

Create a generic subnetwork from Recon 3D

Author(s): Ines Thiele, Susan M. T. Fleming, Systems Biochemistry Group, ICRB, University of Luxembourg

Reviewer(s): Anouk Heiskan, Catherine M. Clancy, Laurent Hellegott, LCIH, University of Luxembourg.

In this tutorial, we show how to create a generic subnetwork from Recon 2D 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

Initiating the OSHA Territory

Initialize the Cobra Toolbox using the `initCobraToolbox` function

% in intercession time

Get the optimization solver

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

```
% set font size to 10pt
```

However, for the analysis of large models such as Recon 3D, it is not recommended to use the "g1pk" package, but rather a commercial-grade solver, such as "mosek". For detailed information, refer to the [Cobra Toolbox solver installation guide](#).

For the analysis of a Recon model, change the solver to "minotaur".

```
salwertName = 'gurobi1';
changeDefaultSolver(salwertName, 'LP');
```

* Curviki interface added to PPT-AB web.

CONCLUSION

Load the model

In this tutorial, the used model is the generic model of human metabolism, Recon 2D [9]. If Recon 2D is not available, use Recon 2 [2] provided in The COBRA Toolbox. Other COBRA models may be downloaded from the [Virtual Metabolic Human](http://www.vital-metabolic.com) website and saved to your preferred directory.

Before proceeding with the simulations, the path for the model needs to be defined

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```
Filename = 'RecentModel.mat'; % If using Weiss 2 model, amend filename.
model = readcModel([currentFilePath 'test' filePath 'models' filePath filename]);
model.create([xsize(model),1,1]) = 'E';
```

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

```
model.L1[7:10] := connecter(model.x_rate, "connecter_x_rate_toTanner") == 0;
model.L1[11:10] := connecter(model.y_rate, "connecter_y_rate_toTanner") == 0;
model.L1[12:10] := connecter(model.x_rate, "connecter_x_rate_toTanner") == 0;
model.L1[13:10] := connecter(model.y_rate, "connecter_y_rate_toTanner") == 0;
DPI = (CTVATCHM["DPI", model.x_rate]);
model.L1[20] = 0;
T0000 = (CTVATCHM["t0000", model.x_rate]);
model.L1[21:1000] = 0;
model.L0[1:1000] = 0;
model.L0[1:1000] = 0;
model.L0[1:1000] = 0;
```

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.)

<code>table.sources[i].testedProc = Proc</code>	<code>= DESTROYedProcSourceName(i)</code>
---	---

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

$$\text{DR_atg_c: } \text{H2a}[x] + \text{atg}[x] \rightarrow \text{adp}[x] + \text{H}[x] + \text{pH}[x]$$

Identify the model reactions that are needed to ensure that all metabolic functions can have a non-zero flux. (Note that this function uses `sparenessFA`, i.e., alternative solutions may exist but are not considered here.) Applicable to Record only.

```

17 ~~~~~
[TestedOutLandV], TestedOutInWaterLandLink, TestedRustCasedLinks, PerCasedLinks) = TestRandomFCIDat(model, 'all', 0)
TestedRust = unique([TestedRustC; TestedRustCasedLinks]);
TestedRustCK = intersect(Lrust, TestedRust);
~~~~~

```

Next we remove all human metabolic reactions (HMRs) (i.e., those reactions originating from HMR 2.0 [2]) and that start with HMR_ that are not needed for the aforementioned tasks. Applicable to Bioco 3 only.

```
17 if !isempty(STARTTIME) || !isEmpty, 'NOGOLF'))
18     NPER = model.L.runs(STARTTIME, 'NPER', model.L.runs);
19     NPER_NBI = GOLF(17) * NPER, NOGOLF(17);
20     model.Lb(17) = ismember(model.L.runs, NPER_NBI) == 0;
21     model.Lub(17) = ismember(model.L.runs, NPER_NBI) == 0;
```

We will also remove all dual module reactions, i.e., those ones with the term "Yeast" in the substrate, month-eliminating box [4]. Applicable to React 3 only.

```

if ~isEmpty(getStringFromFile, "Recon3"))
  DR = model.react(match("Recon", model.subsystems));
  model.isTfIndicible(model.react, DR) = 0;
  model.isTfIndicible(model.react, DR) = 0;
  DR1 = (strcmp("Transport of AcetylCoA", model.subsystems));
  model.isTfIndicible(DR1) = 0;
  model.isTfIndicible(DR1) = 0;
end

```

We will also remove all reactions from the 'Peptide metabolism' subsystem. Applicable to Recon 3 only.

```

if ~isEmpty(getStringFromFile, "Recon3"))
  DR = model.react(match("Peptide metabolism", model.subsystems));
  model.isTfIndicible(model.react, DR) = 0;
  model.isTfIndicible(model.react, DR) = 0;
end

