COBRA Models Overview

This tutorial will reveiw the basic atributes of a COBRA model.

```
clear;
```

Loading COBRA models

There are several to read or load models associated with the COBRA toolbox. They include:

1. Loading a model located in the same directory as the calling program

   model = readCbModel('model name'); # This could be a .mat or .xml (SBML) file, example: *model = readCbModel('e_coli_core.mat');*

```
model = readCbModel('e_coli_core.mat');
```

```
Each model.subSystems{x} is a character array, and this format is retained.
```

2. Loading a model from the BIGG database (BiGG Models (ucsd.edu))

   `loadBiGGModel`(*model_ids*, *format*, *multichoice*). example: *`model = loadBiGGModel('e_coli_core');`*

```
model2 = loadBiGGModel('iJO1366'); % Larger E.coli model
```

```
Each model.subSystems{x} is a character array, and this format is retained.
```

The models available in the BIGG database can be found by the following function (BiGG Models (ucsd.edu)).

```
BIGGmodels = listBiGGModels();
BIGG_Models_List = split(BIGGmodels,"{")
```

```
BIGG_Models_List = 110×1 cell
''
'"results": ['
'"bigg_id": "e_coli_core", "…
'"bigg_id": "iAB_RBC_283", "…
'"bigg_id": "iAF1260", "gene…
'"bigg_id": "iAF1260b", "gen…
'"bigg_id": "iAF692", "gene_…
'"bigg_id": "iAF987", "gene_…
'"bigg_id": "iAM_Pb448", "ge…
'"bigg_id": "iAM_Pc455", "ge…
```

Model Information

The details of the model can be seen as follows

```
model
```

```
model = struct with fields:
              S: [72×95 double]
           mets: {72×1 cell}
              b: [72×1 double]
         csense: [72×1 char]
           rxns: {95×1 cell}
             lb: [95×1 double]
             ub: [95×1 double]
              c: [95×1 double]
      osenseStr: 'max'
          genes: {137×1 cell}
          rules: {95×1 cell}
     metCharges: [72×1 double]
    metFormulas: {72×1 cell}
       metNames: {72×1 cell}
        grRules: {95×1 cell}
     rxnGeneMat: [95×137 double]
       rxnNames: {95×1 cell}
```

The purpose of each of these variables is listed below

- S: The stoichiometric matrix containing the model structure (for large models a sparse format is suggested)
- mets: Identifiers of the metabolites (ex: '13dpg_c', '2pg_c', ...)
- b: The coefficients of the constraints of the metabolites.
- csense: Constraint sense - This field indicates the sense of the b matrix, i.e. if b stands for lower than (‘L’) or greater than (‘G’) or equality constraints (‘E’). It is initialized as a char vector of ‘E’ with the same size as model.mets.
- rxns:Identifiers for the reactions (ex: 'ACALD', 'ACKr', ...)
- lb: The lower bounds for fluxes through the reactions.
- ub: The upper bounds for fluxes through the reactions.
- c: The objective coefficient of the reactions.

- osenseStr: The objective sense to either maximize (‘max) or minimize (‘min’) the value of the objective function.
- genes: Identifiers of the genes in the model (ex: 'b0351', 'b1241', ...)
- rules: GPR rules in evaluateable format for each reaction (e.g. "x(1) | x(2) & x(3)", would indicate the first gene or both the second and third gene are necessary for the respective reaction to carry flux.
- metFormulas: Elemental formula for each metabolite (ex: 'C3H4O10P2', 'C3H4O7P', ...)
- metNames: Full name of each corresponding metabolite (ex: 'D-Glycerate 2-phosphate', '3-Phospho-D-glycerate', ...)
- grRules: A string representation of the GPR rules defined in a readable format.
- rxnGeneMat: Matrix with rows corresponding to reactions and columns corresponding to genes.
- rxnNames: Full name of each corresponding reaction (ex: 'Acetaldehyde dehydrogenase (acetylating)', 'Acetate kinase', ...)
- subSystems: subSystem assignment for each reaction (ex: 'Pyruvate Metabolism', 'Citric Acid Cycle', ...)
- description: The name of the file that holds the model
- modelID: The model ID used by the BIGG database

see [cobratoolbox/COBRAModelFields.md at master · opencobra/cobratoolbox · GitHub]

