

SBGN in Use

Learning and using
Process Description language

Topics

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

Teaching/learning SBGN

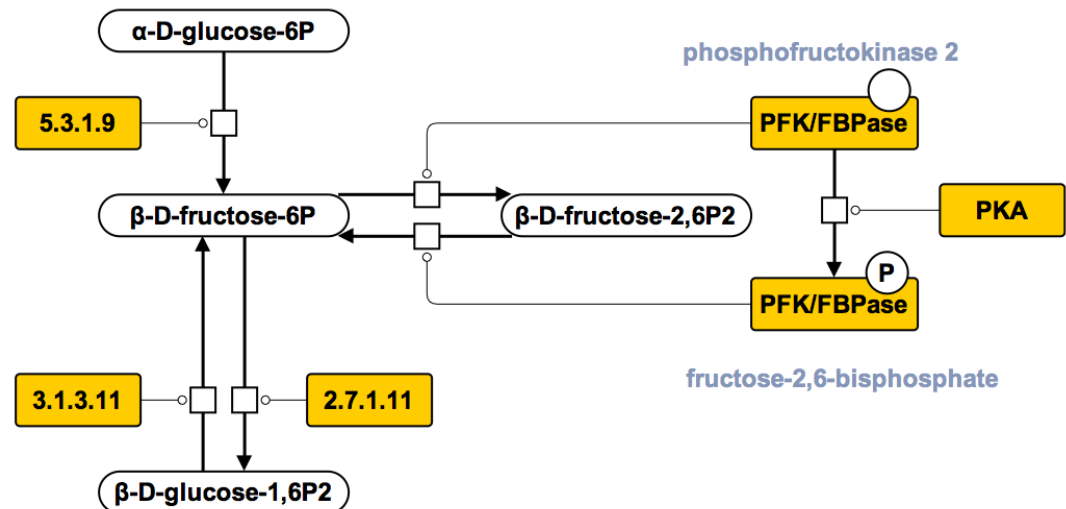
- MSc students, Computational Systems Biology course, School of Informatics, University of Edinburgh
- MSc students, Pathway Reconstruction course, Department of Pathway Medicine, University of Edinburgh

Guidelines

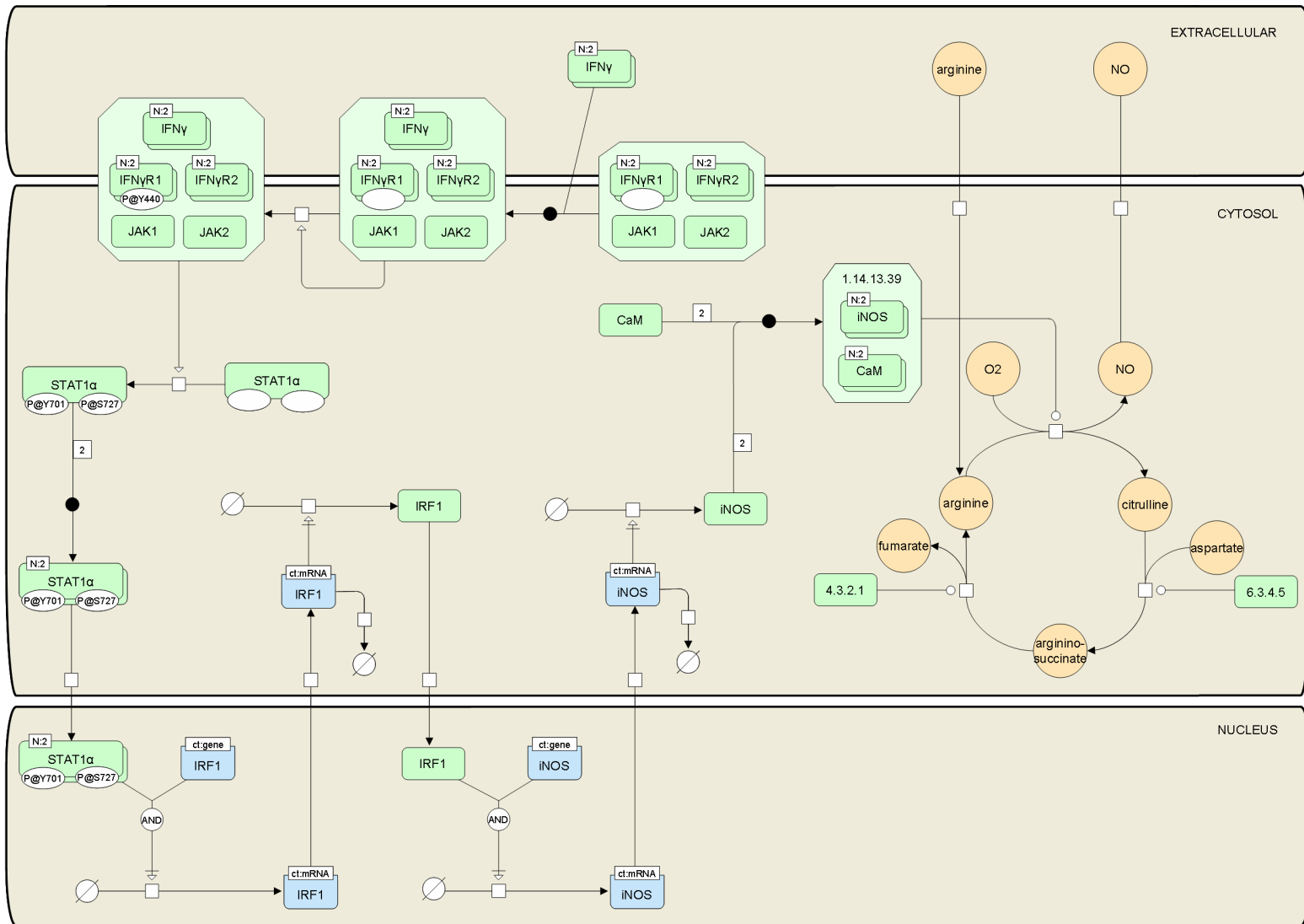
- Good first examples are very important
- Hands-on experience: drawing
- The tool is important (easy-to-create nice-looking diagrams, flexibility)
- Steps
 1. Attempt to visualize a textually described system (1st example)
 2. Redrawing the main example diagram (2nd example)
 3. Pathway reconstruction: 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 activity.
Phosphorylation of the protein is catalyzed by PKA.

