

Create a generic subnetwork from Recon 3D

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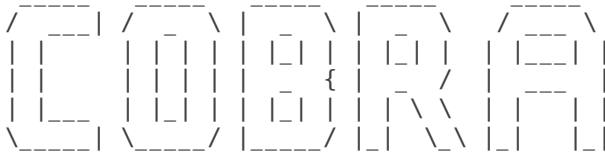
Reviewer(s): Almut Heinken, University of Luxembourg.

In this tutorial, we show how to create a generic subnetwork from Recon 3D that can still perform all metabolic test functions as well as has physiologically defined ATP yield from defined carbon sources. The resulting model does not contain a specified list of reactions, except if they are still needed for the aforementioned tasks, and that is flux consistent.

EQUIPMENT SETUP

If necessary, initialize the cobra toolbox:

```
initCobraToolbox
```



COstraint-Based Reconstruction and Analysis
The COBRA Toolbox - 2017

Documentation:
<http://opencobra.github.io/cobratoolbox>

```
> Checking if git is installed ... Done.
> Checking if the repository is tracked using git ... Done.
> Checking if curl is installed ... Done.
> Checking if remote can be reached ... Done.
> Initializing and updating submodules ... Done.
> Adding all the files of The COBRA Toolbox ... Done.
> Define CB map output... set to svg.
> Retrieving models ... Done.
> TranslateSBML is installed and working properly.
> Configuring solver environment variables ...
- [*---] ILOG_CPLEX_PATH: C:\Program Files\IBM\ILOG\CPLEX_Studio1263\cplex\matlab\x64_win64
- [----] GUROBI_PATH : --> set this path manually after installing the solver ( see instructions )
- [*---] TOMLAB_PATH: C:\tomlab\
- [----] MOSEK_PATH : --> set this path manually after installing the solver ( see instructions )
Done.
> Checking available solvers and solver interfaces ... Done.
> Setting default solvers ... Done.
> Saving the MATLAB path ... Done.
- The MATLAB path was saved in the default location.

> Summary of available solvers and solver interfaces
```

| | Support | LP | MILP | QP | MIQP | NLP | |
|--------------|---------|----|------|----|------|-----|---|
| cplex_direct | full | | 0 | 0 | 0 | 0 | - |
| dqqMinos | full | | 0 | - | - | - | - |
| glpk | full | | 1 | 1 | - | - | - |
| gurobi | full | | 1 | 1 | 1 | 1 | - |
| ibm_cplex | full | | 0 | 0 | 0 | - | - |
| matlab | full | | 1 | - | - | - | 1 |
| mosek | full | | 0 | 0 | 0 | - | - |
| pdco | full | | 1 | - | 1 | - | - |
| quadMinos | full | | 0 | - | - | - | 0 |
| tomlab_cplex | full | | 1 | 1 | 1 | 1 | - |

| | | | | | | |
|--------------|--------------|---|---|---|---|---|
| qpng | experimental | - | - | 1 | - | - |
| tomlab_snopt | experimental | - | - | - | - | 1 |
| gurobi_mex | legacy | 0 | 0 | 0 | 0 | - |
| lindo_old | legacy | 0 | - | - | - | - |
| lindo_legacy | legacy | 0 | - | - | - | - |
| lp_solve | legacy | 1 | - | - | - | - |
| opti | legacy | 0 | 0 | 0 | 0 | 0 |
| ----- | | | | | | |
| Total | - | 6 | 3 | 4 | 2 | 2 |

+ Legend: - = not applicable, 0 = solver not compatible or not installed, 1 = solver installed.

```
> You can solve LP problems using: 'glpk' - 'gurobi' - 'matlab' - 'pdco' - 'tomlab_cplex' - 'lp_solve'
> You can solve MILP problems using: 'glpk' - 'gurobi' - 'tomlab_cplex'
> You can solve QP problems using: 'gurobi' - 'pdco' - 'tomlab_cplex' - 'qpng'
> You can solve MIQP problems using: 'gurobi' - 'tomlab_cplex'
> You can solve NLP problems using: 'matlab' - 'tomlab_snopt'

> Checking for available updates ...
--> You cannot update your fork using updateCobraToolbox(). [940ff8 @ develop].
Please use the MATLAB.devTools (https://github.com/opencobra/MATLAB.devTools).
```

For solving linear programming problems in FBA analysis, certain solvers are required:

```
% changeCobraSolver ('glpk', 'all', 1);
changeCobraSolver ('tomlab_cplex', 'all', 1);
```

```
> Tomlab interface added to MATLAB path.
> Solver for LPproblems has been set to tomlab_cplex.

> Tomlab interface added to MATLAB path.
> Solver for MILPproblems has been set to tomlab_cplex.

> Tomlab interface added to MATLAB path.
> Solver for QPproblems has been set to tomlab_cplex.

> Tomlab interface added to MATLAB path.
> Solver for MIQPproblems has been set to tomlab_cplex.
> Solver tomlab_cplex not supported for problems of type NLP. Currently used: matlab
```

This tutorial can be run with 'glpk' package as linear programming solver, which does not require additional installation and configuration. However, for the analysis of large models, such as Recon 3, it is not recommended to use 'glpk' but rather industrial strength solvers, such as the 'gurobi' package. For detail information, refer to the solver installation guide: <https://github.com/opencobra/cobratoolbox/blob/master/docs/source/installation/solvers.md>

```
warning off MATLAB:subscripting:noSubscriptsSpecified
```

PROCEDURE

Before proceeding with the simulations, the path for the model needs to be set up. In this tutorial, the used model is the generic model of human metabolism, Recon 3 [1]. If Recon 3 is not available, please use Recon 2.

```
if exist('2017_04_28_Recon3dForCurrentDistribution.mat','file')==2
    filename = '2017_04_28_Recon3dForCurrentDistribution.mat';
    load(filename);
    model=modelRecon3model;
    clear modelRecon3model;
```

```

        model.csense(1:size(model.S,1),1)='E';
else
    filename2='Recon2.0model.mat';
    if exist('Recon2.0model.mat','file')==2
        load(filename2);
        model=Recon2model;
        clear Recon2model;
        model.csense(1:size(model.S,1),1)='E';
    end
end
end

```

Set the lower bounds on all biomass reactions and sink/demand reactions to zero.

```

model.lb(find(ismember(model.rxns,'biomass_reaction')))=0;
model.lb(find(ismember(model.rxns,'biomass_maintenance_noTrTr')))=0;
model.lb(find(ismember(model.rxns,'biomass_maintenance')))=0;
DMs = (strmatch('DM_',model.rxns));
model.lb(DMs) = 0;
Sinks = (strmatch('sink_',model.rxns));
model.lb(Sinks) = 0;
model.ub(Sinks) = 1000;

```

Test, which model reactions are needed to ensure that all carbon sources result in a physiologically relevant ATP yield. Note that this function uses sparseFBA, i.e., alternative solutions may exist but are not considered here.

```
[Table_csourcesOri, TestedRxnsC, Perc] = testATPYieldFromCsources(model);
```

Warning: Reaction with the same name already exists in the model, updating the reaction

```
DM_atp_c_h2o(c) + atp(c) -> h(c) + adp(c) + pi(c)
```

Test, which model reactions are needed to ensure that all metabolic functions can have a non-zero flux. Note that this function uses sparseFBA, i.e., alternative solutions may exist but are not considered here.

```
[TestSolutionOri,TestSolutionNameClosedSinks, TestedRxnsClosedSinks, PercClosedSinks] = Test4H
```

