

Create a generic subnetwork from Recon 3D

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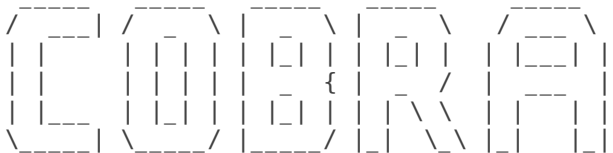
In this tutorial, we show how to create a generic subnetwork from Recon 3D that can still perform all metabolic test functions as well as has physiologically defined ATP yield from defined carbon sources. The resulting model does not contain a specified list of reactions, except if they are still needed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

EQUIPMENT SETUP

Initialize The COBRA Toolbox.

Initialize The Cobra Toolbox using the `initCobraToolbox` function.

```
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 : --> set this path manually after installing the solver ( see instructions )
  - [----] GUROBI_PATH : --> set this path manually after installing the solver ( see instructions )
  - [---*] TOMLAB_PATH: C:\Program Files\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	active		0	0	0	0	-
dqqMinos	active		0	-	-	-	-
glpk	active		1	1	-	-	-
gurobi	active		1	1	1	1	-
ibm_cplex	active		0	0	0	-	-
matlab	active		1	-	-	-	1
mosek	active		0	0	0	-	-

pdco	active	1	-	1	-	-
quadMinos	active	0	-	-	-	0
tomlab_cplex	active	1	1	1	1	-
qpng	passive	-	-	1	-	-
tomlab_snopt	passive	-	-	-	-	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(). [c8bb49 @ tut_createSubnet].
Please use the MATLAB.devTools (https://github.com/opencobra/MATLAB.devTools).
```

Setting the optimization solver.

This tutorial will be run with a 'glpk' package, which is a linear programming ('LP') solver. The 'glpk' package does not require additional installation and configuration.

```
% solverName='glpk';
% solverType='LP';
% changeCobraSolver(solverName,solverType);
```

However, for the analysis of large models, such as Recon 3D, it is not recommended to use the 'glpk' package but rather an industrial strength solver, such as the 'gurobi' package. For detailed information, refer to The Cobra Toolbox [solver installation guide](#).

If tutorial will analyse a Recon model then change solver to gurobi:

```
solverName='gurobi';
solverType='LP';
changeCobraSolver(solverName,solverType);
```

```
> Gurobi interface added to MATLAB path.
```

A solver package may offer different types of optimization programmes to solve a problem. The above example used a LP optimization, other types of optimization programmes include; mixed-integer linear programming ('MILP'), quadratic programming ('QP'), and mixed-integer quadratic programming ('MIQP').

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

PROCEDURE

Load the model.

In this tutorial, the used model is the generic model of human metabolism, Recon 3D [1]. If Recon 3D is not available, please use Recon 2 [2] provided in The Corba Toolbox. Other COBRA models may be downloaded from the [Virtual Metabolic Human](#) webpage and saved to your preferred directory.

Before proceeding with the simulations, the path for the model needs to be set up.

```
pathModel = 'fork-cobratoolbox/test/models/'; % If using Recon 3 model and as necessary, add
filename= 'Recon2.0model.mat'; % If using Recon 3 model, add filename.

if ~isempty(regexpi(filename, 'Recon3'));
    load([pathModel, filename])
    model = modelRecon3model;
    model.csense(1:size(model.S,1),1)='E';
    clear modelRecon3model;
else
    load([pathModel, filename])
    model = Recon2model;
    model.csense(1:size(model.S,1),1)='E';
    clear Recon2model;
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;
```

Identify the model reactions that 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) -> adp(c) + h(c) + pi(c)
```

Identify the model reactions that 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
```

```
test
sink_gly(c) gly(c) <=>
sink_co2(c) co2(c) ->
sink_nh4(c) nh4(c) ->
test
sink_12ppd-S(c) 12ppd-S(c) <=>
sink_mthgxl(c) mthgxl(c) ->
test
sink_12ppd-S(c) 12ppd-S(c) <=>
sink_pyr(c) pyr(c) ->
test
```

```

sink_3pg(c) 3pg(c) <=>
sink_gly(c) gly(c) ->
test
sink_3pg(c) 3pg(c) <=>
sink_ser-L(c) ser-L(c) ->
test
sink_4abut(c) 4abut(c) <=>
sink_succ(m) succ(m) ->
test
sink_4hpro-LT(m) 4hpro-LT(m) <=>
sink_glx(m) glx(m) ->
test
sink_5aop(c) 5aop(c) <=>
sink_pheme(c) pheme(c) ->
test
sink_aact(c) aact(c) <=>
sink_mthgxl(c) mthgxl(c) ->
test
sink_acac(m) acac(m) <=>
sink_acetone(m) acetone(m) ->
test
sink_acac(m) acac(m) <=>
sink_bhb(m) bhb(m) ->
test
sink_acald(c) acald(c) <=>
sink_ac(c) ac(c) ->
test
sink_accoa(c) accoa(c) <=>
sink_pmtcoa(c) pmtcoa(c) ->
test
sink_pmtcoa(c) pmtcoa(c) <=>
sink_malcoa(m) malcoa(m) ->
test
sink_acetone(c) acetone(c) <=>
sink_mthgxl(c) mthgxl(c) ->
test
sink_acgal(c) acgal(c) <=>
sink_udpacgal(c) udpacgal(c) ->
test
sink_acgam(c) acgam(c) <=>
sink_cmpacna(c) cmpacna(c) ->
test
sink_acorn(c) acorn(c) <=>
sink_orn(c) orn(c) ->
test
sink_adrnl(c) adrnl(c) <=>
sink_34dhoxpeg(c) 34dhoxpeg(c) ->
test
sink_akg(m) akg(m) <=>
sink_oaa(m) oaa(m) ->
test
sink_akg(m) akg(m) <=>
sink_glu-L(m) glu-L(m) ->
test
sink_akg(m) akg(m) <=>
test
sink_ala-B(c) ala-B(c) <=>
sink_msa(m) msa(m) ->
test
sink_ala-D(c) ala-D(c) <=>
sink_pyr(c) pyr(c) ->
test
sink_ala-L(c) ala-L(c) <=>
sink_ala-D(c) ala-D(c) ->
test
sink_ala-L(c) ala-L(c) <=>
sink_pyr(c) pyr(c) ->
test

