Analyse properties of conserved moieties

```
tutorial_initConservedMoietyPaths
```

```
modelName = 
'DAS'
projectDir = 
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties'
dataDir = 
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/models/'
softwareDir = 
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/software/'
visDataDir = 
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/visualisation/'
resultsDir = 
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/results/DAS_ConservedMo
rxnfileDir = 
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/mini-ctf/rxns/atom
```

```
if ~recompute
    load([resultsDir  modelName '_ConservedMoietiesAnalysis.mat'])
    return
end
```

Load the atomically resolved models derived from identifyConservedMoieties.m

```
load([resultsDir modelName '_arm.mat'])
```

Basic properties of atomically resolved models

```
disp(arm)
```

```
      MRH: [1×1 struct]
     dATM: [1×1 digraph]
     M2Ai: [11×170 double]
     Ti2R: [176×4 double]
     Ti2I: [176×6 double]
      ATG: [1×1 graph]
      M2A: [11×170 double]
      A2R: [114×4 double]
     A2Ti: [114×176 double]
      I2A: [6×170 double]
      A2I: [114×6 double]
      I2C: [6×56 double]
      C2A: [56×170 double]
      A2C: [114×56 double]
      MTG: [1×1 graph]
      I2M: [6×26 double]
      M2I: [20×6 double]
      M2M: [11×26 double]
      M2R: [20×4 double]
        L: [6×11 double]
```

Load the model, unless it is also saved with the results.

```
if 0
    load([dataDir modelName '.mat'])
    model = iDopaNeuro;
```

```
else
    model=arm.MRH;
end
```

Identify the stoichiometrically consistent subset of the model

```
massBalanceCheck=0;
printLevel=1;
[SConsistentMetBool, SConsistentRxnBool1, SInConsistentMetBool, SInConsistentRxnBool, u
    = findStoichConsistentSubset(model,massBalanceCheck,printLevel);
```

```
--- findStoichConsistentSubset START ----
--- Summary of stoichiometric consistency ----
    11        11     totals.
     0         7     heuristically external.
    11         4     heuristically internal:
    11         4     ... of which are stoichiometrically consistent.
     0         0     ... of which are stoichiometrically inconsistent.
     0         0     ... of which are of unknown consistency.
    11         4     Confirmed stoichiometrically consistent by leak/siphon testing.
--- findStoichConsistentSubset END ----
Warning: Model did not contain a genes field. Building it along with the rules field
Warning: This function can be only be used on a model that has grRules field!\n
```

Remove non-atom mapped part of the model, but keep the external reactions

```
keepRxnBool = getCorrespondingCols(arm.MRH.S, arm.MRH.metAtomMappedBool, true(size(arm.
keepRxnBool = keepRxnBool & ~SConsistentRxnBool1;
removeRxnBool = ~(arm.MRH.rxnAtomMappedBool | keepRxnBool);
model = removeRxns(arm.MRH, arm.MRH.rxns(removeRxnBool));
```

Identify the stoichiometrically consistent subset of the model

```
massBalanceCheck=1;
printLevel=1;
[SConsistentMetBool, SConsistentRxnBool2, SInConsistentMetBool, SInConsistentRxnBool, u
    = findStoichConsistentSubset(model,massBalanceCheck,printLevel);
```

```
--- findStoichConsistentSubset START ----
--- Summary of stoichiometric consistency ----
    11        11     totals.
     0         7     heuristically external.
    11         4     heuristically internal:
    11         4     ... of which are stoichiometrically consistent.
     0         0     ... of which are stoichiometrically inconsistent.
     0         0     ... of which are of unknown consistency.
---
     0         0     heuristically internal 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).
    11         4     Confirmed stoichiometrically consistent by leak/siphon testing.
--- findStoichConsistentSubset END ----
Warning: Model did not contain a genes field. Building it along with the rules field
Warning: This function can be only be used on a model that has grRules field!\n
```

