Generation of a chemoinformatic data base

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INTRODUCTION

The molecular structure of a metabolite in a COBRA model can be represented in various formats such as SMILES InChIs and InChIkeys (See Figure 1), as well as identifiers from various databases such as the Virtual Metabolic Human database [1] (**VMH**), the Human Metabolome Database [2] (**HMDB**), **PubChem** database [3], the Kyoto Encyclopedia of Genes and Genomes [4] (**KEEG**), and the Chemical Entities of Biological Interest [5] (**ChEBI**).

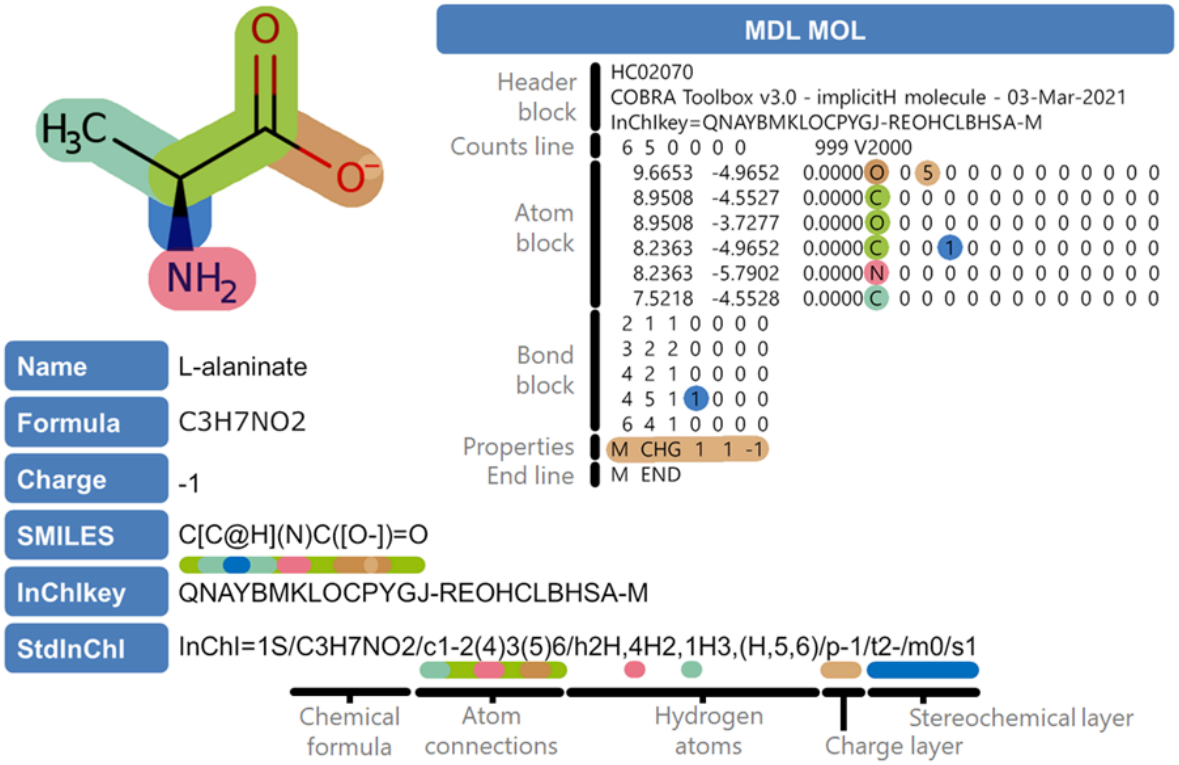


Figure 1. Different chemoinformatic formats

The function generateChemicalDatabase creates a chemoinformatic database using data from a COBRA model (Figure 2). It makes use of a variety of external software, including openBabel [6], MarvinSuite [7], and JAVA. generateChemicalDatabase works even if some of these programs are not installed, but for the best results, all of them should be.

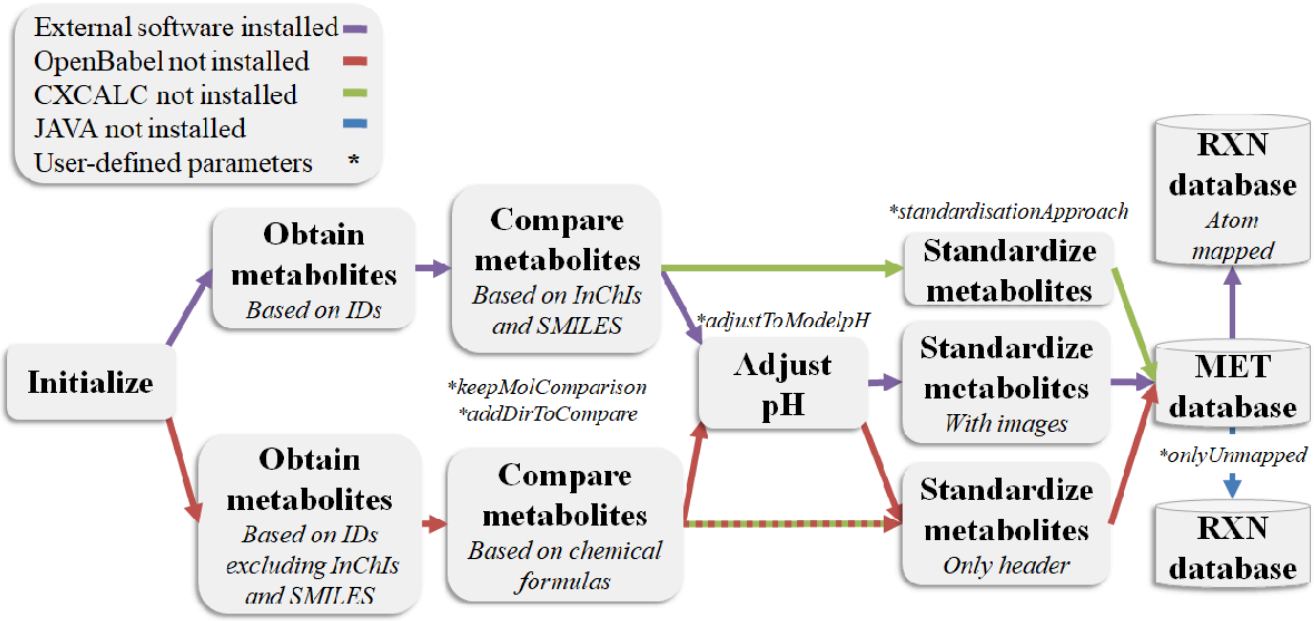


Figure 2. Depending on the system configuration and the user-defined parameters, the pipeline can take various paths.

