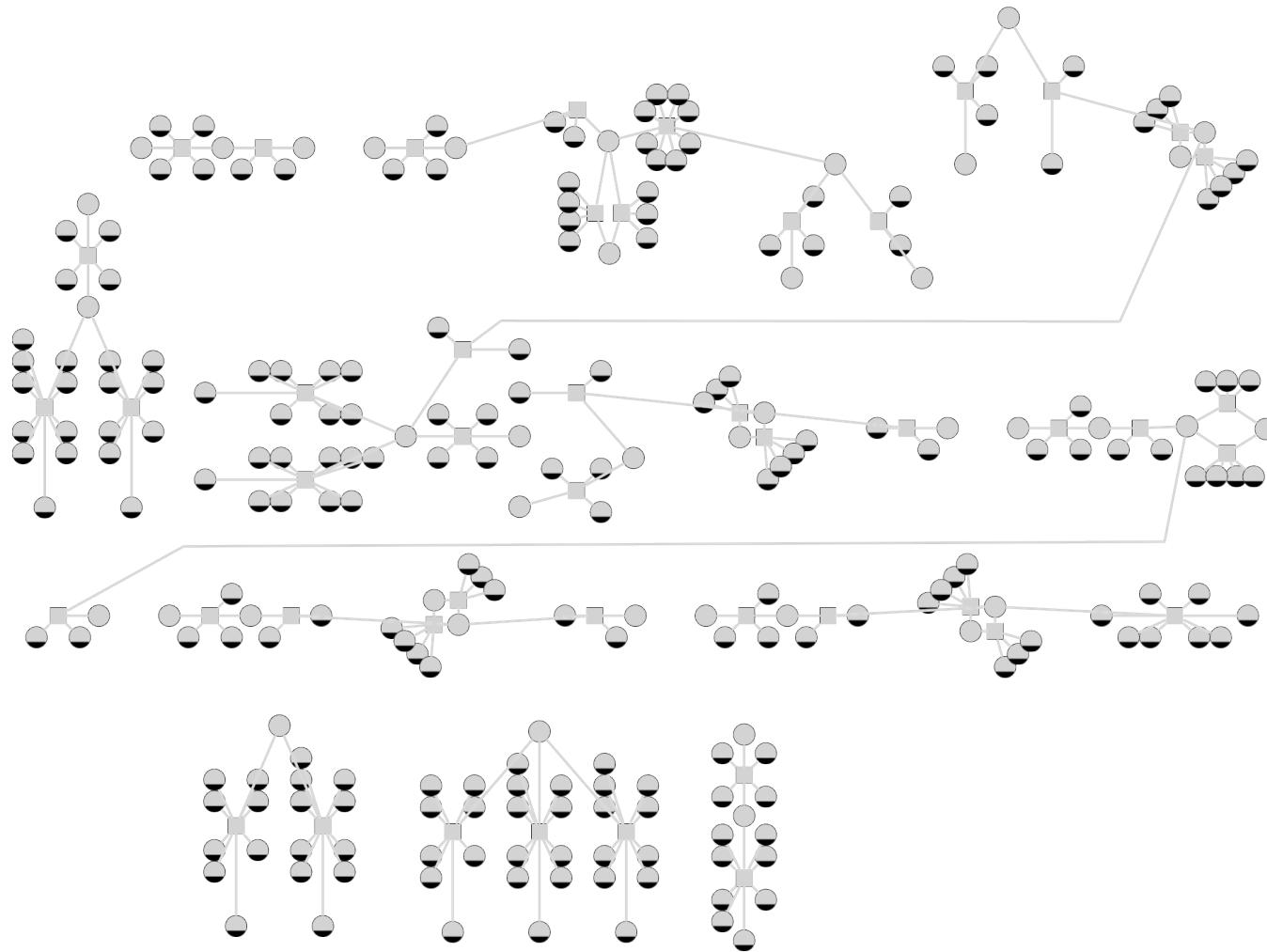




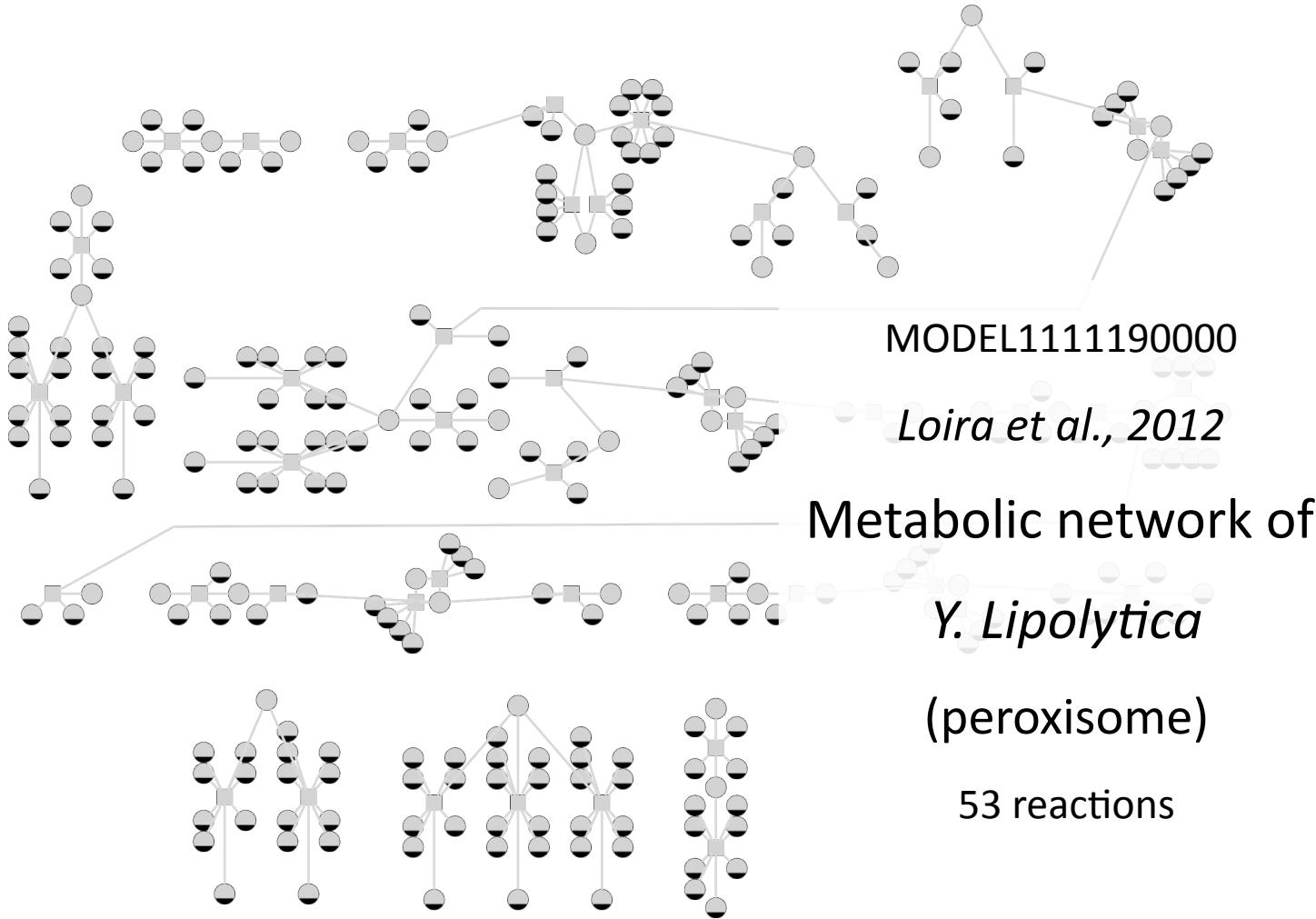
How to represent a generalized metabolic model using SBML and SBGN?

Anna Zhukova and David James Sherman

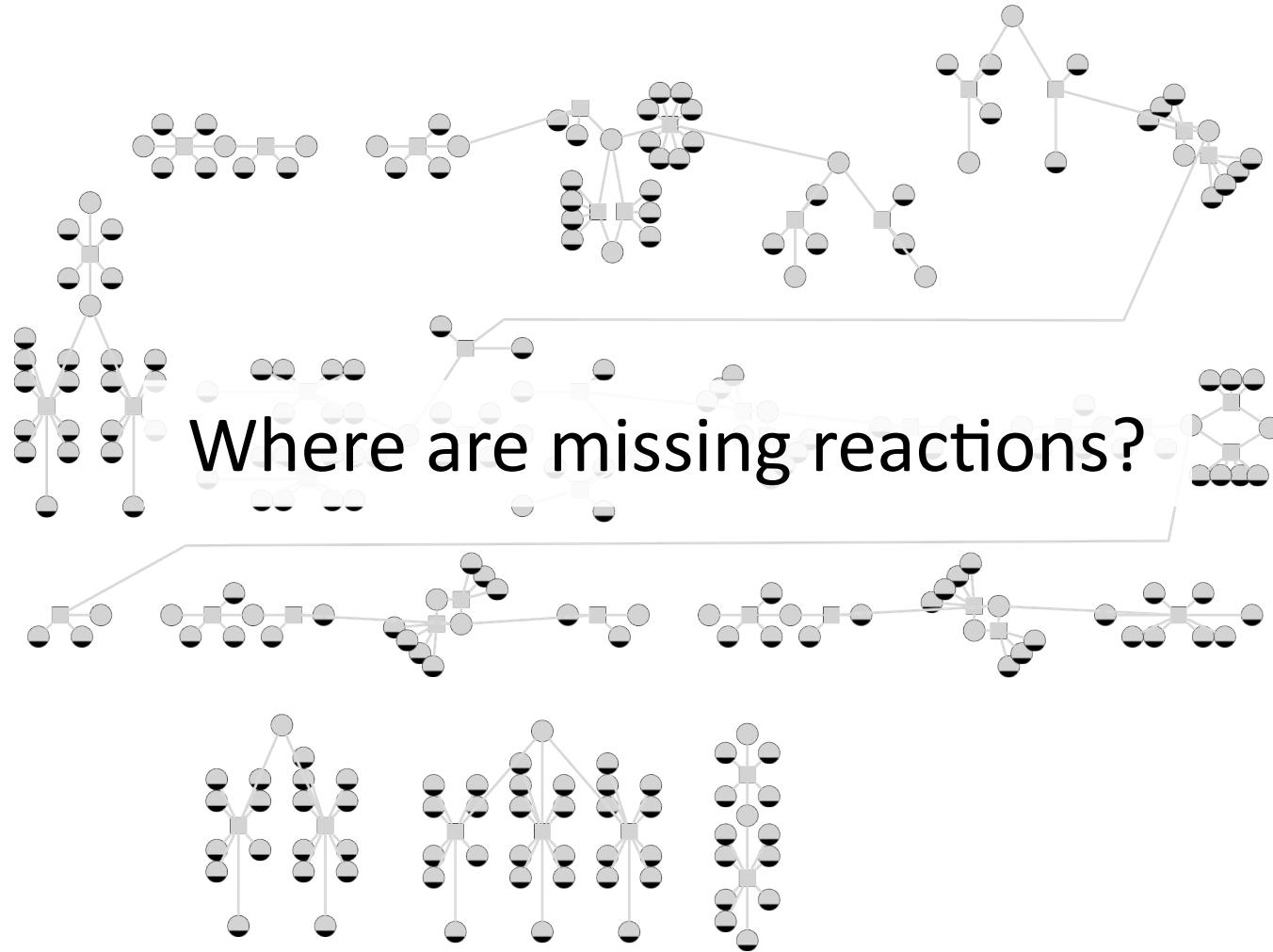
Genome-scale metabolic models are complicated...



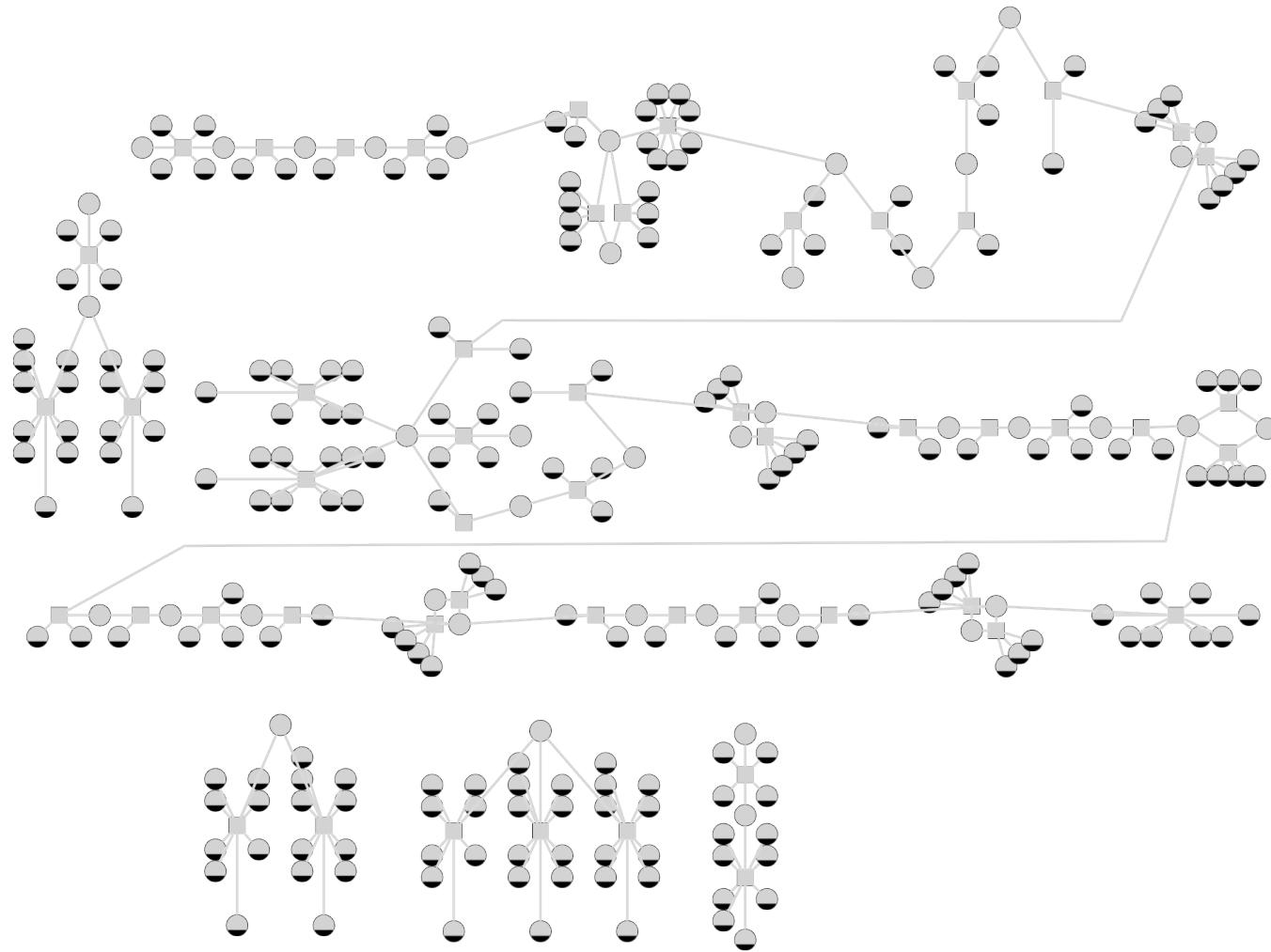
Genome-scale metabolic models are complicated...