Table of model properties

```
rankN=getRankLUSOL(arm.MRH.S(arm.MRH.metAtomMappedBool,arm.MRH.rxnAtomMappedBool));
```

```
Warning: There was an error loading the library "/home/rfleming/work/sbgCloud/code/fork-
cobratoolbox/external/base/solvers/lusol/src/libclusol.so"
Unrecognized function or variable 'libclusol_proto_glnxa64'.
Caught error using lusol interface. Proceeding with matlab LU implementation (slower)
```

```
rankL=getRankLUSOL(arm.L);
```

```
Warning: There was an error loading the library "/home/rfleming/work/sbgCloud/code/fork-
cobratoolbox/external/base/solvers/lusol/src/libclusol.so"
Unrecognized function or variable 'libclusol_proto_glnxa64'.
Caught error using lusol interface. Proceeding with matlab LU implementation (slower)
```

```
rankdATM=getRankLUSOL(incidence(arm.dATM));
```

```
Warning: There was an error loading the library "/home/rfleming/work/sbgCloud/code/fork-
cobratoolbox/external/base/solvers/lusol/src/libclusol.so"
Unrecognized function or variable 'libclusol_proto_glnxa64'.
Caught error using lusol interface. Proceeding with matlab LU implementation (slower)
```

```
rankATG=getRankLUSOL(incidence(arm.ATG));
```

```
Warning: There was an error loading the library "/home/rfleming/work/sbgCloud/code/fork-
cobratoolbox/external/base/solvers/lusol/src/libclusol.so"
Unrecognized function or variable 'libclusol_proto_glnxa64'.
Caught error using lusol interface. Proceeding with matlab LU implementation (slower)
```

```
rankMTG=getRankLUSOL(incidence(arm.MTG));
```

```
Warning: There was an error loading the library "/home/rfleming/work/sbgCloud/code/fork-
cobratoolbox/external/base/solvers/lusol/src/libclusol.so"
Unrecognized function or variable 'libclusol_proto_glnxa64'.
Caught error using lusol interface. Proceeding with matlab LU implementation (slower)
```

```

TT={'Model', 'm+'  , 'Metabolites', size(arm.MRH.S,1);
       ''     , 'm'   , 'Mapped metabolites', nnz(arm.MRH.metAtomMappedBool);
   ''     , 'n+'  , 'Reactions', size(arm.MRH.S,2);
   ''     , ''     ,  'Internal reactions', nnz(SConsistentRxnBool1);
   ''     , ''     ,  'External reactions', nnz(~SConsistentRxnBool1);
   ''     , 'n'   , 'Mapped reactions', nnz(arm.MRH.rxnAtomMappedBool);
   'Mapped model'     , 'm'   , 'size(model.S,1)', rankN;
   ''     , 'n+k'   , 'size(model.S,2)', size(model.S,2);
   ''     , ''     ,  'Internal reactions', nnz(SConsistentRxnBool2);
   ''     , ''     ,  'External reactions', nnz(~SConsistentRxnBool2);
   ''     , 'r'   , 'Rank(N)', rankN;
   ''     , 'm-r' , 'Row rank deficiency(N)', nnz(arm.MRH.metAtomMappedBool) - rankN;
   ''     , ''     ,  'Isomorphism classes', size(arm.L,1);
   ''     , ''     ,  'Independent isomorphism classes', rankL;
   'MTG'  , ''     ,  'Moieties', size(arm.I2M,2);
   ''     , ''     ,  'Moiety transitions', size(arm.M2I,1);
   ''     , ''     ,  'Rank(M)', rankMTG;
  'ATG'   , ''     ,  'Atoms', size(arm.I2A,2);
   ''     , ''     ,  'Atom transitions', size(arm.A2I,1);
   ''     , ''     ,  'Rank(A)', rankATG;
   ''     , ''     ,  'Row rank deficiency(A)', size(arm.I2A,2) - rankATG;
   ''     , ''     ,  'Components', size(arm.C2A,1);
'dATM'    , ''    ,  'Atoms', size(arm.dATM.Nodes,1);
   ''     , ''    ,  'Directed atom transition instances', size(arm.dATM.Edges,1);
   ''     , ''    ,  'Rank(dATM)', rankdATM;
   ''     , ''    ,  'Row rank deficiency(dATM)', size(arm.dATM.Edges,1) - rankdATM;
   ''     , ''    ,  '', NaN;
   };
disp(TT)
```

