An update on Systems Biology Graphical Notation

SBGN Community

Oct. 12, 2015
COMBINE2015, Salt Lake City, Utah

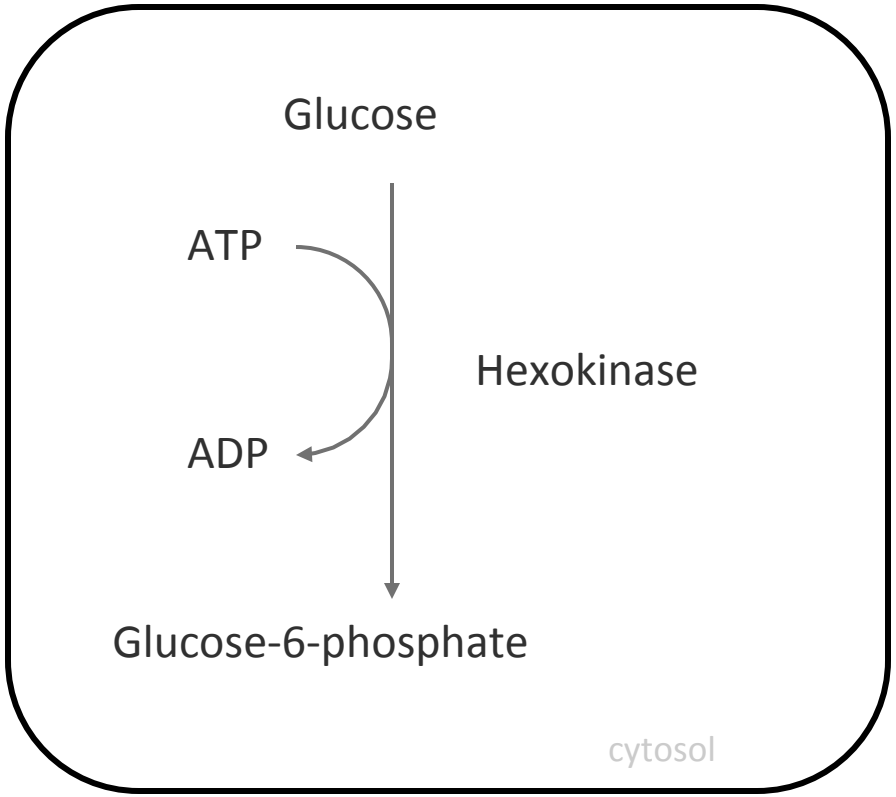
Outline

- Motivation
- Specification development
- Software support

MOTIVATIONS

Pathway Network Diagram

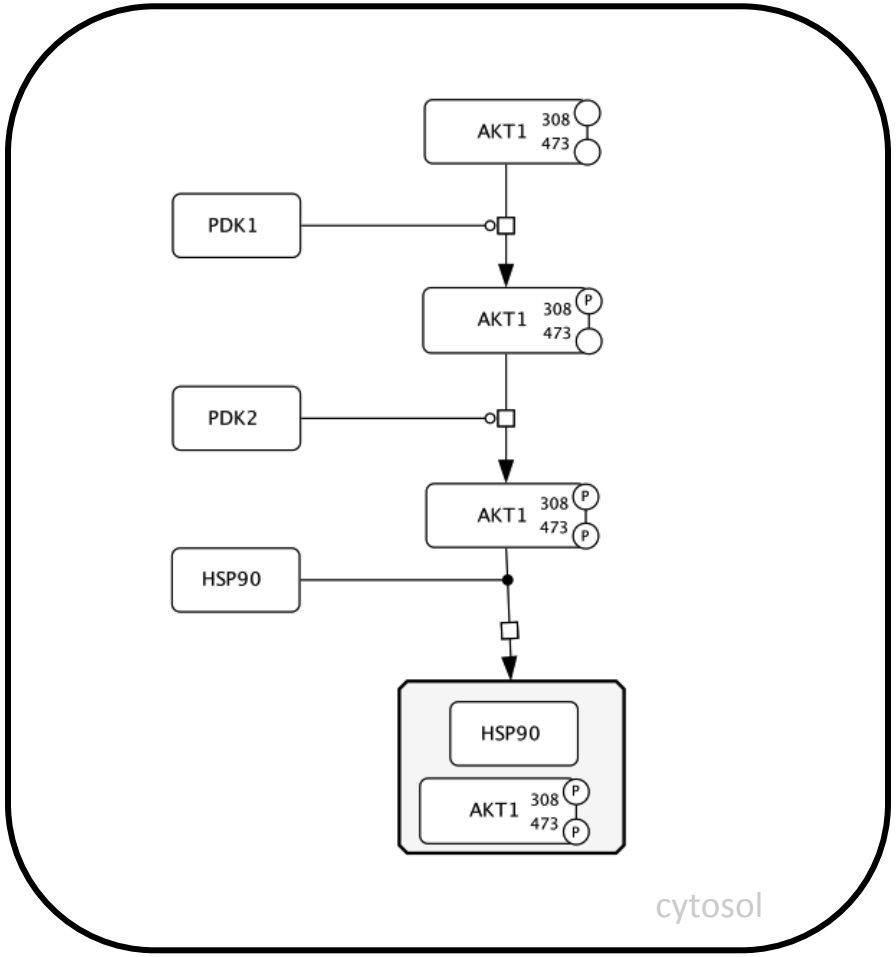
– An easy way to read biological knowledge



- Glucose is converted to glucose -6-phosphate with the consumption of ATP and production of ADP. The process is catalyzed by hexokinase. The reaction occurs in the cytosol of a cell.

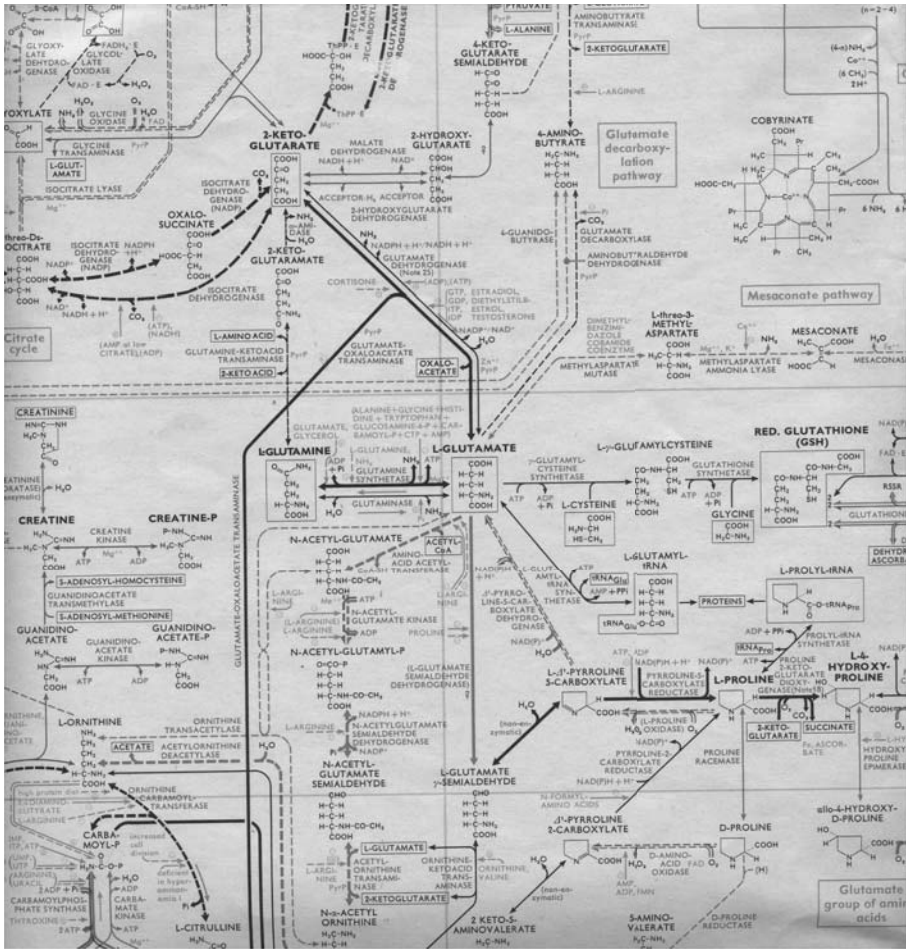
Pathway Network Diagram

– An easy way to read biological knowledge



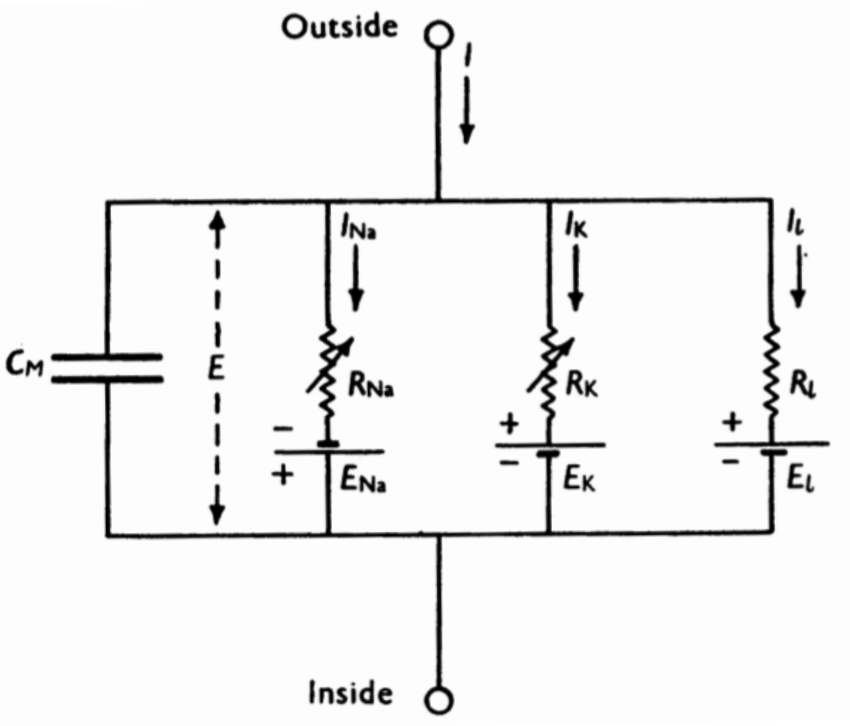
AKT1 is phosphorylated at residue 308 by PDK1. The phosphorylated AKT is then phosphorylated at residue of 473 by PDK2. The second phosphorylation reaction does not happen until the first residue (308) is phosphorylated. When both sites are phosphorylate. All the reactions occur in cytosol.

Pathway diagram has been used a long time ago



A metabolic pathway diagram

From the wall chart of *Biochemical Pathways* created by **Gerhard Michal** (1968)



Electrical circuit diagram representing cell membrane.

From **Hodgkin A.L. and Huxley A.F.** (1952) A quantitative description of membrane current and its application to conduction and excitation in nerve. *J. Physiol*. 117:500-544

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Article

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γCaMKII Shuttles Ca^{2+}/CaM to the Nucleus to Trigger CREB Phosphorylation and Gene Expression

Huan Ma, Rachel D. Groth, Samuel M. Cohen, John F. Emery, Boxing Li, Esthelle Hoedt, Guoan Zhang, Thomas A. Neubert, Richard W. Tsien

DOI: http://dx.doi.org/10.1016/j.cell.2014.09.019 | CrossMark

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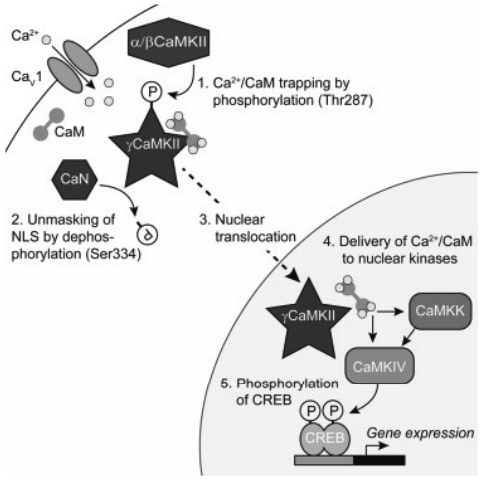
Highlights

- Ca^{2+}/CaM near Ca_V1 channels is delivered into the nucleus by γCaMKII
- Ca^{2+}/CaM provides the crucial signal to activate transcription factor CREB
- βCaMKII phosphorylates γCaMKII at Thr287 to protect the Ca^{2+}/CaM signal
- CaN dephosphorylates γCaMKII at Ser334 to trigger γCaMKII nuclear translocation

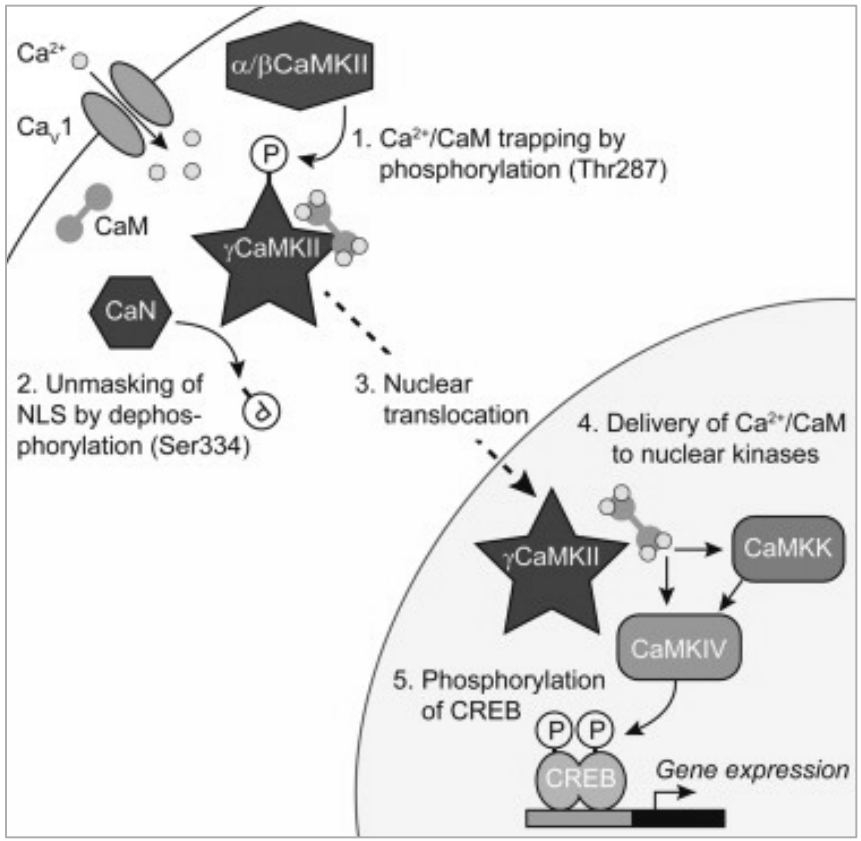
Graphical Abstract



Summary

Activity-dependent CREB phosphorylation and gene expression are critical for long-term neuronal plasticity. Local signaling at Ca_V1 channels triggers these events, but how information is relayed onward to the nucleus remains unclear. Here, we report a mechanism that mediates long-distance communication within cells: a shuttle that transports Ca^{2+}/calmodulin from the surface membrane to the nucleus. We show that the shuttle protein is γCaMKII, its phosphorylation at Thr287 by βCaMKII protects the Ca^{2+}/CaM signal, and CaN triggers its nuclear translocation. Both βCaMKII and CaN act in close proximity to Ca_V1 channels, supporting their dominance, whereas γCaMKII operates as a carrier, not as a kinase. Upon arrival within the nucleus, Ca^{2+}/CaM activates CaMKK and its substrate CaMKIV, the CREB kinase. This mechanism resolves long-standing puzzles about CaM/CaMK-dependent signaling to the nucleus. The significance of the mechanism is emphasized by dysregulation of Ca_V1, γCaMKII, βCaMKII, and CaN in multiple neuropsychiatric disorders.

What are the problems?