```

```

sink_arachd(c) arachd(c) <=>
sink_malcoa(m) malcoa(m) ->
test
sink_arachd(r) arachd(r) <=>
sink_txa2(r) txa2(r) ->
test
sink_arg-L(c) arg-L(c) <=>
sink_creat(c) creat(c) ->
test
sink_arg-L(c) arg-L(c) <=>
sink_glu-L(m) glu-L(m) ->
test
sink_arg-L(c) arg-L(c) <=>
sink_no(c) no(c) ->
test
sink_arg-L(c) arg-L(c) <=>
sink_pcreat(c) pcreat(c) ->
test
sink_ascb-L(c) ascb-L(c) <=>
sink_eryth(c) eryth(c) ->
test
sink_ascb-L(c) ascb-L(c) <=>
sink_lyxnt(c) lyxnt(c) ->
test
sink_ascb-L(c) ascb-L(c) <=>
sink_thrnt(c) thrnt(c) ->
test
sink_ascb-L(c) ascb-L(c) <=>
sink_xylnt(c) xylnt(c) ->
test
sink_asn-L(c) asn-L(c) <=>
sink_oaa(c) oaa(c) ->
test
sink_asp-L(c) asp-L(c) <=>
sink_hco3(c) hco3(c) <=>
sink_arg-L(c) arg-L(c) ->
test
sink_asp-L(c) asp-L(c) <=>
sink_ala-B(c) ala-B(c) ->
test
sink_asp-L(c) asp-L(c) <=>
sink_asn-L(c) asn-L(c) ->
test
sink_asp-L(c) asp-L(c) <=>
sink_argsuc(c) argsuc(c) ->
test
sink_argsuc(c) argsuc(c) <=>
sink_fum(c) fum(c) ->
test
sink_asp-L(c) asp-L(c) <=>
sink_dcamp(c) dcamp(c) ->
test
sink_dcamp(c) dcamp(c) <=>
sink_fum(c) fum(c) ->
test
sink_dcamp(c) dcamp(c) <=>
sink_fum(c) fum(c) ->
test
sink_asp-L(c) asp-L(c) <=>
sink_oaa(c) oaa(c) ->
test
sink_carn(c) carn(c) <=>
sink_ala-B(c) ala-B(c) ->
test
sink_chol(c) chol(c) <=>
sink_dag_hs(c) dag_hs(c) <=>
sink_pe_hs(c) pe_hs(c) ->
test

```

```

sink_chol(m) chol(m) <=>
sink_glyb(m) glyb(m) ->
test
sink_glyb(m) glyb(m) <=>
sink_gly(m) gly(m) ->
test
sink_coke(r) coke(r) <=>
sink_pecgoncoa(r) pecgoncoa(r) ->
test
sink_core2(g) core2(g) <=>
sink_ksii_core2(g) ksii_core2(g) ->
test
sink_core4(g) core4(g) <=>
sink_ksii_core4(g) ksii_core4(g) ->
test
sink_cspg_a(l) cspg_a(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
test
sink_cspg_b(l) cspg_b(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
test
sink_cspg_c(l) cspg_c(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
test
sink_cspg_d(l) cspg_d(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
test
sink_cspg_e(l) cspg_e(l) <=>
sink_gal(l) gal(l) ->
sink_glcur(l) glcur(l) ->
sink_xyl-D(l) xyl-D(l) ->
test
sink_cys-L(c) cys-L(c) <=>
sink_glu-L(c) glu-L(c) <=>
sink_gly(c) gly(c) <=>
sink_gthrd(c) gthrd(c) ->
test
sink_cys-L(c) cys-L(c) <=>
sink_3sala(c) 3sala(c) ->
test
sink_3sala(c) 3sala(c) <=>
sink_so4(c) so4(c) ->
test
sink_cys-L(c) cys-L(c) <=>
sink_hyptaur(c) hyptaur(c) ->
test
sink_Lcystin(c) Lcystin(c) <=>
sink_cys-L(c) cys-L(c) ->
test
sink_dhap(c) dhap(c) <=>
sink_mthgxl(c) mthgxl(c) ->

