

# SBGN-ED – working with the Systems Biology Graphical Notation

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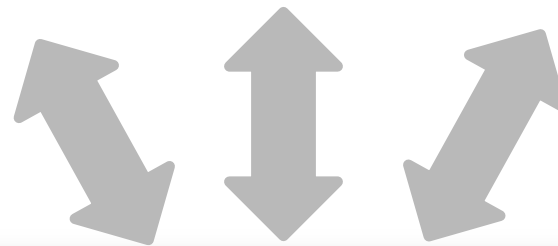


# Working with SBGN

**Creating**  
**Editing**  
**Translating**  
**Validating**

**Exploring**  
**Navigating**

**Data**  
**integrating**  
**Analysing**



**SBGN-ED**

[www.sbgn-ed.org](http://www.sbgn-ed.org)

GML  
GraphML  
SBGN-ML(M1)  
PNG  
JPG  
PDF  
SVG  
PPT  
Web page

GML  
GraphML  
SBGN-ML(M1)

**Import**

**Export**

# Creating and Editing SBGN Maps

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011

The image displays the VANTED V2.0 software interface, which is used for creating and editing SBGN (Systems Biology Graphical Notation) maps. The main window, titled "neuronal\_muscle\_signalling.graphml - view 1", shows a complex biological network diagram. This diagram is divided into three main regions: "synaptic button" (top), "synaptic cleft" (middle), and "muscle cytosol" (bottom). The synaptic button contains nodes for acetyl CoA, ChAT, vAChT, choline, ACh, and synaptic vesicles. The synaptic cleft shows the release of ACh and its interaction with nAChR and AChE. The muscle cytosol depicts the signaling pathway from nAChR to Ca2+, leading to the activation of myosin and actin, resulting in muscle contraction. The interface includes a menu bar (File, Edit, Analysis, Cluster, Edges, Layout, Mapping, Nodes, Window, Help) and a toolbar. On the right side, there are several panels for editing the map, including "Process Description", "Glyph Label", "Entity Pool Nodes", "Auxiliary Units", "Container Nodes", "Reference Nodes", "Process Nodes", "Connecting Arcs", "Logical Operators", "Statements", "Influences", and "Reference Nodes". Each panel contains various icons and controls for modifying the map's elements. At the bottom right, a status bar shows the map's statistics: 21 nodes, 28 edges, 40 MB, and 1 ES.

# Translating SBGN Maps from KEGG

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011

VANTED V2.0

File Edit Analysis Cluster Edges Layout Mapping Nodes Window Help

Metabolism.Carbohydrate Metabolism.Glycolysis \_ Gluconeogenesis - ko0010 - view 1

Metabolism.Carbohydrate Metabolism.Glycolysis \_ Gluconeogenesis - ko...

GLYCOLYSIS / GLUCONEOGENESIS

Starch and sucrose metabolism

D-Glucose 1-phosphate

D-Glucose

alpha-D-Glucose

alpha-D-Glucose 6-phosphate

beta-D-Fructose 6-phosphate

beta-D-Fructose 1,6-bisphosphate

Glycerone phosphate

D-Glyceraldehyde 3-phosphate

2,3-Bisphosphoglycerate

3-Phospho-D-glycerate

2-Phospho-D-glycerate

Phosphoenolpyruvate

Pyruvate

(S)-Lactate

Ethanol

Acetaldehyde

Acetate

Carbon fixation in photosynthetic organisms

Perisphosphate pathway

Citrate cycle (TCA cycle)

