

SBGN Software Support (1) -
Completeness, Exactitude, Validation
Application
CellDesigner™ Ver. 4.1

<http://celldesigner.org>

2010/July

CellDesigner Development Team
The Systems Biology Institute

CellDesigner™ Version 4.1

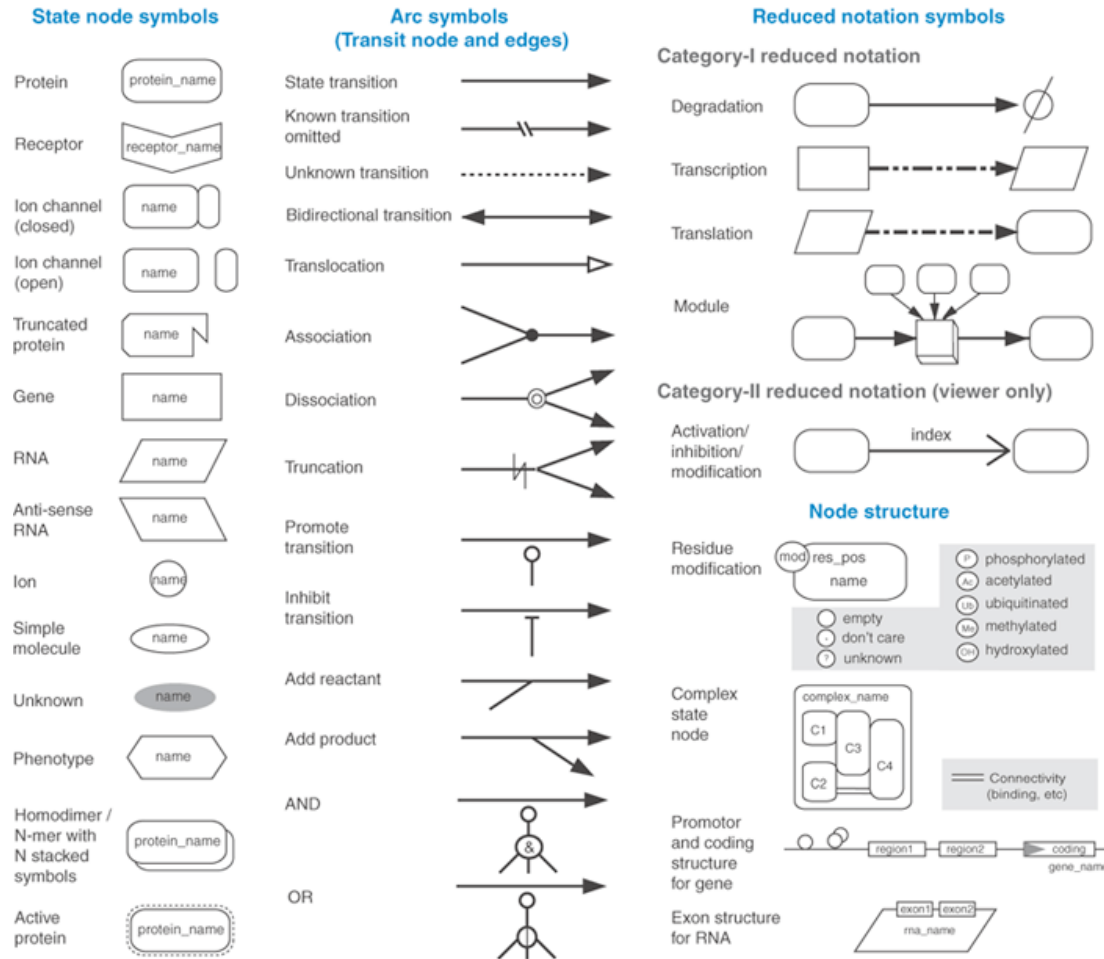
- Instructions for installation:
 - <http://www.celldesigner.org/download.html>
- Instruction for use:
 - CellDesigner 4.1 Help: <http://www.celldesigner.org/help/index.html>
 - CellDesigner 4.1 Startup Guide
<http://www.celldesigner.org/documents/StartupGuide41.pdf>
 - CellDesigner 4.1 : Running CellDesigner's Simulation using Control Panel
<http://www.celldesigner.org/documents/ControlPanel41.pdf>
 - CellDesigner 4.1 : Plugin Tutorial
<http://www.celldesigner.org/documents/PluginTutorial41.pdf>
 - [CellDesigner Plungin API help](#)
(in your installed directory, /document/plugin/index.html)
<http://www.celldesigner.org/plugin/pluginAPI/index.html>

