SEPI_Tryouts_beta3

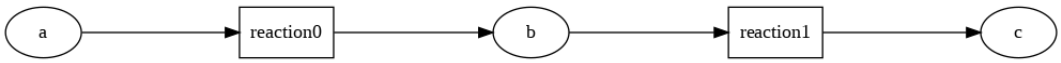
June 27, 2022

[2]:
```
about.
```

[2]:
```
Biocham 4.6.19
Copyright (C) 2003-2020 Inria, EPI Lifeware, Saclay-Île de France, France,
license GNU GPL 2, http://lifeware.inria.fr/biocham4/
```

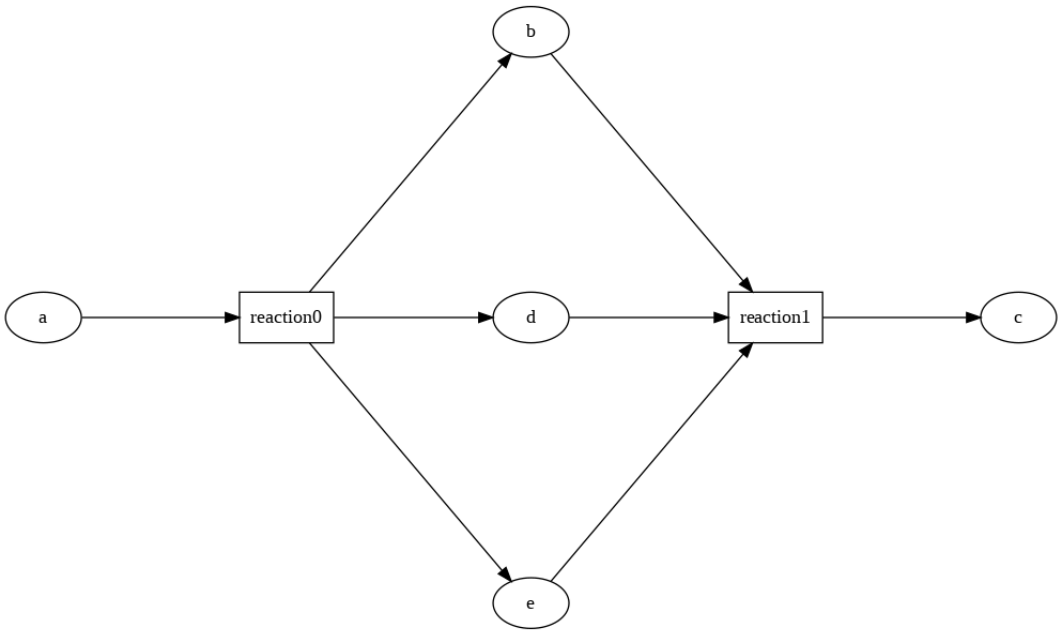
1 0. Playing with SEPI

[3]:
```
clear_model.
new_model(Basic1).
a => b.
b => c.
export_biocham(Basic1.bc).
list_model.
draw_reactions.
```



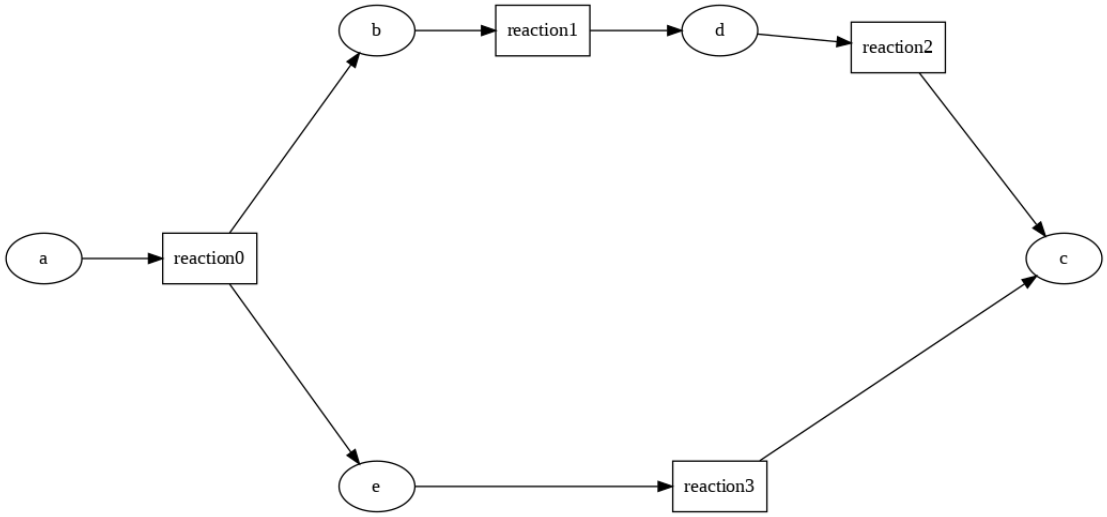
[3]:
```
MA(1) for a=>b.
MA(1) for b=>c.
```

[4]:
```
new_model(Basic2).
a => b+d+e.
b+d+e => c.
export_biocham(Basic2.bc).
list_model.
draw_reactions.
```



[4]:
```
MA(1) for a=>b+d+e.
MA(1) for b+d+e=>c.
```

[5]:
```
new_model(Basic3).
a => b+e.
b => d.
d => c.
e => c.
export_biocham(Basic3.bc).
list_model.
draw_reactions.
```



[5]:
```
MA(1) for a=>b+e.
MA(1) for b=>d.
MA(1) for d=>c.
MA(1) for e=>c.
```

How reductions work on these simple examples : with or without merge restriction

[6]:
```
search_reduction(Basic2.bc, Basic1.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species).
```

[6]:
```
sepi
a -> a
b -> deleted
d -> deleted
e -> b
c -> c
{a => b+d+e} -> {a => b}
{b+d+e => c} -> {b => c}
Number of reductions: 1
```

[7]:
```
search_reduction(Basic2.bc, Basic1.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species, show_support:yes).
```

[7]:
```
sepi
a
e
c
a => b+d+e
b+d+e => c
Number of reductions: 1
```

[16]:
```
search_reduction(Basic2.bc, Basic1.bc, mapping_restriction : [a->a,c->c]).
```

[16]:
```
sepi
a -> a
b -> b
d -> b
e -> b
c -> c
{a => b+d+e} -> {a => b}
{b+d+e => c} -> {b => c}
Number of reductions: 1
```

In the same way, with different paths to the reaction :

[17]:
```
search_reduction(Basic3.bc, Basic1.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species).
```

[17]:
```
sepi
a -> a
b -> deleted
e -> b
d -> deleted
c -> c
{a => b+e} -> {a => b}
{b => d} -> deleted
{d => c} -> {b => c}
{e => c} -> {b => c}
Number of reductions: 1
```

[18]:
```
search_reduction(Basic3.bc, Basic1.bc, mapping_restriction : [a->a,c->c]).
```

[18]:
```
sepi
a -> a
b -> a
e -> b
d -> b
c -> c
{a => b+e} -> deleted
{b => d} -> {a => b}
```

```
{d => c} -> {b => c}
{e => c} -> {b => c}
Number of reductions: 1
```

We can also extract every sepi reduction :

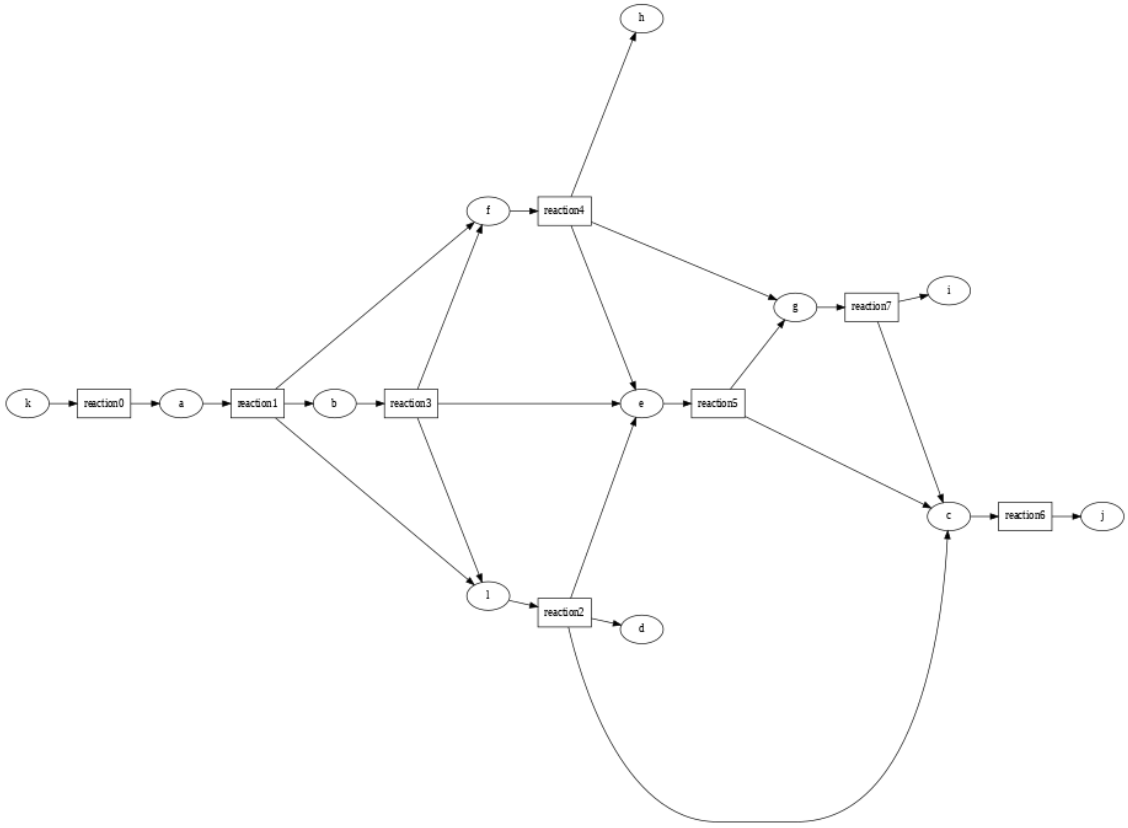
[19]:
```
search_reduction(Basic2.bc, Basic1.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species, all_reductions : yes).
```

[19]:
```
sepi
a -> a
b -> deleted
d -> deleted
e -> b
c -> c
{a => b+d+e} -> {a => b}
{b+d+e => c} -> {b => c}
sepi
a -> a
b -> b
d -> deleted
e -> deleted
c -> c
{a => b+d+e} -> {a => b}
{b+d+e => c} -> {b => c}
sepi
a -> a
b -> deleted
d -> b
e -> deleted
c -> c
{a => b+d+e} -> {a => b}
{b+d+e => c} -> {b => c}
no sepi found
Number of reductions: 3
```

Let's try a more complicated example :

[9]:
```
new_model(Basic4).
k => a.
a => b+f+l.
l => d+e+c.
b => l+e+f.
f => h+e+g.
e => g+c.
c => j.
g => i+c.
export_biocham(Basic4.bc).
```

```
draw_reactions.
```



[10]:
```
search_reduction(Basic4.bc, Basic1.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species).
```