COBRA Reactions Attributes

All of the reactions in the model can be listed as follows

```
model.rxns
```

```
ans = 95×1 cell
'PFK'
'PFL'
'PGI'
'PGK'
'PGL'
'ACALD'
'AKGt2r'
'PGM'
'PIt2r'
'ALCD2x'
```

Printing the reactions and all their attributes

```
rxnIDs = findRxnIDs(model, model.rxns);
Reaction_Abbreviations = model.rxns;
Name = model.rxnNames;
Lower_Bounds = model.lb;
Upper_Bounds = model.ub;
Equations = printRxnFormula(model, model.rxns,0);
Subsystem = model.subSystems;
GPR = findGPRFromRxns(model,rxnIDs);
T = table(Name, Lower_Bounds, Upper_Bounds, Equations,Subsystem,GPR, 'RowNames',Reaction_Abbreviations)
```

T = 95×6 table

	Name	Lower_Bounds	Upper_Bounds	Equations	Subsystem	GPR
1 PFK	'Phosphofru…	0	1000	'atp_c + f6p_c ->…	'Glycolysis/Gluco…	'b3916 or b…
2 PFL	'Pyruvate fo…	0	1000	'pyr_c + coa_c -…	'Pyruvate Metabo…	'((b0902 an…
3 PGI	'Glucose-6-…	-1000	1000	'g6p_c <=> f6p_c '	'Glycolysis/Gluco…	'b4025'
4 PGK	'Phosphogl…	-1000	1000	'3pg_c + atp_c <…	'Glycolysis/Gluco…	'b2926'
5 PGL	'6-phospho…	0	1000	'h2o_c + 6pgl_c …	'Pentose Phosph…	'b0767'
6 ACALD	'Acetaldehy…	-1000	1000	'nad_c + acald_c …	'Pyruvate Metabo…	'b0351 or b…
7 AKGt2r	'2 oxoglutar…	-1000	1000	'h_e + akg_e <=…	'Transport, Extrac…	'b2587'
8 PGM	'Phosphogl…	-1000	1000	'2pg_c <=> 3pg_…	'Glycolysis/Gluco…	'b3612 or b…
9 PIt2r	'Phosphate …	-1000	1000	'h_e + pi_e <=> …	'Inorganic Ion Tra…	'b2987 or b…
10 ALCD2x	'Alcohol de…	-1000	1000	'nad_c + etoh_c …	'Pyruvate Metabo…	'b0356 or b…
11 ACALDt	'Acetaldehy…	-1000	1000	'acald_e <=> ac…	'Transport, Extrac…	's0001'
12 ACKr	'Acetate kin…	-1000	1000	'ac_c + atp_c <=…	'Pyruvate Metabo…	'b3115 or b…
13 PPC	'Phosphoen…	0	1000	'h2o_c + pep_c +…	'Anaplerotic react…	'b3956'
14 ACONTa	'Aconitase (…	-1000	1000	'cit_c <=> h2o_c…	'Citric Acid Cycle'	'b0118 or b…
15 ACONTb	'Aconitase (…	-1000	1000	'h2o_c + acon_C…	'Citric Acid Cycle'	'b0118 or b…
16 ATPM	'ATP mainte…	8.3900	1000	'h2o_c + atp_c -…	'Biomass and ma…	''
17 PPCK	'Phosphoen…	0	1000	'oaa_c + atp_c -…	'Anaplerotic react…	'b3403'
18 ACt2r	'Acetate rev…	-1000	1000	'h_e + ac_e <=> …	'Transport, Extrac…	''
19 PPS	'Phosphoen…	0	1000	'h2o_c + pyr_c + …	'Glycolysis/Gluco…	'b1702'
20 ADK1	'Adenylate …	-1000	1000	'amp_c + atp_c …	'Oxidative Phosp…	'b0474'
21 AKGDH	'2-Oxoglute…	0	1000	'nad_c + akg_c +…	'Citric Acid Cycle'	'b0116 and …
22 ATPS4r	'ATP syntha…	-1000	1000	'4 h_e + pi_c + a…	'Oxidative Phosp…	'((b3736 an…
23 PTAr	'Phosphotra…	-1000	1000	'pi_c + accoa_c …	'Pyruvate Metabo…	'b2297 or b…
24 PYK	'Pyruvate ki…	0	1000	'h_c + pep_c + a…	'Glycolysis/Gluco…	'b1854 or b…
25 BIOMASS_Ecoli_core_w_GAM	'Biomass O…	0	1000	'0.2557 gln__L_c…	'Biomass and ma…	''
26 PYRt2	'Pyruvate tr…	-1000	1000	'h_e + pyr_e <=>…	'Transport, Extrac…	''