Visual Proofs (a)

- that your software supports all or most of SBGN languages

- CellDesigner 4.1 support most of SBGN
Process Description Diagram Level 1.1

Original Notation proposed by Kitano



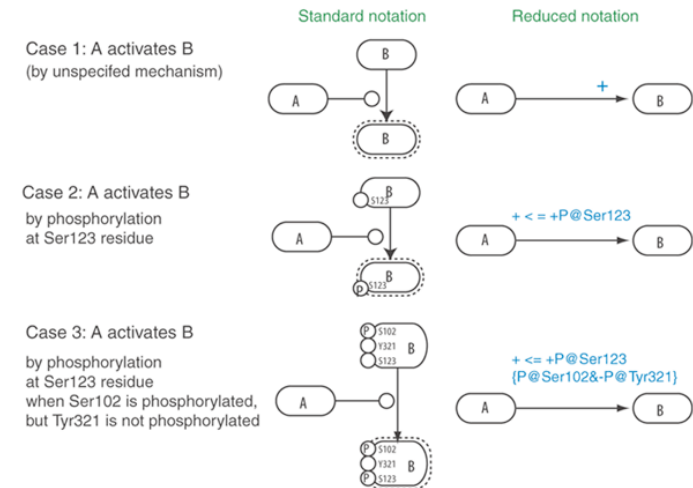
Syntax for index on category-II reduced notation