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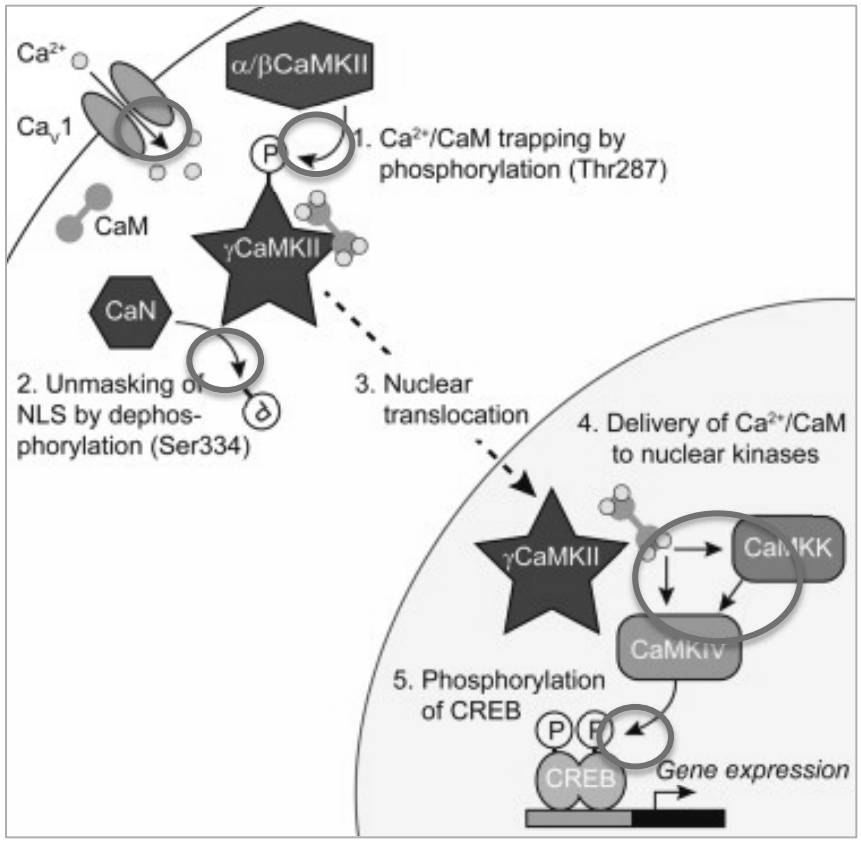

- Graphically ambiguous
  - Glyphs are not defined.
  - It is difficult to interpret the meaning of the diagram without referring to the text.

Ambiguity in Conventional Representation

Ambiguity in Conventional Representation

is transformed into

translocates (X "=" Y)

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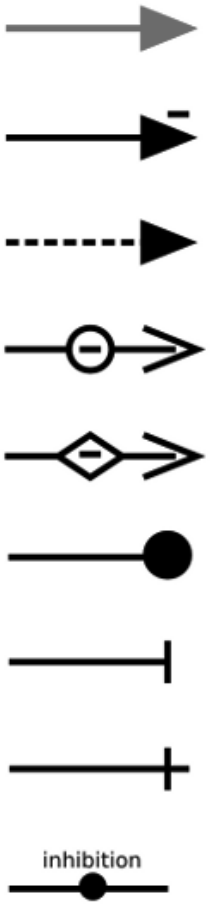

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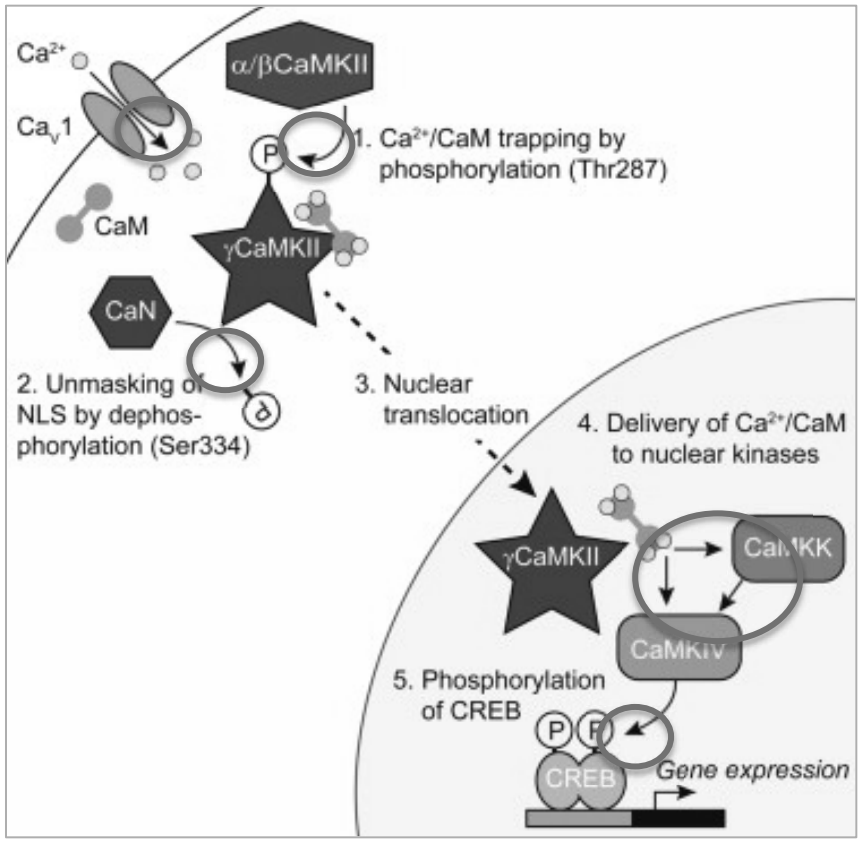

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- Not in computer-readable format

Here comes

The Systems Biology Graphical Notation

http://www.sbgn.org/

History of SBGN

- The SBGN effort was initiated by Professor Hiroaki Kitano.
- The inaugural SBGN workshop was held in Tokyo in February 2006.

The Systems Biology Graphical Notation

Nicolas Le Novère[1], Michael Hucka[2], Huaiyu Mi[3], Stuart Moodie[4], Falk Schreiber[5,6], Anatoly Sorokin[7], Emek Demir[8], Katja Wegner[9], Mirit I Aladjem[10], Sarala M Wimalaratne[11], Frank T Bergman[12], Ralph Gauges[13], Peter Ghazal[4,14], Hideya Kawaji[15], Lu Li[1], Yukiko Matsuoka[16], Alice Villéger[17,18], Sarah E Boyd[19], Laurence Calzone[20], Melanie Courtot[21], Ugur Dogrusoz[22], Tom C Freeman[14,23], Akira Funahashi[24], Samik Ghosh[16], Akiya Jouraku[24], Sohyoung Kim[10], Fedor Kolpakov[25,26], Augustin Luna[10], Sven Sahle[13], Esther Schmidt[1], Steven Watterson[4,22], Guanming Wu[27], Igor Goryanin[4], Douglas B Kell[18,28], Chris Sander[8], Herbert Sauro[12], Jacky L Snoep[29], Kurt Kohn[10] & Hiroaki Kitano[16,30,31]

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NATURE BIOTECHNOLOGY VOLUME 27 NUMBER 8 AUGUST 2009

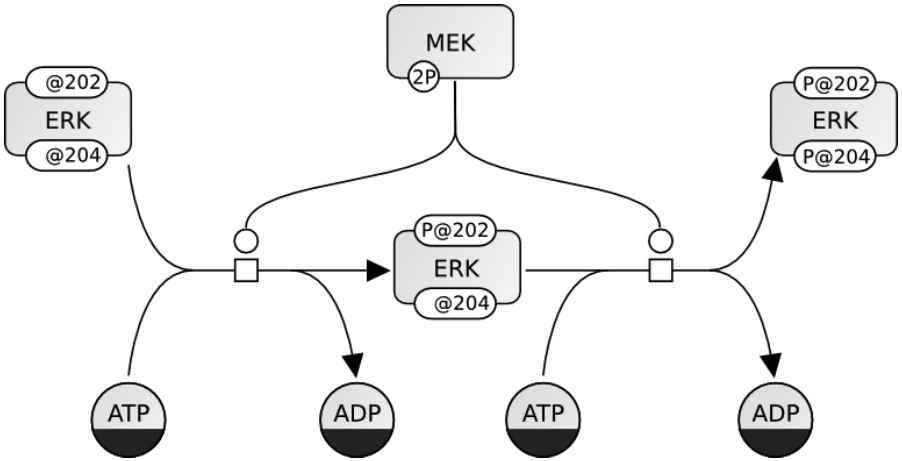
39 authors, 31 affiliations

 SBGN is being developed by a large user community

SPECIFICATION DEVELOPMENT

Three Languages in One Notation

Process Descriptions



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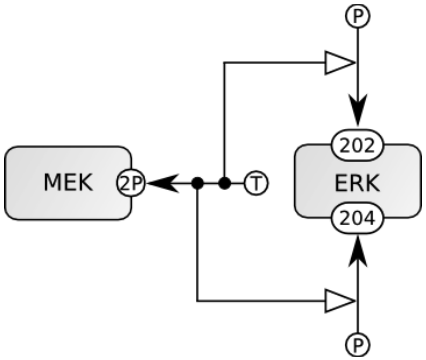
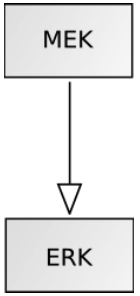
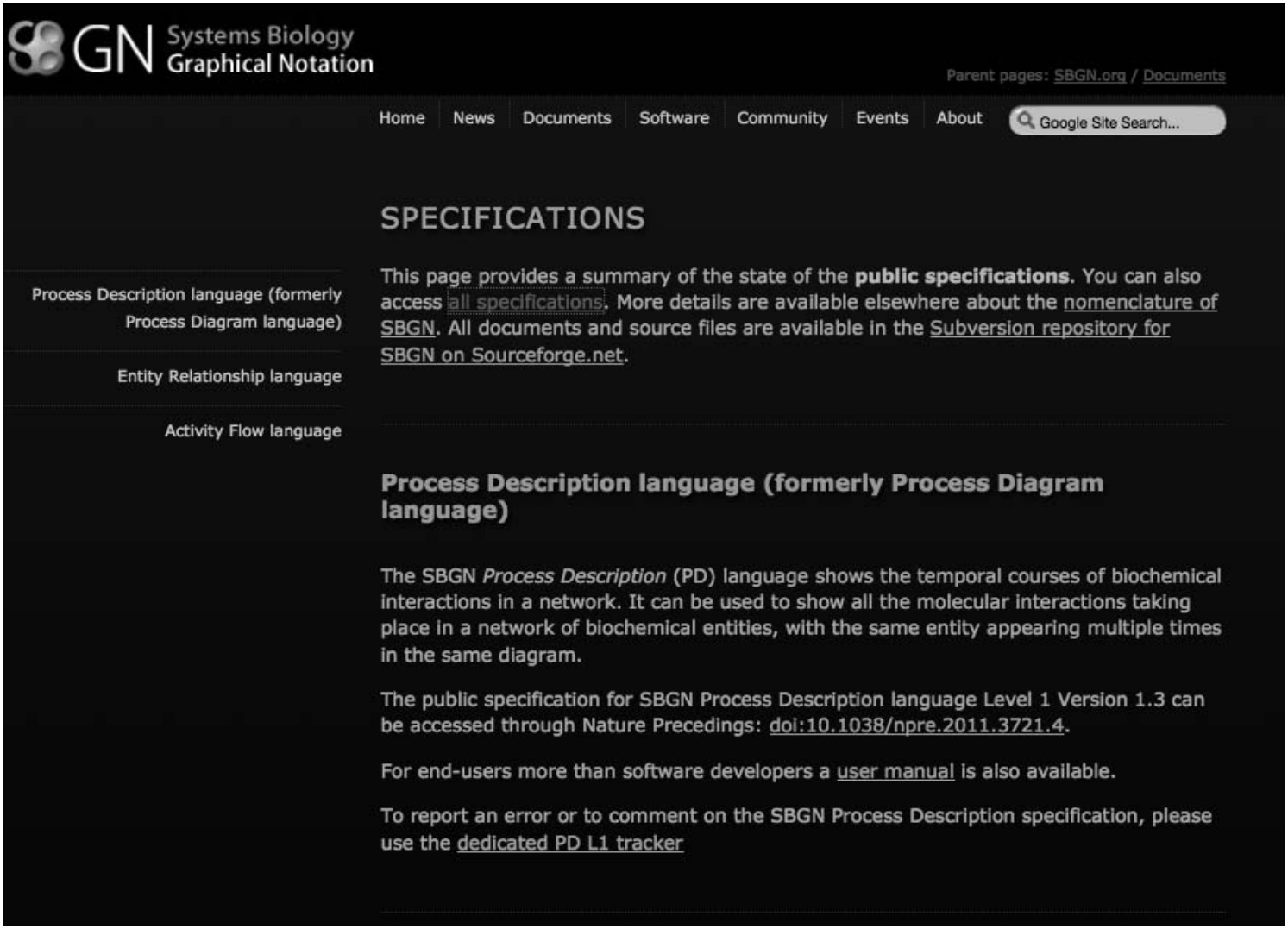


Activity Flows



SBGN Specifications

http://www.sbgn.org/Documents/Specifications



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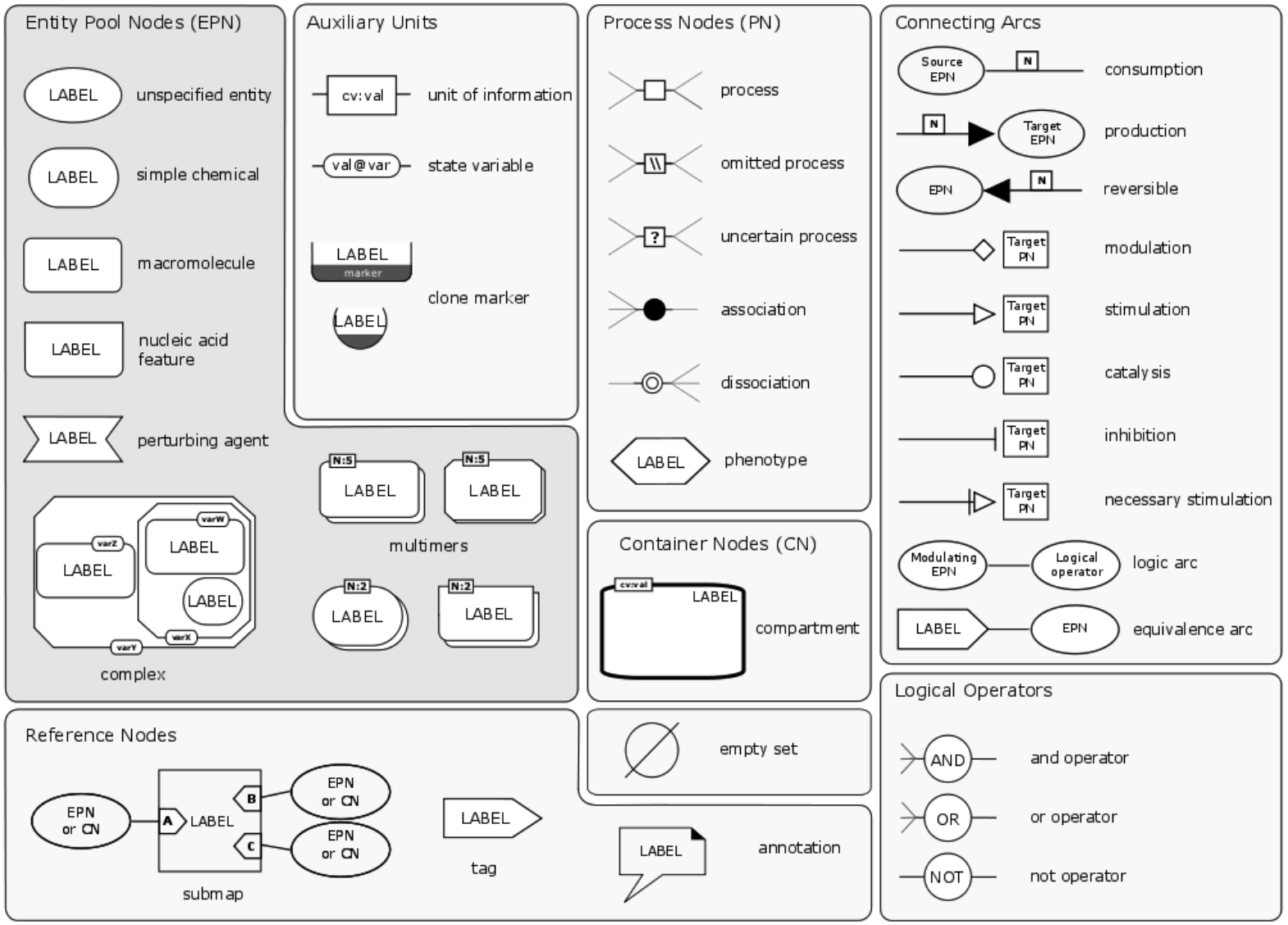