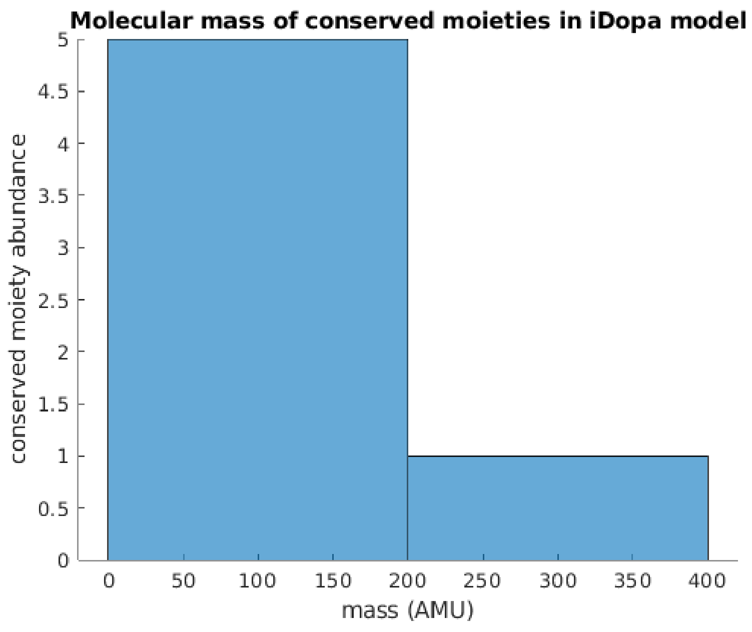
```
    {'Model'       }    {'m+'    }    {'Metabolites'                 }    {[ 11]}
    {0×0 char      }    {'m'     }    {'Mapped metabolites'          }    {[ 11]}
    {0×0 char      }    {'n+'    }    {'Reactions'                   }    {[ 11]}
    {0×0 char      }    {0×0 char}    {'Internal reactions'          }    {[  4]}
    {0×0 char      }    {0×0 char}    {'External reactions'          }    {[  7]}
    {0×0 char      }    {'n'     }    {'Mapped reactions'            }    {[  4]}
    {'Mapped model'}    {'m'     }    {'size(model.S,1)'             }    {[  4]}
    {0×0 char      }    {'n+k'   }    {'size(model.S,2)'             }    {[ 11]}
    {0×0 char      }    {0×0 char}    {'Internal reactions'          }    {[  4]}
    {0×0 char      }    {0×0 char}    {'External reactions'          }    {[  7]}
    {0×0 char      }    {'r'     }    {'Rank(N)'                     }    {[  4]}
    {0×0 char      }    {'m-r'   }    {'Row rank deficiency(N)'      }    {[  7]}
    {0×0 char      }    {0×0 char}    {'Isomorphism classes'         }    {[  6]}
    {0×0 char      }    {0×0 char}    {'Independent isomorphism clas…'}    {[  6]}
    {'MTG'         }    {0×0 char}    {'Moieties'                    }    {[ 26]}
    {0×0 char      }    {0×0 char}    {'Moiety transitions'          }    {[ 20]}
    {0×0 char      }    {0×0 char}    {'Rank(M)'                     }    {[ 20]}
    {'ATG'         }    {0×0 char}    {'Atoms'                       }    {[170]}
    {0×0 char      }    {0×0 char}    {'Atom transitions'            }    {[114]}
    {0×0 char      }    {0×0 char}    {'Rank(A)'                     }    {[114]}
    {0×0 char      }    {0×0 char}    {'Row rank deficiency(A)'      }    {[ 56]}
    {0×0 char      }    {0×0 char}    {'Components'                  }    {[ 56]}
    {'dATM'        }    {0×0 char}    {'Atoms'                       }    {[170]}
    {0×0 char      }    {0×0 char}    {'Directed atom transition ins…'}    {[176]}
    {0×0 char      }    {0×0 char}    {'Rank(dATM)'                  }    {[114]}
    {0×0 char      }    {0×0 char}    {'Row rank deficiency(dATM)'   }    {[ 62]}
    {0×0 char      }    {0×0 char}    {0×0 char                      }    {[NaN]}
```

