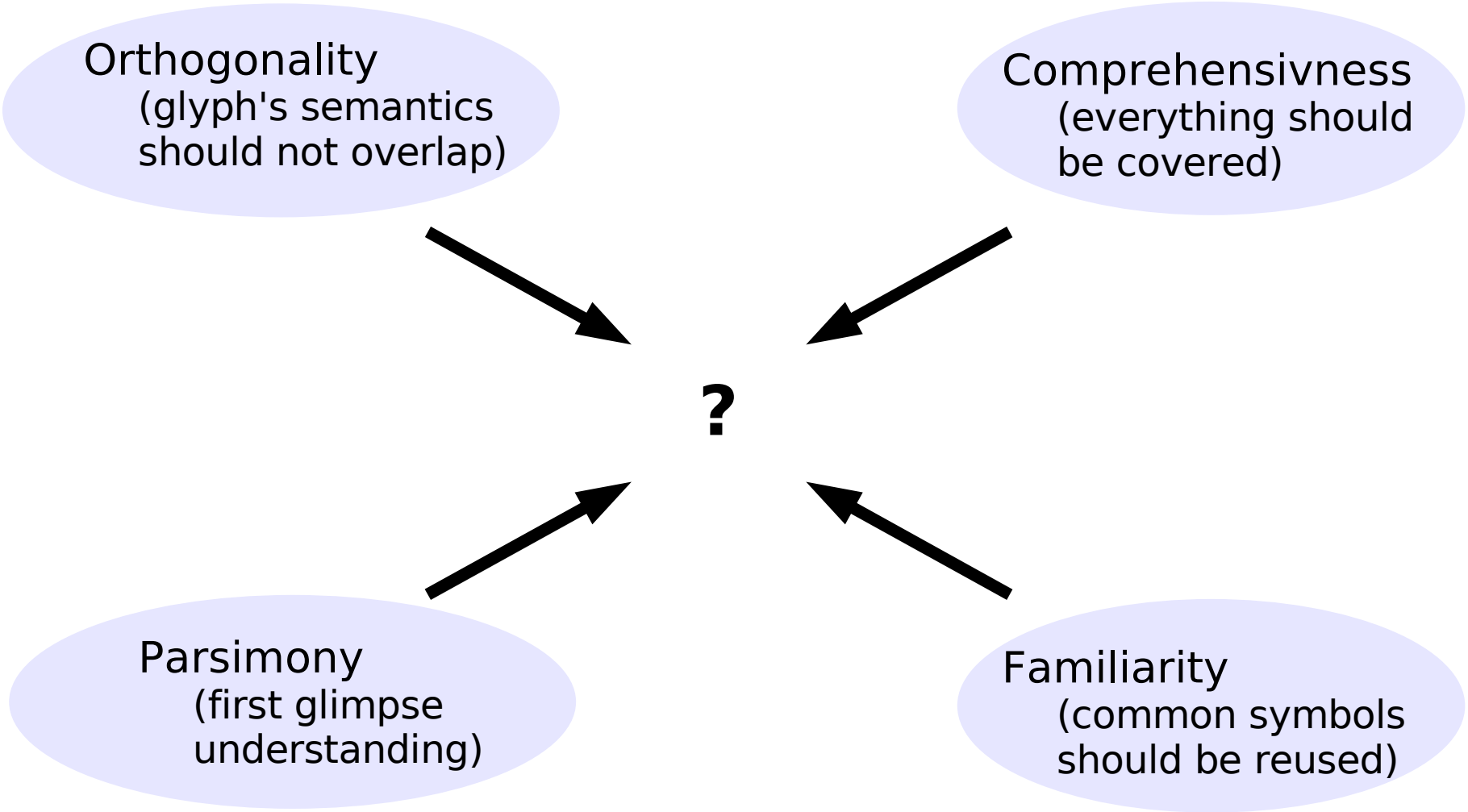
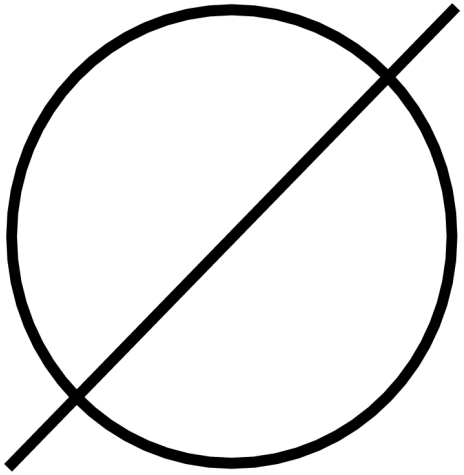
Toward SBGN Level-1 (bis)

The constraints



Preliminary remarks

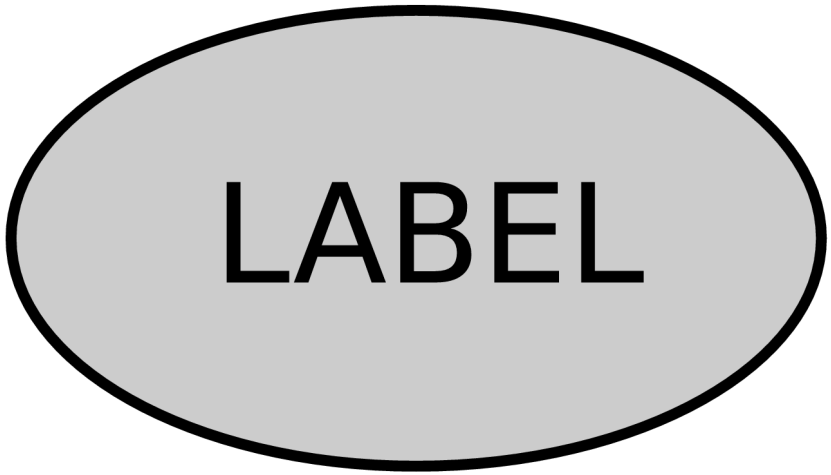
- Process Diagram => State Transition
- SBGN will have ER and ST (agreed in SBGN-1)
- SBGN should be colour independent
- SBGN should be “thickness” independant
- Symbols should be identical in ST and ER as much as possible
- Our audience is not the specialist field but the biologist community: 20-25 basic symbols are the upper boundary for SBGN Level 1 (agreed in SBGN-1)



Should-it be independent of processes?

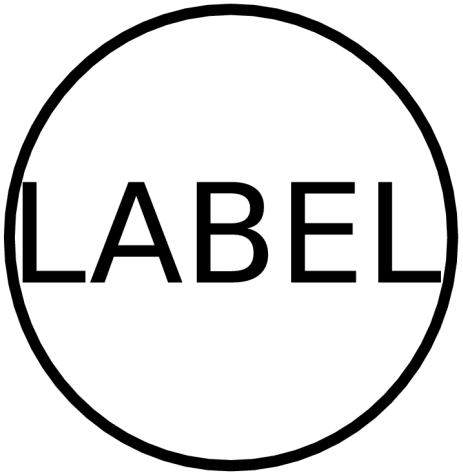
unspecified

Type of a state or an entity that is unknown, or irrelevant in the context. This can be the case if its existence has been inferred indirectly, or if the entity is a commodity created for the needs of a model.

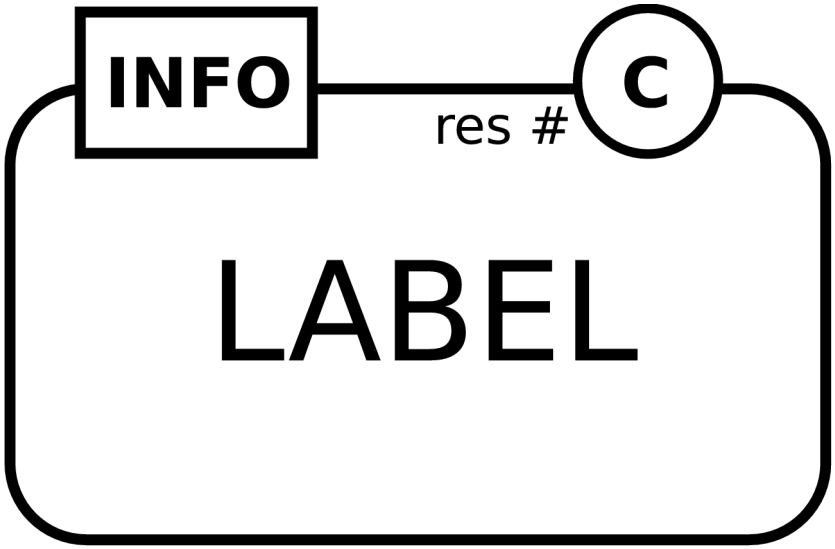


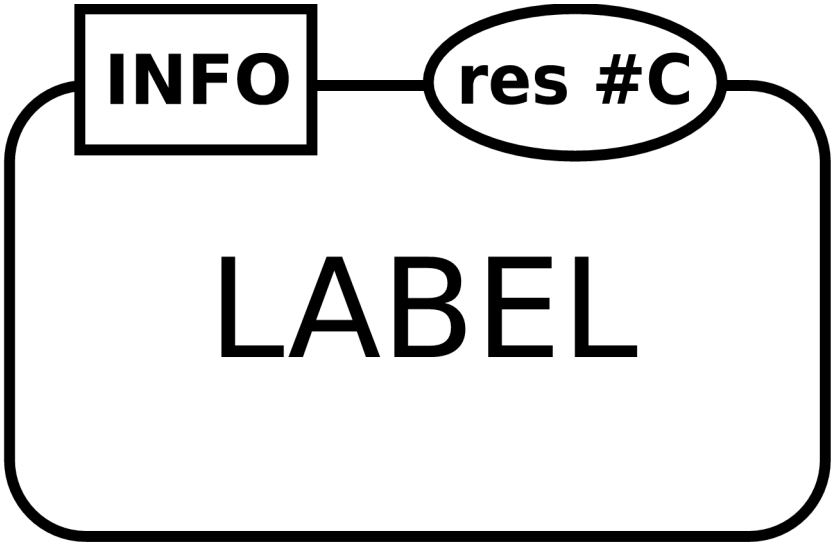
simple chemical

Chemical compound that is not formed by the covalent linking of pseudo-identical residues. Examples of simple chemicals are: an atom, a monoatomic ion, a salt, a radical, a solid metal, a crystal etc.



State or entity built upon the covalent linking of pseudo-identical units. Examples are proteins, nucleic acids (RNA, DNA) or polysaccharides (glycogen, cellulose, starch).

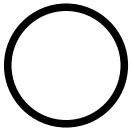




States/entity nodes: modificators

- state variable
  (covalent modification, conformation, isoform ...)

  - covalent modification



empty modification

any modification

unknown modification

phosphorylation (acetylation: Ac, glycosylation: G, hydroxylation: OH, methylation: Me, myristoylation: My, palmytoylation: Pa, phosphorylation: P, prenylation: Pr, protonation: H, sulfation: S, ubiquitination: Ub)

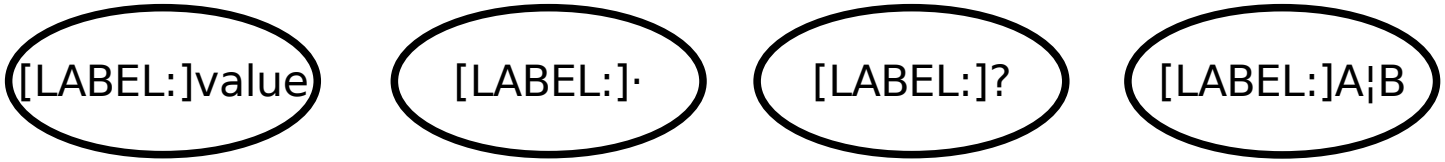
More discussion is needed to evaluate the outreach of the unit of info

The idea of a controlled vocabulary has been proposed to define macromol

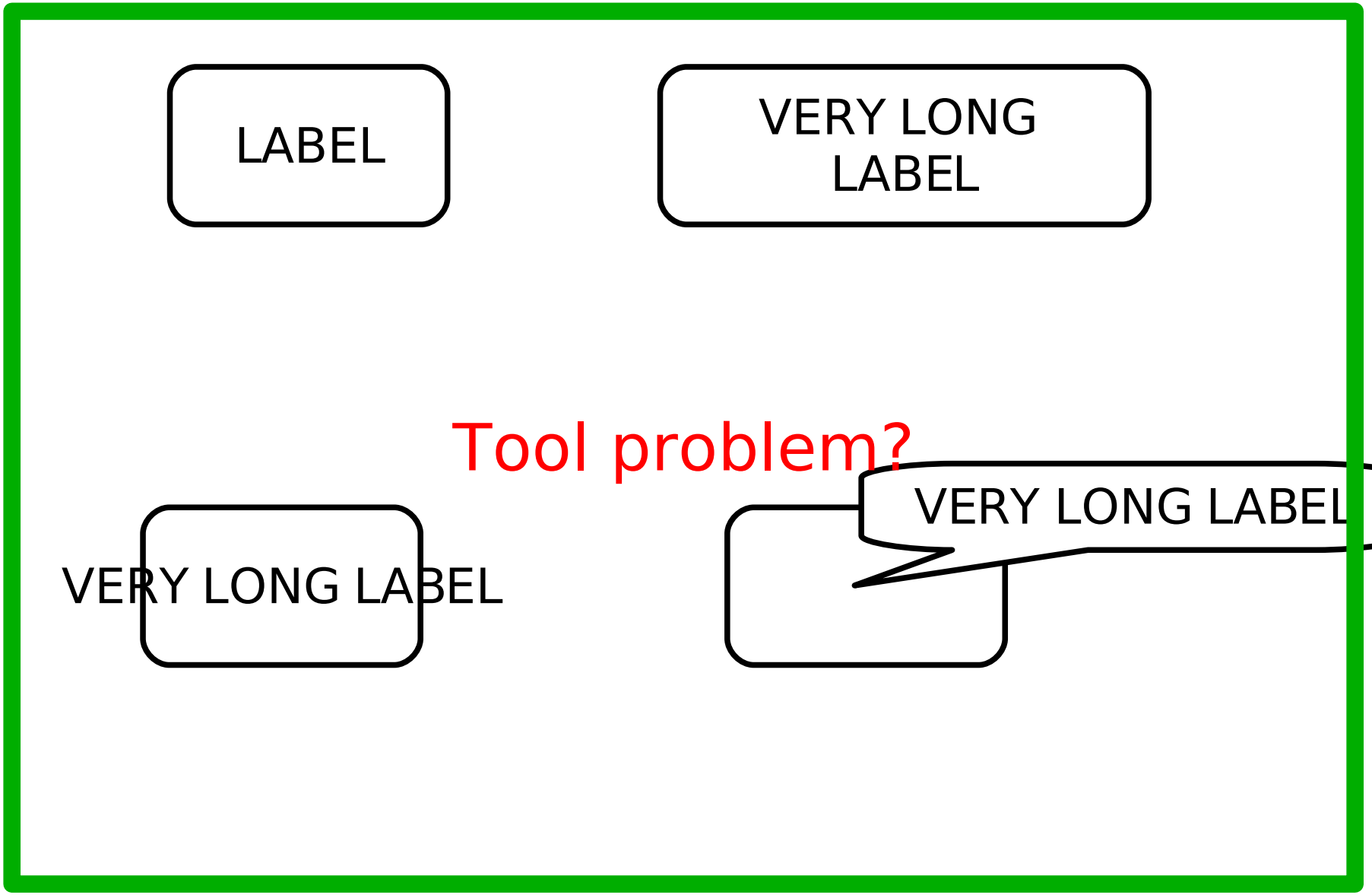
- unit of information
  (binding site, piece of genet info continuous variable)

