SBGN in Use

Learning and using

Process Description language

Topics

- Teaching/learning SBGN
- SBGN PD in Excel
- Representing incomplete information
- Aesthetics

Teaching/learning SBGN

- MSc students, Computational Systems Biology course, School of Informatics, University of Edinburgh

- MSc students, Pathway Reconstruction course, Department of Pathway Medicine, University of Edinburgh

Guidelines

- Good first examples are very important
- Hands-on experience: drawing
- The tool is important (easy-to-create nice-looking diagrams, flexibility)
- Steps
  1. Attempt to visualize a textually described system (1st example)
  2. Redrawing the main example diagram (2nd example)
  3. Pathway reconstruction: visualization in SBGN PD + annotation in Excel

Text to Diagram

Conversion of F6P into F2,6P2 is catalyzed by PFK.
Conversion of F2,6P2 into F6P is catalyzed by FBPase.
Both PFK and FBPase activities are the functions of one
protein. Unphosphorylated protein has PFK activity and
phosphorylated protein has FBPase actiivity.
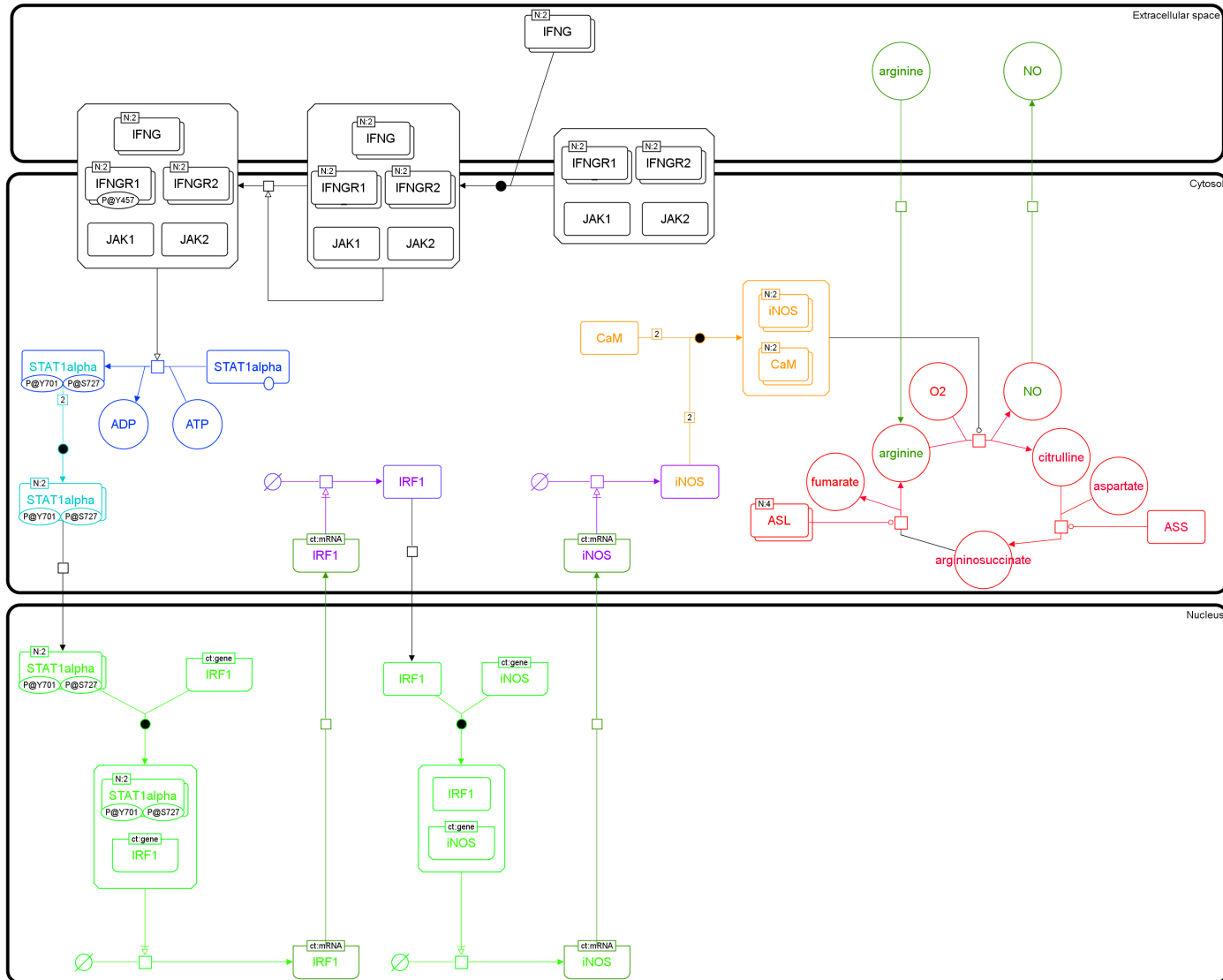Phosphorylation of the protein is catalyzed by PKA.
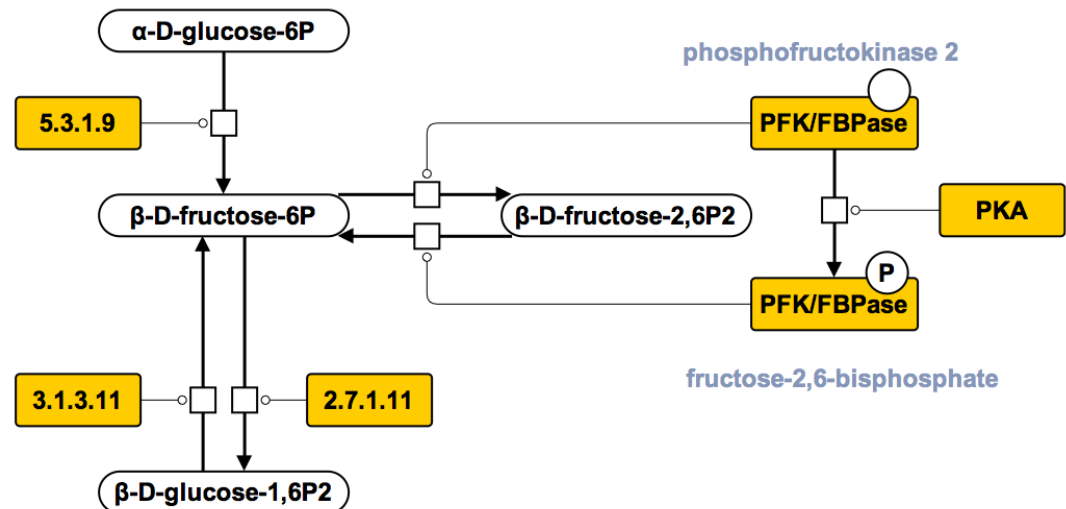
The main example: as many symbols as possible on a small diagram
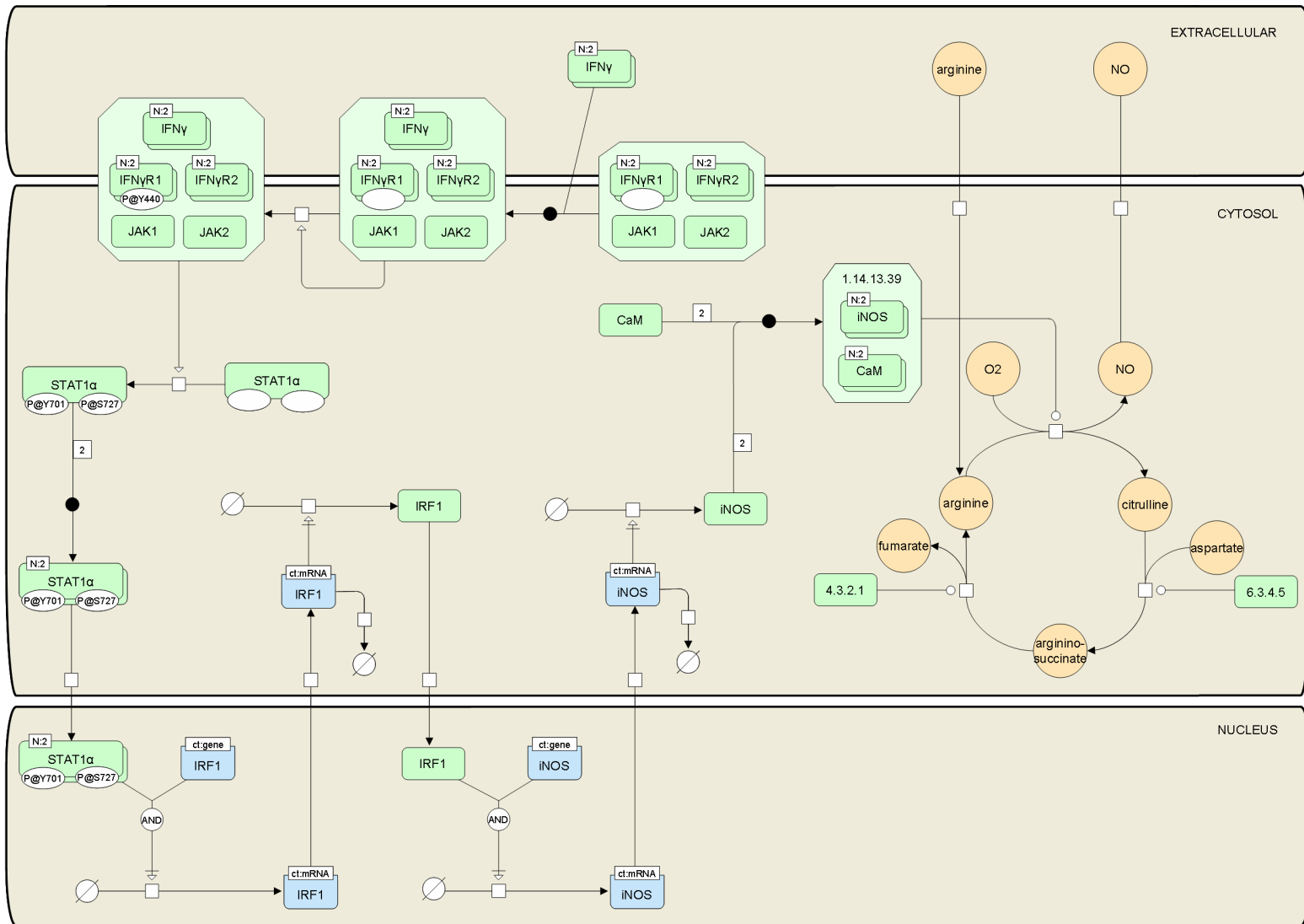
iNOS pathway: the last version