```

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_etha(e) not in model

```

test
sink_dmpp(c) dmpp(c) <=>
sink_ggdp(c) ggdp(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

```

```

test
sink_dna(n) dna(n) <=>
sink_dna5mtc(n) dna5mtc(n) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_dolichol_L(c) dolichol_L(c) <=>
sink_dolmanp_L(r) dolmanp_L(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_dolichol_L(c) dolichol_L(c) <=>
sink_g3m8mpdol_L(r) g3m8mpdol_L(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
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_etha(e) not in model

test
sink_dolichol_U(c) dolichol_U(c) <=>
sink_g3m8mpdol_U(r) g3m8mpdol_U(r) ->
test
sink_dopa(c) dopa(c) <=>
sink_homoval(c) homoval(c) ->
test
sink_etoh(c) etoh(c) <=>
sink_acald(c) acald(c) ->
test
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_etha(e) not in model

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

```

```

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

```

```

sink_ala-B(c) ala-B(c) ->
test
sink_gdp(c) gdp(c) <=>
sink_dgtp(n) dgtp(n) ->
test
sink_gln-L(c) gln-L(c) <=>
sink_hco3(c) hco3(c) <=>
sink_ump(c) ump(c) ->
test
sink_gsn(c) gsn(c) <=>
sink_urate(x) urate(x) ->
test
sink_gua(c) gua(c) <=>
sink_gmp(c) gmp(c) ->
test
sink_hxan(c) hxan(c) <=>
sink_imp(c) imp(c) ->
test
sink_imp(c) imp(c) <=>
sink_atp(c) atp(c) ->
test
sink_imp(c) imp(c) <=>
sink_gtp(c) gtp(c) ->
test
sink_imp(c) imp(c) <=>
sink_urate(x) urate(x) ->
test
sink_prpp(c) prpp(c) <=>
sink_imp(c) imp(c) ->
test
sink_pydx(c) pydx(c) <=>
sink_pydx5p(c) pydx5p(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_thm(c) thm(c) <=>
sink_thmpp(c) thmpp(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_thm(e) thm(e) <=>
sink_thmpp(m) thmpp(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_thmpp(e) thmpp(e) <=>
sink_thmpp(c) thmpp(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_thmpp(m) thmpp(m) ->
test
sink_tyr-L(m) tyr-L(m) <=>
sink_q10(m) q10(m) ->
test
sink_udp(c) udp(c) <=>
sink_dttp(n) dttp(n) ->
test
sink_ump(c) ump(c) <=>
sink_ala-B(c) ala-B(c) ->
test
sink_fru(c) fru(c) <=>
sink_dhap(c) dhap(c) ->
test
sink_fru(c) fru(c) <=>

```



```

sink_g3p(c) g3p(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_fuc-L(c) fuc-L(c) <=>
sink_gdpfuc(c) gdpfuc(c) ->
test
sink_fum(m) fum(m) <=>
sink_oaa(m) oaa(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

```

```

test
sink_glp(c) glp(c) <=>
sink_dtdprmn(c) dtdprmn(c) ->
test
sink_g3p(c) g3p(c) <=>
sink_mthgxl(c) mthgxl(c) ->
test
sink_g6p(c) g6p(c) <=>
sink_r5p(c) r5p(c) ->
test
sink_g6p(c) g6p(c) <=>
sink_ru5p-D(c) ru5p-D(c) ->
test
sink_gal(c) gal(c) <=>
sink_glc-D(c) glc-D(c) ->
test
sink_gal(c) gal(c) <=>
sink_udpgal(c) udpgal(c) ->
test
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_galgalgalthcrm_hs(g) galgalgalthcrm_hs(g) ->
test
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_acgagbside_hs(g) acgagbside_hs(g) ->
test
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_acnacngalgb side_hs(g) acnacngalgb side_hs(g) ->
test
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gdlb2_hs(g) gdlb2_hs(g) ->
test
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gdlc_hs(g) gdlc_hs(g) ->
test
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gplc_hs(g) gplc_hs(g) ->
test
sink_galgluside_hs(g) galgluside_hs(g) <=>
sink_gqlbalph a_hs(g) gqlbalph a_hs(g) ->
test
sink_gam6p(c) gam6p(c) <=>
sink_uacgam(c) uacgam(c) ->
test
sink_gdpmann(c) gdpmann(c) <=>
sink_gdpfuc(c) gdpfuc(c) ->
test
sink_glc-D(c) glc-D(c) <=>
sink_inost(c) inost(c) ->
test
sink_glc-D(c) glc-D(c) <=>
sink_lac-L(c) lac-L(c) ->
sink_atp(c) atp(c) ->
sink_h2o(c) h2o(c) ->
test
sink_glc-D(c) glc-D(c) <=>

