



Metabolic Network Representation in SBGN PD: EC and Identity Gate

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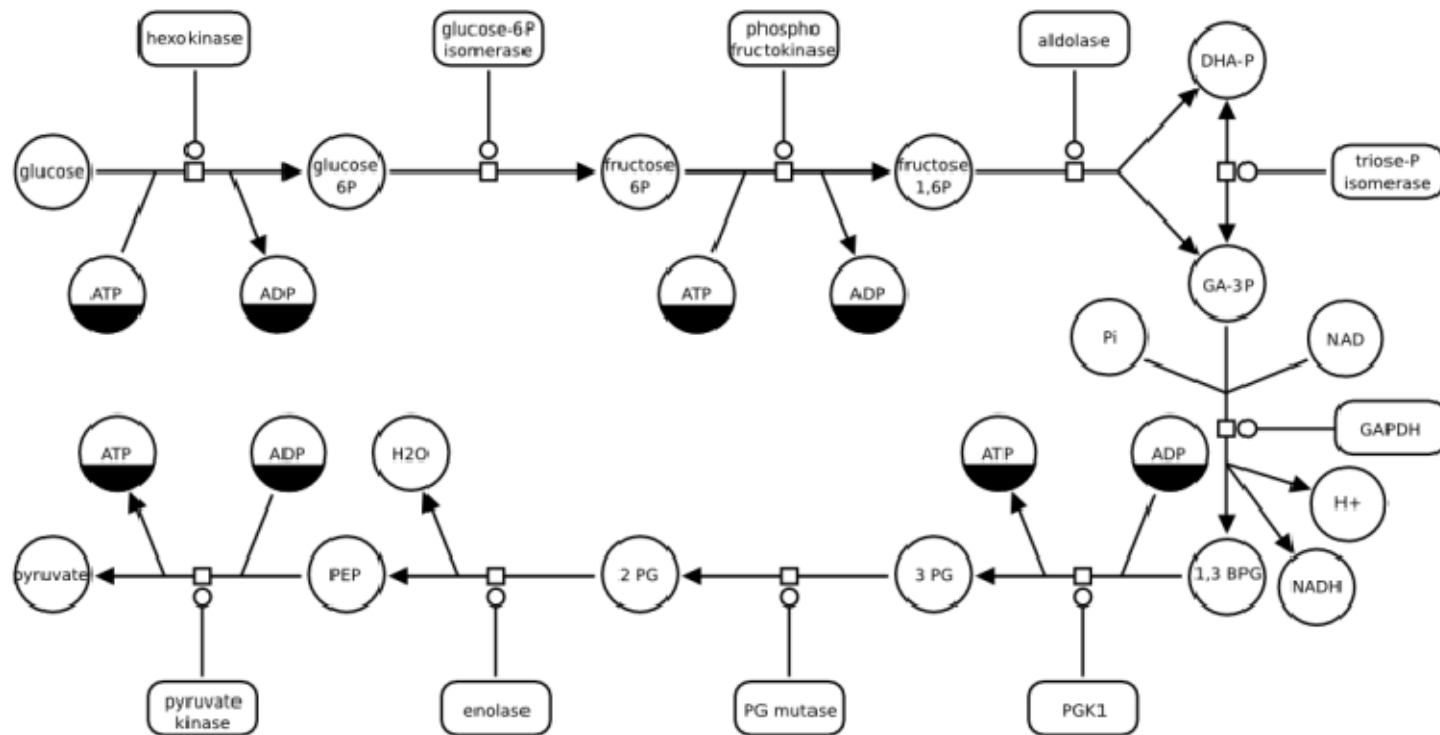




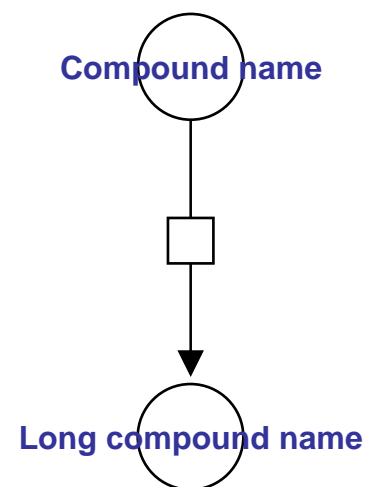
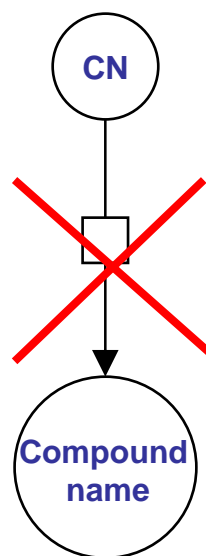
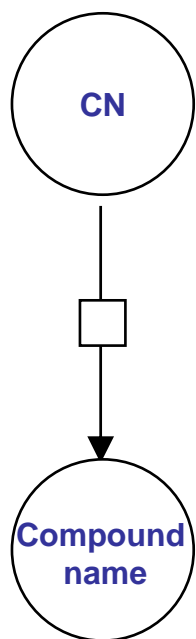
- Proposed new shape for simple chemical
- Proposed new entity: functional gate (EC)
- Proposed new entity: identity gate