	Name	Lower_Bounds	Upper_Bounds	Equations	Subsystem	GPR
27 CO2t	'CO2 transp…	-1000	1000	'co2_e <=> co2_…	'Transport, Extrac…	's0001'
28 RPE	'Ribulose 5-…	-1000	1000	'ru5p__D_c <=> …	'Pentose Phosph…	'b3386 or b…
29 CS	'Citrate synt…	0	1000	'h2o_c + oaa_c +…	'Citric Acid Cycle'	'b0720'
30 RPI	'Ribose-5-p…	-1000	1000	'r5p_c <=> ru5p…	'Pentose Phosph…	'b2914 or b…
31 SUCCt2_2	'Succinate t…	0	1000	'2 h_e + succ_e …	'Transport, Extrac…	'b3528'
32 CYTBD	'Cytochrom…	0	1000	'2 h_c + 0.5 o2_c…	'Oxidative Phosp…	'(b0978 and…
33 D_LACt2	'D lactate tr…	-1000	1000	'h_e + lac__D_e …	'Transport, Extrac…	'b2975 or b…
34 ENO	'Enolase'	-1000	1000	'2pg_c <=> h2o_…	'Glycolysis/Gluco…	'b2779'
35 SUCCt3	'Succinate t…	0	1000	'h_e + succ_c ->…	'Transport, Extrac…	''
36 ETOHt2r	'Ethanol rev…	-1000	1000	'h_e + etoh_e <=…	'Transport, Extrac…	''
37 SUCDi	'Succinate …	0	1000	'q8_c + succ_c -…	'Oxidative Phosp…	'b0721 and …
38 SUCOAS	'Succinyl-C…	-1000	1000	'succ_c + atp_c +…	'Citric Acid Cycle'	'b0728 and …
39 TALA	'Transaldol…	-1000	1000	's7p_c + g3p_c …	'Pentose Phosph…	'b2464 or b…
40 THD2	'NAD(P) tra…	0	1000	'2 h_e + nadh_c …	'Oxidative Phosp…	'b1602 and …
41 TKT1	'Transketol…	-1000	1000	'r5p_c + xu5p__…	'Pentose Phosph…	'b2935 or b…
42 TKT2	'Transketol…	-1000	1000	'xu5p__D_c + e4…	'Pentose Phosph…	'b2935 or b…
43 TPI	'Triose-pho…	-1000	1000	'dhap_c <=> g3p…	'Glycolysis/Gluco…	'b3919'
44 EX_ac_e	'Acetate ex…	0	1000	'ac_e -> '	'Extracellular exc…	''
45 EX_acald_e	'Acetaldehy…	0	1000	'acald_e -> '	'Extracellular exc…	''
46 EX_akg_e	'2-Oxogluta…	0	1000	'akg_e -> '	'Extracellular exc…	''
47 EX_co2_e	'CO2 excha…	-1000	1000	'co2_e <=> '	'Extracellular exc…	''
48 EX_etoh_e	'Ethanol ex…	0	1000	'etoh_e -> '	'Extracellular exc…	''
49 EX_for_e	'Formate ex…	0	1000	'for_e -> '	'Extracellular exc…	''
50 EX_fru_e	'D-Fructose…	0	1000	'fru_e -> '	'Extracellular exc…	''
51 EX_fum_e	'Fumarate e…	0	1000	'fum_e -> '	'Extracellular exc…	''
52 EX_glc__D_e	'D-Glucose …	-10	1000	'glc__D_e <=> '	'Extracellular exc…	''
53 EX_gln__L_e	'L-Glutamin…	0	1000	'gln__L_e -> '	'Extracellular exc…	''
54 EX_glu__L_e	'L-Glutamat…	0	1000	'glu__L_e -> '	'Extracellular exc…	''
55 EX_h_e	'H+ exchan…	-1000	1000	'h_e <=> '	'Extracellular exc…	''
56 EX_h2o_e	'H2O excha…	-1000	1000	'h2o_e <=> '	'Extracellular exc…	''
57 EX_lac__D_e	'D-lactate e…	0	1000	'lac__D_e -> '	'Extracellular exc…	''
58 EX_mal__L_e	'L-Malate e…	0	1000	'mal__L_e -> '	'Extracellular exc…	''
59 EX_nh4_e	'Ammonia e…	-1000	1000	'nh4_e <=> '	'Extracellular exc…	''