Warning: Reaction with the same name already exists in the model, updating the reaction

```

sink_gly(c) gly(c) <=>
sink_co2(c) co2(c) ->
sink_nh4(c) nh4(c) ->
sink_12ppd-S(c) 12ppd-S(c) <=>
sink_mthgxl(c) mthgxl(c) ->
sink_12ppd-S(c) 12ppd-S(c) <=>
sink_pyr(c) pyr(c) ->
sink_3pg(c) 3pg(c) <=>
Warning: Reaction with the same name already exists in the model, updating the reaction
sink_gly(c) gly(c) ->
sink_3pg(c) 3pg(c) <=>
sink_ser-L(c) ser-L(c) ->
sink_4abut(c) 4abut(c) <=>
sink_succ(m) succ(m) ->
sink_4hpro-LT(m) 4hpro-LT(m) <=>
sink_glx(m) glx(m) ->
sink_5aop(c) 5aop(c) <=>
sink_pheme(c) pheme(c) ->
sink_aact(c) aact(c) <=>
sink_mthgxl(c) mthgxl(c) ->
sink_acac(m) acac(m) <=>
sink_acetone(m) acetone(m) ->

```

```
sink_acac(m) acac(m) <=>
sink_bhb(m) bhb(m) ->
sink_acald(c) acald(c) <=>
sink_ac(c) ac(c) ->
sink_accoa(c) accoa(c) <=>
```

Warning: Reaction with the same name already exists in the model, updating the reaction

```
sink_pmtcoa(c) pmtcoa(c) ->
```

Warning: Reaction with the same name already exists in the model, updating the reaction

```
sink_pmtcoa(c) pmtcoa(c) <=>
sink_malcoa(m) malcoa(m) ->
sink_acetone(c) acetone(c) <=>
sink_mthgxl(c) mthgxl(c) ->
sink_acgal(c) acgal(c) <=>
sink_udpacgal(c) udpacgal(c) ->
sink_acgam(c) acgam(c) <=>
sink_cmpacna(c) cmpacna(c) ->
sink_acorn(c) acorn(c) <=>
sink_orn(c) orn(c) ->
sink_adrnl(c) adrnl(c) <=>
sink_34dhoxpeg(c) 34dhoxpeg(c) ->
sink_akg(m) akg(m) <=>
sink_oaa(m) oaa(m) ->
sink_akg(m) akg(m) <=>
sink_glu-L(m) glu-L(m) ->
sink_akg(m) akg(m) <=>
sink_ala-B(c) ala-B(c) <=>
sink_msa(m) msa(m) ->
sink_ala-D(c) ala-D(c) <=>
sink_pyr(c) pyr(c) ->
sink_ala-L(c) ala-L(c) <=>
sink_ala-D(c) ala-D(c) ->
sink_ala-L(c) ala-L(c) <=>
sink_pyr(c) pyr(c) ->
sink_arachd(c) arachd(c) <=>
sink_malcoa(m) malcoa(m) ->
sink_arachd(r) arachd(r) <=>
sink_txa2(r) txa2(r) ->
sink_arg-L(c) arg-L(c) <=>
sink_creat(c) creat(c) ->
sink_arg-L(c) arg-L(c) <=>
sink_glu-L(m) glu-L(m) ->
sink_arg-L(c) arg-L(c) <=>
sink_no(c) no(c) ->
sink_arg-L(c) arg-L(c) <=>
sink_pcreat(c) pcreat(c) ->
sink_ascb-L(c) ascb-L(c) <=>
```

Warning: Metabolite eryth(c) not in model - added to the model

```
sink_eryth(c) eryth(c) ->
```

```
sink_ascb-L(c) ascb-L(c) <=>
```

Warning: Metabolite lyxnt(c) not in model - added to the model

```
sink_lyxnt(c) lyxnt(c) ->
```

```
sink_ascb-L(c) ascb-L(c) <=>
```

```
sink_thrnt(c) thrnt(c) ->
```

```
sink_ascb-L(c) ascb-L(c) <=>
```

Warning: Metabolite xylnt(c) not in model - added to the model

```
sink_xylnt(c) xylnt(c) ->
```

```
sink_asn-L(c) asn-L(c) <=>
```

```
sink_oaa(c) oaa(c) ->
```

```
sink_asp-L(c) asp-L(c) <=>
```

```
sink_hco3(c) hco3(c) <=>
```

```
sink_arg-L(c) arg-L(c) ->
```

```
sink_asp-L(c) asp-L(c) <=>
```

```
sink_ala-B(c) ala-B(c) ->
```

```
sink_asp-L(c) asp-L(c) <=>
```

```
sink_asn-L(c) asn-L(c) ->
```

```
sink_asp-L(c) asp-L(c) <=>
sink_argsuc(c) argsuc(c) ->
sink_argsuc(c) argsuc(c) <=>
sink_fum(c) fum(c) ->
sink_asp-L(c) asp-L(c) <=>
sink_dcamp(c) dcamp(c) ->
sink_dcamp(c) dcamp(c) <=>
sink_fum(c) fum(c) ->
sink_dcamp(c) dcamp(c) <=>
sink_fum(c) fum(c) ->
sink_asp-L(c) asp-L(c) <=>
sink_oaa(c) oaa(c) ->
sink_carn(c) carn(c) <=>
sink_ala-B(c) ala-B(c) ->
```

Warning: Reaction with the same name already exists in the model, updating the reaction

```
sink_chol(c) chol(c) <=>
sink_dag_hs(c) dag_hs(c) <=>
sink_pe_hs(c) pe_hs(c) ->
sink_chol(m) chol(m) <=>
sink_glyb(m) glyb(m) ->
sink_glyb(m) glyb(m) <=>
sink_gly(m) gly(m) ->
sink_coke(r) coke(r) <=>
```

Warning: Metabolite pecgoncoa(r) not in model - added to the model

```
sink_pecgoncoa(r) pecgoncoa(r) ->
sink_core2(g) core2(g) <=>
sink_ksii_core2(g) ksii_core2(g) ->
sink_core4(g) core4(g) <=>
sink_ksii_core4(g) ksii_core4(g) ->
sink_cspg_a(l) cspg_a(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
sink_cspg_b(l) cspg_b(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
sink_cspg_c(l) cspg_c(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
sink_cspg_d(l) cspg_d(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
sink_cspg_e(l) cspg_e(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
sink_cys-L(c) cys-L(c) <=>
sink_glu-L(c) glu-L(c) <=>
```

Warning: Reaction with the same name already exists in the model, updating the reaction

```
sink_gly(c) gly(c) <=>
sink_gthrd(c) gthrd(c) ->
sink_cys-L(c) cys-L(c) <=>
sink_3sala(c) 3sala(c) ->
sink_3sala(c) 3sala(c) <=>
sink_so4(c) so4(c) ->
sink_cys-L(c) cys-L(c) <=>
sink_hyptaur(c) hyptaur(c) ->
sink_Lcystin(c) Lcystin(c) <=>
sink_cys-L(c) cys-L(c) ->
sink_dhap(c) dhap(c) <=>
sink_mthgxl(c) mthgxl(c) ->
```