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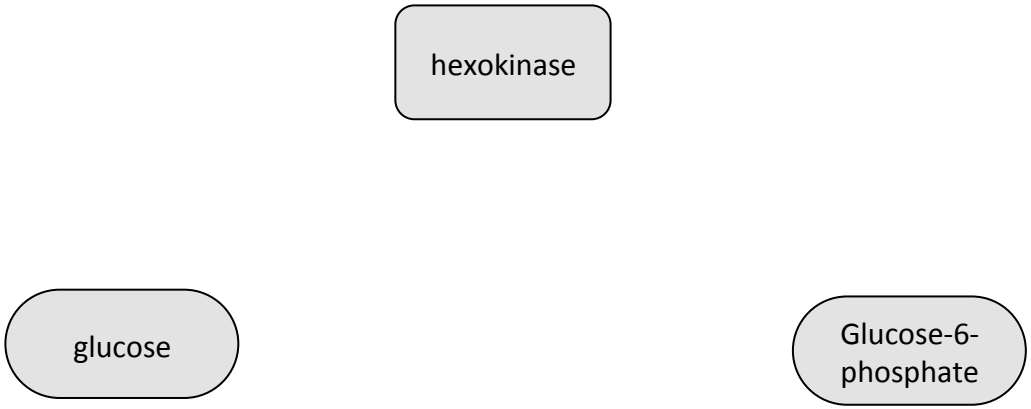

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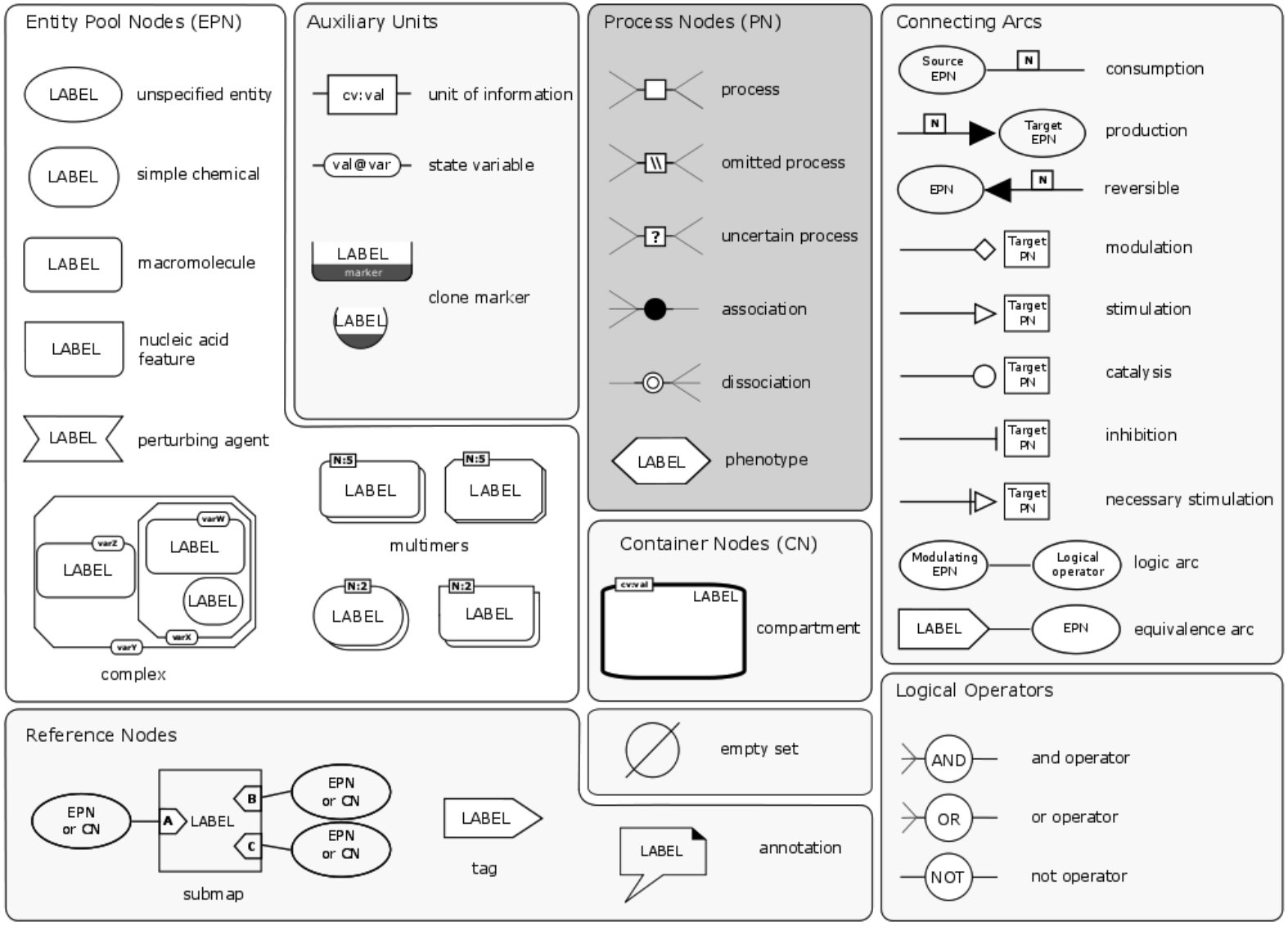

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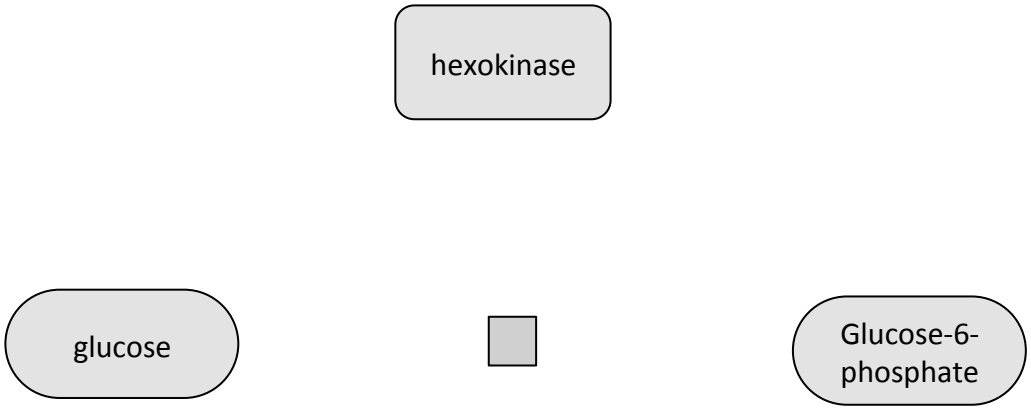

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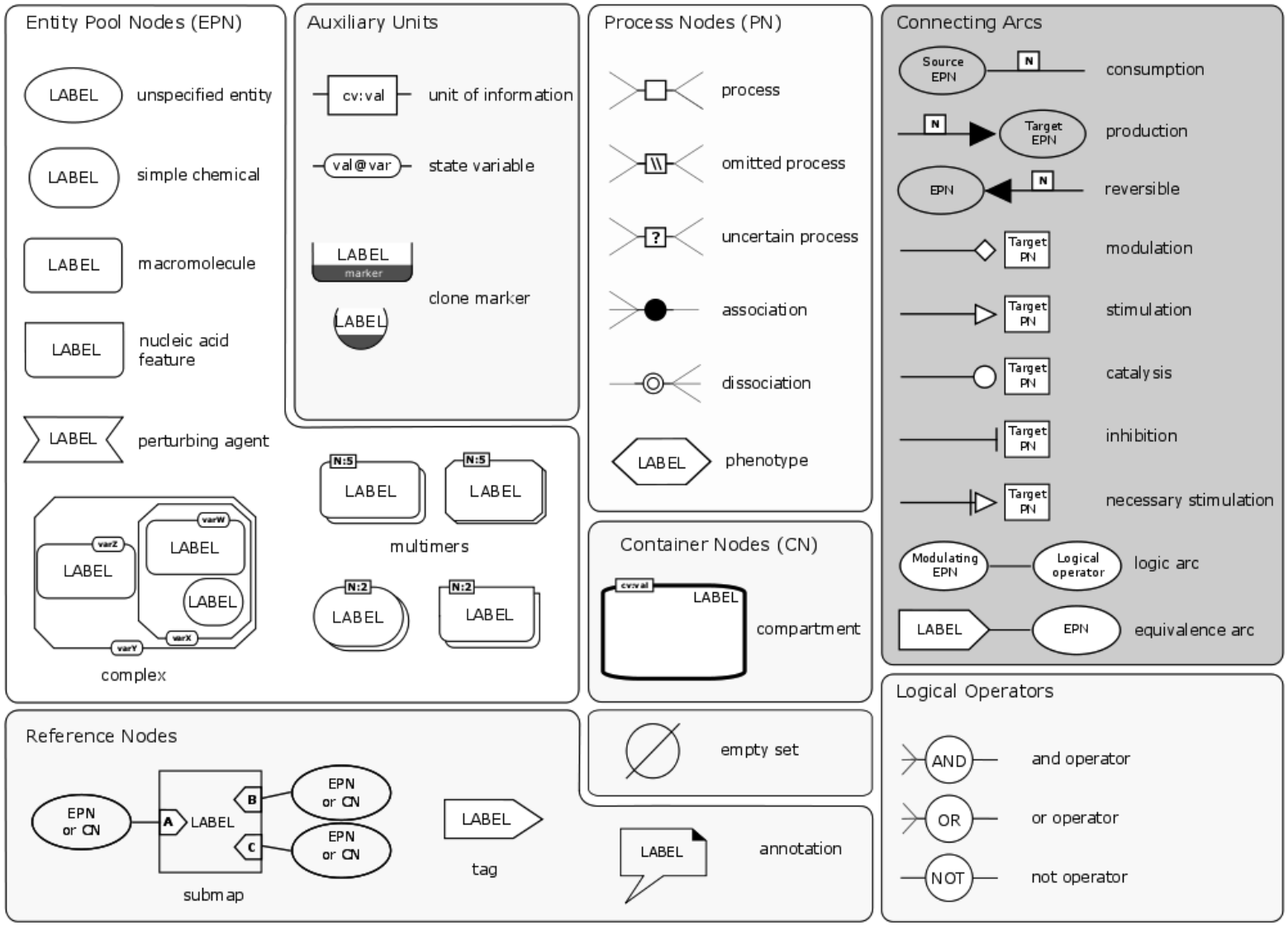

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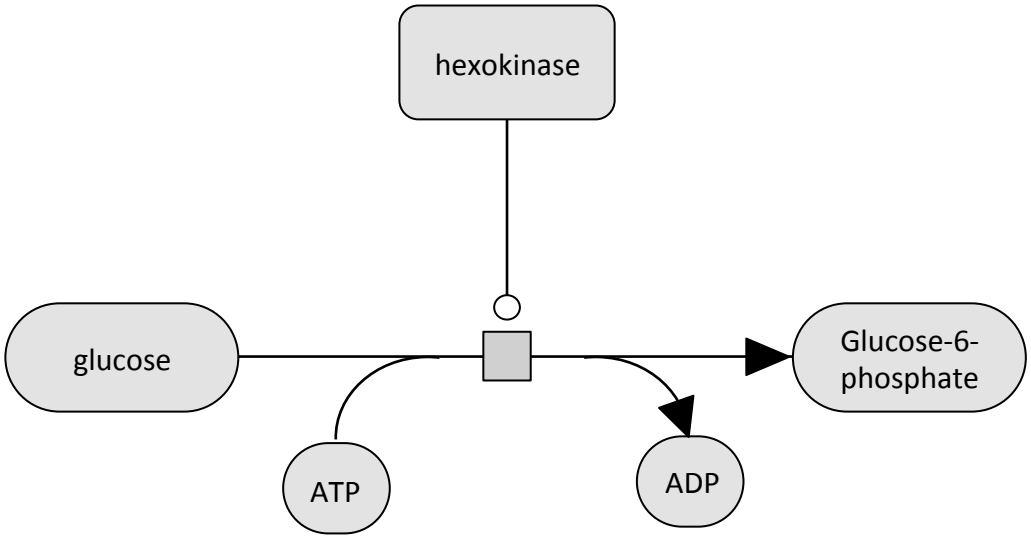

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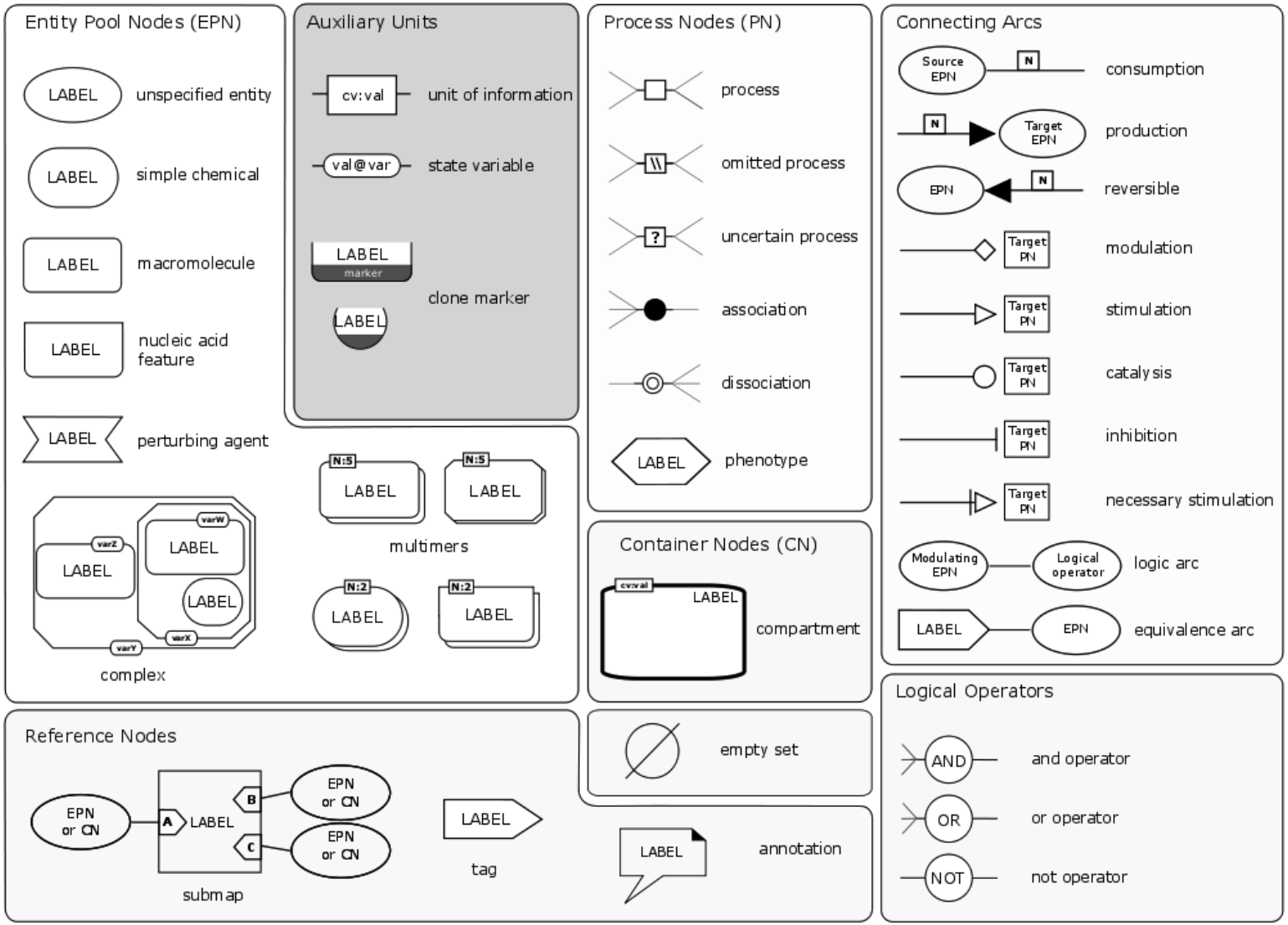

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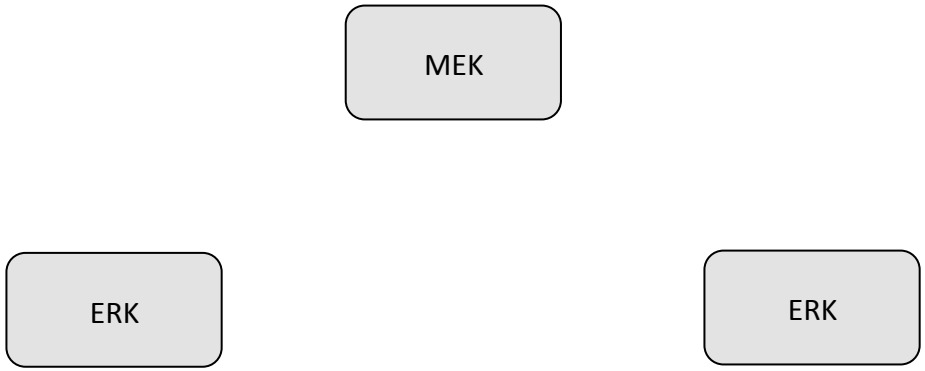