States/entity nodes: modificators

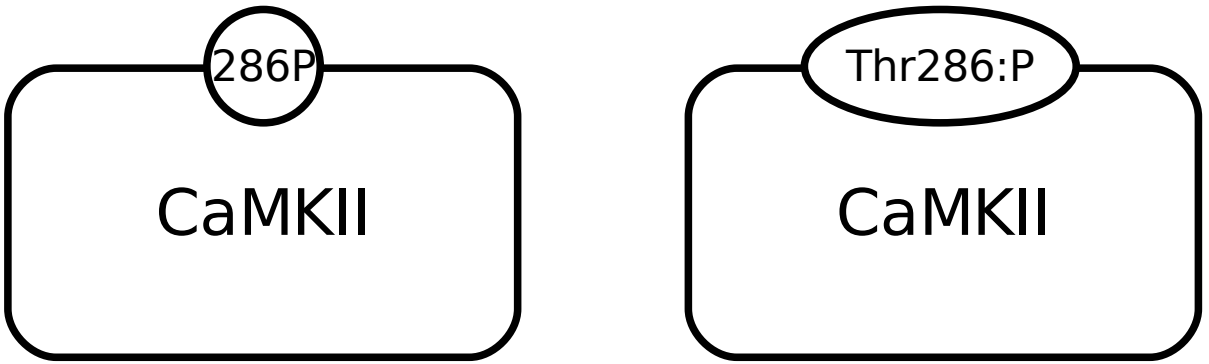
- Can a state variable not be restricted to binary states? What about multiple states, such as inactive, active and desensitised?
- If non-binary, how does ER deal with it?
- Boolean logic on state variables:



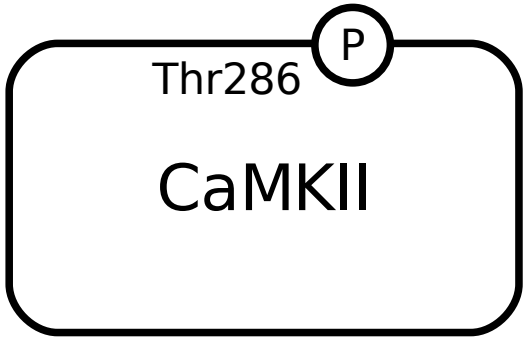
Label of state/entity nodes



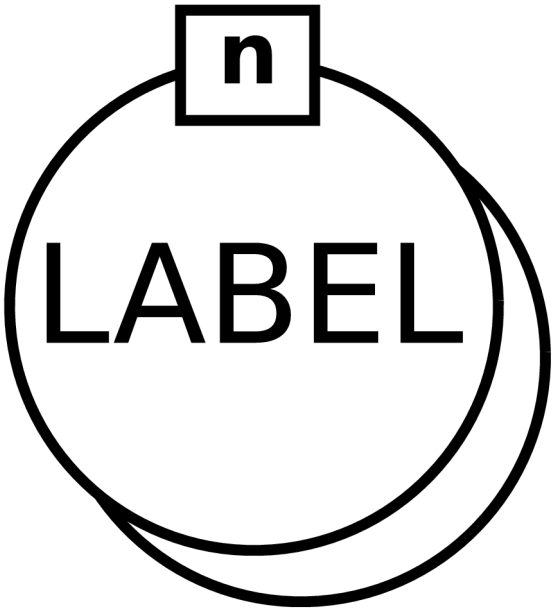
Label of state variables

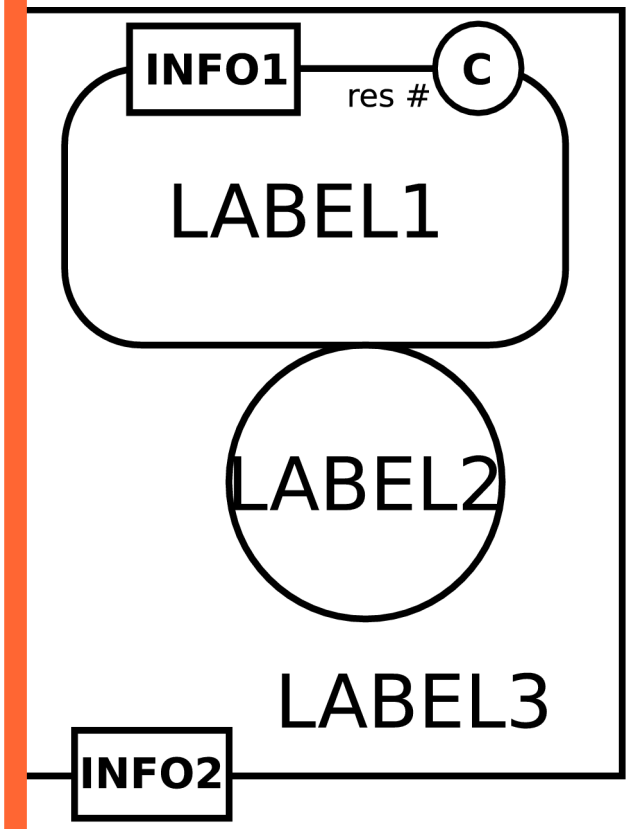


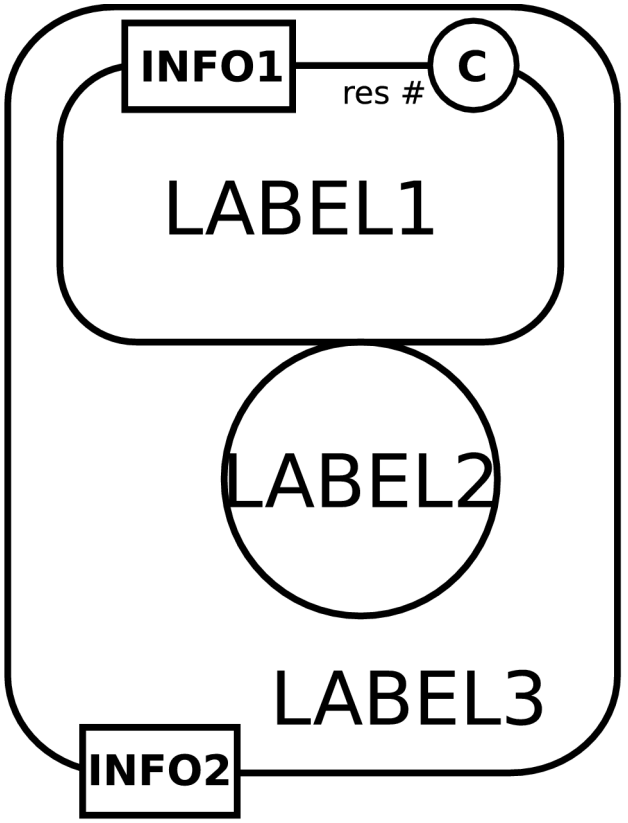
Tool problem?

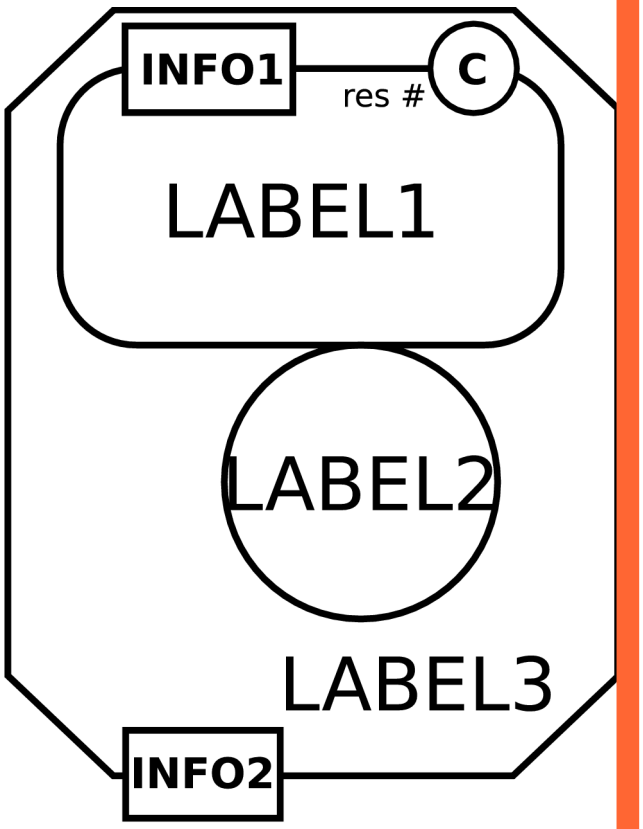



n
LABEL

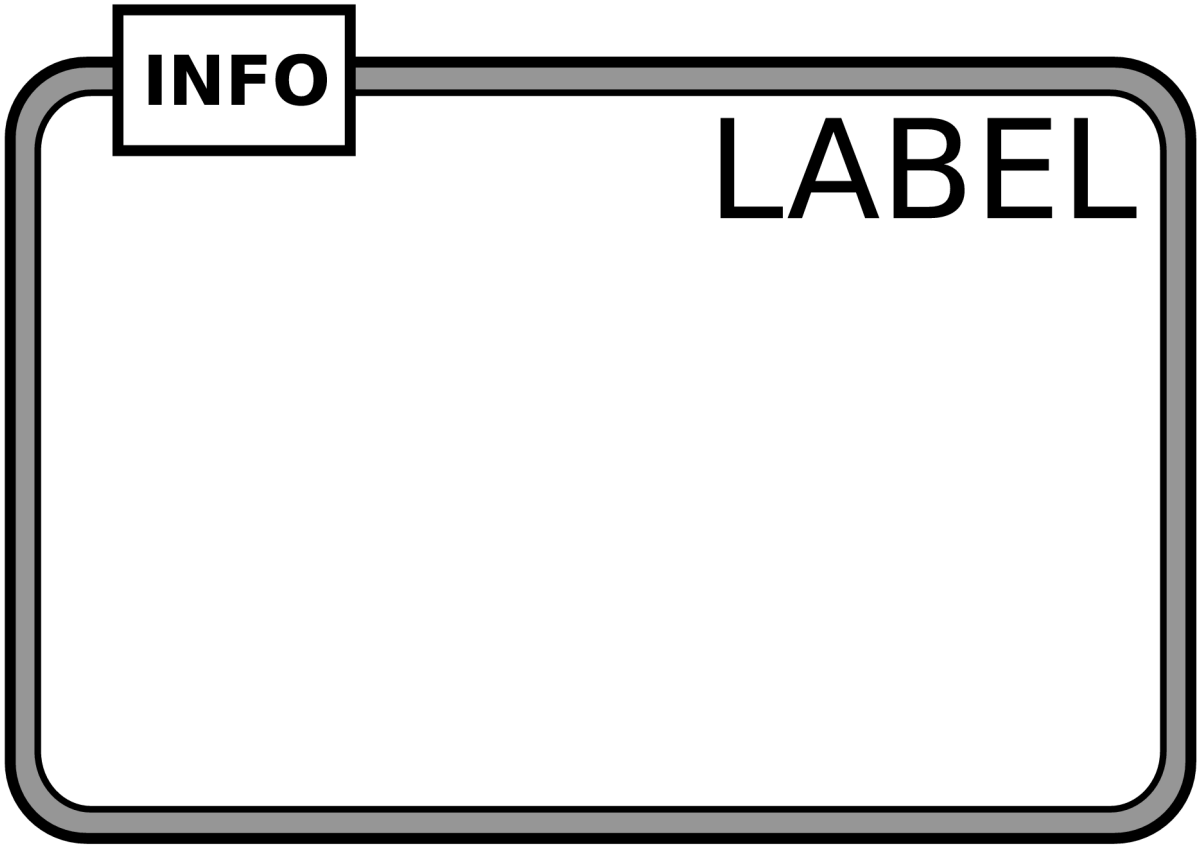

n
LABEL

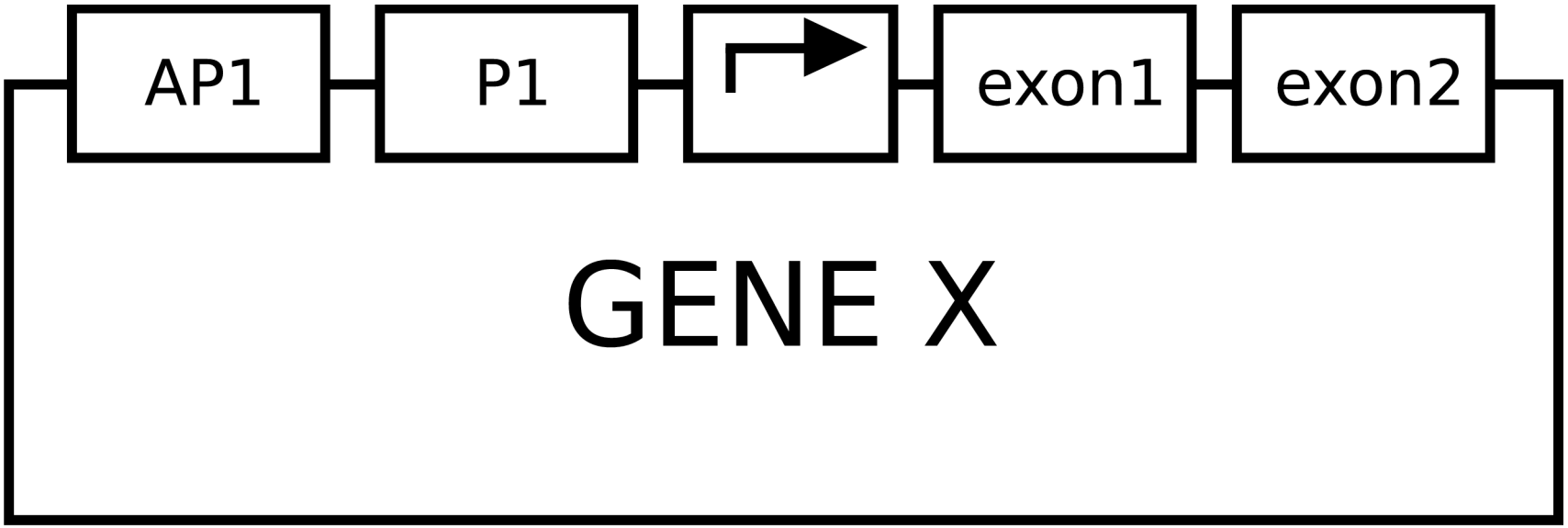




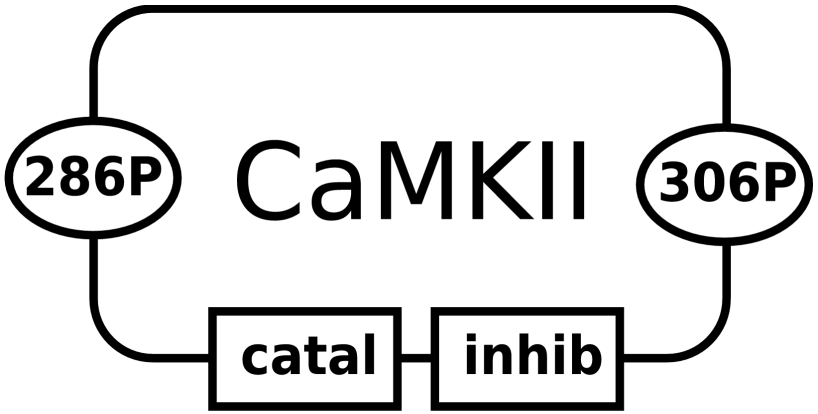


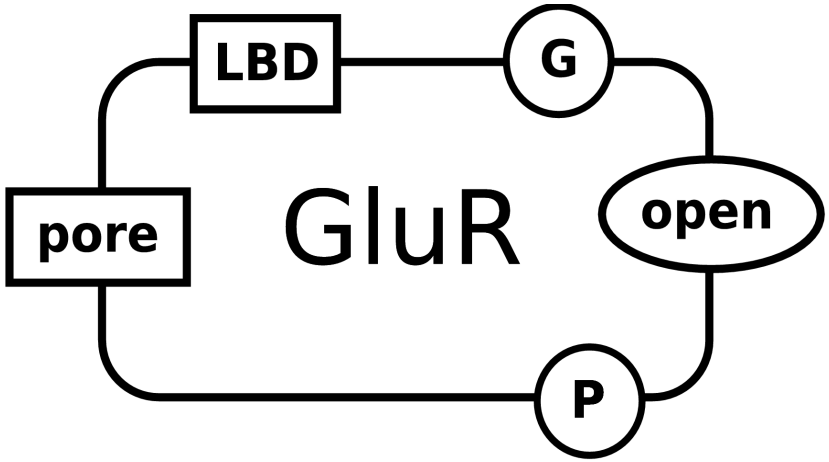
Shape of a complex. Is-it a module?
Is-it a macromolecule? Does-a module always contain processes?