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

```

sink_dmpp(c) dmpp(c) <=>
Warning: Metabolite ggdp(c) not in model - added to the model

sink_ggdp(c) ggdp(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
Warning: Metabolite dna(n) not in model - added to the model

sink_dna(n) dna(n) <=>
Warning: Metabolite dna5mtc(n) not in model - added to the model

sink_dna5mtc(n) dna5mtc(n) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_dolichol_L(c) dolichol_L(c) <=>
Warning: Metabolite dolmanp_L(r) not in model - added to the model

sink_dolmanp_L(r) dolmanp_L(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_dolichol_L(c) dolichol_L(c) <=>
Warning: Metabolite g3m8mpdol_L(r) not in model - added to the model

sink_g3m8mpdol_L(r) g3m8mpdol_L(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_dolichol_U(c) dolichol_U(c) <=>
sink_dolmanp_U(r) dolmanp_U(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_dolichol_U(c) dolichol_U(c) <=>
Warning: Metabolite g3m8mpdol_U(r) not in model - added to the model

sink_g3m8mpdol_U(r) g3m8mpdol_U(r) ->
sink_dopa(c) dopa(c) <=>
sink_homoval(c) homoval(c) ->
sink_etoh(c) etoh(c) <=>
sink_acald(c) acald(c) ->
sink_f6p(c) f6p(c) <=>
sink_g3p(c) g3p(c) <=>
sink_r5p(c) r5p(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_frdp(c) frdp(c) <=>
sink_dolichol_L(r) dolichol_L(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_frdp(c) frdp(c) <=>
sink_dolichol_U(r) dolichol_U(r) ->
sink_ade(c) ade(c) <=>
sink_amp(c) amp(c) ->
sink_adn(c) adn(c) <=>
sink_urate(x) urate(x) ->
sink_adp(c) adp(c) <=>
sink_datp(n) datp(n) ->
sink_cdp(c) cdp(c) <=>
sink_dctp(n) dctp(n) ->
sink_cmp(c) cmp(c) <=>
sink_cytd(c) cytd(c) ->
sink_cytd(c) cytd(c) <=>
sink_ala-B(c) ala-B(c) ->
sink_dcmp(c) dcmp(c) <=>
sink_ala-B(c) ala-B(c) ->
sink_gdp(c) gdp(c) <=>
sink_dgtp(n) dgtp(n) ->
sink_gln-L(c) gln-L(c) <=>

```

```

sink_hco3(c) hco3(c) <=>
sink_ump(c) ump(c) ->
sink_gsn(c) gsn(c) <=>
sink_urate(x) urate(x) ->
sink_gua(c) gua(c) <=>
sink_gmp(c) gmp(c) ->
sink_hxan(c) hxan(c) <=>
sink_imp(c) imp(c) ->
sink_imp(c) imp(c) <=>
sink_atp(c) atp(c) ->
sink_imp(c) imp(c) <=>
sink_gtp(c) gtp(c) ->
sink_imp(c) imp(c) <=>
sink_urate(x) urate(x) ->
sink_prpp(c) prpp(c) <=>
sink_imp(c) imp(c) ->
Warning: Reaction with the same name already exists in the model, updating the reaction
sink_pydx(c) pydx(c) <=>
sink_pydx5p(c) pydx5p(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_thm(c) thm(c) <=>
Warning: Reaction with the same name already exists in the model, updating the reaction
sink_thmpp(c) thmpp(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_thm(e) thm(e) <=>
sink_thmpp(m) thmpp(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_thmpp(e) thmpp(e) <=>
Warning: Reaction with the same name already exists in the model, updating the reaction
sink_thmpp(c) thmpp(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_thmpp(m) thmpp(m) ->
sink_tyr-L(m) tyr-L(m) <=>
sink_q10(m) q10(m) ->
sink_udp(c) udp(c) <=>
sink_dttp(n) dttp(n) ->
sink_ump(c) ump(c) <=>
sink_ala-B(c) ala-B(c) ->
sink_fru(c) fru(c) <=>
sink_dhap(c) dhap(c) ->
sink_fru(c) fru(c) <=>
sink_g3p(c) g3p(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_fuc-L(c) fuc-L(c) <=>
sink_gdpfuc(c) gdpfuc(c) ->
sink_fum(m) fum(m) <=>
sink_oaa(m) oaa(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_glp(c) glp(c) <=>
Warning: Metabolite dtdprmn(c) not in model - added to the model
sink_dtdprmn(c) dtdprmn(c) ->
sink_g3p(c) g3p(c) <=>
sink_mthgxl(c) mthgxl(c) ->
sink_g6p(c) g6p(c) <=>
sink_r5p(c) r5p(c) ->
sink_g6p(c) g6p(c) <=>

```

```

sink_ru5p-D(c) ru5p-D(c) ->
sink_gal(c) gal(c) <=>
sink_glc-D(c) glc-D(c) ->
sink_gal(c) gal(c) <=>
sink_udpgal(c) udpgal(c) ->
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_galgalgalthcrm_hs(g) galgalgalthcrm_hs(g) ->
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_acgagbside_hs(g) acgagbside_hs(g) ->
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_acnacngalgsbside_hs(g) acnacngalgsbside_hs(g) ->
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gdlb2_hs(g) gdlb2_hs(g) ->
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gdlc_hs(g) gdlc_hs(g) ->
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gplc_hs(g) gplc_hs(g) ->
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gqlbalpha_hs(g) gqlbalpha_hs(g) ->
sink_gam6p(c) gam6p(c) <=>
sink_uacgam(c) uacgam(c) ->
sink_gdpmann(c) gdpmann(c) <=>
sink_gdpfuc(c) gdpfuc(c) ->
sink_glc-D(c) glc-D(c) <=>
sink_inost(c) inost(c) ->
sink_glc-D(c) glc-D(c) <=>
sink_lac-L(c) lac-L(c) ->
sink_atp(c) atp(c) ->
sink_h2o(c) h2o(c) ->
sink_glc-D(c) glc-D(c) <=>
sink_lac-D(c) lac-D(c) ->
sink_glc-D(c) glc-D(c) <=>
sink_lcts(g) lcts(g) ->
sink_glc-D(c) glc-D(c) <=>
sink_pyr(c) pyr(c) ->
sink_gln-L(c) gln-L(c) <=>
sink_nh4(c) nh4(c) ->
sink_gln-L(m) gln-L(m) <=>
sink_glu-L(m) glu-L(m) ->
sink_gln-L(m) gln-L(m) <=>
sink_glu-L(m) glu-L(m) ->
sink_glu5sa(c) glu5sa(c) <=>
sink_pro-L(c) pro-L(c) ->
sink_glu-L(c) glu-L(c) <=>
sink_4abut(c) 4abut(c) ->
sink_glu-L(c) glu-L(c) <=>
sink_gln-L(c) gln-L(c) ->
sink_glu-L(c) glu-L(c) <=>
sink_pro-L(c) pro-L(c) ->
sink_glu-L(m) glu-L(m) <=>
sink_akg(m) akg(m) ->
sink_gluside_hs(g) gluside_hs(g) <=>
sink_galgluside_hs(g) galgluside_hs(g) ->
sink_glx(m) glx(m) <=>
sink_glyclt(m) glyclt(m) ->

```

Warning: Reaction with the same name already exists in the model, updating the reaction

```

sink_gly(c) gly(c) <=>
sink_ser-L(c) ser-L(c) ->
sink_ser-L(c) ser-L(c) <=>
sink_pyr(c) pyr(c) ->
sink_glyc(c) glyc(c) <=>
sink_glc-D(c) glc-D(c) ->
sink_glyc(c) glyc(c) <=>
sink_Rtotal(c) Rtotal(c) <=>
sink_Rtotal2(c) Rtotal2(c) <=>
sink_dag_hs(c) dag_hs(c) ->

```

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

sink_glyc(c) glyc(c) <=>
sink_Rtotal(c) Rtotal(c) <=>

Warning: Reaction with the same name already exists in the model, updating the reaction

sink_tag_hs(c) tag_hs(c) ->
sink_glyclt(c) glyclt(c) <=>

Warning: Reaction with the same name already exists in the model, updating the reaction

sink_gly(c) gly(c) ->

Warning: Reaction with the same name already exists in the model, updating the reaction