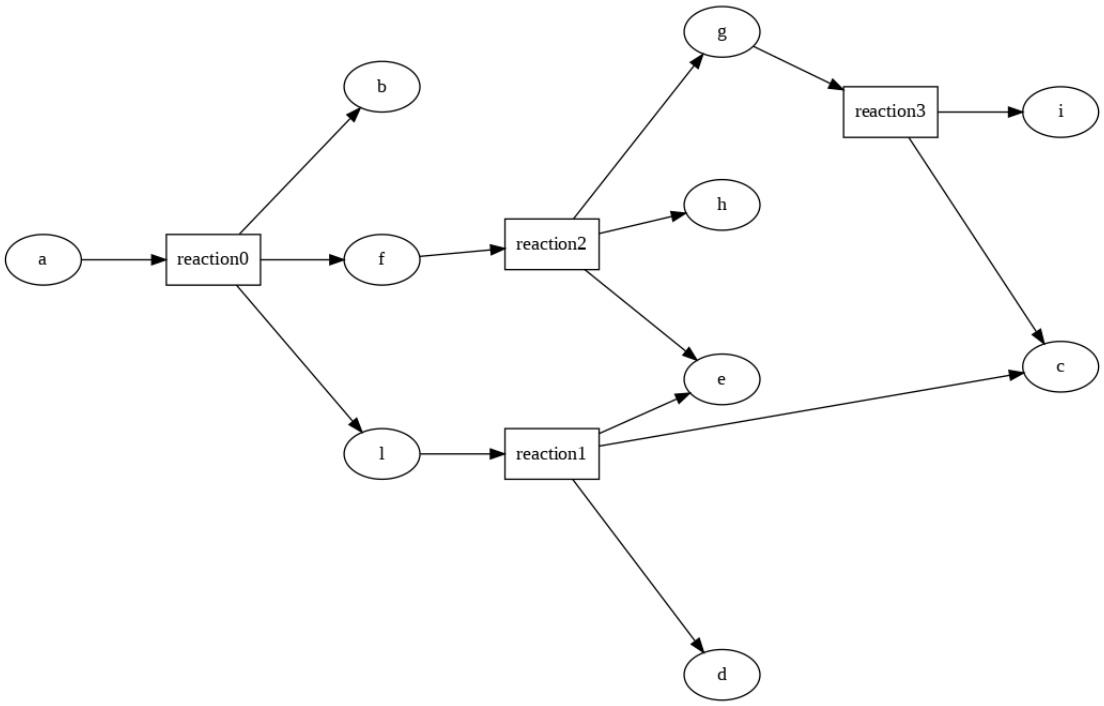
[10]:
```
sepi
k -> deleted
a -> a
b -> deleted
f -> deleted
l -> deleted
c -> c
d -> deleted
e -> deleted
g -> b
h -> deleted
j -> deleted
i -> deleted
{k => a} -> deleted
```

```
{a => b+f+l} -> {a => b}
{l => c+d+e} -> {b => c}
{b => e+f+l} -> deleted
{f => e+g+h} -> {a => b}
{e => c+g} -> deleted
{c => j} -> deleted
{g => c+i} -> {b => c}
Number of reductions: 1
```

[11]:
```
search_reduction(Basic4.bc, Basic1.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species,show_support : yes).
```

[11]:
```
sepi
a
c
g
a => b+f+l
l => c+d+e
f => e+g+h
g => c+i
Number of reductions: 1
```

[12]:
```
new_model.
a => b+f+l.
l => c+d+e.
f => e+g+h.
g => c+i.
draw_reactions.
```



[49]:
```
search_reduction(Basic4.bc, Basic2.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species).
```

[49]:
```
no sepi found
Number of reductions: 0
```

[50]:
```
search_reduction(Basic4.bc, Basic3.bc, mapping_restriction : [a->a,c->c],␣
↪merge_restriction : not_species).
```

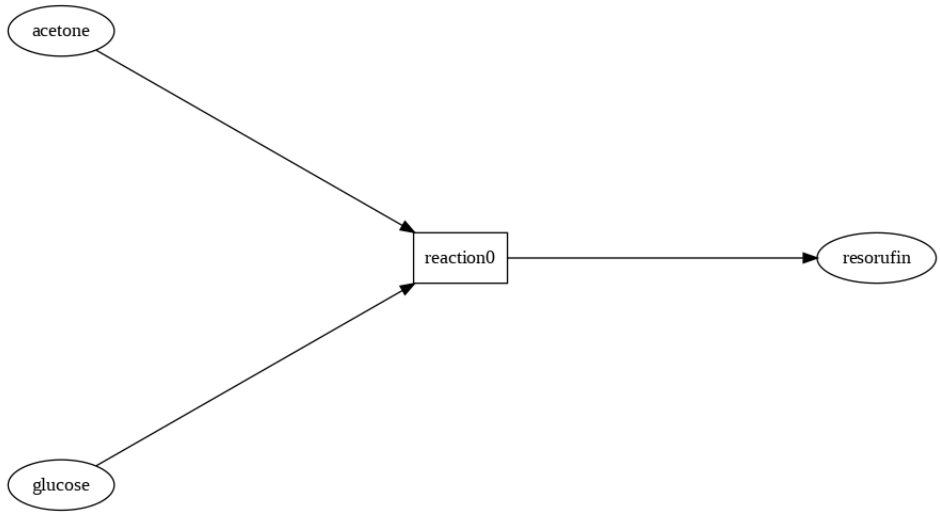
[50]:
```
sepi
k -> deleted
a -> a
b -> deleted
f -> b
l -> e
c -> c
d -> deleted
e -> deleted
g -> d
h -> deleted
j -> deleted
i -> deleted
{k => a} -> deleted
```

```
{a => b+f+l} -> {a => b+e}
{l => c+d+e} -> {e => c}
{b => e+f+l} -> {a => b+e}
{f => e+g+h} -> {b => d}
{e => c+g} -> deleted
{c => j} -> deleted
{g => c+i} -> {d => c}
Number of reductions: 1
```

2 1. First CRNs

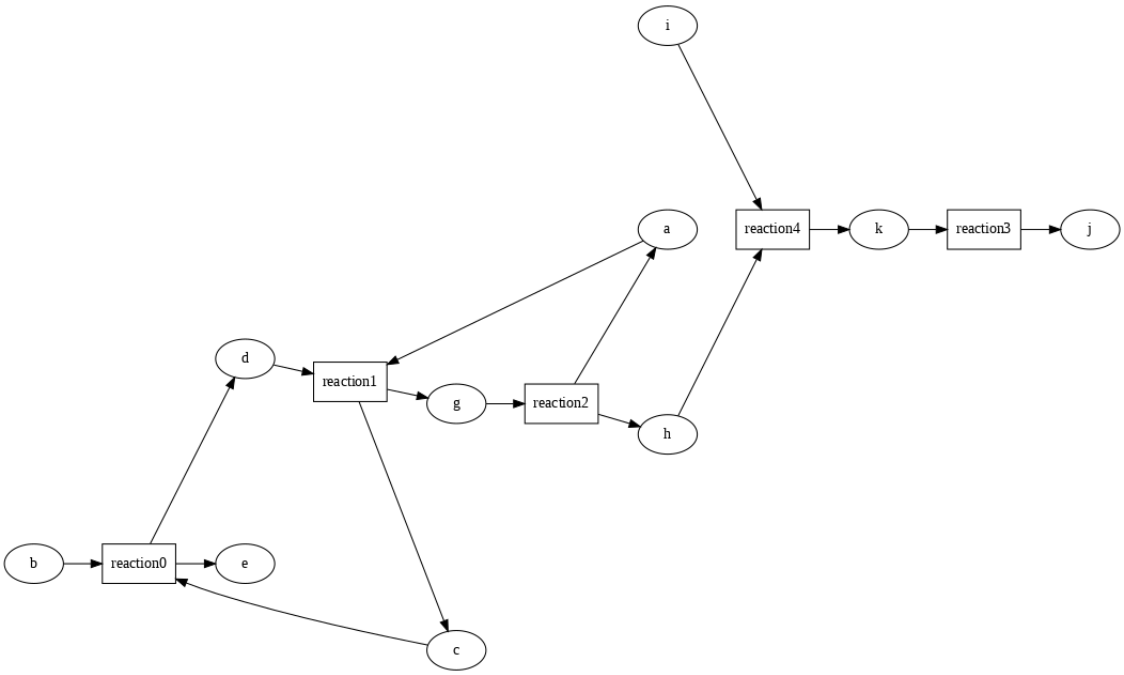
CRNAlexis is the cCRN developped in Alexis' thesis CRNVeryShort is one example of aCRN to concretize : acetone + glucose => resorufin CRNShort is Alexis' CRN but with letters to correspond more to a aCRN CRNLong is an aCRN on which solutions (as SISO*) can be found in BRENDA

[13]:
```
clear_model.
new_model(CRNVeryShort).
acetone+glucose=>resorufin.
export_biocham(CRNVeryShort.bc).
list_model.
draw_reactions.
```



[13]: MA(1) for acetone+glucose=>resorufin.

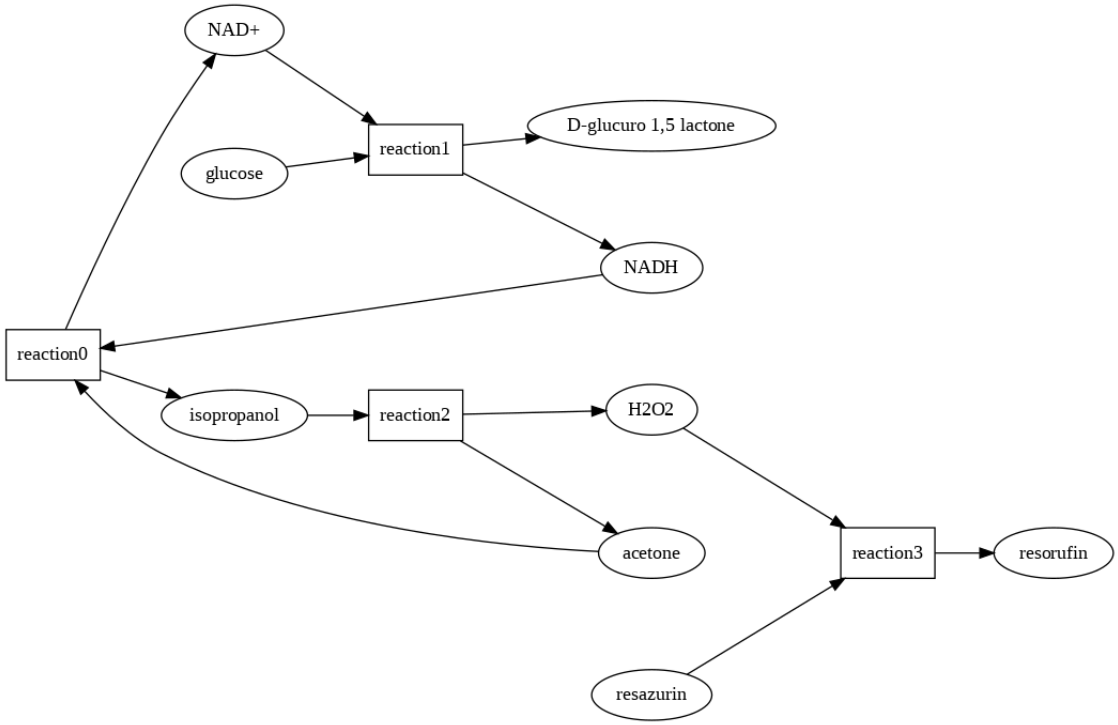
[14]:
```
new_model(CRNlong).
b+c=>d+e.
a+d=>c+g.
g=>a+h.
k=>j.
h+i=>k.
export_biocham(CRNlong.bc).
list_model.
draw_reactions.
```



[14]:
```
MA(1) for b+c=>d+e.
MA(1) for a+d=>c+g.
MA(1) for g=>a+h.
MA(1) for k=>j.
MA(1) for h+i=>k.
```

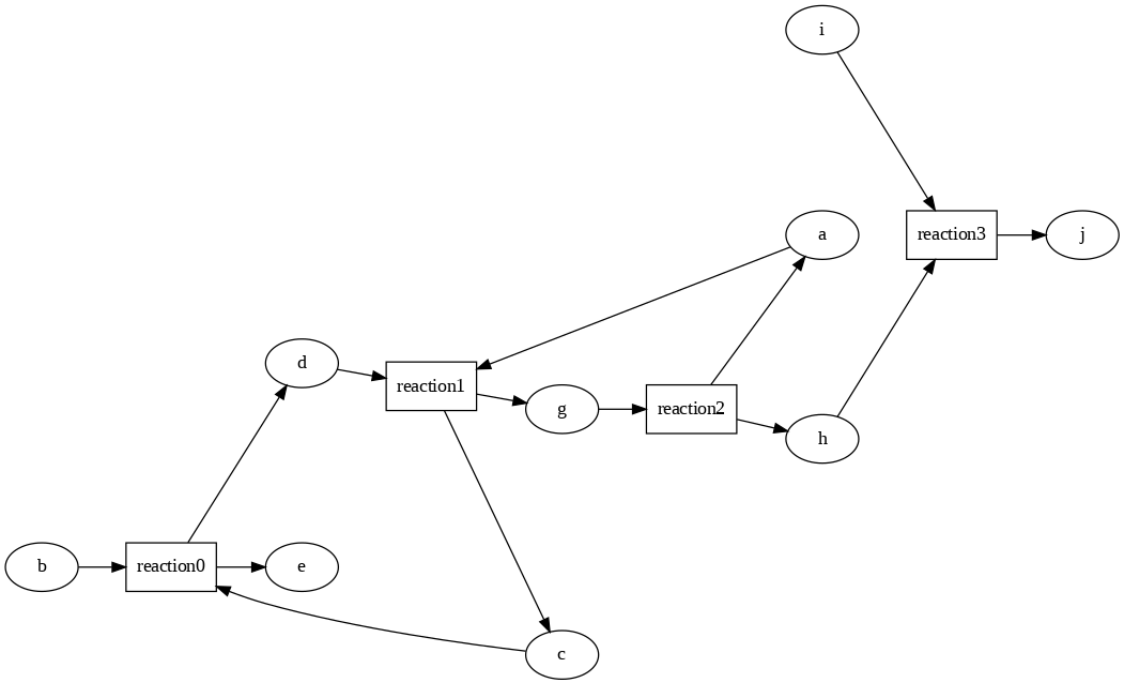
[1]:
```
new_model(CRNAlexis).
NADH+acetone=>'NAD+'+isopropanol.
'NAD+'+glucose=> 'D-glucuro 1,5 lactone' + NADH.
isopropanol=>H2O2+acetone.
H2O2+resazurin=>resorufin.
```

```
export_biocham(CRNAlexis.bc).
list_model.
draw_reactions.
```




```
[1]: MA(1) for NADH+acetone=>'NAD+'+isopropanol.
     MA(1) for 'NAD+'+glucose=>'D-glucuro 1,5 lactone'+NADH.
     MA(1) for isopropanol=>H2O2+acetone.
     MA(1) for H2O2+resazurin=>resorufin.
```

```
[2]: new_model(CRNshort).
     b+c => d+e.
     a+d => c+g.
     g => a+h.
     h+i => j.
     export_biocham(CRNshort.bc).
     list_model.
     draw_reactions.
```