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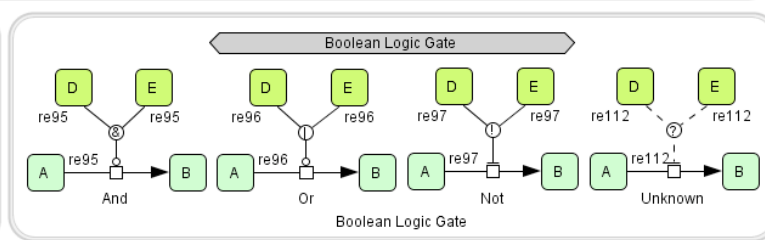
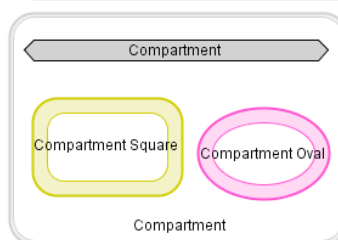
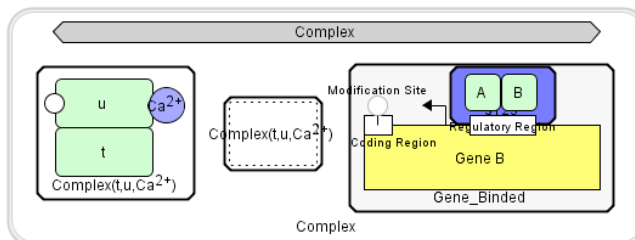
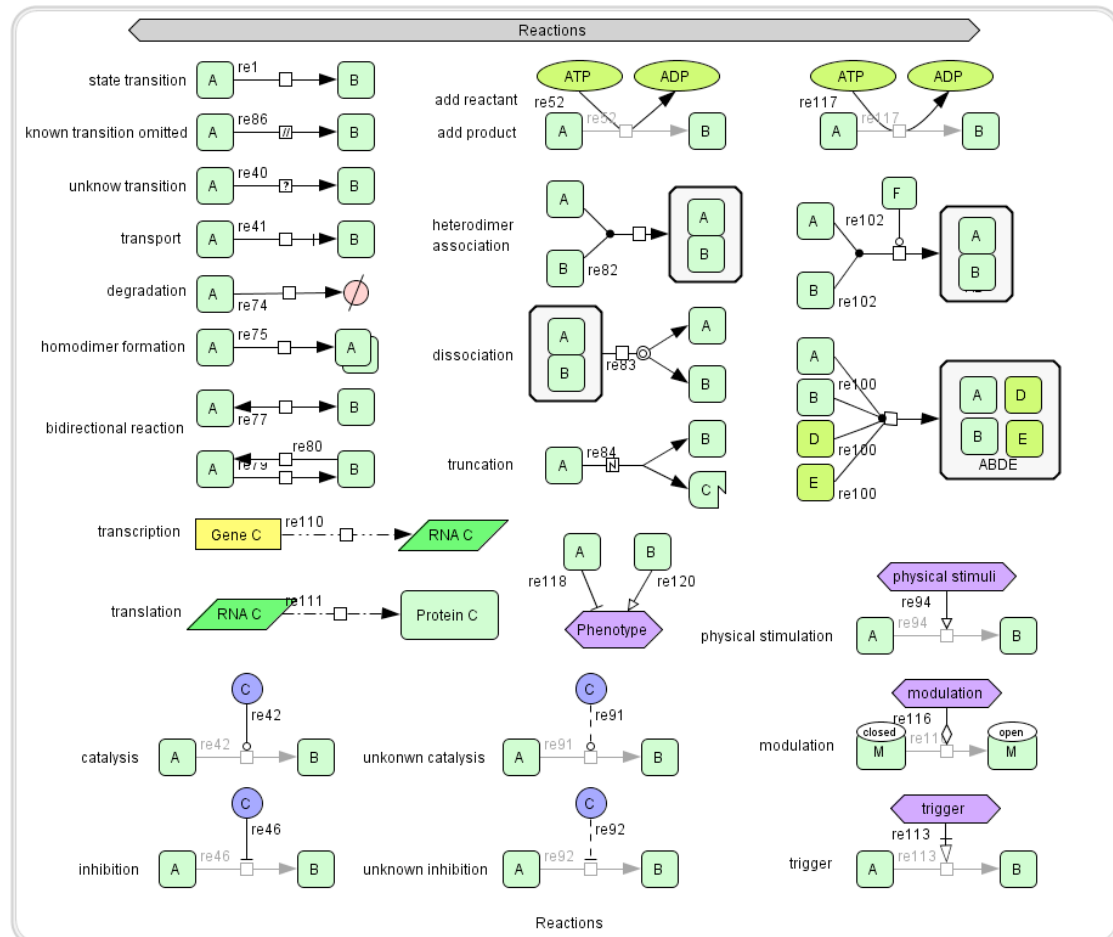
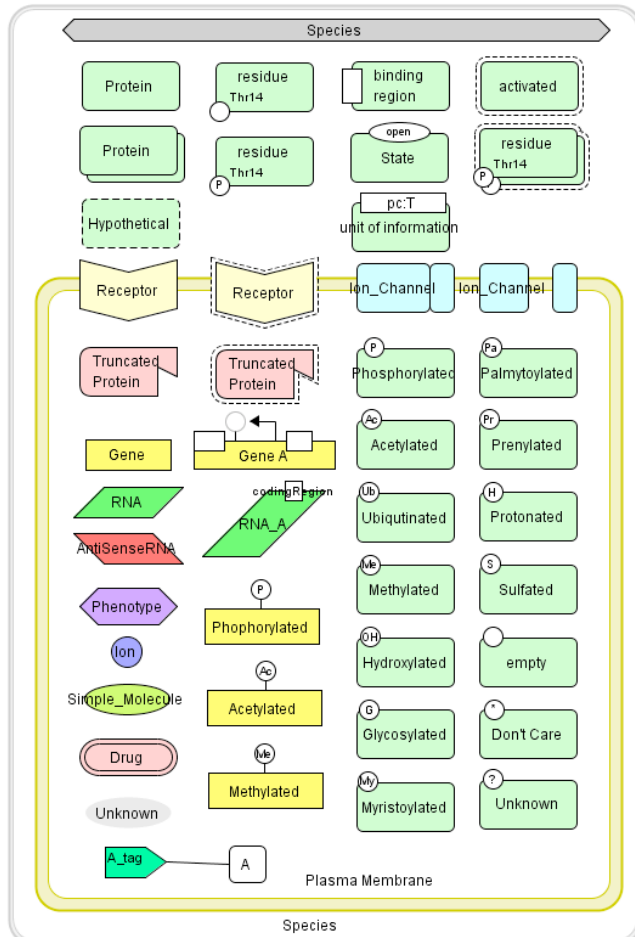
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Result              = TRANSITION ('+' | '-' | empty) '<=' | empty
ImmediateEffect    = TERM_IE
Condition          = empty | '!' TERM_COND '?'
SimpleSentence     = ('+' | '-' | TRANSITION | '?')