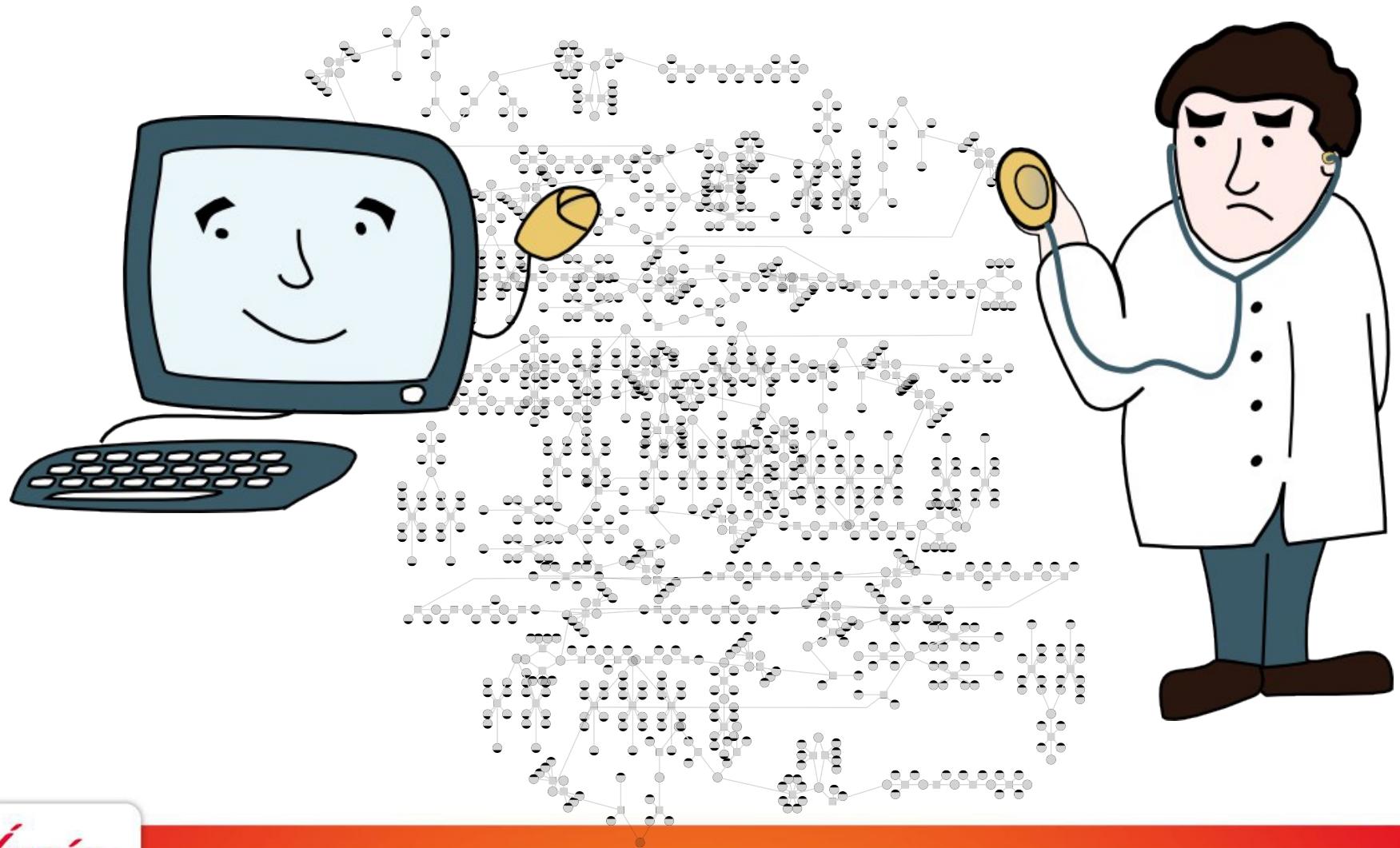
Genome-scale metabolic models are complicated...

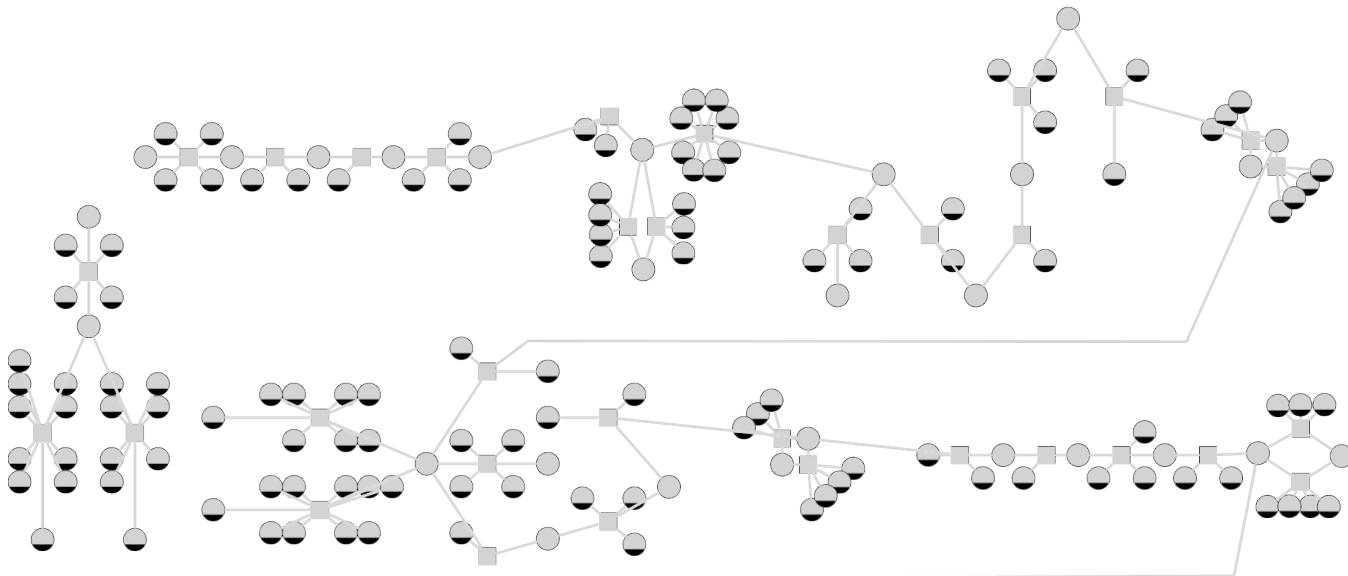


Genome-scale metabolic models are complicated...

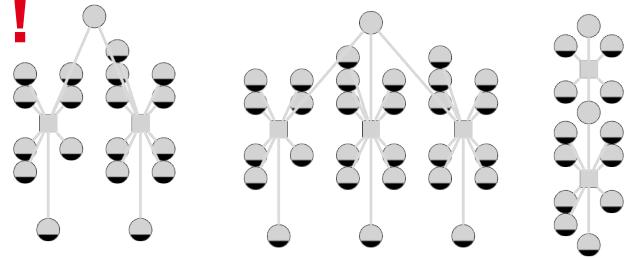


Genome-scale metabolic models are complicated...



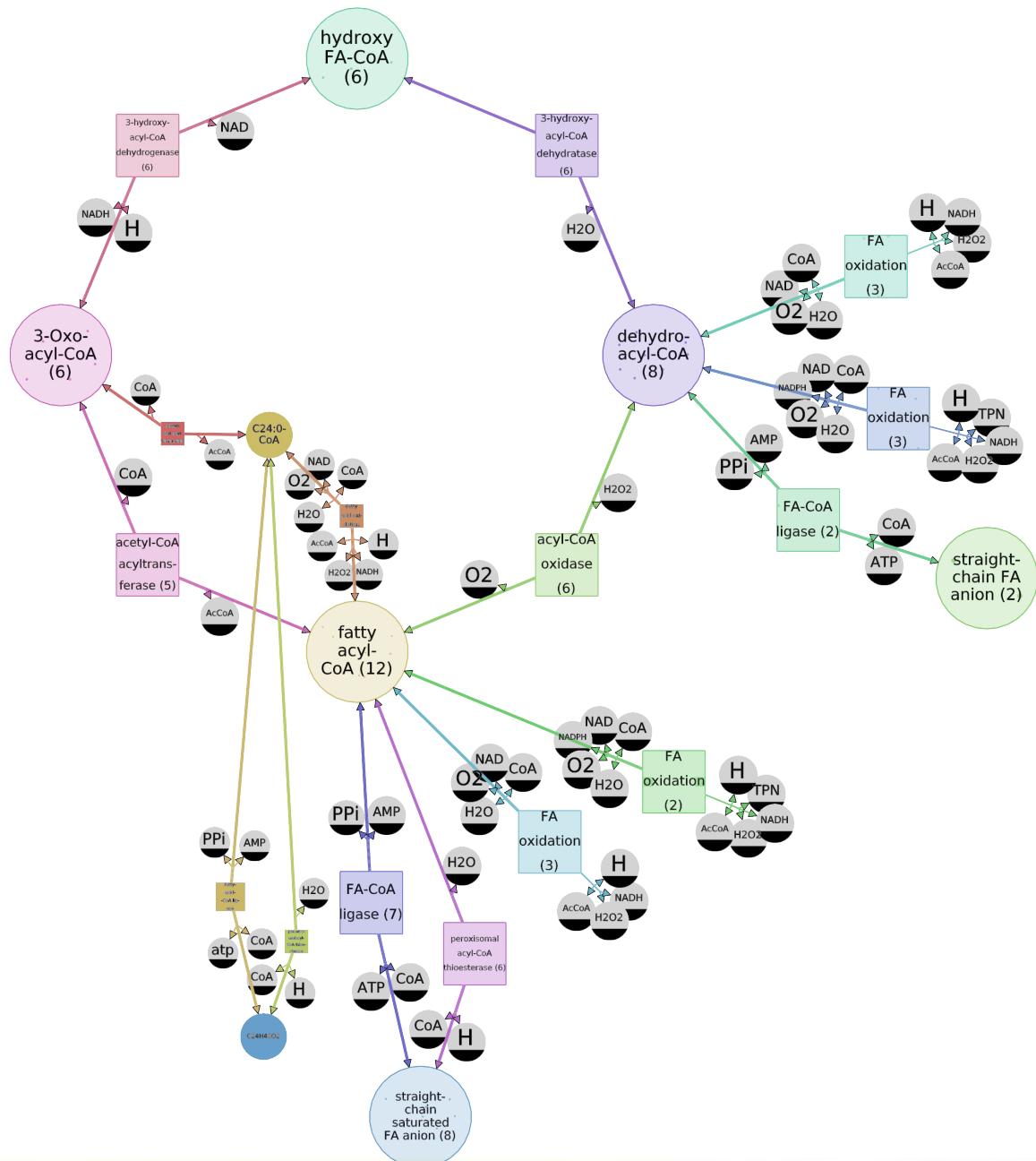


**Let's
generalize !**

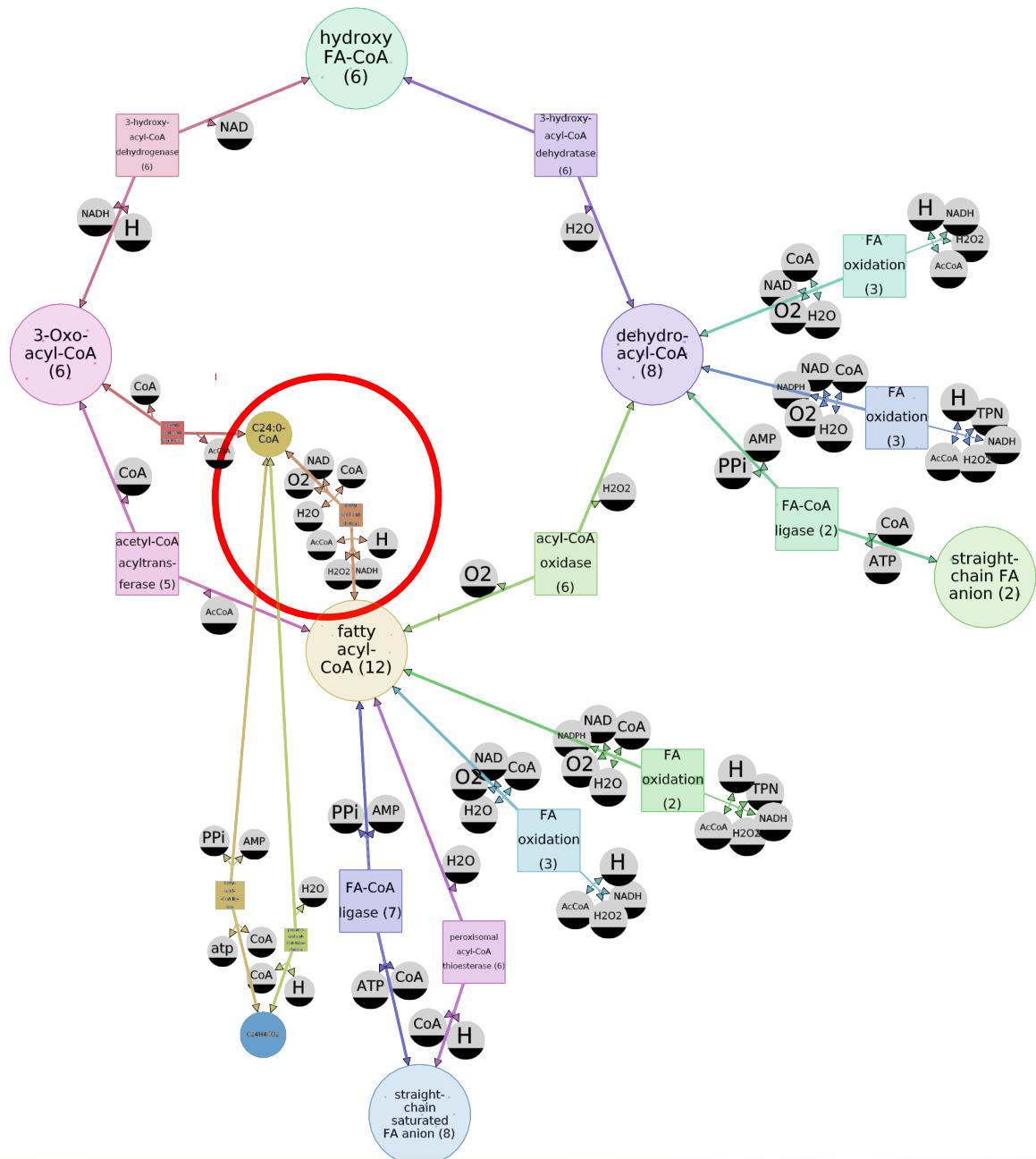


(The figure is produced using the Tulip graph visualization tool.)