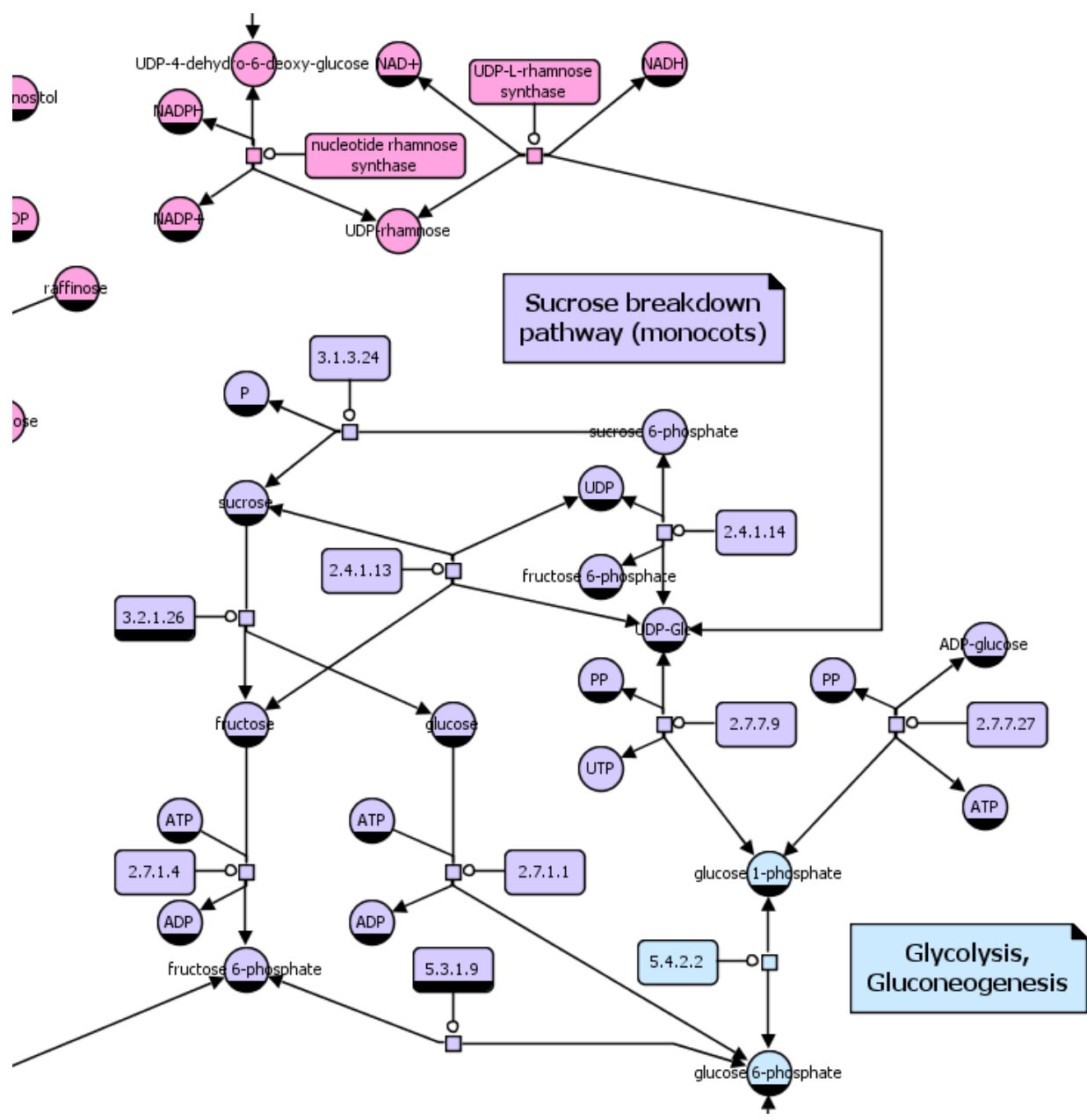


LABEL

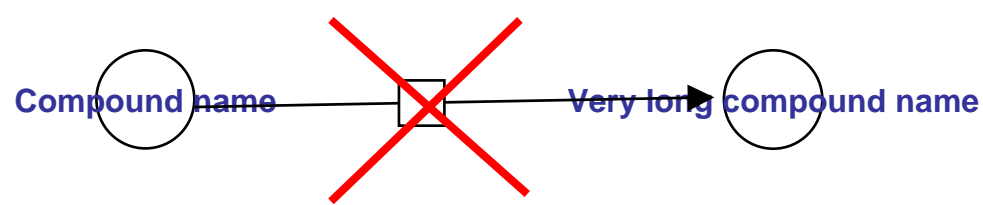
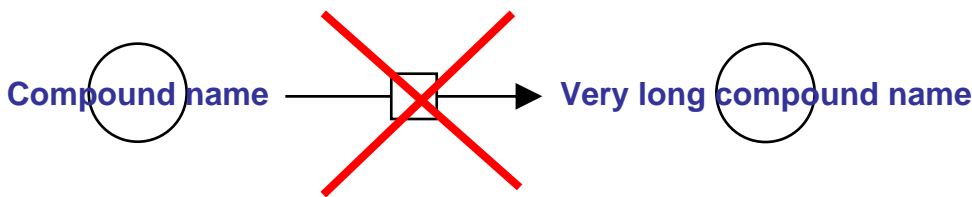
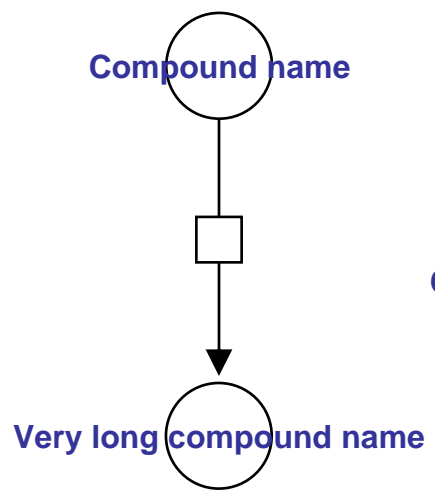
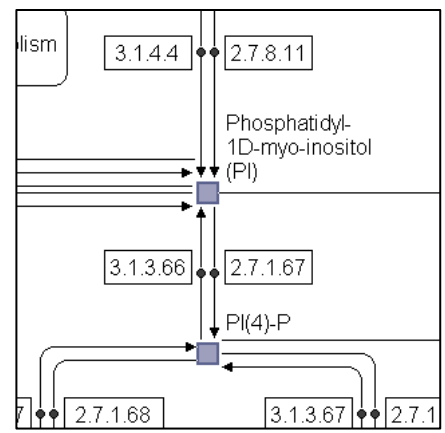
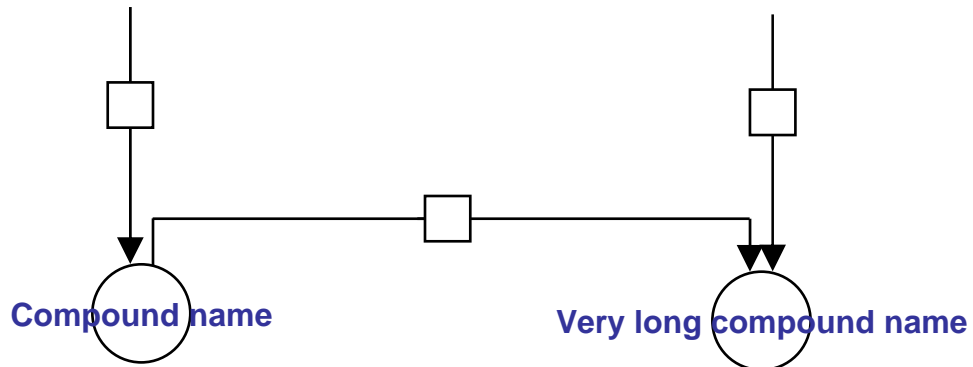