60 EX_o2_e	'O2 exchan…	-1000	1000	'o2_e <=> '	'Extracellular exc…	''
61 EX_pi_e	'Phosphate …	-1000	1000	'pi_e <=> '	'Extracellular exc…	''
62 EX_pyr_e	'Pyruvate e…	0	1000	'pyr_e -> '	'Extracellular exc…	''
63 EX_succ_e	'Succinate …	0	1000	'succ_e -> '	'Extracellular exc…	''
64 FBA	'Fructose-bi…	-1000	1000	'fdp_c <=> dhap…	'Glycolysis/Gluco…	'b2097 or b…
65 FBP	'Fructose-bi…	0	1000	'h2o_c + fdp_c -…	'Glycolysis/Gluco…	'b3925 or b…
66 FORt2	'Formate tr…	0	1000	'h_e + for_e -> h…	'Transport, Extrac…	'b0904 or b…
67 FORt	'Formate tr…	-1000	0	'for_e <=> for_c '	'Transport, Extrac…	'b0904 or b…
68 FRD7	'Fumarate r…	0	1000	'q8h2_c + fum_c …	'Oxidative Phosp…	'b4151 and …
69 FRUpts2	'Fructose tr…	0	1000	'pep_c + fru_e ->…	'Transport, Extrac…	'b1817 and …
70 FUM	'Fumarase'	-1000	1000	'h2o_c + fum_c …	'Citric Acid Cycle'	'b1612 or b…
71 FUMt2_2	'Fumarate t…	0	1000	'2 h_e + fum_e -…	'Transport, Extrac…	'b3528'
72 G6PDH2r	'Glucose 6-…	-1000	1000	'nadp_c + g6p_c …	'Pentose Phosph…	'b1852'
73 GAPD	'Glyceralde…	-1000	1000	'nad_c + pi_c + g…	'Glycolysis/Gluco…	'b1779'
74 GLCpts	'D-glucose t…	0	1000	'glc__D_e + pep_…	'Transport, Extrac…	'(b2417 and…
75 GLNS	'Glutamine …	0	1000	'glu__L_c + nh4_…	'Glutamate Meta…	'b3870 or b…
76 GLNabc	'L-glutamin…	0	1000	'gln__L_e + h2o_…	'Transport, Extrac…	'b0811 and …
77 GLUDy	'Glutamate …	-1000	1000	'glu__L_c + h2o_…	'Glutamate Meta…	'b1761'
78 GLUN	'Glutaminase'	0	1000	'gln__L_c + h2o_…	'Glutamate Meta…	'b1812 or b…
79 GLUSy	'Glutamate …	0	1000	'gln__L_c + h_c …	'Glutamate Meta…	'b3212 and …
80 GLUt2r	'L glutamat…	-1000	1000	'glu__L_e + h_e …	'Transport, Extrac…	'b4077'
81 GND	'Phosphogl…	0	1000	'nadp_c + 6pgc_…	'Pentose Phosph…	'b2029'
82 H2Ot	'H2O transp…	-1000	1000	'h2o_e <=> h2o_…	'Transport, Extrac…	'b0875 or s…
83 ICDHyr	'Isocitrate d…	-1000	1000	'icit_c + nadp_c …	'Citric Acid Cycle'	'b1136'
84 ICL	'Isocitrate ly…	0	1000	'icit_c -> glx_c + …	'Anaplerotic react…	'b4015'
85 LDH_D	'D-lactate d…	-1000	1000	'lac__D_c + nad_…	'Pyruvate Metabo…	'b2133 or b…
86 MALS	'Malate synt…	0	1000	'glx_c + h2o_c + …	'Anaplerotic react…	'b4014 or b…
87 MALt2_2	'Malate tran…	0	1000	'2 h_e + mal__L_…	'Transport, Extrac…	'b3528'
88 MDH	'Malate deh…	-1000	1000	'mal__L_c + nad…	'Citric Acid Cycle'	'b3236'
89 ME1	'Malic enzy…	0	1000	'mal__L_c + nad…	'Anaplerotic react…	'b1479'
90 ME2	'Malic enzy…	0	1000	'mal__L_c + nad…	'Anaplerotic react…	'b2463'
91 NADH16	'NADH deh…	0	1000	'4 h_c + nadh_c …	'Oxidative Phosp…	'b2276 and …

