C972C973C974C975C976C977C978C979C980C981C982C983C984C985C986C987C988C989C990C991C992C993C994C995C996C997C998C999

[illegible]

[illegible]



INACTE\_u Isolaic acid dehydrogenase (mito)  
 INH0a inosine kinase, mitochondrial  
 INH1L inosine facilitated transport from lysosome  
 INH1M inosine facilitated transport into mitochondria  
 INP0P inosine polyphosphate transport (IMP)  
 IOX0g potassium transport via proton antiport  
 LACT1g D-glactosidase, lysosomal  
 LCA2a L-lactate dehydrogenase, mitochondrial  
 LCA3a L-lactate dehydrogenase, mitochondrial  
 LCT0L lactose transport from cytosol to lysosome (via autophagolysosis)  
 LCYT2Tc L-cysteine:2-methylthio amine transferase, mitochondrial  
 LDH\_La L-lactate dehydrogenase  
 LHC0T0B1r leucine:histidine transfer  
 LINCPT1 carnitine D-palmitoyltransferase  
 LINCPT2 transport into the mitochondria (carnitine)  
 LINC0B0 transport into the mitochondria (carnitine)  
 LIP0L Lipase transport via sodium symport  
 L\_LACTm L-lactate transport via diffusion (cytosol to mitochondria)  
 LMS0D cytochrome P450 lauric acid 14-alpha-demethylase (CYP4)  
 LSL L-serine S formation  
 LTC0L L-tryptophan decarboxylase  
 LTP0T1a histidine-tyrosine N-methyltransferase, nuclear  
 LTP0T2a histidine-tyrosine N-methyltransferase, nuclear  
 LTP0T3a histidine-tyrosine N-methyltransferase, nuclear  
 MALT0r MALT transaminase, endoplasmic reticulum  
 MGMT2c MGT phosphoethanolamine transferase, endoplasmic reticulum  
 MALT1g alpha-glucosidase, lysosomal  
 MNG\_0B1r mannosidase II, endoplasmic reticulum (glucosylated-producing)  
 MNG\_1B0r mannosidase II, endoplasmic reticulum (glucosylated-producing)  
 MNG\_0B1r mannosidase II, endoplasmic reticulum (glucosylated-producing)  
 MNG\_1C0r mannosidase II, endoplasmic reticulum (glucosylated-producing)  
 MNG0a mannosamine oxidase (L-4-methylphenol)  
 MCDy Methyl-Cad decarboxylase peroxisomal  
 MCD1S Methyl-Cad-BCP transacylase  
 MCD2a Methyl-Cad-BCP transacylase, mitochondrial  
 MELAT0B0C Melanin:oxygen 2,3-di-oxygenase (indole-decylating)  
 MEND0r Melanin transporter, endoplasmic reticulum  
 MESC0a Mescanoyl-Cad pyruvate-lyase  
 MGL0a methylglucosamine, mitochondrial  
 M1340PK inositol-1,3,4,5,6-pentakisphosphate 2-kinase  
 M1340PI inositol-1,3,4,5,6-pentakisphosphate nuclear transport (diffusion)  
 M1340PKa inositol-1,3,4,5-triphosphate 0-kinase, nucleus  
 M1340PKa inositol-1,3,4,6-tetrakisphosphate 3-kinase, nucleus  
 M1340PI 1D-Myo-Inositol 1,3,4,6-tetrakisphosphate nuclear transport (diffusion)  
 M1340PK inositol-1,3,6-triphosphate 0-kinase  
 M1340PKa inositol-1,4,5,6- tetrakisphosphate 3-kinase, nucleus  
 M1340PKa inositol-1,4,5-triphosphate 0-kinase, nucleus  
 M1340PKa inositol-1,4,5-triphosphate 3-kinase, nucleus  
 M1340PK inositol-1,4,5,6-tetrakisphosphate 3-kinase  
 MCT0Tc 2-methylsuccinate dehydrogenase  
 MEND0PI inositol hexakisphosphate nuclear transport (diffusion)  
 MGL0c Melanodextrin glucosidase (melaninase)  
 MGL1g Melanodextrin glucosidase (melaninase), lysosome  
 MNC Methylmethyl-Cad decarboxylase  
 MNC2y Methylmethyl-Cad decarboxylase, peroxisomal  
 MND0 M-D-oxymethylsuccinate:ADP oxidoreductase  
 MND0a M-D-oxymethylsuccinate:ADP oxidoreductase (x)  
 NDK NDK kinase  
 NADPH NADP nucleoside  
 NAL1g sodium proton antiporter (NaH in 1:1)  
 NDK0a nucleoside-diphosphate kinase (ATP:GDP), mitochondrial  
 NDK2a nucleoside-diphosphate kinase (ATP:GDP), mitochondrial  
 NDK0a nucleoside-diphosphate kinase (ATP:GDP), mitochondrial  
 N1P0C2D0B1e nucleoside transport  
 NPM0T nucleoside-nucleotide adenylyltransferase, mitochondrial  
 NPMTC0C D-Methylsuccinate:oxygen oxidoreductase (deaminating)  
 NMTa nucleoside-nucleotide adenylyltransferase, mitochondrial  
 NUNCPT1 carnitine D-palmitoyltransferase  
 NUNCPT2 carnitine transferase  
 NUNC0B0 transport into the mitochondria (carnitine)  
 NTD12 D'-nucleoside (GDP)  
 NTD21 D'-nucleoside (GMP), lysosome  
 NTD2a D'-nucleoside (GMP), mitochondrial  
 NTD31 D'-nucleoside (GDP), lysosome  
 NTD41 D'-nucleoside (GMP), lysosome  
 NTD51 D'-nucleoside (GDP), lysosome  
 NTD61 D'-nucleoside (GMP), lysosome  
 NTD71 D'-nucleoside (GMP), lysosome  
 NTD81 D'-nucleoside (GDP), lysosome  
 NTD91 D'-nucleoside (GMP), lysosome