**Let's
generalize !**

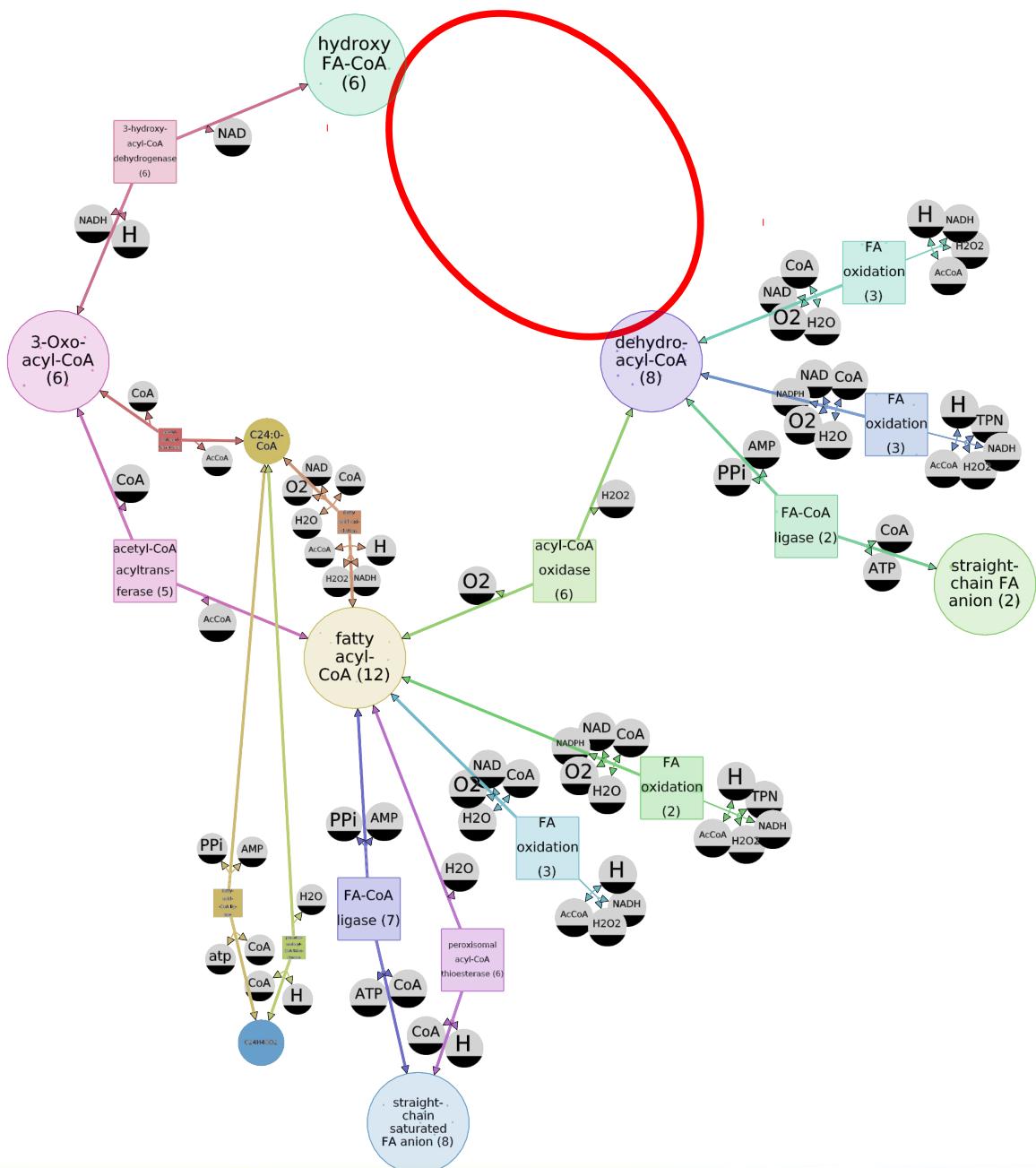


**Let's
generalize !**



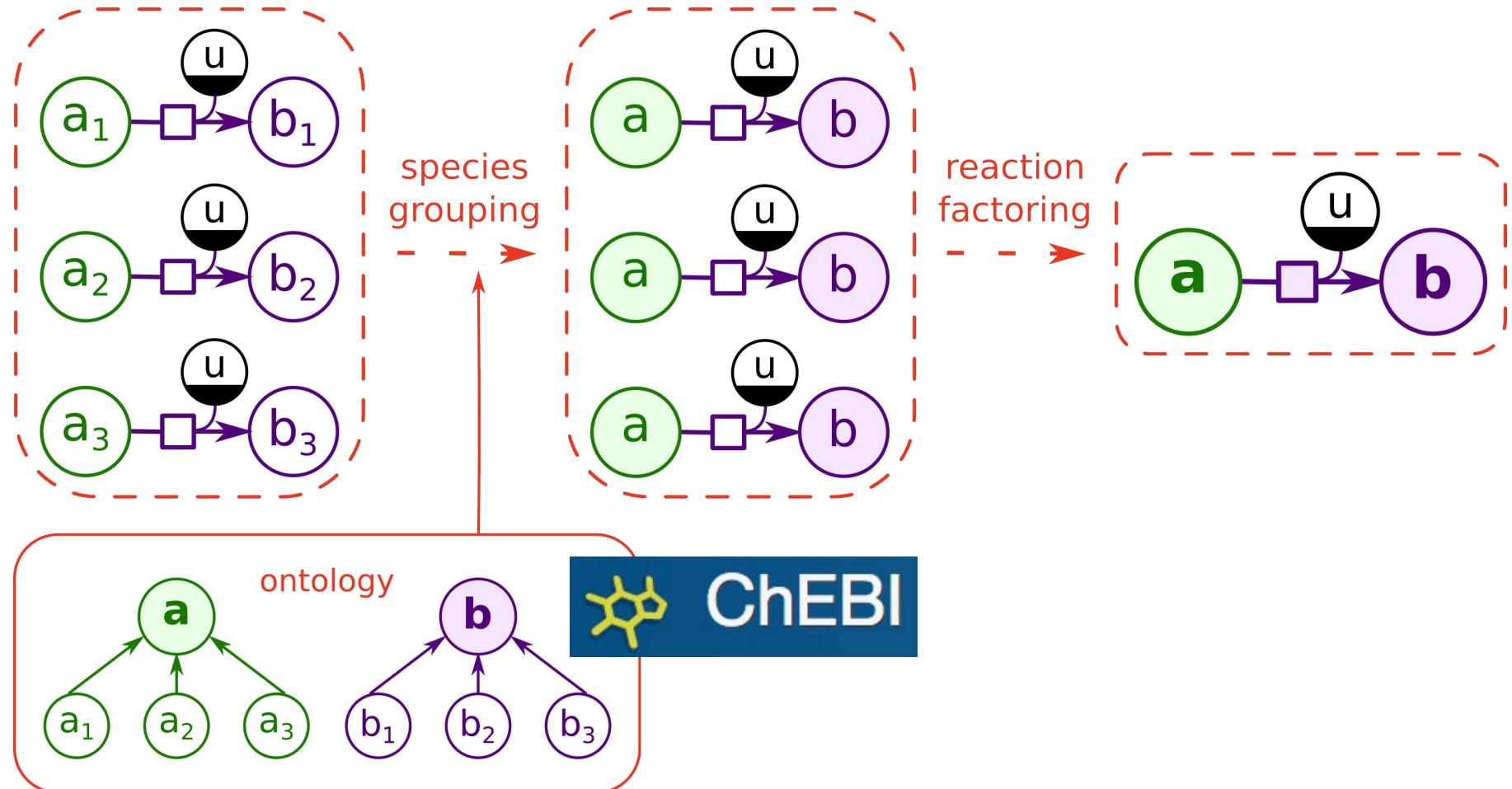
(The figure is produced using the Tulip graph visualization tool.)

**Let's
generalize !**

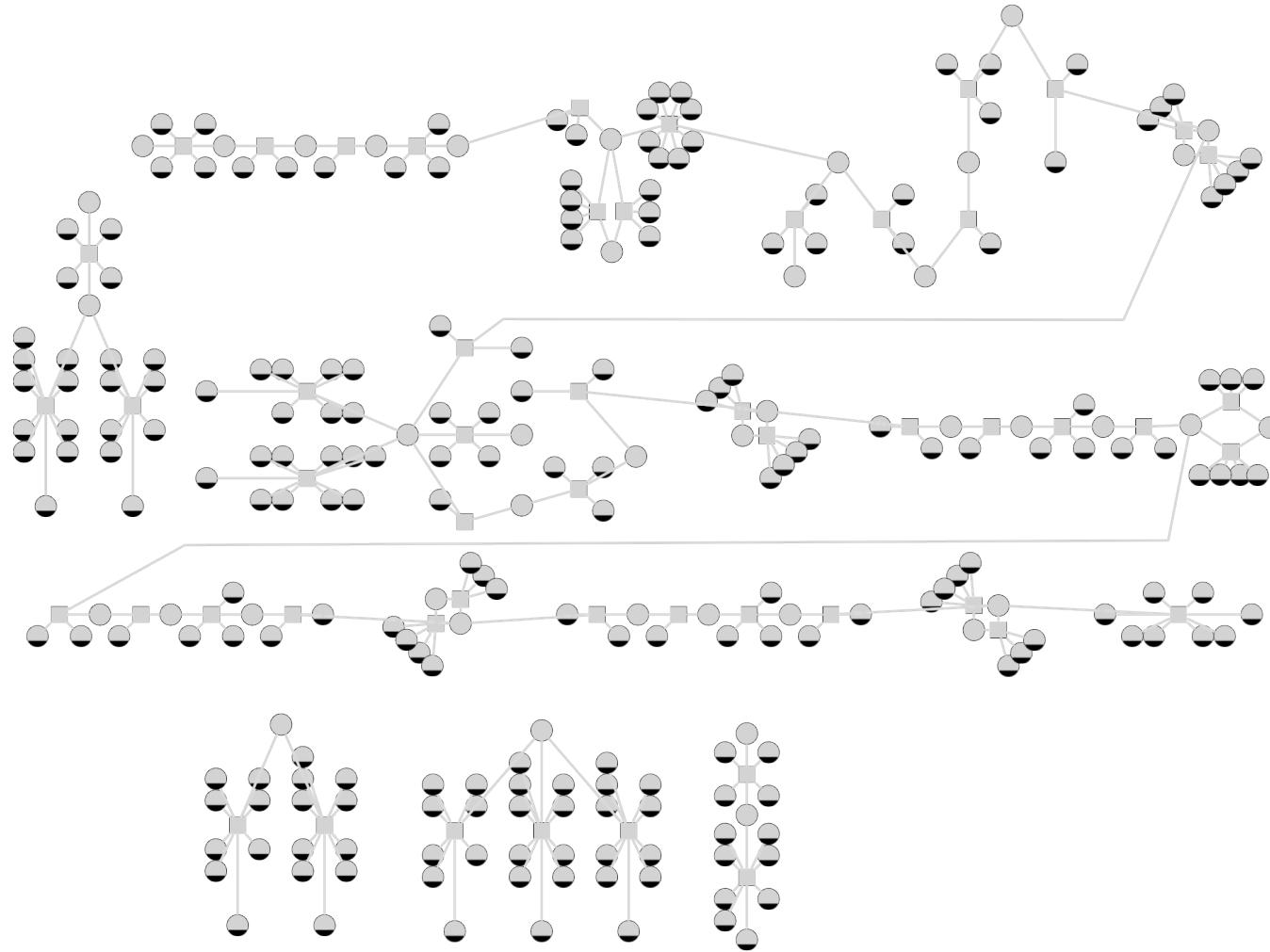


(The figure is produced using the Tulip graph visualization tool.)

Generalization method (simplified)