http://sourceforge.net/apps/mediawiki/sbgnbricks

SBGN PD in Excel

Developing a database
with SBGN PD compatibility

SBGN PD symbols -> Text

Group	Element	Example
Entity Pool Nodes	unspecified entity	
Entity Pool Nodes	simple chemical	Default
Entity Pool Nodes	macromolecule	[mt:prot]STAT1alpha<P@Y701,S727>
Entity Pool Nodes	macromolecule multimer	[mt:prot]STAT1alpha<P@Y701,S727>[N:2]
Entity Pool Nodes	nucleic acid feature	[ct:gene]iNOS
Entity Pool Nodes	nucleic acid feature	[ct:mRNA]iNOS
Entity Pool Nodes	perturbing agent	
Entity Pool Nodes	source/sink	Ø Ø
Entity Pool Nodes	complex	{ [mt:prot]iNOS[N:2]; [mt:prot]CaM[N:2] }
Auxiliary Units	unit of information	[mt:prot]
Auxiliary Units	state variable	<P@Y701,S727>
Auxiliary Units	clone marker	Automatically
Process Nodes	process	>> process >>, << process >>
Process Nodes	omitted process	>>\\>>, <<\\>>
Process Nodes	uncertain process	>>?>>, <<?>>
Process Nodes	association	>> association >>
Process Nodes	dissociation	>> dissociation >>
Connecting Arcs	consumtion	Input column
Connecting Arcs	production	Output column
Connecting Arcs	modulation	Modulation column
Connecting Arcs	stimulation	Stimulation column
Connecting Arcs	catalysis	Catalysis column
Connecting Arcs	inhibition	Inhibition column
Connecting Arcs	necessary stimulation	Necessary stimulation column