Compound name inside shape

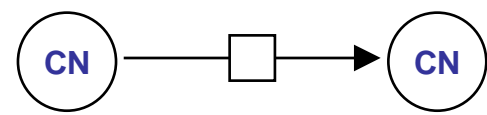




Compound name

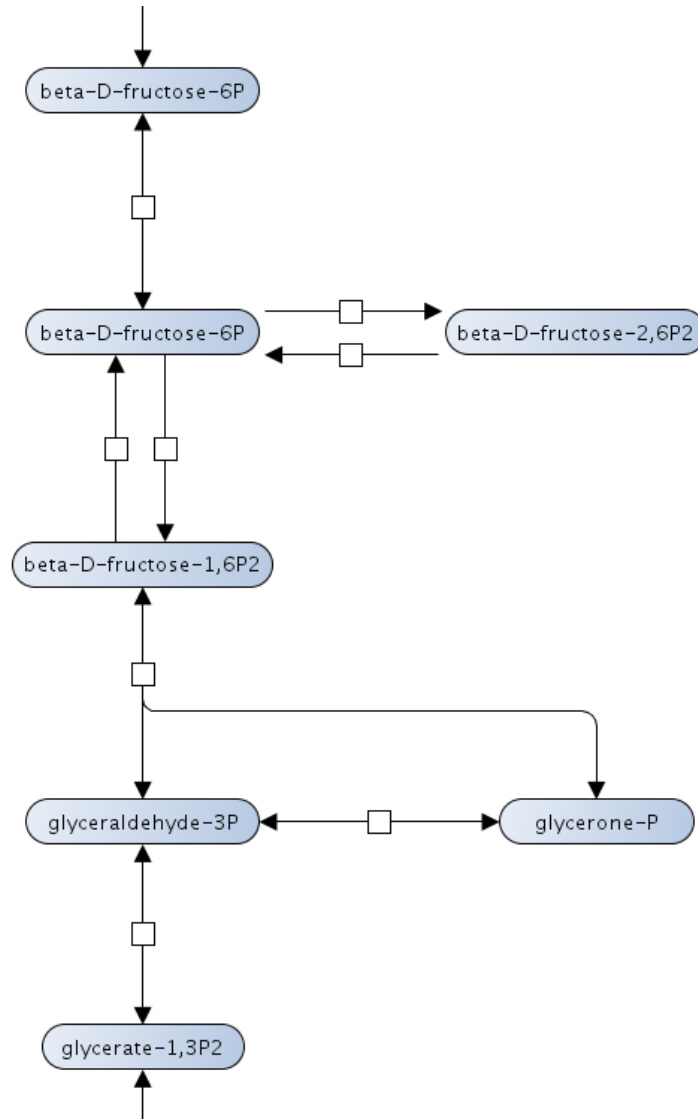


Additional work is required in order to prepare abbreviation for each compound



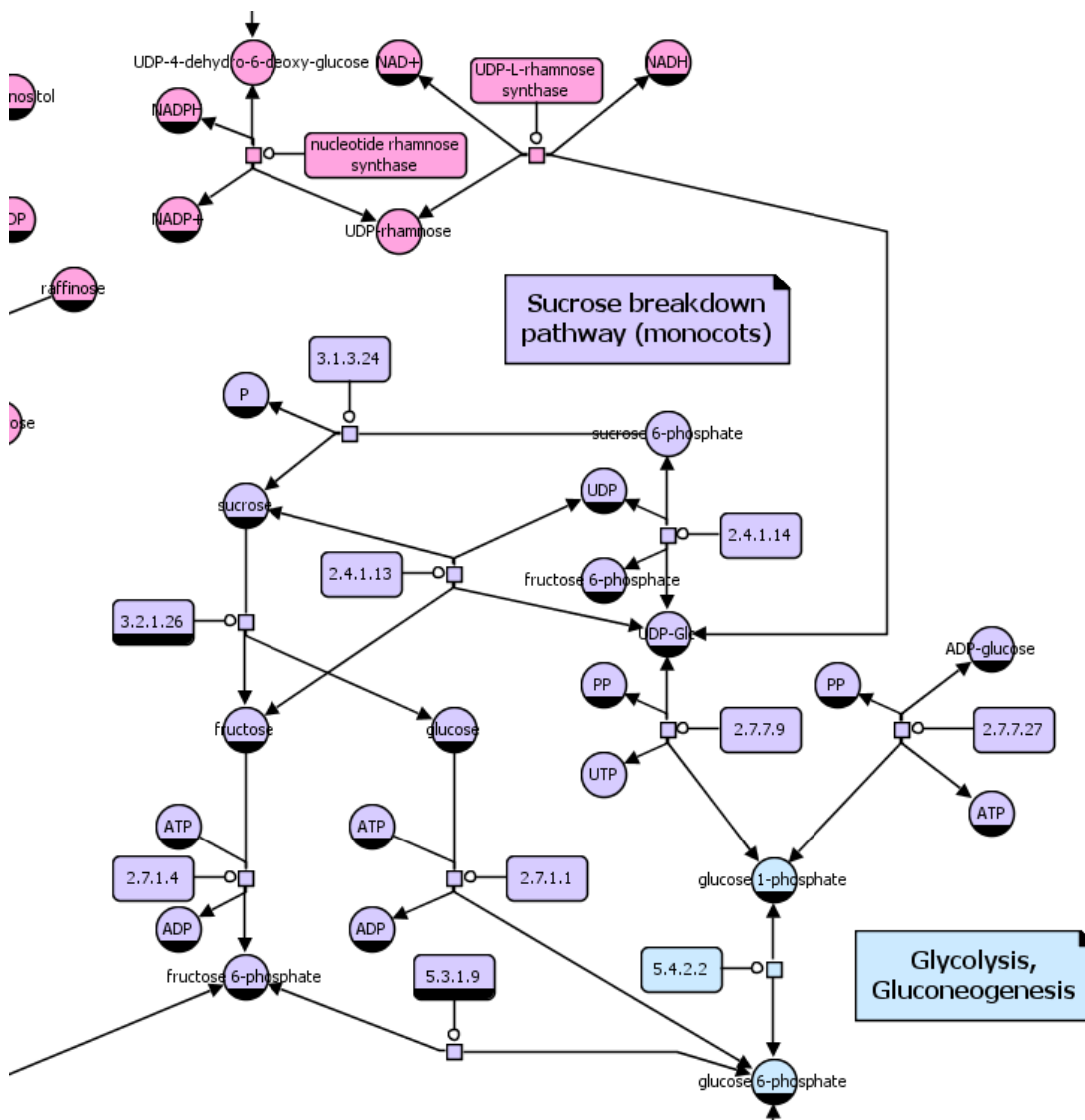
It is going to be more difficult to read maps with abbreviations instead of common compound names

Proposed new shape for simple chemical entity

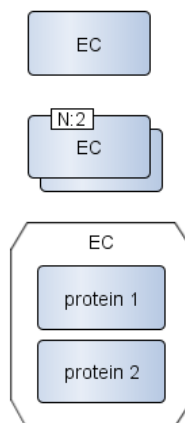
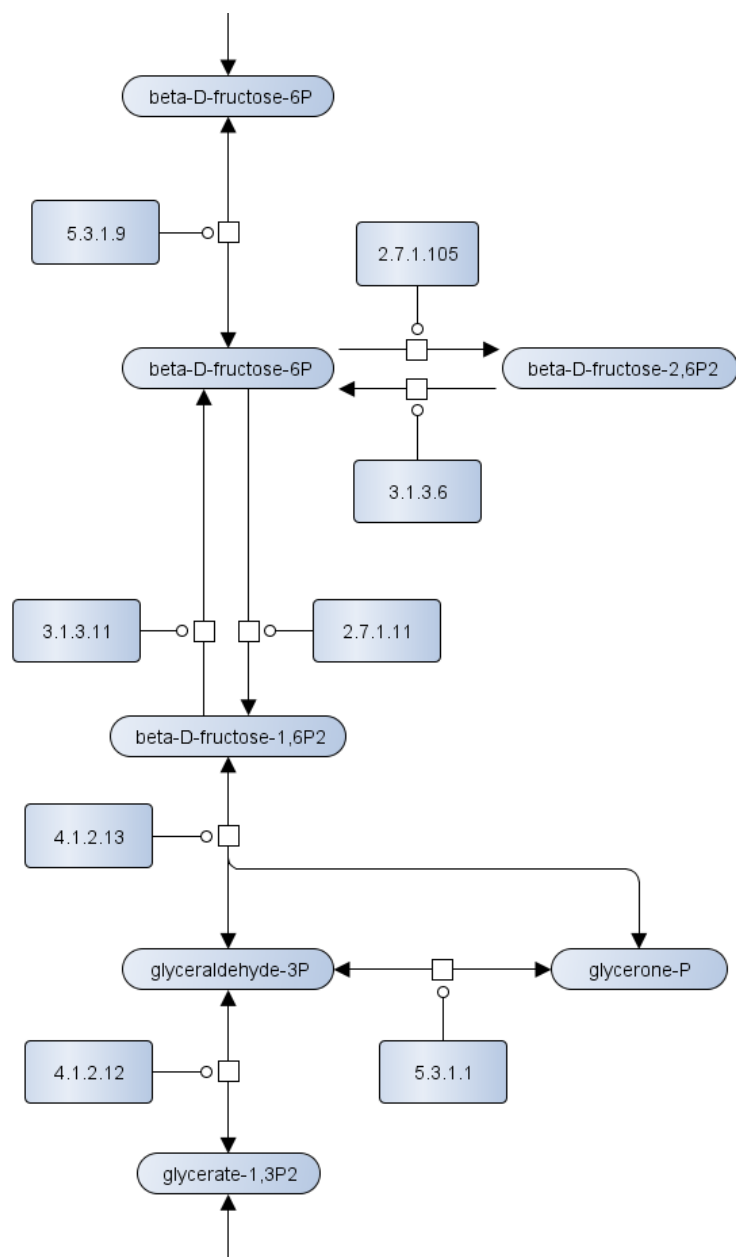