sink_glygn2(c) glygn2(c) <=>

sink_glc-D(c) glc-D(c) ->

sink_glygn2(e) glygn2(e) <=>

sink_glc-D(e) glc-D(e) ->

sink_glx(c) glx(c) <=>

sink_oxa(c) oxa(c) ->

sink_ha(l) ha(l) <=>

sink_acgam(l) acgam(l) ->

sink_glcur(l) glcur(l) ->

sink_his-L(c) his-L(c) <=>

sink_glu-L(c) glu-L(c) ->

sink_his-L(c) his-L(c) <=>

sink_hista(c) hista(c) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

sink_hista(c) hista(c) <=>

sink_3mlda(c) 3mlda(c) ->

sink_hista(c) hista(c) <=>

sink_im4act(c) im4act(c) ->

sink_hmgcoa(x) hmgcoa(x) <=>

sink_chsterol(r) chsterol(r) ->

sink_hmgcoa(x) hmgcoa(x) <=>

sink_frdp(x) frdp(x) ->

sink_hmgcoa(x) hmgcoa(x) <=>

sink_xoldiolone(r) xoldiolone(r) ->

sink_hmgcoa(x) hmgcoa(x) <=>

sink_xoltritol(c) xoltritol(c) ->

sink_hpyr(c) hpyr(c) <=>

sink_2pg(c) 2pg(c) ->

sink_hpyr(c) hpyr(c) <=>

sink_glyclt(c) glyclt(c) ->

sink_hpyr(c) hpyr(c) <=>

sink_glyc-S(c) glyc-S(c) ->

sink_hspg(l) hspg(l) <=>

sink_gal(l) gal(l) ->

sink_glcur(l) glcur(l) ->

sink_xyl-D(l) xyl-D(l) ->

sink_hyptaur(c) hyptaur(c) <=>

sink_taur(x) taur(x) ->

sink_ile-L(c) ile-L(c) <=>

sink_accoa(c) accoa(c) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

sink_inost(c) inost(c) <=>

sink_pail_hs(c) pail_hs(c) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

sink_inost(c) inost(c) <=>

sink_pail45p_hs(c) pail45p_hs(c) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

sink_inost(c) inost(c) <=>

sink_pail4p_hs(c) pail4p_hs(c) ->

sink_inost(c) inost(c) <=>

```

sink_xu5p-D(c) xu5p-D(c) ->
sink_ipdp(x) ipdp(x) <=>
sink_sql(r) sql(r) ->
sink_itacon(m) itacon(m) <=>
sink_pyr(m) pyr(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_ksi(l) ksi(l) <=>
sink_man(l) man(l) ->
sink_acgam(l) acgam(l) ->
sink_ksii_core2(l) ksii_core2(l) <=>
sink_Ser/Thr(l) Ser/Thr(l) ->
sink_ksii_core4(l) ksii_core4(l) <=>
sink_Ser/Thr(l) Ser/Thr(l) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
Warning: Metabolite l2fn2m2masn(g) not in model - added to the model

sink_l2fn2m2masn(g) l2fn2m2masn(g) <=>
Warning: Metabolite ksi(g) not in model - added to the model

sink_ksi(g) ksi(g) ->
sink_lac-L(c) lac-L(c) <=>
sink_glc-D(c) glc-D(c) ->
sink_Lcyst(c) Lcyst(c) <=>
sink_taur(x) taur(x) ->
sink_leu-L(c) leu-L(c) <=>
sink_accoa(c) accoa(c) ->
sink_lys-L(c) lys-L(c) <=>
sink_accoa(m) accoa(m) ->
sink_lys-L(x) lys-L(x) <=>
sink_aacoa(m) aacoa(m) ->
Warning: Metabolite m8masn(r) not in model - added to the model

sink_m8masn(r) m8masn(r) <=>
Warning: Metabolite nm4masn(g) not in model - added to the model

sink_nm4masn(g) nm4masn(g) ->
sink_man(c) man(c) <=>
sink_gdpmann(c) gdpmann(c) ->
sink_man6p(c) man6p(c) <=>
sink_kdn(c) kdn(c) ->
sink_mescon(m) mescon(m) <=>
sink_pyr(m) pyr(m) ->
sink_met-L(c) met-L(c) <=>
sink_cys-L(c) cys-L(c) ->
sink_mil45p(c) mil45p(c) <=>
sink_inost(c) inost(c) ->
sink_msa(m) msa(m) <=>
sink_ala-B(m) ala-B(m) ->
sink_mthgxl(c) mthgxl(c) <=>
sink_l2ppd-S(c) l2ppd-S(c) ->
sink_mthgxl(c) mthgxl(c) <=>
sink_lac-D(c) lac-D(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_n2m2nmasn(l) n2m2nmasn(l) <=>
sink_man(l) man(l) ->
sink_acgam(l) acgam(l) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
Warning: Metabolite nm4masn(g) not in model - added to the model

sink_nm4masn(g) nm4masn(g) <=>
Warning: Metabolite l2fn2m2masn(g) not in model - added to the model

sink_l2fn2m2masn(g) l2fn2m2masn(g) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

```

Warning: Metabolite nm4masn(g) not in model - added to the model

sink_nm4masn(g) nm4masn(g) <=>

Warning: Metabolite n2m2nmasn(g) not in model - added to the model

sink_n2m2nmasn(g) n2m2nmasn(g) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

Warning: Metabolite nm4masn(g) not in model - added to the model

sink_nm4masn(g) nm4masn(g) <=>

Warning: Metabolite s2l2fn2m2masn(g) not in model - added to the model

sink_s2l2fn2m2masn(g) s2l2fn2m2masn(g) ->

sink_o2s(c) o2s(c) <=>

sink_h2o2(c) h2o2(c) ->

sink_h2o2(c) h2o2(c) <=>

sink_o2(c) o2(c) <=>

sink_h2o(c) h2o(c) ->

sink_orn(c) orn(c) <=>

sink_nh4(c) nh4(c) ->

sink_orn(c) orn(c) <=>

sink_ptrc(c) ptrc(c) ->

sink_orn(c) orn(c) <=>

sink_spmc(c) spmc(c) ->

sink_orn(c) orn(c) <=>

sink_sprm(c) sprm(c) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

sink_pail_hs(c) pail_hs(c) <=>

sink_gpi_prot_hs(r) gpi_prot_hs(r) ->

sink_pail45p_hs(c) pail45p_hs(c) <=>

sink_mil45p(c) mil45p(c) ->

sink_phe-L(c) phe-L(c) <=>

sink_pac(c) pac(c) ->

sink_phe-L(c) phe-L(c) <=>

sink_pacald(c) pacald(c) ->

sink_phe-L(c) phe-L(c) <=>

sink_peamn(c) peamn(c) ->

sink_phe-L(c) phe-L(c) <=>

sink_phaccoa(c) phaccoa(c) ->

sink_phe-L(c) phe-L(c) <=>

sink_pheacgln(c) pheacgln(c) ->

sink_phe-L(c) phe-L(c) <=>

sink_phpyr(c) phpyr(c) ->

sink_phe-L(c) phe-L(c) <=>

sink_tyr-L(c) tyr-L(c) ->

sink_pheme(c) pheme(c) <=>

sink_bilirub(c) bilirub(c) ->

sink_phytcoa(x) phytcoa(x) <=>

sink_dmnoncoa(m) dmnoncoa(m) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

Warning: Reaction with the same name already exists in the model, updating the reaction

sink_pmtcoa(c) pmtcoa(c) <=>

sink_crmp_hs(c) crmp_hs(c) ->

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

Warning: Reaction with the same name already exists in the model, updating the reaction