**NB017169** protein tyrosine kinase [Lysine transport (nucleus to ER)]  
**NTVW18** Na/Gluide triphosphate pyrophosphorylase (dtp)  
**NTVW11** Na/Gluide triphosphate pyrophosphorylase (slp)  
**NTVP9** Na/Gluide triphosphate pyrophosphorylase (slp)  
**P4S3A5** cytochrome P450 3A5  
**P4S6A1r** cytochrome p450 P450 3A13  
**P4S6B1r** cytochrome P450 3B5  
**P4S6F1C1r** cytochrome p450 F1C1/F2  
**P4S6F1C1r** cytochrome p450 F1C1/F2  
**P4S6F1R1r** cytochrome p450 F1R  
**P4S6L7R1r** cytochrome p450 7A1/1A2/B1  
**PC1P02G** Procollagen-Lysine 1, 2-oxoglutarate 5-dehydrogenase  
**PDS15** 3',5'-cyclic-nucleotide phosphodiesterase,Gelgi  
**PDS16** 3',5'-cyclic-nucleotide phosphodiesterase, Gelgi  
**PL\_H1g** phosphatidylcholine:serine scramblase  
**PFCCGG3D1Y** Pseudomonas Cu transporter (ER)  
**PEPGT15e** peptide (Tyrosine) nuclear transport via diffusion  
**PGE1r** Prostaglandin-H 2-oxygenase [Precursor]  
**PGE1r** Prostaglandin H synthase  
**PGLYCP** Phosphoglycerate phosphatase  
**PHB1A1** phenylalanine transaminase  
**PHB1A2** phenylalanine transaminase (x)  
**PHB1ACn** phosphatidylcholine/ 3-bisphosphate phospholipase C, nucleus  
**PHGPBRc** phosphatidylcholine/ 3-phosphate 3-kinase, endoplasmic reticulum  
**PHGPBRc** phosphatidylcholine/ 3-phosphate 3-kinase, endoplasmic reticulum  
**PD12c** phosphate transporter, mitochondrial  
**PLA2** phospholipase A2  
**PLXTP19r** protein tyrosine peptidase (endoplasmic reticulum)  
**PM1121A8Ph** 3-diphosphoinositol-1,2,3,4,5-pentabiphosphate dihydrophosphatase  
**PM1121A8Ph** 3-diphosphoinositol-1,2,3,4,5-pentabiphosphate dihydrophosphatase, nucleus  
**PM1130A8Ph** diphosphoinositol-3,4,5-bis-trisubstrate dihydrophosphatase  
**PM1130A8Ph** diphosphoinositol-3,4,5-bis-trisubstrate dihydrophosphatase, nucleus  
**PNK2c** penicillinase kinase (mitochondrial)  
**PPA2** isomeric triphosphatase  
**PPA2c** isomeric triphosphatase, mitochondrial  
**PPM1121A8Pt** 3-diphosphoinositol pentabiphosphate nuclear transport (diffusion)  
**PPM1130A8Pt** phosphatidylcholine/ tetra-biphosphate nuclear transport (diffusion)  
**PPPR** pyruvate:cytochrome oxidoreductase (hydroxylating,decarboxylating)  
**PPPTN** Isomeric triphosphate transport through nuclear pore  
**PPSGAG21r** L-Proline, 2-oxoglutarate:cytochrome oxidoreductase (4-hydroxylating) (ER)  
**PROD1Zr** D-proline reductase transport via proton symport  
**PROD1Zr** D-proline reductase transport via proton symport (lysosome)  
**PROD1Zr** L-proline reductase transport via proton symport (lysosome)  
**PROL1Zr** L-proline transport, mitochondrial  
**PPMKGADHDr** Propenyl-Cou hydrolyase (x)  
**PL\_H1er** phosphatidylcholine scramblase  
**PL\_H1ig** phosphatidylcholine scramblase  
**PTE1c** peroxisomal asyl-CoA thioesterase  
**PTE1c** peroxisomal asyl-CoA thioesterase  
**PTNP1** 8-pyrenyltetrahydropyran synthase  
**PTNP1r** 8-pyrenyltetrahydropyran synthase, nuclear  
**PTNG1Zr** Malonate acetyltransferase  
**PUPBP1r** Pyridoxamine 3'-phosphate transport via diffusion, mitochondria  
**PUGXP1r** Pyridoxal 3'-phosphate transport via diffusion, mitochondria  
**PVLALDDe** Pevalil aldehyde:NAD+ oxidoreductase  
**PVLALDDe** Pevalil aldehyde:NAD+ oxidoreductase (x)  
**QU1LVN** Quinolinate Synthase (Eukaryotic)  
**R1ir** Retinoate transport, nuclear  
**RAB\_K\_2** R-vibrio kinase  
**RETNCO** Retinoyl CoA formation  
**RSTT\_2\_R total** Fluo 2 position.  
**RSTT\_3\_R total** Fluo 3 position.  
**RSTT1\_R total** Fluo  
**RSTT2\_R total** Fluo  
**RSTT3\_R total** Fluo  
**RSTT4\_R total** Fluo  
**RSTT5\_R total** Fluo  
**RSTT6\_R total** Fluo  
**RTTSL1CBMP1T** carnitine fatty-acyl transferase  
**RTTSL1CBMP1T** R group transport into the mitochondria  
**RTTSL1CBM1** R group transport into the mitochondria  
**RTTSL1CBMP1T** carnitine fatty-acyl transferase  
**RTTSL1CBMP1T** R group transport into the mitochondria  
**RTTSL1CBM1** R group transport into the mitochondria  
**RTTSL1CBMP1T** carnitine fatty-acyl transferase  
**RTTSL1CBMP1T** R group transport into the mitochondria  
**RTTSL1CBM1** R group transport into the mitochondria  
**Maria1ig** fatty acid intracellular transport  
**S2T1g** chondroitin 2-sulfotransferase, Golgi  
**S2T2g** chondroitin 2-sulfotransferase, Golgi  
**S2T3r** uronyl 2-sulfotransferase, Golgi