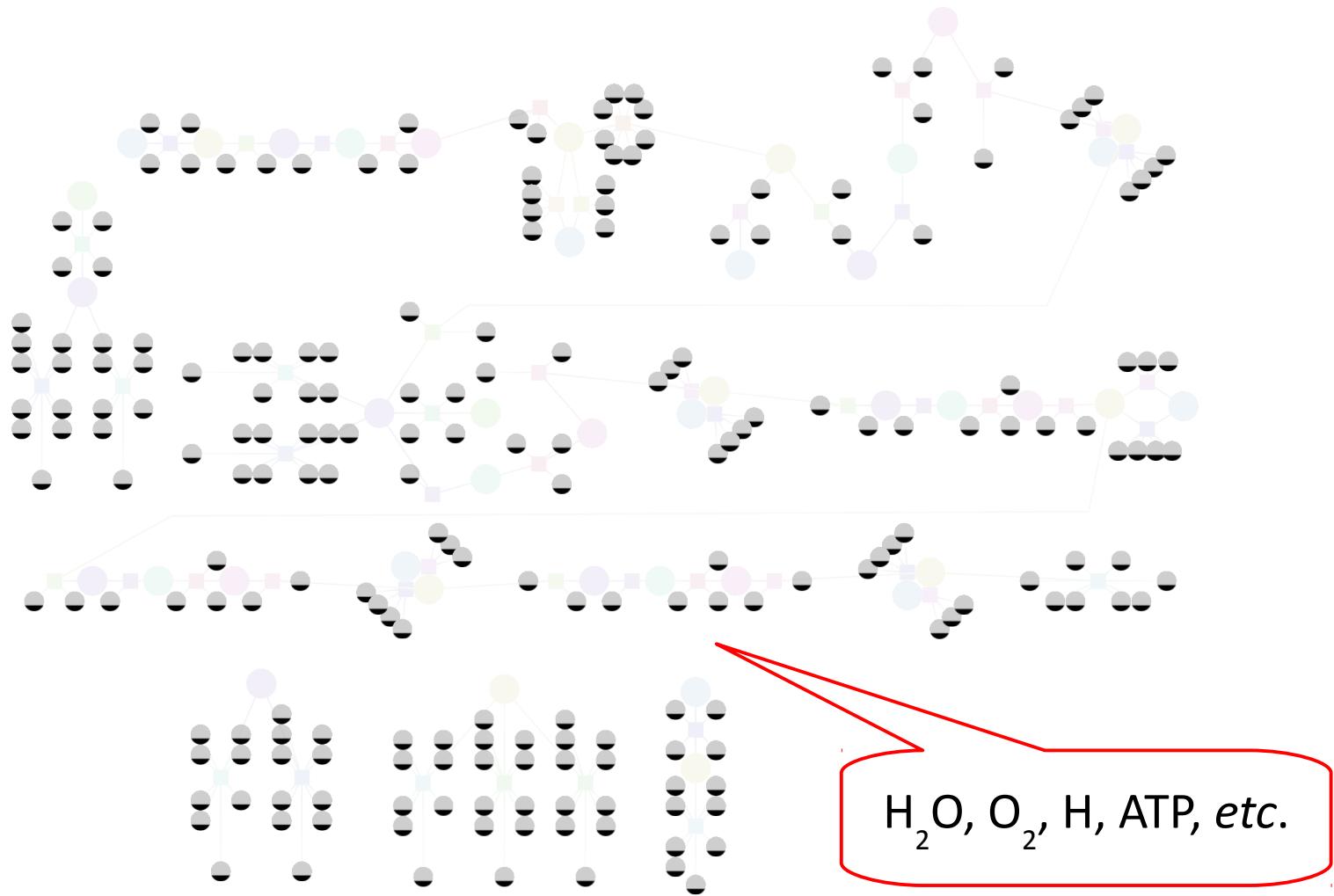


Generalization method: species

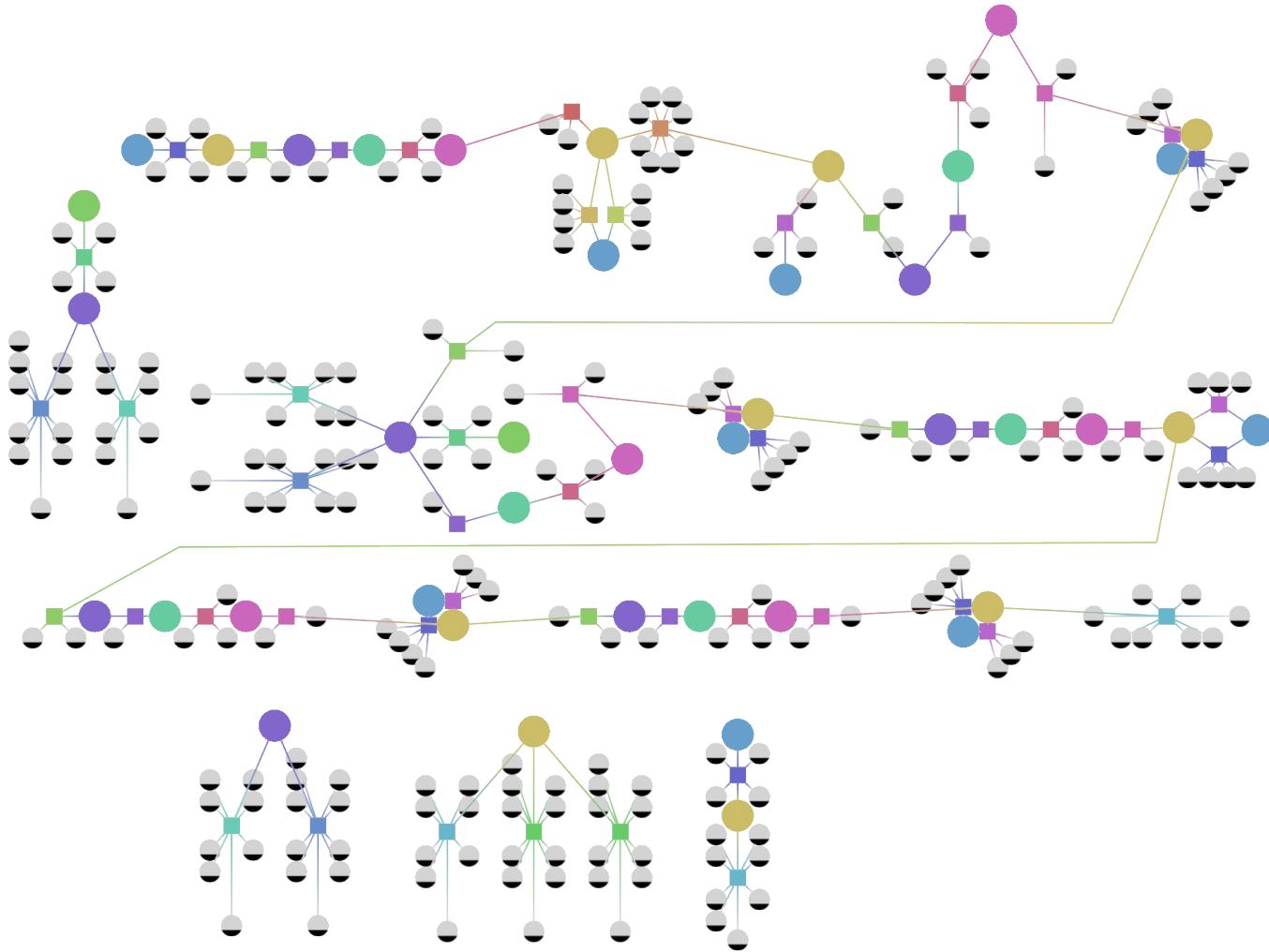


(The figure is produced using the Tulip graph visualization tool.)

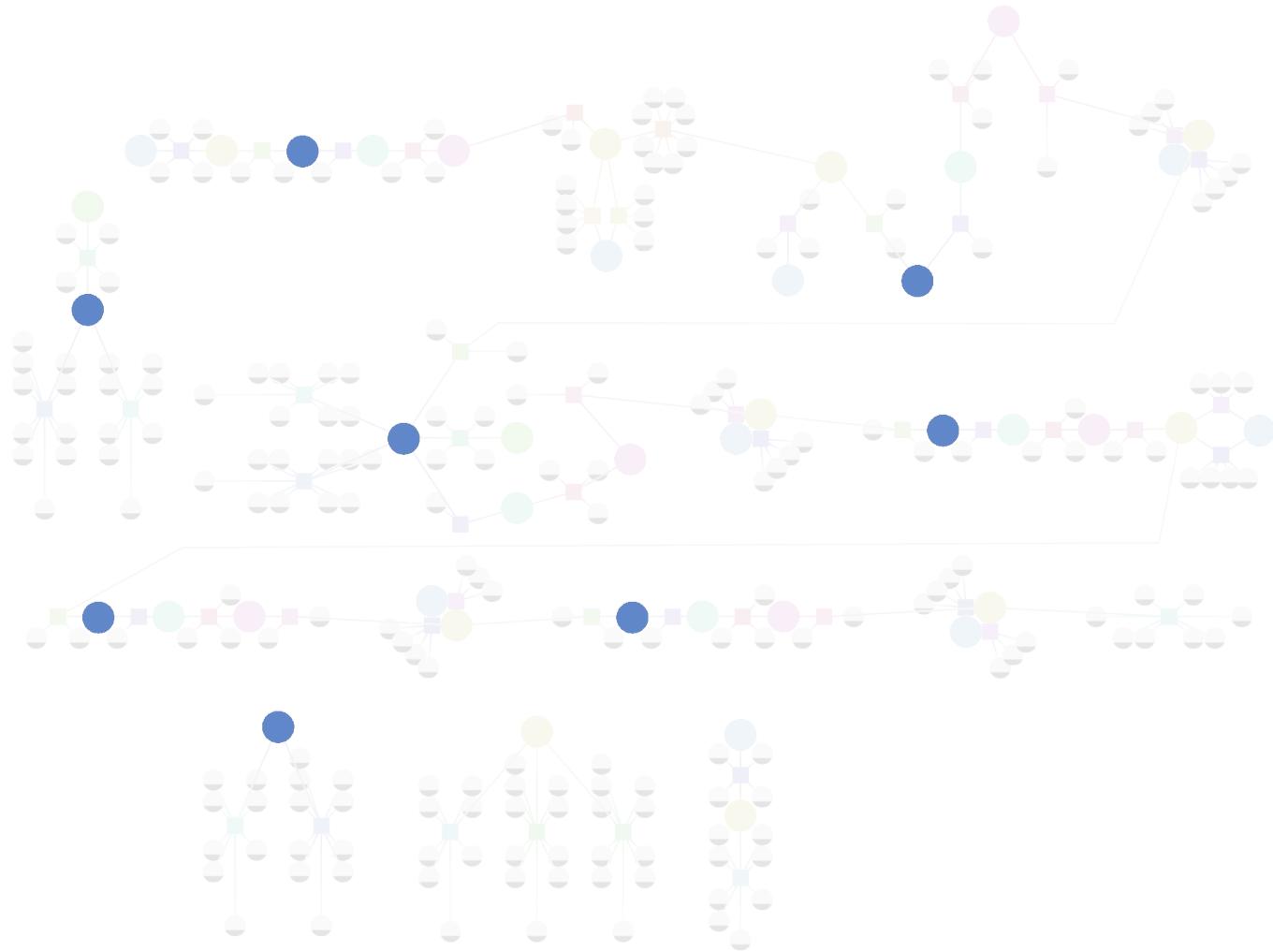
Generalization method: ubiquitous species