The function compares the molecular structure information from various sources for each metabolite, and the molecular structure from the source with the highest score is considered correct. The disimilarity comparison is performed by calculating the euclidean distances of all molecular structures obtained. The following criteria are used to assign the score:

Comparison	Max score	Description
Comparability to other databases	1	Divides the number of unique identifiers by the number of repeated instances of an identifier to compare the similarity between sources. The dissimilarity test does not take into account sources that do not have an identifier.
Chemical formula	10	The chemical formula indicated in the COBRA model is compared to the chemical formula obtained from the source. It gives a score of 10 if there is a match and an 8 if match with no hydrogen atoms.
InChI layers	11	Compares the information layer between the InChIs obtained. It starts with a score of 4, and each layer has a score of 1.

The goal of the comparison is to obtain a larger number of atomically balanced metabolic reactions. The Reaction Decoder Tool algorithm [8] (**RDT**) is used to obtain the atom mappings of each metabolic reaction. Finally, the atom mapping data is used to calculate the number of bonds formed or broken in a metabolic reaction, as well as the energy required to break the bond. The information gathered is incorporated into the COBRA model.

We will obtain chemoinformatic data on the Ecoli core model in this tutorial. The identifiers will be added using the `addMetInfoInCBmodel` function.

Generate chemoinformatic database

Clean up the workspace and configure the user directory.

```
clear
if ispc
    userDir = winqueryreg('HKEY_CURRENT_USER',...
        ['Software\Microsoft\Windows\CurrentVersion\' ...
         'Explorer\Shell Folders'],'Personal');
else
    userDir = char(java.lang.System.getProperty('user.home'));
end
```

Load the ecoli core model.

```
load ecoli_core_model.mat
model.mets = regexprep(model.mets, '\-', '\_');
```

Add chemoinformatic information from an external file to the ecoli core model, such as SMILES, InChIs, or different database identifiers.

```
dataFile = which('chemoinformaticDatabaseTutorial.mlx')
```

```
dataFile =
'/Users/gpreciat/work/code/cobratoolbox/tutorials/dataIntegration/chemoinformaticDatabase/chemoinformatic
```

```
inputData = regexprep(dataFile, 'chemoinformaticDatabaseTutorial.mlx', 'metaboliteIds.x
replace = false;
[model, hasEffect] = addMetInfoInCBmodel(model, inputData, replace);
```

The user-defined parameters in the function `generateChemicalDatabase` will activate various processes. Each parameter is described in detail below:

- **outputDir**: The path to the directory containing the RXN files with atom mappings (default: current directory)
- **printlevel**: Verbose level
- **standardisationApproach**: String containing the type of standardisation for the molecules (default: 'explicitH' if openBabel [6] is installed, otherwise default: 'basic'):

1. explicitH: Normal chemical graphs;
2. implicitH: Hydrogen suppressed chemical graph;
3. neutral: Chemical graphs with protonated molecules;
4. basic: Update the header.

- **keepMolComparison**: Logic value for comparing MDL MOL files from various sources (default: FALSE)
- **onlyUnmapped**: Logic value to select create only unmapped MDL RXN files (default: FALSE).
- **adjustToModelpH**: Logic value used to determine whether a molecule's pH must be adjusted in accordance with the COBRA model. (default: TRUE, requires MarvinSuite [7]).
- **addDirsToCompare**: Cell(s) with the path to directory to an existing database (default: empty).
- **dirNames**: Cell(s) with the name of the directory(ies) (default: empty).

- **debug**: Logical value used to determine whether or not the results of different points in the function will be saved for debugging (default: empty).

```
options.outputDir = [userDir '/work/code/ctf/databases/ecoliDB'];
options.printlevel = 1;
options.debug = true;
options.standardisationApproach = 'explicitH';
options.adjustToModelpH = true;
options.keepMolComparison = true;
options.dirsToCompare = {'~/work/code/ctf/mets/molFiles'};
options.onlyUnmapped = false;
options.dirNames = {'VMH'};
```