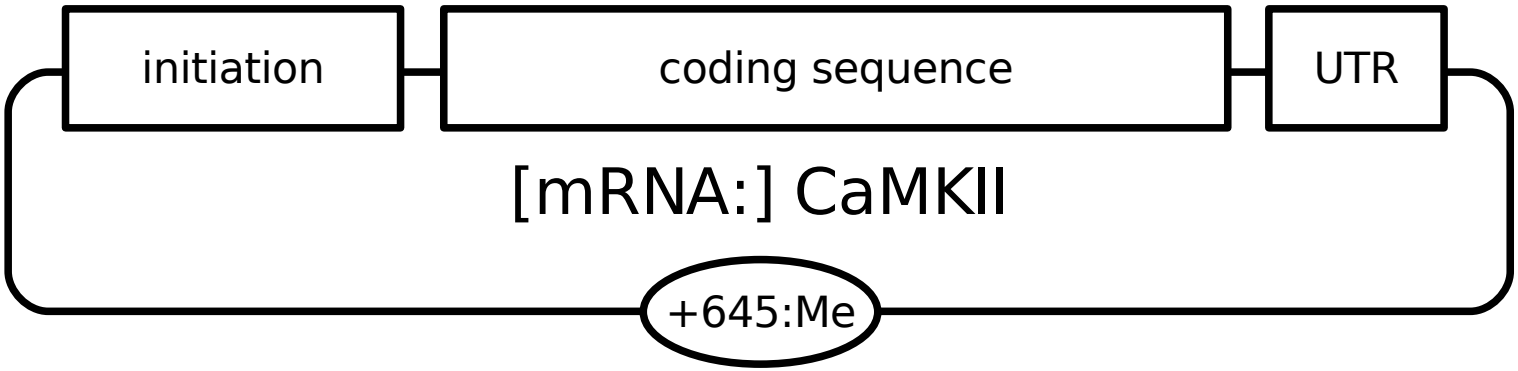

INFO
LABEL


AP1
P1
exon1
exon2
GENE X

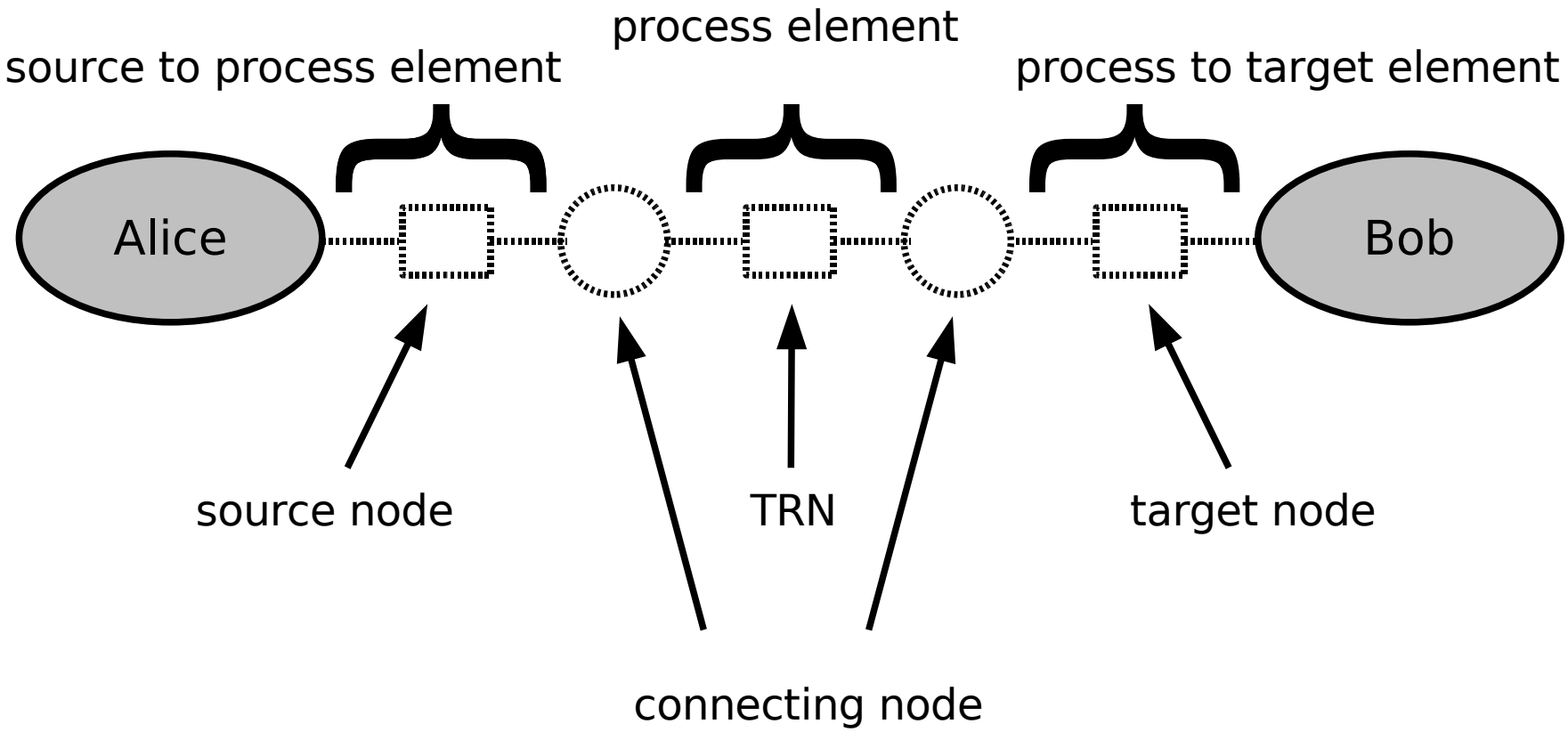
Complex SENs



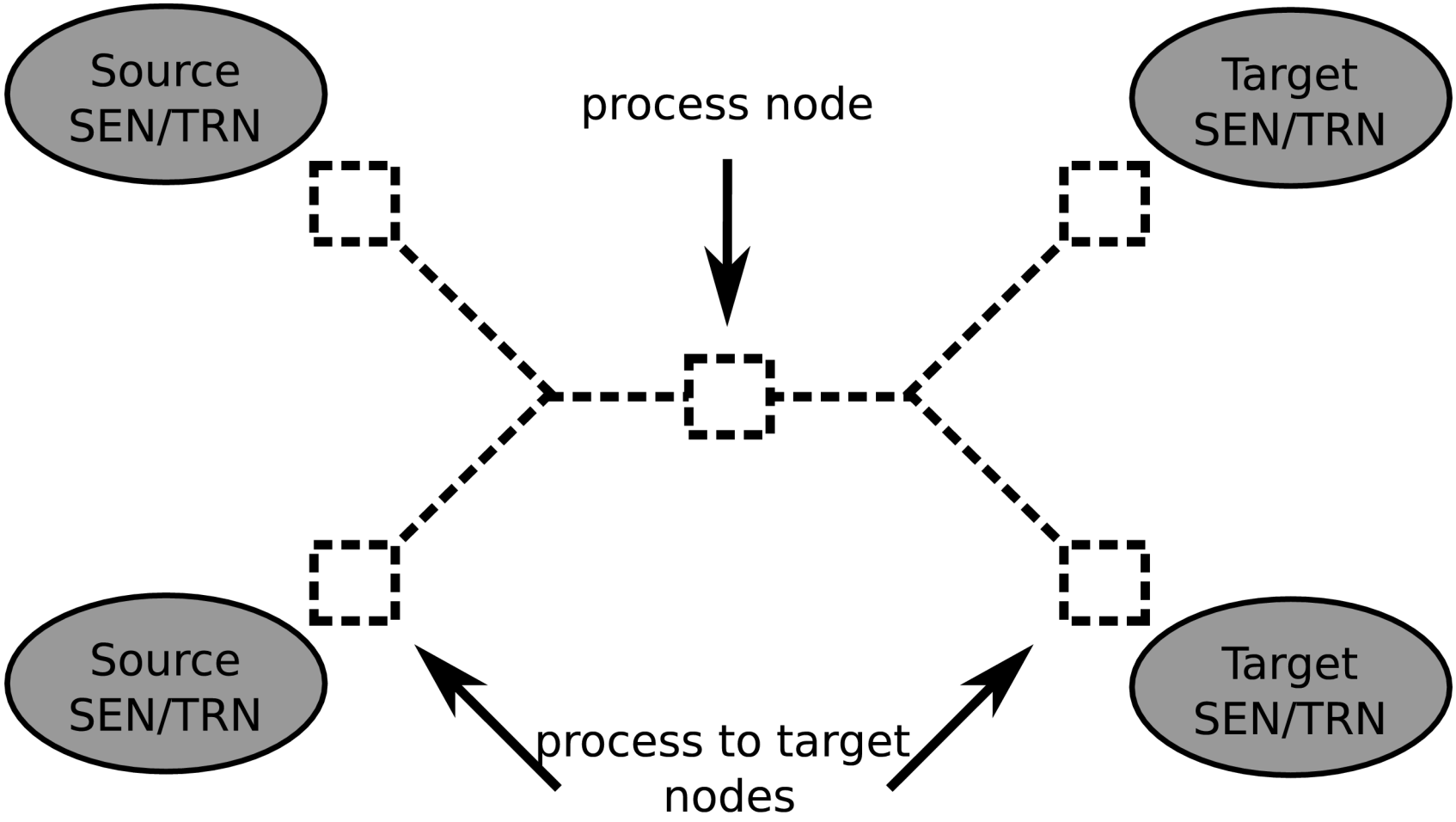




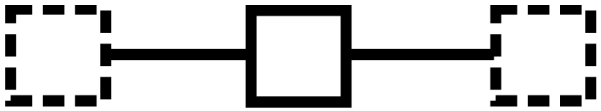
Structure of a process



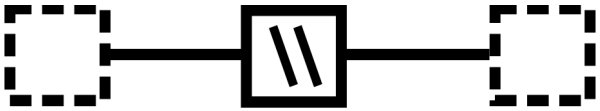
Structure of a process



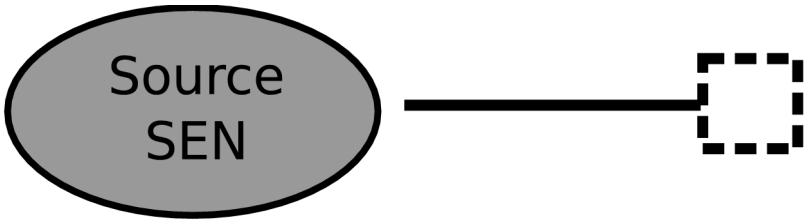
process transforming a set of states or entities in another set of states or entities

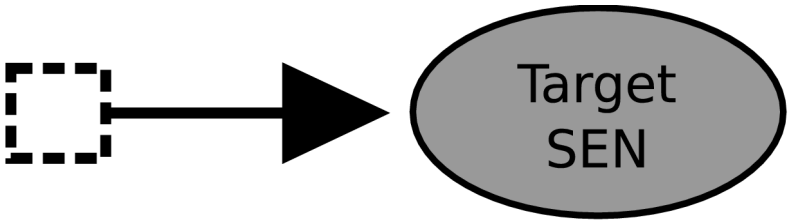


processes that are known to exist, but are omitted from the diagram for the sake of clarity or parsimony

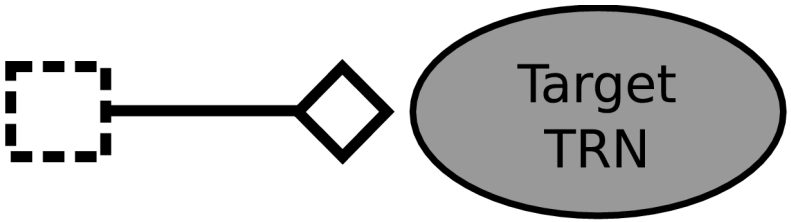


processes that may not exist ...


Source
SEN

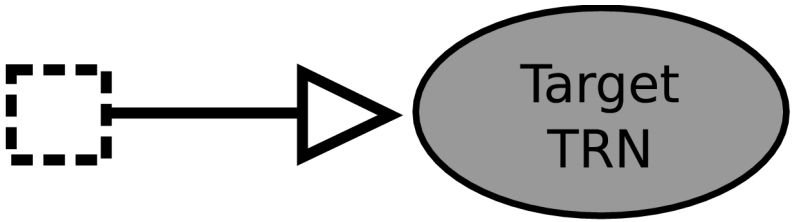

Target
SEN

transition that affects the flux of a process represented by the target TRN. Such a modulation can affect the process *positively or negatively* or even both ways depending on the conditions, for instance the concentration of the intervening participants



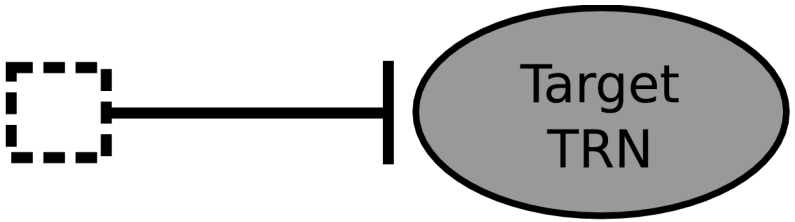
What is a modulation?

transition that affects **positively** the flux of a process represented by the target TRN

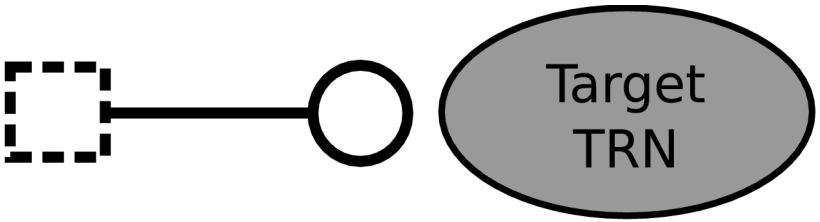


What is a stimulation?

transition that affects **negatively** the flux of a process represented by the target TRN

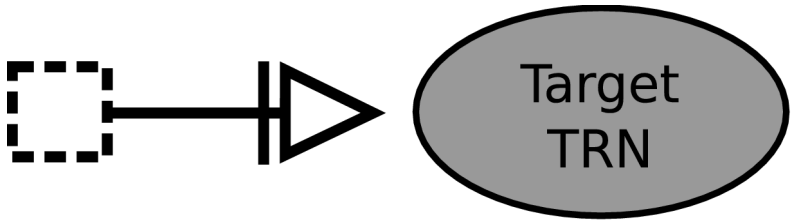


particular case of stimulation. The positive effect on the transition is due to the lowering of the activation energy of a reaction.