1. Short names for entity pool nodes

Entity Marker / Alias / Short Name	Entity Definition
"STAT1alphaP"	[mt:prot]STAT1alpha<P@Y701,S727>
"STAT1alphaP*2"	[mt:prot]STAT1alpha<P@Y701,S727>[N:2]
"IFNGR_complex"	{ [mt:prot]INFG[N:2]; [mt:prot]INFGR1[N:2]; [mt:prot]INFGR2[N:2]; [mt:prot]JAK1; [mt:prot]JAK2 }
"IFNGR_active"	{ [mt:prot]INFG[N:2]; [mt:prot]INFGR1<P@Y440>[N:2]; [mt:prot]INFGR2*2; [mt:prot]JAK1; [mt:prot]JAK2 }
"iNOS"	[mt:prot]iNOS
"iNOS gene"	[ct:gene]iNOS
"iNOS mRNA"	[ct:mRNA]iNOS
"iNOS-CaM"	{ [mt:prot]iNOS[N:2]; [mt:prot]CaM[N:2] }

[LABEL]   unit of information
<LABEL>   state variable
{complex description}   complex

"SHORT_NAME"

2. Stimulation/inhibition and logic gates

Input	Process Type and Direction	Output	Stimulation	Catalysis	Necessary Stimulation	Inhibition
arginine +O2	>> process >>	citruline + NO		"iNOS-CaM"		
"STAT1alpha"	>> process >>	"STAT1alpha2P"	"IFNGR_active"			
"empty set"	>> process >>	"IRF1_mRNA"			"STAT1alpha2P" AND "IRF1_gene"	

One line – one process
plus all the connected links
(activation/inhibition etc.)

Incomplete knowledge representation

Uncertain connections
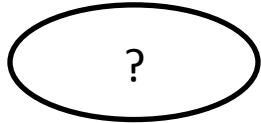
Unspecified entity

Unknown/unspecified macromolecule

Unknown/unspecified macromolecule

Uncertain process

Omitted process
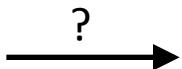
Uncertain activation/inhibition
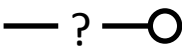
Aestetics