```

```

sink_lac-D(c) lac-D(c) ->
test
sink_glc-D(c) glc-D(c) <=>
sink_lcts(g) lcts(g) ->
test
sink_glc-D(c) glc-D(c) <=>
sink_pyr(c) pyr(c) ->
test
sink_gln-L(c) gln-L(c) <=>
sink_nh4(c) nh4(c) ->
test
sink_gln-L(m) gln-L(m) <=>
sink_glu-L(m) glu-L(m) ->
test
sink_gln-L(m) gln-L(m) <=>
sink_glu-L(m) glu-L(m) ->
test
sink_glu5sa(c) glu5sa(c) <=>
sink_pro-L(c) pro-L(c) ->
test
sink_glu-L(c) glu-L(c) <=>
sink_4abut(c) 4abut(c) ->
test
sink_glu-L(c) glu-L(c) <=>
sink_gln-L(c) gln-L(c) ->
test
sink_glu-L(c) glu-L(c) <=>
sink_pro-L(c) pro-L(c) ->
test
sink_glu-L(m) glu-L(m) <=>
sink_akg(m) akg(m) ->
test
sink_gluside_hs(g) gluside_hs(g) <=>
sink_galgluside_hs(g) galgluside_hs(g) ->
test
sink_glx(m) glx(m) <=>
sink_glyclt(m) glyclt(m) ->
test
sink_gly(c) gly(c) <=>
sink_ser-L(c) ser-L(c) ->
test
sink_ser-L(c) ser-L(c) <=>
sink_pyr(c) pyr(c) ->
test
sink_glyc(c) glyc(c) <=>
sink_glc-D(c) glc-D(c) ->
test
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_etha(e) not in model

test
sink_glyc(c) glyc(c) <=>
sink_Rtotal(c) Rtotal(c) <=>
sink_tag_hs(c) tag_hs(c) ->
test
sink_glyclt(c) glyclt(c) <=>
sink_gly(c) gly(c) ->
test
sink_glygn2(c) glygn2(c) <=>
sink_glc-D(c) glc-D(c) ->
test
sink_glygn2(e) glygn2(e) <=>
sink_glc-D(e) glc-D(e) ->
test

```

```
sink_glx(c) glx(c) <=>
sink_oxa(c) oxa(c) ->
test
sink_ha(l) ha(l) <=>
sink_acgam(l) acgam(l) ->
sink_glc(l) glc(l) ->
test
sink_his-L(c) his-L(c) <=>
sink_glu-L(c) glu-L(c) ->
test
sink_his-L(c) his-L(c) <=>
sink_hista(c) hista(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model
```

```
test
sink_hista(c) hista(c) <=>
sink_3mlda(c) 3mlda(c) ->
test
sink_hista(c) hista(c) <=>
sink_im4act(c) im4act(c) ->
test
sink_hmgcoa(x) hmgcoa(x) <=>
sink_chsterol(r) chsterol(r) ->
test
sink_hmgcoa(x) hmgcoa(x) <=>
sink_frdp(x) frdp(x) ->
test
sink_hmgcoa(x) hmgcoa(x) <=>
sink_xoldiolone(r) xoldiolone(r) ->
test
sink_hmgcoa(x) hmgcoa(x) <=>
sink_xoltriol(c) xoltriol(c) ->
test
sink_hpyr(c) hpyr(c) <=>
sink_2pg(c) 2pg(c) ->
test
sink_hpyr(c) hpyr(c) <=>
sink_glyclt(c) glyclt(c) ->
test
sink_hpyr(c) hpyr(c) <=>
sink_glyc-S(c) glyc-S(c) ->
test
sink_hspg(l) hspg(l) <=>
sink_gal(l) gal(l) ->
sink_glc(l) glc(l) ->
sink_xyl-D(l) xyl-D(l) ->
test
sink_hyptaur(c) hyptaur(c) <=>
sink_taur(x) taur(x) ->
test
sink_ile-L(c) ile-L(c) <=>
sink_accoa(c) accoa(c) ->
```

```
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model
```

```
test
sink_inost(c) inost(c) <=>
sink_pail_hs(c) pail_hs(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model
test
sink_inost(c) inost(c) <=>
sink_pail45p_hs(c) pail45p_hs(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model
test
```

```

sink_inost(c) inost(c) <=>
sink_pail4p_hs(c) pail4p_hs(c) ->
test
sink_inost(c) inost(c) <=>
sink_xu5p-D(c) xu5p-D(c) ->
test
sink_ipdp(x) ipdp(x) <=>
sink_sql(r) sql(r) ->
test
sink_itacon(m) itacon(m) <=>
sink_pyr(m) pyr(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_ksi(l) ksi(l) <=>
sink_man(l) man(l) ->
sink_acgam(l) acgam(l) ->
test
sink_ksii_core2(l) ksii_core2(l) <=>
sink_Ser/Thr(l) Ser/Thr(l) ->
test
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_etha(e) not in model

test
sink_l2fn2m2masn(g) l2fn2m2masn(g) <=>
sink_ksi(g) ksi(g) ->
test
sink_lac-L(c) lac-L(c) <=>
sink_glc-D(c) glc-D(c) ->
test
sink_Lcyst(c) Lcyst(c) <=>
sink_taur(x) taur(x) ->
test
sink_leu-L(c) leu-L(c) <=>
sink_accoa(c) accoa(c) ->
test
sink_lys-L(c) lys-L(c) <=>
sink_accoa(m) accoa(m) ->
test
sink_lys-L(x) lys-L(x) <=>
sink_aacoa(m) aacoa(m) ->
test
sink_m8masn(r) m8masn(r) <=>
sink_nm4masn(g) nm4masn(g) ->
test
sink_man(c) man(c) <=>
sink_gdpmann(c) gdpmann(c) ->
test
sink_man6p(c) man6p(c) <=>
sink_kdn(c) kdn(c) ->
test
sink_mescon(m) mescon(m) <=>
sink_pyr(m) pyr(m) ->
test
sink_met-L(c) met-L(c) <=>
sink_cys-L(c) cys-L(c) ->
test
sink_mil45p(c) mil45p(c) <=>
sink_inost(c) inost(c) ->
test
sink_msa(m) msa(m) <=>
sink_ala-B(m) ala-B(m) ->
test
sink_mthgxl(c) mthgxl(c) <=>