TERM_IE            = RESIDUE_IE | TERM_IE OP TERM_IE
TERM_COND         = RESIDUE_COND | TERM_COND OP TERM_COND
RESIDUE_IE        = ('+' | '-') MODIFICATION ('@' TYPE [0-9]+ SUBUNIT | empty)
RESIDUE_COND     = ('-' | empty) MODIFICATION '@' TYPE [0-9]+
OP                = ('&' | '|')
MODIFICATION      = (P | Me | Ac | Ub | Hy) | (P | M | A | U | H)
TYPE              = (Tyr | Ser | Thr) | (Y | S | T)
SUBUNIT           = empty | '/' SUBUNIT_NAME
TRANSITION        = [a-zA-Z][0-9]*
SUBUNIT_NAME      = [a-zA-Z0-9]+
    
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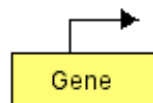
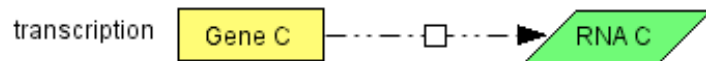
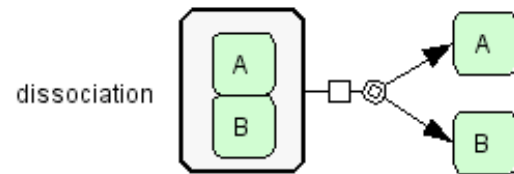
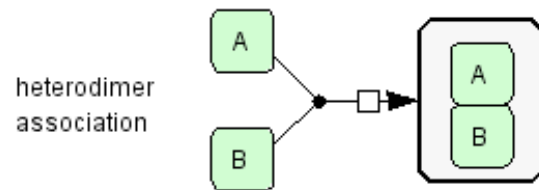
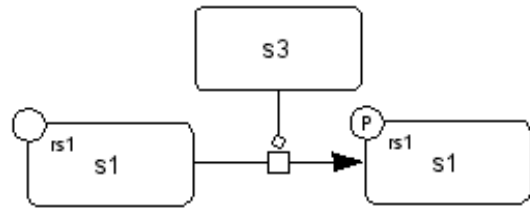
Kitano, H. et al. "Using process diagrams for the graphical representation of biological networks", *Nature Biotechnology* **23**(8), 961 - 966 (2005)