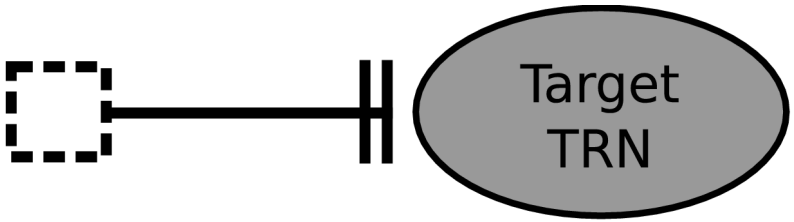
trigger (absolute stimulation)

stimulation that is necessary for a process to take place



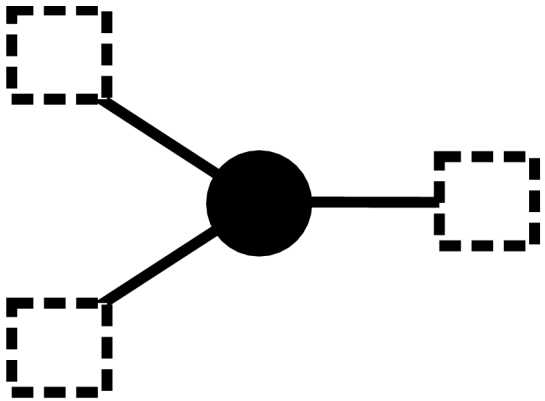
Do-we need trigger? Is trigger equal to ab solute stimulation?

process that move a *state variab*le back to its default value

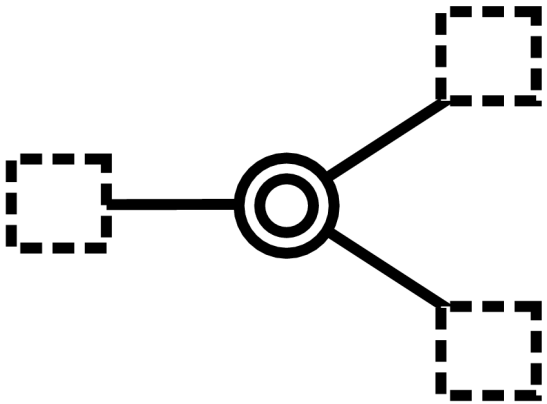


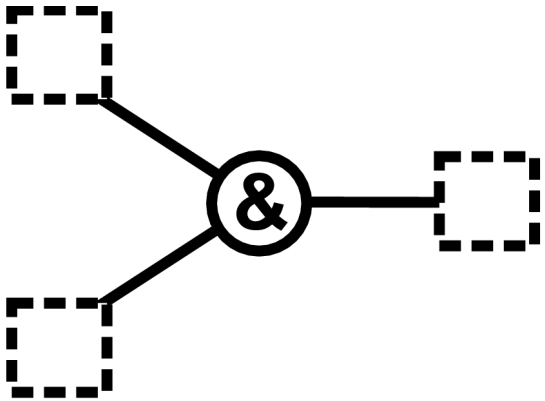
Do-we need reset? Is reset equal to absolute inhibition?

non-covalent binding of the biological objects represented by the SENs into a larger complex

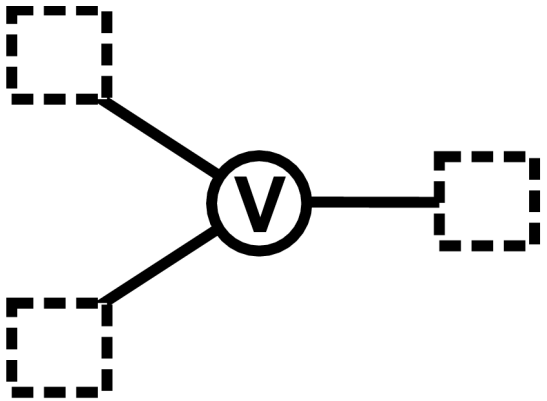


rupture of a non-covalent binding between the biological entities represented by the SENs