```

```

sink_12ppd-S(c) 12ppd-S(c) ->
test
sink_mthgxl(c) mthgxl(c) <=>
sink_lac-D(c) lac-D(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
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_etha(e) not in model

test
sink_nm4masn(g) nm4masn(g) <=>
sink_l2fn2m2masn(g) l2fn2m2masn(g) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_nm4masn(g) nm4masn(g) <=>
sink_n2m2nmasn(g) n2m2nmasn(g) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_nm4masn(g) nm4masn(g) <=>
sink_s2l2fn2m2masn(g) s2l2fn2m2masn(g) ->
test
sink_o2s(c) o2s(c) <=>
sink_h2o2(c) h2o2(c) ->
test
sink_h2o2(c) h2o2(c) <=>
sink_o2(c) o2(c) <=>
sink_h2o(c) h2o(c) ->
test
sink_orn(c) orn(c) <=>
sink_nh4(c) nh4(c) ->
test
sink_orn(c) orn(c) <=>
sink_ptrc(c) ptrc(c) ->
test
sink_orn(c) orn(c) <=>
sink_spmd(c) spmd(c) ->
test
sink_orn(c) orn(c) <=>
sink_sprm(c) sprm(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_pail_hs(c) pail_hs(c) <=>
sink_gpi_prot_hs(r) gpi_prot_hs(r) ->
test
sink_pail45p_hs(c) pail45p_hs(c) <=>
sink_mil45p(c) mil45p(c) ->
test
sink_phe-L(c) phe-L(c) <=>
sink_pac(c) pac(c) ->
test
sink_phe-L(c) phe-L(c) <=>
sink_pacald(c) pacald(c) ->
test
sink_phe-L(c) phe-L(c) <=>
sink_peamn(c) peamn(c) ->
test
sink_phe-L(c) phe-L(c) <=>
sink_phaccoa(c) phaccoa(c) ->

```

```

test
sink_phe-L(c) phe-L(c) <=>
sink_pheacgln(c) pheacgln(c) ->
test
sink_phe-L(c) phe-L(c) <=>
sink_phpyr(c) phpyr(c) ->
test
sink_phe-L(c) phe-L(c) <=>
sink_tyr-L(c) tyr-L(c) ->
test
sink_pheme(c) pheme(c) <=>
sink_bilirub(c) bilirub(c) ->
test
sink_phytcoa(x) phytcoa(x) <=>
sink_dmnoncoa(m) dmnoncoa(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_pmtcoa(c) pmtcoa(c) <=>
sink_crmphs(c) crmp_hs(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_pmtcoa(c) pmtcoa(c) <=>
sink_sphmyln_hs(c) sphmyln_hs(c) ->
test
sink_ppcoa(m) ppcoa(m) <=>
sink_succoa(m) succoa(m) ->
test
sink_pro-L(c) pro-L(c) <=>
sink_glu-L(c) glu-L(c) ->
test
sink_ptrc(c) ptrc(c) <=>
sink_ala-B(c) ala-B(c) ->
test
sink_ptrc(c) ptrc(c) <=>
sink_spmc(c) spmc(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

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

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