sink_pmtcoa(c) pmtcoa(c) <=>

sink_sphmyln_hs(c) sphmyln_hs(c) ->

sink_ppcoa(m) ppcoa(m) <=>

sink_succoa(m) succoa(m) ->

sink_pro-L(c) pro-L(c) <=>

sink_glu-L(c) glu-L(c) ->

sink_ptrc(c) ptrc(c) <=>

sink_ala-B(c) ala-B(c) ->

```

sink_ptrc(c) ptrc(c) <=>
sink_spmd(c) spmd(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_pyr(c) pyr(c) <=>
sink_fadh2(m) fadh2(m) <=>
sink_fad(m) fad(m) ->
sink_h(m) h(m) ->
sink_pyr(c) pyr(c) <=>
sink_lac-D(c) lac-D(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_pyr(c) pyr(c) <=>
sink_nad(m) nad(m) ->
sink_h(m) h(m) ->
sink_pyr(c) pyr(c) <=>
sink_accoa(m) accoa(m) ->
sink_nadh(m) nadh(m) ->
sink_co2(c) co2(c) ->
sink_pyr(c) pyr(c) <=>
sink_ala-L(c) ala-L(c) ->
sink_ala-L(c) ala-L(c) <=>
sink_pyr(c) pyr(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_s2l2fn2m2masn(l) s2l2fn2m2masn(l) <=>
sink_man(l) man(l) ->
sink_acgam(l) acgam(l) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_Ser/Thr(g) Ser/Thr(g) <=>
sink_udpacgal(g) udpacgal(g) <=>
sink_core2(g) core2(g) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_Ser/Thr(g) Ser/Thr(g) <=>
sink_udpacgal(g) udpacgal(g) <=>
sink_core4(g) core4(g) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_Ser/Thr(g) Ser/Thr(g) <=>
sink_udpacgal(g) udpacgal(g) <=>
sink_Tn_antigen(g) Tn_antigen(g) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_Ser/Thr(g) Ser/Thr(g) <=>
sink_udpacgal(g) udpacgal(g) <=>
sink_sTn_antigen(g) sTn_antigen(g) ->
sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>
sink_cs_pre(g) cs_pre(g) ->
sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>
sink_cspg_a(g) cspg_a(g) ->
sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>
sink_cspg_c(g) cspg_c(g) ->
sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>
sink_cspg_d(g) cspg_d(g) ->
sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>
sink_cspg_e(g) cspg_e(g) ->
sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>
sink_hspg(g) hspg(g) ->
sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>
sink_cspg_b(g) cspg_b(g) ->
sink_ser-L(c) ser-L(c) <=>

```

```
sink_cys-L(c) cys-L(c) ->
sink_so4(c) so4(c) <=>
sink_paps(c) paps(c) ->
sink_spmd(c) spmd(c) <=>
sink_sprm(c) sprm(c) ->
sink_srtm(c) srtm(c) <=>
Warning: Metabolite f5hoxkyn(c) not in model - added to the model
```

```
sink_f5hoxkyn(c) f5hoxkyn(c) ->
sink_srtm(c) srtm(c) <=>
sink_fna5moxam(c) fna5moxam(c) ->
sink_srtm(c) srtm(c) <=>
Warning: Metabolite nmthsrtm(c) not in model - added to the model
```

```
sink_nmthsrtm(c) nmthsrtm(c) ->
sink_succoa(m) succoa(m) <=>
sink_oaa(m) oaa(m) ->
sink_taur(x) taur(x) <=>
sink_tchola(x) tchola(x) ->
sink_thcholstoic(x) thcholstoic(x) <=>
sink_gchola(x) gchola(x) ->
sink_thcholstoic(x) thcholstoic(x) <=>
sink_tchola(x) tchola(x) ->
sink_trp-L(c) trp-L(c) <=>
sink_ppcoa(c) ppcoa(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_accoa(c) accoa(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_anth(c) anth(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_id3acald(c) id3acald(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_kynate(c) kynate(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_melatn(c) melatn(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_Lfmkynr(c) Lfmkynr(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_Lkynr(c) Lkynr(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_nformanth(c) nformanth(c) ->
sink_srtm(c) srtm(c) <=>
```

Warning: Metabolite 5moxact(c) not in model - added to the model

```
sink_5moxact(c) 5moxact(c) ->
sink_srtm(c) srtm(c) <=>
sink_6hoxmelatn(c) 6hoxmelatn(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_quln(c) quln(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_srtm(c) srtm(c) ->
sink_Tyr-ggn(c) Tyr-ggn(c) <=>
```

Warning: Reaction with the same name already exists in the model, updating the reaction

```
sink_glygn2(c) glygn2(c) ->
sink_tyr-L(c) tyr-L(c) <=>
sink_34hpp(c) 34hpp(c) ->
sink_tyr-L(c) tyr-L(c) <=>
sink_4hphac(c) 4hphac(c) ->
sink_tyr-L(c) tyr-L(c) <=>
sink_adrnl(c) adrnl(c) ->
sink_tyr-L(c) tyr-L(c) <=>
sink_dopa(c) dopa(c) ->
sink_tyr-L(c) tyr-L(c) <=>
sink_fum(c) fum(c) ->
sink_acac(c) acac(c) ->
sink_tyr-L(c) tyr-L(c) <=>
sink_melanin(c) melanin(c) ->
sink_tyr-L(c) tyr-L(c) <=>
```

```
sink_nrpphr(c) nrpphr(c) ->
sink_uacgam(c) uacgam(c) <=>
sink_udpglcur(c) udpglcur(c) <=>
sink_ha(e) ha(e) ->
sink_uacgam(c) uacgam(c) <=>
```

Warning: Metabolite m8masn(r) not in model - added to the model

```
sink_m8masn(r) m8masn(r) ->
sink_udpglcur(c) udpglcur(c) <=>
sink_xu5p-D(c) xu5p-D(c) ->
sink_ura(c) ura(c) <=>
sink_ala-B(c) ala-B(c) ->
sink_val-L(c) val-L(c) <=>
sink_3aib(c) 3aib(c) ->
sink_val-L(c) val-L(c) <=>
sink_succoa(m) succoa(m) ->
sink_xoltritol(m) xoltritol(m) <=>
sink_thcholstoic(m) thcholstoic(m) ->
sink_xylu-D(c) xylu-D(c) <=>
sink_glyclt(c) glyclt(c) ->
```

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

FBA =

```
    full: [10600×1 double]
    obj: 4.0000
    rcost: [10600×1 double]
    dual: [5835×1 double]
    solver: 'tomlab_cplex'
    algorithm: 'default'
    stat: 1
    origStat: 1
    time: 0.4470
    basis: [16435×1 double]
    x: [10600×1 double]
    f: 4.0000
    y: [5835×1 double]
    w: [10600×1 double]
    v: [10600×1 double]
```

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_ca2(e) not in model

```
sink_pyr(m) pyr(m) ->
sink_pyr(c) pyr(c) ->
sink_pyr(c) pyr(c) ->
sink_ala-L(c) ala-L(c) ->
sink_pyr(c) pyr(c) ->
sink_ala-L(c) ala-L(c) ->
sink_ala-L(c) ala-L(c) ->
sink_ala-L(c) ala-L(c) ->
sink_gln-L(c) gln-L(c) ->
sink_gln-L(c) gln-L(c) ->
sink_gln-L(c) gln-L(c) ->
sink_gln-L(c) gln-L(c) ->
sink_ala-L(c) ala-L(c) ->
sink_gln-L(c) gln-L(c) ->
sink_ala-L(c) ala-L(c) ->
sink_gln-L(c) gln-L(c) ->
sink_ala-L(c) ala-L(c) ->
sink_gln-L(c) gln-L(c) ->
sink_ala-L(c) ala-L(c) ->
sink_orn(c) orn(c) ->
sink_pro-L(c) pro-L(c) ->
sink_ptrc(c) ptrc(c) ->
sink_gln-L(c) gln-L(c) ->
sink_sprm(c) sprm(c) ->
```

```

sink_spmd(c) spmd(c) ->
sink_ptrc(c) ptrc(c) ->
Warning: Reaction with the same name already exists in the model, updating the reaction
Warning: Metabolite pcreat[e] not in model - added to the model
EX_pcreat(e) pcreat[e] ->
sink_creat(c) creat(c) ->
sink_pcreat(c) pcreat(c) ->
sink_lac-L(c) lac-L(c) ->
Warning: Reaction with the same name already exists in the model, updating the reaction
sink_glygn2(c) glygn2(c) ->
sink_e4p(c) e4p(c) ->
sink_mag-hs(c) mag-hs(c) ->
sink_glyc(c) glyc(c) ->
sink_accoa(m) accoa(m) ->
sink_accoa(m) accoa(m) ->
sink_accoa(m) accoa(m) ->
sink_dhap(c) dhap(c) ->
sink_amp(c) amp(c) ->
sink_imp(c) imp(c) ->
sink_prpp(c) prpp(c) <=>
sink_gmp(c) gmp(c) ->
sink_imp(c) imp(c) ->
sink_thym(c) thym(c) ->
sink_cmp(c) cmp(c) ->
sink_dtmp(c) dtmp(c) ->
sink_citr-L(c) citr-L(c) <=>
sink_arg-L(c) arg-L(c) ->
sink_cys-L(c) cys-L(c) <=>
sink_taur(c) taur(c) ->
Warning: Reaction with the same name already exists in the model, updating the reaction
sink_gly(c) gly(c) <=>
sink_orn(c) orn(c) ->
sink_citr-L(c) citr-L(c) <=>
sink_urea(c) urea(c) ->
Warning: Reaction with the same name already exists in the model, updating the reaction
sink_gly(c) gly(c) <=>
sink_gthrd(c) gthrd(c) ->
sink_pro-L(c) pro-L(c) <=>
sink_4abut(c) 4abut(c) ->
sink_pro-L(c) pro-L(c) <=>
sink_orn(c) orn(c) ->
sink_met-L(c) met-L(c) <=>
sink_hcys-L(c) hcys-L(c) ->
sink_hcys-L(c) hcys-L(c) <=>
sink_met-L(c) met-L(c) ->
sink_hcys-L(c) hcys-L(c) <=>
sink_cys-L(c) cys-L(c) ->
sink_lys-L(c) lys-L(c) <=>
sink_glu-L(c) glu-L(c) ->
sink_trp-L(c) trp-L(c) <=>
sink_trypta(c) trypta(c) ->
sink_kynate(c) kynate(c) <=>
sink_nicrnt(c) nicrnt(c) ->
sink_pyr(c) pyr(c) <=>
sink_lac-L(c) lac-L(c) ->
sink_gal(c) gal(c) <=>
sink_udpg(c) udpg(c) ->
sink_fru(c) fru(c) <=>
sink_lac-L(c) lac-L(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_malcoa(c) malcoa(c) <=>
sink_eicostetcoa(c) eicostetcoa(c) ->
sink_accoa(c) accoa(c) <=>