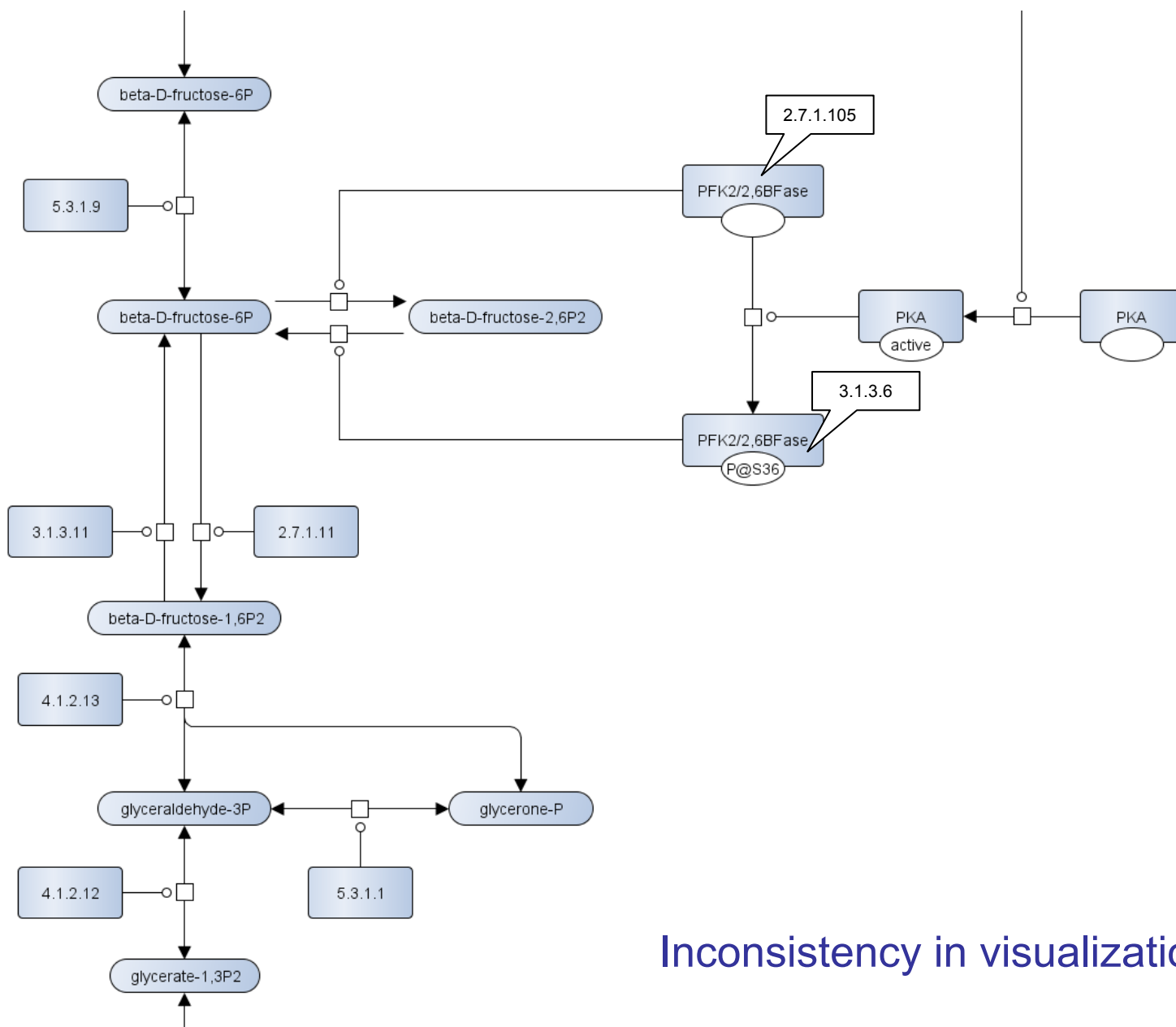
EC



EC is the most compact and informative way to show protein function on a metabolic diagram