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c0766 [malonyl-acyl-carrier protein][malonyl-CoA C-acyltransferase] acarbonylating, acetyl- and acetyl-reducing and thiamine-hydrolysi  
 c0767 Tetradecanoyl-[acyl-carrier protein][malonyl-acyl-carrier-protein] C-acyltransferase [decarbonylating] Fatty acid biosynthesis EC:2.3.  
 c0768 Decanoyl-[acyl-carrier protein][malonyl-CoA C-acyltransferase] acarbonylating, acetyl- and acetyl-reducing and thiamine-hydrolysi  
 c0769 Decanoyl-[acyl-carrier protein][malonyl-acyl-carrier-protein] C-acyltransferase [decarbonylating] Fatty acid biosynthesis EC:2.3.  
 c0769 [3R]-5-Hydroxydecanoyl-[acyl-carrier-protein] NADP+ oxidoreductase Fatty acid biosynthesis EC:2.3.1.20  
 c0770 [3R]-5-Hydroxydecanoyl-[acyl-carrier-protein] hydro-lyase Fatty acid biosynthesis EC:2.3.1.25  
 c0771 Tetradecanoyl-[acyl-carrier protein][malonyl-CoA C-acyltransferase] decarbonylating, acetyl- and acetyl-reducing and thiamine-hydro  
 c0772 Tetradecanoyl-[acyl-carrier protein][malonyl-acyl-carrier-protein] C-acyltransferase [decarbonylating] Fatty acid biosynthesis EC  
 c0773 Hexadecanoyl-[acyl-carrier protein][malonyl-acyl-carrier-protein] C-acyltransferase [decarbonylating] Fatty acid biosynthesis EC:2.3.  
 c0775 Pyrimidinopyrimidine nucleoside triphosphate 7,8-B,9-dihydrolase Purate biosynthesis EC:3.5.5.36  
 c0776 c0776  
 c0777 GTP 7,8-B,9-dihydrolase Purate biosynthesis EC:3.5.5.36  
 c0778 c0778  
 c0788 sphingosine-2-phosphate palmitaldehyde-lyase sphingolipid metabolism EC:6.3.2.27  
 c0800 Virtual reaction/potential definition  
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 c0805 Vesicular transport  
 c0806 Vesicular transport  
 c0807 Vesicular transport  
 c0808 Vesicular transport  
 c0825 Vesicular transport  
 c0826 Transport reaction  
 c0839 Facilitated transport reaction  
 c0836 Facilitated transport reaction  
 c0825 Vesicular transport  
 c0827 Free diffusion  
 c0836 Facilitated transport reaction  
 c0892 Na+/bile acid cotransporter Active transport  
 c0888 Facilitated diffusion  
 c0885 Facilitated diffusion  
 c0882 Facilitated diffusion  
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 c0884 Facilitated diffusion  
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 c0886 Facilitated diffusion  
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 c0839 Major Facilitator(MF) TCRB:J.A.38.6.7  
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 c0842 Vesicular transport  
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 c0844 Facilitated transport reaction  
 c0847 Vesicular transport  
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 c0875 Transport reaction  
 c0873 Transport reaction  
 c0876 Vesicular transport  
 c0876 Facilitated transport reaction  
 c0877 Vesicular transport  
 c0888 Vesicular transport  
 c0882 Vesicular transport  
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 c0892 Albumin Protein assembly  
 c0893 serpin peptidase inhibitor, clade A (alpha-1 antiproteinase, antitrypsin), member 3 Protein assembly  
 c0894 serpin peptidase inhibitor, clade A (alpha-1 antiproteinase, antitrypsin), member 1 Protein assembly  
 c0895 apolipoprotein B Protein assembly  
 c0896 NADH dehydrogenase (ubiquinone) 1, alpha/beta subcomplex, 1 Protein assembly  
 c0897 ACP Protein assembly  
 c0896 Apo-CII Protein assembly  
 c0899 Apo-CII Protein assembly  
 c0900 Apo-CIII Protein assembly  
 c0905 Fibrinogen alpha chain Protein assembly  
 c0902 Haptoglobin Protein assembly  
 c0903 Plasminogen Protein assembly  
 c0904 Prothrombin Protein assembly  
 c0905 TN Protein assembly  
 c0912 Apo-B Protein assembly  
 c0913 Apo-AI Protein assembly  
 c0927 Transport reaction  
 c0926 Transport reaction