```

We will use the method FASTCORE, 'fastcore', to ensure a flux-consistent subnetwork [8].

```

getSgList = 2e-8;
getSgMethod = 'fastcore';
getSgMethod = 'fastcore';
getSgList = 2;
[fluxConsistentReactions, fluxConsistentReactions, fluxConsistentReactions, fluxConsistentReactions, modelOut] = findFluxConsistentSubnet(model,
    3100 Total reactions.
    3200 Reversible reactions.
    4100 Irreversible reactions.
    5000 Flux consistent reactions, without flipping.
    5200 Flux inconsistent irreversible reactions, without flipping.
    5370 Flux inconsistent reactions, without flipping.
    5217 Flux consistent reactions.
    5217 Flux inconsistent reversible reactions left to flip.
    5218 Flux consistent reactions.
    5218 Flux inconsistent reversible reactions left to flip.
    5219 Flux consistent reactions.
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    5220 Flux consistent reactions.
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    5221 Flux consistent reactions.
    5221 Flux inconsistent reversible reactions left to flip.
    5222 Flux consistent reactions.
    5222 Flux inconsistent reversible reactions left to flip.
    5223 Flux consistent reactions.
    5223 Flux inconsistent reversible reactions left to flip.

```

And remove the flux inconsistent reactions from the model.

```

model.isConsistent = removeReactions(model, model.react(find(FluxConsistentReactions)));

```

We will now update the GPR associations.

```

model.isConsistent.genes = [];
model.isConsistent.reactions = [];
model.isConsistent.genes = model.isConsistent.genes;
for i = 1 : length(model.isConsistent.genes)
  if ~isEmpty(model.isConsistent.genes(i))
    model.isConsistent = changeGeneAssociations(model.isConsistent, model.isConsistent.react(i), model.isConsistent.genes(i));
  end
end

```

```

New gene 809.1 added to model.
New gene 26.1 added to model.
New gene 316.2 added to model.
New gene 316.1 added to model.
New gene 3391.1 added to model.
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New gene 2572.1 added to model
New gene 2572.2 added to model
New gene 2880.1 added to model
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New gene 8799.1 added to model
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New gene 9821.1 added to model
New gene 1181.4 added to model
New gene 1181.2 added to model
New gene 1181.3 added to model
New gene 1181.1 added to model
New gene 342886.1 added to model
New gene 1138.1 added to model
New gene 9488.1 added to model
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New gene 17.1 added to model
New gene 41291877.1 added to model

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New gene AAG77088.1 added to model
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New gene Z1881186.1 added to model
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New gene K43872.1 added to model
New gene K18898.1 added to model
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New gene K1838.1 added to model
New gene AAG9523.1 added to model
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[illegible]

```

New group 21832.1 added to model
New group 21837.1 added to model
New group 21299.1 added to model
New group 21297.5 added to model
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New group 43152.1 added to model
New group 43153.1 added to model
New group 43139.1 added to model
New group 13101.1 added to model
New group 43151.2 added to model
New group 91877.5 added to model
New group 219968.1 added to model
New group 43154.5 added to model
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New group 13137.1 added to model
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New group 91799.1 added to model
New group 915748.1 added to model
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New group 131497.1 added to model
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New group 131051.1 added to model
New group 2314.1 added to model
New group 43131.1 added to model
New group 44101.1 added to model
New group 3903.1 added to model
New group 43931.1 added to model
New group 20801.1 added to model
New group 9161.1 added to model

```

Save the resulting model

```
save("subgraphviz.rtfm-act", "node/consistent")
```

Size of the original ResNet model

```

jMet, nMet) = size(Model.S)
fprintf('Model Size: %d\n', nMet); fprintf('Model Size: %d\n', nMet);
total = 0;

```

Year	Area	Value	Unit
1990	2000	1000	kg

Size of the resulting Beacon sub-network:

```

[mpet,mpas] = size(nodesInNetwork.S);
for i=1:'size(nodesInNetwork','Nodes'),'Nodes'; for j=1:'size(nodesInNetwork','mpet','mpas'); total = 0;

```

Jahr	Brutto	Netto
2010	5205	5205

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

References

- [1] Iwure, E., et al. Recon 3D: A resource enabling a three-dimensional view of gene variation in human metabolism. *unpublished*, 2017.
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- [3] Madhugoyal, K., Aggar, R., Kamg, C., et al. (2014) Genome-scale metabolic modelling of hepatocytes reveals serine deficiency in patients with non-alcoholic fatty liver disease. *Nat. commun.*, 5, 3082.
- [4] Sahoo, S., Harasiddhi HS, Fleming RM, Thiele I. Modeling the effects of commonly used drugs on human metabolism. *FEBS J*. 2016;Jan(362):297-307.
- [5] Vlassara, N, Pacheco MF, Sawyer T. Fast reconstruction of compact context-specific metabolic network models. *PLoS Comput Biol*. 2016;Jan(10):1.