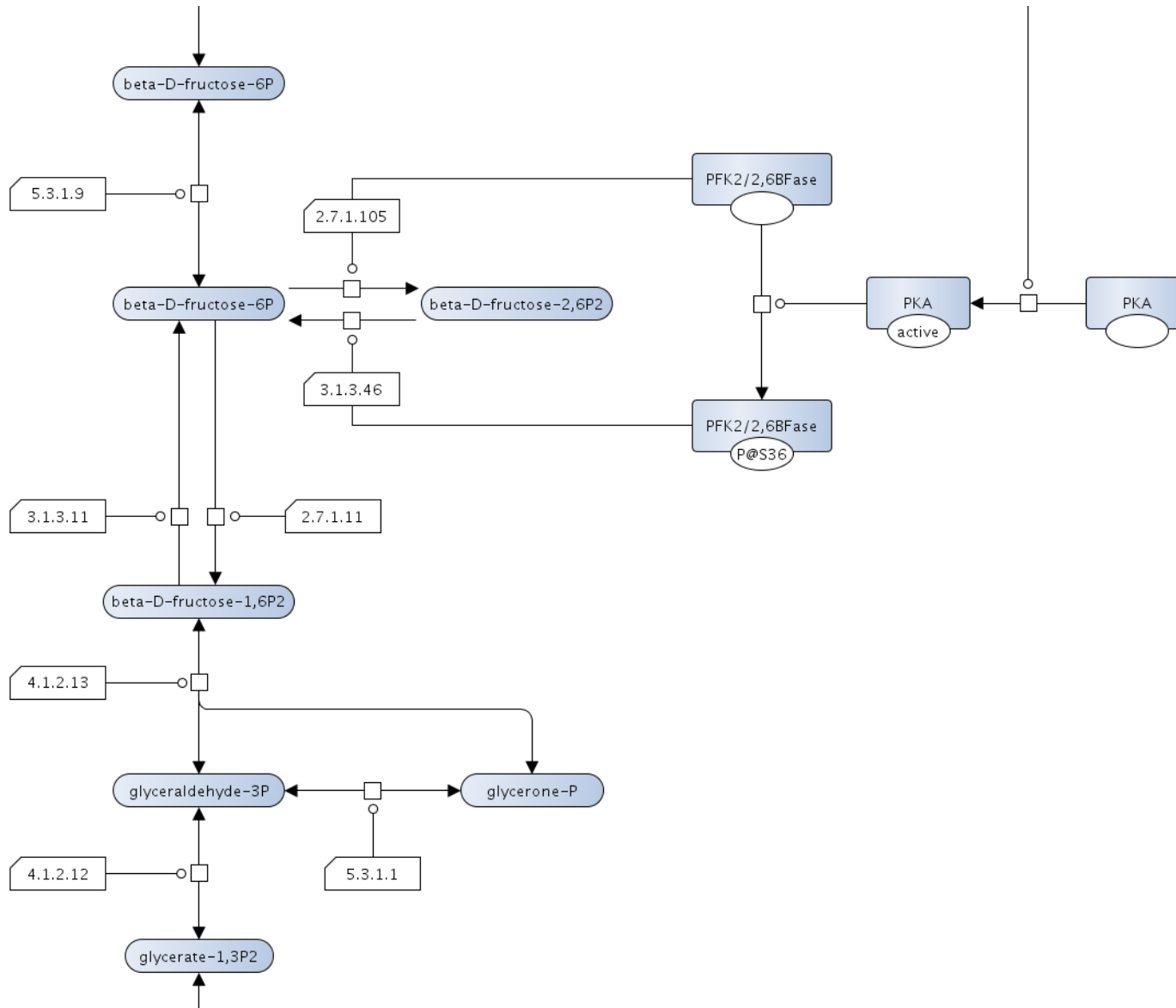


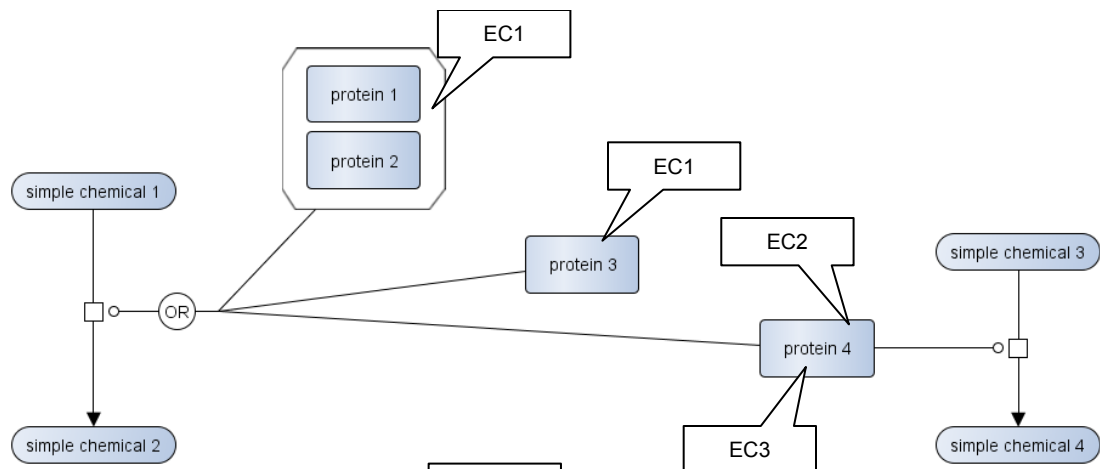
EC is shown as a generic protein, that could symbolize a protein, or a multimer, or a complex



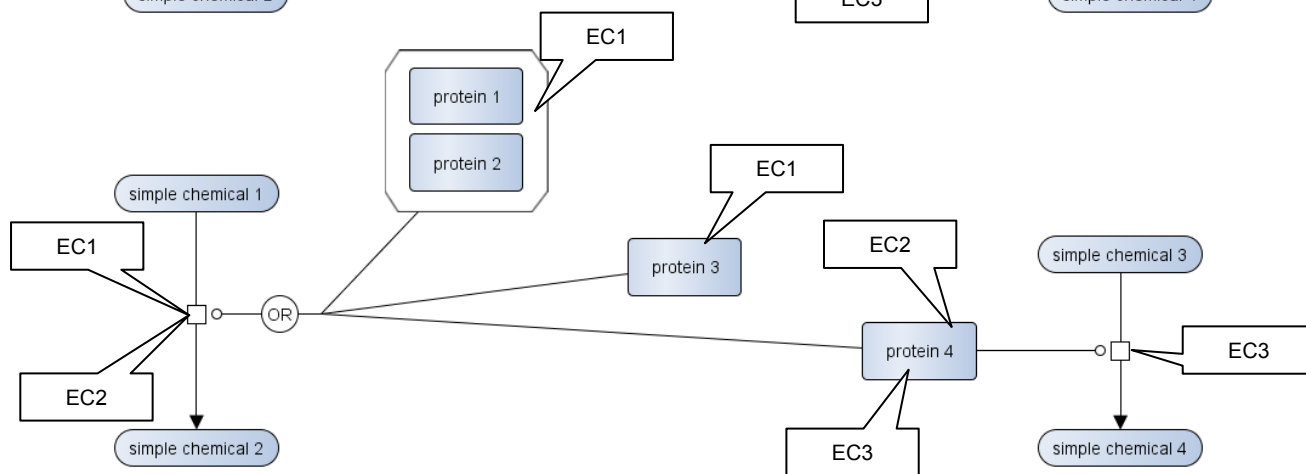
Inconsistency in visualization

Proposed new entity: functional gate





ambiguous

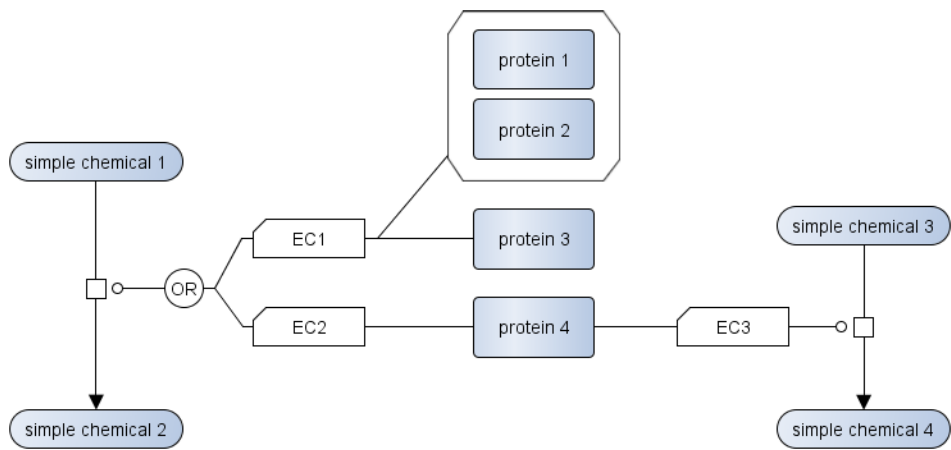


unambiguous

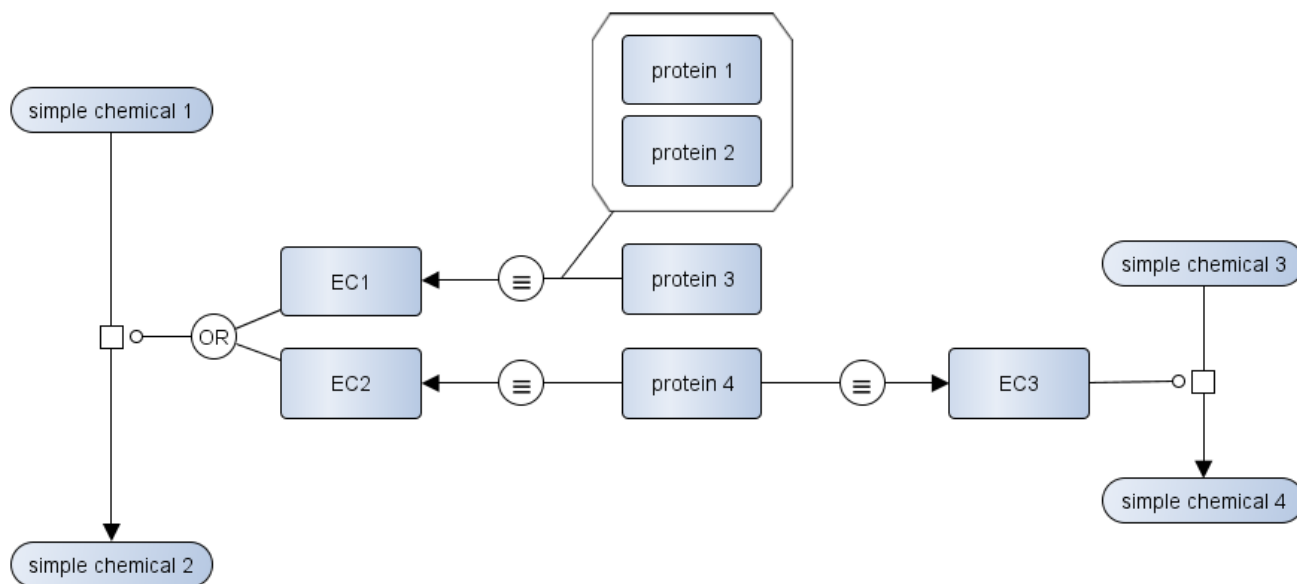
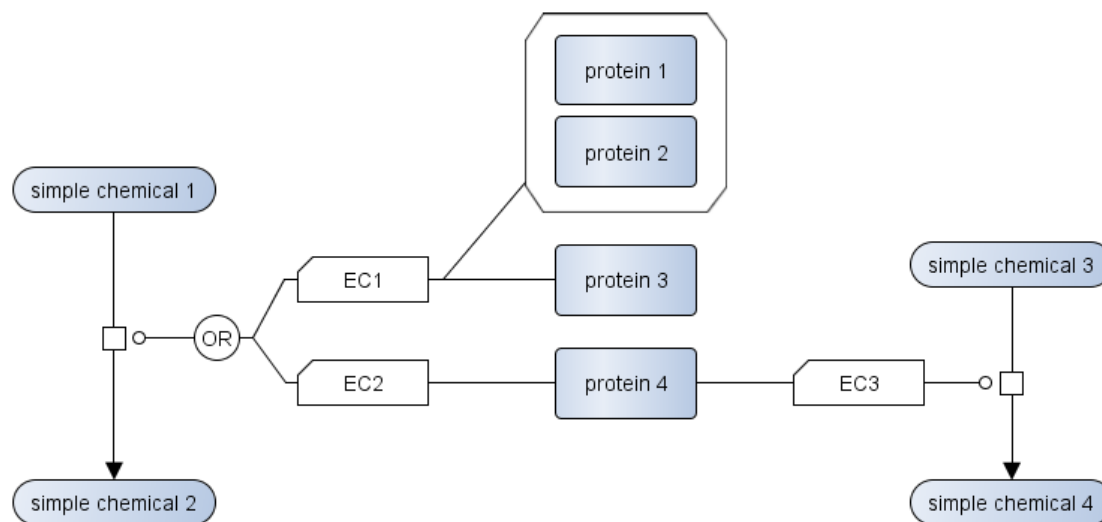
difficult to read