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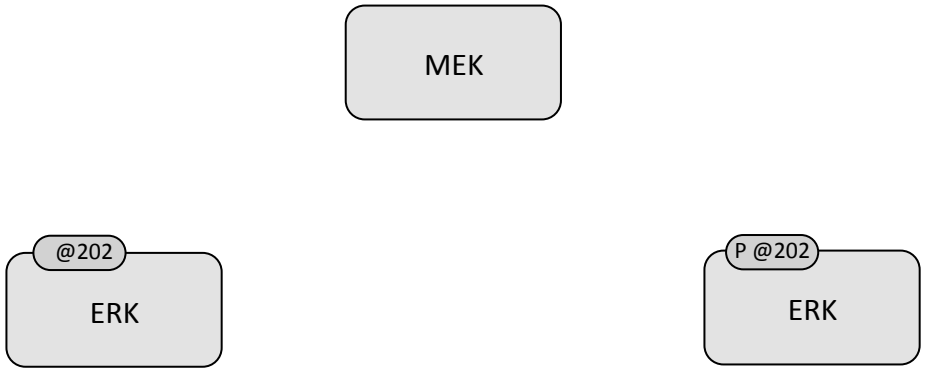

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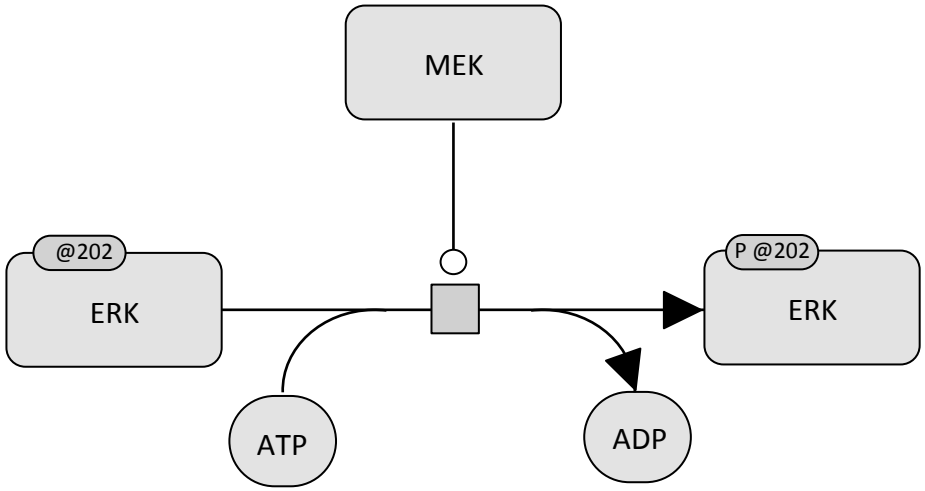

PD Example

Cell

γCaMKII Shuttles Ca^{2+}/CaM to the Nucleus to Trigger CREB Phosphorylation and Gene Expression

Huan Ma,[1,*] Rachel D. Groth,[3] Samuel M. Cohen,[1] John F. Emery,[1] Boxing Li,[1] Esthelle Hoedt,[2] Guoan Zhang,[2] Thomas A. Neubert,[2] and Richard W. Tsien[1,*]
[1]Department of Neuroscience and Physiology, Neuroscience Institute, NYU Langone Medical Center, New York, NY 10016, USA
[2]Department of Biochemistry and Molecular Pharmacology and Skirball Institute, NYU Langone Medical Center, New York, NY 10016, USA
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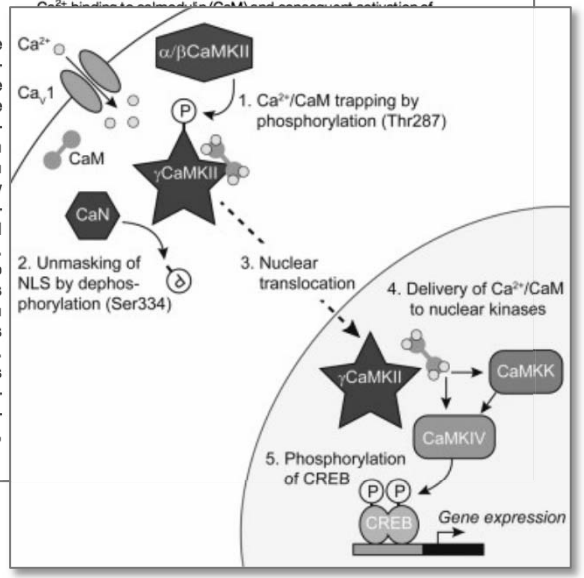
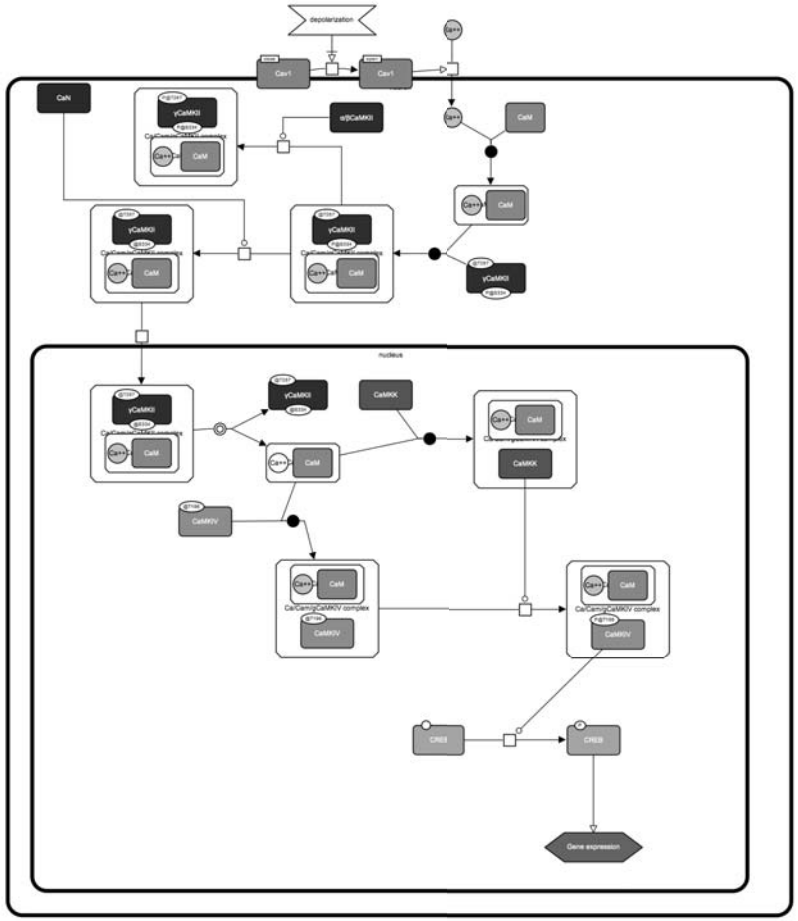
http://dx.doi.org/10.1016/j.cell.2014.09.019

SUMMARY

Activity-dependent CREB phosphorylation and gene expression are critical for long-term neuronal plasticity. Local signaling at Ca_V1 channels triggers these events, but how information is relayed onward to the nucleus remains unclear. Here, we report a mechanism that mediates long-distance communication within cells: a shuttle that transports Ca^{2+}/calmodulin from the surface membrane to the nucleus. We show that the shuttle protein is γCaMKII, its phosphorylation at Thr287 by βCaMKII protects the Ca^{2+}/CaM signal, and CaN triggers its nuclear translocation. Both βCaMKII and CaN act in close proximity to Ca_V1 channels, supporting their dominance, whereas γCaMKII operates as a carrier, not as a kinase. Upon arrival within the nucleus, Ca^{2+}/CaM activates CaMKK and its substrate CaMKIV, the CREB kinase. This mechanism resolves long-standing puzzles about CaM/CaMK-dependent signaling to the nucleus. The significance of the mechanism is emphasized by dysregulation of Ca_V1, γCaMKII, βCaMKII, and CaN in multiple neuropsychiatric disorders.





SBGN-PD

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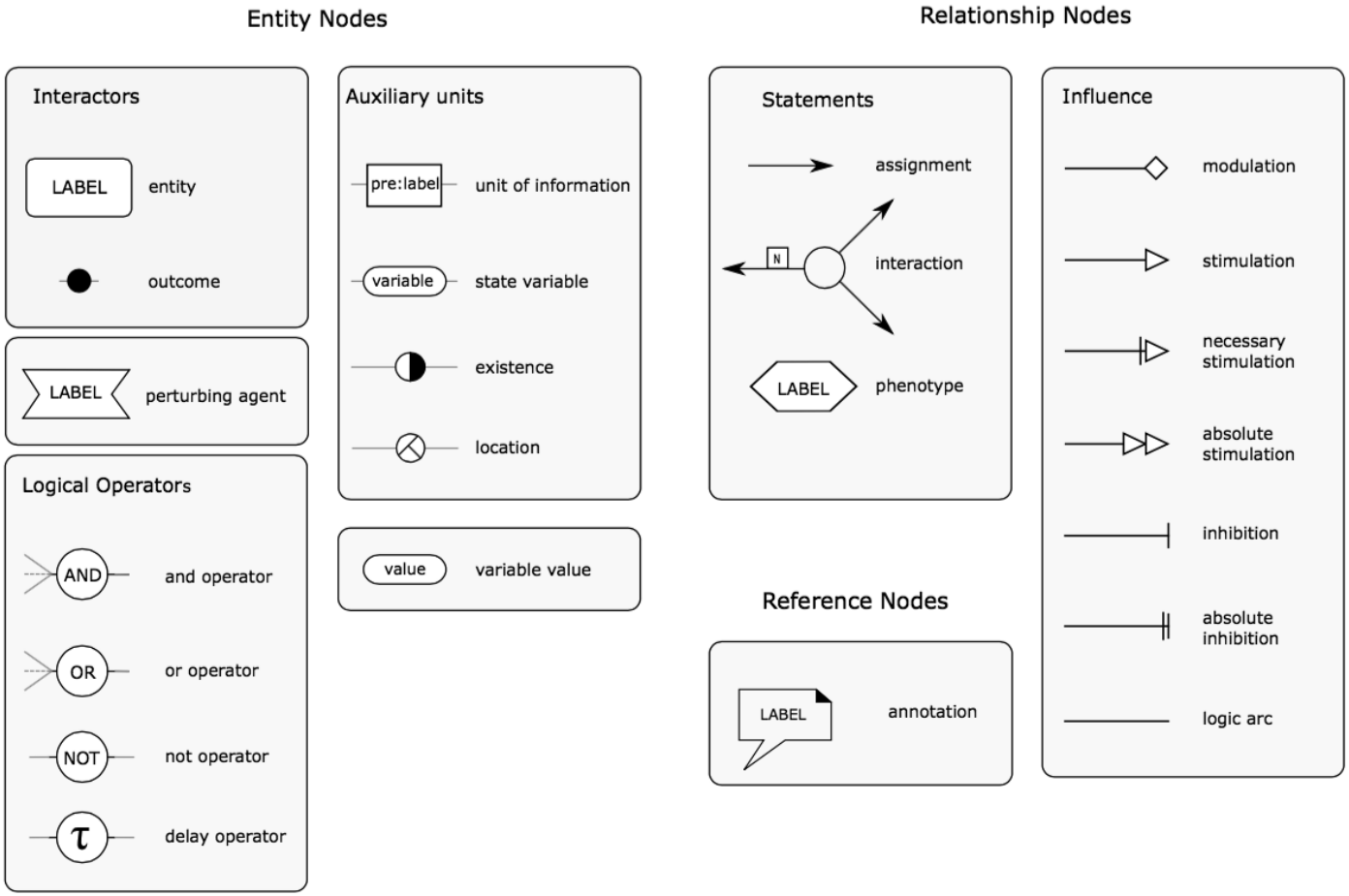

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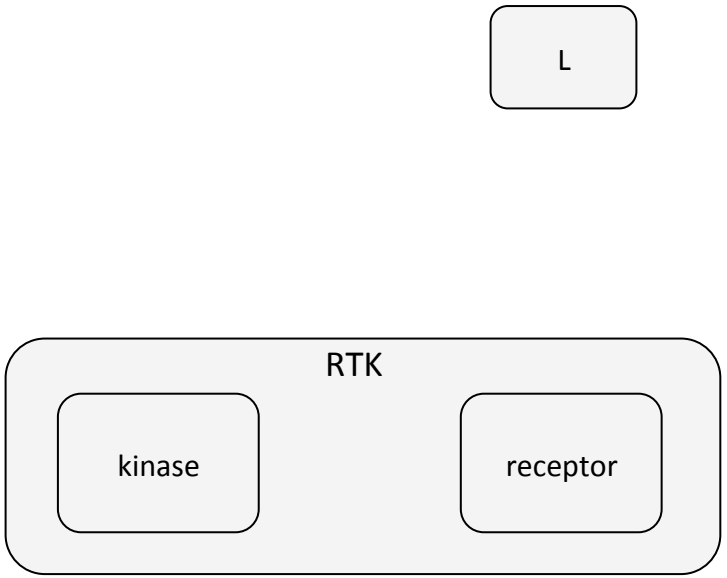

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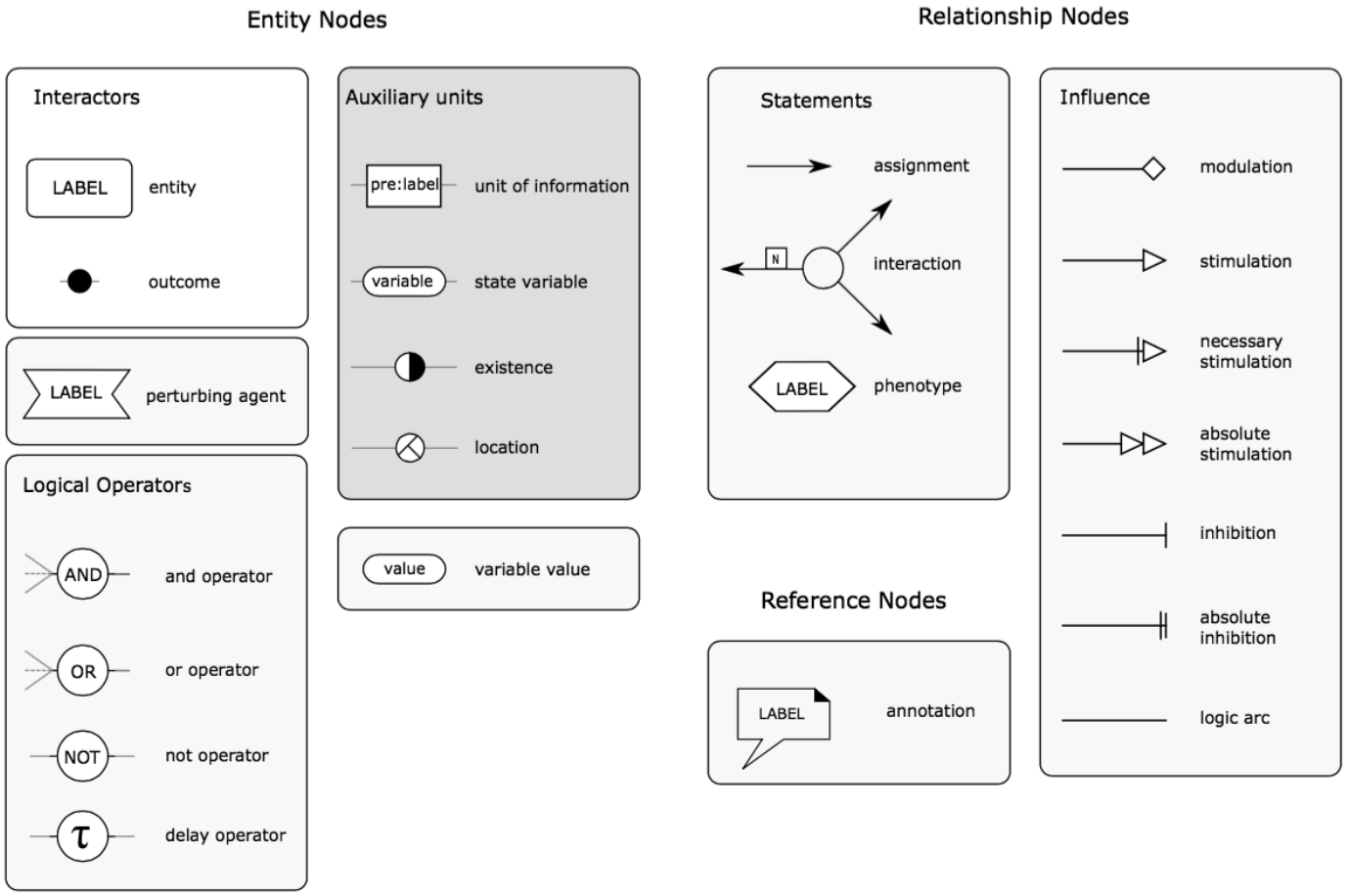