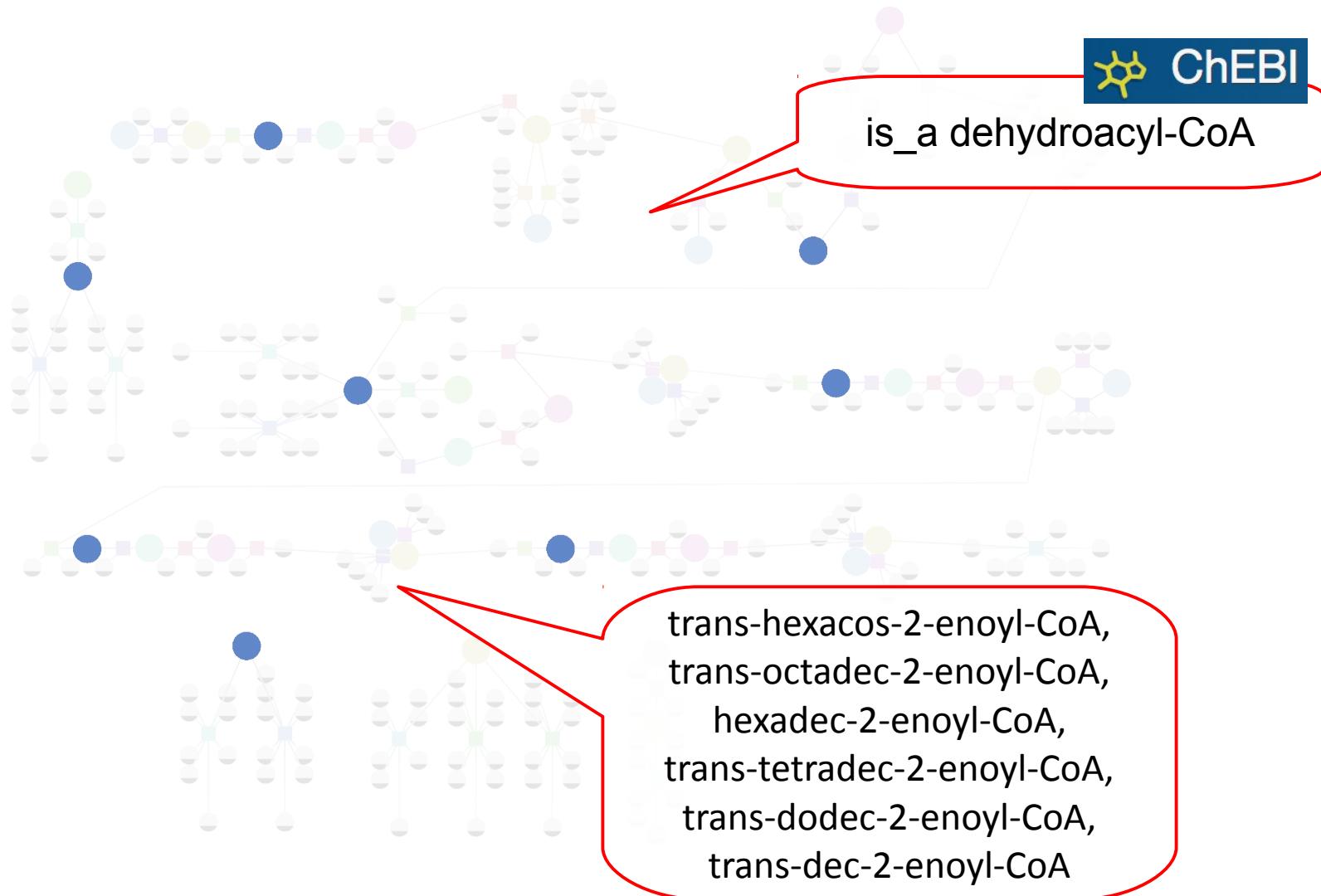
Generalization method: species



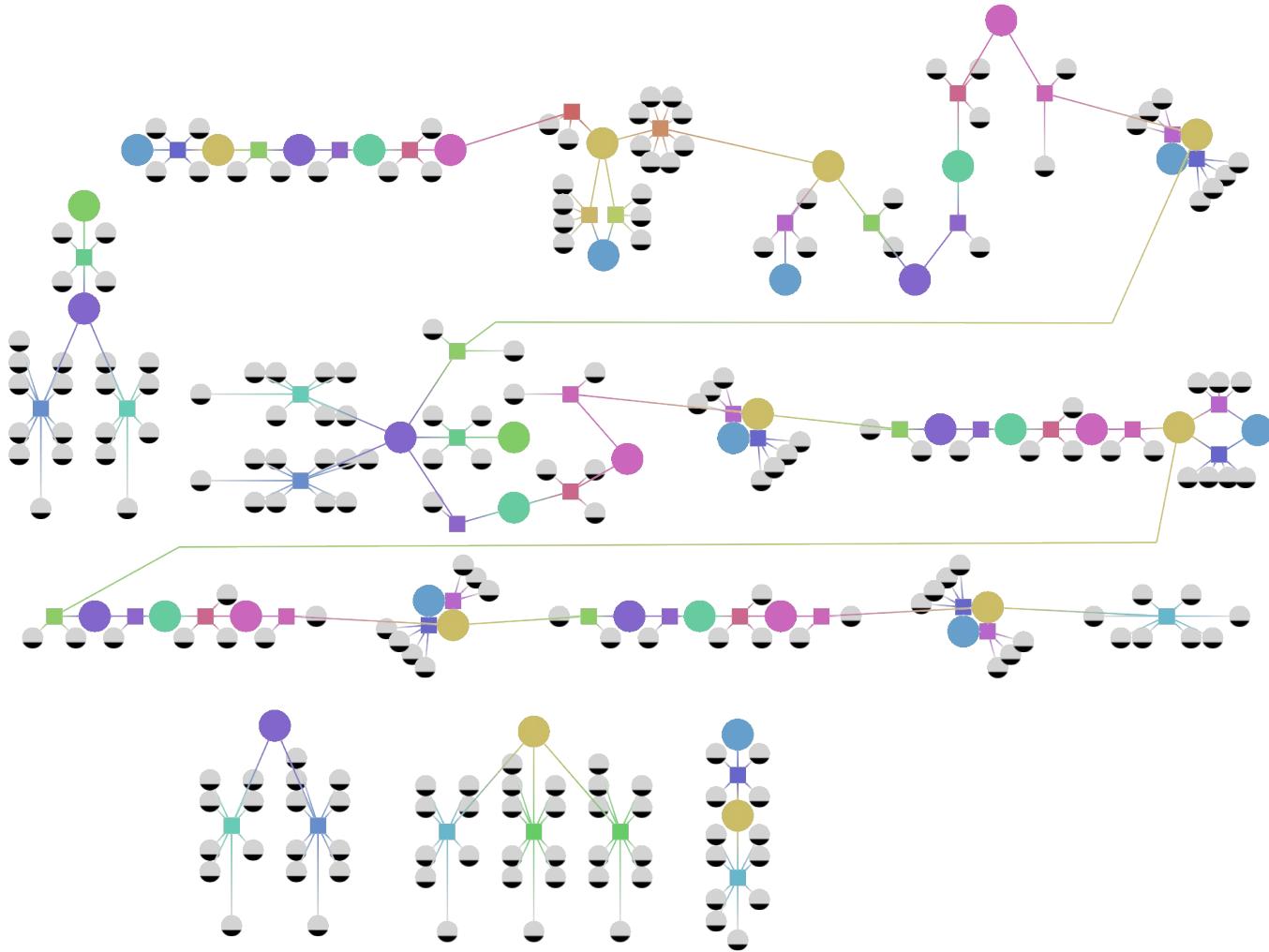
Generalization method: species grouping



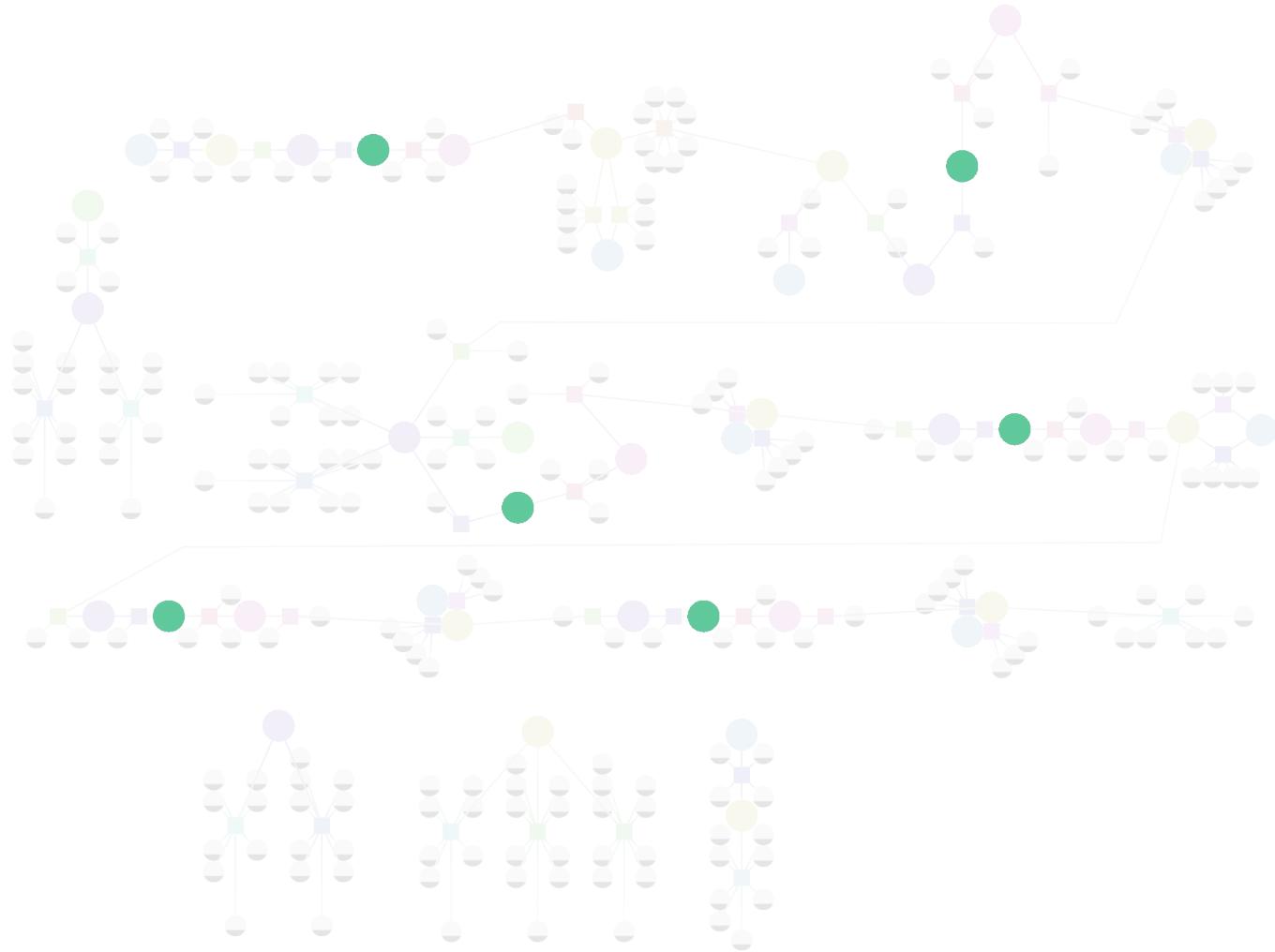
Generalization method: species grouping



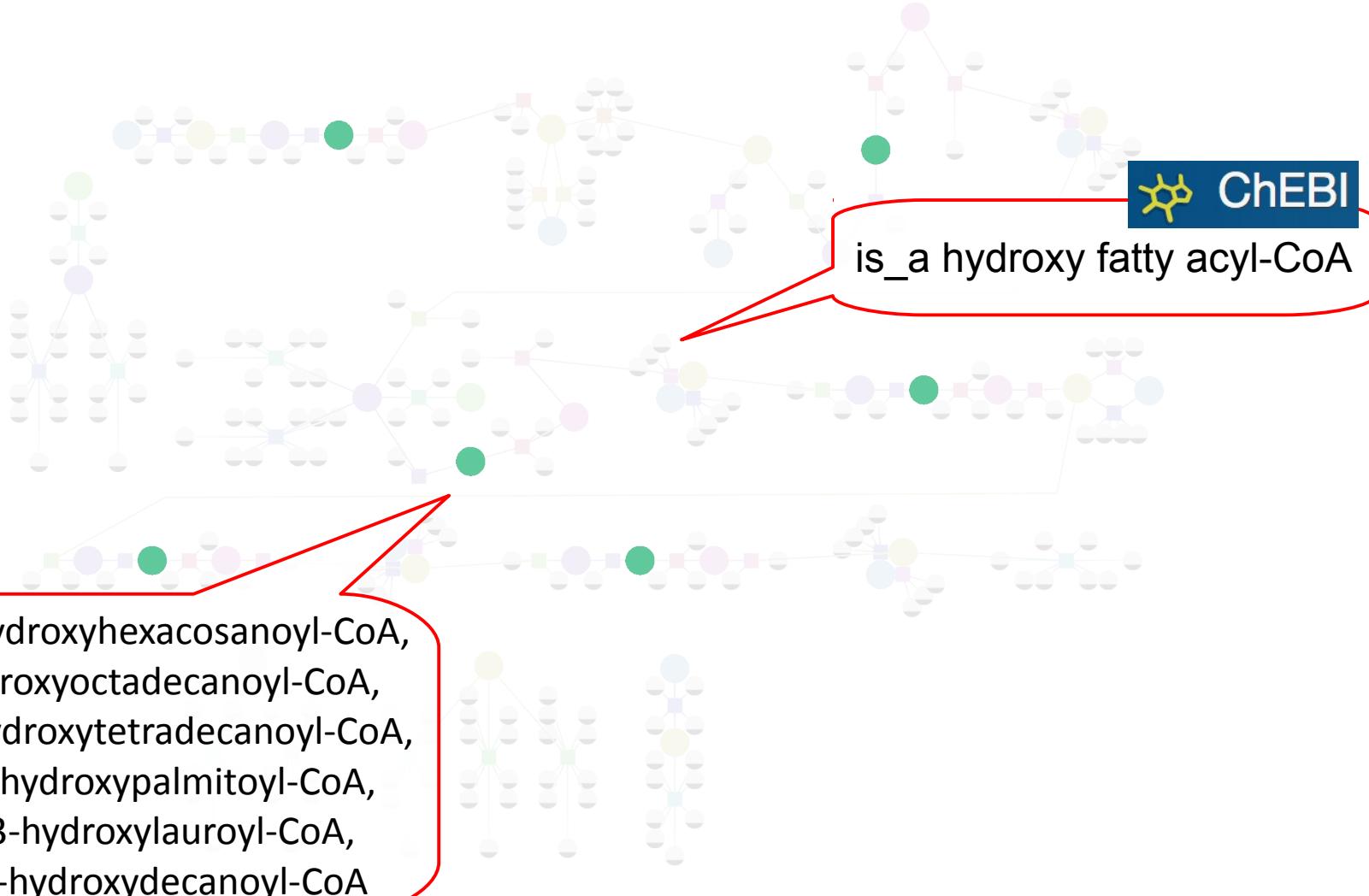
Generalization method: species



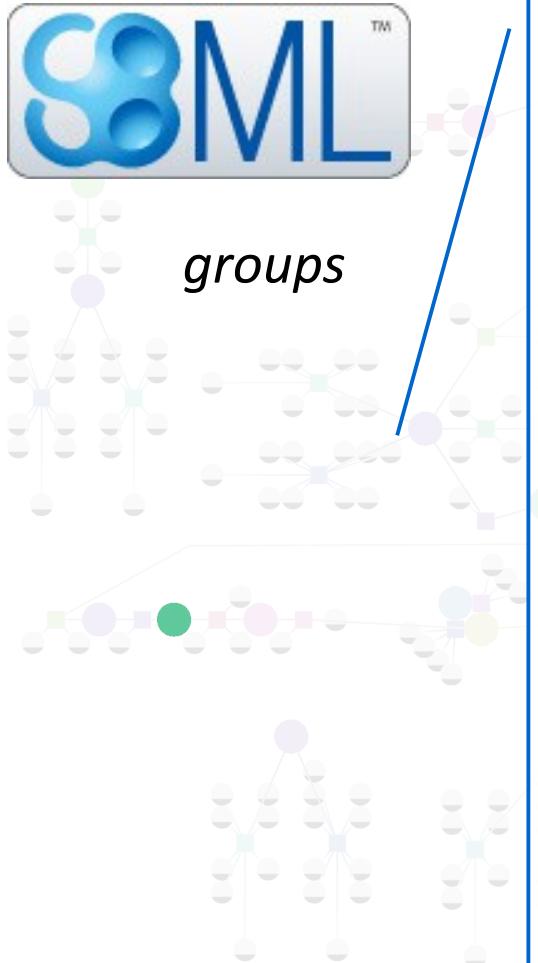
Generalization method: species grouping



Generalization method: species grouping



Representation?



```
<group id="g1" kind="classification" met...
<listOfMembers sboTerm="SBO:0000248"
  <member idRef="s_0048"/>
  <member idRef="s_0054"/>
  ...
  <member idRef="s_0236"/>
</listOfMembers>
<annotation>
  <rdf:RDF xmlns:rdf=...
    <rdf:Description rdf:about="#m_g1">
      <bqbiol:is>
        <rdf:Bag>
          <rdf:li rdf:resource=
            "http://ident../chebi:37671"/>
        ...
      </rdf:Bag>
    </rdf:Description>
  </annotation>

```

Representation?



groups

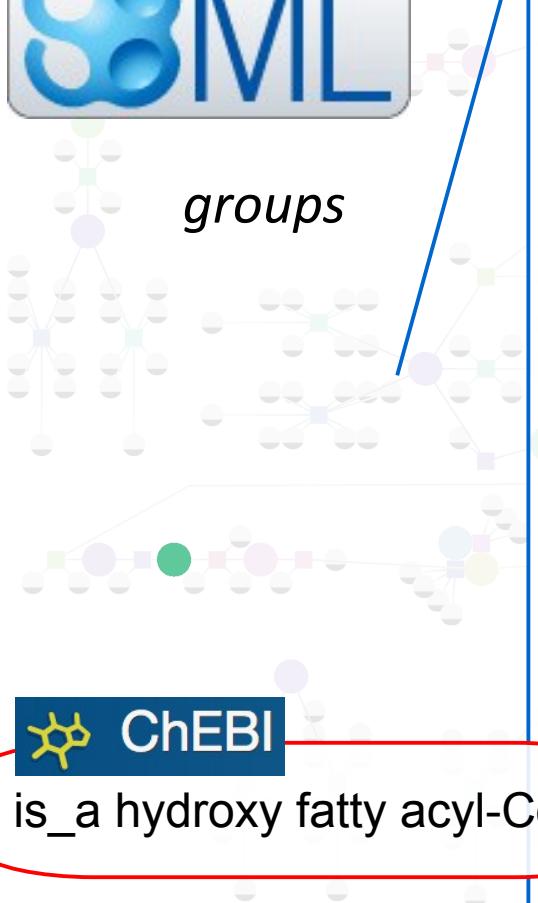
(S)-3-hydroxyhexacosanoyl-CoA,
3-hydroxyoctadecanoyl-CoA,
(S)-3-hydroxytetradecanoyl-CoA,
(S)-3-hydroxypalmitoyl-CoA,
(S)-3-hydroxylauroyl-CoA,
(S)-3-hydroxydecanoyl-CoA

```
<group id="g1" kind="classification" met...
<listOfMembers sboTerm="SBO:0000248"
<member idRef="s_0048"/>
<member idRef="s_0054"/>
...
<member idRef="s_0236"/>
</listOfMembers>
<annotation>
<rdf:RDF xmlns:rdf=...
<rdf:Description rdf:about="#m_g1">
<bqbiol:is>
<rdf:Bag>
<rdf:li rdf:resource=
"http://ident../chebi:37671"/>
...
...
```

Representation?



groups



is_a hydroxy fatty acyl-CoA

```
<group id="g1" kind="classification" met...
<listOfMembers sboTerm="SBO:0000248"
  <member idRef="s_0048"/>
  <member idRef="s_0054"/>
  ...
  <member idRef="s_0236"/>
</listOfMembers>
<annotation>
  <rdf:RDF xmlns:rdf=...
    <rdf:Description rdf:about="#m_g1">
      <bqbiol:is>
        <rdf:Bag>
          <rdf:li rdf:resource=
            "http://ident../chebi:37671"/>
        ...
      </rdf:Bag>
    </rdf:Description>
  </annotation>
</group>
```

Representation?