Properties of conserved moieties

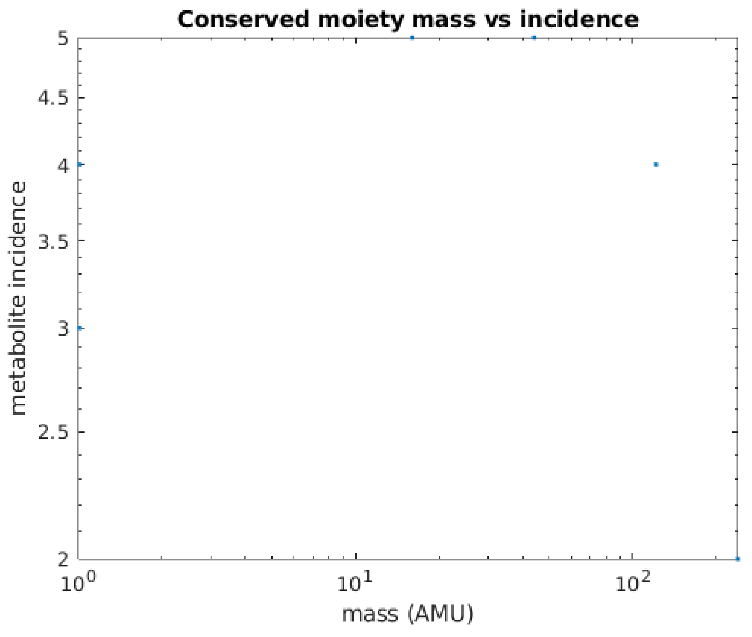
```
[moietyMasses, knownmoietyMasses, unknownElements, Ematrix, elements] = getMolecularMas
[metMasses, knownmetMasses, unknownElements, Ematrix, elements] = getMolecularMass(mode
```

Compare the distributions of the molecular moietyMasses

```
figure
hold on
h = histogram(moietyMasses);
xlabel('mass (AMU)')
ylabel('conserved moiety abundance')
title('Molecular mass of conserved moieties in iDopa model')
```

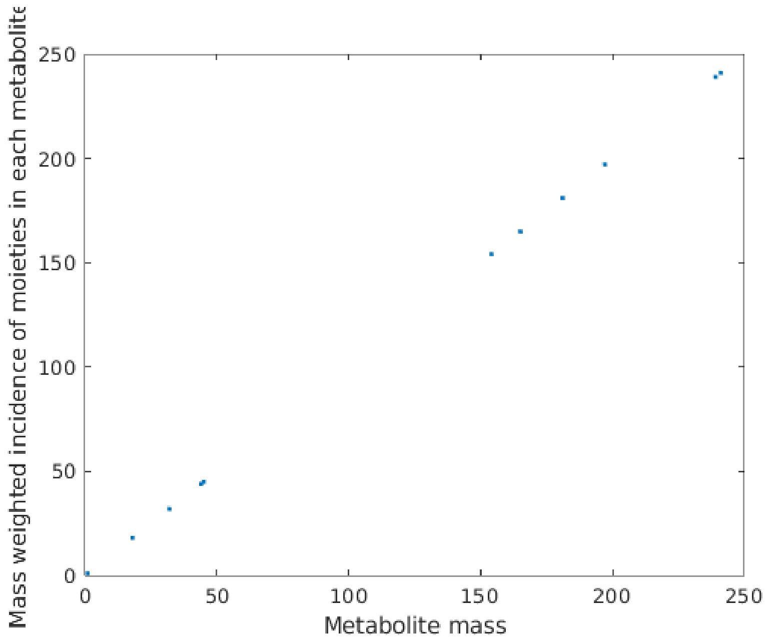


```
%h2.BinWidth = 0.25;
figure
moietyIncidence = sum(arm.L~=0,2);
loglog(moietyMasses,moietyIncidence,'.')
title('Conserved moiety mass vs incidence')
xlabel('mass (AMU)')
ylabel('metabolite incidence')
```



The metabolite mass vs mass weighted incidence of moieties in each metabolite should be a straight line trough the origin if all of the moieties that make up a metabolite are present and the formula for the metabolite is correct. Sometimes the metabolite formula is ambiguous, e.g., FULLR in the formula, so the mass will be incorrect.

```
figure
approxMetMasses = arm.L'*moietyMasses;
plot(metMasses,approxMetMasses,'.')
xlabel('Metabolite mass')
ylabel('Mass weighted incidence of moieties in each metabolite')
```



```
massDifference = abs(approxMetMasses-metMasses)./metMasses;
bool=massDifference >0.1;
n=1;
C = cell(nnz(bool),6);
for i=1:size(model.S,1)
    if bool(i)
        C(n,:)={i, massDifference(i),model.mets{i},model.metFormulas{i},metMasses(i),ap
        n=n+1;
    end
end
C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','massDifference','mets','metFormula','metMass','app
disp(T)
```