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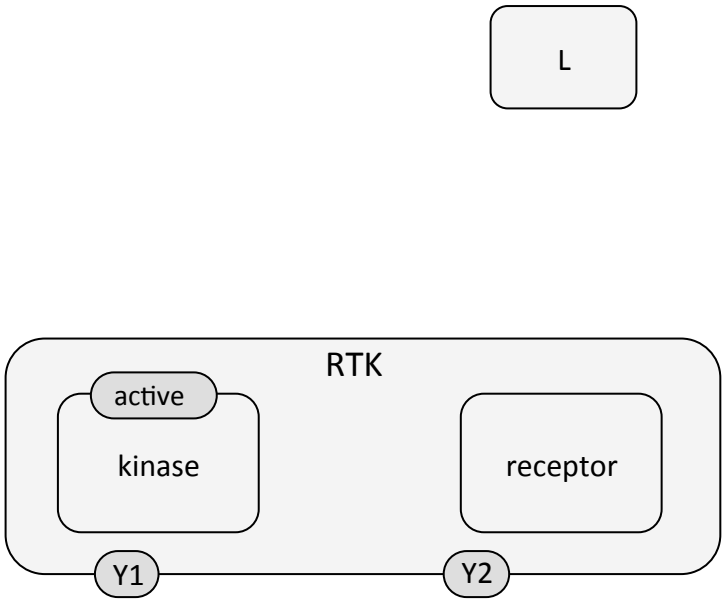

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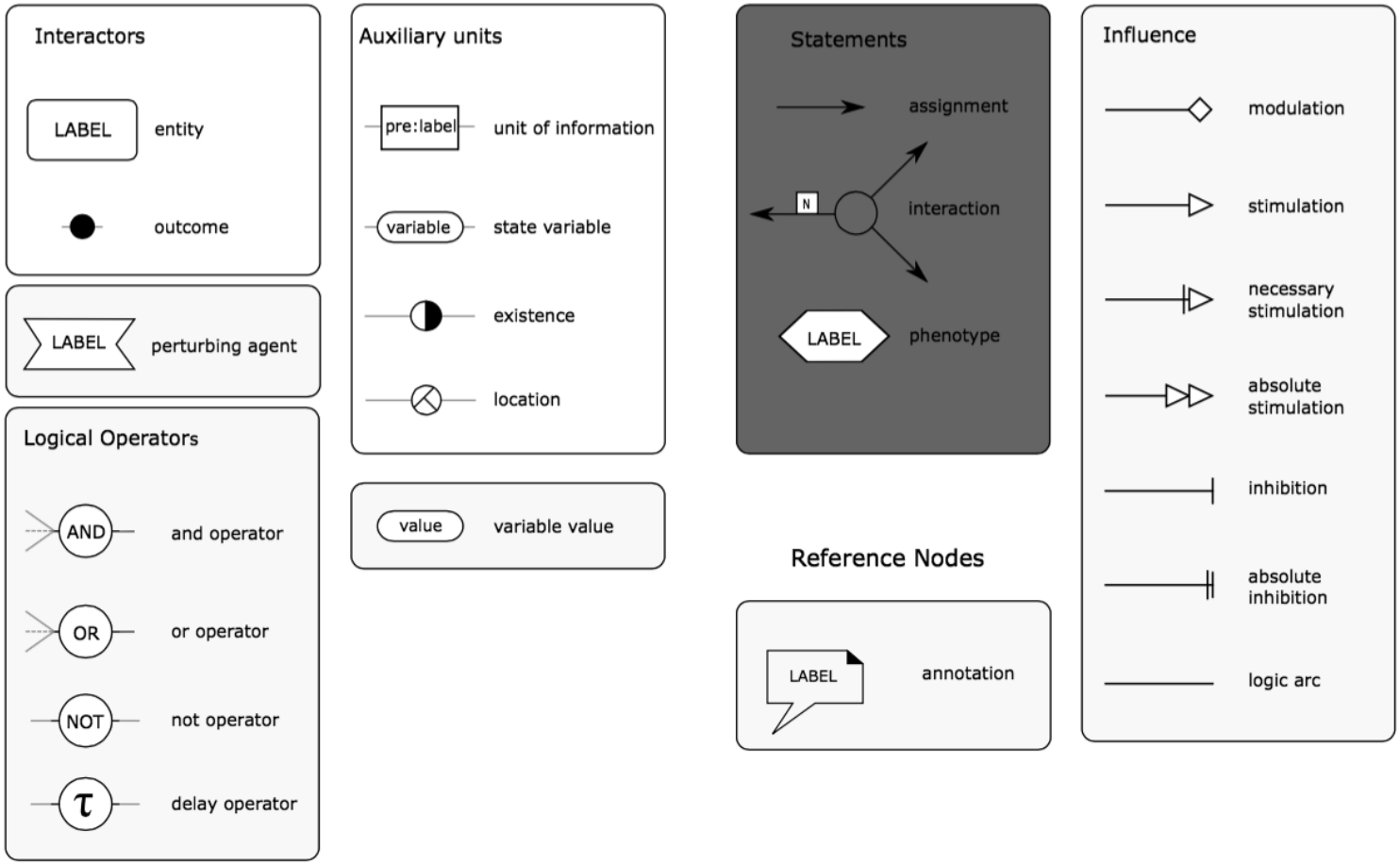

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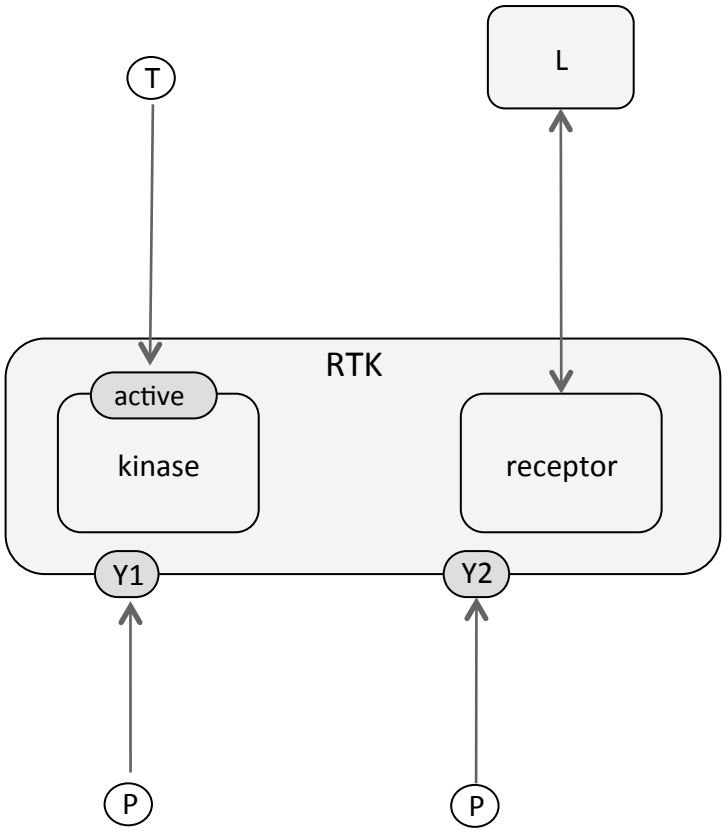

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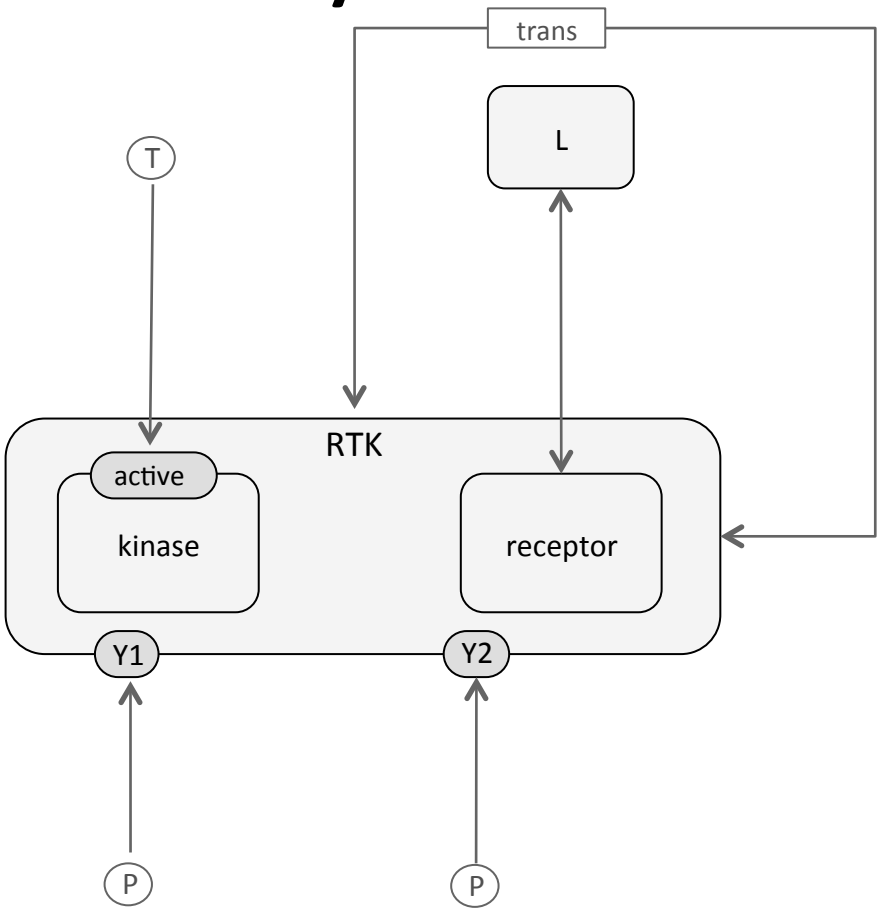

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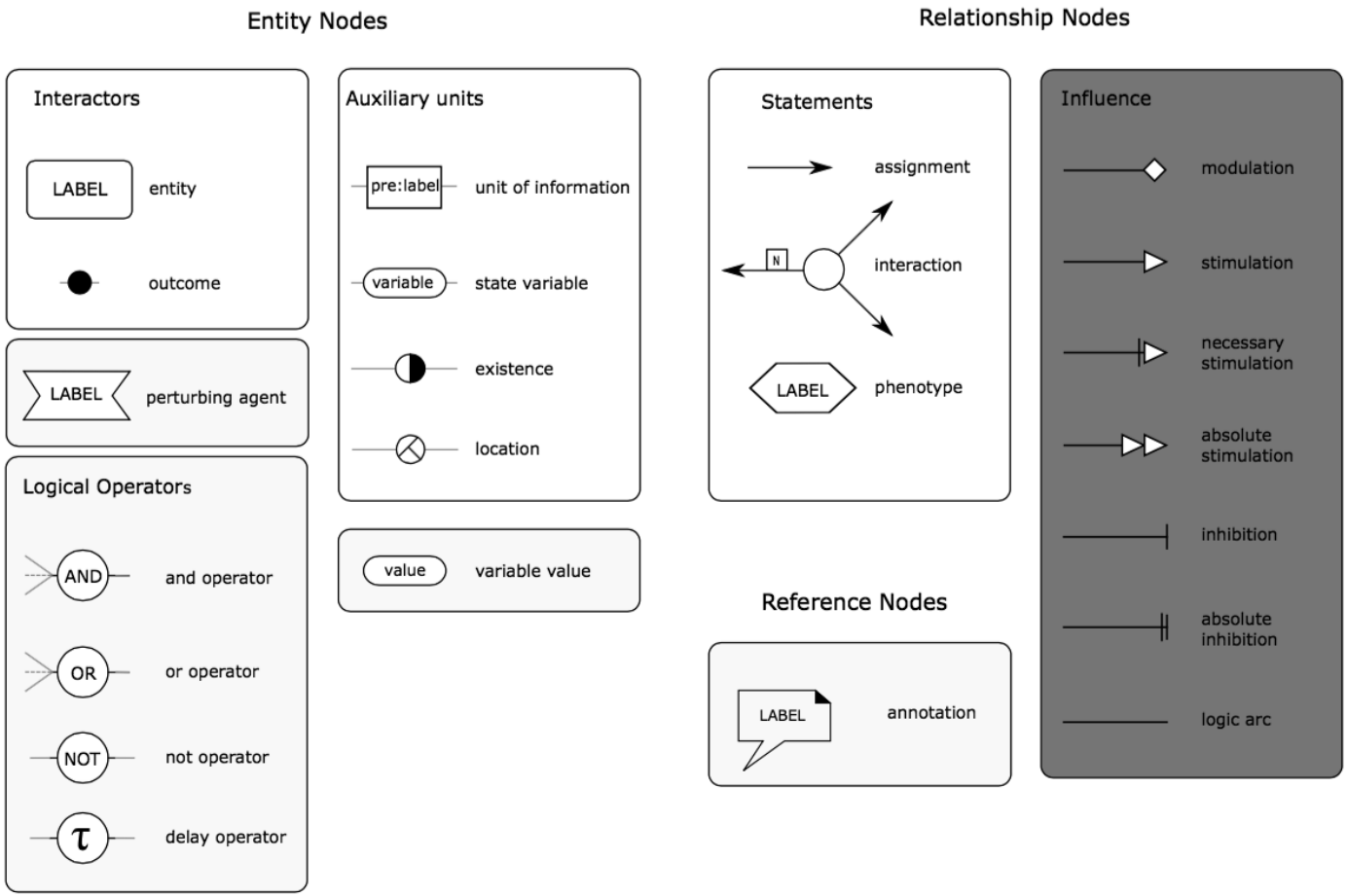

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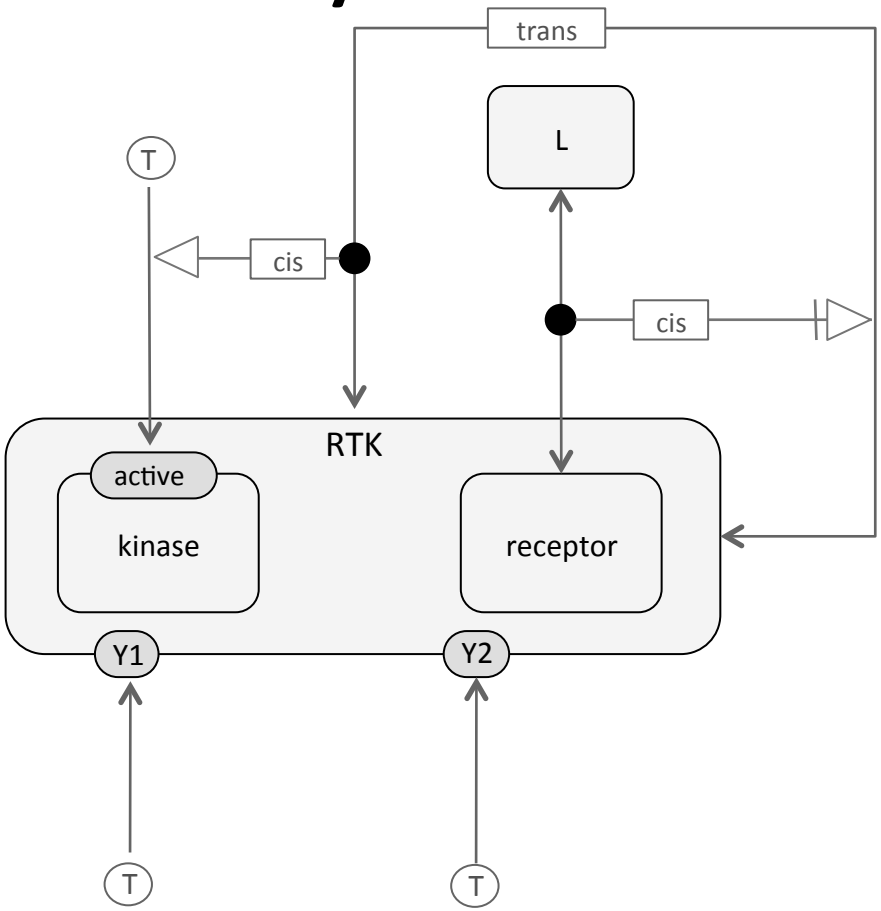