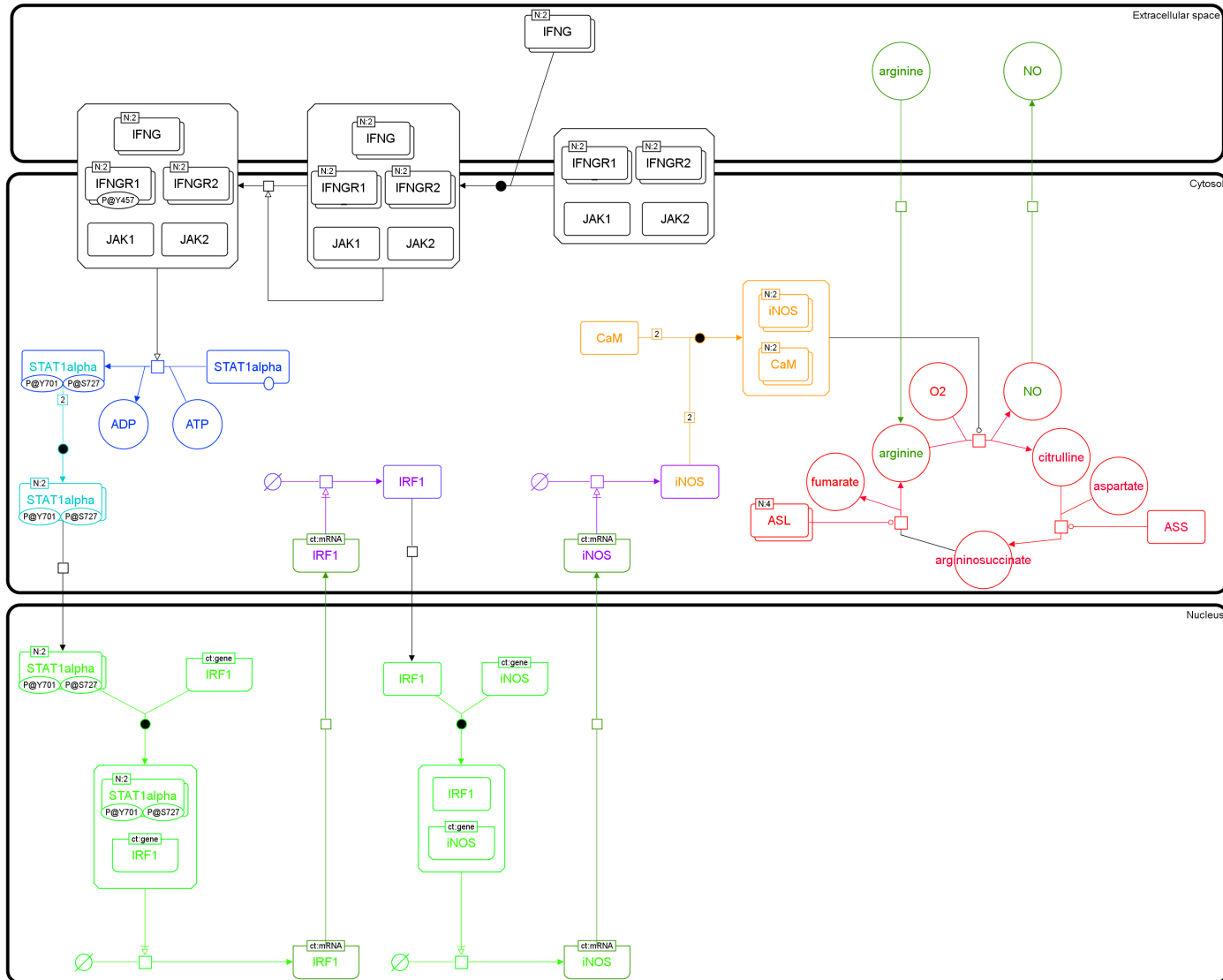


The main example: as many symbols as possible on a small diagram



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

"STAT1alphaP"

"STAT1alphaP*2"

"IFNGR_complex"

"IFNGR_active"

"iNOS"

"iNOS gene"

"iNOS mRNA"

"iNOS-CaM"

Entity Definition

[mt:prot]STAT1alpha<P@Y701,S727>

[mt:prot]STAT1alpha<P@Y701,S727>[N:2]

{ [mt:prot]INFG[N:2]; [mt:prot]INFG1[N:2]; [mt:prot]INFG2[N:2];

[mt:prot]JAK1; [mt:prot]JAK2 }

{ [mt:prot]INFG[N:2]; [mt:prot]INFG1<P@Y440>[N:2]; [mt:prot]INFG2*2;

[mt:prot]JAK1; [mt:prot]JAK2 }

[mt:prot]iNOS

[ct:gene]iNOS

[ct:mRNA]iNOS

{ [mt:prot]iNOS[N:2]; [mt:prot]CaM[N:2] }

[LABEL]

unit of information

<LABEL>

state variable

{complex description}

complex

"SHORT_NAME"

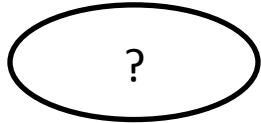
2. Stimulation/inhibition and logic gates

Input	Process Type and Direction	Output	Stimulation	Catalysis	Necessary Stimulation	Inhibi tion
arginine + O ₂	>> 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