Readability

- The smallest font size

- Default shape size/font size

- Layout

- Patterns

- Irregularities

P@Y701 — P@S727

STAT1

P@Y701 — P@S727

STAT1

P@Y701 — P@S727

STAT1

45°

R

H

8R<H<12R
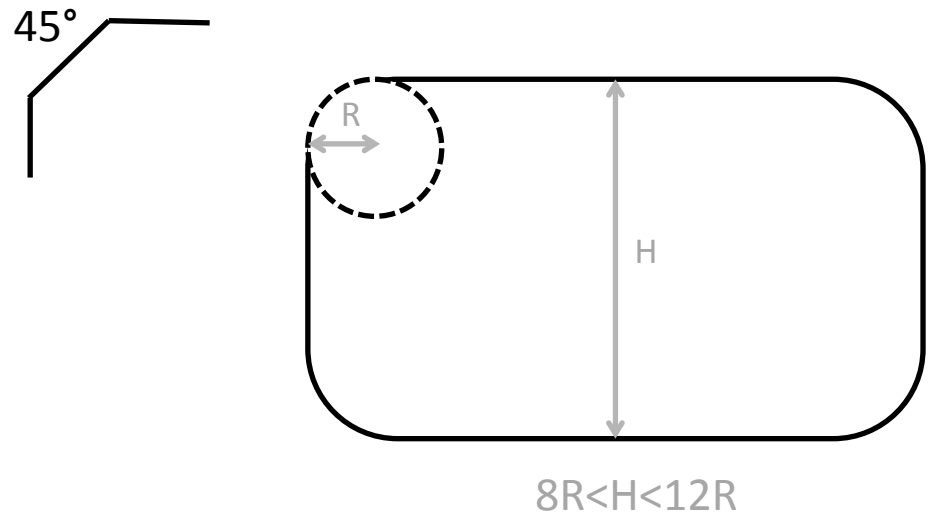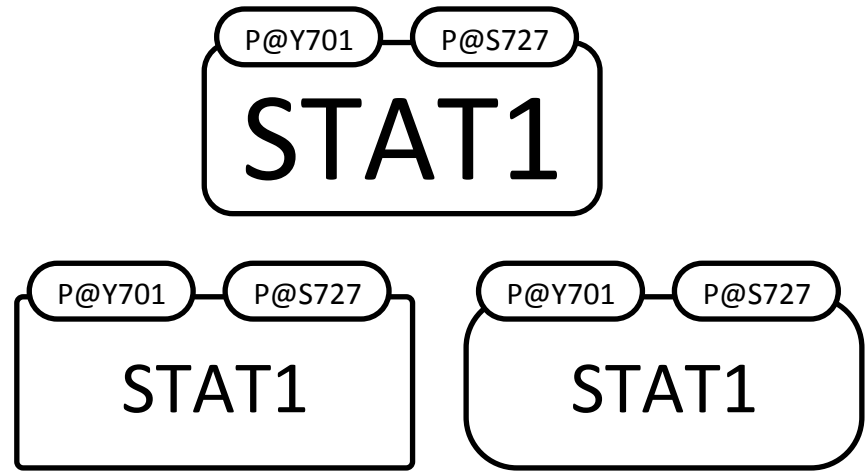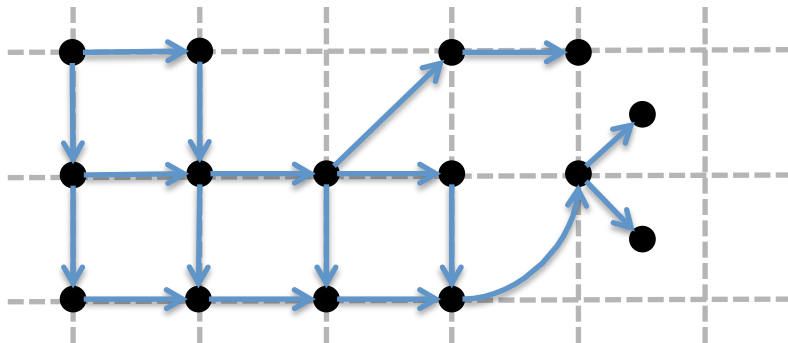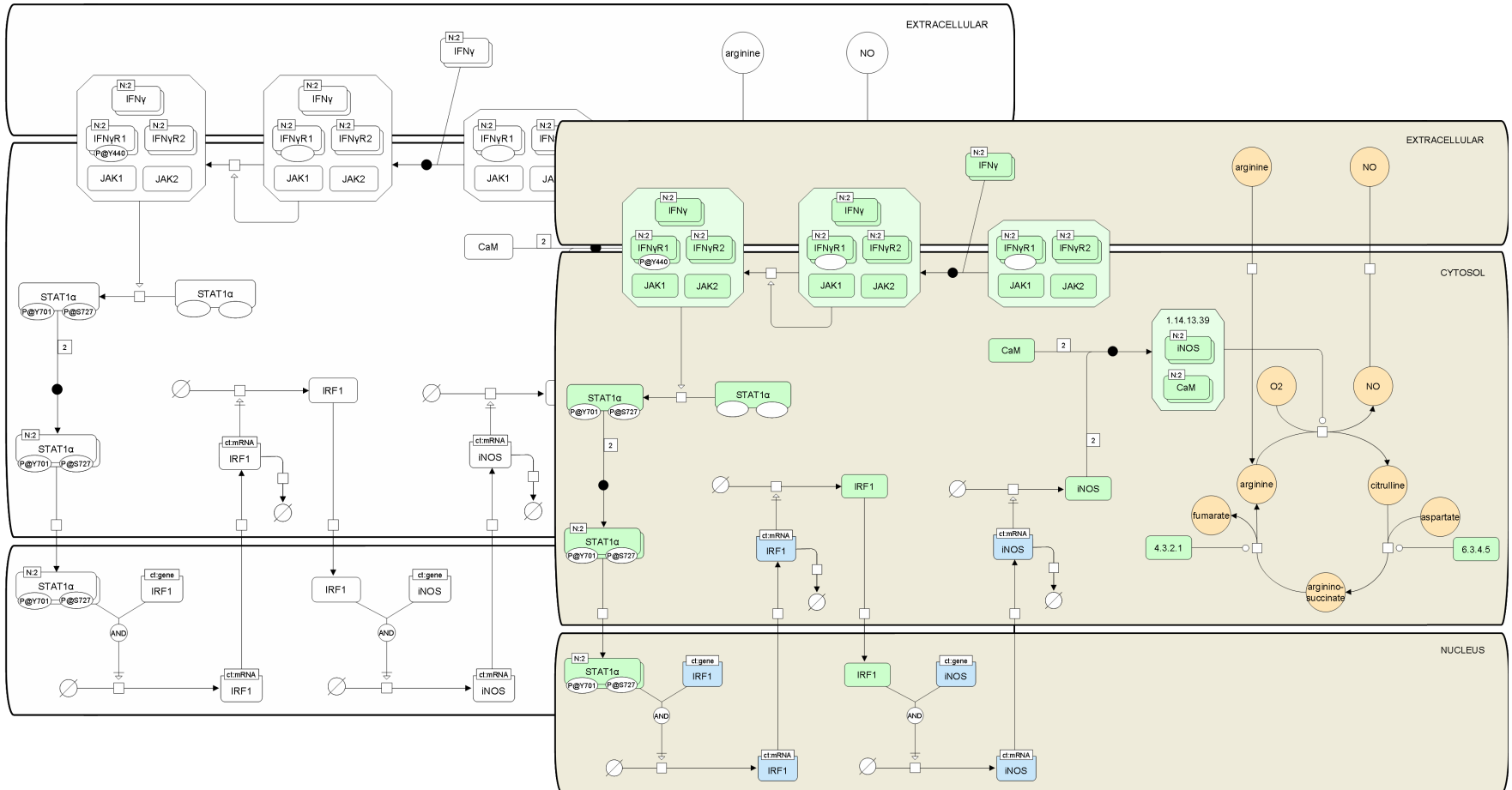
Colours?