*Graph
quotient node*

hydroxy
FA-CoA.
(6)

Representation?

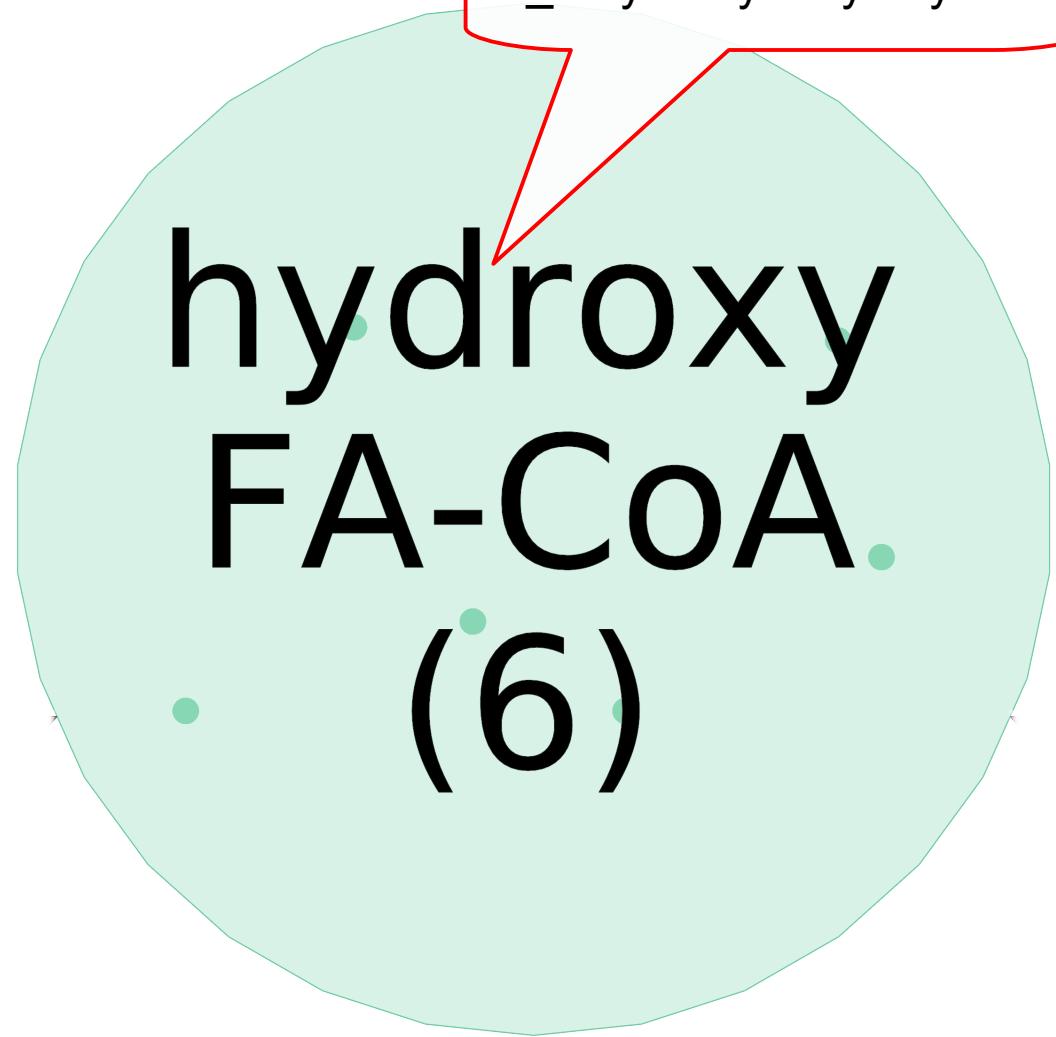
*Graph
quotient node*

(S)-3-hydroxyhexacosanoyl-CoA,
3-hydroxyoctadecanoyl-CoA,
(S)-3-hydroxytetradecanoyl-CoA,
(S)-3-hydroxypalmitoyl-CoA,
(S)-3-hydroxylauroyl-CoA,
(S)-3-hydroxydecanoyl-CoA

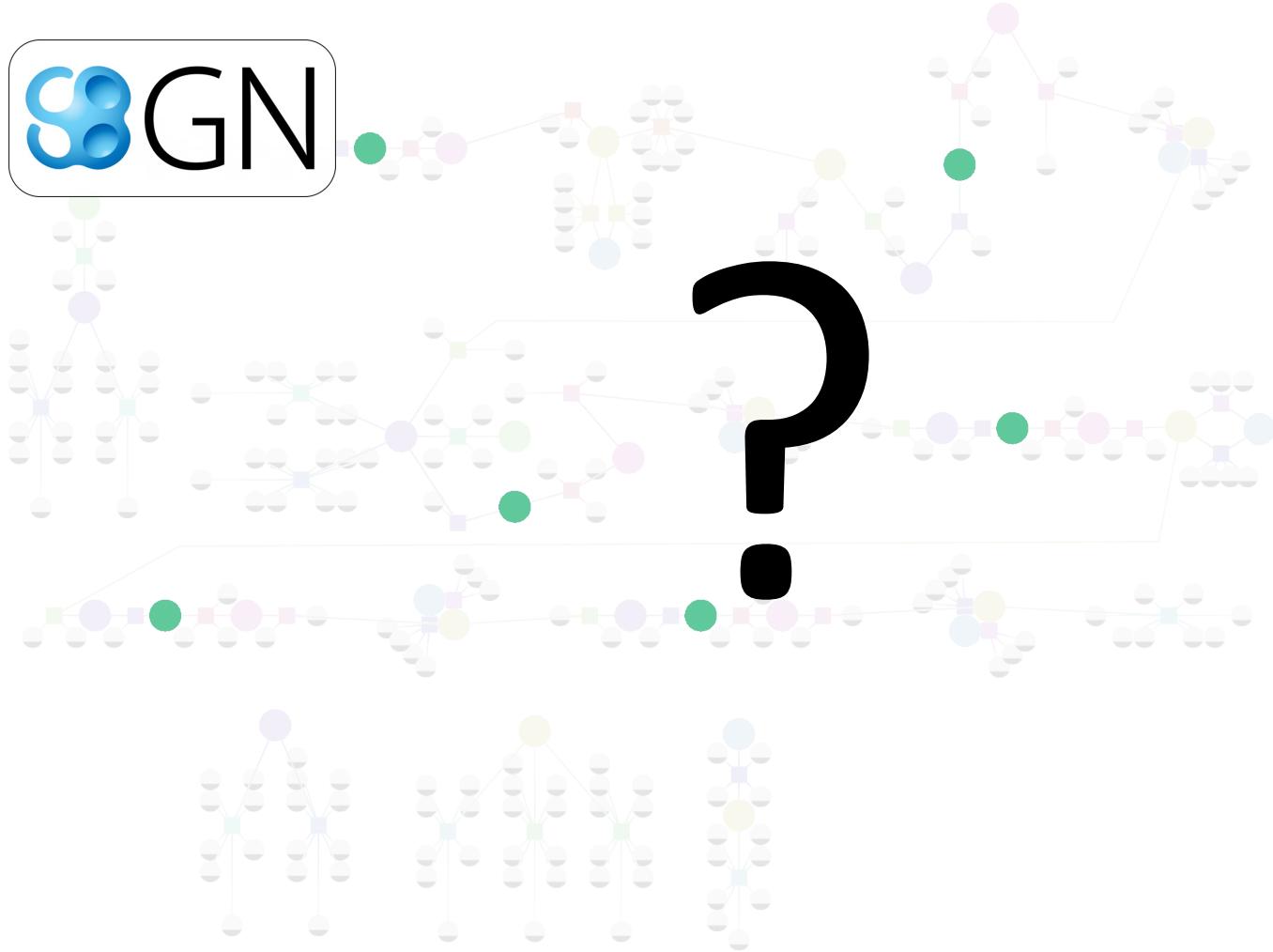
hydroxy
FA-CoA.
(6)

Representation?

*Graph
quotient node*



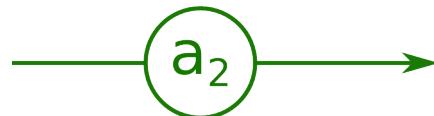
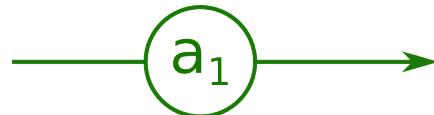
Representation?



Representation?



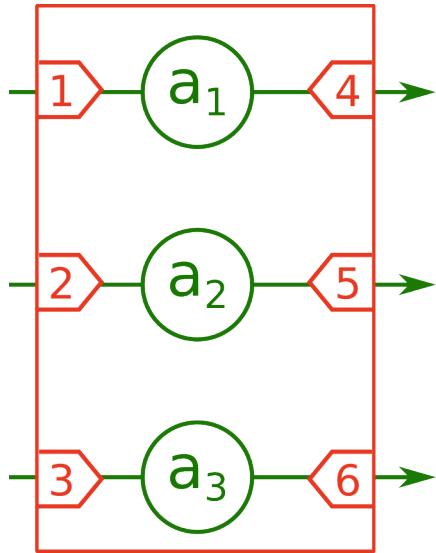
submap



Representation?



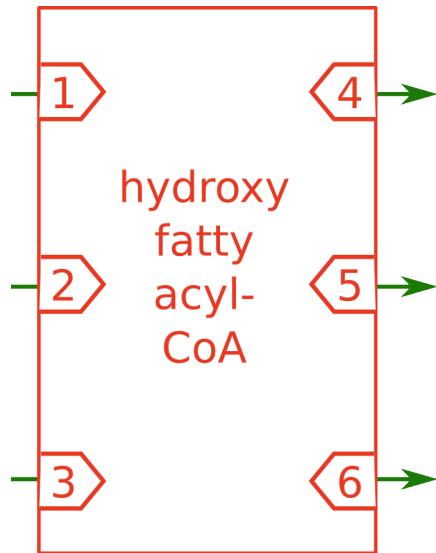
submap



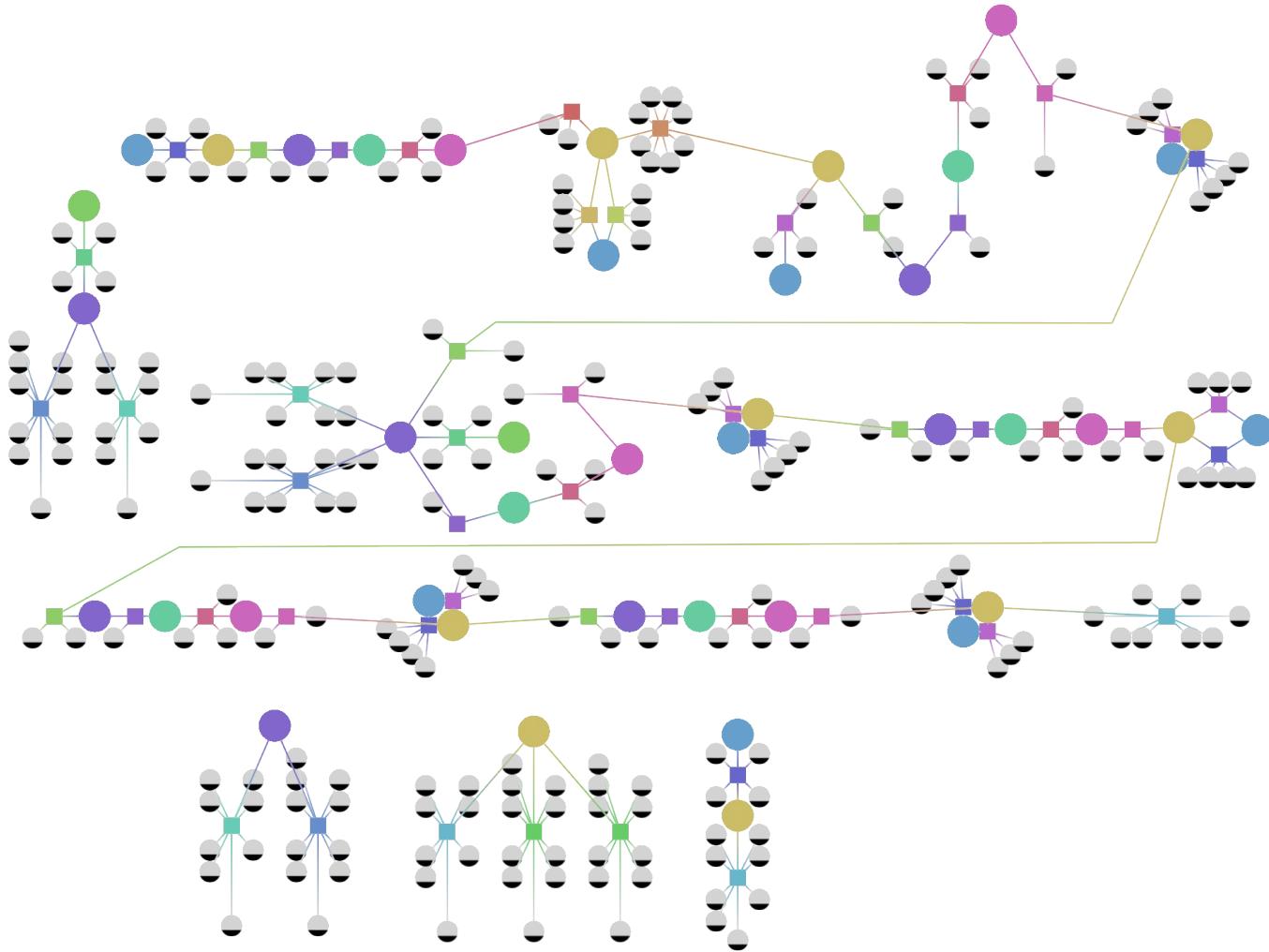
Representation?