	Name	Lower_Bounds	Upper_Bounds	Equations	Subsystem	GPR
92 NADTRHD	'NAD trans…	0	1000	'nad_c + nadph_…	'Oxidative Phosp…	'b3962 or (b…
93 NH4t	'Ammonia r…	-1000	1000	'nh4_e <=> nh4_…	'Inorganic Ion Tra…	's0001 or b…
94 O2t	'O2 transpo…	-1000	1000	'o2_e <=> o2_c '	'Transport, Extrac…	's0001'
95 PDH	'Pyruvate d…	0	1000	'nad_c + pyr_c + …	'Glycolysis/Gluco…	'b0114 and …

COBRA Metabolite Attributes

The metabolites included in a COBRA model can be found as follows

```
model.mets
```

```
ans = 72×1 cell
'glc__D_e'
'gln__L_c'
'gln__L_e'
'glu__L_c'
'glu__L_e'
'glx_c'
'h2o_c'
'h2o_e'
'h_c'
'h_e'
```

Printing metabolite attributes

```
Metabolite_Abbreviations = model.mets;
Metabolite_Name = model.metNames;
Metabolite_Formulas = model.metFormulas;
T = table(Metabolite_Name, Metabolite_Formulas,'RowNames',Metabolite_Abbreviations)
```