Metabolites with mass most similar to the mass of the moiety they contain

```
[minimalMassMetabolite, minimalMassFraction, numMinimalMassMetabolites] = representativ
if ~isfield(model,'metNames')
    model.metNames = model.mets;
end
```

High molecular weight moieties that are present in many metabolites.

```
massWeightedIncidence=diag(moietyMasses)*arm.L*ones(size(arm.L,2),1);
[massWeightedIncidenceSorted, xi] = sort(massWeightedIncidence,'descend');
bool=false(size(arm.L,1),1);
bool(xi(1:min(length(xi),30)))=1;
C = cell(nnz(bool),9);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(strcmp(minimalMassMetabolite{i},model.mets));
        C(n,1:9) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Minima
size(T,1)
```

```
ans = 6
```

```
disp(T)
```

```
    index    metabolites    rxns    moietyformula      mass     Minimalmassmetabolite      Name        Fo
    _____    ___________    ____    _____________    ______    _____________________    __________    ____

      3           2           6     {'C9H13N5O3'}     239.1          {'dhbpt'}          {'dhbpt'}    {'C9H
      1           4           8     {'C8H11N'   }    121.09          {'dopa' }          {'dopa' }    {'C8H
      2           5          11     {'CO2'      }     43.99          {'co2'  }          {'co2'  }    {'CO2
      6           5          12     {'O'        }    15.995          {'h2o'  }          {'h2o'  }    {'H2O
      4           4          11     {'H'        }    1.0078          {'h'    }          {'h'    }    {'H'
      5           3           8     {'H'        }    1.0078          {'h2o'  }          {'h2o'  }    {'H2O
```

Moieties that are present in a near maximal number of metabolites.

```
bool=moietyIncidence>=100;
C = cell(nnz(bool),9);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(strcmp(minimalMassMetabolite{i},model.mets));
        C(n,1:9) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,2,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Minima
size(T,1)
```

```
ans = 0
```

```
disp(T)
```

Moieties that are present in a moderate number of metabolites.

```
bool= moietyIncidence>=10 & moietyIncidence<=100;
C = cell(nnz(bool),9);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(strcmp(minimalMassMetabolite{i},model.mets));
        C(n,1:9) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,9,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Minima
size(T,1)
```

```
ans = 0
```

```
disp(T)
```

Moieties that are present in a small number of metabolites.

```
bool= moietyIncidence>2 & moietyIncidence<=10;
C = cell(nnz(bool),9);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(strcmp(minimalMassMetabolite{i},model.mets));
        C(n,1:9) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Minima
size(T,1)
```

```
ans = 5
```

```
disp(T)
```

```
    index    metabolites    rxns    moietyformula     mass      Minimalmassmetabolite       Name        Form
    _____    ___________    ____    _____________    ______    _____________________    _________    _____

      1           4           8      {'C8H11N'}      121.09          {'dopa'}           {'dopa'}    {'C8H1
      2           5          11      {'CO2'   }       43.99          {'co2' }           {'co2' }    {'CO2'
      6           5          12      {'O'     }      15.995          {'h2o' }           {'h2o' }    {'H2O'
      4           4          11      {'H'     }      1.0078          {'h'   }           {'h'   }    {'H'
      5           3           8      {'H'     }      1.0078          {'h2o' }           {'h2o' }    {'H2O'
```

Moieties that are present in a minimal number of metabolites.

```
bool=moietyIncidence==2;
C = cell(nnz(bool),11);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(arm.L(i,:)~=0);
        C(n,1:11) = {i,moietyFormulae{i},moietyMasses(i),model.mets{ind(1)},model.metNa
        n=n+1;
    end
end

C=sortrows(C,3,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','moietyformula','mass','met1','name1','formula1','m
size(T,1)
```

```
ans = 1
```

```
disp(T)
```

```
    index    moietyformula    mass       met1          name1          formula1          met2          name2
    _____    _____________    _____    _________    _________    _____________    _________    _________

      3      {'C9H13N5O3'}    239.1    {'thbpt'}    {'thbpt'}    {'C9H15N5O3'}    {'dhbpt'}    {'dhbpt'}
```