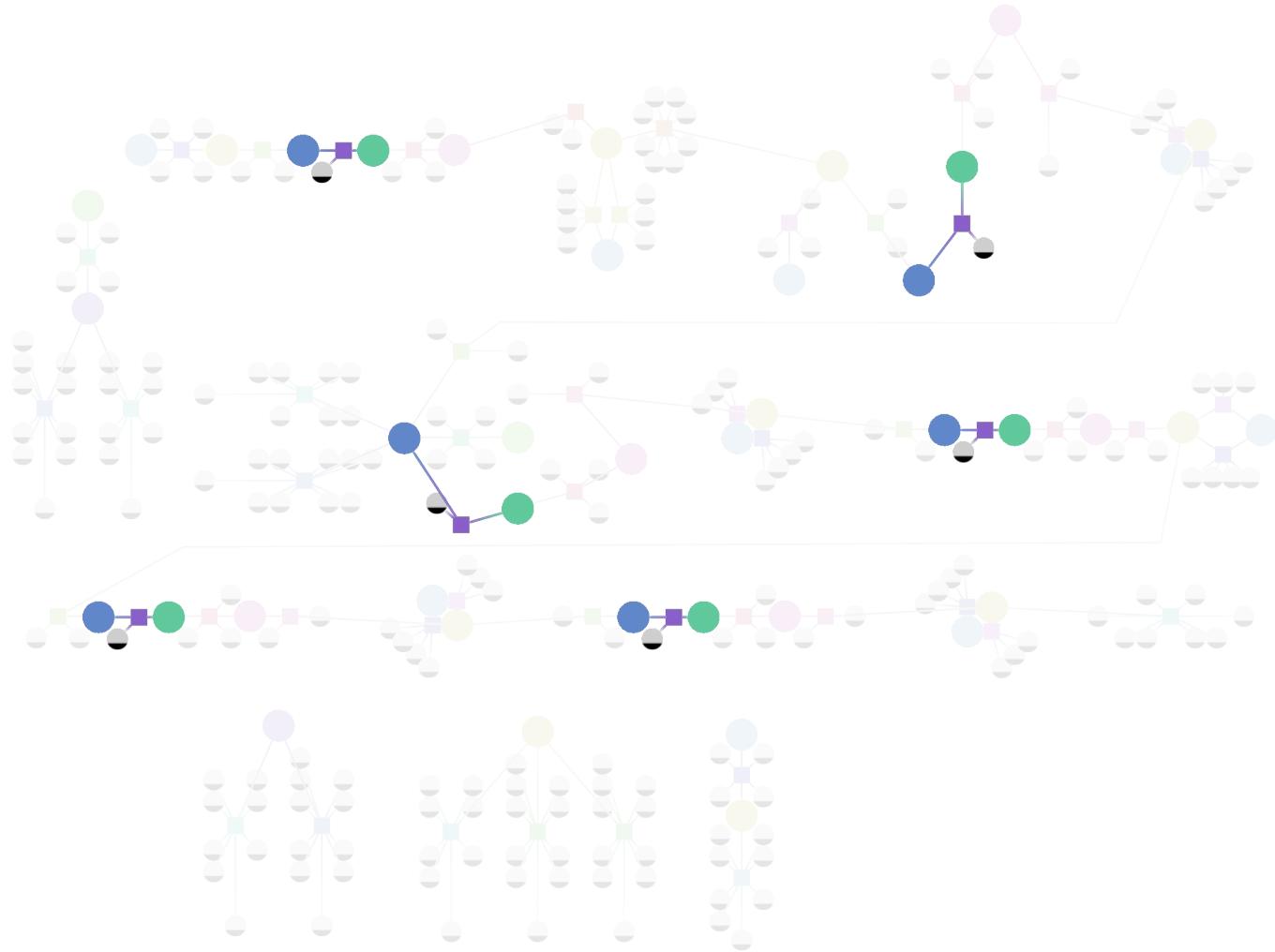
submap



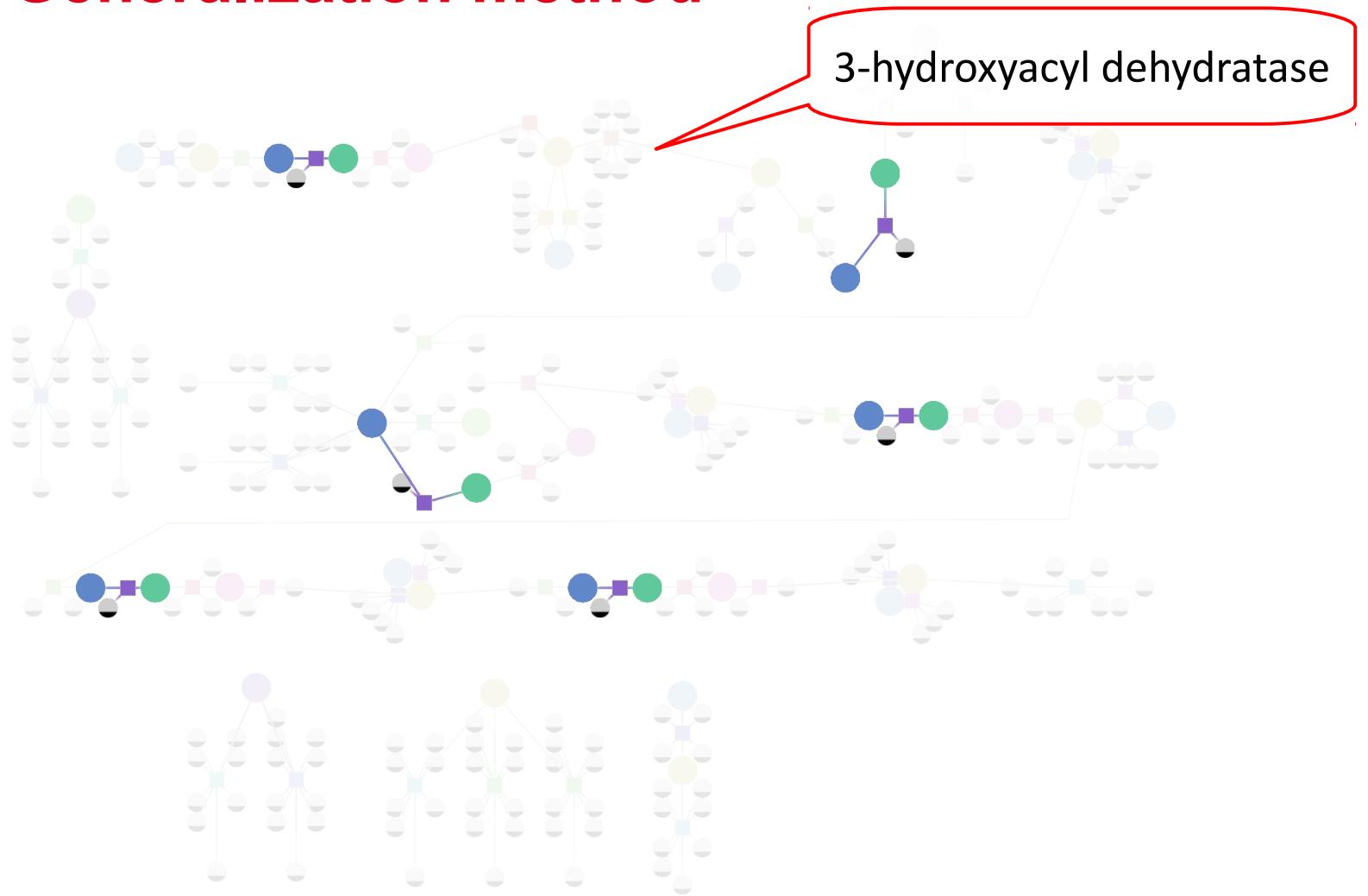
Generalization method



Generalization method



Generalization method



Generalization method

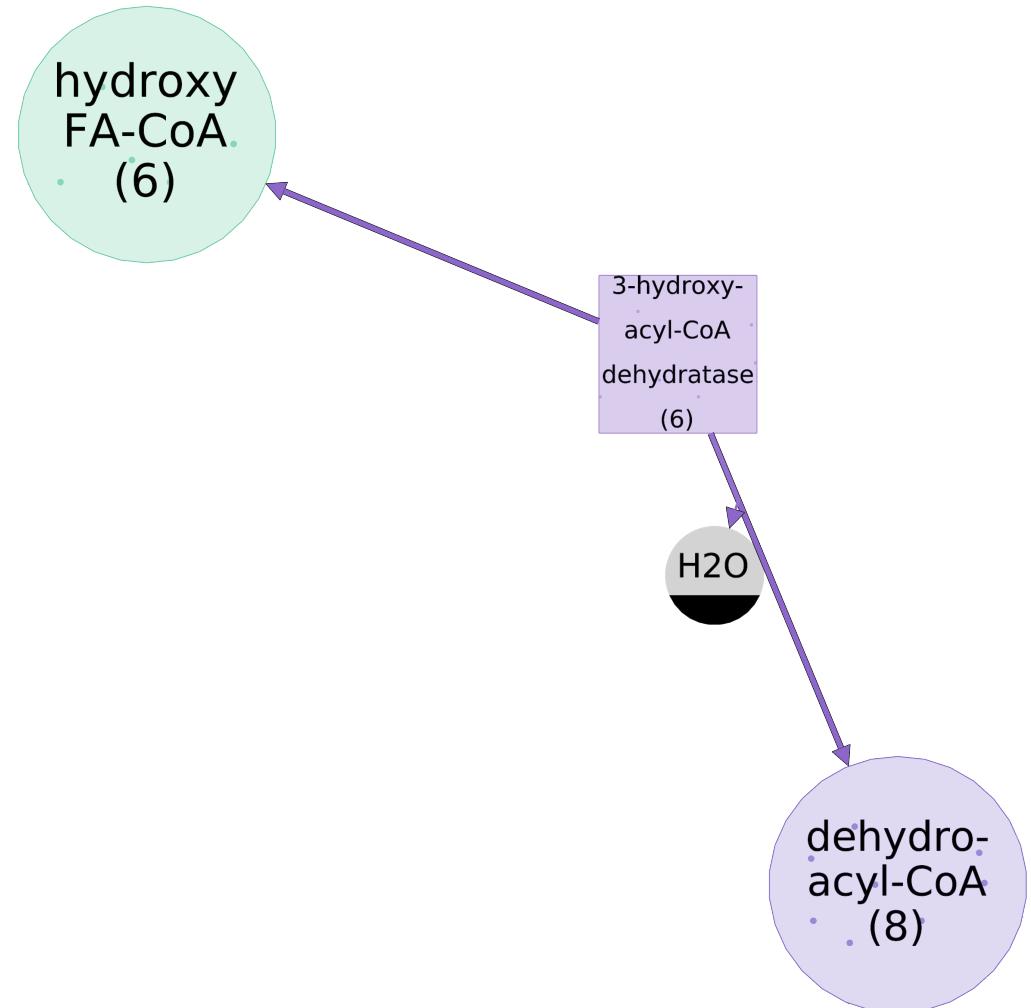


groups

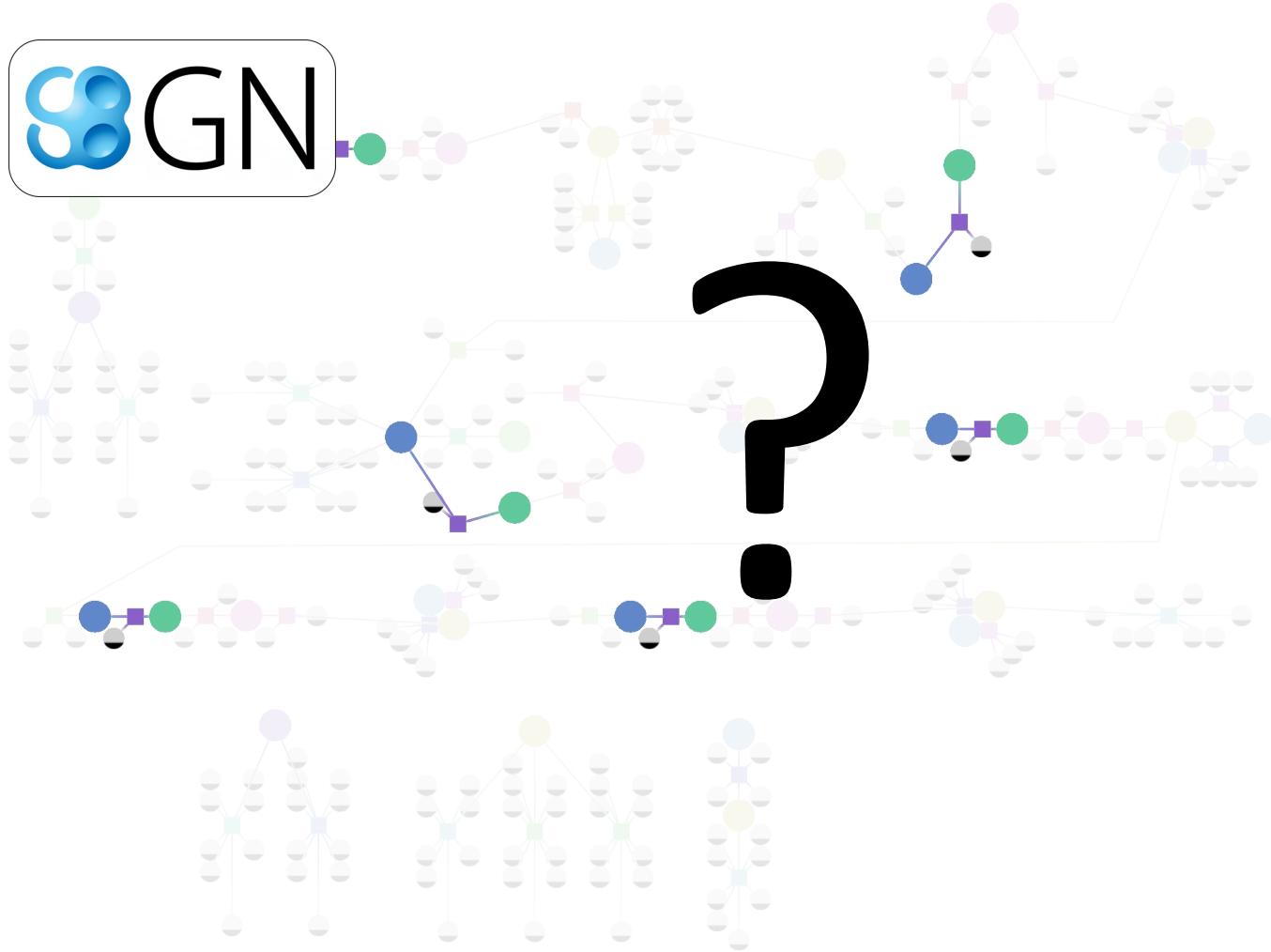
```
<listOfGroups xmlns="http://www.sbml.org/sbml/level2/version1/groups/1.0.0">
  <group id="g1" kind="collection" metaid="1">
    <listOfMembers>
      <member idRef="r_0049"/>
      <member idRef="r_0050"/>
      ...
      <member idRef="r_0054"/>
    </listOfMembers>
  </group>
```