CellDesigner Graphical Notation

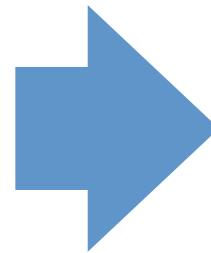
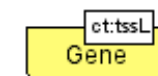
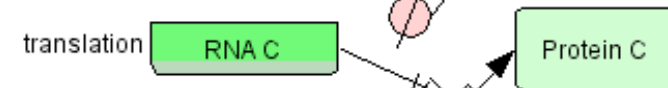
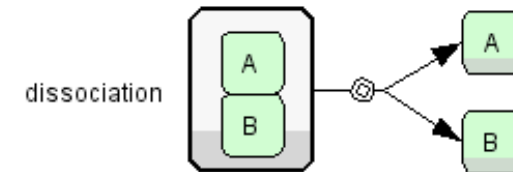
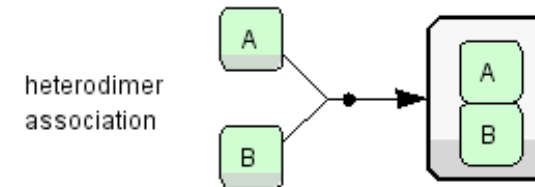
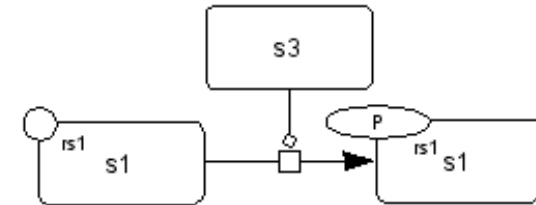