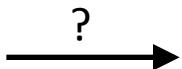
Unknown/unspecified macromolecule



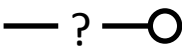
Uncertain process



Omitted process



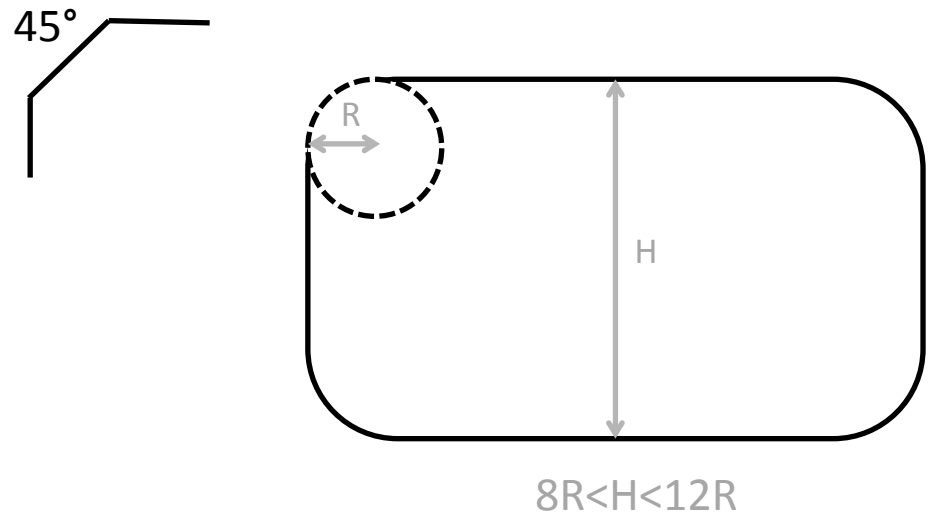
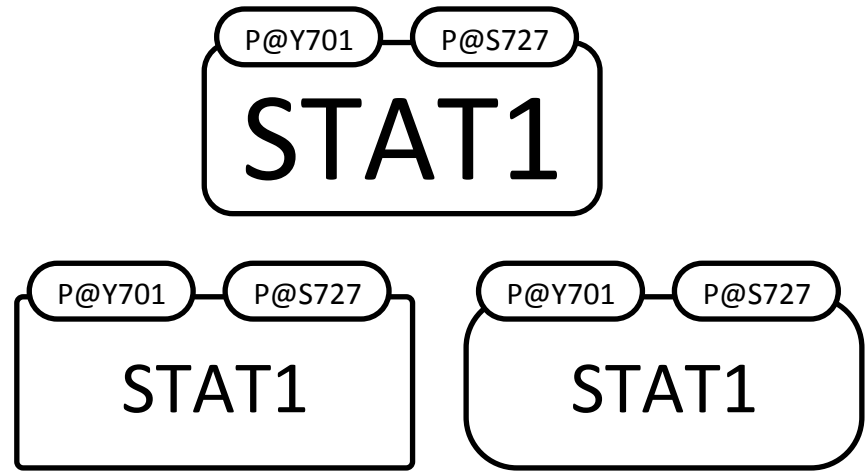
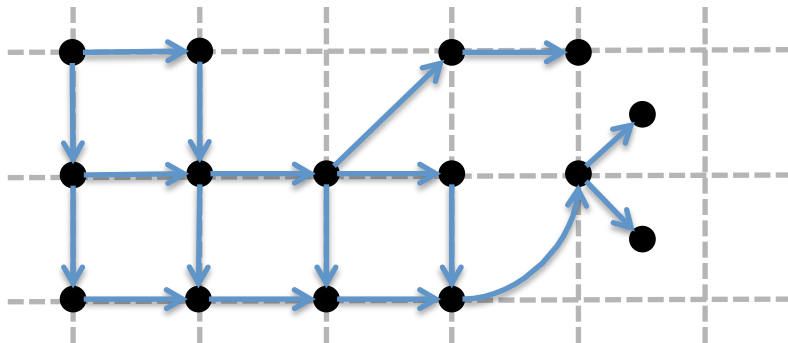
Uncertain activation/inhibition