T = 72×2 table

	Metabolite_Name	Metabolite_Formulas
1 glc__D_e	'D-Glucose'	'C6H12O6'
2 gln__L_c	'L-Glutamine'	'C5H10N2O3'
3 gln__L_e	'L-Glutamine'	'C5H10N2O3'
4 glu__L_c	'L-Glutamate'	'C5H8NO4'
5 glu__L_e	'L-Glutamate'	'C5H8NO4'
6 glx_c	'Glyoxylate'	'C2H1O3'
7 h2o_c	'H2O H2O'	'H2O'
8 h2o_e	'H2O H2O'	'H2O'
9 h_c	'H+'	'H'
10 h_e	'H+'	'H'
11 icit_c	'Isocitrate'	'C6H5O7'
12 lac__D_c	'D-Lactate'	'C3H5O3'
13 lac__D_e	'D-Lactate'	'C3H5O3'
14 mal__L_c	'L-Malate'	'C4H4O5'
15 mal__L_e	'L-Malate'	'C4H4O5'
16 nad_c	'Nicotinamide adenine din…	'C21H26N7O14P2'
17 nadh_c	'Nicotinamide adenine din…	'C21H27N7O14P2'
18 nadp_c	'Nicotinamide adenine din…	'C21H25N7O17P3'
19 nadph_c	'Nicotinamide adenine din…	'C21H26N7O17P3'
20 nh4_c	'Ammonium'	'H4N'
21 13dpg_c	'3-Phospho-D-glyceroyl p…	'C3H4O10P2'
22 nh4_e	'Ammonium'	'H4N'
23 o2_c	'O2 O2'	'O2'
24 2pg_c	'D-Glycerate 2-phosphate'	'C3H4O7P'
25 o2_e	'O2 O2'	'O2'
26 3pg_c	'3-Phospho-D-glycerate'	'C3H4O7P'
27 oaa_c	'Oxaloacetate'	'C4H2O5'
28 pep_c	'Phosphoenolpyruvate'	'C3H2O6P'
29 6pgc_c	'6-Phospho-D-gluconate'	'C6H10O10P'
30 pi_c	'Phosphate'	'HO4P'
31 6pgl_c	'6-phospho-D-glucono-1,…	'C6H9O9P'
32 pi_e	'Phosphate'	'HO4P'
33 ac_c	'Acetate'	'C2H3O2'
34 pyr_c	'Pyruvate'	'C3H3O3'
35 pyr_e	'Pyruvate'	'C3H3O3'
36 q8_c	'Ubiquinone-8'	'C49H74O4'
37 q8h2_c	'Ubiquinol-8'	'C49H76O4'
38 r5p_c	'Alpha-D-Ribose 5-phosp…	'C5H9O8P'

	Metabolite_Name	Metabolite_Formulas
39 ru5p__D_c	'D-Ribulose 5-phosphate'	'C5H9O8P'
40 ac_e	'Acetate'	'C2H3O2'
41 acald_c	'Acetaldehyde'	'C2H4O'
42 s7p_c	'Sedoheptulose 7-phosph…	'C7H13O10P'
43 acald_e	'Acetaldehyde'	'C2H4O'
44 accoa_c	'Acetyl-CoA'	'C23H34N7O17P3S'
45 succ_c	'Succinate'	'C4H4O4'
46 succ_e	'Succinate'	'C4H4O4'
47 succoa_c	'Succinyl-CoA'	'C25H35N7O19P3S'
48 acon_C_c	'Cis-Aconitate'	'C6H3O6'
49 xu5p__D_c	'D-Xylulose 5-phosphate'	'C5H9O8P'
50 actp_c	'Acetyl phosphate'	'C2H3O5P'
51 adp_c	'ADP C10H12N5O10P2'	'C10H12N5O10P2'
52 akg_c	'2-Oxoglutarate'	'C5H4O5'
53 akg_e	'2-Oxoglutarate'	'C5H4O5'
54 amp_c	'AMP C10H12N5O7P'	'C10H12N5O7P'
55 atp_c	'ATP C10H12N5O13P3'	'C10H12N5O13P3'
56 cit_c	'Citrate'	'C6H5O7'
57 co2_c	'CO2 CO2'	'CO2'
58 co2_e	'CO2 CO2'	'CO2'
59 coa_c	'Coenzyme A'	'C21H32N7O16P3S'
60 dhap_c	'Dihydroxyacetone phosp…	'C3H5O6P'
61 e4p_c	'D-Erythrose 4-phosphate'	'C4H7O7P'
62 etoh_c	'Ethanol'	'C2H6O'
63 etoh_e	'Ethanol'	'C2H6O'
64 f6p_c	'D-Fructose 6-phosphate'	'C6H11O9P'
65 fdp_c	'D-Fructose 1,6-bisphosp…	'C6H10O12P2'
66 for_c	'Formate'	'CH1O2'
67 for_e	'Formate'	'CH1O2'
68 fru_e	'D-Fructose'	'C6H12O6'
69 fum_c	'Fumarate'	'C4H2O4'
70 fum_e	'Fumarate'	'C4H2O4'
71 g3p_c	'Glyceraldehyde 3-phosp…	'C3H5O6P'
72 g6p_c	'D-Glucose 6-phosphate'	'C6H11O9P'