Classification of conserved moieties

```
moietyTypes = classifyMoieties(arm.L, model.S);
```

An 'Internal' moiety is one that either does not participate in any exchange reaction or is conserved by all exchange reactions

```
isInternalMoiety = strcmp('Internal',moietyTypes);
bool = isInternalMoiety;
C = cell(nnz(bool),8);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(arm.L(i,:)~=0);
        C(n,1:8) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Exampl
size(T,1)
```

```
ans = 1
```

```
disp(T)
```

```
    index    metabolites    rxns    moietyformula     mass     Examplemet    Examplename    Exampleformula
    _____    ___________    ____    _____________    _____    __________    ___________    ______________

      3           2          6      {'C9H13N5O3'}    239.1    {'thbpt'}      {'thbpt'}     {'C9H15N5O3'}
```

A 'Transitive' moiety is one that is only found in primary metabolites

```
isTransititiveMoiety= strcmp('Transitive',moietyTypes);
bool = isTransititiveMoiety;
C = cell(nnz(bool),9);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(strcmp(minimalMassMetabolite{i},model.mets));
        C(n,1:9) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,9,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Minima
size(T,1)
```

```
ans = 3
```

```
disp(T)
```

```
    index    metabolites    rxns    moietyformula     mass      Minimalmassmetabolite      Name        Form
    _____    ___________    ____    _____________    ______    _____________________    _________    ______

      2           5          11      {'CO2'    }      43.99          {'co2' }           {'co2' }    {'CO2'
      6           5          12      {'O'      }     15.995          {'h2o' }           {'h2o' }    {'H2O'
      1           4           8      {'C8H11N'}      121.09          {'dopa'}           {'dopa'}    {'C8H1
```

An 'Integrative' moiety is one that is not conserved in the open network and found in both primary and secondary metabolites.

```
bool= strcmp('Integrative',moietyTypes);
C = cell(nnz(bool),8);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(arm.L(i,:)~=0);
        C(n,1:8) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Exampl
size(T,1)
```

```
ans = 2
```

```
disp(T)
```

```
    index    metabolites    rxns    moietyformula     mass      Examplemet    Examplename    Exampleformula
    _____    ___________    ____    _____________    ______    __________    ___________    ______________

      4           4          11         {'H'}        1.0078    {'thbpt'}      {'thbpt'}     {'C9H15N5O3'}
      5           3           8         {'H'}        1.0078    {'thbpt'}      {'thbpt'}     {'C9H15N5O3'}
```

Mitochondrially localised moieties

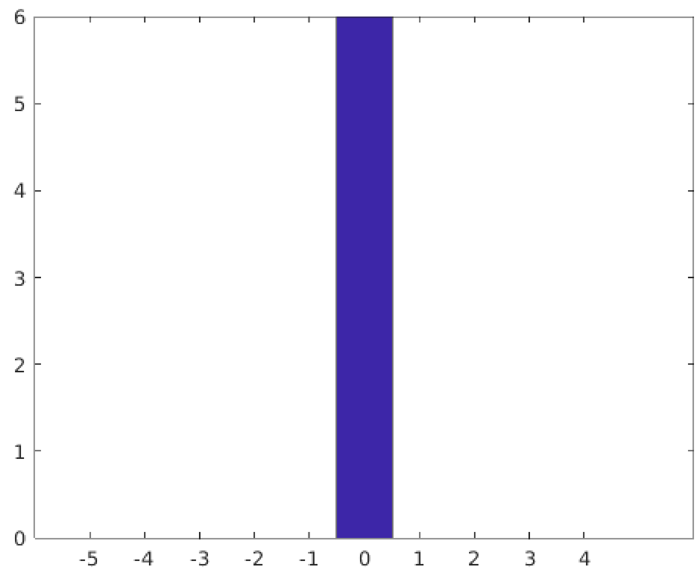
```
[compartments, uniqueCompartments] = getCompartment(model.mets);
isMitochondrial=strcmp('m',compartments);
nnz(isMitochondrial)
```

```
ans = 0
```

```
isCompletelyMitochondrialMoiety = ~any(arm.L(:,~isMitochondrial),2);
nnz(isCompletelyMitochondrialMoiety)
```

```
ans = 6
```

```
mitochondrialMoietyFraction = sum(arm.L(:,isMitochondrial),2)./sum(arm.L,2);
figure;
title('Fraction of moiety incidence that is mitochondrial')
hist(mitochondrialMoietyFraction)
```



```
bool= mitochondrialMoietyFraction==1;
C = cell(nnz(bool),8);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(arm.L(i,:)~=0);
        C(n,1:8) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
```

```
end

C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Exampl
size(T,1)
```

```
ans = 0
```

```
disp(T)
```