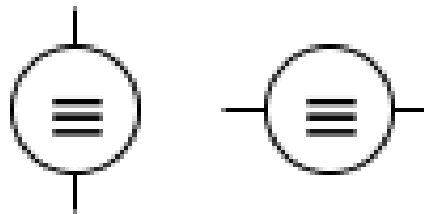
unambiguous

easy to read

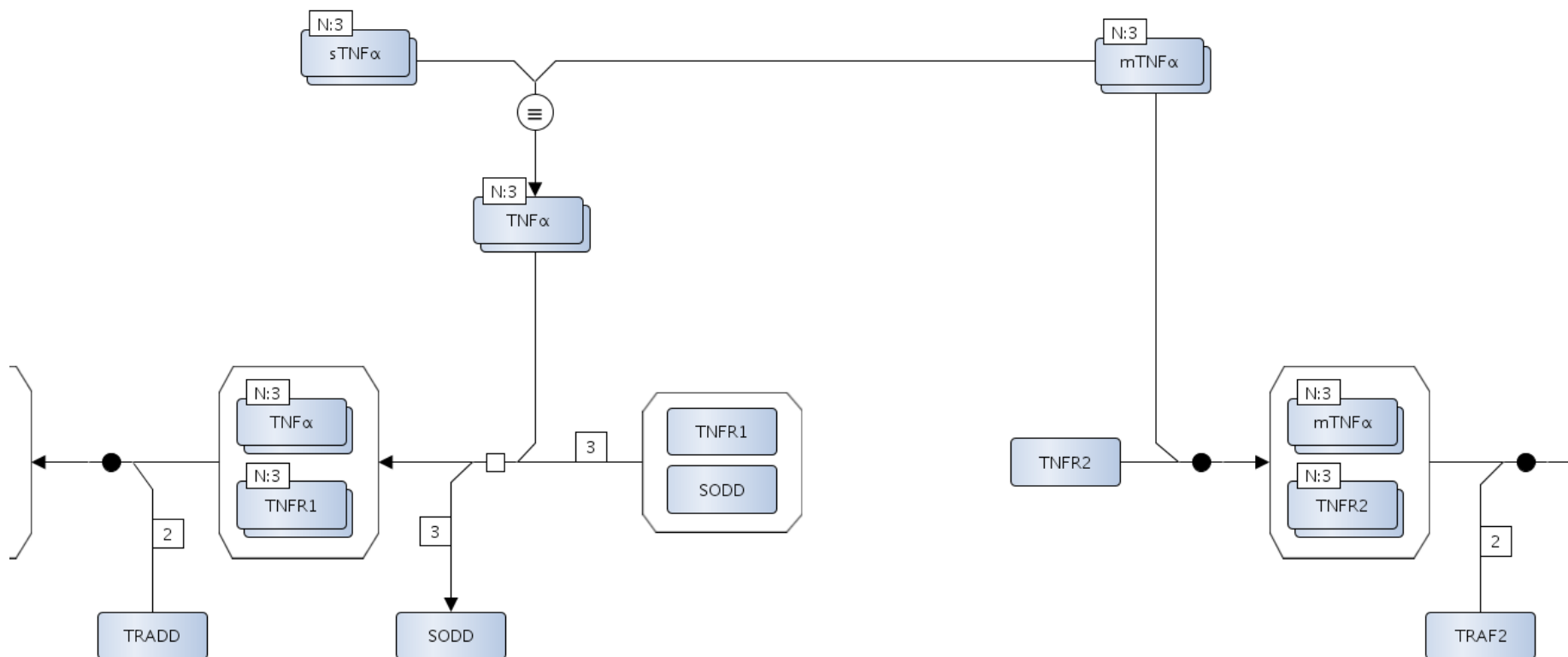


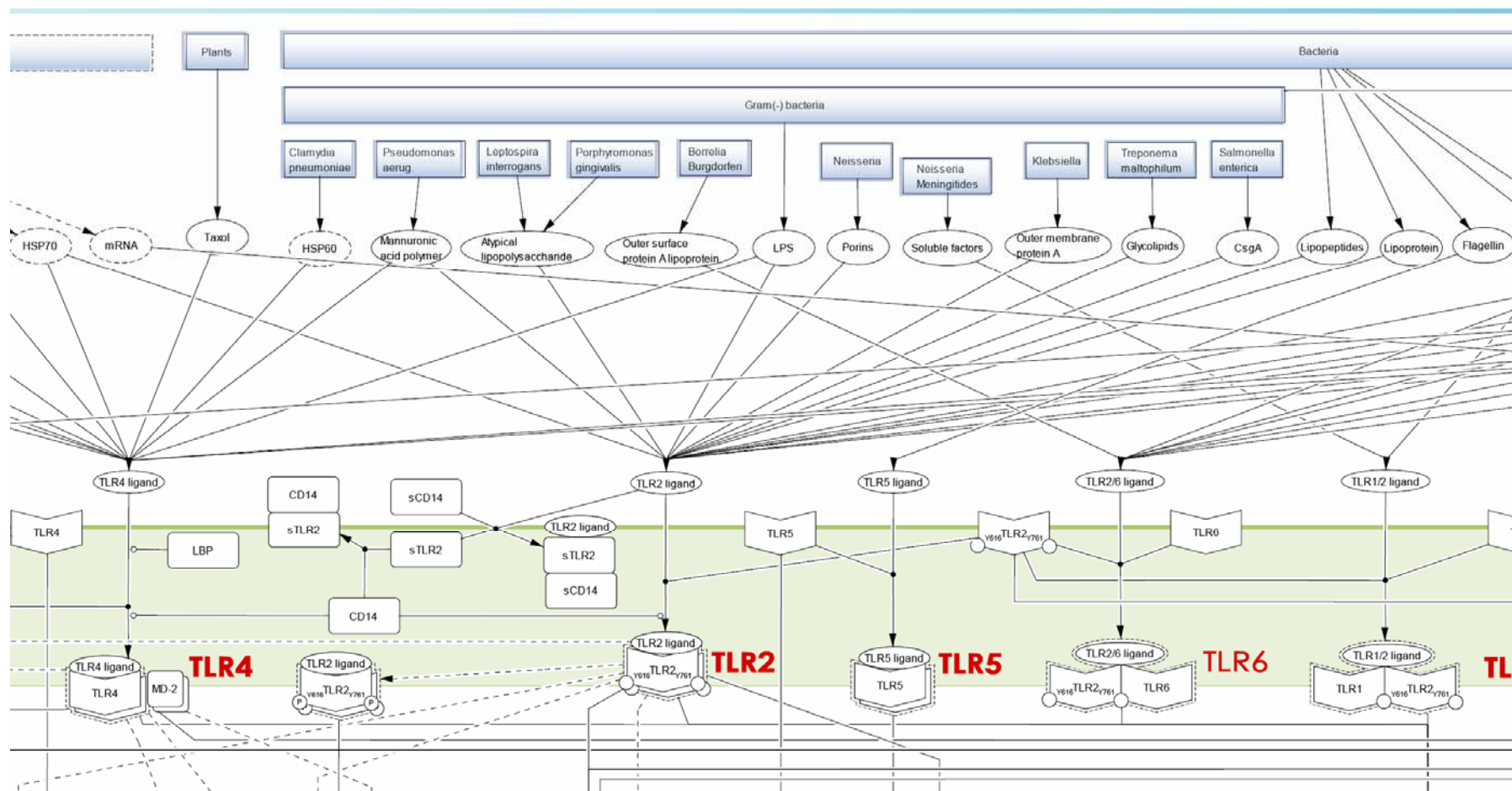
Using identity gate instead of functional gate