```

```

sink_chsterol(r) cholesterol(r) ->
sink_inost(c) inost(c) <=>
sink_glac(r) glac(r) ->
sink_pail_hs(c) pail_hs(c) <=>
sink_pail4p_hs(c) pail4p_hs(c) ->
sink_arachd(c) arachd(c) <=>
sink_prostgh2(c) prostgh2(c) ->
sink_arachd(c) arachd(c) <=>
sink_prostgd2(r) prostgd2(r) ->
sink_arachd(c) arachd(c) <=>
sink_prostge2(r) prostge2(r) ->
sink_arachd(c) arachd(c) <=>
sink_prostgi2(r) prostgi2(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_25hvitd3(m) 25hvitd3(m) <=>
sink_2425dhvitd3(m) 2425dhvitd3(m) ->
sink_caro(c) caro(c) <=>
sink_retinal(c) retinal(c) ->
Warning: Model already has the same reaction you tried to add: sink_glu_L(c)

```

```

DM_pro-L(m) pro-L(m) ->
sink_retinol-cis-11(c) retinol-cis-11(c) <=>
sink_retinal(c) retinal(c) ->
sink_pail_hs(c) pail_hs(c) <=>
sink_pchol-hs(c) pchol-hs(c) ->
sink_pail_hs(c) pail_hs(c) <=>
sink_pe_hs(c) pe_hs(c) ->
sink_pail_hs(c) pail_hs(c) <=>
sink_ps-hs(c) ps-hs(c) ->
sink_pail_hs(c) pail_hs(c) <=>
sink_g3pc(c) g3pc(c) ->
sink_dag_hs(c) dag_hs(c) <=>
sink_pchol-hs(c) pchol-hs(c) ->
sink_dag_hs(c) dag_hs(c) <=>
sink_pe_hs(c) pe_hs(c) ->
sink_dag_hs(c) dag_hs(c) <=>
sink_clpn-hs(c) clpn-hs(c) ->
sink_dag_hs(c) dag_hs(c) <=>
sink_pgp-hs(c) pgp-hs(c) ->
sink_bhb(m) bhbm(m) <=>
sink_acac(m) acac(m) ->
sink_mal-L(m) mal-L(m) <=>
sink_pyr(m) pyr(m) ->
sink_glu-L(c) glu-L(c) <=>
sink_gln-L(c) gln-L(c) ->
sink_cys-L(c) cys-L(c) <=>
Warning: Reaction with the same name already exists in the model, updating the reaction

sink_coa(c) coa(c) ->
sink_occoa(m) occoa(m) <=>
sink_accoa(m) accoa(m) ->
Warning: Reaction with the same name already exists in the model, updating the reaction

sink_lnlncgcoa(c) lnlncgcoa(c) <=>
sink_dlnlncgcoa(c) dlnlncgcoa(c) ->
Warning: Reaction with the same name already exists in the model, updating the reaction

sink_chol(c) chol(c) <=>
sink_ach(c) ach(c) ->
sink_pyr(m) pyr(m) <=>
sink_oaa(m) oaa(m) ->
sink_crtn(c) crtn(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model

sink_arachd(c) arachd(c) <=>
sink_leuktrE4(c) leuktrE4(c) ->
Warning: Reaction EX_cbl1(e) not in model

```



```
Warning: Reaction EX_ca2(e) not in model
sink_arachd(c) arachd(c) <=>
sink_C06314(c) C06314(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_ca2(e) not in model
sink_nrpphr(c) nrpphr(c) <=>
sink_3mox4hoxm(c) 3mox4hoxm(c) ->
sink_sbt-D(c) sbt-D(c) <=>
sink_fru(c) fru(c) ->
sink_accoa(m) accoa(m) ->
sink_succoa(m) succoa(m) ->
```

```
TestedRxns = unique([TestedRxnsC; TestedRxnsClosedSinks]);
TestedRxnsX = intersect(model.rxns,TestedRxns);
```

In this example, we aim to remove all HMR reactions (i.e., those reactions originating from HMR 2.0 [2] and that start with 'HMR_') that are not needed for the aforementioned tasks.

```
HMR = model.rxns(strmatch('HMR_',model.rxns));
HMR_NE = setdiff(HMR,TestedRxnsX);
model.lb(find(ismember(model.rxns,HMR_NE))) = 0;
model.ub(find(ismember(model.rxns,HMR_NE))) = 0;
```

We will also remove all drug module reactions, i.e., those ones with the term 'Xeno' in the subsystem, mostly originating from [3].

```
DM = model.rxns(strmatch('Xeno',model.subSystems));
model.lb(find(ismember(model.rxns,DM))) = 0;
model.ub(find(ismember(model.rxns,DM))) = 0;
DMt = (strmatch('Transport of Xenobiotic',model.rxnNames));
model.lb(DMt) = 0;
model.ub(DMt) = 0;
```

We will also remove all reactions from the 'Peptide metabolism' subsystem.

```
DM = model.rxns(strmatch('Peptide metabolism',model.subSystems));
model.lb(find(ismember(model.rxns,DM))) = 0;
model.ub(find(ismember(model.rxns,DM))) = 0;
```

Now we will ensure that the reversibility of each reaction is in accordance to the defined lower bound.

```
model.rev(find(model.lb<0))=1;
model.rev(find(model.lb>=0))=0;
```