Transitive moiety, of sufficient mass, with moderate incidence

```
isTransititiveMoiety= strcmp('Transitive',moietyTypes);
isModerateIncidence = moietyIncidence>=7 & moietyIncidence<=100;
isSufficientMass = moietyMasses > 2;
isSufficientMinimalMassFraction = minimalMassFraction > 0.1;
bool = isTransititiveMoiety & isModerateIncidence & isSufficientMass & isSufficientMini
C = cell(nnz(bool),9);
n=1;
for i=1:size(arm.L,1)
    if bool(i)
        ind = find(strcmp(minimalMassMetabolite{i},model.mets));
        C(n,1:9) = {i,nnz(arm.L(i,:)),nnz(model.S((arm.L(i,:)~=0)',:)~=0),moietyFormula
        n=n+1;
    end
end

C=sortrows(C,9,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','metabolites','rxns','moietyformula','mass','Minima
size(T,1)
```

```
ans = 0
```

```
disp(T)
```

Individual moiety subnetwork

Examine the metabolites and reactions in an individual moiety subnetwork.

```
ind = min(size(arm.L,1),32);% anth moiety
mBool=arm.L(ind,:)~=0;
nnz(mBool)
```

```
ans = 5
```

```
rBool = getCorrespondingCols(model.S, mBool, true(size(model.S,2),1), 'inclusive');
nnz(rBool)
```

```
ans = 6
```

Metabolites

```
bool=mBool;
C = cell(nnz(bool),5);
n=1;
for i=1:size(model.S,1)
    if bool(i)
        C(n,1:5) = {i,model.mets{i},model.metNames{i},model.metFormulas{i},metMasses(i
        n=n+1;
    end
end
C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','met','name','formula','mass'};
disp(T)
```

```
    index        met            name          formula         mass 
    _____    ___________    ___________    ____________    ______

      7      {'34dhphe'}    {'34dhphe'}    {'C9H11NO4'}    197.07
      4      {'tyr_L'  }    {'tyr_L'  }    {'C9H11NO3'}    181.07
      9      {'dopa'   }    {'dopa'   }    {'C8H12NO2'}    154.09
      3      {'o2'     }    {'o2'     }    {'O2'      }     31.99
      6      {'h2o'    }    {'h2o'    }    {'H2O'     }    18.011
```

Reactions

```
formulas = printRxnFormula(model, model.rxns(rBool));
```

```
R1     phe_L + thbpt + o2     ->    tyr_L + dhbpt + h2o 
R2     thbpt + o2 + tyr_L     ->    dhbpt + h2o + 34dhphe 
R3     34dhphe + h     ->    dopa + co2 
EX_o2     o2     <=> 
EX_h2o     h2o     -> 
EX_dopa     dopa     -> 
```

```
return
```

Another Individual moiety subnetwork

Specify the index of a particular moiety

```
ind = min(size(arm.L,1),215);% Nicotinate moiety in iDopaNeuro1.
mBool=arm.L(ind,:)~=0;
nnz(mBool)
rBool = getCorrespondingCols(model.S, mBool, true(size(model.S,2),1), 'inclusive');
nnz(rBool)
```

Metabolites

```
bool=mBool;
C = cell(nnz(bool),5);
n=1;
for i=1:size(model.S,1)
    if bool(i)
        C(n,1:5) = {i,model.mets{i},model.metNames{i},model.metFormulas{i},metMasses(i
        n=n+1;
    end
```

```
end
C=sortrows(C,5,'descend');
T=cell2table(C);
T.Properties.VariableNames={'index','met','name','formula','mass'};
disp(T)
```

Reactions

```
formulas = printRxnFormula(model, model.rxns(rBool));
```

Save analysis results

```
save([resultsDir  modelName '_ConservedMoietiesAnalysis.mat'])
```