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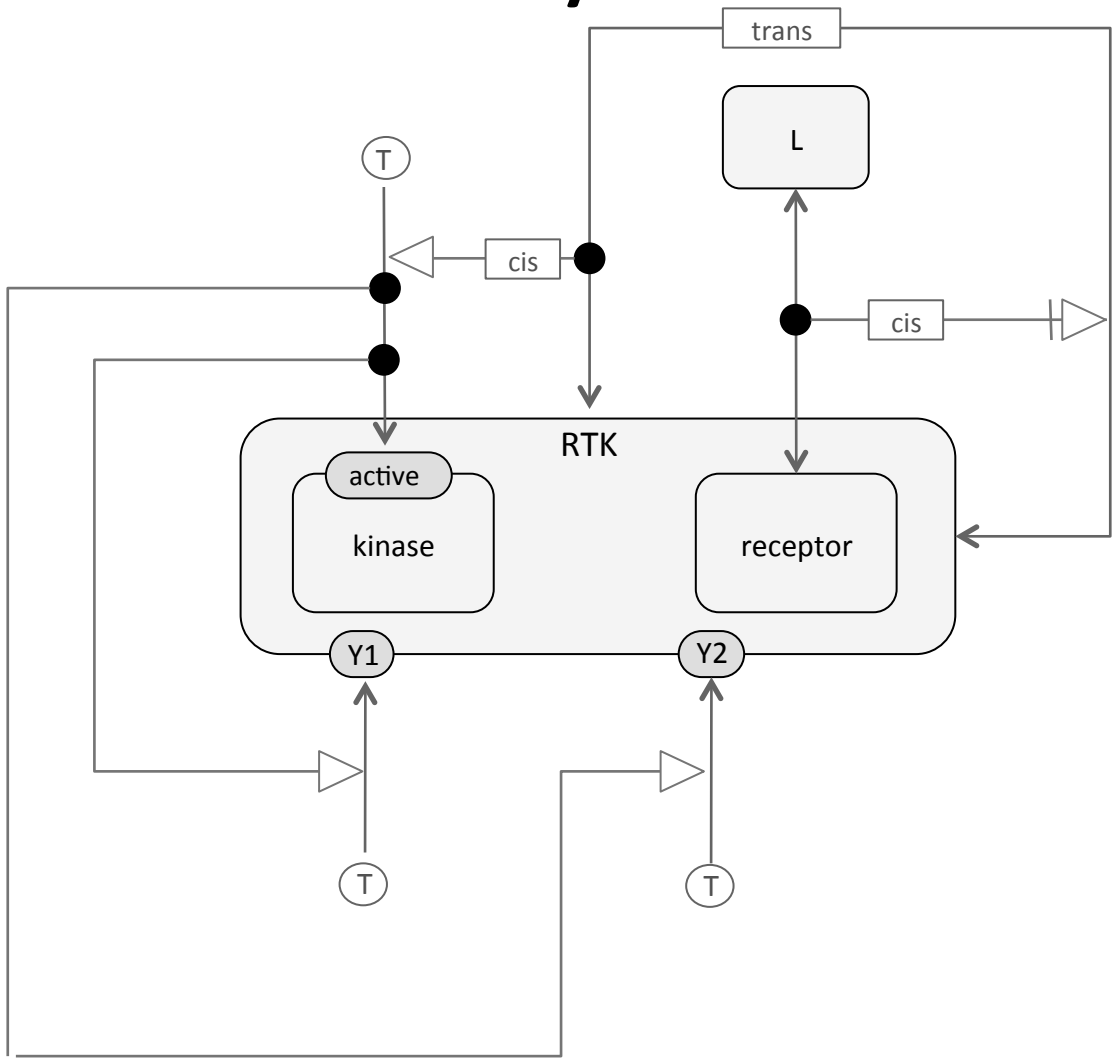

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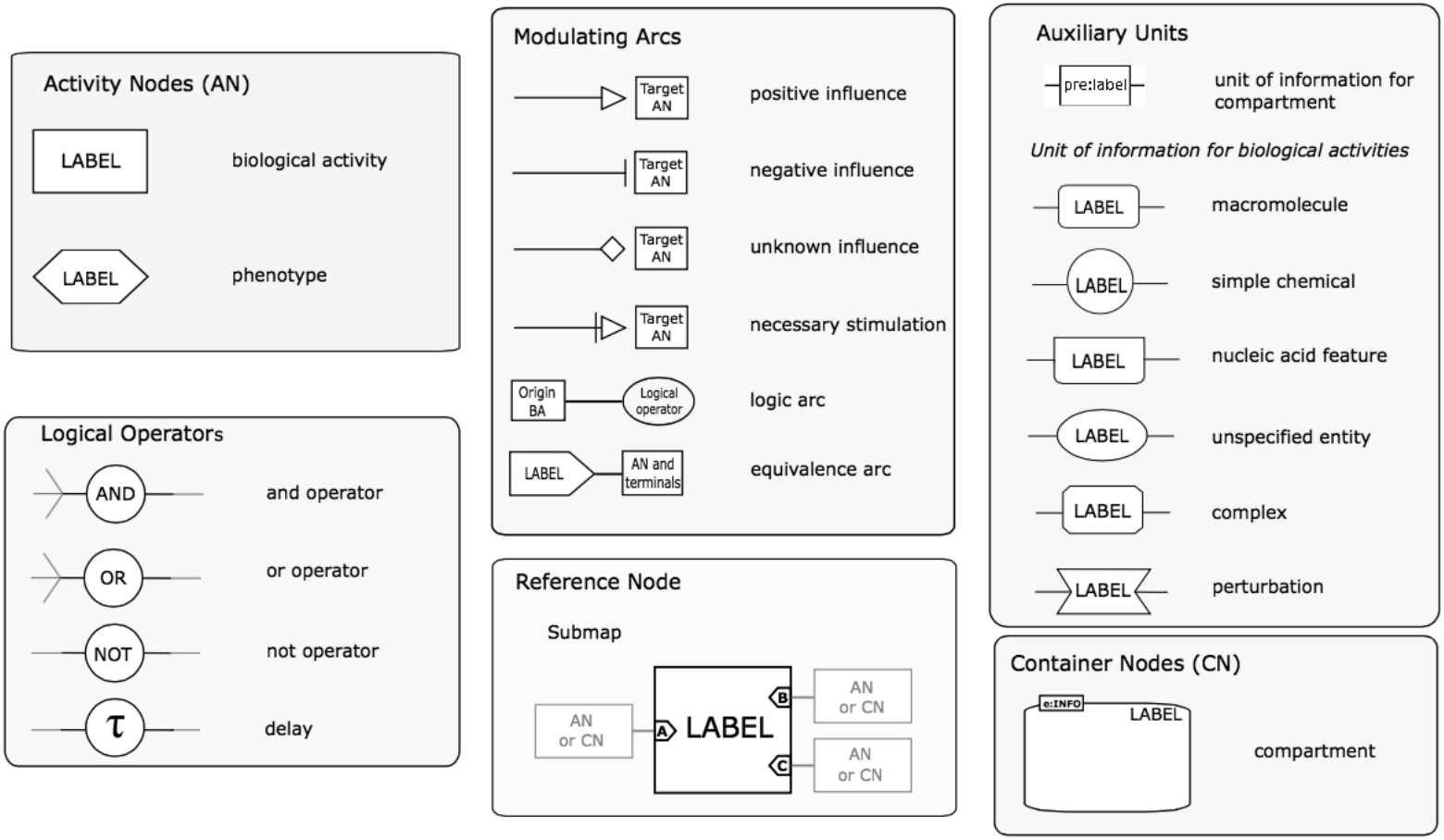
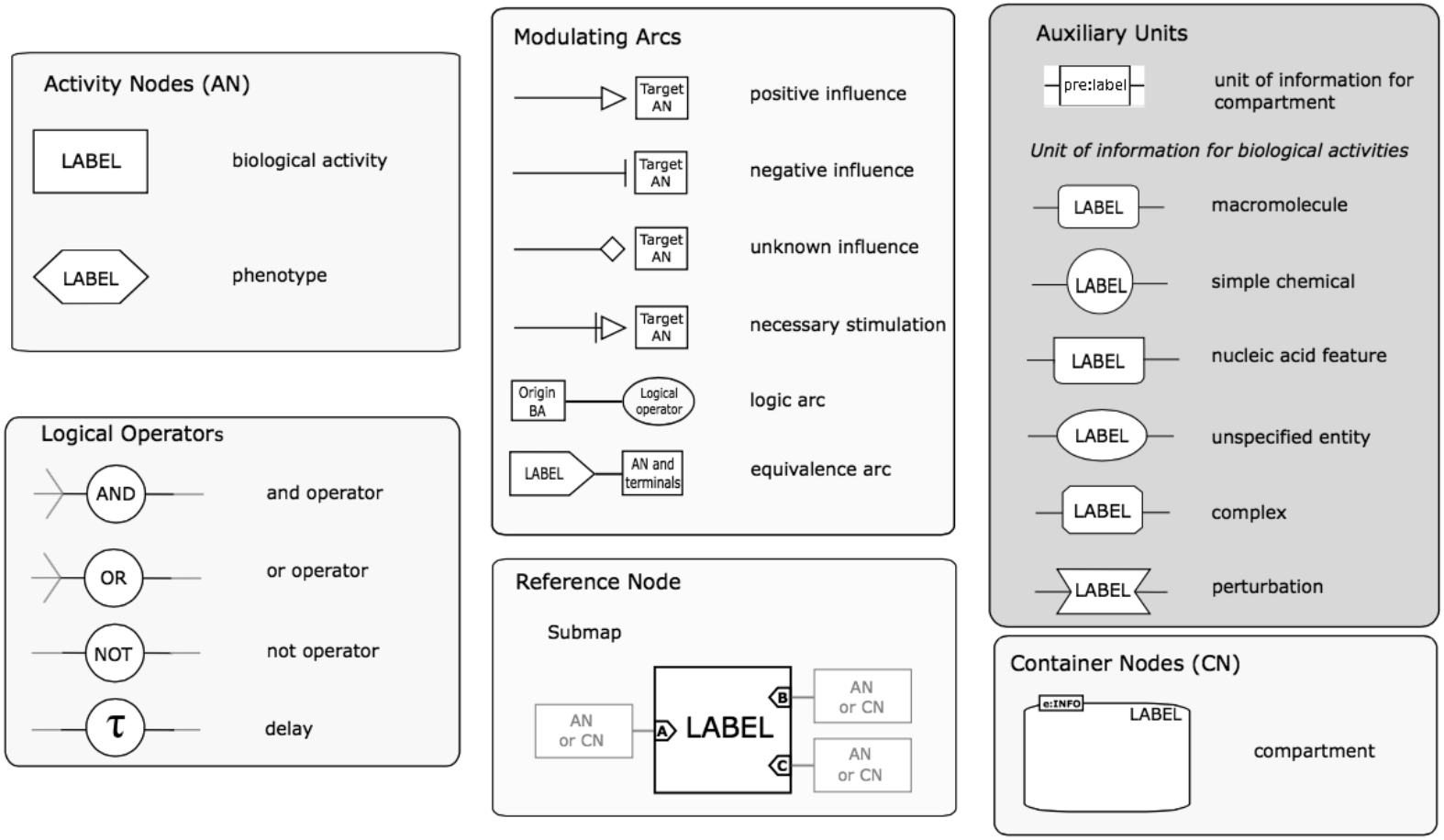
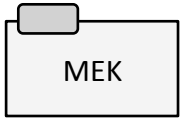


