MERGED Collapse All Readme 2021-11-23 15:20

Independent Section

Contains tests that are independent of the class of modeled organism, a model's complexity or

Specific Section

Covers general statistics and specific aspects of a metabolic network that are not universally

Consistency

Stoichiometric Consistency

Stoichiometric inconsistency violates universal cc 1. Molecular masses are always positive, and 2. C side of a reaction the mass is conserved. A single incorrectly defined reaction can lead to stoichiom inconsistency in the model, and consequently to unconserved metabolites. Similar to insufficient c this may give rise to cycles which either produce r nothing or consume mass from the model. Impler This test uses an implementation of the algorithm presented in section 3.1 by Gevorgyan, A., M. G Pc and D. A Fell. "Detection of Stoichiometric Inconsi Biomolecular Models." Bioinformatics 24, no. 19 (2245. doi: 10.1093/bioinformatics/btn425

This model's stoichiometry inconsistent

```
false
```

Mass Balance

This will exclude biomass, exchange and demand as they are unbalanced by definition. It will also fa reactions where at least one metabolite does not formula defined. In steady state, for each metabol sum of influx equals the sum of efflux. Hence the masses of both sides of any model reaction have equal. Reactions where at least one metabolite dc have a formula are not considered to be balanced though the remaining metabolites participating in reaction might be. Implementation: For each reac isn't a boundary or biomass reaction check if each metabolite has a non-zero elements attribute and calculate if the overall element balance of reactan products is equal to zero.

A total of 1255 (46.72%) reactions are mass unba with at least one of the metabolites not having a f the overall mass not equal to 0: r_4342, r_4343, r_ r_4349, r_4352, ...

SBML

SBML Level and Version Errored

This test reports if the model file is represented in the latest edition (level) of the Systems Biology Markup Language (SBML) which is Level 3, and at least version 1. Implementation: The level and version are parsed directly from the SBML document.

```
null
```

FBC enabled Errored

The Flux Balance Constraints (FBC) Package extends SBML with structured and semantic descriptions for domain-specific model components such as flux bounds, multiple linear objective functions, gene-protein-reaction associations, metabolite chemical formulas, charge and related annotations which are relevant for parameterized GEMs and FBA models. The SBML and constraint-based modeling communities collaboratively develop this package and update it based on user input. Implementation: Parse the state of the FBC plugin from the SBML document.

```
null
```

Basic Information

Model Identifier MERGED

The MIRIAM guidelines require a model to be identified via an ID. Further, the ID will be displayed on the memote snapshot report, which helps to

Charge Balance

This will exclude biomass, exchange and demand as they are unbalanced by definition. It will also fa reactions where at least one metabolite does not charge defined. In steady state, for each metaboli of influx equals the sum of efflux. Hence the net c both sides of any model reaction have to be equal Reactions where at least one metabolite does not charge are not considered to be balanced, even th remaining metabolites participating in the reactio be. Implementation: For each reaction that isn't a or biomass reaction check if each metabolite has charge attribute and if so calculate if the overall s charges of reactants and products is equal to zero

A total of 686 (25.54%) reactions are charge unba with at least one of the metabolites not having a c the overall charge not equal to 0: r_4342, r_4344, r r_0477, r_0478, ...


```
["r_4342","r_4344","r_4352","r_0477","r
r_0490","r_0502","r_0503","r_0512","r_0
0525","r_0530","r_0531","r_0534","r_053
```


Metabolite Connectivity

Disconnected metabolites are not part of any reac model. They are most likely left-over from the reco process, but may also point to network and knowl gaps. Implementation: Check for any metabolites cobra.Model object with emtpy reaction attribute.

A total of 1 (0.04%) metabolites are not associate reaction of the model: m_0035


```
["m_0035"]
```


Unbounded Flux In Default Medium

A large fraction of model reactions able to carry u flux under default conditions indicates problems v reaction directionality, missing cofactors, incorrec transport reactions and more. Implementation: W changing the default constraints run flux variabilit From the FVA results identify those reactions that equal to the model's maximal or minimal flux.

A fraction of 14.32% of the non-blocked reactions

attribute, this value is parsed from the "id" attribute of the <model> tag in the SBML file e.g. <model fbc:strict="true" id="iJO1366">.

The model ID is MERGED


```
"MERGED"
```


Total Metabolites 2,338

To be useful a metabolic model should consist at least of a few metabolites that are converted by reactions. This test simply checks if there are more than zero metabolites. Implementation: Check if the cobra.Model object has non-empty "metabolites" attribute, this list is populated from the list of sbml:listOfSpecies which should contain at least one sbml:species.

2338 metabolites are defined in the model.


```
["m_0001","m_0002","m_0003","m_0
004","m_0005","m_0006","m_0007",
"m_0008","m_0009","m_0010","m_00
```


Total Reactions 2,844

To be useful a metabolic model should consist at least of a few reactions. This test simply checks if there are more than zero reactions. Implementation: Check if the cobra.Model object has non-empty "reactions" attribute, this list is populated from the list of sbml:listOfReactions which should contain at least one sbml:reaction.

2844 reactions are defined in the model.


```
["r_0003","r_0005","r_0006","r_0
007","r_0012","r_0013","r_0014",
"r_0016","r_0017","r_0018","r_00
```


Total Genes 935