```

Warning: Reaction EX_etha(e) not in model

test

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_etha(e) not in model

test

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_etha(e) not in model

test

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_etha(e) not in model

test

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_etha(e) not in model

test

sink_Ser/Thr(g) Ser/Thr(g) <=>

sink_udpacgal(g) udpacgal(g) <=>

sink_sTn_antigen(g) sTn_antigen(g) ->

test

sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>

sink_cs_pre(g) cs_pre(g) ->

test

sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>

sink_cspg_a(g) cspg_a(g) ->

test

sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>

sink_cspg_c(g) cspg_c(g) ->

test

sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>

sink_cspg_d(g) cspg_d(g) ->

test

sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>

sink_cspg_e(g) cspg_e(g) ->

test

sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>

sink_hspg(g) hspg(g) ->

test

sink_Ser-Gly/Ala-X-Gly(r) Ser-Gly/Ala-X-Gly(r) <=>

sink_cspg_b(g) cspg_b(g) ->

test

sink_ser-L(c) ser-L(c) <=>

sink_cys-L(c) cys-L(c) ->

test

sink_so4(c) so4(c) <=>

sink_paps(c) paps(c) ->

test

sink_spmd(c) spmd(c) <=>

sink_sprm(c) sprm(c) ->

test

sink_srtn(c) srtn(c) <=>

sink_f5hoxkyn(c) f5hoxkyn(c) ->

test

sink_srtn(c) srtn(c) <=>

```

sink_fna5moxam(c) fna5moxam(c) ->
test
sink_srtm(c) srtm(c) <=>
sink_nmthsrtn(c) nmthsrtn(c) ->
test
sink_succoa(m) succoa(m) <=>
sink_oaa(m) oaa(m) ->
test
sink_taur(x) taur(x) <=>
sink_tchola(x) tchola(x) ->
test
sink_thcholstoic(x) thcholstoic(x) <=>
sink_gchola(x) gchola(x) ->
test
sink_thcholstoic(x) thcholstoic(x) <=>
sink_tchola(x) tchola(x) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_ppcoa(c) ppcoa(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_accoa(c) accoa(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_anth(c) anth(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_id3acald(c) id3acald(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_kynate(c) kynate(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_melatn(c) melatn(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_Lfmkynr(c) Lfmkynr(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_Lkynr(c) Lkynr(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_nformanth(c) nformanth(c) ->
test
sink_srtm(c) srtm(c) <=>
sink_5moxact(c) 5moxact(c) ->
test
sink_srtm(c) srtm(c) <=>
sink_6hoxmelatn(c) 6hoxmelatn(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_quln(c) quln(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_srtm(c) srtm(c) ->
test
sink_Tyr-ggn(c) Tyr-ggn(c) <=>
sink_glygn2(c) glygn2(c) ->
test
sink_tyr-L(c) tyr-L(c) <=>
sink_34hpp(c) 34hpp(c) ->
test
sink_tyr-L(c) tyr-L(c) <=>
sink_4hphac(c) 4hphac(c) ->
test
sink_tyr-L(c) tyr-L(c) <=>
sink_adrnl(c) adrnl(c) ->
test

```



```

sink_tyr-L(c) tyr-L(c) <=>
sink_dopa(c) dopa(c) ->
test
sink_tyr-L(c) tyr-L(c) <=>
sink_fum(c) fum(c) ->
sink_acac(c) acac(c) ->
test
sink_tyr-L(c) tyr-L(c) <=>
sink_melanin(c) melanin(c) ->
test
sink_tyr-L(c) tyr-L(c) <=>
sink_nrpphr(c) nrpphr(c) ->
test
sink_uacgam(c) uacgam(c) <=>
sink_udpglcur(c) udpglcur(c) <=>
sink_ha(e) ha(e) ->
test
sink_uacgam(c) uacgam(c) <=>
sink_m8masn(r) m8masn(r) ->
test
sink_udpglcur(c) udpglcur(c) <=>
sink_xu5p-D(c) xu5p-D(c) ->
test
sink_ura(c) ura(c) <=>
sink_ala-B(c) ala-B(c) ->
test
sink_val-L(c) val-L(c) <=>
sink_3aib(c) 3aib(c) ->
test
sink_val-L(c) val-L(c) <=>
sink_succoa(m) succoa(m) ->
test
sink_xoltriol(m) xoltriol(m) <=>
sink_thcholstoic(m) thcholstoic(m) ->
test
sink_xylu-D(c) xylu-D(c) <=>
sink_glyclt(c) glyclt(c) ->

```

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_etha(e) not in model

FBA =

```

    full: [7440x1 double]
    obj: 17.9030
    rcost: [7440x1 double]
    dual: [5063x1 double]
    solver: 'gurobi'
    algorithm: 'default'
    stat: 1
    origStat: 'OPTIMAL'
    time: 0.1420
    basis: [1x1 struct]
        x: [7440x1 double]
        f: 17.9030
        y: [5063x1 double]
        w: [7440x1 double]
        v: [7440x1 double]

```

Warning: Reaction EX_cbl1(e) not in model

Warning: Reaction EX_etha(e) not in model

```

test
sink_pyr(m) pyr(m) ->
test
sink_pyr(c) pyr(c) ->
test
sink_pyr(c) pyr(c) ->
test
sink_ala-L(c) ala-L(c) ->

```

```

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

```

Warning: Metabolite pcreat[e] not in model - added to the model

```

test
EX_pcreat(e) pcreat[e] <=>
sink_creat(c) creat(c) ->
test
sink_pcreat(c) pcreat(c) ->
test
sink_lac-L(c) lac-L(c) ->
test
sink_glygn2(c) glygn2(c) ->
test
sink_e4p(c) e4p(c) ->
test
sink_mag-hs(c) mag-hs(c) ->
test
sink_glyc(c) glyc(c) ->
test
sink_accoa(m) accoa(m) ->
test