Generalization method

*Graph
quotient nodes*



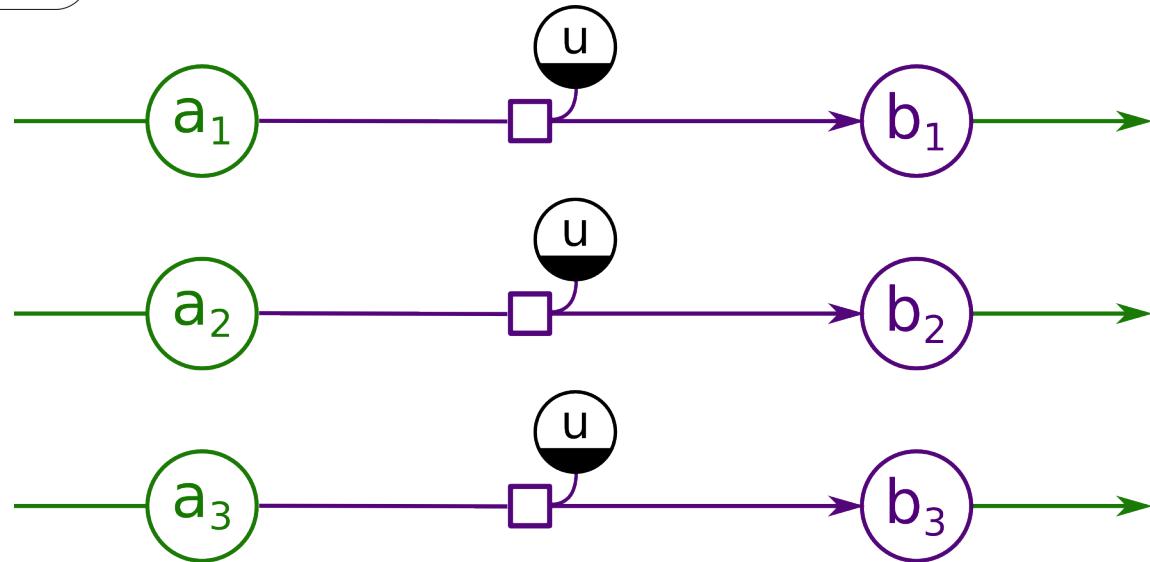
Generalization method



Generalization method



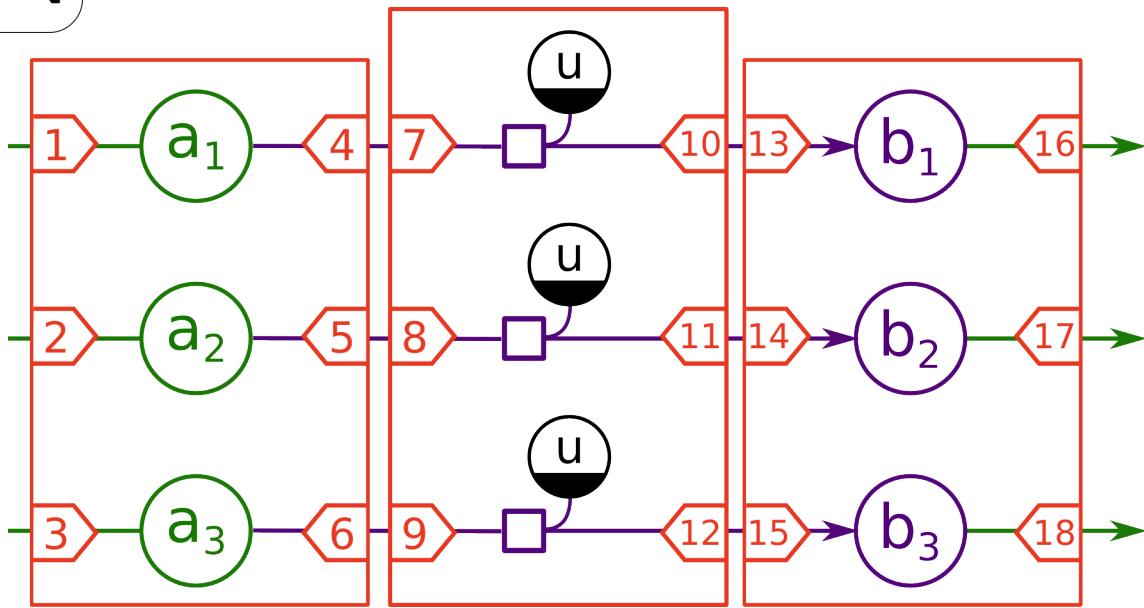
submap



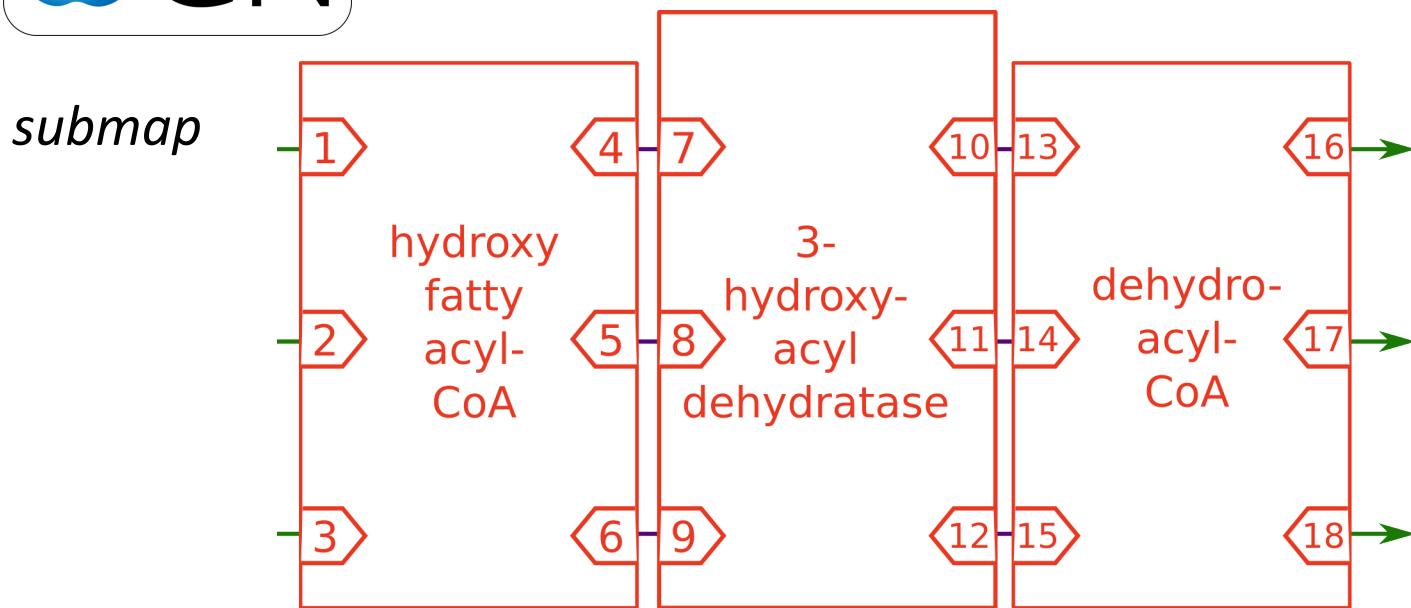
Generalization method



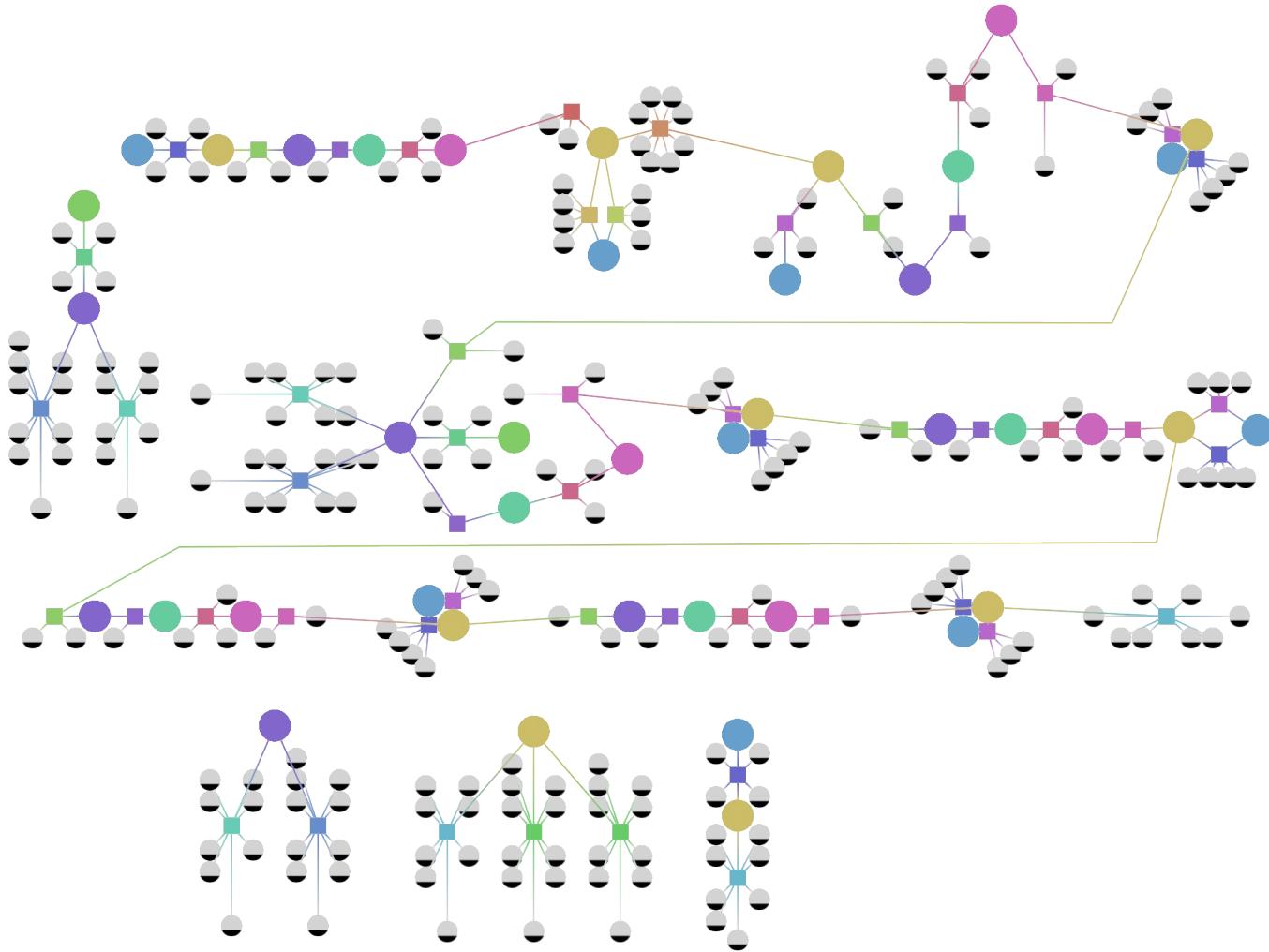
submap



Generalization method



Generalization method



Result

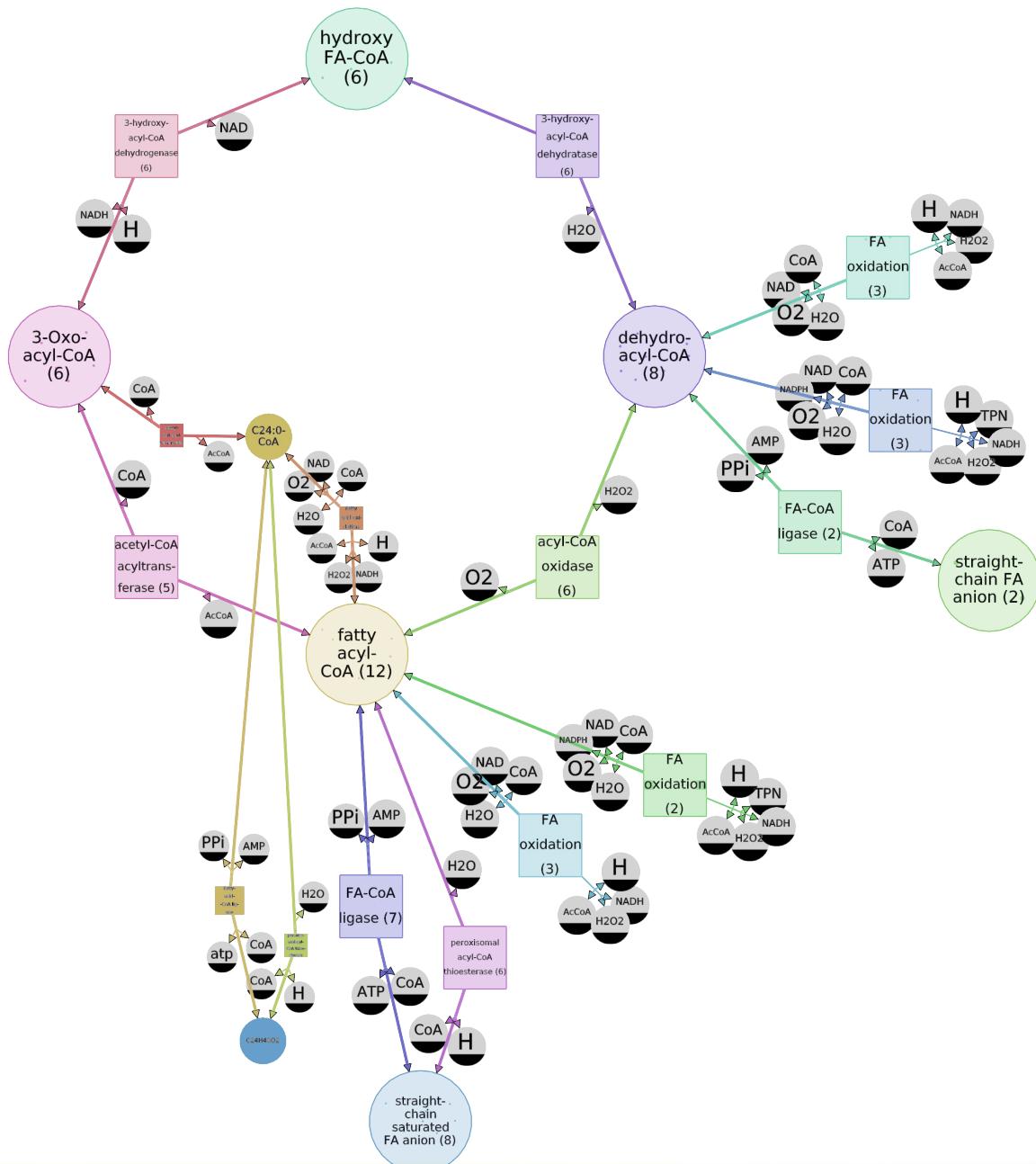


groups

```
<listOfGroups xmlns="http://www.sbml.org/sbml/level2/version1/groups/1.0.0">
  <group id="g1">
    ...
  </group>
  <group id="g2">
    ...
  </group>
  ...
</listOfGroups>
```

Result

Graph quotient nodes



(The figure is produced using the Tulip graph visualization tool.)

Acknowledgements

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Bordeaux, France

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Pascal Durrens
Florian Lajus
Witold Dyrka
Razanne Issa

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and community
*all over the world***

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Nicolas Rodriguez Sarah Keating

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