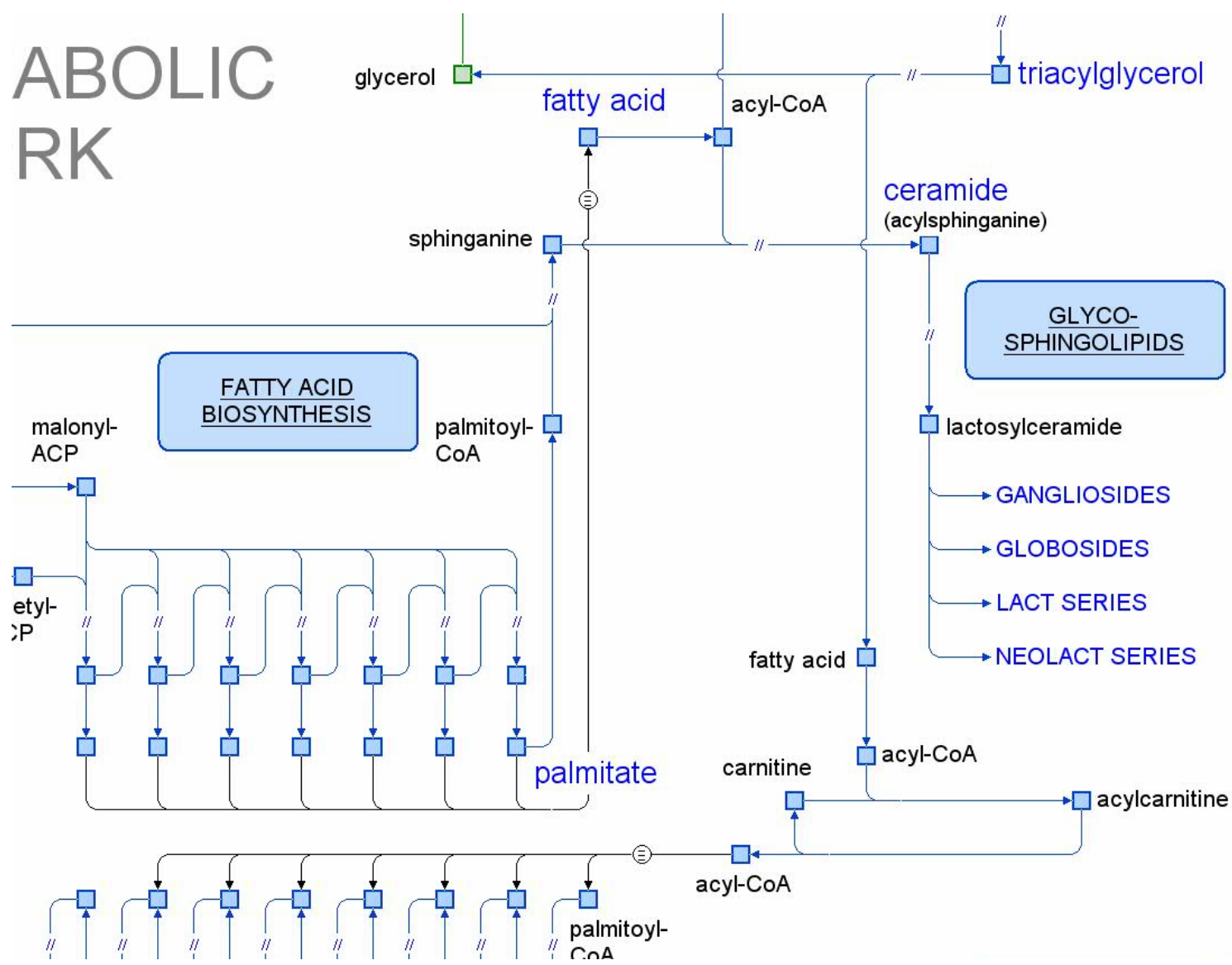


Identity gate

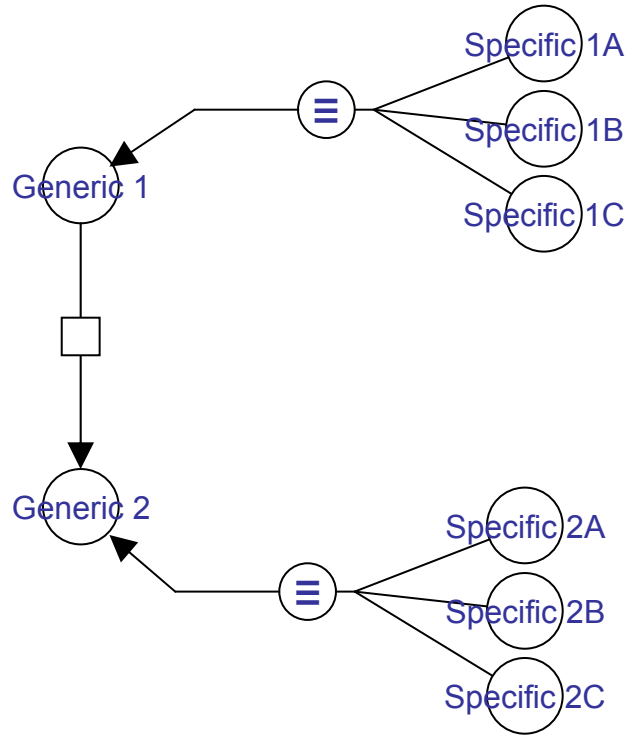




ABOLIC RK



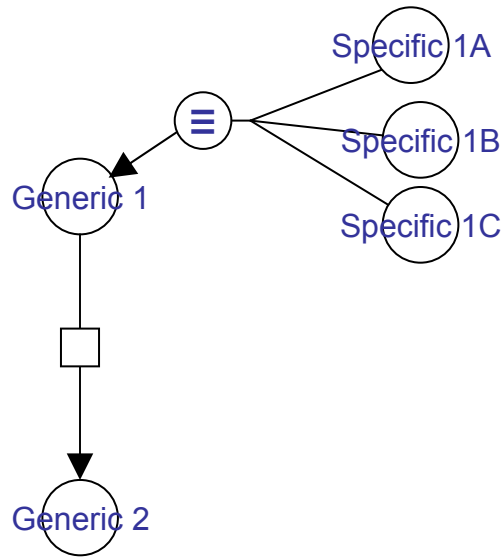
Potentially using identity gates might cause ambiguity