```

```
sink_accoa(m) accoa(m) ->
test
sink_accoa(m) accoa(m) ->
test
sink_dhap(c) dhap(c) ->
test
sink_amp(c) amp(c) ->
test
sink_imp(c) imp(c) ->
test
sink_prpp(c) prpp(c) <=>
sink_gmp(c) gmp(c) ->
test
sink_imp(c) imp(c) ->
test
sink_thym(c) thym(c) ->
test
sink_cmp(c) cmp(c) ->
test
sink_dtmp(c) dtmp(c) ->
test
sink_citr-L(c) citr-L(c) <=>
sink_arg-L(c) arg-L(c) ->
test
sink_cys-L(c) cys-L(c) <=>
sink_taur(c) taur(c) ->
test
sink_gly(c) gly(c) <=>
sink_orn(c) orn(c) ->
test
sink_citr-L(c) citr-L(c) <=>
sink_urea(c) urea(c) ->
test
sink_gly(c) gly(c) <=>
sink_gthrd(c) gthrd(c) ->
test
sink_pro-L(c) pro-L(c) <=>
sink_4abut(c) 4abut(c) ->
test
sink_pro-L(c) pro-L(c) <=>
sink_orn(c) orn(c) ->
test
sink_met-L(c) met-L(c) <=>
sink_hcys-L(c) hcys-L(c) ->
test
sink_hcys-L(c) hcys-L(c) <=>
sink_met-L(c) met-L(c) ->
test
sink_hcys-L(c) hcys-L(c) <=>
sink_cys-L(c) cys-L(c) ->
test
sink_lys-L(c) lys-L(c) <=>
sink_glu-L(c) glu-L(c) ->
test
sink_trp-L(c) trp-L(c) <=>
sink_trypta(c) trypta(c) ->
test
sink_kynate(c) kynate(c) <=>
sink_nicrnt(c) nicrnt(c) ->
test
sink_pyr(c) pyr(c) <=>
sink_lac-L(c) lac-L(c) ->
test
sink_gal(c) gal(c) <=>
sink_udpg(c) udpg(c) ->
test
sink_fru(c) fru(c) <=>
```

```

sink_lac-L(c) lac-L(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_malcoa(c) malcoa(c) <=>
sink_eicostetcoa(c) eicostetcoa(c) ->
test
sink_accoa(c) accoa(c) <=>
sink_chsterol(r) chsterol(r) ->
test
sink_inost(c) inost(c) <=>
sink_glac(r) glac(r) ->
test
sink_pail_hs(c) pail_hs(c) <=>
sink_pail4p_hs(c) pail4p_hs(c) ->
test
sink_arachd(c) arachd(c) <=>
sink_prostgh2(c) prostgh2(c) ->
test
sink_arachd(c) arachd(c) <=>
sink_prostgd2(r) prostgd2(r) ->
test
sink_arachd(c) arachd(c) <=>
sink_prostge2(r) prostge2(r) ->
test
sink_arachd(c) arachd(c) <=>
sink_prostgi2(r) prostgi2(r) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_25hvitd3(m) 25hvitd3(m) <=>
sink_2425dhvitd3(m) 2425dhvitd3(m) ->
test
sink_caro(c) caro(c) <=>
sink_retinal(c) retinal(c) ->
test
DM_glu-L(c) glu-L(c) ->
test
DM_pro-L(m) pro-L(m) ->
test
sink_retinol-cis-11(c) retinol-cis-11(c) <=>
sink_retinal(c) retinal(c) ->
test
sink_pail_hs(c) pail_hs(c) <=>
sink_pchol-hs(c) pchol-hs(c) ->
test
sink_pail_hs(c) pail_hs(c) <=>
sink_pe_hs(c) pe_hs(c) ->
test
sink_pail_hs(c) pail_hs(c) <=>
sink_ps-hs(c) ps-hs(c) ->
test
sink_pail_hs(c) pail_hs(c) <=>
sink_g3pc(c) g3pc(c) ->
test
sink_dag_hs(c) dag_hs(c) <=>
sink_pchol-hs(c) pchol-hs(c) ->
test
sink_dag_hs(c) dag_hs(c) <=>
sink_pe_hs(c) pe_hs(c) ->
test
sink_dag_hs(c) dag_hs(c) <=>
sink_clpn-hs(c) clpn-hs(c) ->
test
sink_dag_hs(c) dag_hs(c) <=>
sink_pgp-hs(c) pgp-hs(c) ->

```

```

test
sink_bhb(m) bhbm(m) <=>
sink_acac(m) acac(m) ->
test
sink_mal-L(m) mal-L(m) <=>
sink_pyr(m) pyr(m) ->
test
sink_glu-L(c) glu-L(c) <=>
sink_gln-L(c) gln-L(c) ->
test
sink_cys-L(c) cys-L(c) <=>
sink_coa(c) coa(c) ->
test
sink_occoa(m) occoa(m) <=>
sink_accoa(m) accoa(m) ->
test
sink_lnlncgcoa(c) lnlncgcoa(c) <=>
sink_dlnlcgcoa(c) dlnlcgcoa(c) ->
test
sink_chol(c) chol(c) <=>
sink_ach(c) ach(c) ->
test
sink_pyr(m) pyr(m) <=>
sink_oaa(m) oaa(m) ->
test
sink_crtm(c) crt(m) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

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

test
sink_arachd(c) arachd(c) <=>
sink_C06314(c) C06314(c) ->
Warning: Reaction EX_cbl1(e) not in model
Warning: Reaction EX_etha(e) not in model

test
sink_nrpphr(c) nrpphr(c) <=>
sink_3mox4hoxm(c) 3mox4hoxm(c) ->
test
sink_sbt-D(c) sbt-D(c) <=>
sink_fru(c) fru(c) ->
test
sink_accoa(m) accoa(m) ->
test
sink_succoa(m) succoa(m) ->