CellDesigner SBGN Viewer

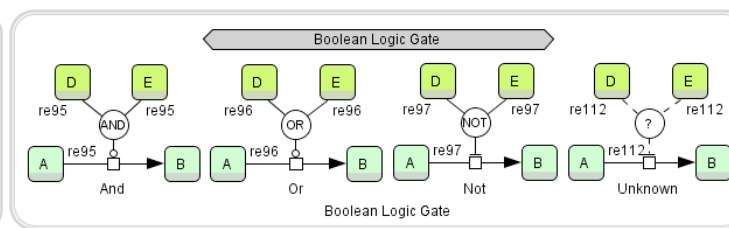
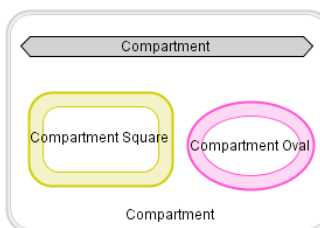
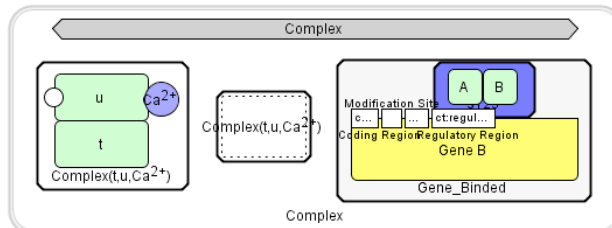
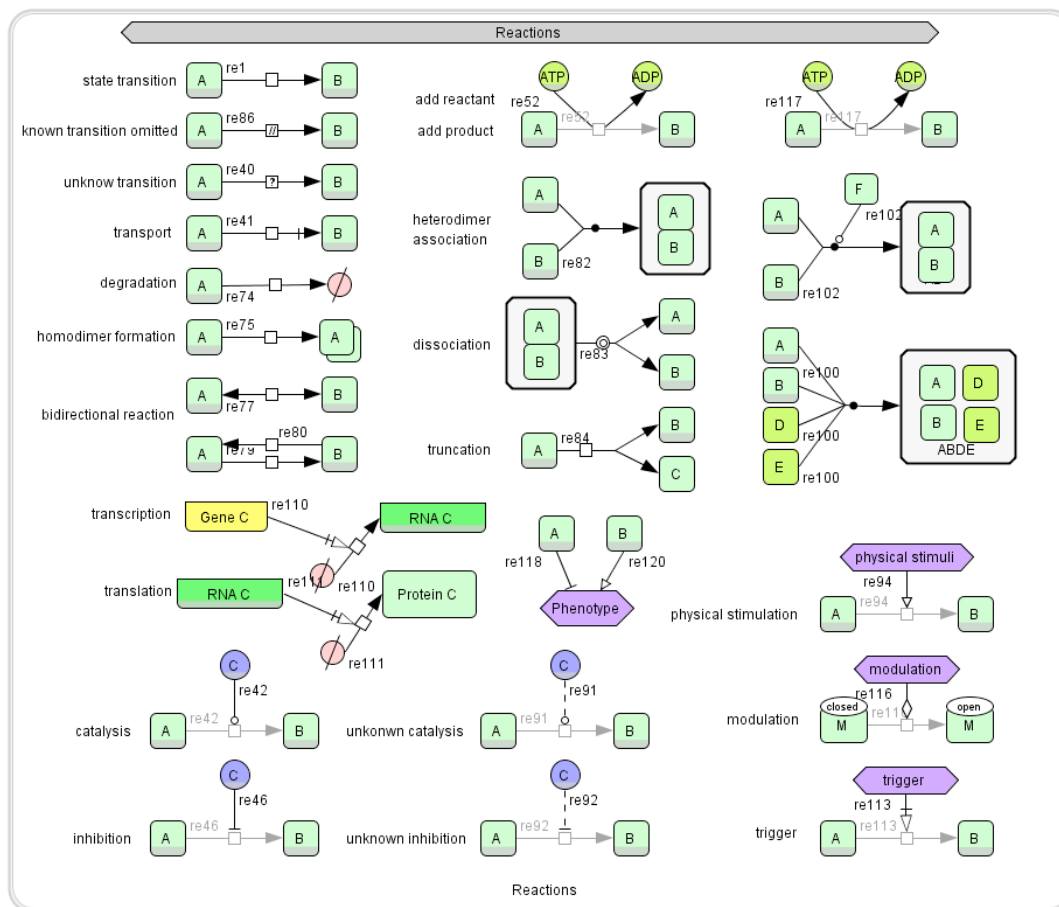
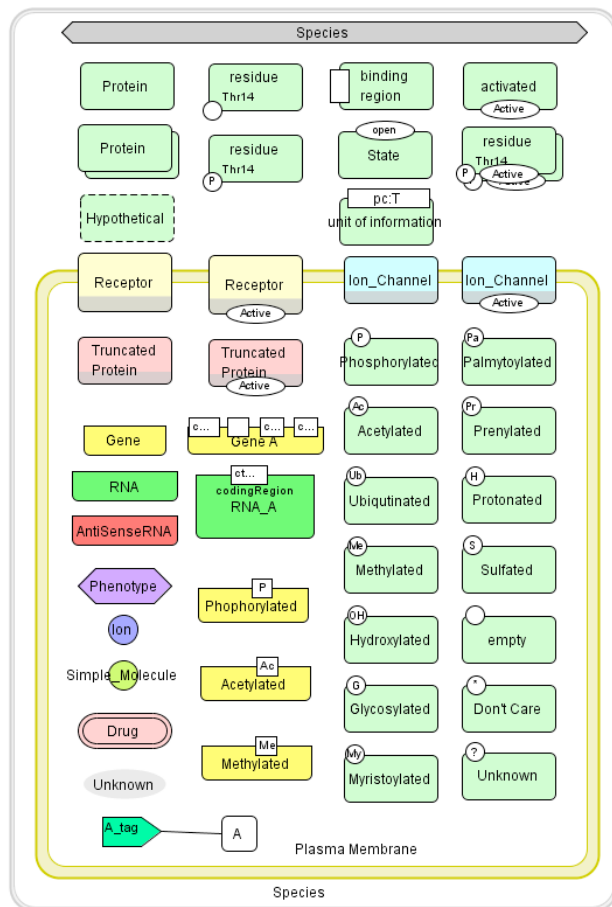
CellDesigner view