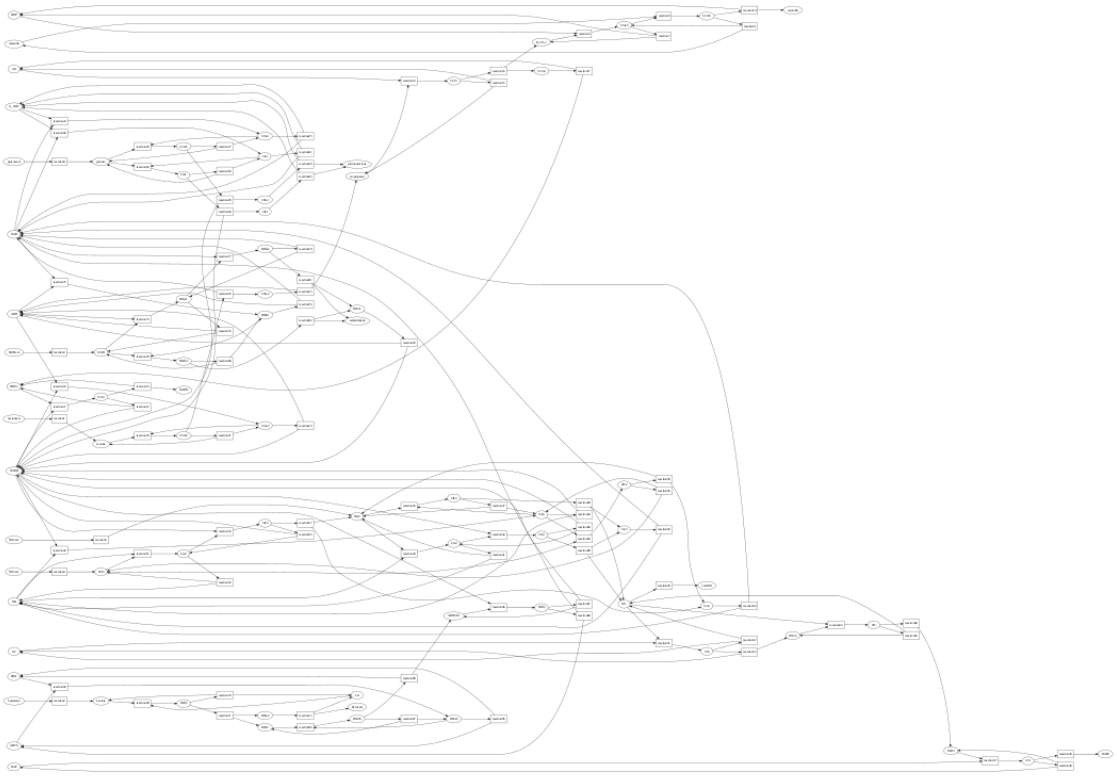


[2]:
```
MA(1) for b+c=>d+e.
MA(1) for a+d=>c+g.
MA(1) for g=>a+h.
MA(1) for h+i=>j.
```

[55]:
```
% list_models.
```

We'll be using the following subset of reactions for the rest of the notebook :

[3]:
```
clear_model.
load(library:examples/modalINF473L/catalog.bc).
export_biocham(Catalog.bc).
draw_reactions.
```



3 2. First SEPI examples on basic CRNs to understand functionnalities

Another example, this time a SEPI with a simple contraction :

[4]:
```
search_reduction(CRNlong.bc, CRNAlexis.bc, mapping_restriction : [a->acetone,␣
↪b->glucose, j->resorufin], merge_restriction : not_species).
```

[4]:
```
sepi
b -> glucose
c -> NAD+
d -> NADH
e -> D-glucuro 1,5 lactone
a -> acetone
g -> isopropanol
h -> H2O2
k -> deleted
j -> resorufin
i -> resazurin
{b+c => d+e} -> {NAD++glucose => D-glucuro 1,5 lactone+NADH}
{a+d => c+g} -> {NADH+acetone => NAD++isopropanol}
{g => a+h} -> {isopropanol => H2O2+acetone}
```

```
{k => j} -> {H2O2+resazurin => resorufin}
{h+i => k} -> {H2O2+resazurin => resorufin}
Number of reductions: 1
```

In the same fashion, we can also see that with the bigger CRNlong :

[30]:
```
search_reduction(CRNlong.bc, CRNVeryShort.bc, mapping_restriction :␣
↪[a->acetone, b->glucose, j->resorufin], merge_restriction : not_species).
```

[30]:
```
sepi
b -> glucose
c -> deleted
d -> deleted
e -> deleted
a -> acetone
g -> deleted
h -> deleted
i -> deleted
k -> deleted
j -> resorufin
{b+c => d+e} -> {acetone+glucose => resorufin}
{a+d => c+g} -> {acetone+glucose => resorufin}
{g => a+h} -> deleted
{h+i => k} -> deleted
{k => j} -> {acetone+glucose => resorufin}
Number of reductions: 1
```

This cell's goal is to show that Alexis' CRN is indeed a SEPI of the VeryShort, meaning it is a solution to it's concretization

[5]:
```
search_reduction(CRNAlexis.bc, CRNVeryShort.bc, mapping_restriction :␣
↪[acetone->acetone, glucose->glucose, resorufin->resorufin],␣
↪merge_restriction : not_species).
```

[5]:
```
sepi
NADH -> deleted
acetone -> acetone
NAD+ -> deleted
isopropanol -> deleted
glucose -> glucose
D-glucuro 1,5 lactone -> deleted
H2O2 -> deleted
resazurin -> deleted
resorufin -> resorufin
{NADH+acetone => NAD++isopropanol} -> {acetone+glucose => resorufin}
{NAD++glucose => D-glucuro 1,5 lactone+NADH} -> {acetone+glucose => resorufin}
{isopropanol => H2O2+acetone} -> deleted
{H2O2+resazurin => resorufin} -> {acetone+glucose => resorufin}
```

```
Number of reductions: 1
```

4 3. Implementation of these principles to search real CRNs in the catalog

Below : SEPI search of a concretization isomorphic to Alexis'

[6]:
```
search_reduction(Catalog.bc, CRNshort.bc, mapping_restriction : [acetone->a,␣
↪glucose->b, resorufin->j], merge_restriction : not_species).
```

[6]:
```
sepi
glucoseext -> deleted
glucose -> b
acetoneext -> deleted
acetone -> a
Lactateext -> deleted
Lactate -> e
EtOHext -> deleted
EtOH -> i
NO3ext -> deleted
NO3 -> deleted
NO2ext -> deleted
NO2 -> deleted
HRP -> deleted
H_2O_2 -> deleted
CCia5 -> deleted
resazurin -> deleted
CCib5 -> deleted
resorufin -> j
HRP2 -> deleted
NADH -> deleted
CCf4 -> deleted
NADN -> deleted
AO -> deleted
isopropanol -> deleted
CCf3 -> deleted
CCio3 -> deleted
ADH -> h
CCia2 -> deleted
CCib2 -> deleted
CCfa2 -> deleted
NAD -> deleted
G_1DH -> deleted
CCia1 -> deleted
CCib1 -> deleted
CCfa1 -> deleted
```

```
gluconolacrone -> deleted
NO -> deleted
volatNO -> deleted
O2 -> deleted
Cf6 -> deleted
NO2b -> deleted
Cf5 -> deleted
N2O3 -> deleted
DAF -> deleted
Cf4 -> deleted
DAFF -> deleted
NR -> deleted
Cia3 -> deleted
Cib3 -> deleted
Cfa3 -> deleted
Cfb3 -> deleted
Cio3 -> deleted
Cia2 -> deleted
Cfa2 -> deleted
Cfb2 -> deleted
Cio2 -> deleted
Cia1 -> deleted
Cib1 -> deleted
Cfa1 -> deleted
ABTSOX -> g
DDf3 -> deleted
ABTS -> deleted
LO -> deleted
DDf2 -> deleted
DDio2 -> deleted
H2O2 -> deleted
Pyruvate -> deleted
DDia1 -> deleted
DDib1 -> deleted
DDfa1 -> deleted
DDfb1 -> deleted
DDio1 -> deleted
acetaldehyde -> deleted
POD -> c
DDia5 -> deleted
DDib5 -> d
{glucoseext => glucose} -> deleted
{acetoneext => acetone} -> deleted
{Lactateext => Lactate} -> deleted
{EtOHext => EtOH} -> deleted
{NO3ext => NO3} -> deleted
{NO2ext => NO2} -> {a+d => c+g}
```

```
{HRP+H_2O_2 => CCia5} -> deleted
{CCia5 => HRP+H_2O_2} -> deleted
{CCia5+resazurin => CCib5} -> {h+i => j}
{CCib5 => CCia5+resazurin} -> {b+c => d+e}
{CCib5 => HRP+resorufin} -> {h+i => j}
{HRP2+NADH => CCf4} -> deleted
{CCf4 => HRP2+NADH} -> deleted
{CCf4 => HRP2+NADN} -> deleted
{AO+isopropanol => CCf3} -> deleted
{CCf3 => AO+isopropanol} -> {a+d => c+g}
{CCf3 => CCio3+H_2O_2} -> deleted
{CCio3 => AO+HRP2} -> deleted
{ADH+NADH => CCia2} -> deleted
{CCia2 => ADH+NADH} -> deleted
{CCia2+acetone => CCib2} -> {a+d => c+g}
{CCib2 => CCia2+acetone} -> {g => a+h}
{CCib2 => CCfa2+NAD} -> deleted
{CCfa2 => ADH+isopropanol} -> deleted
{G_1DH+NAD => CCia1} -> deleted
{CCia1 => G_1DH+NAD} -> {h+i => j}
{CCia1+glucose => CCib1} -> deleted
{CCib1 => CCia1+glucose} -> deleted
{CCib1 => CCfa1+NADH} -> deleted
{CCfa1 => G_1DH+gluconolacrone} -> deleted
{NO => volatNO} -> deleted
{NO+O2 => Cf6} -> deleted
{Cf6 => NO+O2} -> deleted
{Cf6 => NO2b+O2} -> deleted
{NO+NO2b => Cf5} -> deleted
{Cf5 => NO+NO2b} -> deleted
{Cf5 => N2O3} -> deleted
{DAF+N2O3 => Cf4} -> deleted
{Cf4 => DAF+N2O3} -> deleted
{Cf4 => DAFF} -> deleted
{NO2+NR => Cia3} -> deleted
{Cia3 => NO2+NR} -> deleted
{NADH+NR => Cib3} -> deleted
{Cib3 => NADH+NR} -> deleted
{Cia3+NADH => Cfa3} -> deleted
{Cib3+NO2 => Cfb3} -> {h+i => j}
{Cfa3 => Cia3+NADH} -> deleted
{Cfb3 => Cib3+NO2} -> deleted
{Cfa3 => Cio3+NO} -> deleted
{Cfb3 => Cio3+NO} -> deleted
{Cio3 => NAD+NR} -> deleted
{NO3+NR => Cia2} -> deleted
{Cia2 => NO3+NR} -> deleted
```

```
{Cia2+NADH => Cfa2} -> deleted
{Cib3+NO3 => Cfb2} -> deleted
{Cfa2 => Cia2+NADH} -> deleted
{Cfb2 => Cib3+NO3} -> deleted
{Cfa2 => Cio2+NO2} -> deleted
{Cfb2 => Cio2+NO2} -> deleted
{Cio2 => NAD+NR} -> deleted
{G_1DH+NAD => Cia1} -> deleted
{Cia1 => G_1DH+NAD} -> deleted
{Cia1+glucose => Cib1} -> {b+c => d+e}
{Cib1 => Cia1+glucose} -> deleted
{Cib1 => Cfa1+NADH} -> {b+c => d+e}
{Cfa1 => G_1DH+gluconolacrone} -> deleted
{ABTSOX+NADH => DDf3} -> {g => a+h}
{DDf3 => ABTSOX+NADH} -> deleted
{DDf3 => ABTS+NAD} -> {b+c => d+e}
{LO+Lactate => DDf2} -> deleted
{DDf2 => LO+Lactate} -> {b+c => d+e}
{DDf2 => DDio2+H2O2} -> deleted
{DDio2 => LO+Pyruvate} -> deleted
{ADH+EtOH => DDia1} -> deleted
{DDia1 => ADH+EtOH} -> deleted
{ADH+NAD => DDib1} -> {h+i => j}
{DDib1 => ADH+NAD} -> {g => a+h}
{DDia1+NAD => DDfa1} -> deleted
{DDib1+EtOH => DDfb1} -> {h+i => j}
{DDfa1 => DDia1+NAD} -> deleted
{DDfb1 => DDib1+EtOH} -> deleted
{DDfa1 => DDio1+acetaldehyde} -> deleted
{DDfb1 => DDio1+acetaldehyde} -> {g => a+h}
{DDio1 => ADH+NADH} -> deleted
{ABTS+POD => DDia5} -> {b+c => d+e}
{DDia5 => ABTS+POD} -> deleted
{DDia5+H2O2 => DDib5} -> {b+c => d+e}
{DDib5 => DDia5+H2O2} -> deleted
{DDib5 => ABTSOX+POD} -> {a+d => c+g}
Number of reductions: 1
```