Use the function generateChemicalDatabase

```
info = generateChemicalDatabase(model, options);
```

```
------------------------------------------------------------
CHEMICAL DATABASE
------------------------------------------------------------

Generating a chemical database with the following options:

                  outputDir: '/Users/gpreciat/work/code/ctf/databases/ecoliDB'
                 printlevel: 1
                      debug: 1
    standardisationApproach: 'explicitH'
            adjustToModelpH: 1
          keepMolComparison: 1
              dirsToCompare: {'~/work/code/ctf/mets/molFiles/'}
               onlyUnmapped: 0
                   dirNames: {'VMH'}

------------------------------------------------------------
Obtaining MOL files from chemical databases ...

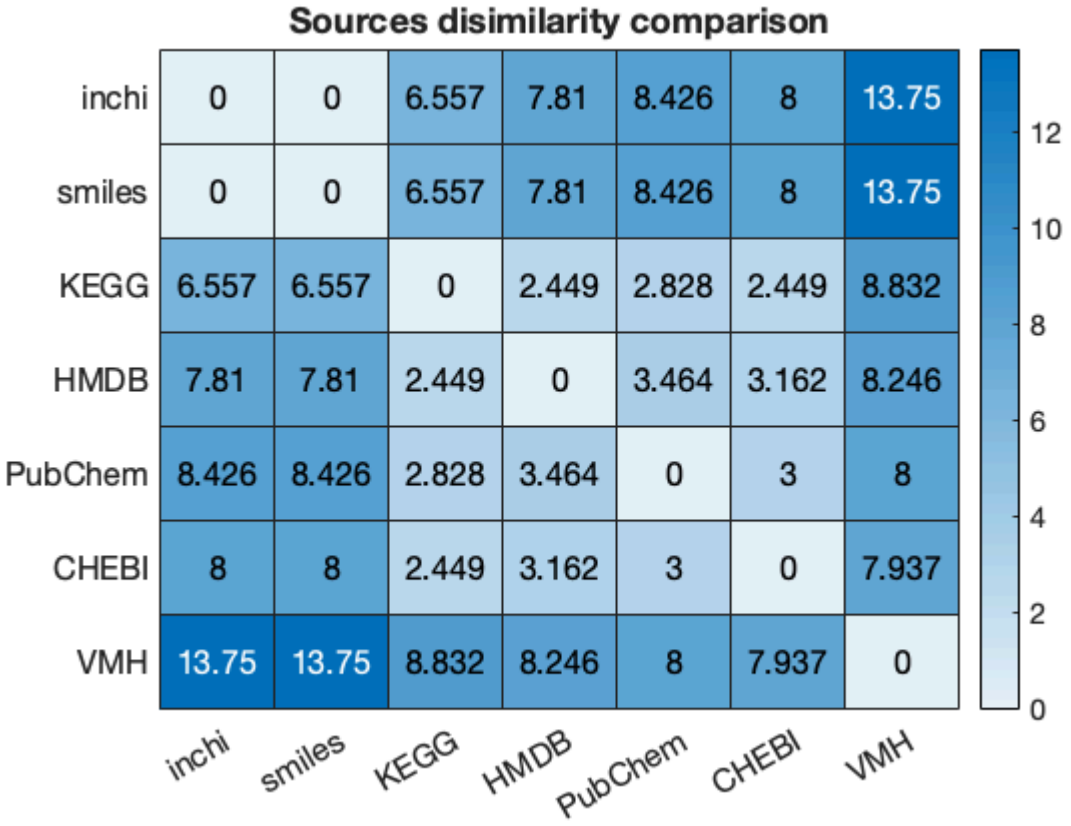
inchi:
molCollectionReport = struct with fields:
              noOfMets: 54
       noOfMetsWithMol: 50
    noOfMetsWithoutMol: 4
              coverage: 92.5926
smiles:
molCollectionReport = struct with fields:
              noOfMets: 54
       noOfMetsWithMol: 50
    noOfMetsWithoutMol: 4
              coverage: 92.5926
KEGG:
molCollectionReport = struct with fields:
              noOfMets: 54
       noOfMetsWithMol: 49
    noOfMetsWithoutMol: 5
              coverage: 90.7407
HMDB:
molCollectionReport = struct with fields:
```

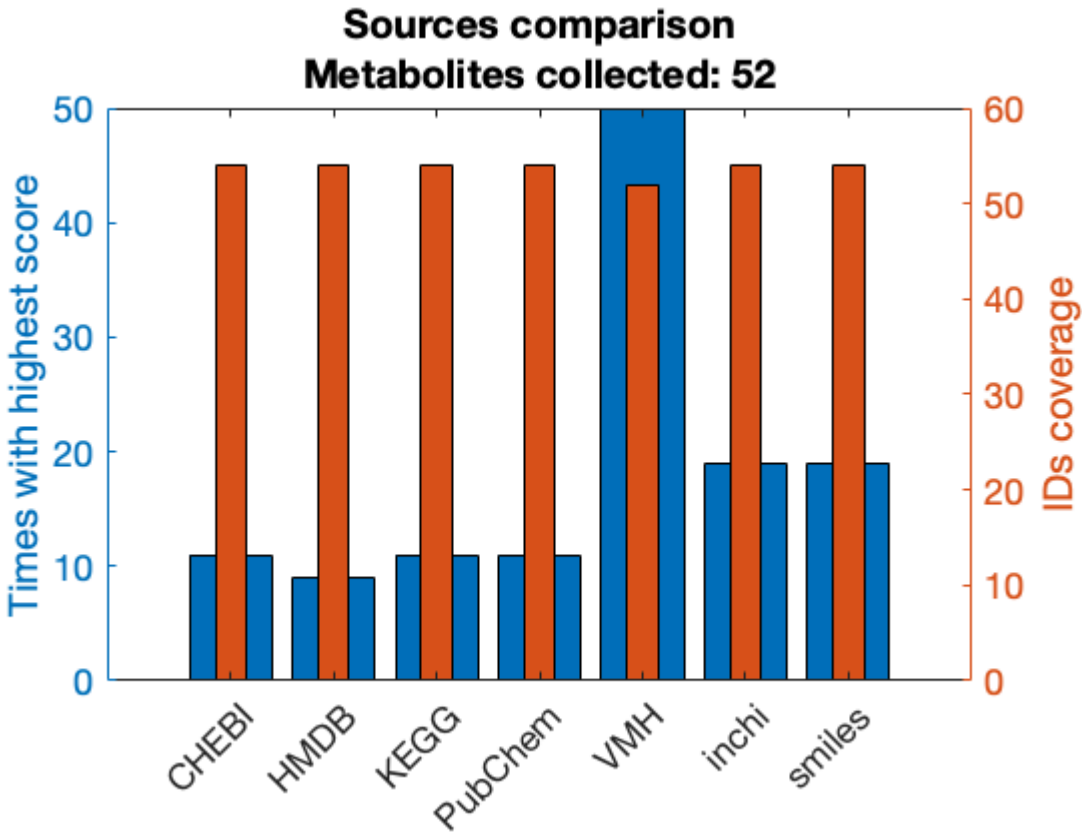
```
            noOfMets: 54
       noOfMetsWithMol: 51
    noOfMetsWithoutMol: 3
            coverage: 94.4444
PubChem:
molCollectionReport = struct with fields:
            noOfMets: 54
       noOfMetsWithMol: 50
    noOfMetsWithoutMol: 4
            coverage: 92.5926
CHEBI:
molCollectionReport = struct with fields:
            noOfMets: 54
       noOfMetsWithMol: 48
    noOfMetsWithoutMol: 6
            coverage: 88.8889
```

```
Comparing information from sources ...
  52×8 table
```