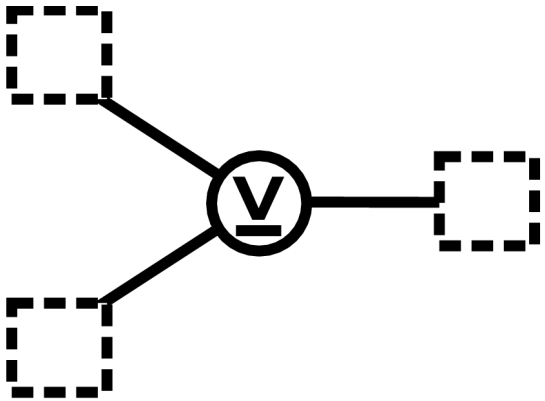




or ∧

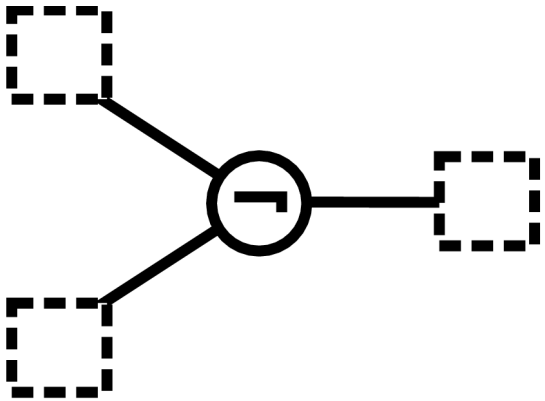


or

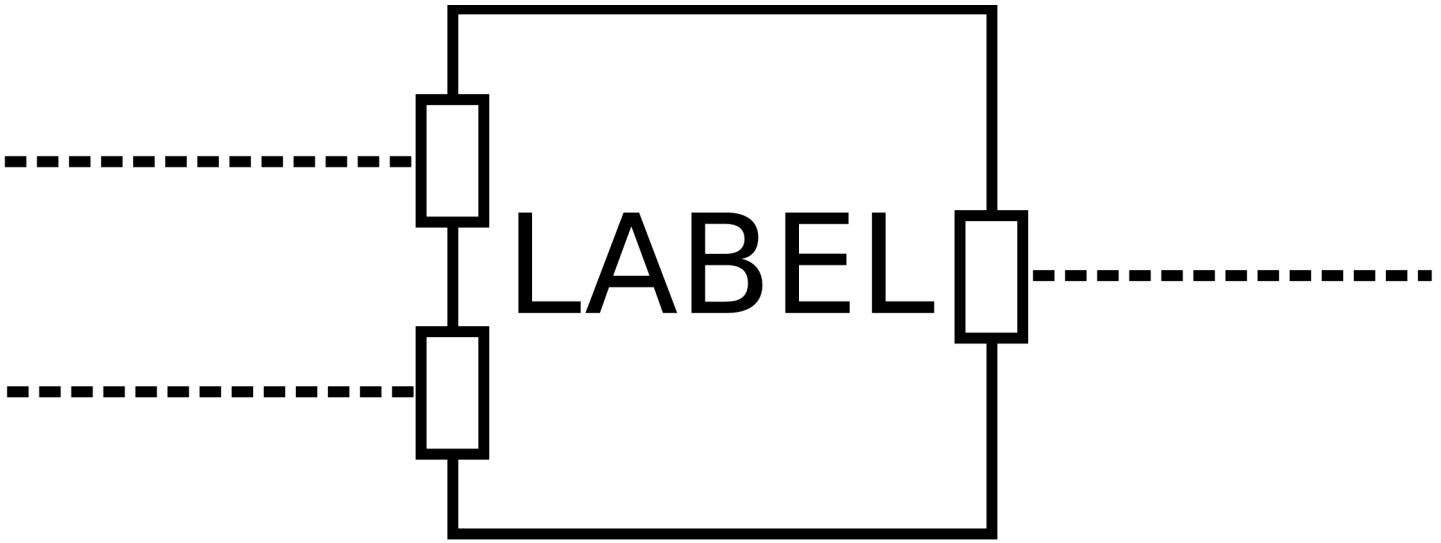


or ⊕

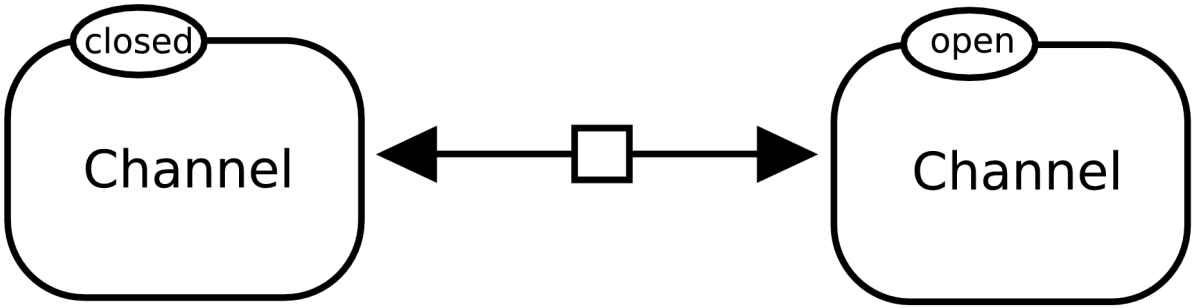
not



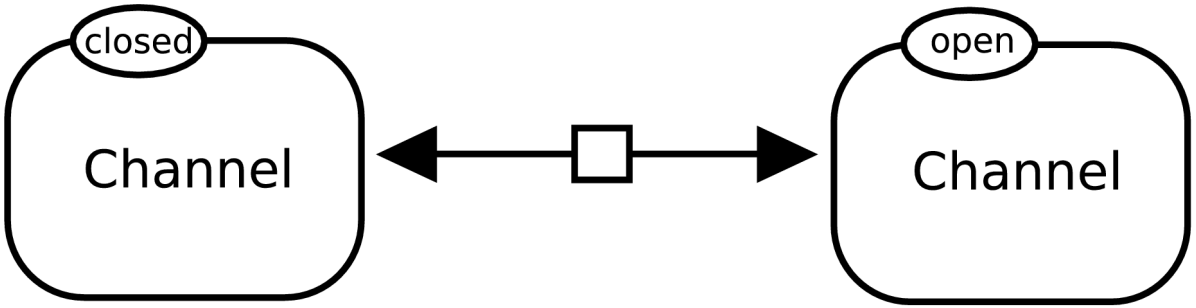
or


LABEL

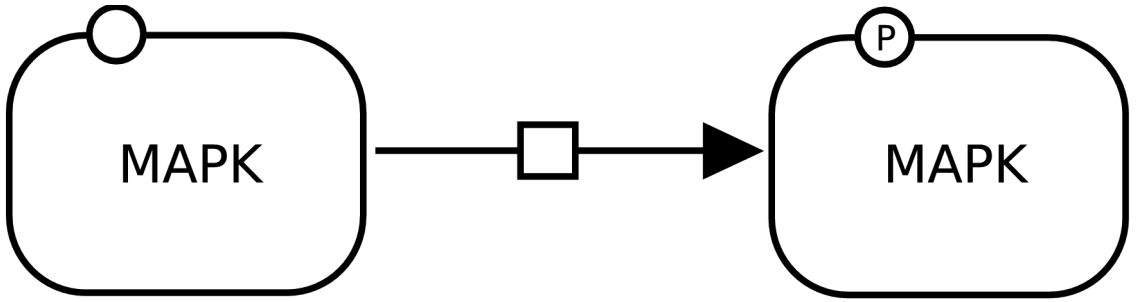
transition



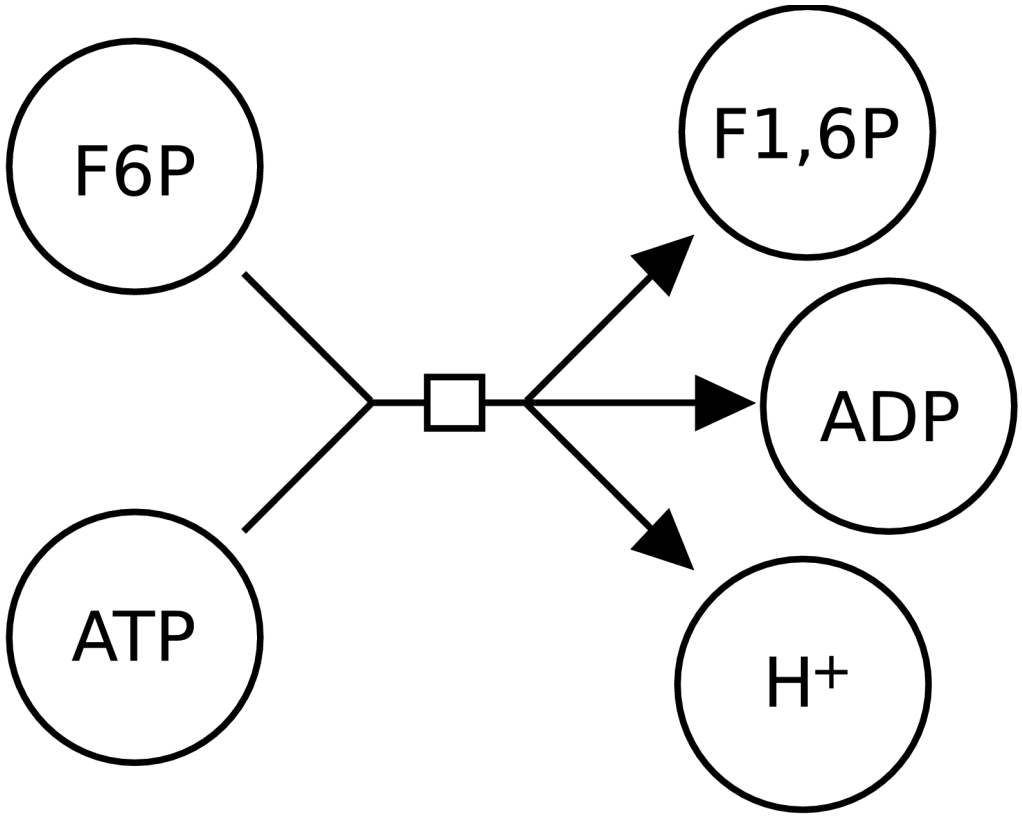
transition

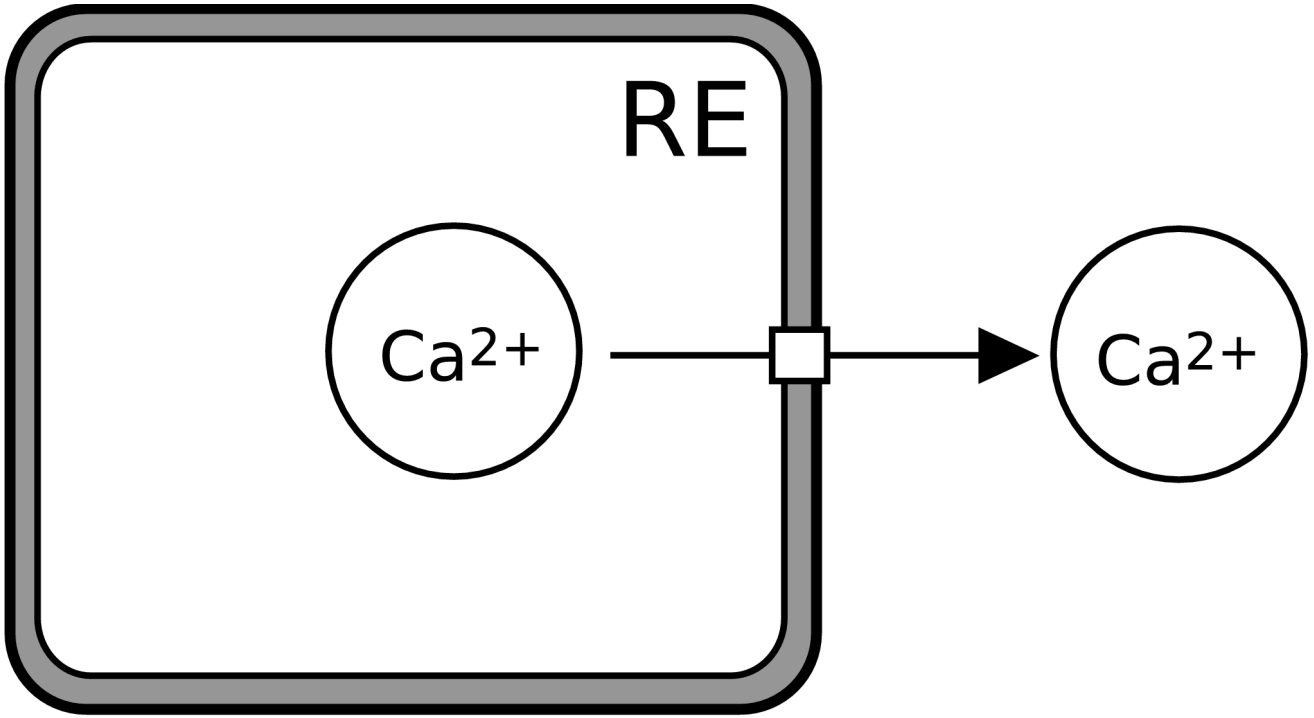


transition



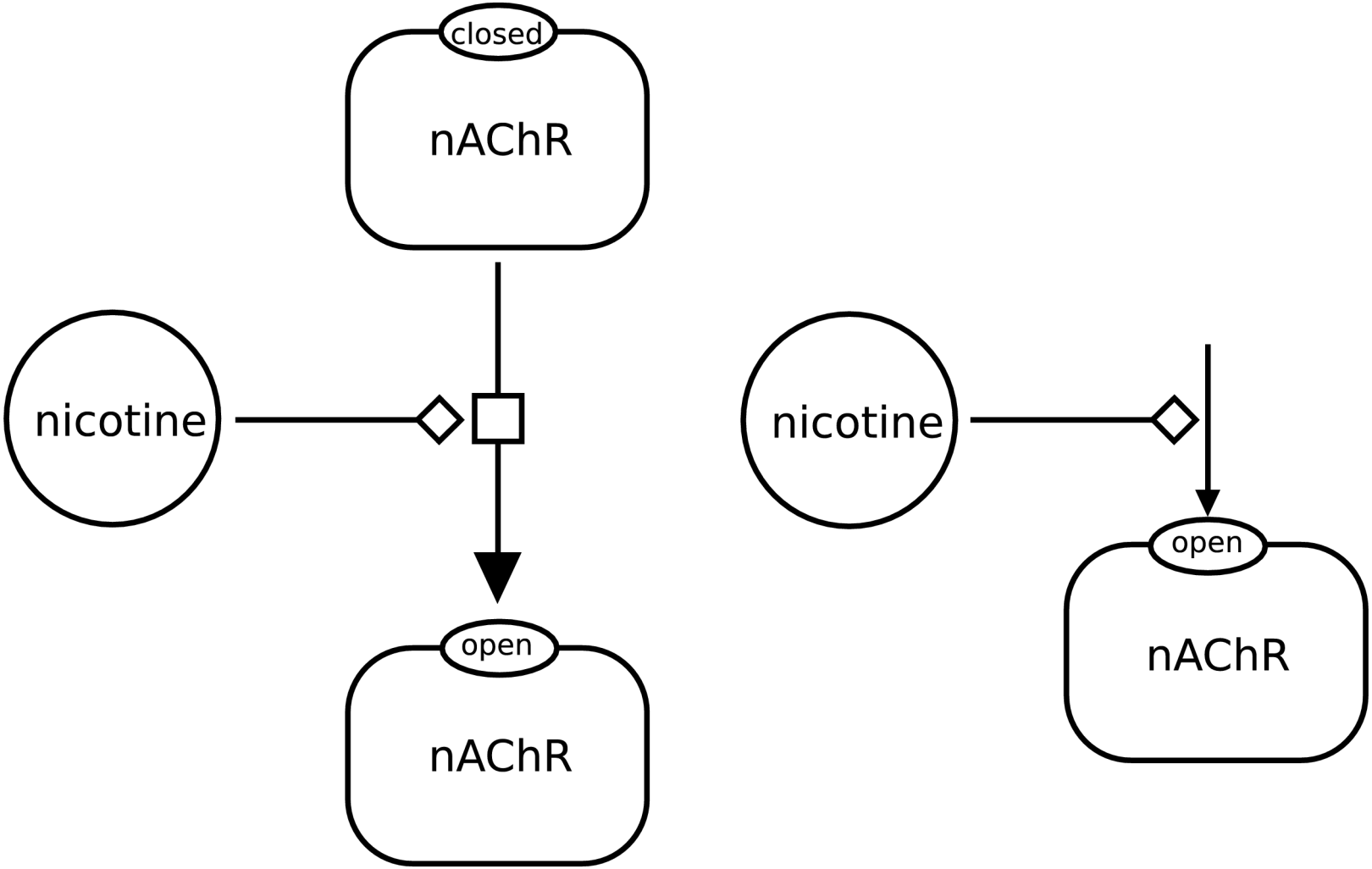
transition



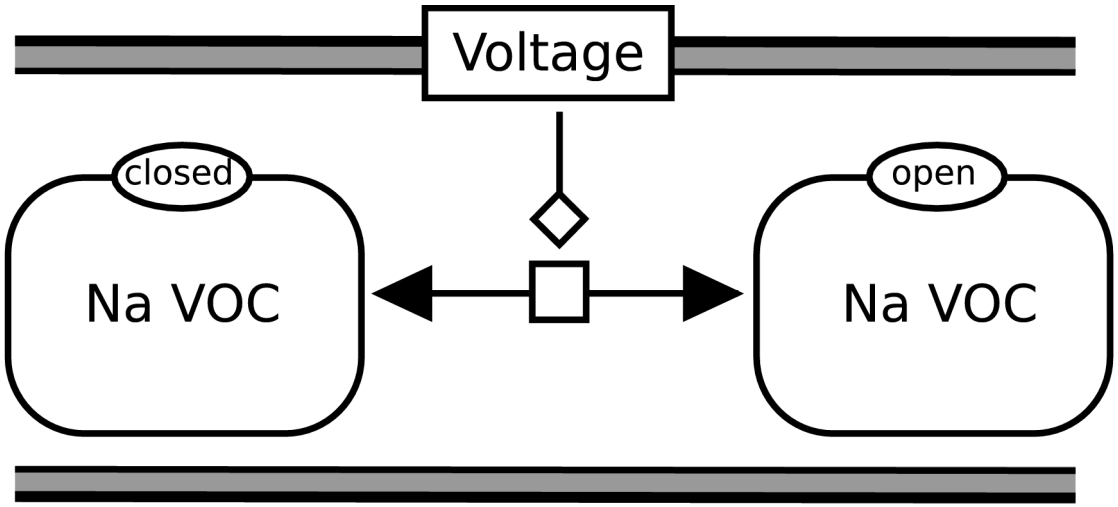


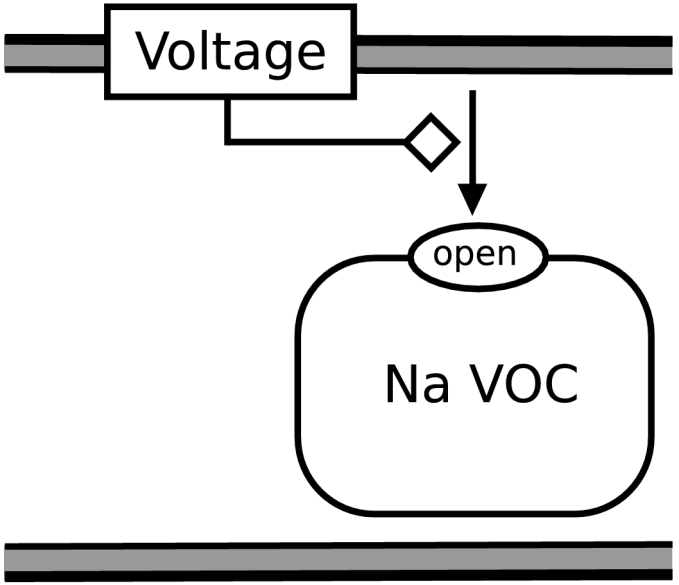
rewrite with the proper compartment, and a version later with the active transport