We will use fastcc [4], to ensure a flux-consistent subnetwork.

```
param.epsilon=1e-4;
param.modeFlag=0;
%param.method='null_fastcc';
param.method='fastcc';
printLevel=3;
[fluxConsistentMetBool,fluxConsistentRxnBool,fluxInConsistentMetBool,fluxInConsistentRxnBool,m
```

```
10600 Total reactions
4402 Reversible reactions.
6198 Irreversible reactions.
7453 Flux consistent reactions, without flipping.
```

```
2020 Flux inconsistent irreversible reactions, without flipping.
1127 Flux inconsistent reactions, without flipping.
7706 Flux consistent reactions.
874 Flux inconsistent reversible reactions left to flip.
7709 Flux consistent reactions.
871 Flux inconsistent reversible reactions left to flip.
7711 Flux consistent reactions.
869 Flux inconsistent reversible reactions left to flip.
7715 Flux consistent reactions.
855 Flux inconsistent reversible reactions left to flip.
7717 Flux consistent reactions.
833 Flux inconsistent reversible reactions left to flip.
7719 Flux consistent reactions.
720 Flux inconsistent reversible reactions left to flip.
7721 Flux consistent reactions.
718 Flux inconsistent reversible reactions left to flip.
```

And remove the flux inconsistent reactions from the model.

```
modelConsistent = removeRxns(model,model.rxns(find(fluxInConsistentRxnBool)));
```

We will now update the GPR associations.

```
modelConsistent.genes = [];
modelConsistent.rxnGeneMat = [];
modelGrRule = modelConsistent.grRules;
for i = 1 : length(modelGrRule)
    if ~isempty(modelGrRule{i})
        modelConsistent = changeGeneAssociation(modelConsistent,modelConsistent.rxns{i},modelGrRule{i});
    end
end
```

```
New gene 8639.1 added to model
New gene 26.1 added to model
New gene 314.2 added to model
New gene 314.1 added to model
New gene 1591.1 added to model
New gene 10993.1 added to model
New gene 6818.1 added to model
New gene 89874.1 added to model
New gene 92483.1 added to model
New gene 3948.2 added to model
New gene 55293.1 added to model
New gene 3945.1 added to model
New gene 3939.1 added to model
New gene 160287.1 added to model
New gene 3948.1 added to model
New gene 9123.1 added to model
New gene 9194.1 added to model
New gene 6566.1 added to model
New gene 57835.3 added to model
New gene 8671.1 added to model
New gene 57835.2 added to model
New gene 57835.1 added to model
New gene 57835.4 added to model
New gene 4967.2 added to model
New gene 1738.1 added to model
New gene 8050.1 added to model
New gene 1743.1 added to model
New gene 4967.1 added to model
New gene 130.1 added to model
```

New gene 127.1 added to model
New gene 125.1 added to model
New gene 124.1 added to model
New gene 131.1 added to model
New gene 126.1 added to model
New gene 128.1 added to model
New gene 137872.1 added to model
New gene 1312.1 added to model
New gene 1312.2 added to model
New gene 117247.1 added to model
New gene 218.1 added to model
New gene 222.1 added to model
New gene 220.1 added to model
New gene 221.1 added to model
New gene 3242.1 added to model
New gene 18.1 added to model
New gene 18.2 added to model
New gene 2531.1 added to model
New gene 23498.1 added to model
New gene 55268.1 added to model
New gene 51166.1 added to model
New gene 883.1 added to model
New gene 51166.2 added to model
New gene 1644.1 added to model
New gene 4128.1 added to model
New gene 4129.1 added to model
New gene 10165.1 added to model
New gene 8604.1 added to model
New gene 51380.1 added to model
New gene 2571.1 added to model
New gene 2572.1 added to model
New gene 2571.2 added to model
New gene 2805.1 added to model
New gene 2806.1 added to model
New gene 8659.1 added to model
New gene 8659.2 added to model
New gene 4363.1 added to model
New gene 6822.1 added to model
New gene 6573.1 added to model
New gene 6573.2 added to model
New gene 316.1 added to model
New gene 6570.1 added to model
New gene 6571.1 added to model
New gene 2348.5 added to model
New gene 2348.3 added to model
New gene 2348.1 added to model
New gene 2348.6 added to model
New gene 2352.1 added to model
New gene 2348.4 added to model
New gene 2348.2 added to model
New gene 4125.1 added to model
New gene 53947.1 added to model
New gene 51146.1 added to model
New gene 28.1 added to model
New gene 206358.1 added to model
New gene 6529.1 added to model
New gene 6538.1 added to model
New gene 6540.1 added to model
New gene 6539.1 added to model
New gene 38.1 added to model

New gene 3032.1 added to model
New gene 10449.1 added to model
New gene 3030.1 added to model
New gene 39.1 added to model
New gene 30.1 added to model
New gene 32.1 added to model
New gene 9197.1 added to model
New gene 84532.1 added to model
New gene 79611.1 added to model
New gene 64841.1 added to model
New gene 55577.1 added to model
New gene 5238.1 added to model
New gene 162417.1 added to model
New gene 43.1 added to model
New gene 43.2 added to model
New gene 6572.1 added to model
New gene 47.1 added to model
New gene 47.2 added to model
New gene 54187.1 added to model
New gene 26503.1 added to model
New gene 140838.1 added to model
New gene 54.1 added to model
New gene 51205.1 added to model
New gene 36.1 added to model
New gene 34.1 added to model
New gene 80724.1 added to model
New gene 35.1 added to model
New gene 84129.1 added to model
New gene 27034.1 added to model
New gene 28976.1 added to model
New gene 3712.1 added to model
New gene 134526.1 added to model
New gene 51.1 added to model
New gene 51.2 added to model
New gene 95.1 added to model
New gene 50.1 added to model
New gene 48.1 added to model
New gene 8309.1 added to model
New gene 52.1 added to model
New gene 52.3 added to model
New gene 52.2 added to model
New gene 55.1 added to model
New gene 788.1 added to model
New gene 55902.1 added to model
New gene 65985.1 added to model
New gene 55902.2 added to model
New gene 438.1 added to model
New gene 1571.1 added to model
New gene 100.1 added to model
New gene 3177.1 added to model
New gene 205.3 added to model
New gene 205.1 added to model
New gene 204.1 added to model
New gene 204.3 added to model
New gene 204.2 added to model
New gene 205.2 added to model
New gene 26289.1 added to model
New gene 26289.2 added to model

New gene 50808.1 added to model
New gene 262.1 added to model
New gene 112.1 added to model
New gene 55811.1 added to model
New gene 109.1 added to model
New gene 112.2 added to model
New gene 114.1 added to model
New gene 108.1 added to model
New gene 113.1 added to model
New gene 107.1 added to model
New gene 196883.1 added to model
New gene 115.1 added to model
New gene 111.1 added to model
New gene 2030.1 added to model
New gene 9154.2 added to model
New gene 9154.1 added to model
New gene 64078.1 added to model
New gene 9153.1 added to model
New gene 952.1 added to model
New gene 1375.1 added to model
New gene 1375.3 added to model
New gene 1375.4 added to model
New gene 126129.1 added to model
New gene 1374.1 added to model
New gene 1375.2 added to model
New gene 1376.1 added to model
New gene 9060.1 added to model
New gene 9061.1 added to model
New gene 158.1 added to model
New gene 158.2 added to model
New gene 79369.1 added to model
New gene 10678.1 added to model
New gene 11041.1 added to model
New gene 146712.1 added to model
New gene 374907.1 added to model
New gene 93010.1 added to model
New gene 374907.2 added to model
New gene 10678.2 added to model
New gene 10331.1 added to model
New gene 79814.1 added to model
New gene 10555.1 added to model
New gene 137964.1 added to model
New gene 56895.1 added to model
New gene 56894.2 added to model
New gene 56894.1 added to model
New gene 55326.1 added to model
New gene 10554.1 added to model
New gene 129642.1 added to model
New gene 64902.1 added to model
New gene 64850.1 added to model
New gene 189.1 added to model
New gene 3073.1 added to model
New gene 3074.1 added to model
New gene 10606.1 added to model
New gene 8402.1 added to model
New gene 1468.1 added to model
New gene 64849.1 added to model
New gene 64849.2 added to model
New gene 1645.1 added to model
New gene 1109.1 added to model
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New gene 23464.1 added to model
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New gene 211.1 added to model
New gene 54407.1 added to model
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New gene 57393.1 added to model
New gene 59272.1 added to model
New gene 2875.1 added to model
New gene 84706.1 added to model
New gene 92745.1 added to model
New gene 10991.1 added to model
New gene 284273.2 added to model
New gene 284273.1 added to model
New gene 10327.1 added to model
New gene 10327.2 added to model
New gene 216.1 added to model
New gene 8854.2 added to model
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New gene 10317.4 added to model
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New gene 10317.3 added to model
New gene 10317.2 added to model
New gene 10317.5 added to model
New gene 84002.1 added to model
New gene 570.1 added to model
New gene 3141.1 added to model
New gene 140679.1 added to model
New gene 8424.1 added to model
New gene 53630.1 added to model
New gene 622.2 added to model
New gene 622.3 added to model
New gene 622.1 added to model
New gene 23743.1 added to model
New gene 635.1 added to model
New gene 10599.1 added to model
New gene 1244.1 added to model
New gene 8714.1 added to model
New gene 28234.1 added to model
New gene 645.1 added to model
New gene 644.1 added to model
New gene 10380.1 added to model
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New gene 2538.1 added to model
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New gene 873.1 added to model