```

```

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

```

Next we remove all human metabolic reactions (HMRs) (i.e., those reactions originating from HMR 2.0 [3] and that start with 'HMR_') that are not needed for the aforementioned tasks. Applicable to Recon 3 only.

```

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 [4]. Applicable to Recon 3 only.

```
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. Applicable to Recon 3 only.

```
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 the method FASTCORE, 'fastcc', to ensure a flux-consistent subnetwork [5].

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

```
7440 Total reactions
3260 Reversible reactions.
4180 Irreversible reactions.
5091 Flux consistent reactions, without flipping.
1266 Flux inconsistent irreversible reactions, without flipping.
1083 Flux inconsistent reactions, without flipping.
5235 Flux consistent reactions.
 939 Flux inconsistent reversible reactions left to flip.
5237 Flux consistent reactions.
 937 Flux inconsistent reversible reactions left to flip.
5241 Flux consistent reactions.
 933 Flux inconsistent reversible reactions left to flip.
5245 Flux consistent reactions.
 929 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},modelg
```

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 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 4967.1 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 4967.2 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 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 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 4128.1 added to model

New gene 4129.1 added to model
New gene 8659.1 added to model
New gene 8659.2 added to model
New gene 6799.1 added to model
New gene 6817.3 added to model
New gene 6799.2 added to model
New gene 6818.2 added to model
New gene 6817.2 added to model
New gene 6818.1 added to model
New gene 6817.1 added to model
New gene 6817.4 added to model
New gene 6818.3 added to model
New gene 6817.5 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 65985.1 added to model
New gene 28.1 added to model
New gene 223.1 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 39.1 added to model
New gene 3030.1 added to model
New gene 3032.1 added to model
New gene 30.1 added to model
New gene 31.1 added to model
New gene 32.1 added to model
New gene 9197.1 added to model
New gene 55902.1 added to model
New gene 55902.2 added to model
New gene 84532.1 added to model
New gene 5973.1 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 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 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 3658.1 added to model
New gene 48.1 added to model
New gene 50.1 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 788.1 added to model
New gene 1571.1 added to model
New gene 112611.1 added to model
New gene 98.1 added to model
New gene 97.2 added to model
New gene 97.1 added to model
New gene 100.1 added to model
New gene 3177.1 added to model
New gene 122481.1 added to model
New gene 203.1 added to model
New gene 26289.1 added to model
New gene 26289.2 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 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 132.1 added to model
New gene 132.2 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 11164.1 added to model
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New gene 9060.1 added to model
New gene 9061.1 added to model
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New gene 158.2 added to model
New gene 159.1 added to model
New gene 122622.1 added to model
New gene 122622.2 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 10331.1 added to model
New gene 10678.2 added to model
New gene 51005.1 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 64902.1 added to model
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New gene 10768.2 added to model
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New gene 471.1 added to model
New gene 10606.1 added to model
New gene 8402.1 added to model
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New gene 383.1 added to model
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New gene 435.1 added to model
New gene 445.1 added to model
New gene 445.2 added to model
New gene 83884.1 added to model
New gene 10166.1 added to model
New gene 410.1 added to model
New gene 427.1 added to model
New gene 427.2 added to model
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New gene 8705.1 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 53630.1 added to model
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New gene 56052.1 added to model
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New gene 635.1 added to model
New gene 10599.1 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
New gene 686.1 added to model
New gene 8884.1 added to model
New gene 80704.1 added to model
New gene 51733.1 added to model
New gene 7108.1 added to model
New gene 50814.1 added to model
New gene 3295.1 added to model
New gene 6307.1 added to model
New gene 492.1 added to model
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New gene 493.1 added to model
New gene 10257.1 added to model
New gene 10057.2 added to model
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New gene 847.1 added to model
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New gene 8760.1 added to model
New gene 10390.1 added to model
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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
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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 8714.1 added to model
New gene 55349.1 added to model
New gene 1120.2 added to model
New gene 1119.1 added to model
New gene 1120.1 added to model
New gene 1119.2 added to model
New gene 60482.1 added to model
New gene 6582.1 added to model
New gene 6584.1 added to model
New gene 6582.2 added to model
New gene 6820.1 added to model
New gene 19.1 added to model
New gene 10948.1 added to model
New gene 27159.2 added to model
New gene 171425.1 added to model
New gene 171425.2 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 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
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```

Save the resulting model.

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

Size of the original Recon model:

```
[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
5063   7440  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
2910   5245  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.

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