CellDesigner SBGN view

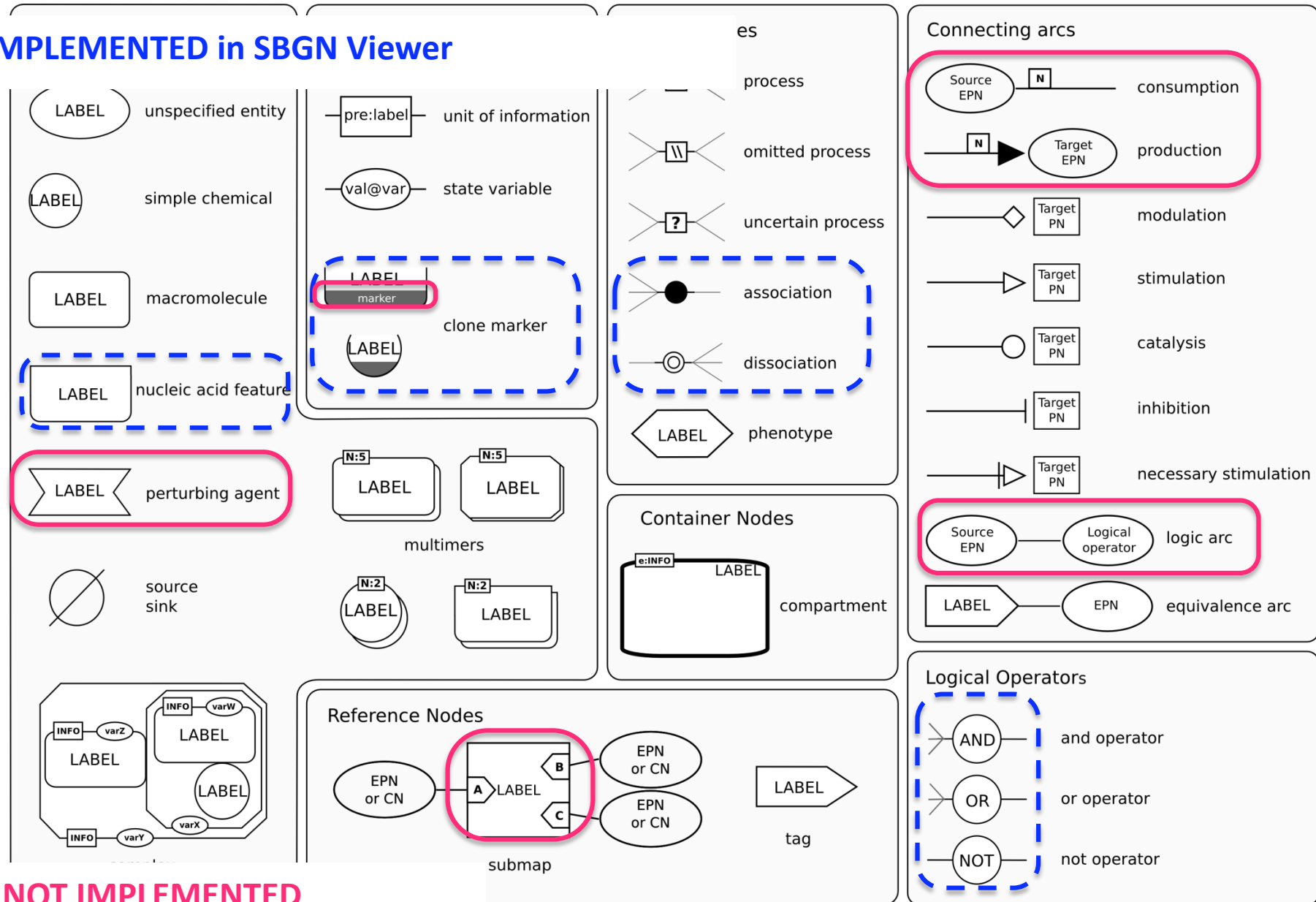


Converting CD to SBGN PD view



SBGN PD Level 1.1 implemented in Viewer

IMPLEMENTED in SBGN Viewer



NOT IMPLEMENTED

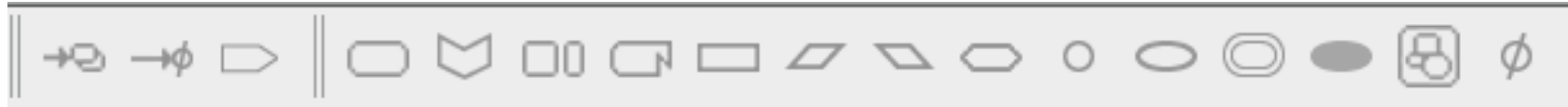
Visual Proofs (b)

- that your software uses the languages accurately, following not only the glyphs but also the syntax and semantics.