mets	sourceWithHighestScore	metNames
"13dpg"	"VMH"	"3-Phospho-D-glyceroyl phosphate"
"2pg"	"VMH"	"D-Glycerate 2-phosphate"
"3pg"	"VMH"	"3-Phospho-D-glycerate"
"6pgc"	"VMH"	"6-Phospho-D-gluconate"
"6pgl"	"VMH"	"6-phospho-D-glucono-1,5-lactone"
"ac"	"inchi smiles VMH"	"Acetate"
"acald"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"Acetaldehyde"
"accoa"	"VMH"	"Acetyl-CoA"
"adp"	"VMH"	"ADP"
"akg"	"inchi smiles VMH"	"2-Oxoglutarate"
"amp"	"VMH"	"AMP"
"atp"	"VMH"	"ATP"
"cit"	"inchi smiles VMH"	"Citrate"
"co2"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"CO2"
"coa"	"VMH"	"Coenzyme A"
"dhap"	"inchi smiles VMH"	"Dihydroxyacetone phosphate"
"e4p"	"VMH"	"D-Erythrose 4-phosphate"
"etoh"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"Ethanol"
"f6p"	"VMH"	"D-Fructose 6-phosphate"
"fdp"	"VMH"	"D-Fructose 1,6-bisphosphate"
"for"	"inchi smiles VMH"	"Formate"
"fru"	"KEGG HMDB PubChem CHEBI VMH"	"D-Fructose"
"fum"	"VMH"	"Fumarate"
"g3p"	"VMH"	"Glyceraldehyde 3-phosphate"
"g6p"	"VMH"	"D-Glucose 6-phosphate"
"glc_D"	"KEGG PubChem CHEBI VMH"	"D-Glucose"
"gln_L"	"KEGG HMDB PubChem CHEBI VMH"	"L-Glutamine"
"glu_L"	"VMH"	"L-Glutamate"
"glx"	"inchi smiles VMH"	"Glyoxylate"
"h"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"H+"
"h2o"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"H2O"
"icit"	"inchi smiles VMH"	"Isocitrate"
"lac_D"	"VMH"	"D-Lactate"
"mal_L"	"VMH"	"L-Malate"
"nad"	"KEGG PubChem CHEBI"	"Nicotinamide adenine dinucleotide"
"nadh"	"VMH"	"Nicotinamide adenine dinucleotide - reduce
"nadp"	"KEGG PubChem CHEBI"	"Nicotinamide adenine dinucleotide phosphat
"nadph"	"VMH"	"Nicotinamide adenine dinucleotide phosphat
"nh4"	"inchi smiles VMH"	"Ammonium"
"o2"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"O2"
"oaa"	"inchi smiles VMH"	"Oxaloacetate"

"pep"	"inchi smiles VMH"	"Phosphoenolpyruvate"
"pi"	"inchi smiles VMH"	"Phosphate"
"pyr"	"inchi smiles VMH"	"Pyruvate"
"r5p"	"VMH"	"alpha-D-Ribose 5-phosphate"
"ru5p_D"	"VMH"	"D-Ribulose 5-phosphate"
"s7p"	"VMH"	"Sedoheptulose 7-phosphate"
"succ"	"inchi smiles VMH"	"Succinate"
"succoa"	"VMH"	"Succinyl-CoA"
"xu5p_D"	"VMH"	"D-Xylulose 5-phosphate"
"actp"	"VMH"	"Acetyl phosphate"
"q8h2"	"HMDB VMH"	"Ubiquinol-8"






```
Adjusting pH based on the model's chemical formula ...

adjustedpH:
  52×13 table
```