modulations

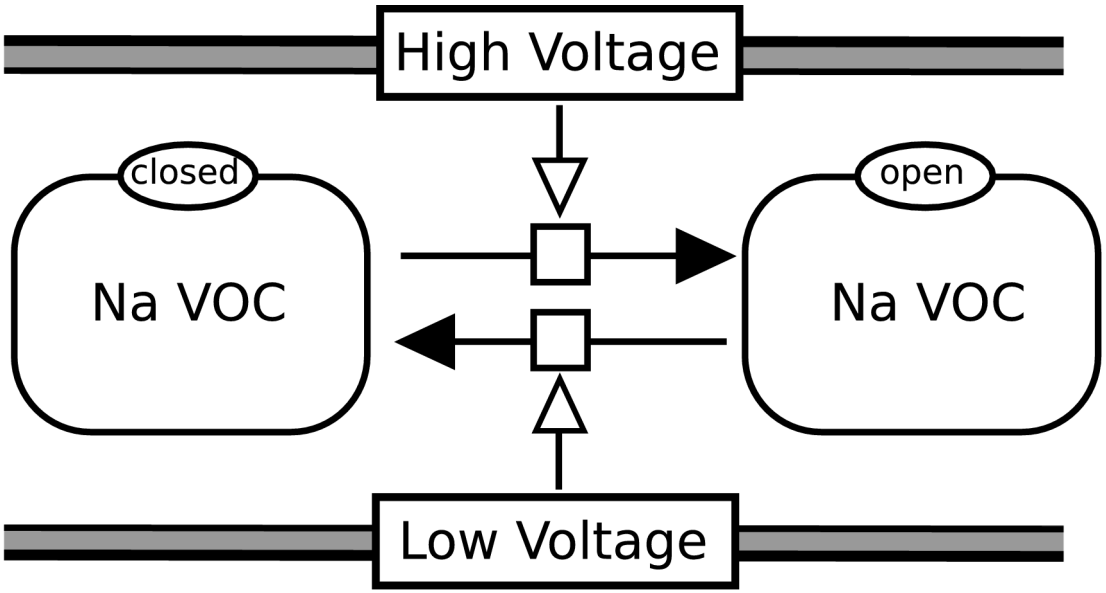


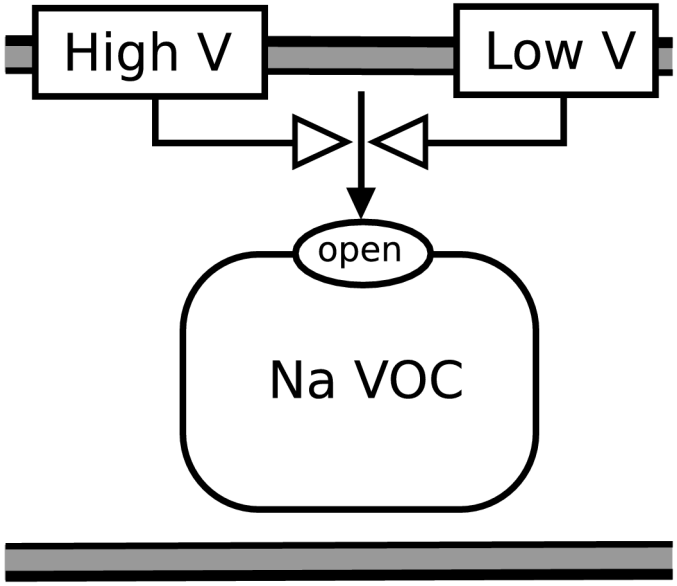
modulation



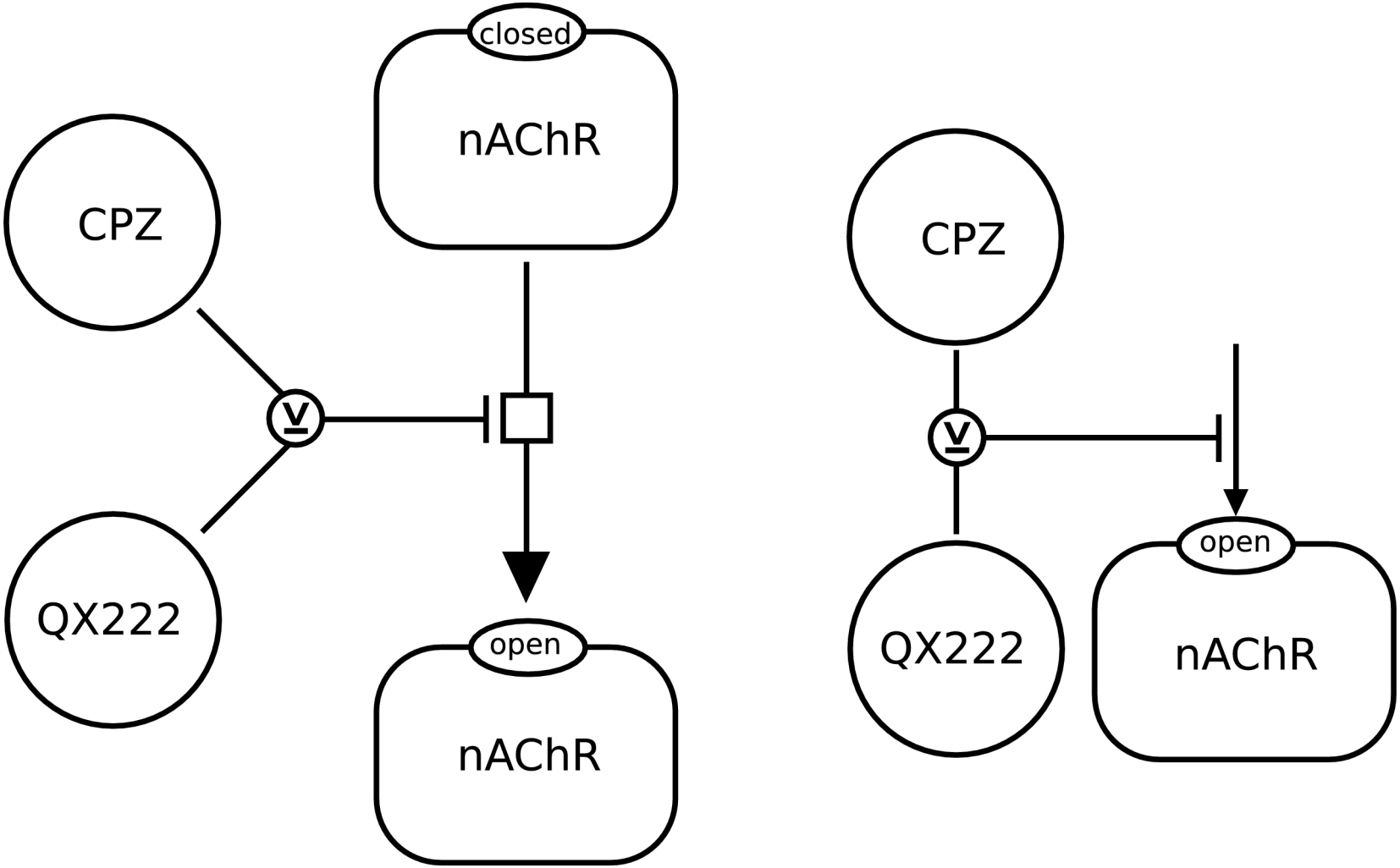


modulation

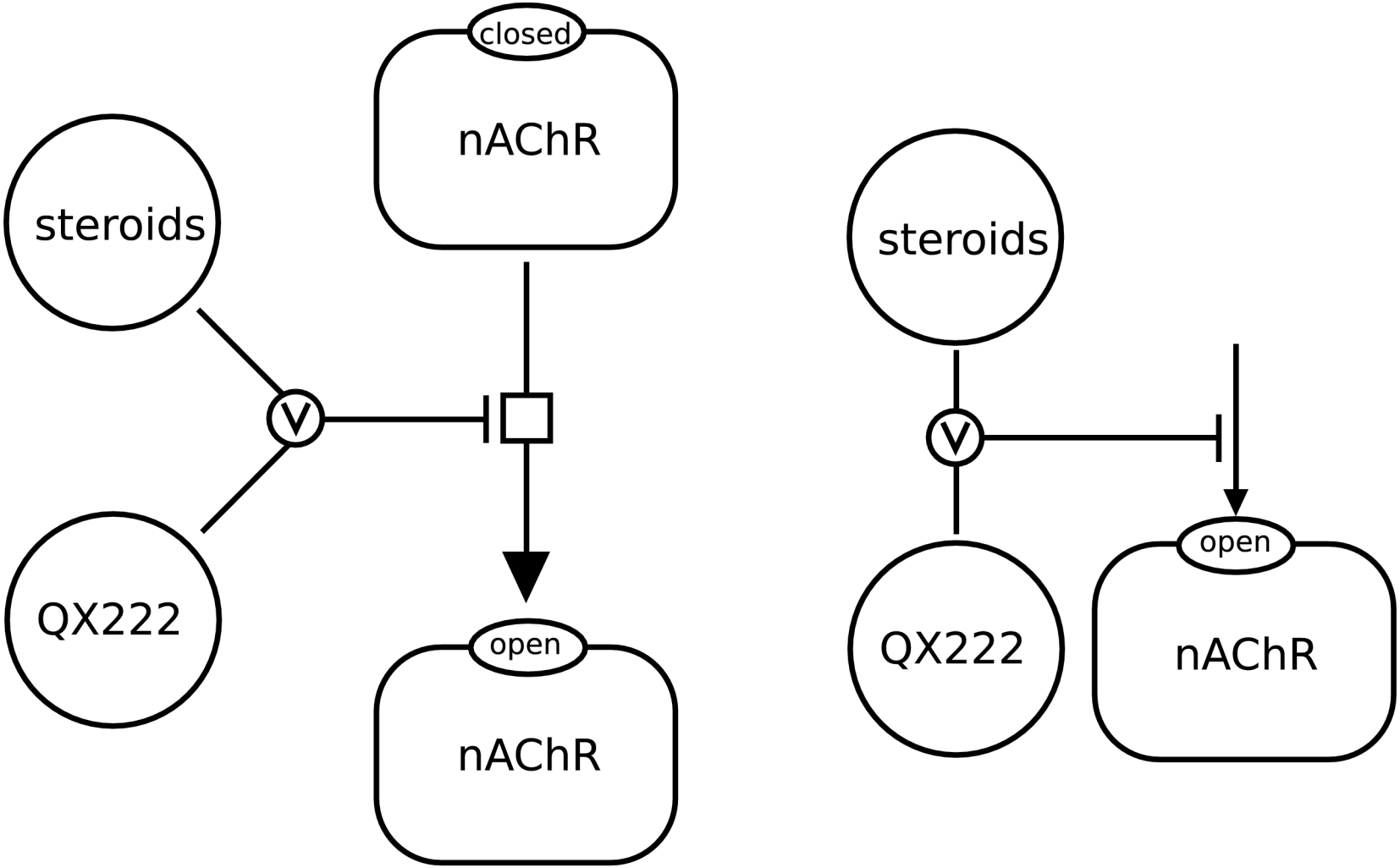

High Voltage
closed
Na VOC
open
Na VOC
Low Voltage


High V
Low V
open
Na VOC

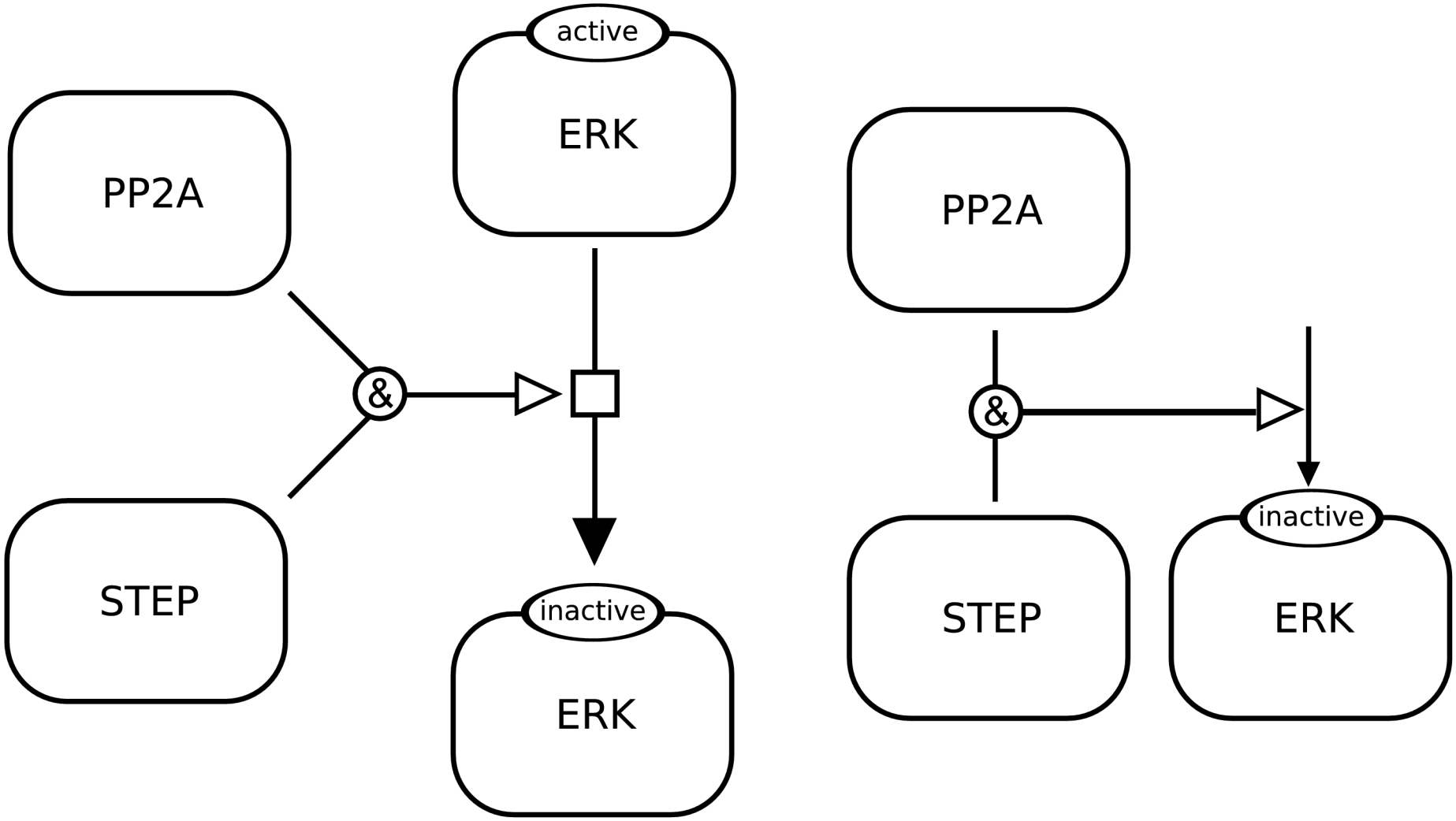
inhibition