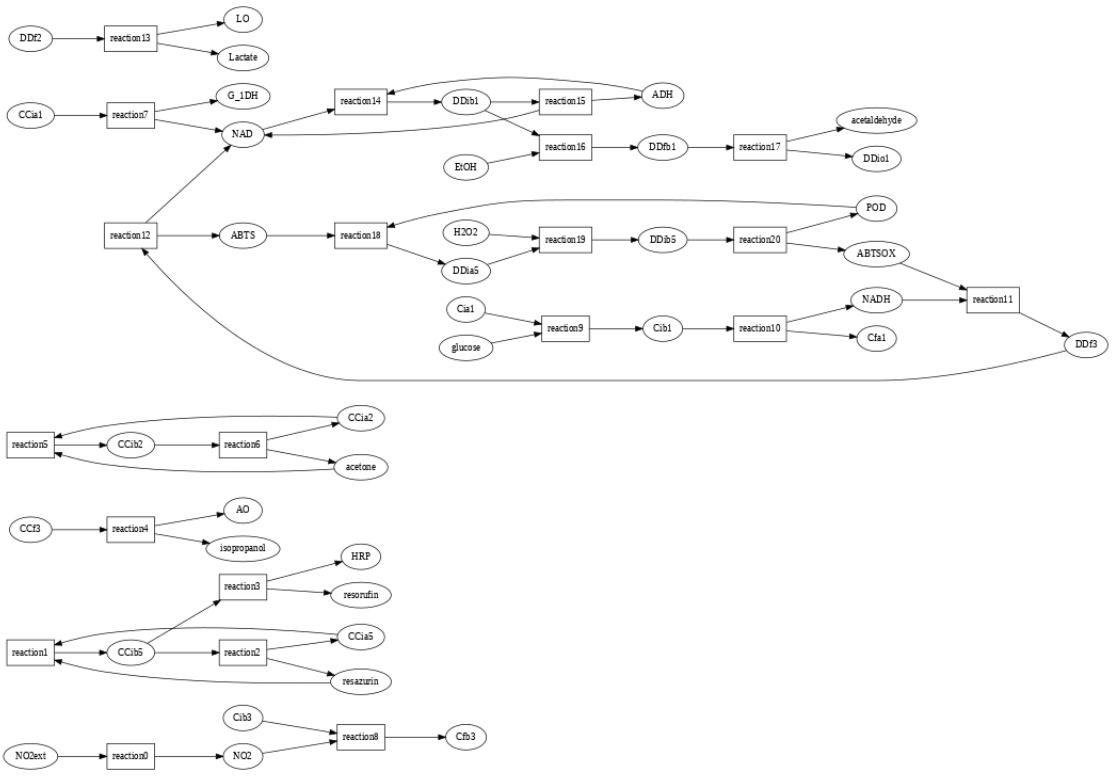
[7]:
```
search_reduction(Catalog.bc, CRNshort.bc, mapping_restriction : [acetone->a,␣
↪glucose->b, resorufin->j], merge_restriction : not_species, show_support :␣
↪yes).
```

[7]:
```
sepi
glucose
acetone
Lactate
EtOH
```

```
resorufin
ADH
ABTSOX
POD
DDib5
NO2ext => NO2
CCia5+resazurin => CCib5
CCib5 => CCia5+resazurin
CCib5 => HRP+resorufin
CCf3 => AO+isopropanol
CCia2+acetone => CCib2
CCib2 => CCia2+acetone
CCia1 => G_1DH+NAD
Cib3+NO2 => Cfb3
Cia1+glucose => Cib1
Cib1 => Cfa1+NADH
ABTSOX+NADH => DDf3
DDf3 => ABTS+NAD
DDf2 => LO+Lactate
ADH+NAD => DDib1
DDib1 => ADH+NAD
DDib1+EtOH => DDfb1
DDfb1 => DDio1+acetaldehyde
ABTS+POD => DDia5
DDia5+H2O2 => DDib5
DDib5 => ABTSOX+POD
Number of reductions: 1
```

[8]:
```
new_model.
NO2ext => NO2.
CCia5+resazurin => CCib5.
CCib5 => CCia5+resazurin.
CCib5 => HRP+resorufin.
CCf3 => AO+isopropanol.
CCia2+acetone => CCib2.
CCib2 => CCia2+acetone.
CCia1 => G_1DH+NAD.
Cib3+NO2 => Cfb3.
Cia1+glucose => Cib1.
Cib1 => Cfa1+NADH.
ABTSOX+NADH => DDf3.
DDf3 => ABTS+NAD.
DDf2 => LO+Lactate.
ADH+NAD => DDib1.
DDib1 => ADH+NAD.
DDib1+EtOH => DDfb1.
DDfb1 => DDio1+acetaldehyde.
```

```
ABTS+POD => DDia5.
DDia5+H2O2 => DDib5.
DDib5 => ABTSOX+POD.
draw_reactions.
```



Same search but with an additional step before resorufin (analoguous to the solutions found with the SISO* heuristic algorithms).

[9]:
```
search_reduction(Catalog.bc, CRNlong.bc, mapping_restriction : [acetone->a,␣
↪glucose->b, resorufin->j], merge_restriction : not_species).
```

[9]:
```
sepi
glucoseext -> deleted
glucose -> b
acetoneext -> deleted
acetone -> a
Lactateext -> deleted
Lactate -> deleted
EtOHext -> deleted
EtOH -> i
NO3ext -> deleted
NO3 -> deleted
NO2ext -> deleted
```

```
NO2 -> deleted
HRP -> deleted
H_2O_2 -> h
CCia5 -> deleted
resazurin -> deleted
CCib5 -> deleted
resorufin -> j
HRP2 -> deleted
NADH -> k
CCf4 -> deleted
NADN -> deleted
AO -> deleted
isopropanol -> deleted
CCf3 -> deleted
CCio3 -> deleted
ADH -> deleted
CCia2 -> deleted
CCib2 -> deleted
CCfa2 -> deleted
NAD -> deleted
G_1DH -> deleted
CCia1 -> g
CCib1 -> deleted
CCfa1 -> deleted
gluconolacrone -> deleted
NO -> c
volatNO -> deleted
O2 -> deleted
Cf6 -> deleted
NO2b -> deleted
Cf5 -> deleted
N2O3 -> deleted
DAF -> deleted
Cf4 -> deleted
DAFF -> deleted
NR -> deleted
Cia3 -> deleted
Cib3 -> deleted
Cfa3 -> deleted
Cfb3 -> deleted
Cio3 -> deleted
Cia2 -> deleted
Cfa2 -> deleted
Cfb2 -> deleted
Cio2 -> deleted
Cia1 -> deleted
Cib1 -> deleted
```

```
Cfa1 -> deleted
ABTSOX -> e
DDf3 -> deleted
ABTS -> deleted
LO -> deleted
DDf2 -> deleted
DDio2 -> deleted
H2O2 -> deleted
Pyruvate -> deleted
DDia1 -> deleted
DDib1 -> deleted
DDfa1 -> deleted
DDfb1 -> deleted
DDio1 -> deleted
acetaldehyde -> deleted
POD -> d
DDia5 -> deleted
DDib5 -> deleted
{glucoseext => glucose} -> deleted
{acetoneext => acetone} -> deleted
{Lactateext => Lactate} -> {h+i => k}
{EtOHext => EtOH} -> deleted
{NO3ext => NO3} -> deleted
{NO2ext => NO2} -> deleted
{HRP+H_2O_2 => CCia5} -> {h+i => k}
{CCia5 => HRP+H_2O_2} -> {g => a+h}
{CCia5+resazurin => CCib5} -> {h+i => k}
{CCib5 => CCia5+resazurin} -> {h+i => k}
{CCib5 => HRP+resorufin} -> {k => j}
{HRP2+NADH => CCf4} -> {k => j}
{CCf4 => HRP2+NADH} -> deleted
{CCf4 => HRP2+NADN} -> deleted
{AO+isopropanol => CCf3} -> {g => a+h}
{CCf3 => AO+isopropanol} -> {h+i => k}
{CCf3 => CCio3+H_2O_2} -> deleted
{CCio3 => AO+HRP2} -> deleted
{ADH+NADH => CCia2} -> deleted
{CCia2 => ADH+NADH} -> deleted
{CCia2+acetone => CCib2} -> {a+d => c+g}
{CCib2 => CCia2+acetone} -> {g => a+h}
{CCib2 => CCfa2+NAD} -> deleted
{CCfa2 => ADH+isopropanol} -> deleted
{G_1DH+NAD => CCia1} -> {a+d => c+g}
{CCia1 => G_1DH+NAD} -> {g => a+h}
{CCia1+glucose => CCib1} -> deleted
{CCib1 => CCia1+glucose} -> deleted
{CCib1 => CCfa1+NADH} -> deleted
```

```
{CCfa1 => G_1DH+gluconolacrone} -> deleted
{NO => volatNO} -> deleted
{NO+O2 => Cf6} -> deleted
{Cf6 => NO+O2} -> {a+d => c+g}
{Cf6 => NO2b+O2} -> deleted
{NO+NO2b => Cf5} -> {b+c => d+e}
{Cf5 => NO+NO2b} -> deleted
{Cf5 => N2O3} -> deleted
{DAF+N2O3 => Cf4} -> deleted
{Cf4 => DAF+N2O3} -> deleted
{Cf4 => DAFF} -> deleted
{NO2+NR => Cia3} -> deleted
{Cia3 => NO2+NR} -> deleted
{NADH+NR => Cib3} -> deleted
{Cib3 => NADH+NR} -> deleted
{Cia3+NADH => Cfa3} -> deleted
{Cib3+NO2 => Cfb3} -> deleted
{Cfa3 => Cia3+NADH} -> deleted
{Cfb3 => Cib3+NO2} -> deleted
{Cfa3 => Cio3+NO} -> deleted
{Cfb3 => Cio3+NO} -> deleted
{Cio3 => NAD+NR} -> deleted
{NO3+NR => Cia2} -> deleted
{Cia2 => NO3+NR} -> deleted
{Cia2+NADH => Cfa2} -> deleted
{Cib3+NO3 => Cfb2} -> deleted
{Cfa2 => Cia2+NADH} -> deleted
{Cfb2 => Cib3+NO3} -> deleted
{Cfa2 => Cio2+NO2} -> deleted
{Cfb2 => Cio2+NO2} -> deleted
{Cio2 => NAD+NR} -> deleted
{G_1DH+NAD => Cia1} -> deleted
{Cia1 => G_1DH+NAD} -> deleted
{Cia1+glucose => Cib1} -> {b+c => d+e}
{Cib1 => Cia1+glucose} -> deleted
{Cib1 => Cfa1+NADH} -> deleted
{Cfa1 => G_1DH+gluconolacrone} -> deleted
{ABTSOX+NADH => DDf3} -> deleted
{DDf3 => ABTSOX+NADH} -> deleted
{DDf3 => ABTS+NAD} -> deleted
{LO+Lactate => DDf2} -> deleted
{DDf2 => LO+Lactate} -> deleted
{DDf2 => DDio2+H2O2} -> deleted
{DDio2 => LO+Pyruvate} -> deleted
{ADH+EtOH => DDia1} -> deleted
{DDia1 => ADH+EtOH} -> deleted
{ADH+NAD => DDib1} -> deleted
```

```
{DDib1 => ADH+NAD} -> deleted
{DDia1+NAD => DDfa1} -> deleted
{DDib1+EtOH => DDfb1} -> {h+i => k}
{DDfa1 => DDia1+NAD} -> deleted
{DDfb1 => DDib1+EtOH} -> deleted
{DDfa1 => DDio1+acetaldehyde} -> deleted
{DDfb1 => DDio1+acetaldehyde} -> deleted
{DDio1 => ADH+NADH} -> {h+i => k}
{ABTS+POD => DDia5} -> {a+d => c+g}
{DDia5 => ABTS+POD} -> deleted
{DDia5+H2O2 => DDib5} -> deleted
{DDib5 => DDia5+H2O2} -> deleted
{DDib5 => ABTSOX+POD} -> {b+c => d+e}
Number of reductions: 1
```