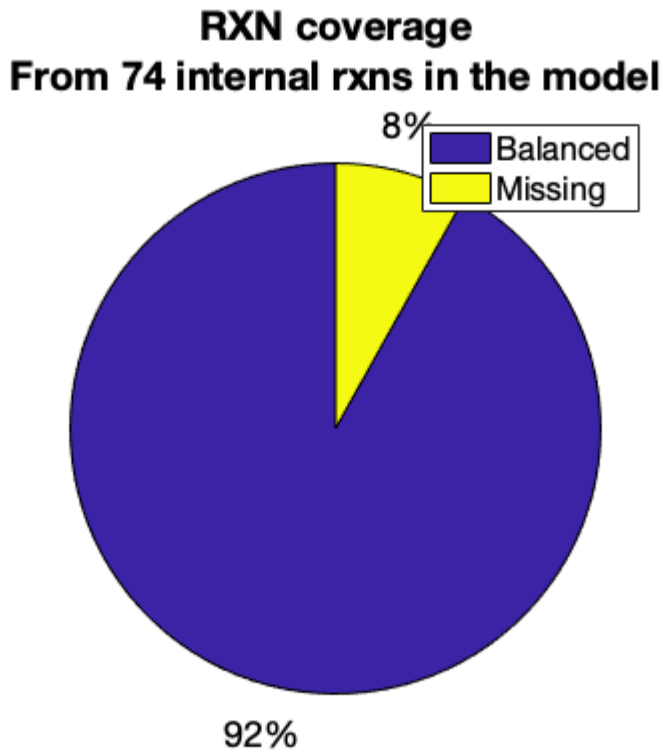
mets	sourceWithHighestScore	metNames
"13dpg"	"VMH"	"3-Phospho-D-glyceroyl phosphate"
"2pg"	"VMH"	"D-Glycerate 2-phosphate"
"3pg"	"VMH"	"3-Phospho-D-glycerate"
"6pgc"	"VMH"	"6-Phospho-D-gluconate"
"6pgl"	"VMH"	"6-phospho-D-glucono-1,5-lactone"
"ac"	"inchi smiles VMH"	"Acetate"
"acald"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"Acetaldehyde"
"accoa"	"VMH"	"Acetyl-CoA"
"adp"	"VMH"	"ADP"
"akg"	"inchi smiles VMH"	"2-Oxoglutarate"
"amp"	"VMH"	"AMP"
"atp"	"VMH"	"ATP"
"cit"	"inchi smiles VMH"	"Citrate"
"co2"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"CO2"
"coa"	"VMH"	"Coenzyme A"
"dhap"	"inchi smiles VMH"	"Dihydroxyacetone phosphate"
"e4p"	"VMH"	"D-Erythrose 4-phosphate"
"etoh"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"Ethanol"
"f6p"	"VMH"	"D-Fructose 6-phosphate"
"fdp"	"VMH"	"D-Fructose 1,6-bisphosphate"
"for"	"inchi smiles VMH"	"Formate"
"fru"	"KEGG HMDB PubChem CHEBI VMH"	"D-Fructose"
"fum"	"VMH"	"Fumarate"
"g3p"	"VMH"	"Glyceraldehyde 3-phosphate"
"g6p"	"VMH"	"D-Glucose 6-phosphate"
"glc_D"	"KEGG PubChem CHEBI VMH"	"D-Glucose"
"gln_L"	"KEGG HMDB PubChem CHEBI VMH"	"L-Glutamine"

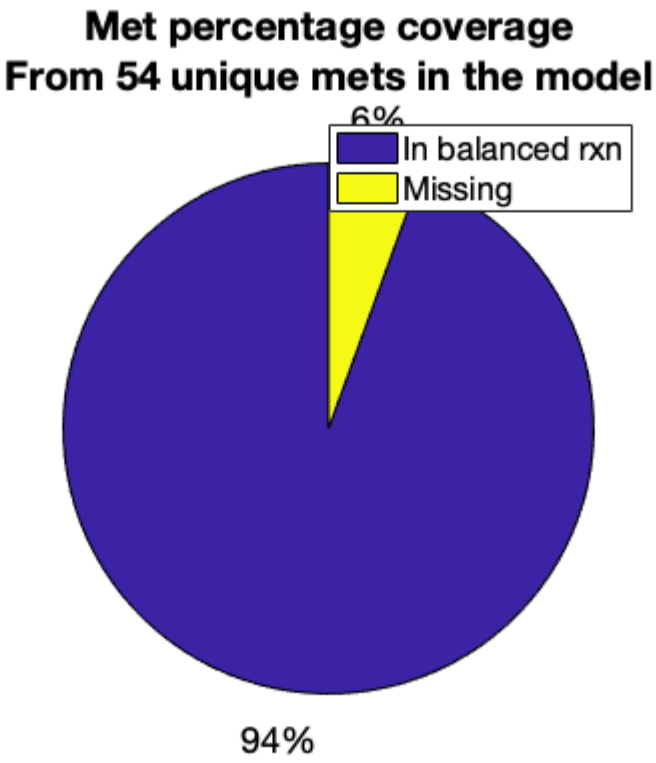
"glu_L"	"VMH"	"L-Glutamate"
"glx"	"inchi smiles VMH"	"Glyoxylate"
"h"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"H+"
"h2o"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"H2O"
"icit"	"inchi smiles VMH"	"Isocitrate"
"lac_D"	"VMH"	"D-Lactate"
"mal_L"	"VMH"	"L-Malate"
"nad"	"KEGG PubChem CHEBI"	"Nicotinamide adenine dinucleotide"
"nadh"	"VMH"	"Nicotinamide adenine dinucleotide - reduce
"nadp"	"KEGG PubChem CHEBI"	"Nicotinamide adenine dinucleotide phosphat
"nadph"	"VMH"	"Nicotinamide adenine dinucleotide phosphat
"nh4"	"inchi smiles VMH"	"Ammonium"
"o2"	"inchi smiles KEGG HMDB PubChem CHEBI VMH"	"O2"
"oaa"	"inchi smiles VMH"	"Oxaloacetate"
"pep"	"inchi smiles VMH"	"Phosphoenolpyruvate"
"pi"	"inchi smiles VMH"	"Phosphate"
"pyr"	"inchi smiles VMH"	"Pyruvate"
"r5p"	"VMH"	"alpha-D-Ribose 5-phosphate"
"ru5p_D"	"VMH"	"D-Ribulose 5-phosphate"
"s7p"	"VMH"	"Sedoheptulose 7-phosphate"
"succ"	"inchi smiles VMH"	"Succinate"
"succoa"	"VMH"	"Succinyl-CoA"
"xu5p_D"	"VMH"	"D-Xylulose 5-phosphate"
"actp"	"VMH"	"Acetyl phosphate"
"q8h2"	"HMDB VMH"	"Ubiquinol-8"

```
Standardizing 52 MOL files ...
 52×4 table
```