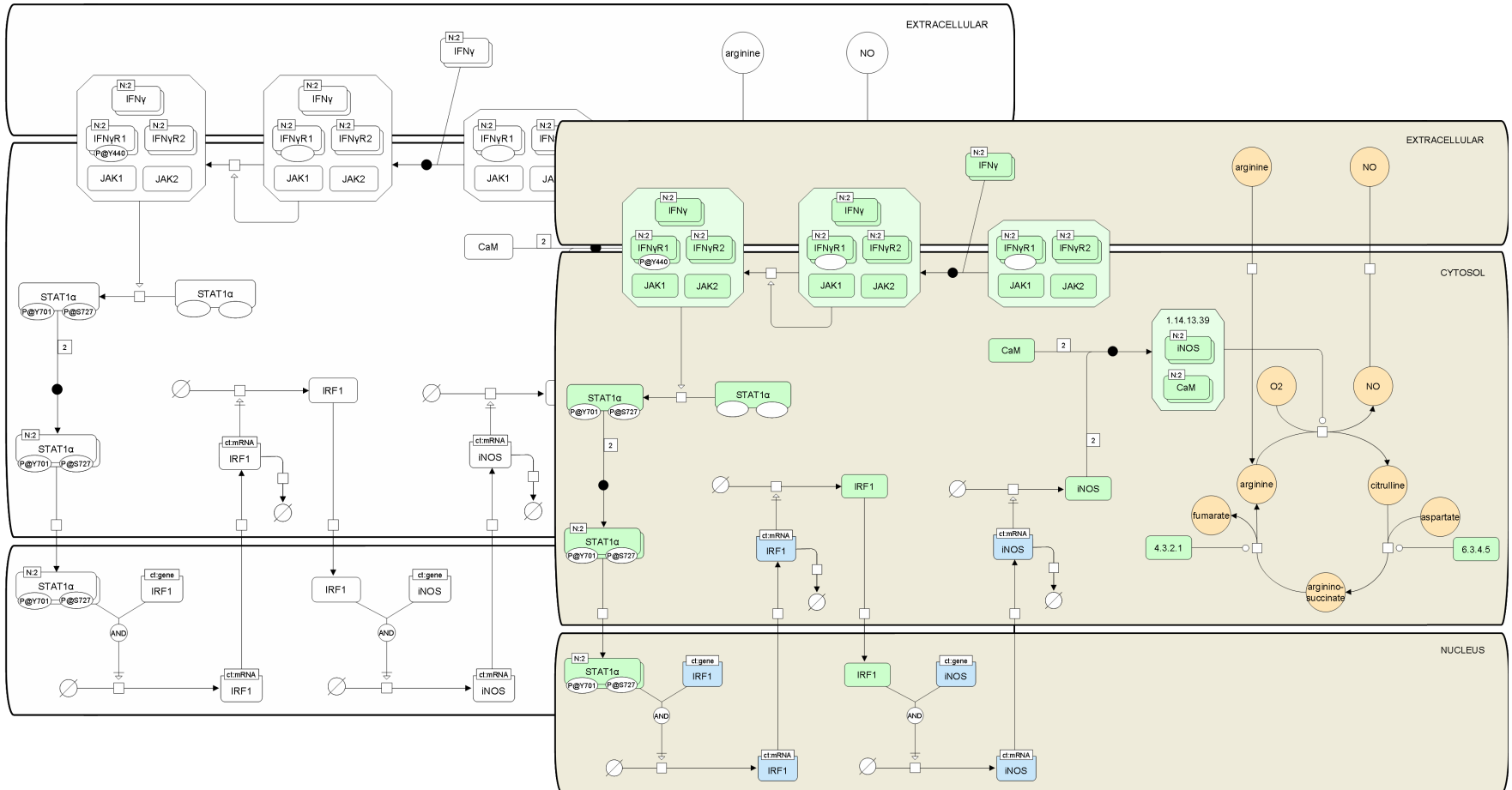
Aesthetics

Readability

- The smallest font size
- Default shape size/font size
- Layout
- Patterns
- Irregularities



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/>

The screenshot displays the Color Scheme Designer web application. At the top, the title "Color Scheme Designer" is shown, along with copyright information "2002-2010 © Petr Stanicek • Version 3.5 • NEWS". A navigation bar includes buttons for "Undo", "Redo", "Random", "Colorblind", "Color space", "Export", and "Help". Below the navigation bar, there are six icons representing different color schemes: "mono", "complement", "triad", "tetrad", "analogic" (which is selected), and "accented analogic". To the right of these icons, a horizontal bar displays four color swatches: orange, yellow, red, and brown. Below this bar, the "Scheme ID" is shown as "0B527w0w0w0w0". On the far right, a vertical banner reads "CREATE FREE STUNNING WEBSITES GO >>". The main interface is divided into two sections. The left section features a color wheel with a "Hue: 38°" and "Angle: 45°" display. A tooltip over the wheel states: "Primary color hue. Click and drag the spot around the color wheel to change the value. Double-click to type the numeric value." The right section shows a 3x3 grid of color swatches, with the center swatch being a bright yellow. At the bottom left, the RGB values are listed: "R: 100 %", "G: 52 %", "B: 0 %". At the bottom right, the RGB value "FF8500" is displayed, and a "Show sample text" button is visible.

Color Scheme Designer

2002-2010 © Petr Stanicek • Version 3.5 • NEWS

Undo Redo Random Colorblind Color space Export Help

mono complement triad tetrad analogic accented analogic

Scheme ID: 0B527w0w0w0w0

CREATE FREE STUNNING WEBSITES GO >>

Hue: 38° Angle: 45°

opposite

warm

cold

Primary color hue. Click and drag the spot around the color wheel to change the value. Double-click to type the numeric value.