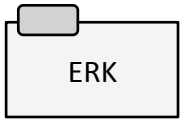
SBGN Activity Flow

Activity Flow Reference Card

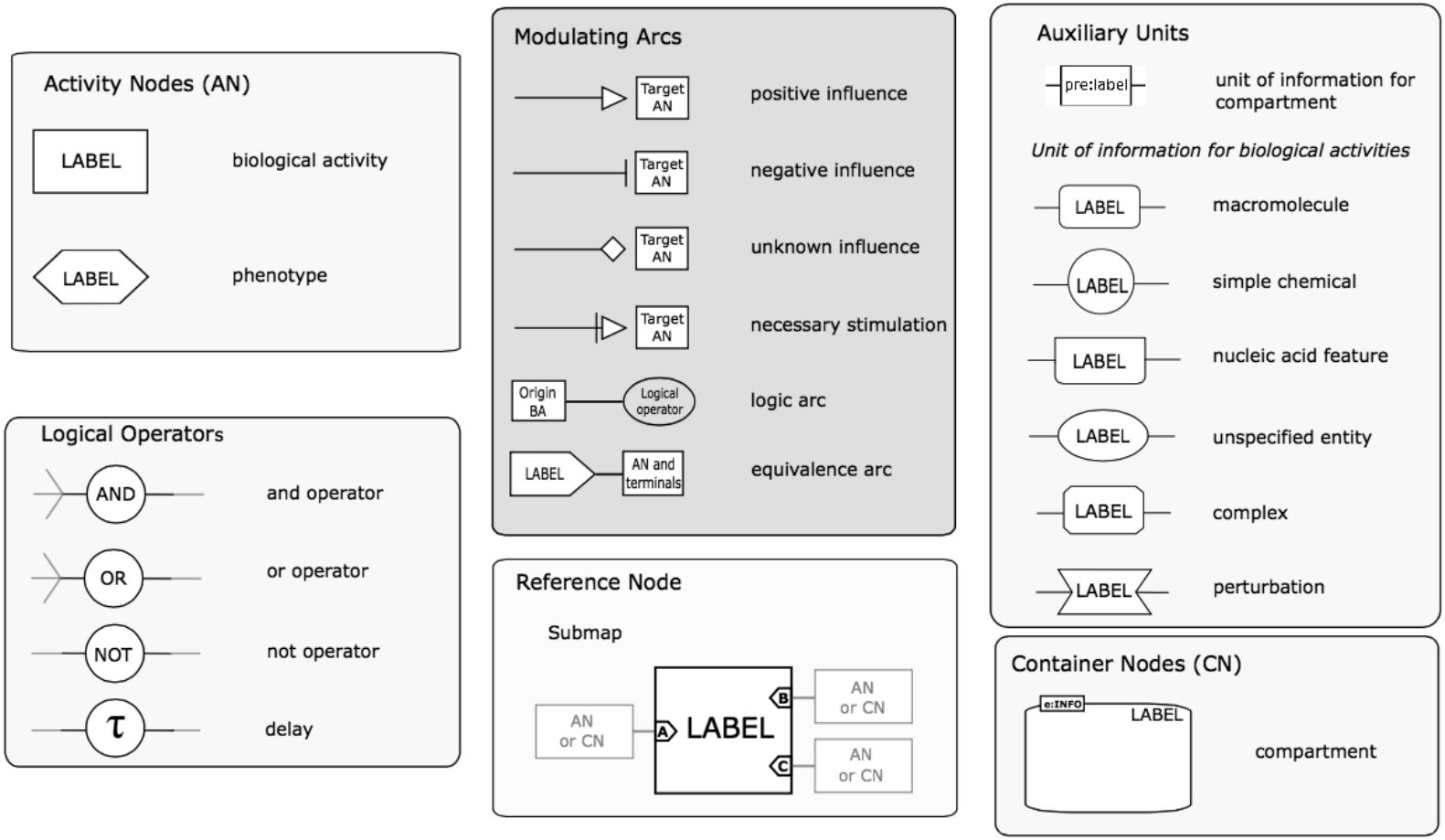


SBGN Activity Flow

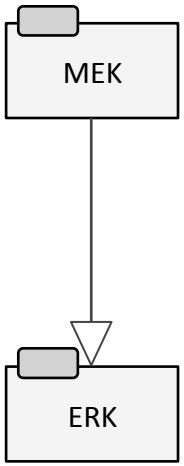




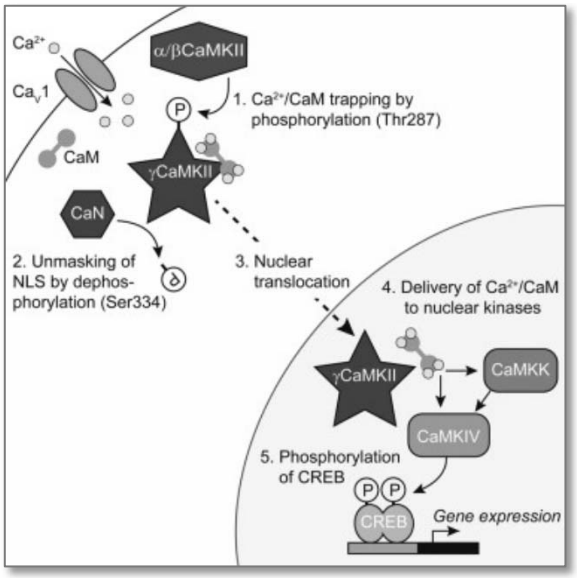
Activity Flow Reference Card

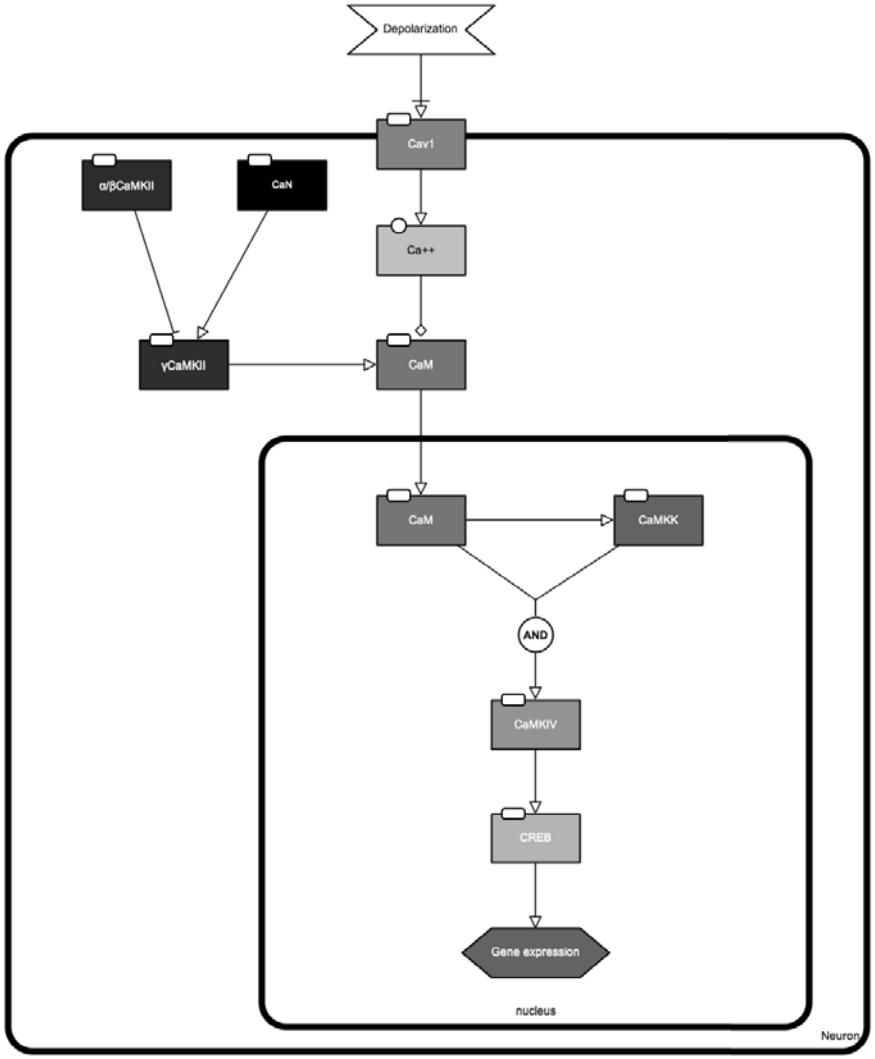


SBGN Activity Flow



AF Example

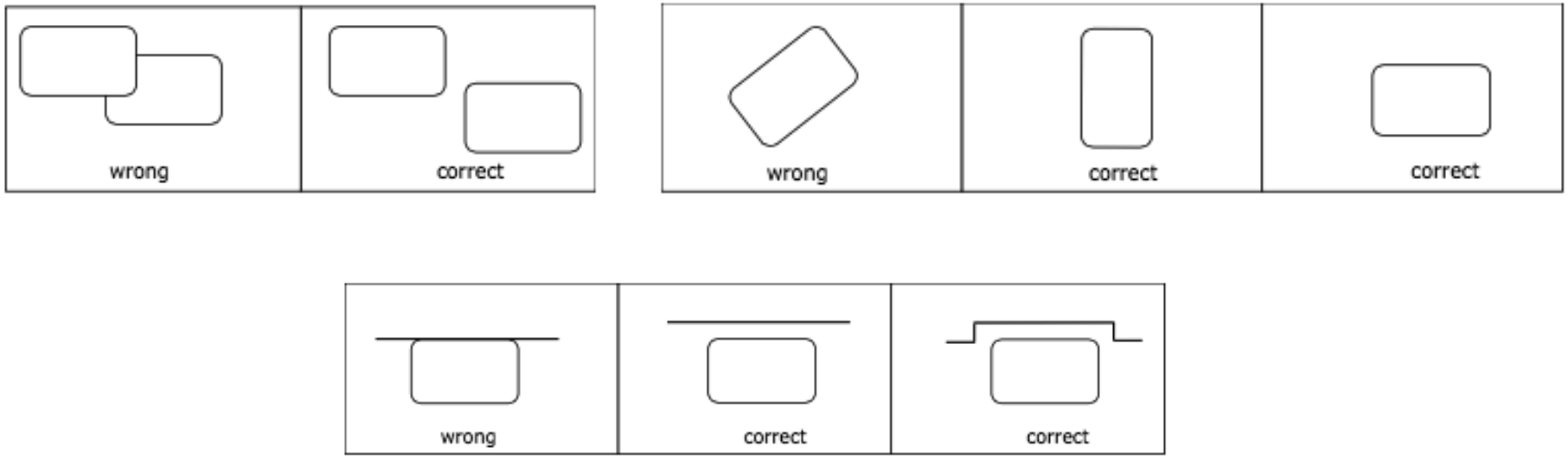




SBGN-AF

Semantics and Layout Rules

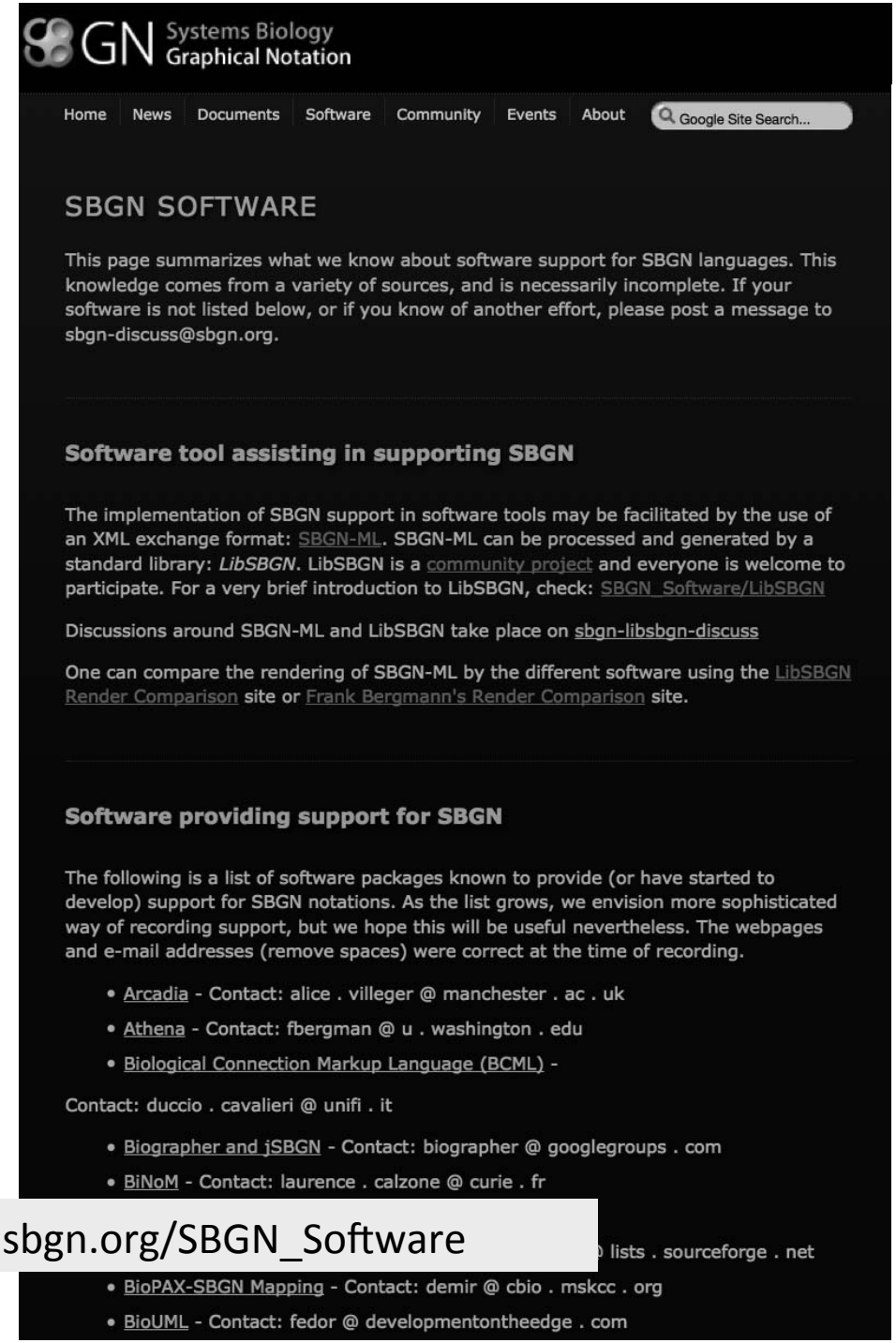
- All SBGN concepts are mapped to Systems Biology Ontology (SBO) terms.
- Layout rules



Current Status

- SBGN-PD
  - Current release: Level 1 Version 1.3
  - Candidate release: Level 1 Version 2 (end of 2015)
- SBGN-ER
  - Current release: Level 1 Version 2
- SBGN-AF
  - Current release: Level 1 Version 1.2

SOFTWARE SUPPORT



http://www.sbgn.org/SBGN_Software

SBGN-ML and LibSBGN

BIOINFORMATICS ORIGINAL PAPER Vol. 28 no. 15 2012, pages 2016–2021
doi:10.1093/bioinformatics/bts270

Systems Biology Advance Access publication May 10, 2012

Software support for SBGN maps: SBGN-ML and LibSBGN

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Associate Editor: Trey Ideker

ABSTRACT

Motivation: LibSBGN is a software library for reading, writing and manipulating Systems Biology Graphical Notation (SBGN) maps stored using the recently developed SBGN-ML file format. The library (available in C++ and Java) makes it easy for developers to add SBGN support to their tools, whereas the file format facilitates the exchange of maps between compatible software applications. The library also supports validation of maps, which simplifies the task of ensuring compliance with the detailed SBGN specifications. With this effort we hope to increase the adoption of SBGN in bioinformatics tools, ultimately enabling more researchers to visualize biological knowledge in a precise and unambiguous manner.

Availability and implementation: Milestone 2 was released in December 2011. Source code, example files and binaries are freely available under the terms of either the LGPL v2.1+ or Apache v2.0 open source licenses from http://libsbgn.sourceforge.net.

Contact: sbgn-libsbgn@lists.sourceforge.net

Received on December 13, 2011; revised on April 24, 2012; accepted on May 1, 2012

1 INTRODUCTION

The Systems Biology Graphical Notation (SBGN, Le Novère *et al.*, 2009) facilitates the representation and exchange of complex biological knowledge in a concise and unambiguous manner: as standardized pathway maps. It has been developed and supported by a vibrant community of biologists, biochemists, software developers, bioinformaticians and pathway databases experts.

SBGN is described in detail in the online specifications (see http://sbgn.org/Documents/Specifications). Here we summarize its concepts only briefly. SBGN defines three orthogonal visual languages: Process Description (PD), Entity Relationship (ER) and Activity Flow (AF). SBGN maps must follow the visual vocabulary, syntax and layout rules of one of these languages. The choice of language depends on the type of pathway or process being depicted and the amount of available information. The PD language, which originates from Kitano's Process Diagrams (Kitano *et al.*, 2005) and the related CellDesigner tool (Funahashi *et al.*, 2008), is equivalent to a bipartite graph (with a few exceptions) with one type of nodes representing pools of biological entities, and a second type of nodes representing biological processes such as biochemical reactions, transport, binding and degradation. Arcs represent consumption, production or control, and can only connect nodes of differing types. The PD language is very suitable for metabolic pathways, but struggles to concisely depict the combinatorial complexity of certain proteins with many phosphorylation states. The ER language, on the other hand, is inspired by Kohn's Molecular Interaction Maps (Kohn *et al.*, 2006), and describes relations between biomolecules. In ER, two entities can be linked with an interaction arc. The outcome of an interaction (for example, a protein complex), is considered an entity in itself, represented by a black dot, which can engage in further interactions. Thus ER represents dependencies between interactions, or putting it differently, it can represent which interaction is necessary for another one to take place. Interactions are possible between two or more entities, which make ER maps roughly equivalent to a hypergraph in which an arc can connect more than two nodes. ER is more concise than PD when it comes to representing protein modifications and protein interactions, although it is less capable when it comes to presenting biochemical reactions. Finally, the third language in the SBGN family is AF, which

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- Community project started in 2009
  - facilitate development of SBGN supporting tools
  - increase interoperability between these tools
- Electronic implementation of SBGN
  - exchange format for SBGN maps: **SBGN-ML**
    - XML schema based
    - express semantics, relationships and geometry
  - software library to interact with SBGN maps: **LibSBGN**
    - object model and API (C++, C#, Java)
    - key features: reading, writing, validation
    - libSBGN python was released recently after the HOARMONY 2015

SBGN-ML and LibSBGN

Wiki http://www.sbgn.org/LibSBGN
SourceForge project http://sourceforge.net/projects/libsbgn/
Mailing list sbgn-libsbgn@lists.sourceforge.net

Tools supporting SBGN-ML
http://www.sbgn.org/LibSBGN/ClientTools

Databases supporting SBGN-ML
Path2Models, PANTHER Pathway, Reactome, MetaCrop

Rendering comparison pipeline
http://libsbgn.sourceforge.net/render_comparison/

libSBGN python
https://github.com/matthiaskoenig/libsbgn-python

SBGN-ED

BIOINFORMATICS APPLICATIONS NOTE Vol. 26 no. 18 2010, pages 2340–2341
doi:10.1093/bioinformatics/btq407

Systems biology

Advance Access publication July 13, 2010

Editing, validating and translating of SBGN maps

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Associate Editor: Trey Ideker

ABSTRACT

Motivation: The recently proposed Systems Biology Graphical Notation (SBGN) provides a standard for the visual representation of biochemical and cellular processes. It aims to support more efficient and accurate communication of biological knowledge between different research communities in the life sciences. However, to increase the use of SBGN, tools for editing, validating and translating SBGN maps are desirable.

Results: We present SBGN-ED, a tool which allows the creation of all three types of SBGN maps from scratch or the editing of existing maps, the validation of these maps for syntactical and semantical correctness, the translation of networks from the KEGG and MetaCrop databases into SBGN and the export of SBGN maps into several file and image formats.

Availability: SBGN-ED is freely available from http://vanted.ipk-gatersleben.de/addons/sbgn-ed. The web site contains also tutorials and example files.

Contact: schreibe@ipk-gatersleben.de

Received on March 16, 2010; revised on June 18, 2010; accepted on July 6, 2010

1 INTRODUCTION

The Systems Biology Graphical Notation (SBGN; http://sbgn.org) (Le Novère *et al.*, 2009) is an emerging standard for the visual representation of biological networks. This standardization aims to improve information exchange and to support the collaborative creation of large maps based on individual modules. Such unified graphical representation should overcome the current situation in which many different styles of networks are used in biochemical, biological and medical books, articles and online resources. Especially in the growing field of systems biology, where increasingly complex and large networks have to be investigated, SBGN offers a promising approach for creating more intuitive and unambiguous visualizations.

Three different views of biological processes cover different levels of detail:

(1) *Process Description* (PD), which shows the temporal dependencies of biological interactions in a network in detail;
(2) *Entity Relationship* (ER), which displays the relationships in which a given entity participates in a network (without consideration of temporal aspects); and
(3) *Activity Flow* (AF), which shows the flow of information between biological entities in a network in an abstract way.

*To whom correspondence should be addressed.

Drawing large interaction maps is a time-consuming task. To enhance the usability of SBGN, tool support for creating, editing and validating such maps is required. Currently, several tools support or have started to consider SBGN, for an overview see http://sbgn.org/SBGN_Software.