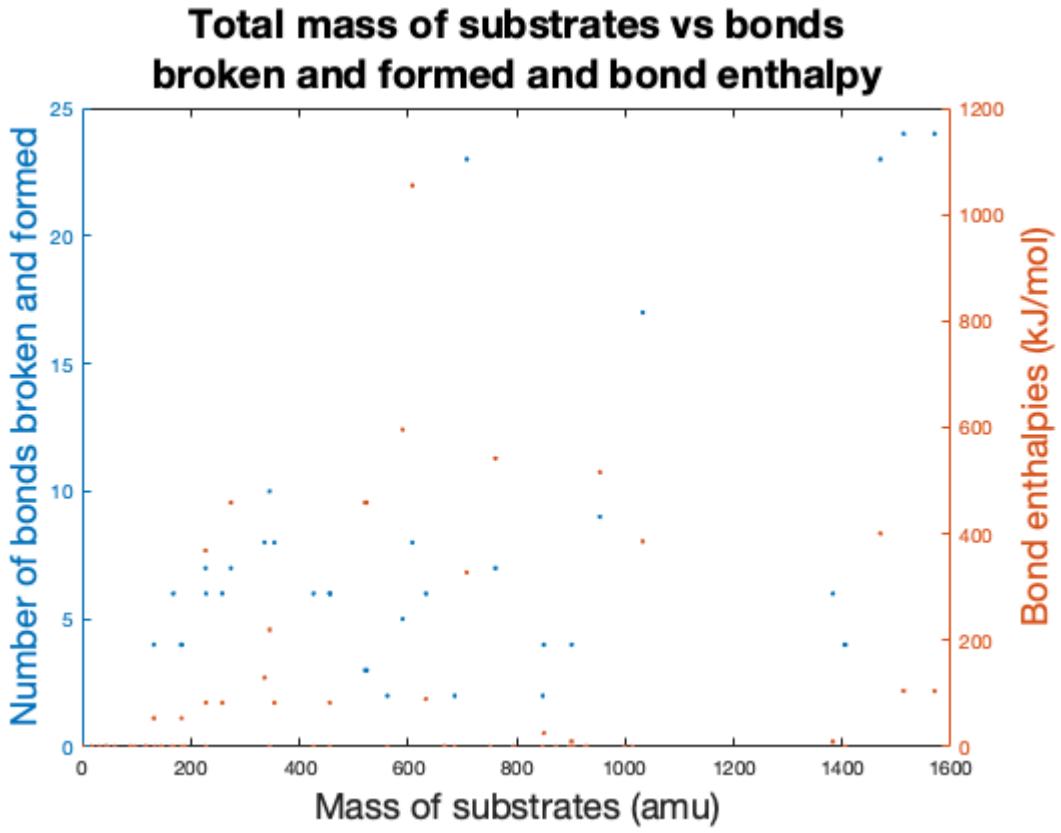
mets	InChIKeys	
"13dpg"	"InChIKey=LJQLQCAXBUHEAZ-UWTATZPHSA-J"	"InChI=1S/C3H8O10P2/c4-2(1-12-14(6,7)8)3(5)13-1
"2pg"	"InChIKey=GXIURPTVHJPJLF-UWTATZPHSA-K"	"InChI=1S/C3H7O7P/c4-1-2(3(5)6)10-11(7,8)9/h2,4
"3pg"	"InChIKey=OSJPPGNTCRNQQC-UWTATZPHSA-K"	"InChI=1S/C3H7O7P/c4-2(3(5)6)1-10-11(7,8)9/h2,4
"6pgc"	"InChIKey=BIRSGZKFKXLSJQ-SQOUGZDYSA-K"	"InChI=1S/C6H13O10P/c7-2(1-16-17(13,14)15)3(8)4
"6pgl"	"InChIKey=IJOJIVNDFQSGAB-SQOUGZDYSA-L"	"InChI=1S/C6H11O9P/c7-3-2(1-14-16(11,12)13)15-6
"ac"	"InChIKey=QTBSBXVTEAMEQO-UHFFFAOYSA-M"	"InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)/p-1"
"acald"	"InChIKey=IKHGUXGNUITLKF-UHFFFAOYSA-N"	"InChI=1S/C2H4O/c1-2-3/h2H,1H3"
"accoa"	"InChIKey=ZSLZBFCDCINBPY-ZSJPKINUSA-J"	"InChI=1S/C23H38N7O17P3S/c1-12(31)51-7-6-25-14(
"actp"	"InChIKey=LIPOUNRJVLNBCD-UHFFFAOYSA-L"	"InChI=1S/C2H5O5P/c1-2(3)7-8(4,5)6/h1H3,(H2,4,5
"adp"	"InChIKey=XTWYTFMLZFPYCI-KQYNXXCUSA-K"	"InChI=1S/C10H15N5O10P2/c11-8-5-9(13-2-12-8)15(
"akg"	"InChIKey=KPGXRSRHYNQIFN-UHFFFAOYSA-L"	"InChI=1S/C5H6O5/c6-3(5(9)10)1-2-4(7)8/h1-2H2,(
"amp"	"InChIKey=UDMBCSSLTHHNCD-KQYNXXCUSA-L"	"InChI=1S/C10H14N5O7P/c11-8-5-9(13-2-12-8)15(3-
"atp"	"InChIKey=ZKHQWZAMYRWXGA-KQYNXXCUSA-J"	"InChI=1S/C10H16N5O13P3/c11-8-5-9(13-2-12-8)15(
"cit"	"InChIKey=KRKNYBCHXYNGOX-UHFFFAOYSA-K"	"InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10
"co2"	"InChIKey=CURLTUGMZLYLDI-UHFFFAOYSA-N"	"InChI=1S/CO2/c2-1-3"
"coa"	"InChIKey=RGJOEKWQDUBAIZ-IBOSZNHHSA-J"	"InChI=1S/C21H36N7O16P3S/c1-21(2,16(31)19(32)24
"dhap"	"InChIKey=GNGACRATGGDKBX-UHFFFAOYSA-L"	"InChI=1S/C3H7O6P/c4-1-3(5)2-9-10(6,7)8/h4H,1-2
"e4p"	"InChIKey=NGHMDNPXVRFFGS-IUYQGCFVSA-L"	"InChI=1S/C4H9O7P/c5-1-3(6)4(7)2-11-12(8,9)10/h
"etoh"	"InChIKey=LFQSCWFLJHTTHZ-UHFFFAOYSA-N"	"InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3"
"f6p"	"InChIKey=GSXOAOHZAIYLCY-HSUXUTPPSA-L"	"InChI=1S/C6H13O9P/c7-1-3(8)5(10)6(11)4(9)2-15-
"fdp"	"InChIKey=RNBGYGVWRKECFJ-VRPWFDPXSA-J"	"InChI=1S/C6H14O12P2/c7-4-3(1-16-19(10,11)12)18
"for"	"InChIKey=BDAGIHXWWSANSR-UHFFFAOYSA-M"	"InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3)/p-1"
"fru"	"InChIKey=RFSUNEUAIZKAJO-ARQDHWQXSA-N"	"InChI=1S/C6H12O6/c7-1-3-4(9)5(10)6(11,2-8)12-3
"fum"	"InChIKey=VZCYOOQTPOCHFL-OWOJBTEDSA-L"	"InChI=1S/C4H4O4/c5-3(6)1-2-4(7)8/h1-2H,(H,5,6)
"g3p"	"InChIKey=LXJXRIRHZLFYRP-VKHMYHEASA-L"	"InChI=1S/C3H7O6P/c4-1-3(5)2-9-10(6,7)8/h1,3,5H
"g6p"	"InChIKey=NBSCHQHZLSJFNQ-GASJEMHNSA-L"	"InChI=1S/C6H13O9P/c7-3-2(1-14-16(11,12)13)15-6
"glc_D"	"InChIKey=WQZGKKKJIJFFOK-GASJEMHNSA-N"	"InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2
"gln_L"	"InChIKey=ZDXPYRJPNDTMRX-VKHMYHEASA-N"	"InChI=1S/C5H10N2O3/c6-3(5(9)10)1-2-4(7)8/h3H,1
"glu_L"	"InChIKey=WHUUTDBJXJRKMK-VKHMYHEASA-M"	"InChI=1S/C5H9NO4/c6-3(5(9)10)1-2-4(7)8/h3H,1-2
"glx"	"InChIKey=HHLFWLYXYJOTON-UHFFFAOYSA-M"	"InChI=1S/C2H2O3/c3-1-2(4)5/h1H,(H,4,5)/p-1"
"h"	"InChIKey=GPRLSGONYQIRFK-UHFFFAOYSA-N"	"InChI=1S/p+1"
"h2o"	"InChIKey=XLYOFNOQVPJJNP-UHFFFAOYSA-N"	"InChI=1S/H2O/h1H2"