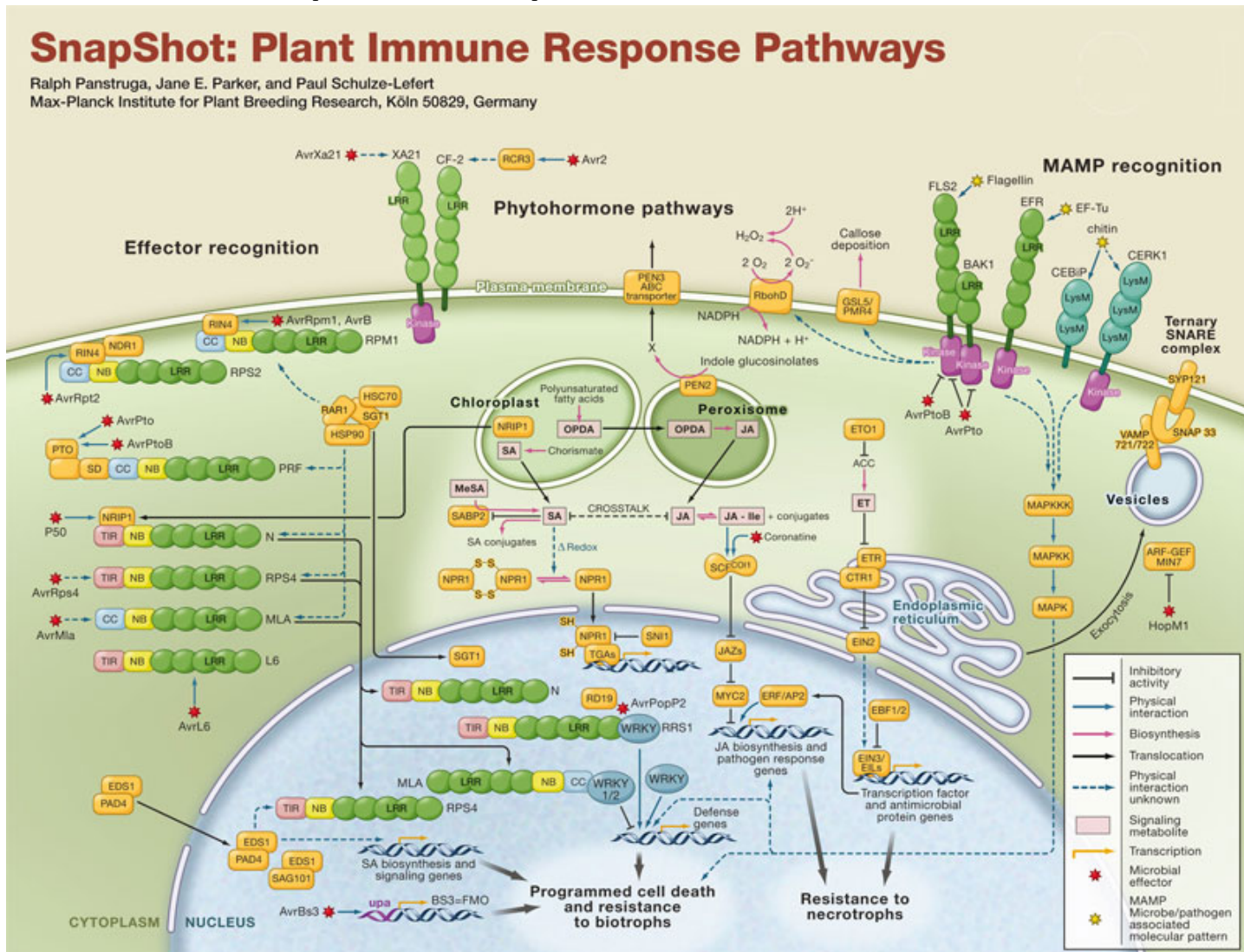
R: 100 %
G: 52 %
B: 0 %

RGB: FF8500

Show sample text

Adopting any existing colour scheme?

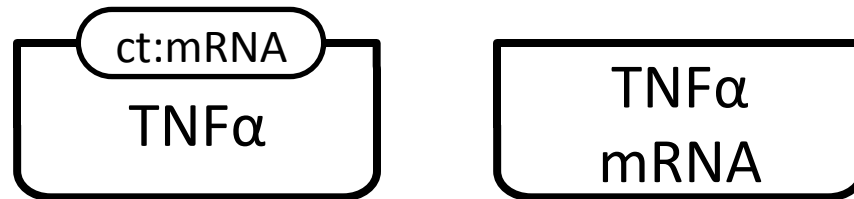
<http://snapshots.cell.com/>



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