COBRA Gene Attributes

The genes included in a COBRA model can be found as follows

```
model.genes
```

```
ans = 137×1 cell
'b1241'
'b0351'
's0001'
'b1849'
'b3115'
'b2296'
'b1276'
'b0118'
'b0474'
'b0116'
```

The attributes of the genes can be found in the model are as follows

```
Gene_Abbreviations = model.genes;
Gene_IDs = findGeneIDs(model, model.genes);
GPR = findGPRFromRxns(model,rxnIDs);
Metabolite_Name = model.metNames;
Metabolite_Formulas = model.metFormulas;
T = table(Gene_IDs,'RowNames',Gene_Abbreviations)
```

```
T = 137×1 table
```

	Gene_IDs
1 b1241	1
2 b0351	2
3 s0001	3
4 b1849	4
5 b3115	5
6 b2296	6

	Gene_IDs
7 b1276	7
8 b0118	8
9 b0474	9
10 b0116	10
11 b0727	11
12 b0726	12
13 b2587	13
14 b0356	14
15 b1478	15
16 b3734	16
17 b3733	17
18 b3736	18
19 b3737	19
20 b3739	20
21 b3738	21
22 b3735	22
23 b3731	23
24 b3732	24
25 b0720	25
26 b0733	26
27 b0734	27
28 b0979	28
29 b0978	29
30 b3603	30
31 b2975	31
32 b2779	32
33 b2925	33
34 b1773	34
35 b2097	35
36 b3925	36
37 b4232	37
38 b2492	38
39 b0904	39
40 b4152	40
41 b4154	41
42 b4153	42
43 b4151	43
44 b1819	44
45 b1817	45
46 b2416	46
47 b2415	47
48 b1818	48
49 b1611	49
50 b4122	50
51 b1612	51
52 b3528	52
53 b1852	53
54 b1779	54
55 b1101	55
56 b2417	56
57 b1621	57
58 b1297	58
59 b3870	59
60 b0809	60
61 b0811	61
62 b0810	62
63 b1761	63
64 b1524	64
65 b0485	65
66 b1812	66
67 b3213	67
68 b3212	68
69 b4077	69
70 b2029	70
71 b0875	71

	Gene_IDs
72 b1136	72
73 b4015	73
74 b1380	74
75 b2133	75
76 b4014	76
77 b2976	77
78 b3236	78
79 b1479	79
80 b2463	80
81 b2281	81
82 b2277	82
83 b2280	83
84 b2286	84
85 b2287	85
86 b2284	86
87 b2276	87
88 b2282	88
89 b2279	89
90 b2283	90
91 b2285	91
92 b2288	92
93 b2278	93
94 b1603	94
95 b3962	95
96 b1602	96
97 b0451	97
98 b0114	98
99 b0115	99
100 b3916	100

General Model Information

Model Compartments

The compartments that can be supported by teh COBRA toolbox are

```
getDefaultCompartments
```

```
ans = 1×12 cell
'c'          'm'          'v'          'x'          'e'          't'          'g'          'r'          'n'          'p'          'l'          'u'
```

Model Objective Function

The active objective function is found by

```
checkObjective(model)
```

```
summaryT = 23×5 table
```

	Coefficient	Metabolite	metID	Reaction	RxnID
1	-0.2557	gln__L_c	2	BIOMASS_Ecol…	25
2	-4.9414	glu__L_c	4	BIOMASS_Ecol…	25
3	-59.8100	h2o_c	7	BIOMASS_Ecol…	25
4	59.8100	h_c	9	BIOMASS_Ecol…	25
5	-3.5470	nad_c	16	BIOMASS_Ecol…	25
6	3.5470	nadh_c	17	BIOMASS_Ecol…	25
7	13.0279	nadp_c	18	BIOMASS_Ecol…	25
8	-13.0279	nadph_c	19	BIOMASS_Ecol…	25
9	-1.4960	3pg_c	26	BIOMASS_Ecol…	25
10	-1.7867	oaa_c	27	BIOMASS_Ecol…	25
11	-0.5191	pep_c	28	BIOMASS_Ecol…	25
12	59.8100	pi_c	30	BIOMASS_Ecol…	25
13	-2.8328	pyr_c	34	BIOMASS_Ecol…	25
14	-0.8977	r5p_c	38	BIOMASS_Ecol…	25
15	-3.7478	accoa_c	44	BIOMASS_Ecol…	25
16	59.8100	adp_c	51	BIOMASS_Ecol…	25
17	4.1182	akg_c	52	BIOMASS_Ecol…	25
18	-59.8100	atp_c	55	BIOMASS_Ecol…	25
19	3.7478	coa_c	59	BIOMASS_Ecol…	25
20	-0.3610	e4p_c	61	BIOMASS_Ecol…	25