- CellDesigner provides the set of icons which draws the exact glyphs as well as arcs with syntax and semantics

Parts Icons

Nodes



Arcs + Process Nodes



Modification Arcs



Logic Operators



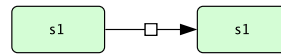
Macros = Basic Pattern

Macro Icons

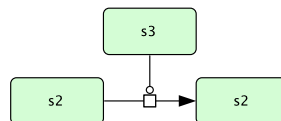


MACROS

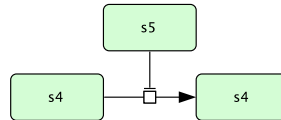
Macro1: State Transition



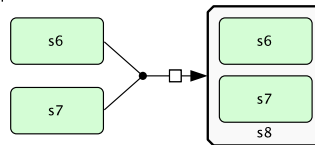
Macro2: Catalysis



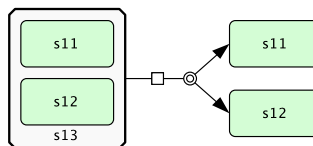
Macro3: Inhibition



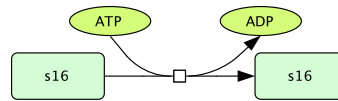
Macro4: Association



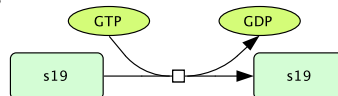
Macro5: Dissociation



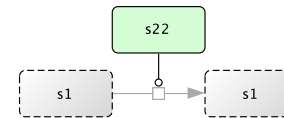
Macro6: ATP_ADG



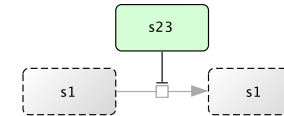
Macro7: GTP_GDP



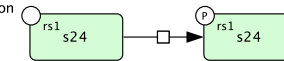
Macro8: Add Catalysis



Macro9: Add Inhibition



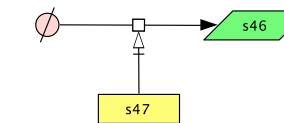
Macro10: Phosphorylation



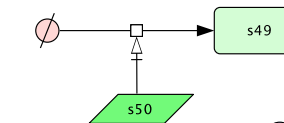
Macro11: Add/Edit Residue Modification



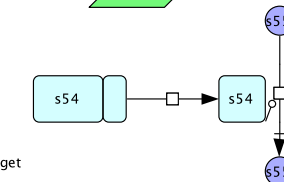
Macro12: Transcription



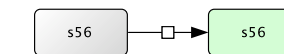
Macro13: Translation



Macro14: Ion Channel



Macro15: Reaction Target



Visual Proofs (c)

- that is able to catch or correct mistakes made by users.

- Although there is no explicit verification function, CellDesigner provides real-time guidance to the user by preventing semantically incorrect representations. It guides the user not to draw the wrong arcs : for example, Modification arcs cannot be connected other than process nodes.

CellDesigner 4.1

Development Team

- Samik Ghosh (SBI)
- Yukiko Matsuoka (SBI)
- Yosuke Seto (SBI)
- Hiroaki Kitano (SBI)
- Akira Funahashi (Keio Univ.)
- Akiya Jouraku (Keio Univ.*)
- Norihiro Kikuchi (MKI)
- CellDesigner Applet
 - Huaiyu Mi (SBI)
 - Anushya Muruganujan (SRI)
- SBML ODE Solver
 - Rainer Mache (Univ. Vienna)
 - Christopher Flamm (Univ. Vienna)
- Copasi
 - Ralph Gauges (Univ. Heidelberg)
 - Sven Sahle (Univ. Heidelberg)
 - Ursula Kummer (Univ. Heidelberg)
- SABIO-RK
 - Martin Golebiewski (EML, Germany)
- SBW
 - Frank Bergmann (Univ. Washington)
 - Herbert Sauro (Univ. Washington)
- SBML
 - SBML community
- SBGN
 - SBGN Community