r0109 Transport reaction  
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 r0112 Transport reaction  
 r0113 Transport reaction  
 r0114 methylsterol monooxygenase Biosynthesis of steroids EC:1.14.14.72  
 r0115 hydroxysteroid (17-beta) dehydrogenase 7 Biosynthesis of steroids EC:1.1.1.178  
 r0116 steroid-16alpha-carboxylate 3-dehydrogenase (decarboxylating) Biosynthesis of steroids EC:1.1.1.179  
 r0117 NAD(P)-dependent steroid dehydrogenase-like EC:1.1.1.179  
 r0148 Vesicular transport  
 r0149 Biosynthesis of steroids Enzyme catalyzed  
 r0239 Vesicular transport  
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 r0293 EC:6.2.1.3  
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 r0299 HMG Protein assembly  
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 r0314 fatty acid synthase Polyunsaturated fatty acid biosynthesis EC:2.3.1.85  
 r0315 fatty acid synthase Polyunsaturated fatty acid biosynthesis EC:2.3.1.85  
 r0316 fatty acid synthase Polyunsaturated fatty acid biosynthesis EC:2.3.1.85  
 r0317 oleoyl-CoA hydratase EC:2.3.1.85  
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 r0321 gamma-glutamyl hydrolase EC:3.4.19.9  
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 r0392 amylase-1,6-glucosidase, 4-alpha-glucanotransferase EC:3.2.2.1.33  
 r0393 EC:3.2.1.31  
 r0394 EC:3.2.1.31  
 r0395 carnitine acetyltransferase EC:2.3.1.7  
 r0396 EC:3.2.1.31  
 r0399 carnitine acetyltransferase EC:2.3.1.7  
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 r0403 Protein degradation  
 r0411 O-Galactoyl-6-acetyl-6-galactosaminyl-10-acetylneuraminyl-10- galactosyl-6-glucosylamide galactohydrolase EC:3.2.1.23  
 r0418 [acyl-carrier-protein] 3-pantetheine-phosphatidyltransferase Pantetheinate and CoA biosynthesis EC:1.3.1.4.14  
 r0419 2-Oxoglutarate 3-epigallocatechin-3-O-gallate 2-oxidoreductase Pyridoxine metabolism EC:1.17.4.1  
 r0422 2-Oxoglutarate 3-epigallocatechin-3-O-gallate 2-oxidoreductase Pyridoxine metabolism EC:1.17.4.1  
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 r0427 Transport reaction  
 r0428 Transport reaction  
 r0443 Active transport  
 r0445 Transport reaction  
 r0447 headonatalADP+ delta2-oxidoreductase EC:1.3.1.27  
 r0468 Facilitated transport reaction  
 r0472 long-chain-acyl-CoA dehydrogenase EC:1.3.1.96.33  
 r0474 EC:4.2.1.27  
 r0477 EC:1.1.1.35  
 r0479 EC:2.3.1.38  
 r0483 EC:2.3.1.38  
 r0485 Glycoside-Pectinase-Hexuronide (GPH)Cation Symporter TC26:2.3.28.1.1  
 r0487 Glycoside-Pectinase-Hexuronide (GPH)Cation Symporter TC26:2.3.28.1.1  
 r0489 Glycoside-Pectinase-Hexuronide (GPH)Cation Symporter TC26:2.3.28.1.1  
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 r0532 ATP-binding Casorin (ABC) TC26:3.4.1.288.15  
 r0533 ATP-binding Casorin (ABC) TC26:3.4.1.288.15  
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| 0016769 | 0016770 |
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[illegible]



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





```

%save the model with open exchanges as the default generic
%model
model load (open)
if prctave == 0
    fprintf('no\n')
    %open external reactions in stoichiometrically and flux consistent. A flux balance model generated from a re
end
end
save([result if isfalse '_consistent.mat'], 'model')
end

```

## REFERENCES

- Georgyan, A., Postman, M. G., Fell D., Detection of stoichiometric inconsistencies in biodecoute models. *Bioinformatics*, 26(78)2069–81, 2008.
- Fleming, R.M.T., et al., Cardinality optimisation in constraint-based modeling -Application to Recon 3D (submitted), 2017.
- Brunk, S. et al: Recon 3D: A resource enabling a three-dimensional view of gene variation in human metabolism. (submitted) 2017.