"icit"	"InChIKey=ODBLHEXUDAPZAU-UHFFFAOYSA-K"	"InChI=1S/C6H8O7/c7-3(8)1-2(5(10)11)4(9)6(12)13
"lac_D"	"InChIKey=JVTAAEKCZFNVCJ-REOHCLBHSA-M"	"InChI=1S/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)
"mal_L"	"InChIKey=BJEPYKJPYRNKOW-REOHCLBHSA-L"	"InChI=1S/C4H6O5/c5-2(4(8)9)1-3(6)7/h2,5H,1H2,(
"nad"	"InChIKey=BAWFJGJZGIEFAR-NNYOXOHSSA-M"	"InChI=1S/C21H27N7O14P2/c22-17-12-19(25-7-24-17
"nadh"	"InChIKey=BOPGDPNILDQYTO-NNYOXOHSSA-L"	"InChI=1S/C21H29N7O14P2/c22-17-12-19(25-7-24-17
"nadp"	"InChIKey=XJLXINKUBYWONI-NNYOXOHSSA-K"	"InChI=1S/C21H28N7O17P3/c22-17-12-19(25-7-24-17
"nadph"	"InChIKey=ACFIXJIJDZMPPO-NNYOXOHSSA-J"	"InChI=1S/C21H30N7O17P3/c22-17-12-19(25-7-24-17
"nh4"	"InChIKey=QGZKDVFQNNGYKY-UHFFFAOYSA-O"	"InChI=1S/H3N/h1H3/p+1"
"o2"	"InChIKey=MYMOFIZGZYHOMD-UHFFFAOYSA-N"	"InChI=1S/O2/c1-2"
"oaa"	"InChIKey=KHPXUQMNIQBQEV-UHFFFAOYSA-L"	"InChI=1S/C4H4O5/c5-2(4(8)9)1-3(6)7/h1H2,(H,6,7
"pep"	"InChIKey=DTBNBXWJWCWCIK-UHFFFAOYSA-K"	"InChI=1S/C3H5O6P/c1-2(3(4)5)9-10(6,7)8/h1H2,(H
"pi"	"InChIKey=NBIIXXVUZAFLBC-UHFFFAOYSA-L"	"InChI=1S/H3O4P/c1-5(2,3)4/h(H3,1,2,3,4)/p-2"
"pyr"	"InChIKey=LCTONWCANYUPML-UHFFFAOYSA-M"	"InChI=1S/C3H4O3/c1-2(4)3(5)6/h1H3,(H,5,6)/p-1"
"q8h2"	"InChIKey=LOJUQFSPYHMHEO-SGHXUWJISA-N"	"InChI=1S/C49H76O4/c1-36(2)20-13-21-37(3)22-14-






```
Obtaining RInChIes and reaction SMILES ...
Found biomass reaction: Biomass_Ecoli_core_N(w/GAM)-Nmet2
ATP maintenance reaction is not considered an exchange reaction by default. It should be mass balanced:
ATPM atp[c] + h2o[c]  -> adp[c] + h[c] + pi[c]
```




```
95×4 table
```