Here we present SBGN-ED, a Vanted (Junker *et al.*, 2006) add-on for editing, validating and translating of SBGN maps. SBGN-ED contains a unique combination of features from SBGN map creation and editing to syntactic and semantic validation of SBGN maps, to automatic translation of existing non-SBGN networks from KEGG (Kanehisa *et al.*, 2010) and MetaCrop (Grafahrend-Belau *et al.*, 2008) into SBGN, and to the export of SBGN maps in different file and image formats. Furthermore, all methods of the Vanted system for integration and network-based analysis of high-throughput data, data visualization and network layout as well as constraint-based model simulation are fully accessible to the SBGN maps. The Vanted system and the SBGN-ED add-on form a comprehensive platform for SBGN-supported analysis and visualization of biological networks.

2 METHODS

SBGN-ED is an add-on for Vanted (Junker *et al.*, 2006). Vanted is an open source software that offers the loading and editing of networks, allows the integration of different *omics data and provides a variety of functions for data mapping and processing, statistical analysis and visualization. The main functions of SBGN-ED are:

(1) SBGN map creation and editing;
(2) SBGN map validation; and
(3) the translation of networks into SBGN.

These SBGN maps can then be exported into different file and image formats such as GML, GraphML, PDF, SVG, PNG, PNG/HTML image maps and JPG. The following subsections describe the methodology of important functions such as validation and translation.

2.1 Editing

SBGN maps can be created from scratch or loaded from files. The relevant functionality for editing such maps is similar to well-established editing methods for networks (see typical network analysis and graph drawing tools) and allows the addition, removal and alteration of SBGN symbols (nodes and edges), the alteration of the size, color, label and other attributes of map elements, and the alteration of the layout of the map manually or automatically.

Following the SBGN specification, SBGN-ED supports all SBGN symbols (nodes and edges) as well as special connectors defined within glyphs (e.g. ports sticking out of process nodes). These connectors are dynamically adapted during the drawing of a map according to user interaction. For each SBGN language (PD, ER and AF), a side panel contains

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- editing, validating and translating of SBGN maps
- add-on for VANTED
- supports all three SBGN languages
- supports SBGN-ML
- http://www.sbgn-ed.org

SBGN-ED

SBGN-ED **Editing, Translating and Validating of SBGN Maps**

Overview **Download & Installation** **Tutorials** **Example Files** **Copyright & Contact**

Overview

The Systems Biology Graphical Notation (SBGN, http://sbgn.org) is an emerging standard for graphical representations of biochemical and cellular processes studied in systems biology. This standardisation helps to communicate biological knowledge more efficient and accurate between different research communities in the life sciences. However, to support SBGN, tools for editing, validating and translating of SBGN maps are necessary.

We present SBGN-ED, a VANTED add-on which allows to create and edit all three types of SBGN maps, that is Process Description, Entity Relationship and Activity Flow, to validate these maps according to the SBGN specifications, to translate maps from the KEGG pathway database into SBGN, and to export SBGN maps into several file and image formats.

The VANTED system (**V**isualisation and **A**nalysis of **Net**works containing **E**xperimental **D**ata) is an open source software that offers the possibility to load and edit graphs, which may represent biological pathways or functional hierarchies. It allows to integrate different *omics data into the functional context and provides a variety of functions for data mapping and processing, statistical analysis, and visualisation. With the VANTED Add-on interface it is easily possible to extend the functionality of the software.

News

31/08/2015 - SBGN-ED 1.5.1 released

- compatible with VANTED 2.5
- bug fixes

24/10/2013 - SBGN-ED 1.5 released

- SBGN Process Description (PD) to SBGN Activity Flow (AF) translation added
- bug fixes

16/08/2013 - SBGN-ED 1.4 released

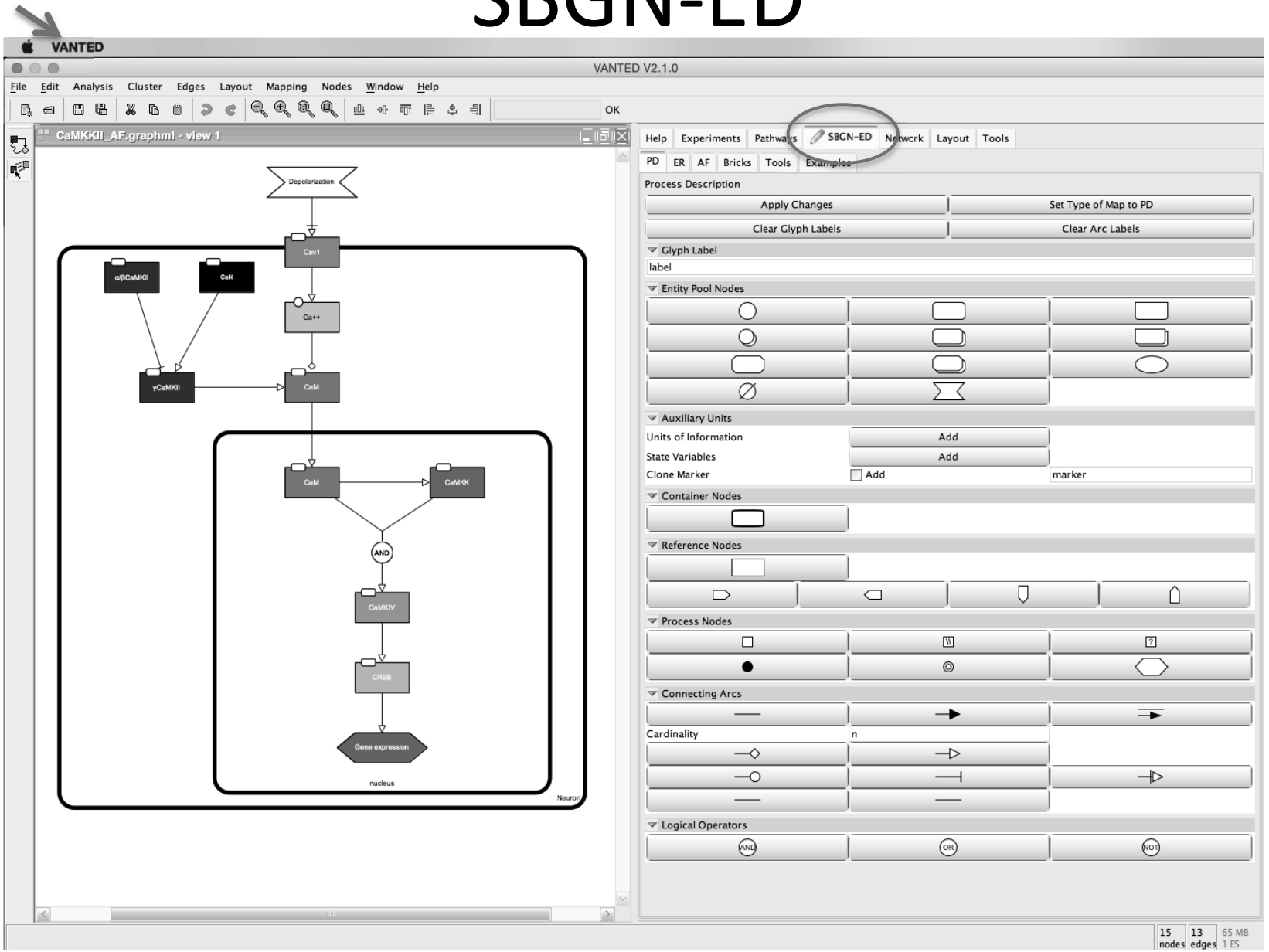
- KEGG to SBGN translation with Constraint Layout added
- SBGN bricks added
- simple SBML to SBGN translation added
- bug fixes

07/08/2012 - SBGN-ED 1.3 released

- compatible with VANTED 2.1.0
- bug fixes

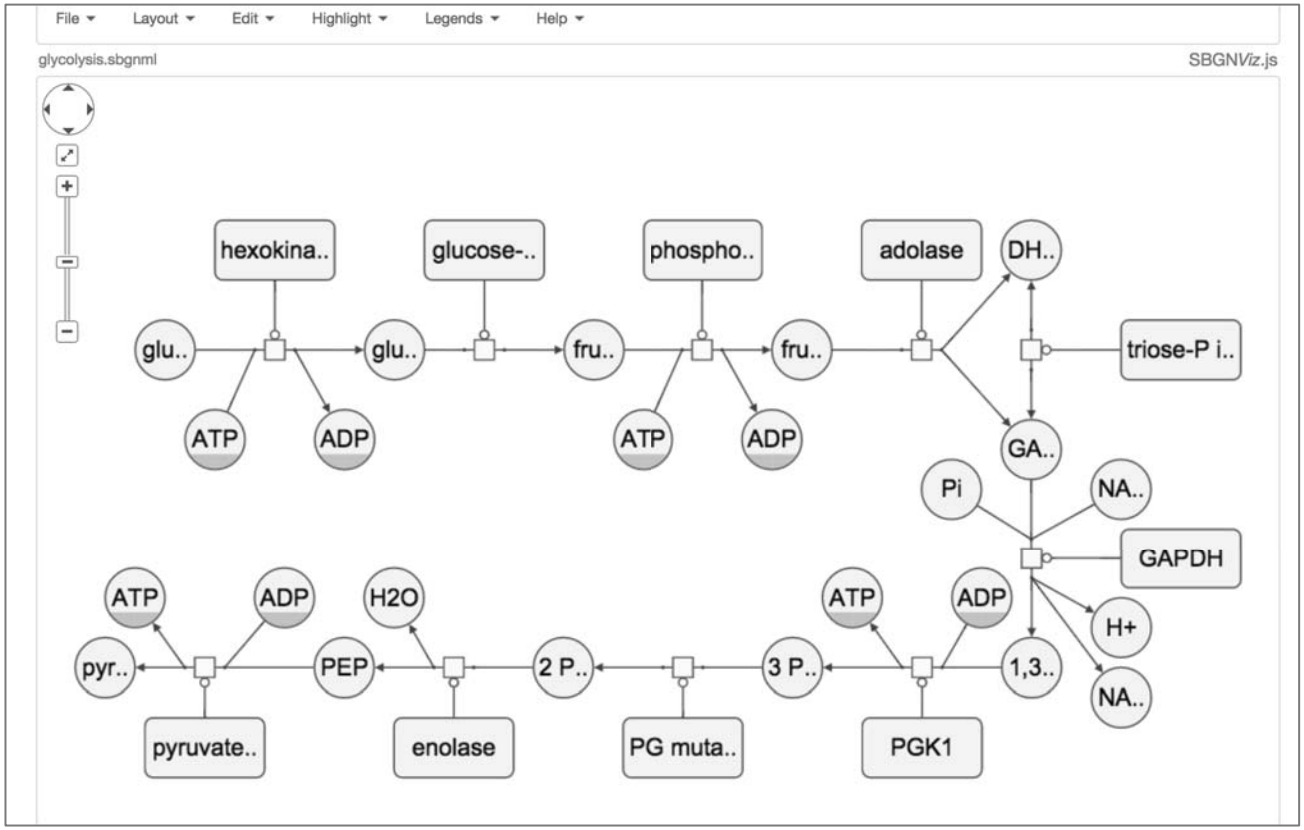
Czauderna *et al.*, Editing, Validating, and Translating of SBGN Maps, *Bioinformatics* (2010)

SBGN-ED


VANTED
VANTED V2.1.0
File Edit Analysis Cluster Edges Layout Mapping Nodes Window Help
OK
CaMKKII_AF.graphml - view 1
Depolarization
Cav1
α/βCaMKII
CaN
Ca++
γCaMKII
CaM
CaM
CaMKK
AND
CaMKIV
CREB
Gene expression
nucleus
Neuron
Help Experiments Pathways SBGN-ED Network Layout Tools
PD ER AF Bricks Tools Examples
Process Description
Apply Changes
Set Type of Map to PD
Clear Glyph Labels
Clear Arc Labels
Glyph Label
label
Entity Pool Nodes
Auxiliary Units
Units of Information
Add
State Variables
Add
Clone Marker
Add
marker
Container Nodes
Reference Nodes
Process Nodes
Connecting Arcs
Cardinality
n
Logical Operators
AND
OR
NOT
15 nodes
13 edges
65 MB
1 ES

SBGN*Viz*: a web based SBGN viewer

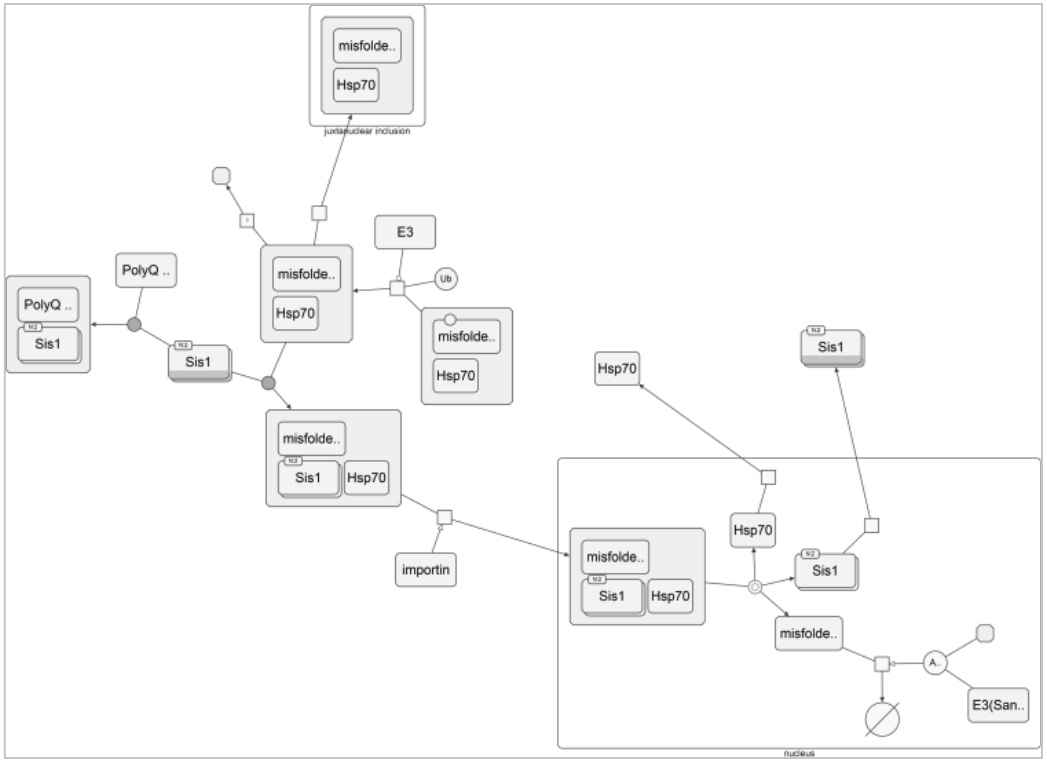
- Read/write SBGN-ML, display in SBGN-PD
- Full support for compound structures including auto-layout
- Save as static images
- Code URL: https://github.com/PathwayCommons/sbgnviz-js

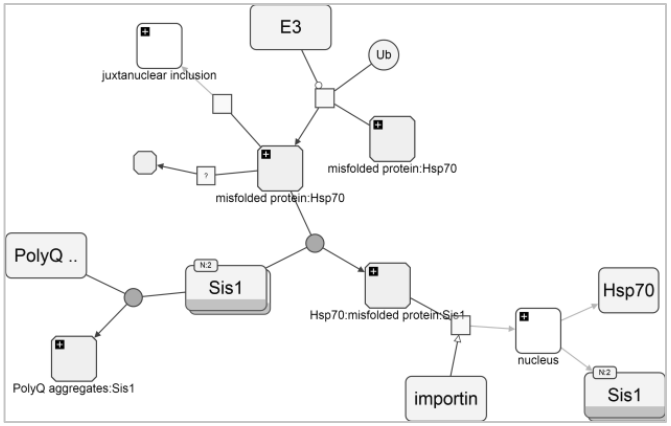


M. Sari, I. Bahceci, U. Dogrusoz, S.O. Sumer, B.A. Aksoy, O. Babur, E. Demir, "SBGNViz: a tool for visualization and complexity management of SBGN process description maps", PLoS ONE, 10(6), e0128985, 2015.

SBGN*Viz*: a web based SBGN viewer

- Complexity management operations to show/hide selected and collapse/expand compound structures





M. Sari, I. Bahceci, U. Dogrusoz, S.O. Sumer, B.A. Aksoy, O. Babur, E. Demir, "SBGNViz: a tool for visualization and complexity management of SBGN process description maps", PLoS ONE, 10(6), e0128985, 2015.

What's next?

- Continue to support the community to incorporate SBGN functionality.
  - Level 2 specification - easier support of a diverse community.
  - Community support – SBOL, Gene Ontology, etc.
  - Software support
  - Community outreach
  - Funding

Acknowledgements

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Acknowledgements

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