SEPI search to find a regular solution to the acetone∧ glucose = resorufin CRN

[10]:
```
search_reduction(Catalog.bc, CRNVeryShort.bc, mapping_restriction :␣
↪[acetone->acetone, glucose->glucose, resorufin->resorufin],␣
↪merge_restriction : not_species).
```

[10]:
```
sepi
glucoseext -> deleted
glucose -> glucose
acetoneext -> deleted
acetone -> acetone
Lactateext -> deleted
Lactate -> deleted
EtOHext -> deleted
EtOH -> deleted
NO3ext -> deleted
NO3 -> deleted
NO2ext -> deleted
NO2 -> deleted
HRP -> deleted
H_2O_2 -> deleted
CCia5 -> deleted
resazurin -> deleted
CCib5 -> deleted
resorufin -> resorufin
HRP2 -> deleted
NADH -> deleted
CCf4 -> deleted
NADN -> deleted
AO -> deleted
isopropanol -> deleted
CCf3 -> deleted
```

```
CCio3 -> deleted
ADH -> deleted
CCia2 -> deleted
CCib2 -> deleted
CCfa2 -> deleted
NAD -> deleted
G_1DH -> deleted
CCia1 -> deleted
CCib1 -> deleted
CCfa1 -> deleted
gluconolacrone -> deleted
NO -> deleted
volatNO -> deleted
O2 -> deleted
Cf6 -> deleted
NO2b -> deleted
Cf5 -> deleted
N2O3 -> deleted
DAF -> deleted
Cf4 -> deleted
DAFF -> deleted
NR -> deleted
Cia3 -> deleted
Cib3 -> deleted
Cfa3 -> deleted
Cfb3 -> deleted
Cio3 -> deleted
Cia2 -> deleted
Cfa2 -> deleted
Cfb2 -> deleted
Cio2 -> deleted
Cia1 -> deleted
Cib1 -> deleted
Cfa1 -> deleted
ABTSOX -> deleted
DDf3 -> deleted
ABTS -> deleted
LO -> deleted
DDf2 -> deleted
DDio2 -> deleted
H2O2 -> deleted
Pyruvate -> deleted
DDia1 -> deleted
DDib1 -> deleted
DDfa1 -> deleted
DDfb1 -> deleted
DDio1 -> deleted
```

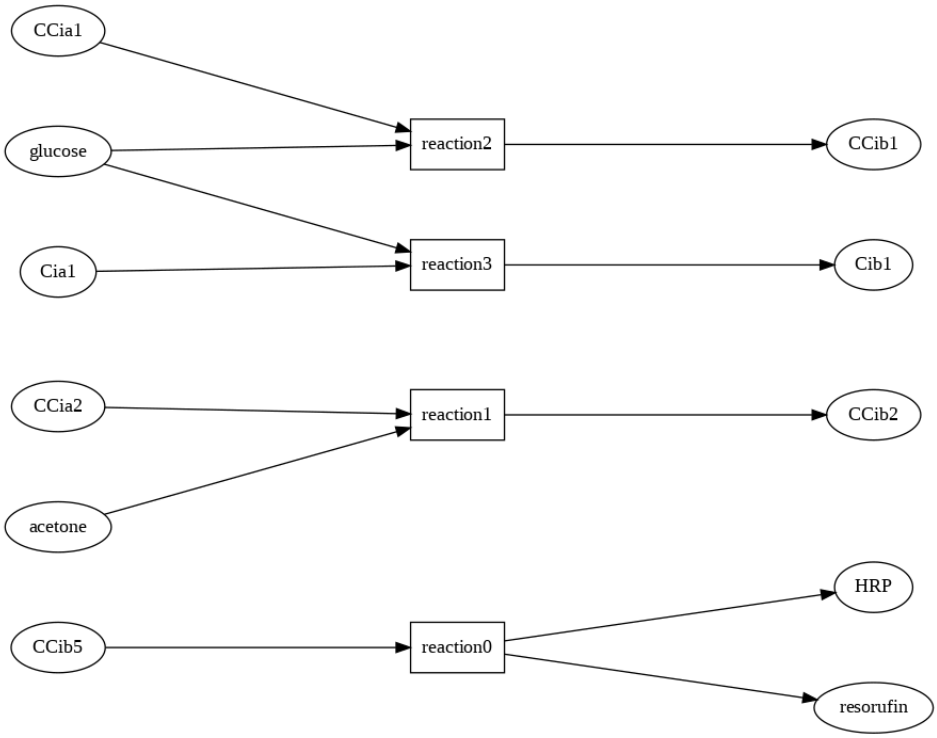
```
acetaldehyde -> deleted
POD -> deleted
DDia5 -> deleted
DDib5 -> deleted
{glucoseext => glucose} -> deleted
{acetoneext => acetone} -> deleted
{Lactateext => Lactate} -> deleted
{EtOHext => EtOH} -> deleted
{NO3ext => NO3} -> deleted
{NO2ext => NO2} -> deleted
{HRP+H_2O_2 => CCia5} -> deleted
{CCia5 => HRP+H_2O_2} -> deleted
{CCia5+resazurin => CCib5} -> deleted
{CCib5 => CCia5+resazurin} -> deleted
{CCib5 => HRP+resorufin} -> {acetone+glucose => resorufin}
{HRP2+NADH => CCf4} -> deleted
{CCf4 => HRP2+NADH} -> deleted
{CCf4 => HRP2+NADN} -> deleted
{AO+isopropanol => CCf3} -> deleted
{CCf3 => AO+isopropanol} -> deleted
{CCf3 => CCio3+H_2O_2} -> deleted
{CCio3 => AO+HRP2} -> deleted
{ADH+NADH => CCia2} -> deleted
{CCia2 => ADH+NADH} -> deleted
{CCia2+acetone => CCib2} -> {acetone+glucose => resorufin}
{CCib2 => CCia2+acetone} -> deleted
{CCib2 => CCfa2+NAD} -> deleted
{CCfa2 => ADH+isopropanol} -> deleted
{G_1DH+NAD => CCia1} -> deleted
{CCia1 => G_1DH+NAD} -> deleted
{CCia1+glucose => CCib1} -> {acetone+glucose => resorufin}
{CCib1 => CCia1+glucose} -> deleted
{CCib1 => CCfa1+NADH} -> deleted
{CCfa1 => G_1DH+gluconolacrone} -> deleted
{NO => volatNO} -> deleted
{NO+O2 => Cf6} -> deleted
{Cf6 => NO+O2} -> deleted
{Cf6 => NO2b+O2} -> deleted
{NO+NO2b => Cf5} -> deleted
{Cf5 => NO+NO2b} -> deleted
{Cf5 => N2O3} -> deleted
{DAF+N2O3 => Cf4} -> deleted
{Cf4 => DAF+N2O3} -> deleted
{Cf4 => DAFF} -> deleted
{NO2+NR => Cia3} -> deleted
{Cia3 => NO2+NR} -> deleted
{NADH+NR => Cib3} -> deleted
```

```
{Cib3 => NADH+NR} -> deleted
{Cia3+NADH => Cfa3} -> deleted
{Cib3+NO2 => Cfb3} -> deleted
{Cfa3 => Cia3+NADH} -> deleted
{Cfb3 => Cib3+NO2} -> deleted
{Cfa3 => Cio3+NO} -> deleted
{Cfb3 => Cio3+NO} -> deleted
{Cio3 => NAD+NR} -> deleted
{NO3+NR => Cia2} -> deleted
{Cia2 => NO3+NR} -> deleted
{Cia2+NADH => Cfa2} -> deleted
{Cib3+NO3 => Cfb2} -> deleted
{Cfa2 => Cia2+NADH} -> deleted
{Cfb2 => Cib3+NO3} -> deleted
{Cfa2 => Cio2+NO2} -> deleted
{Cfb2 => Cio2+NO2} -> deleted
{Cio2 => NAD+NR} -> deleted
{G_1DH+NAD => Cia1} -> deleted
{Cia1 => G_1DH+NAD} -> deleted
{Cia1+glucose => Cib1} -> {acetone+glucose => resorufin}
{Cib1 => Cia1+glucose} -> deleted
{Cib1 => Cfa1+NADH} -> deleted
{Cfa1 => G_1DH+gluconolacrone} -> deleted
{ABTSOX+NADH => DDf3} -> deleted
{DDf3 => ABTSOX+NADH} -> deleted
{DDf3 => ABTS+NAD} -> deleted
{LO+Lactate => DDf2} -> deleted
{DDf2 => LO+Lactate} -> deleted
{DDf2 => DDio2+H2O2} -> deleted
{DDio2 => LO+Pyruvate} -> deleted
{ADH+EtOH => DDia1} -> deleted
{DDia1 => ADH+EtOH} -> deleted
{ADH+NAD => DDib1} -> deleted
{DDib1 => ADH+NAD} -> deleted
{DDia1+NAD => DDfa1} -> deleted
{DDib1+EtOH => DDfb1} -> deleted
{DDfa1 => DDia1+NAD} -> deleted
{DDfb1 => DDib1+EtOH} -> deleted
{DDfa1 => DDio1+acetaldehyde} -> deleted
{DDfb1 => DDio1+acetaldehyde} -> deleted
{DDio1 => ADH+NADH} -> deleted
{ABTS+POD => DDia5} -> deleted
{DDia5 => ABTS+POD} -> deleted
{DDia5+H2O2 => DDib5} -> deleted
{DDib5 => DDia5+H2O2} -> deleted
{DDib5 => ABTSOX+POD} -> deleted
Number of reductions: 1
```

[11]:
```
search_reduction(Catalog.bc, CRNVeryShort.bc, mapping_restriction :␣
↪[acetone->acetone, glucose->glucose, resorufin->resorufin],␣
↪merge_restriction : not_species, show_support : yes).
```

[11]:
```
sepi
glucose
acetone
resorufin
CCib5 => HRP+resorufin
CCia2+acetone => CCib2
CCia1+glucose => CCib1
Cia1+glucose => Cib1
Number of reductions: 1
```

[12]:
```
new_model.
CCib5 => HRP+resorufin.
CCia2+acetone => CCib2.
CCia1+glucose => CCib1.
Cia1+glucose => Cib1.
draw_reactions.
```



AVOID USING, former usage but network is too large Smart1Subset is made out of every reaction with an enzyme involved in the first solution heuristically found, and at least one metabolite in it

[32]:
```
clear_model.
load(library:examples/sepi/BrendaBiochamReactionsSmart1SubsetM.bc).
draw_reactions.
```

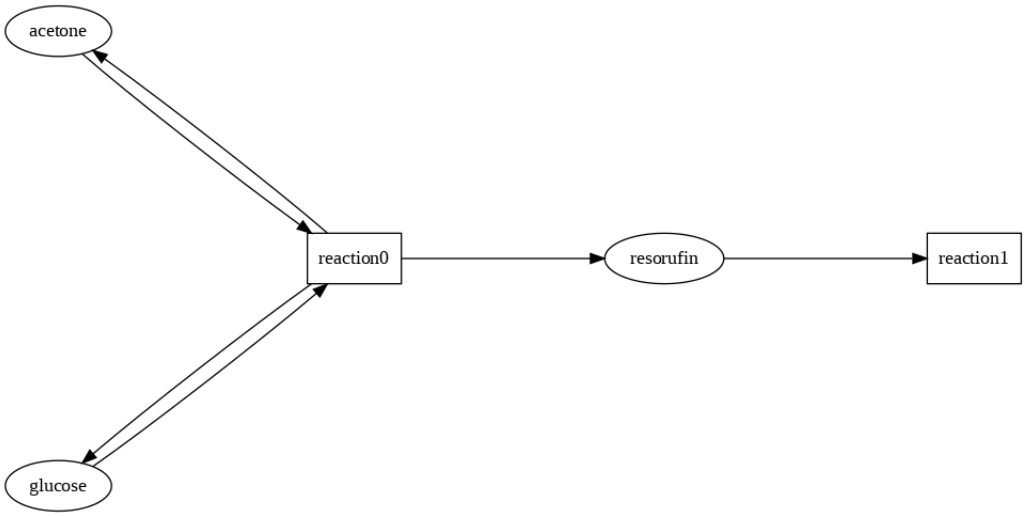
[ ]:
```
search_reduction(library:examples/sepi/BrendaBiochamReactionsSmart1SubsetM.bc,␣
↪CRNlong.bc, timeout : 10000000000000000000000000, stats : yes,␣
↪merge_restriction : not_species, mapping_restriction : [m286->a, m33->b,␣
↪m25014->j]).
```

5 4. Bigger examples of concretization : GluONe, LacOH and GluNOx

These three logical circuits can be read as : GluONe → Resorufin = glucose∧acetone et NADH = glucose ∧(1-acetone) LacOH → NADH = EtOH et ABTSOX = Lactate∧(1-EtOH) GluNOx → DAFF = glucose∧NOx et NADH = glucose∧(1-NOx) We will mostly focus on the none NADH branches.