rxns	rxnNames
'ACALD'	'acetaldehyde dehydrogenase (acetylating)'
'ACALDt'	'acetaldehyde reversible transport'
'ACKr'	'acetate kinase'
'ACONTa'	'aconitase (half-reaction A, Citrate hydro-lyase)'
'ACONTb'	'aconitase (half-reaction B, Isocitrate hydro-lyase)'
'ACt2r'	'acetate reversible transport via proton symport'
'ADK1'	'adenylate kinase'
'AKGDH'	' 2-Oxogluterate dehydrogenase'
'AKGt2r'	' 2-oxoglutarate reversible transport via symport'
'ALCD2x'	'alcohol dehydrogenase (ethanol)'
'ATPM'	'ATP maintenance requirement'
'ATPS4r'	'ATP synthase (four protons for one ATP)'
'Biomass_Ecoli_core_N(w/GAM)-Nmet2'	'core E. coli biomass equation (Neidhardt Based with GAM, N me
'CO2t'	'CO2 transporter via diffusion'
'CS'	'citrate synthase'
'CYTBD'	'cytochrome oxidase bd (ubiquinol-8: 2 protons)'
'D-LACt2'	'D-lactate transport via proton symport'
'ENO'	'enolase'
'ETOHt2r'	'ethanol reversible transport via proton symport'
'EX_ac(e)'	'Acetate exchange'
'EX_acald(e)'	'Acetaldehyde exchange'
'EX_akg(e)'	' 2-Oxoglutarate exchange'
'EX_co2(e)'	'CO2 exchange'
'EX_etoh(e)'	'Ethanol exchange'
'EX_for(e)'	'Formate exchange'
'EX_fru(e)'	'D-Fructose exchange'
'EX_fum(e)'	'Fumarate exchange'
'EX_glc(e)'	'D-Glucose exchange'
'EX_gln-L(e)'	'L-Glutamine exchange'
'EX_glu-L(e)'	'L-Glutamate exchange'
'EX_h2o(e)'	'H2O exchange'
'EX_h(e)'	'H+ exchange'
'EX_lac-D(e)'	'D-lactate exchange'
'EX_mal-L(e)'	'L-Malate exchange'
'EX_nh4(e)'	'Ammonia exchange'
'EX_o2(e)'	'O2 exchange'
'EX_pi(e)'	'Phosphate exchange'
'EX_pyr(e)'	'Pyruvate exchange'
'EX_succ(e)'	'Succinate exchange'
'FBA'	'fructose-bisphosphate aldolase'
'FBP'	'fructose-bisphosphatase'
'FORt2'	'formate transport in via proton symport'
'FORti'	'formate transport via diffusion'
'FRD7'	'fumarate reductase'
'FRUpts2'	'Fructose transport via PEP:Pyr PTS (f6p generating)'
'FUM'	'fumarase'
'FUMt2_2'	'Fumarate transport via proton symport (2 H)'
'G6PDH2r'	'glucose 6-phosphate dehydrogenase'
'GAPD'	'glyceraldehyde-3-phosphate dehydrogenase'
'GLCpts'	'D-glucose transport via PEP:Pyr PTS'
'GLNS'	'glutamine synthetase'
'GLNabc'	'L-glutamine transport via ABC system'
'GLUDy'	'glutamate dehydrogenase (NADP)'
'GLUN'	'glutaminase'
'GLUSy'	'glutamate synthase (NADPH)'
'GLUt2r'	'L-glutamate transport via proton symport, reversible'
'GND'	'phosphogluconate dehydrogenase'
'H2Ot'	'H2O transport via diffusion'
'ICDHyr'	'isocitrate dehydrogenase (NADP)'
'ICL'	'Isocitrate lyase'
'LDH_D'	'D-lactate dehydrogenase'

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  'MALS'                                  'malate synthase'
  'MALt2_2'                               'Malate transport via proton symport (2 H)'
  'MDH'                                   'malate dehydrogenase'
  'ME1'                                   'malic enzyme (NAD)'
  'ME2'                                   'malic enzyme (NADP)'
  'NADH16'                                'NADH dehydrogenase (ubiquinone-8 & 3 protons)'
  'NADTRHD'                               'NAD transhydrogenase'
  'NH4t'                                  'ammonia reversible transport'
  'O2t'                                   'o2 transport (diffusion)'
  'PDH'                                   'pyruvate dehydrogenase'
  'PFK'                                   'phosphofructokinase'
  'PFL'                                   'pyruvate formate lyase'
  'PGI'                                   'glucose-6-phosphate isomerase'
  'PGK'                                   'phosphoglycerate kinase'
  'PGL'                                   ' 6-phosphogluconolactonase'
  'PGM'                                   'phosphoglycerate mutase'
  'PIt2r'                                 'phosphate reversible transport via symport'
  'PPC'                                   'phosphoenolpyruvate carboxylase'
  'PPCK'                                  'phosphoenolpyruvate carboxykinase'
  'PPS'                                   'phosphoenolpyruvate synthase'
  'PTAr'                                  'phosphotransacetylase'
  'PYK'                                   'pyruvate kinase'
  'PYRt2r'                                'pyruvate reversible transport via proton symport'
  'RPE'                                   'ribulose 5-phosphate 3-epimerase'
  'RPI'                                   'ribose-5-phosphate isomerase'
  'SUCCt2_2'                              'succinate transport via proton symport (2 H)'
  'SUCCt3'                                'succinate transport out via proton antiport'
  'SUCDi'                                 'succinate dehydrogenase (irreversible)'
  'SUCOAS'                                'succinyl-CoA synthetase (ADP-forming)'
  'TALA'                                  'transaldolase'
  'THD2'                                  'NAD(P) transhydrogenase'
  'TKT1'                                  'transketolase'
  'TKT2'                                  'transketolase'
  'TPI'                                   'triose-phosphate isomerase'

Diary written to: /Users/gpreciat/work/code/ctf/databases/ecoliDB
generateChemicalDatabase run is complete.
```

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