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New gene 10423.2 added to model
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New gene 8760.1 added to model
New gene 10390.1 added to model
New gene 56994.1 added to model
New gene 64781.1 added to model
New gene 64781.2 added to model
New gene 10087.1 added to model
New gene 6565.1 added to model
New gene 9023.1 added to model
New gene 1103.4 added to model
New gene 1103.2 added to model
New gene 1103.3 added to model
New gene 1103.1 added to model
New gene 162466.1 added to model
New gene 5130.1 added to model
New gene 9468.1 added to model
New gene 6579.1 added to model
New gene 6554.1 added to model
New gene 6555.1 added to model
New gene 8714.3 added to model
New gene 8647.1 added to model
New gene 8714.2 added to model
New gene 55349.1 added to model
New gene 1120.2 added to model
New gene 1119.1 added to model
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New gene 1119.2 added to model
New gene 60482.1 added to model
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New gene 6584.1 added to model
New gene 6582.2 added to model
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New gene 27159.2 added to model
New gene 9058.1 added to model
New gene 6576.1 added to model
New gene 1159.1 added to model
New gene 1160.1 added to model
New gene 548596.1 added to model
New gene 1152.1 added to model
New gene 1158.1 added to model
New gene 5172.1 added to model
New gene 65010.1 added to model
New gene 65010.3 added to model
New gene 65010.2 added to model
New gene 54675.1 added to model
New gene 10559.1 added to model
New gene 55907.1 added to model
New gene 8034.1 added to model
New gene 8824.1 added to model
New gene 51805.1 added to model
New gene 51004.1 added to model
New gene 51004.2 added to model
New gene 10229.1 added to model
New gene 9245.1 added to model
New gene 2650.1 added to model

New gene 51301.1 added to model
New gene 192134.1 added to model
New gene 6535.1 added to model
New gene 386757.1 added to model
New gene 1384.1 added to model
New gene 6583.1 added to model
New gene 1431.1 added to model
New gene 1431.2 added to model
New gene 54677.1 added to model
New gene 1384.2 added to model
New gene 1384.3 added to model
New gene 8140.1 added to model
New gene 23428.1 added to model
New gene 23428.2 added to model
New gene 1036.1 added to model
New gene 124935.1 added to model
New gene 23657.1 added to model
New gene 978.1 added to model
New gene 57379.1 added to model
New gene 7371.1 added to model
New gene 83549.1 added to model
New gene 51727.1 added to model
New gene 129607.1 added to model
New gene 9162.1 added to model
New gene 1607.1 added to model
New gene 8525.2 added to model
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New gene 9551.1 added to model
New gene 522.4 added to model
New gene 522.2 added to model
New gene 515.3 added to model
New gene 522.1 added to model
New gene 517.1 added to model
New gene 516.1 added to model
New gene 518.1 added to model
New gene 539.1 added to model
New gene 267020.1 added to model
New gene 27109.1 added to model

New gene 7384.1 added to model
New gene 7388.1 added to model
New gene 4519.1 added to model
New gene 29796.2 added to model
New gene 10975.1 added to model
New gene 7385.1 added to model
New gene 7386.1 added to model
New gene 1537.1 added to model
New gene 27089.1 added to model
New gene 7381.1 added to model
New gene 29796.1 added to model
New gene 9016.1 added to model
New gene 7352.2 added to model
New gene 7352.1 added to model
New gene 7351.1 added to model
New gene 9016.2 added to model
New gene 9481.1 added to model

New gene 4715.1 added to model
New gene 4720.1 added to model
New gene 4719.1 added to model
New gene 4700.1 added to model
New gene 55967.1 added to model
New gene 4709.1 added to model
New gene 4710.1 added to model

New gene 4726.1 added to model
New gene 4718.1 added to model
New gene 4696.1 added to model
New gene 4694.1 added to model
New gene 374291.1 added to model
New gene 4728.1 added to model
New gene 4712.2 added to model
New gene 4717.1 added to model
New gene 4705.1 added to model
New gene 4725.1 added to model
New gene 4716.1 added to model
New gene 4537.1 added to model
New gene 7991.1 added to model
New gene 4722.1 added to model
New gene 4541.1 added to model
New gene 4539.1 added to model
New gene 4707.1 added to model
New gene 4701.1 added to model
New gene 4723.1 added to model
New gene 4698.1 added to model
New gene 4538.1 added to model
New gene 4697.1 added to model
New gene 51079.1 added to model
New gene 4714.1 added to model
New gene 4704.1 added to model
New gene 126328.1 added to model
New gene 4711.1 added to model
New gene 4724.1 added to model
New gene 4713.1 added to model
New gene 4536.1 added to model
New gene 4695.1 added to model
New gene 4702.1 added to model
New gene 4708.1 added to model
New gene 4535.1 added to model
New gene 4731.2 added to model
New gene 4706.1 added to model
New gene 4729.1 added to model
New gene 4540.1 added to model
New gene 7991.2 added to model
New gene 4731.1 added to model
New gene 4712.1 added to model
New gene 54539.1 added to model

New gene 1351.1 added to model
New gene 1347.1 added to model
New gene 1329.1 added to model
New gene 1327.1 added to model
New gene 341947.1 added to model
New gene 9167.1 added to model
New gene 1350.1 added to model
New gene 4512.1 added to model
New gene 1349.1 added to model
New gene 1339.1 added to model
New gene 1345.1 added to model
New gene 4513.1 added to model
New gene 9377.1 added to model
New gene 125965.1 added to model
New gene 4514.1 added to model
New gene 170712.1 added to model
New gene 1346.1 added to model
New gene 1340.1 added to model
New gene 84701.1 added to model
New gene 1337.1 added to model

Save the resulting model.

```
save('SubNetworkRecon.mat','modelConsistent')
```

Size of the original Recon:

```
[nMet,nRxn] = size(model.S);  
fprintf('%6s\t%6s\n','#mets','#rxns'); fprintf('%6u\t%6u\t%s%\n',nMet,nRxn,' total in Recon')
```

```
#mets  #rxns  
5835   10600  total in Recon
```

Size of the resulting Recon subnetwork:

```
[nMet,nRxn] = size(modelConsistent.S);  
fprintf('%6s\t%6s\n','#mets','#rxns'); fprintf('%6u\t%6u\t%s%\n',nMet,nRxn,' total in Recon s
```

```
#mets  #rxns  
3991   7721  total in Recon subnetwork
```

Consider to evaluate the resulting model with the tutorial `modelProperties` and `modelSanityChecks` to ensure proper functioning of the generic subnetwork of Recon.

References

- [1] Brunk, E. et al. Recon 3D: A resource enabling a three-dimensional view of gene variation in human metabolism. (submitted) 2017.
- [2] HMR 2.0
- [3] Drug module.
- [4] FastCore.