5.1 GluONe

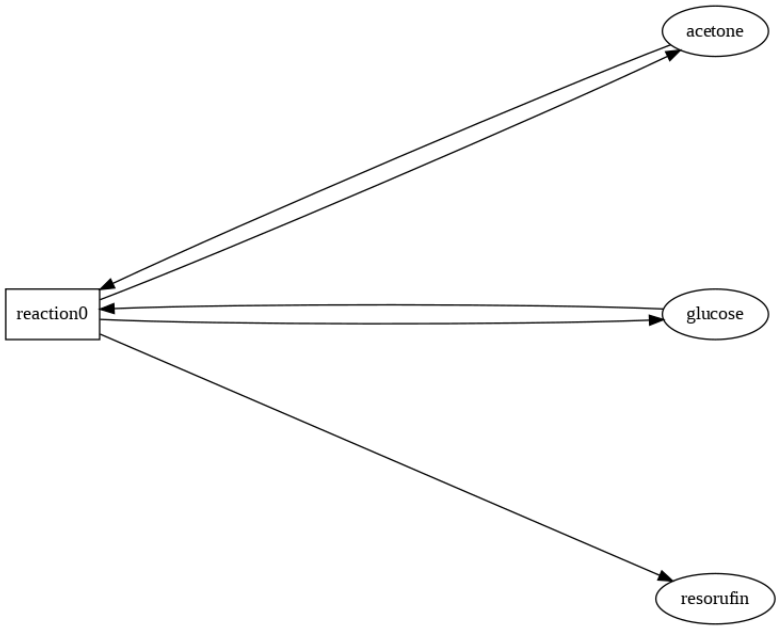
[23]:
```
clear_model.
%add_function( resorufin = (acetone * glucose), NADH = (glucose * (1 -␣
 ↪acetone))).
stabilize_expression(acetone*glucose-resorufin,resorufin,[acetone=1,glucose=1]).
%stabilize_expression(ABTSOX-lactate*(1-EtOH),ABTSOX,[lactate=1,EtOH=0,ABTSOX=1]).
 ↪
export_biocham(GluONe.bc).
list_model.
draw_reactions.
```



[23]:
```
MA(1.0) for acetone+glucose=>acetone+glucose+resorufin.
MA(1.0) for resorufin=>_.
initial_state(acetone=1).
initial_state(glucose=1).
```

A simplified aCRN without the resorufin→_ , as it leads to some issues :

[22]:
```
new_model(GluONe_Simple).
acetone+glucose=>acetone+glucose+resorufin.
export_biocham(GluONe_Simple.bc).
draw_reactions.
```



[24]:
```
search_reduction(Catalog.bc, GluONe_Simple.bc, mapping_restriction :␣
↪[acetone->acetone, glucose->glucose, resorufin->resorufin],␣
↪merge_restriction : not_species).
```

[24]:
```
sepi
glucoseext -> deleted
glucose -> glucose
acetoneext -> deleted
acetone -> acetone
Lactateext -> deleted
Lactate -> deleted
EtOHext -> deleted
EtOH -> deleted
NO3ext -> deleted
NO3 -> deleted
NO2ext -> deleted
NO2 -> deleted
HRP -> deleted
H_2O_2 -> deleted
CCia5 -> deleted
resazurin -> deleted
CCib5 -> deleted
resorufin -> resorufin
```

```
HRP2 -> deleted
NADH -> deleted
CCf4 -> deleted
NADN -> deleted
AO -> deleted
isopropanol -> deleted
CCf3 -> deleted
CCio3 -> deleted
ADH -> deleted
CCia2 -> deleted
CCib2 -> deleted
CCfa2 -> deleted
NAD -> deleted
G_1DH -> deleted
CCia1 -> deleted
CCib1 -> deleted
CCfa1 -> deleted
gluconolacrone -> deleted
NO -> deleted
volatNO -> deleted
O2 -> deleted
Cf6 -> deleted
NO2b -> deleted
Cf5 -> deleted
N2O3 -> deleted
DAF -> deleted
Cf4 -> deleted
DAFF -> deleted
NR -> deleted
Cia3 -> deleted
Cib3 -> deleted
Cfa3 -> deleted
Cfb3 -> deleted
Cio3 -> deleted
Cia2 -> deleted
Cfa2 -> deleted
Cfb2 -> deleted
Cio2 -> deleted
Cia1 -> deleted
Cib1 -> deleted
Cfa1 -> deleted
ABTSOX -> deleted
DDf3 -> deleted
ABTS -> deleted
LO -> deleted
DDf2 -> deleted
DDio2 -> deleted
```

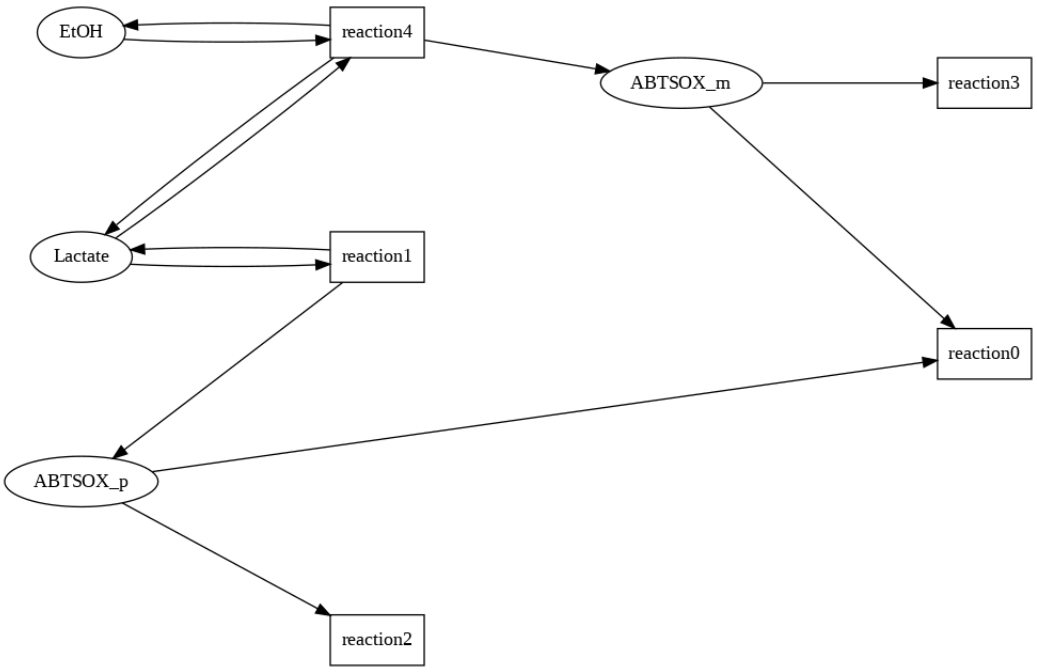
```
H2O2 -> deleted
Pyruvate -> deleted
DDia1 -> deleted
DDib1 -> deleted
DDfa1 -> deleted
DDfb1 -> deleted
DDio1 -> deleted
acetaldehyde -> deleted
POD -> deleted
DDia5 -> deleted
DDib5 -> deleted
{glucoseext => glucose} -> {acetone+glucose => acetone+glucose+resorufin}
{acetoneext => acetone} -> {acetone+glucose => acetone+glucose+resorufin}
{Lactateext => Lactate} -> deleted
{EtOHext => EtOH} -> deleted
{NO3ext => NO3} -> deleted
{NO2ext => NO2} -> deleted
{HRP+H_2O_2 => CCia5} -> deleted
{CCia5 => HRP+H_2O_2} -> deleted
{CCia5+resazurin => CCib5} -> deleted
{CCib5 => CCia5+resazurin} -> deleted
{CCib5 => HRP+resorufin} -> {acetone+glucose => acetone+glucose+resorufin}
{HRP2+NADH => CCf4} -> deleted
{CCf4 => HRP2+NADH} -> deleted
{CCf4 => HRP2+NADN} -> deleted
{AO+isopropanol => CCf3} -> deleted
{CCf3 => AO+isopropanol} -> deleted
{CCf3 => CCio3+H_2O_2} -> deleted
{CCio3 => AO+HRP2} -> deleted
{ADH+NADH => CCia2} -> deleted
{CCia2 => ADH+NADH} -> deleted
{CCia2+acetone => CCib2} -> {acetone+glucose => acetone+glucose+resorufin}
{CCib2 => CCia2+acetone} -> {acetone+glucose => acetone+glucose+resorufin}
{CCib2 => CCfa2+NAD} -> deleted
{CCfa2 => ADH+isopropanol} -> deleted
{G_1DH+NAD => CCia1} -> deleted
{CCia1 => G_1DH+NAD} -> deleted
{CCia1+glucose => CCib1} -> {acetone+glucose => acetone+glucose+resorufin}
{CCib1 => CCia1+glucose} -> {acetone+glucose => acetone+glucose+resorufin}
{CCib1 => CCfa1+NADH} -> deleted
{CCfa1 => G_1DH+gluconolacrone} -> deleted
{NO => volatNO} -> deleted
{NO+O2 => Cf6} -> deleted
{Cf6 => NO+O2} -> deleted
{Cf6 => NO2b+O2} -> deleted
{NO+NO2b => Cf5} -> deleted
{Cf5 => NO+NO2b} -> deleted
```

{Cf5 => N2O3} -> deleted
{DAF+N2O3 => Cf4} -> deleted
{Cf4 => DAF+N2O3} -> deleted
{Cf4 => DAFF} -> deleted
{NO2+NR => Cia3} -> deleted
{Cia3 => NO2+NR} -> deleted
{NADH+NR => Cib3} -> deleted
{Cib3 => NADH+NR} -> deleted
{Cia3+NADH => Cfa3} -> deleted
{Cib3+NO2 => Cfb3} -> deleted
{Cfa3 => Cia3+NADH} -> deleted
{Cfb3 => Cib3+NO2} -> deleted
{Cfa3 => Cio3+NO} -> deleted
{Cfb3 => Cio3+NO} -> deleted
{Cio3 => NAD+NR} -> deleted
{NO3+NR => Cia2} -> deleted
{Cia2 => NO3+NR} -> deleted
{Cia2+NADH => Cfa2} -> deleted
{Cib3+NO3 => Cfb2} -> deleted
{Cfa2 => Cia2+NADH} -> deleted
{Cfb2 => Cib3+NO3} -> deleted
{Cfa2 => Cio2+NO2} -> deleted
{Cfb2 => Cio2+NO2} -> deleted
{Cio2 => NAD+NR} -> deleted
{G_1DH+NAD => Cia1} -> deleted
{Cia1 => G_1DH+NAD} -> deleted
{Cia1+glucose => Cib1} -> {acetone+glucose => acetone+glucose+resorufin}
{Cib1 => Cia1+glucose} -> {acetone+glucose => acetone+glucose+resorufin}
{Cib1 => Cfa1+NADH} -> deleted
{Cfa1 => G_1DH+gluconolacrone} -> deleted
{ABTSOX+NADH => DDf3} -> deleted
{DDf3 => ABTSOX+NADH} -> deleted
{DDf3 => ABTS+NAD} -> deleted
{LO+Lactate => DDf2} -> deleted
{DDf2 => LO+Lactate} -> deleted
{DDf2 => DDio2+H2O2} -> deleted
{DDio2 => LO+Pyruvate} -> deleted
{ADH+EtOH => DDia1} -> deleted
{DDia1 => ADH+EtOH} -> deleted
{ADH+NAD => DDib1} -> deleted
{DDib1 => ADH+NAD} -> deleted
{DDia1+NAD => DDfa1} -> deleted
{DDib1+EtOH => DDfb1} -> deleted
{DDfa1 => DDia1+NAD} -> deleted
{DDfb1 => DDib1+EtOH} -> deleted
{DDfa1 => DDio1+acetaldehyde} -> deleted
{DDfb1 => DDio1+acetaldehyde} -> deleted

```
{DDio1 => ADH+NADH} -> deleted
{ABTS+POD => DDia5} -> deleted
{DDia5 => ABTS+POD} -> deleted
{DDia5+H2O2 => DDib5} -> deleted
{DDib5 => DDia5+H2O2} -> deleted
{DDib5 => ABTSOX+POD} -> deleted
Number of reductions: 1
```