Leave it up to users without offering a default colour scheme?
Will a nice default colour scheme help to promote SBGN?

Default colour scheme?
http://colorschemedesigner.com/

Adopting any existing colour scheme?
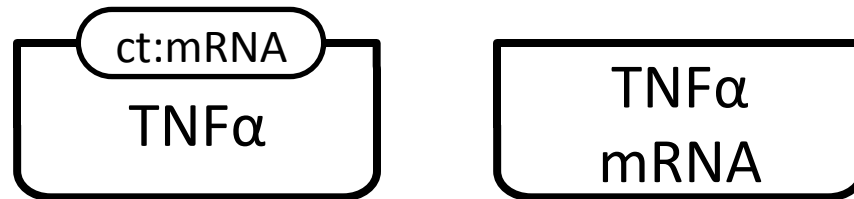## http://snapshots.cell.com/
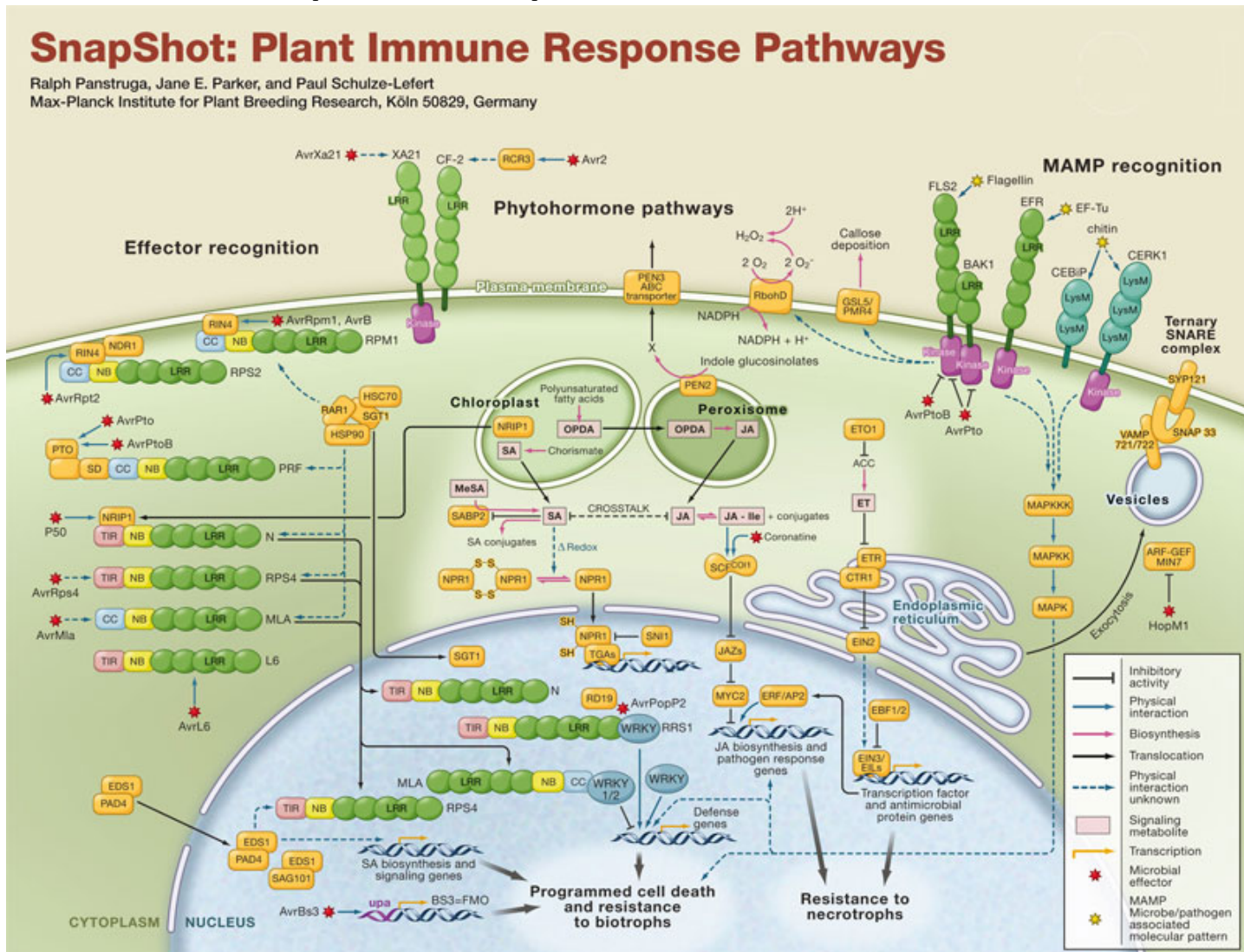
Example diagrams

What kind of examples?

Can use and have to use

The same information can be represented in different ways
and the set of the examples should reflect that

Thank you

SBGN-9

Edinburgh, 29 Apr – 2 May, 2013