	Coefficient	Metabolite	metID	Reaction	RxnID
21	-0.0709	f6p_c	64	BIOMASS_Ecol…	25
22	-0.1290	g3p_c	71	BIOMASS_Ecol…	25
23	-0.2050	g6p_c	72	BIOMASS_Ecol…	25

```
ans = 1×1 cell array
    {'BIOMASS_Ecoli_core_w_GAM'}
```

Model Uptake (model medium)

Print all the reactions that have lower bounds that allow for substrate uptake. The numbers at the end are the reaction ID of the listed exchange reactions

```
uptakeInd = printUptakeBound(model)
```

```
EX_co2_e                      -1000
EX_glc__D_e                     -10
EX_h_e                        -1000
EX_h2o_e                      -1000
EX_nh4_e                      -1000
EX_o2_e                       -1000
EX_pi_e                       -1000
uptakeInd = 7×1
    47
    52
    55
    56
    59
    60
    61
```

Model Exchange, Sink and Demand Reactions

FInd exchange reactions in the model. **selExc** – Boolean vector indicating whether each reaction in model is exchange or not. **selUpt** – Boolean vector indicating whether each reaction in model is nutrient uptake or not. Exchange reactions: These reactions are unbalanced, extra-organism reactions that represent the supply to or removal of metabolites from the extra-organism “space”.Demand reaction – When the consumption reaction(s) of a metabolite is not known or outside the scope of the reconstruction it can be represented by this unbalanced, intracellular reaction (e.g., 1 A -->). Sink reaction – When the synthesis reaction(s) of a metabolite is not known or outside the scope of the reconstruction its discharge can be represented by this unbalanced, intracellular reaction (e.g., 1 A <-->). Exchange reactions start with "EX_", demand reactions start with "DM_", and sink reactions start with "SK_".

```
[selExc, selUpt] = findExcRxns(model2);
model2.rxns(selExc)
```

```
ans = 330×1 cell
'EX_cm_e'
'EX_cmp_e'
'EX_co2_e'
'EX_cobalt2_e'
'DM_4crsol_c'
'DM_5drib_c'
'DM_aacald_c'
'DM_amob_c'
'DM_mthf_c'
'EX_colipa_e'
```

The reactions that are available for uptake

```
model2.rxns(selUpt)
```

```
ans = 25×1 cell
'EX_co2_e'
'EX_cobalt2_e'
'EX_glc__D_e'
'EX_h_e'
'EX_h2o_e'
'EX_k_e'
'EX_cu2_e'
'EX_mg2_e'
'EX_mn2_e'
'EX_mobd_e'
```

COBRA Subsystems

The subsystems found in a model can be found with the following function

```
getModelSubSystems(model)
```

```
ans = 11×1 cell
```

```
'Anaplerotic reactions'
'Biomass and maintenance fun…
'Citric Acid Cycle'
'Extracellular exchange'
'Glutamate Metabolism'
'Glycolysis/Gluconeogenesis'
'Inorganic Ion Transport and…
'Oxidative Phosphorylation'
'Pentose Phosphate Pathway'
'Pyruvate Metabolism'
```

Is a reaction in a subsystem

```
isReactionInSubSystem(model, {'ACALD';'ACKr'}, {'Pyruvate Metabolism'})
```

```
ans = 2×1 logical array
   1
   1
```

Model Visualization

A simple way to visualize a model is to use the Escher (Escher) tools. The Escher website discusses how to load different COBRA models and their maps. An example of the *E.coli* core model map is shown below.