5.2 LacOH

[15]:
```
clear_model.
%add_function(NADH = EtOH, ABTSOX = (1-EtOH)*Lactate).
%compile_function(NADH = EtOH, ABTSOX = (1-EtOH)*Lactate).
%stabilize_expression(NADH - EtOH, (1 - EtOH) * Lactate - ABTSOX, [NADH=1,
 ↪EtOH=1, ABTSOX=1, Lactate=1]).
%stabilize_expression(NADH - EtOH, NADH, [NADH=1,EtOH=1,Lactate=1]).
stabilize_expression(Lactate*(1-EtOH)-ABTSOX, ABTSOX, [Lactate=1, EtOH=1,
 ↪ABTSOX=1]).
export_biocham(LacOH.bc).
list_model.
draw_reactions.
```



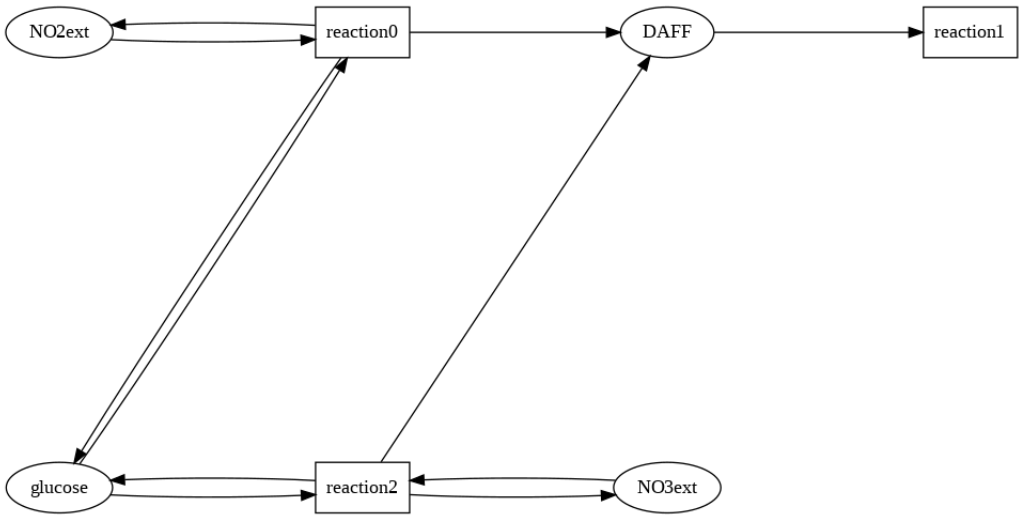
[15]:
```
MA(fast) for ABTSOX_m+ABTSOX_p=>_.
MA(1.0) for Lactate=>ABTSOX_p+Lactate.
MA(1.0) for ABTSOX_p=>_.
MA(1.0) for ABTSOX_m=>_.
MA(1.0) for EtOH+Lactate=>ABTSOX_m+EtOH+Lactate.
initial_state(ABTSOX_p=1).
initial_state(Lactate=1).
initial_state(EtOH=1).
parameter(
  fast = 1000
).
```

[16]:
```
search_reduction(Catalog.bc, LacOH.bc, mapping_restriction : [Lactate->Lactate,
↪EtOH->EtOH, ABTSOX->ABTSOX_p], merge_restriction : not_species).
```

[16]:
```
no sepi found
Number of reductions: 0
```

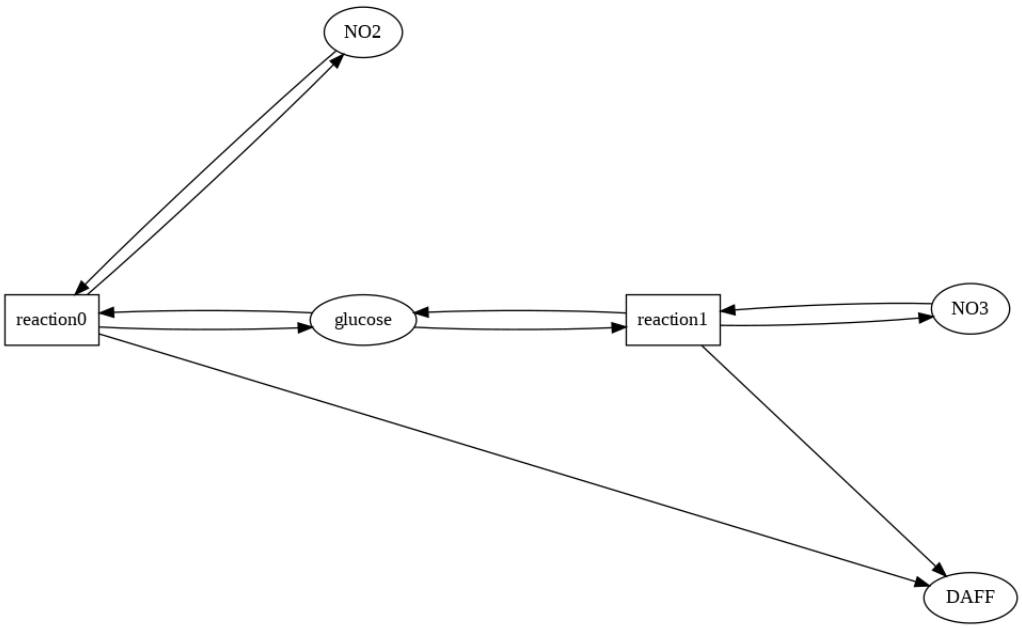
5.3 GluNOx

[29]:
```
clear_model.
%add_function( NADH = glucose*(1-NOx), DAFF = glucose*NOx).
stabilize_expression(DAFF-glucose*(NO2ext+NO3ext),DAFF,[glucose=1,NO2ext=1,NO3ext=0]).
↪
export_biocham(GluNOx.bc).
list_model.
draw_reactions.
```



[29]:
```
MA(1.0) for NO2ext+glucose=>DAFF+NO2ext+glucose.
MA(1.0) for DAFF=>_.
MA(1.0) for NO3ext+glucose=>DAFF+NO3ext+glucose.
initial_state(glucose=1).
initial_state(NO2ext=1).
```

[30]:
```
clear_model.
NO2+glucose=>DAFF+NO2+glucose.
NO3+glucose=>DAFF+NO3+glucose.
export_biocham(GluNOx_Simple.bc).
draw_reactions.
```

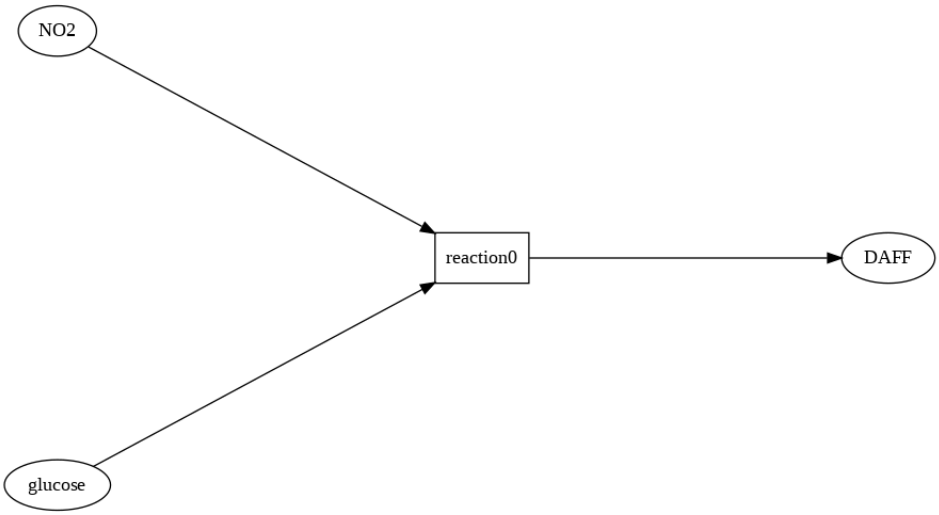


[33]:
```
search_reduction(Catalog.bc, GluNOx_Simple.bc, mapping_restriction :␣
↪[NO2->NO2,NO3->NO3, glucose->glucose, DAFF->DAFF], merge_restriction :␣
↪not_species).
```

[33]:
```
no sepi found
Number of reductions: 0
```

[ ]:
```
search_reduction(Catalog.bc, GluNOx.bc, mapping_restriction : [NO->NO,NO2->NO2,␣
↪glucose->glucose, DAFF->DAFF], merge_restriction : not_species).
```

[46]:
```
clear_model.
NO2 + glucose => DAFF.
%NO + glucose => DAFF.
%NO2 + glucose => DAFF + NO2 + glucose.
%DAFF=>_.
%NO3 + glucose => DAFF + NO3 + glucose.
export_biocham(CRNVeryShort2.bc).
draw_reactions.
```



[48]:
```
search_reduction(Catalog.bc, CRNVeryShort2.bc, mapping_restriction : [NO2->NO2,␣
↪glucose->glucose, DAFF->DAFF], merge_restriction : not_species).
```

[48]:
```
sepi
glucoseext -> deleted
glucose -> glucose
acetoneext -> deleted
acetone -> deleted
Lactateext -> deleted
Lactate -> deleted
EtOHext -> deleted
EtOH -> deleted
NO3ext -> deleted
NO3 -> deleted
NO2ext -> deleted
NO2 -> NO2
HRP -> deleted
H_2O_2 -> deleted
CCia5 -> deleted
resazurin -> deleted
CCib5 -> deleted
resorufin -> deleted
HRP2 -> deleted
```

```
NADH -> deleted
CCf4 -> deleted
NADN -> deleted
AO -> deleted
isopropanol -> deleted
CCf3 -> deleted
CCio3 -> deleted
ADH -> deleted
CCia2 -> deleted
CCib2 -> deleted
CCfa2 -> deleted
NAD -> deleted
G_1DH -> deleted
CCia1 -> deleted
CCib1 -> deleted
CCfa1 -> deleted
gluconolacrone -> deleted
NO -> deleted
volatNO -> deleted
O2 -> deleted
Cf6 -> deleted
NO2b -> deleted
Cf5 -> deleted
N2O3 -> deleted
DAF -> deleted
Cf4 -> deleted
DAFF -> DAFF
NR -> deleted
Cia3 -> deleted
Cib3 -> deleted
Cfa3 -> deleted
Cfb3 -> deleted
Cio3 -> deleted
Cia2 -> deleted
Cfa2 -> deleted
Cfb2 -> deleted
Cio2 -> deleted
Cia1 -> deleted
Cib1 -> deleted
Cfa1 -> deleted
ABTSOX -> deleted
DDf3 -> deleted
ABTS -> deleted
LO -> deleted
DDf2 -> deleted
DDio2 -> deleted
H2O2 -> deleted
```

```
Pyruvate -> deleted
DDia1 -> deleted
DDib1 -> deleted
DDfa1 -> deleted
DDfb1 -> deleted
DDio1 -> deleted
acetaldehyde -> deleted
POD -> deleted
DDia5 -> deleted
DDib5 -> deleted
{glucoseext => glucose} -> deleted
{acetoneext => acetone} -> deleted
{Lactateext => Lactate} -> deleted
{EtOHext => EtOH} -> deleted
{NO3ext => NO3} -> deleted
{NO2ext => NO2} -> deleted
{HRP+H_2O_2 => CCia5} -> deleted
{CCia5 => HRP+H_2O_2} -> deleted
{CCia5+resazurin => CCib5} -> deleted
{CCib5 => CCia5+resazurin} -> deleted
{CCib5 => HRP+resorufin} -> deleted
{HRP2+NADH => CCf4} -> deleted
{CCf4 => HRP2+NADH} -> deleted
{CCf4 => HRP2+NADN} -> deleted
{AO+isopropanol => CCf3} -> deleted
{CCf3 => AO+isopropanol} -> deleted
{CCf3 => CCio3+H_2O_2} -> deleted
{CCio3 => AO+HRP2} -> deleted
{ADH+NADH => CCia2} -> deleted
{CCia2 => ADH+NADH} -> deleted
{CCia2+acetone => CCib2} -> deleted
{CCib2 => CCia2+acetone} -> deleted
{CCib2 => CCfa2+NAD} -> deleted
{CCfa2 => ADH+isopropanol} -> deleted
{G_1DH+NAD => CCia1} -> deleted
{CCia1 => G_1DH+NAD} -> deleted
{CCia1+glucose => CCib1} -> {NO2+glucose => DAFF}
{CCib1 => CCia1+glucose} -> deleted
{CCib1 => CCfa1+NADH} -> deleted
{CCfa1 => G_1DH+gluconolacrone} -> deleted
{NO => volatNO} -> deleted
{NO+O2 => Cf6} -> deleted
{Cf6 => NO+O2} -> deleted
{Cf6 => NO2b+O2} -> deleted
{NO+NO2b => Cf5} -> deleted
{Cf5 => NO+NO2b} -> deleted
{Cf5 => N2O3} -> deleted
```