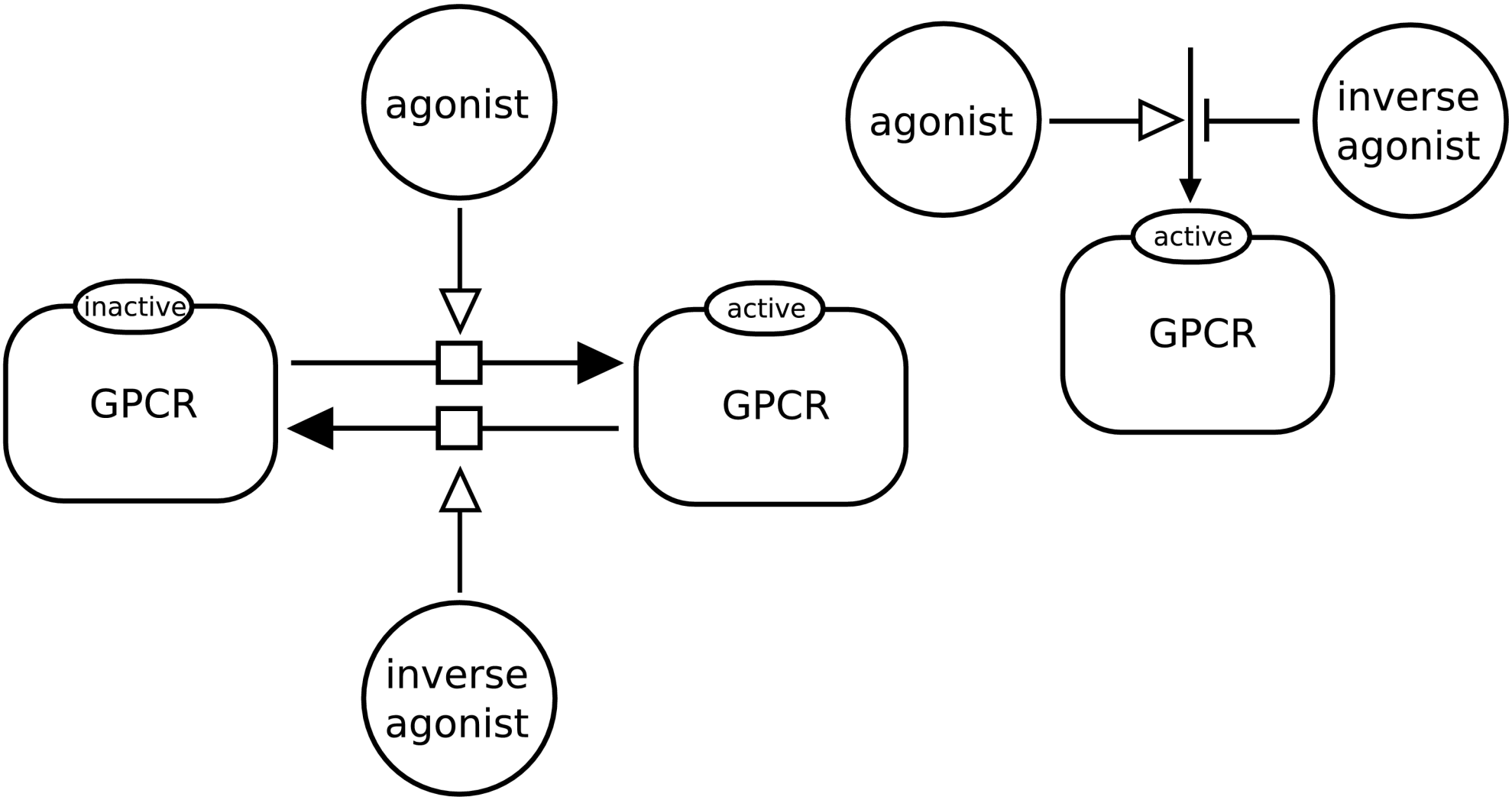
inhibition


closed
nAChR
steroids
QX222
open
nAChR
steroids
QX222
open
nAChR

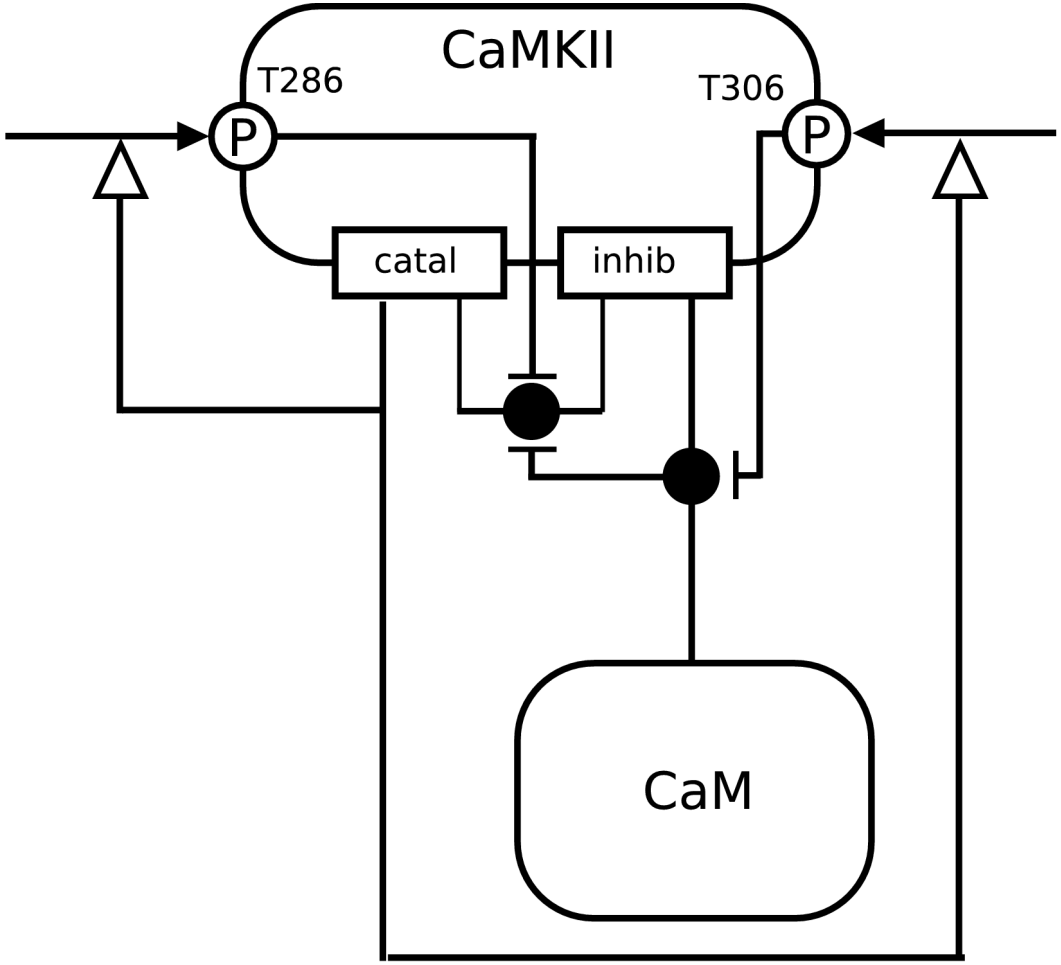
stimulation



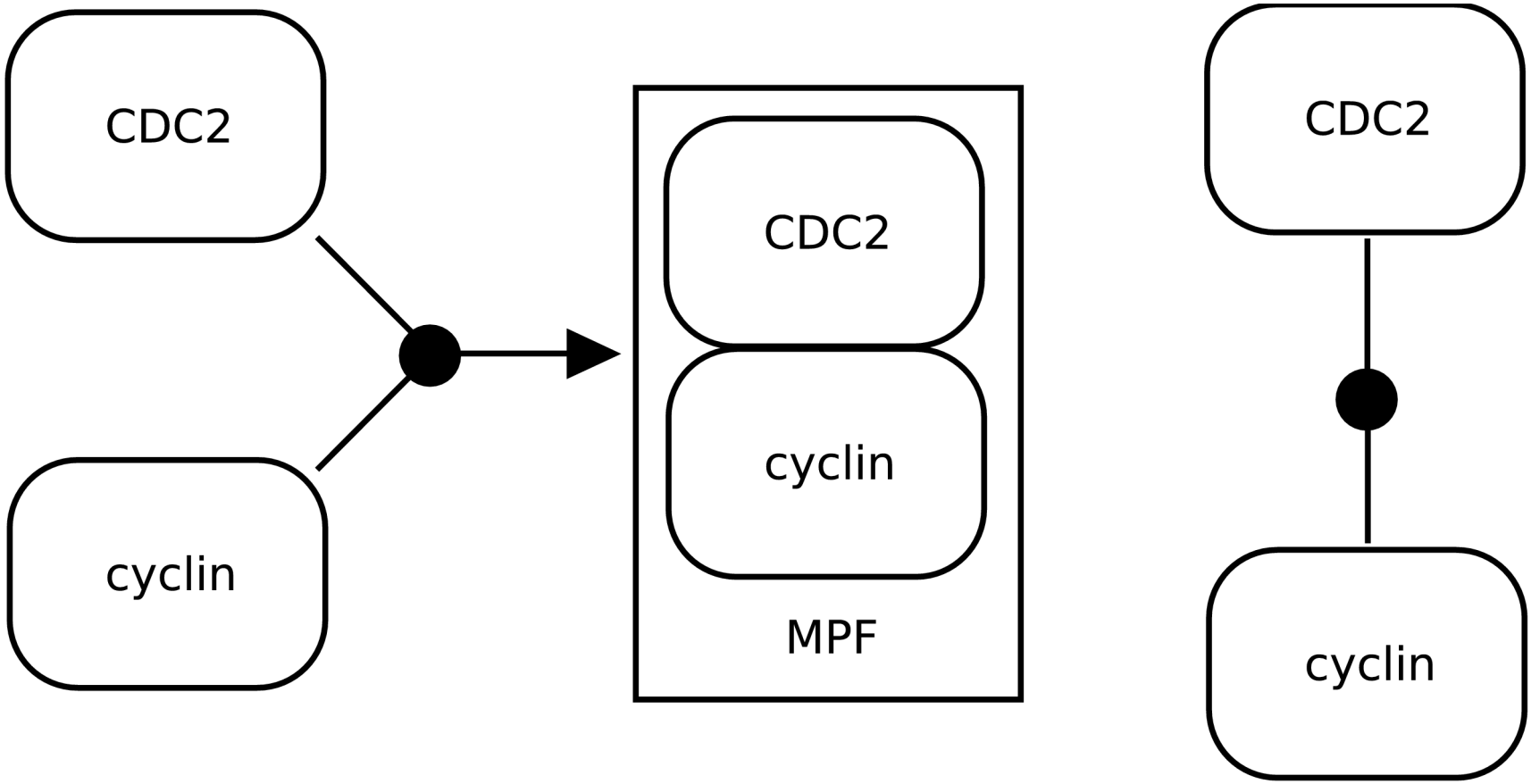
modulations



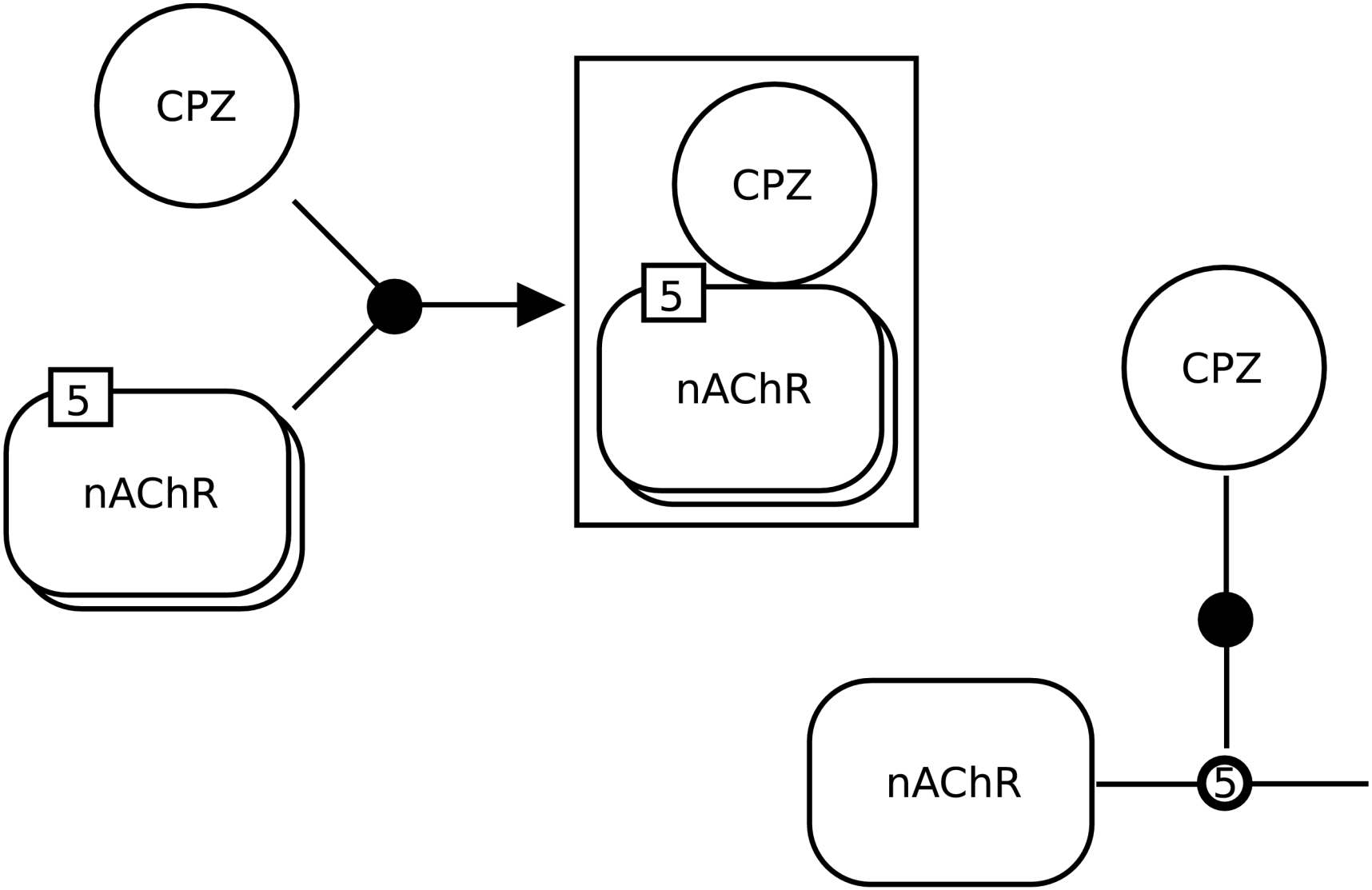
modulations



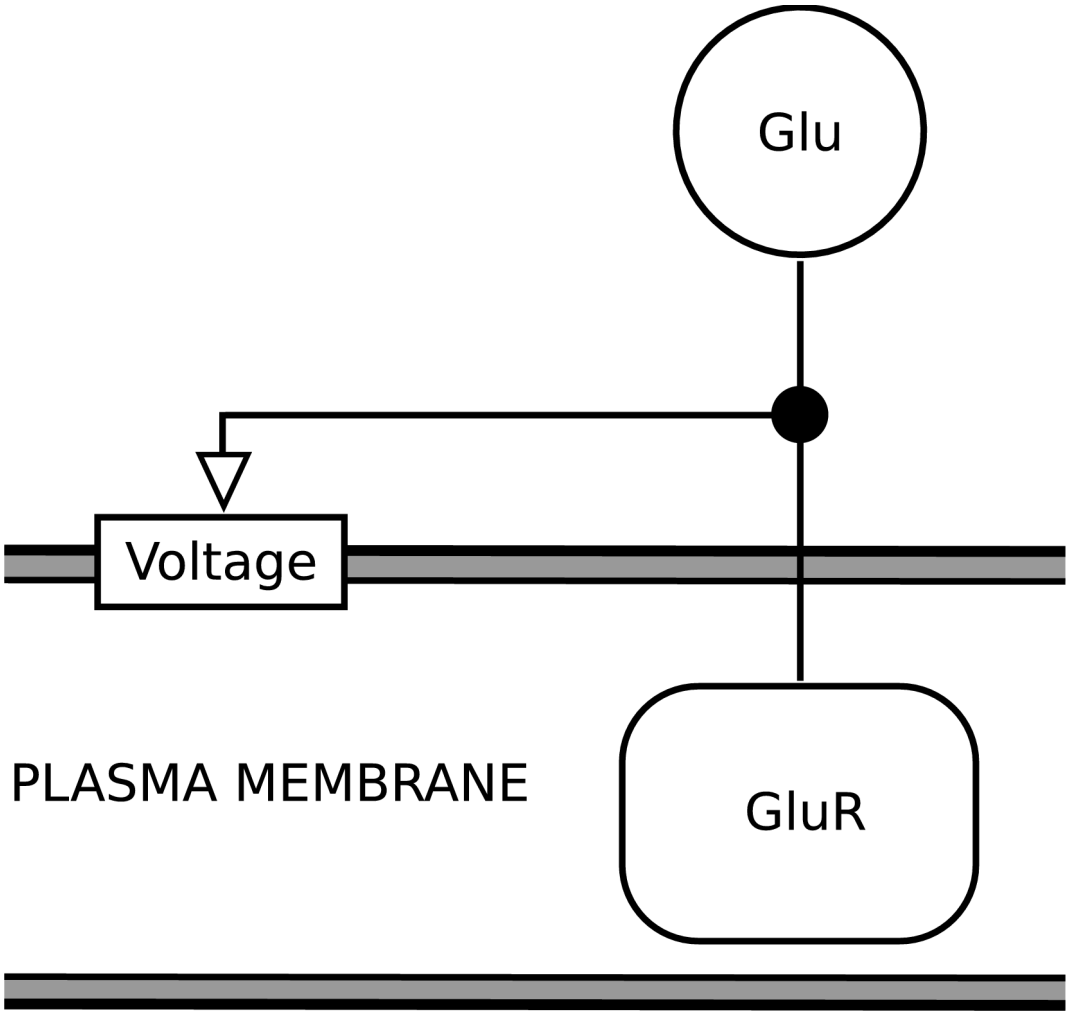
association