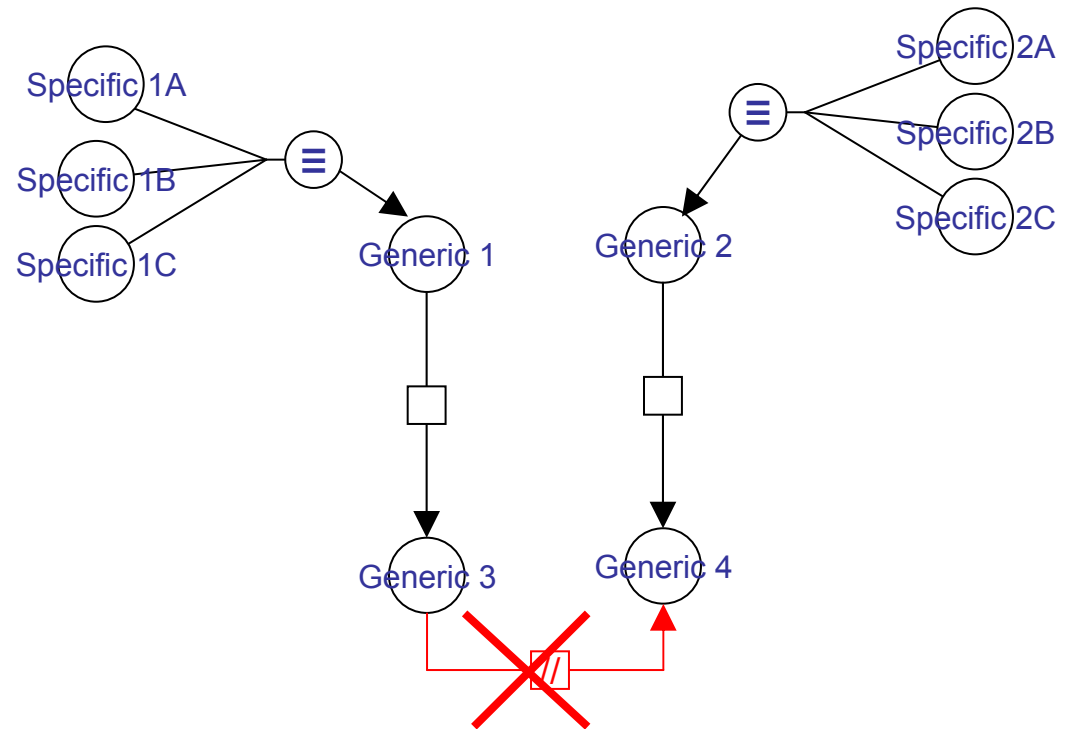
~~1A -> 2A
1A -> 2B
1A -> 2C
1B -> 2A
1B -> 2B
1B -> 2C
1C -> 2A
1C -> 2B
1C -> 2C~~

1A -> 2A
1B -> 2B
1C -> 2C

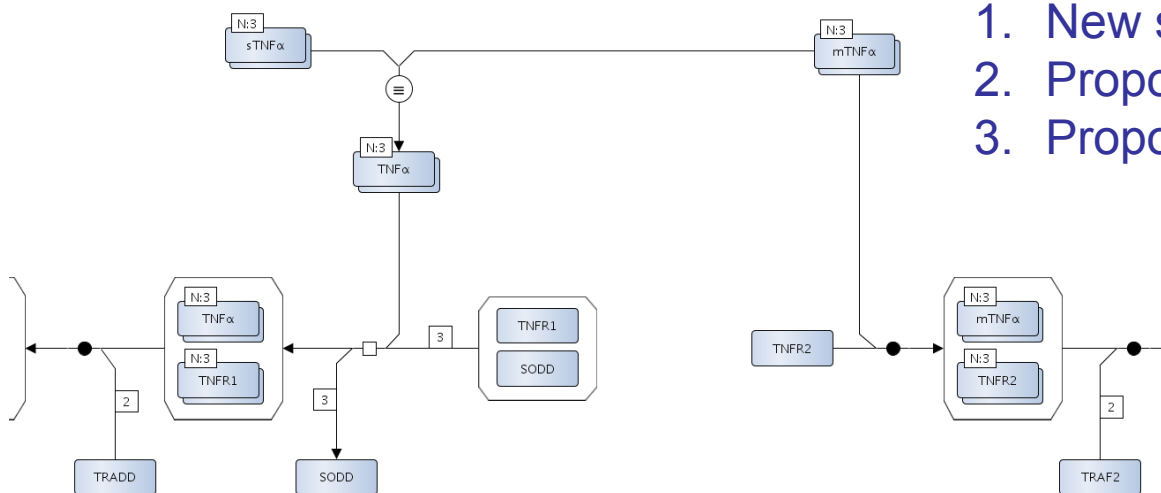
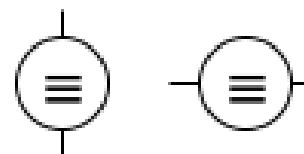
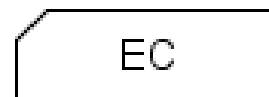
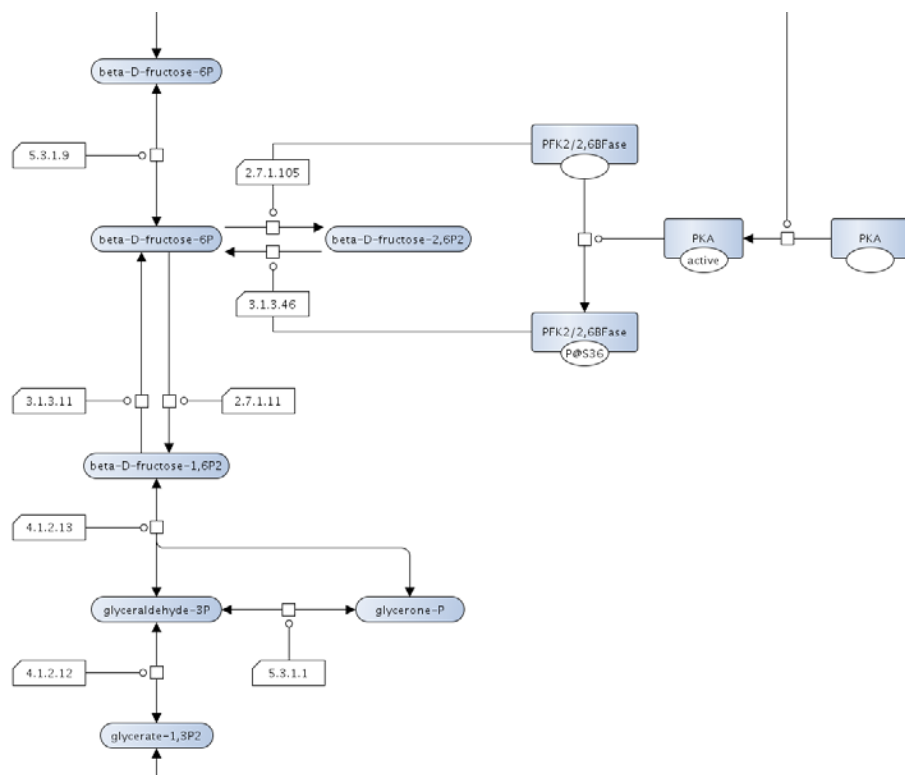
Possible solution: introducing restrictions



Only 1 identity gate on a map



Many unconnected inputs



1. New shape for simple chemicals
2. Proposed new entity: functional gate
3. Proposed new entity: identity gate

Acknowledgments



Stuart Moodie
Anatoly Sorokin
Igor Goryanin



Thank you