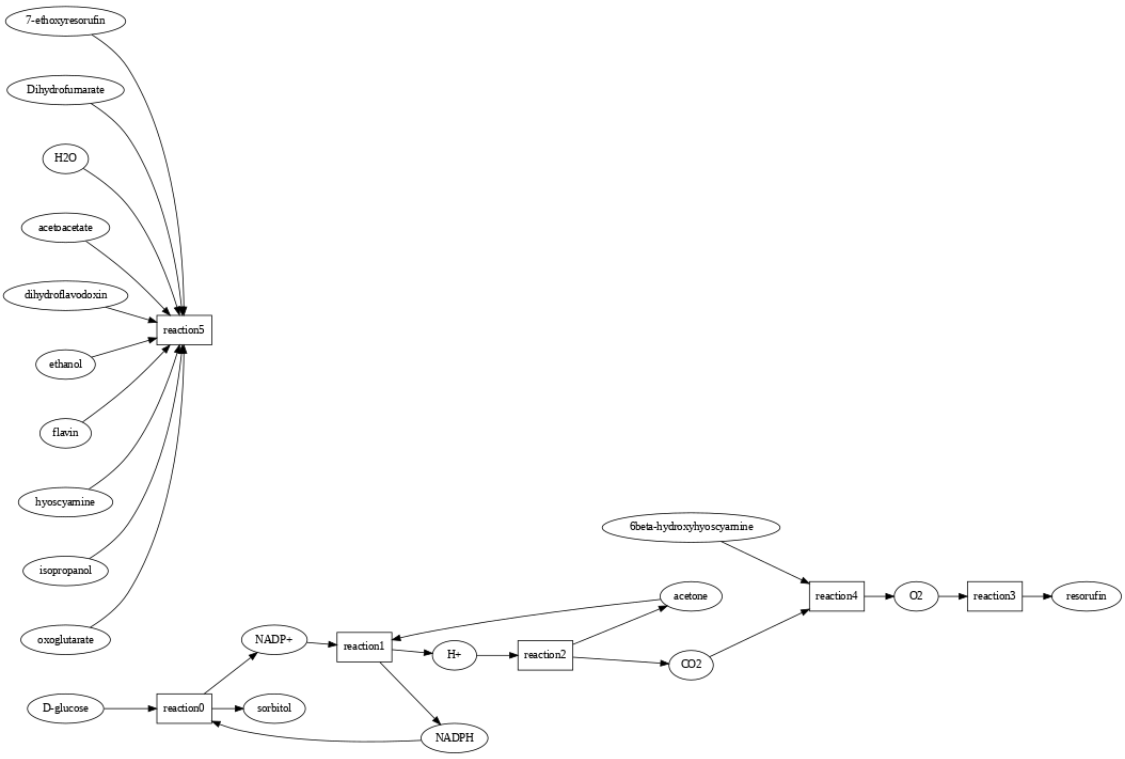
{DAF+N2O3 => Cf4} -> deleted
{Cf4 => DAF+N2O3} -> deleted
{Cf4 => DAFF} -> {NO2+glucose => DAFF}
{NO2+NR => Cia3} -> {NO2+glucose => DAFF}
{Cia3 => NO2+NR} -> deleted
{NADH+NR => Cib3} -> deleted
{Cib3 => NADH+NR} -> deleted
{Cia3+NADH => Cfa3} -> deleted
{Cib3+NO2 => Cfb3} -> {NO2+glucose => DAFF}
{Cfa3 => Cia3+NADH} -> deleted
{Cfb3 => Cib3+NO2} -> deleted
{Cfa3 => Cio3+NO} -> deleted
{Cfb3 => Cio3+NO} -> deleted
{Cio3 => NAD+NR} -> deleted
{NO3+NR => Cia2} -> deleted
{Cia2 => NO3+NR} -> deleted
{Cia2+NADH => Cfa2} -> deleted
{Cib3+NO3 => Cfb2} -> deleted
{Cfa2 => Cia2+NADH} -> deleted
{Cfb2 => Cib3+NO3} -> deleted
{Cfa2 => Cio2+NO2} -> deleted
{Cfb2 => Cio2+NO2} -> deleted
{Cio2 => NAD+NR} -> deleted
{G_1DH+NAD => Cia1} -> deleted
{Cia1 => G_1DH+NAD} -> deleted
{Cia1+glucose => Cib1} -> {NO2+glucose => DAFF}
{Cib1 => Cia1+glucose} -> deleted
{Cib1 => Cfa1+NADH} -> deleted
{Cfa1 => G_1DH+gluconolacrone} -> deleted
{ABTSOX+NADH => DDf3} -> deleted
{DDf3 => ABTSOX+NADH} -> deleted
{DDf3 => ABTS+NAD} -> deleted
{LO+Lactate => DDf2} -> deleted
{DDf2 => LO+Lactate} -> deleted
{DDf2 => DDio2+H2O2} -> deleted
{DDio2 => LO+Pyruvate} -> deleted
{ADH+EtOH => DDia1} -> deleted
{DDia1 => ADH+EtOH} -> deleted
{ADH+NAD => DDib1} -> deleted
{DDib1 => ADH+NAD} -> deleted
{DDia1+NAD => DDfa1} -> deleted
{DDib1+EtOH => DDfb1} -> deleted
{DDfa1 => DDia1+NAD} -> deleted
{DDfb1 => DDib1+EtOH} -> deleted
{DDfa1 => DDio1+acetaldehyde} -> deleted
{DDfb1 => DDio1+acetaldehyde} -> deleted
{DDio1 => ADH+NADH} -> deleted

```
{ABTS+POD => DDia5} -> deleted
{DDia5 => ABTS+POD} -> deleted
{DDia5+H2O2 => DDib5} -> deleted
{DDib5 => DDia5+H2O2} -> deleted
{DDib5 => ABTSOX+POD} -> deleted
Number of reductions: 1
```

6 5. SISO Solutions

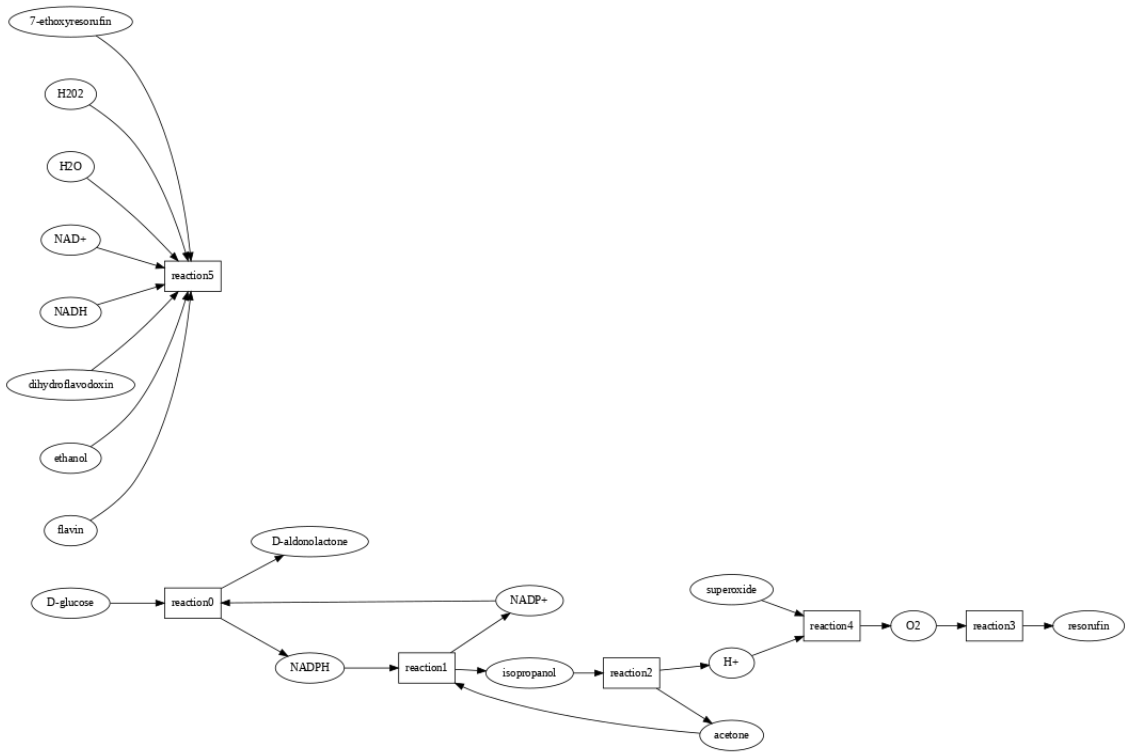
[13]:
```
new_model(CRNlong).
'D-glucose'+'NADPH'=>'NADP+'+'sorbitol'. %aldose reductase
'acetone'+'NADP+'=>'NADPH'+'H+'. %alcohol dehydrogenase (NADP+)
'H+'=>'acetone'+'CO2'. %2-oxopropyl-CoM reductase (carboxylating)
'O2'=>'resorufin'. %unspecific monooxygenase
'CO2'+'6beta-hydroxyhyoscyamine'=>'O2'. %hyoscyamine (6S)-dioxygenase
'dihydroflavodoxin'+'7-ethoxyresorufin'+'H2O'+'ethanol'+'flavin'+'acetoacetate'+'Dihydrofumara
 ↪=> _. %espèces envirronantes

export_biocham(CRNlong.bc).
list_model.
draw_reactions.
```



[13]:
```
MA(1) for 'D-glucose'+NADPH=>'NADP+'+sorbitol.
MA(1) for 'NADP+'+acetone=>'H+'+NADPH.
MA(1) for 'H+'=>CO2+acetone.
MA(1) for O2=>resorufin.
MA(1) for '6beta-hydroxyhyoscyamine'+CO2=>O2.
MA(1) for '7-ethoxyresorufin'+Dihydrofumarate+H2O+acetoacetate+dihydroflavodoxin
+ethanol+flavin+hyoscyamine+isopropanol+oxoglutarate=>_.
```

[16]:
```
new_model(CRNlong).
'D-glucose'+'NADP+'=>'NADPH'+'D-aldonolactone'.
'acetone'+'NADPH'=>'NADP+'+'isopropanol'.
'isopropanol'=>'acetone'+'H+'.
'O2'=>'resorufin'.
'H+'+'superoxide'=>'O2'.
'dihydroflavodoxin'+'7-ethoxyresorufin'+'H2O'+'ethanol'+'flavin'+'NAD+'+'NADH'+'H2O2'␣
↪=> _.
export_biocham(CRNlong.bc).
list_model.
draw_reactions.
```



[16]:
```
MA(1) for 'D-glucose'+'NADP+'=>'D-aldonolactone'+NADPH.
MA(1) for NADPH+acetone=>'NADP+'+isopropanol.
MA(1) for isopropanol=>'H+'+acetone.
```

```
MA(1) for O2=>resorufin.
MA(1) for 'H+'+superoxide=>O2.
MA(1) for
'7-ethoxyresorufin'+H2O2+H2O+'NAD+'+NADH+dihydroflavodoxin+ethanol+flavin=>_.
```