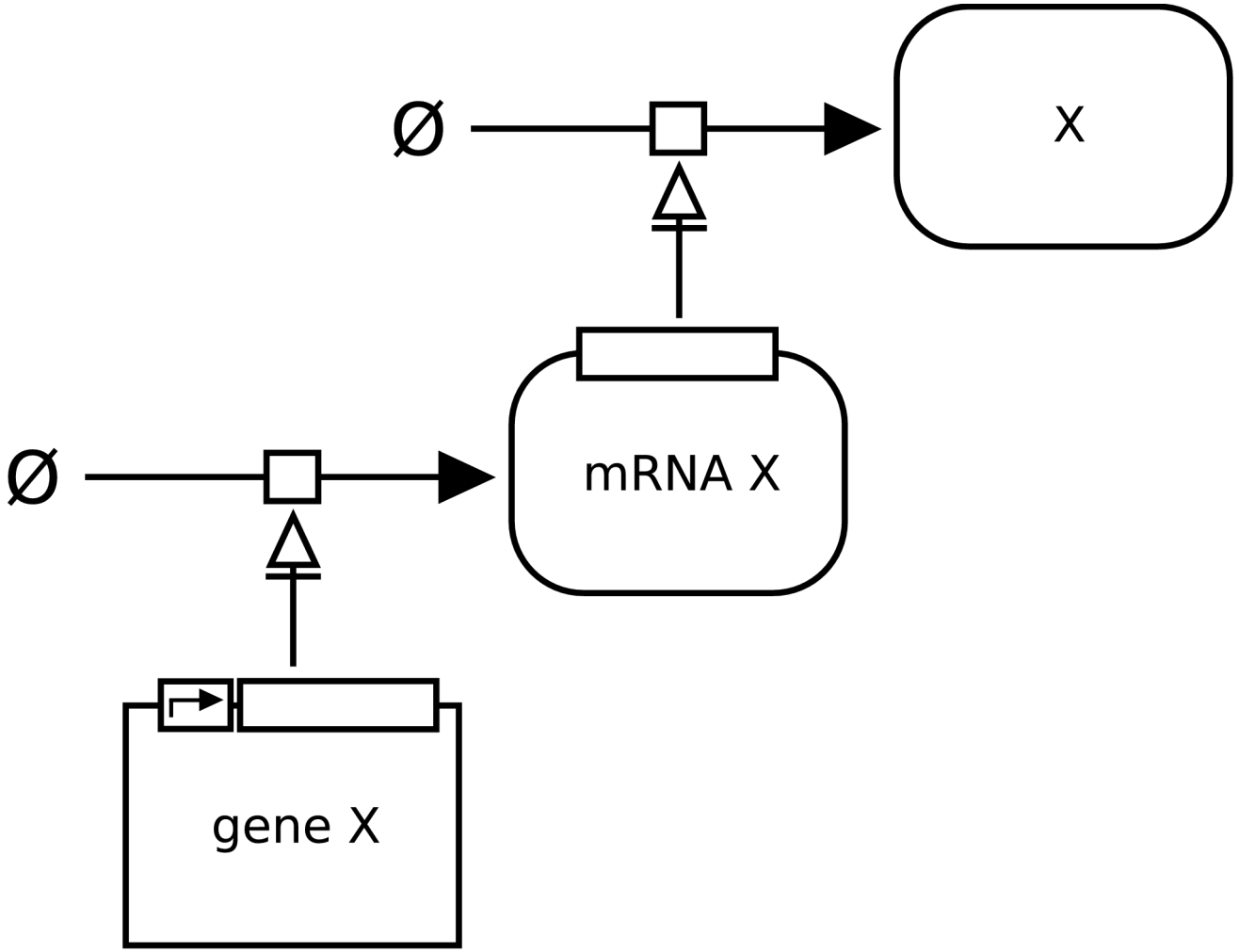
association



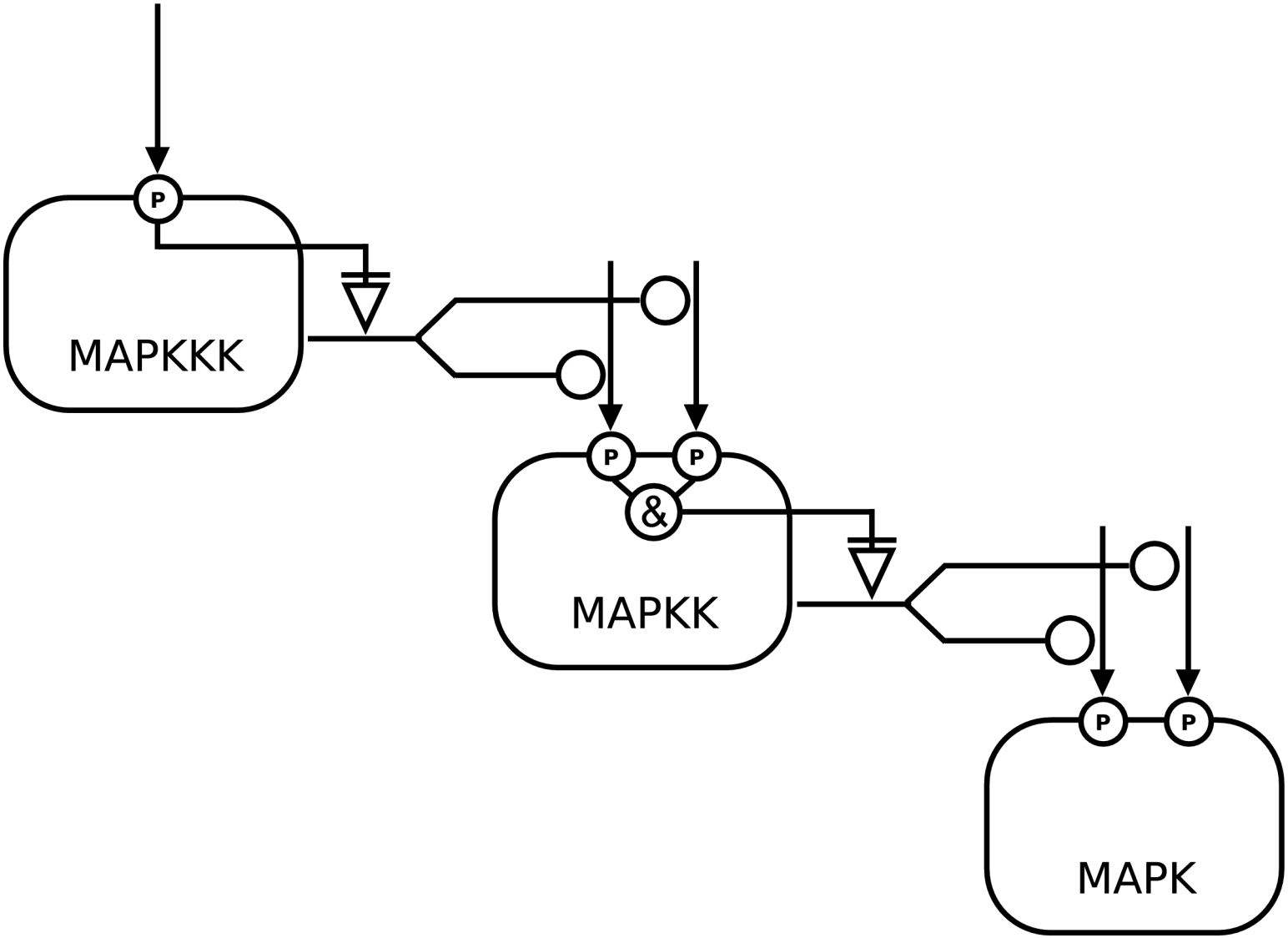
association-stimulation



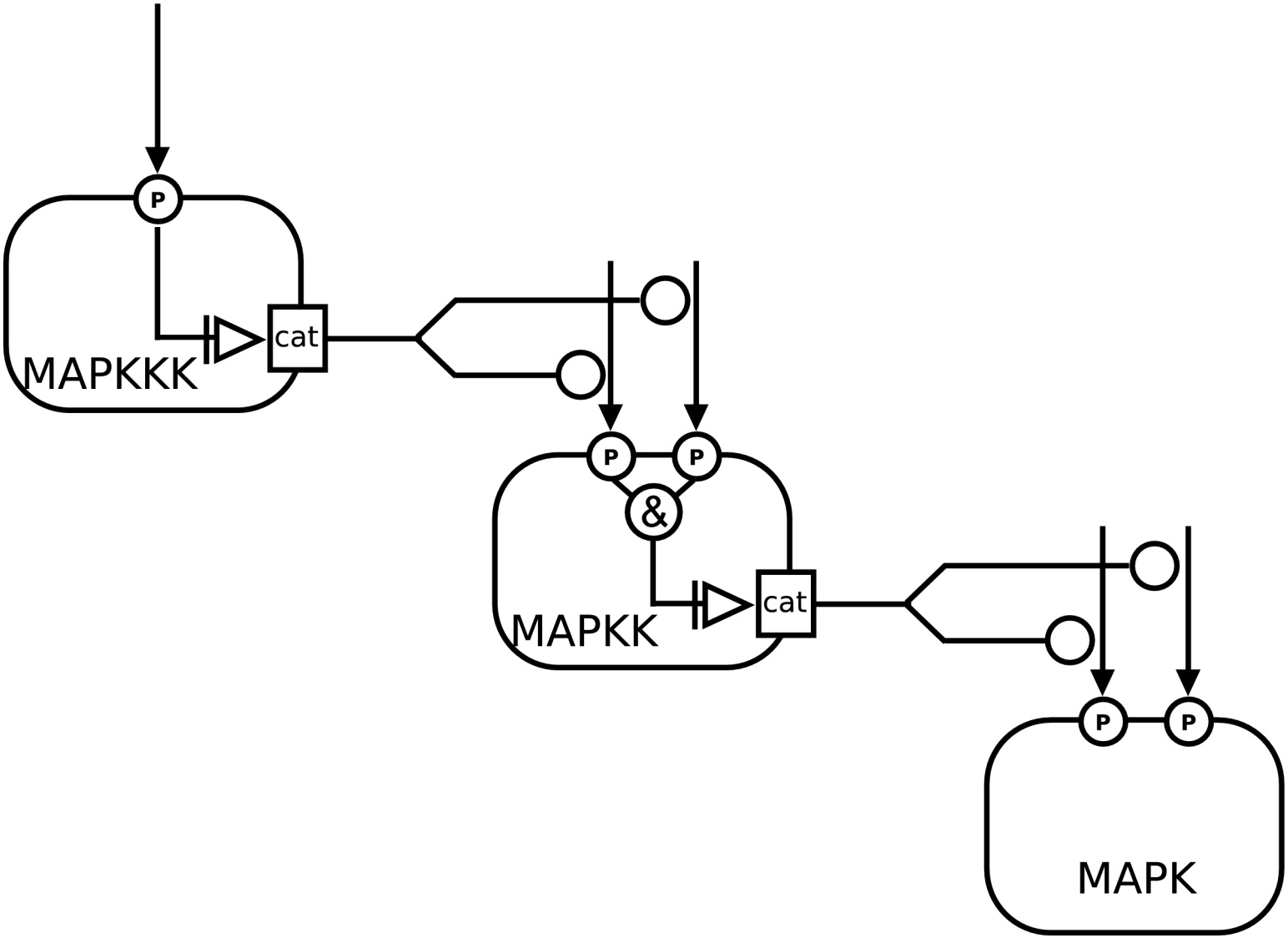
trigger



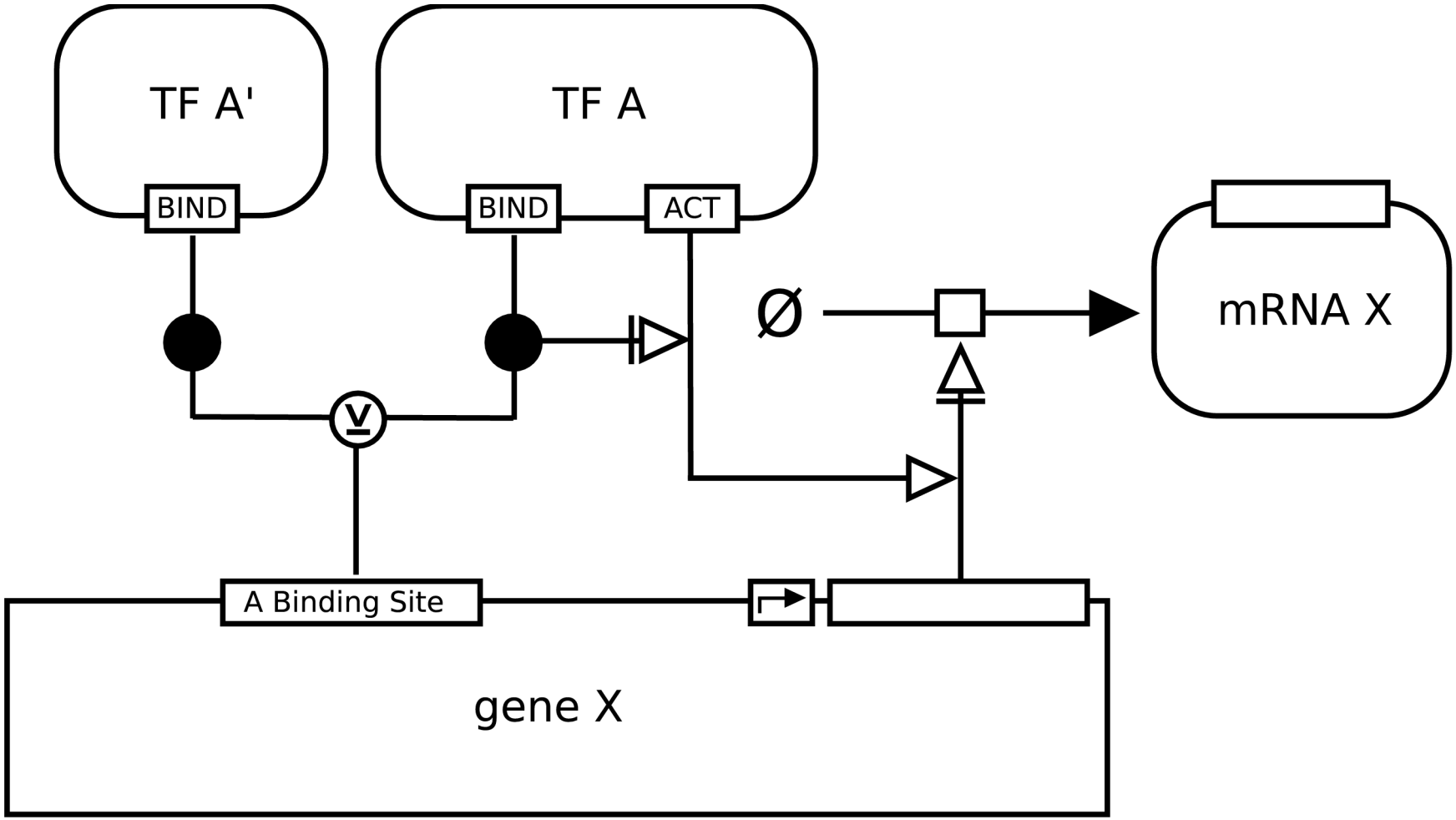
trigger

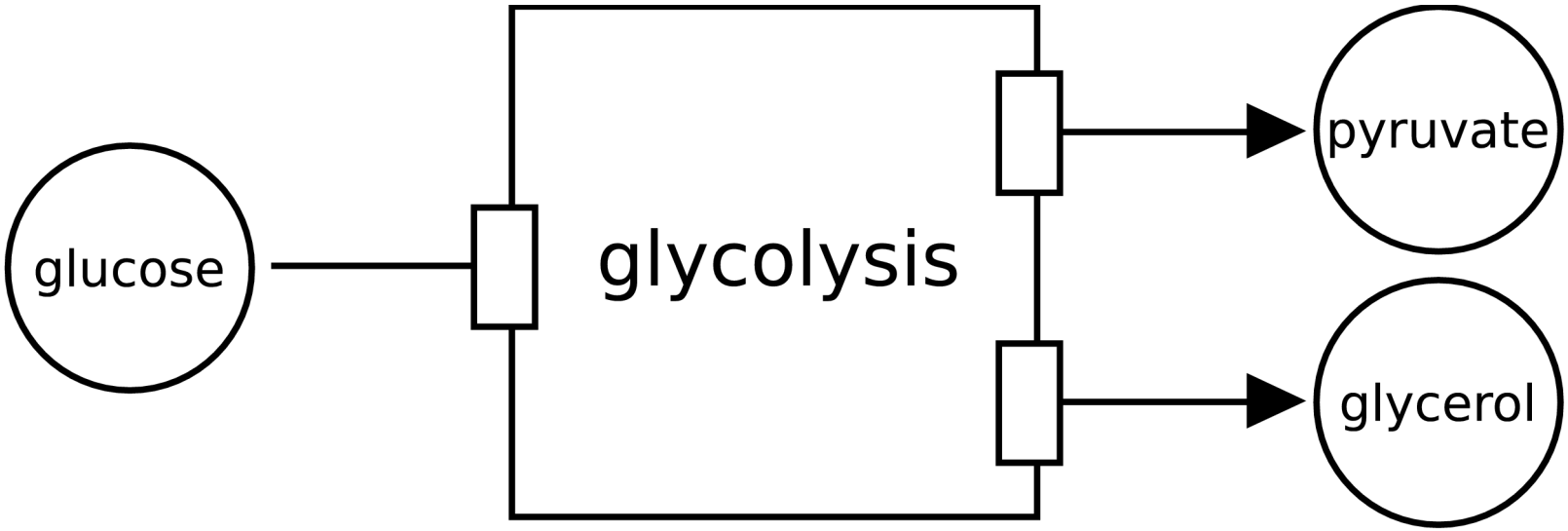


trigger



a bit of everything




glucose
glycolysis
pyruvate
glycerol