Pyruvate metabolism

Propanoate metabolism

Validation

Validate

Remove Validation Annotations

Translation

Translate KEGG to SBGN

Update

Update map from SBGN-ED 1.0.8 or older

95 nodes 129 edges 1071 MB 2 ES

# Validating SBGN Maps

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011

VANTED V2.0

File Edit Analysis Cluster Edges Layout Mapping Nodes Window Help

Energy Metabolism.C4-metabolism (NADP-ME subtype).gml - view 1

mesophyll cell bundle sheath cell

cytosol cytosol

membrane membrane

plastid plastid

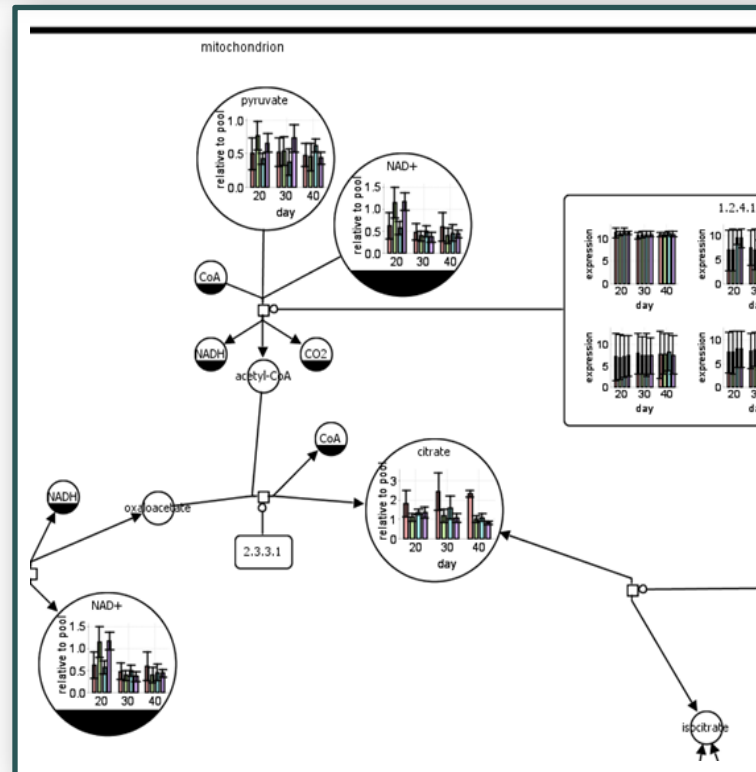
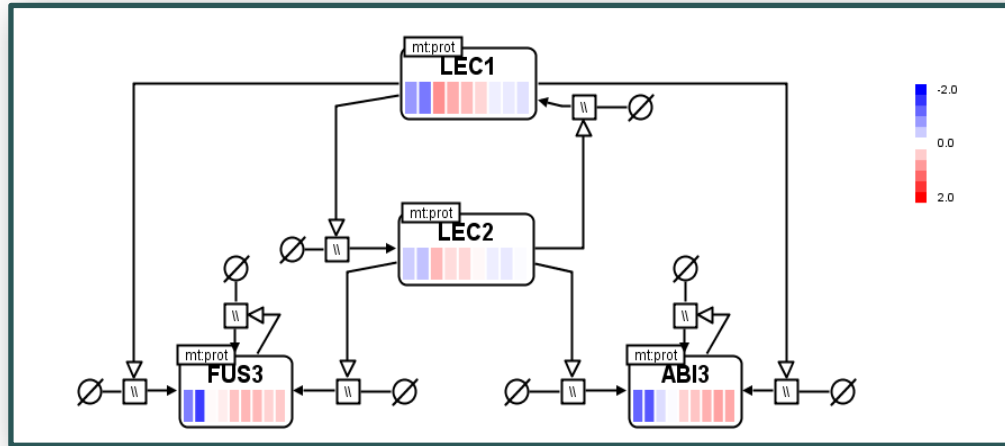
Validation succeeded

Process Description Map is valid.

OK

62 nodes 56 edges 1 ES

# Data Integrating and Analysing in SBGN Maps



## **Current version** (see [www.sbgn-ed.org](http://www.sbgn-ed.org))

- ▶ Improved user interaction
- ▶ More export possibilities
  - ▶ Powerpoint
  - ▶ Webpages
  - ▶ SBGN-ML(M1)

## **Next version** (under development)

- ▶ More importers
  - ▶ SBML (all up to L3V1) (JSBML)
  - ▶ BioPAX (L2,L3) (Paxtools V4)
- ▶ Automatic layout
- ▶ More interaction possibilities

More export possibilities (SBML and BioPAX) planed, but needs validation of user changes!

# Layout

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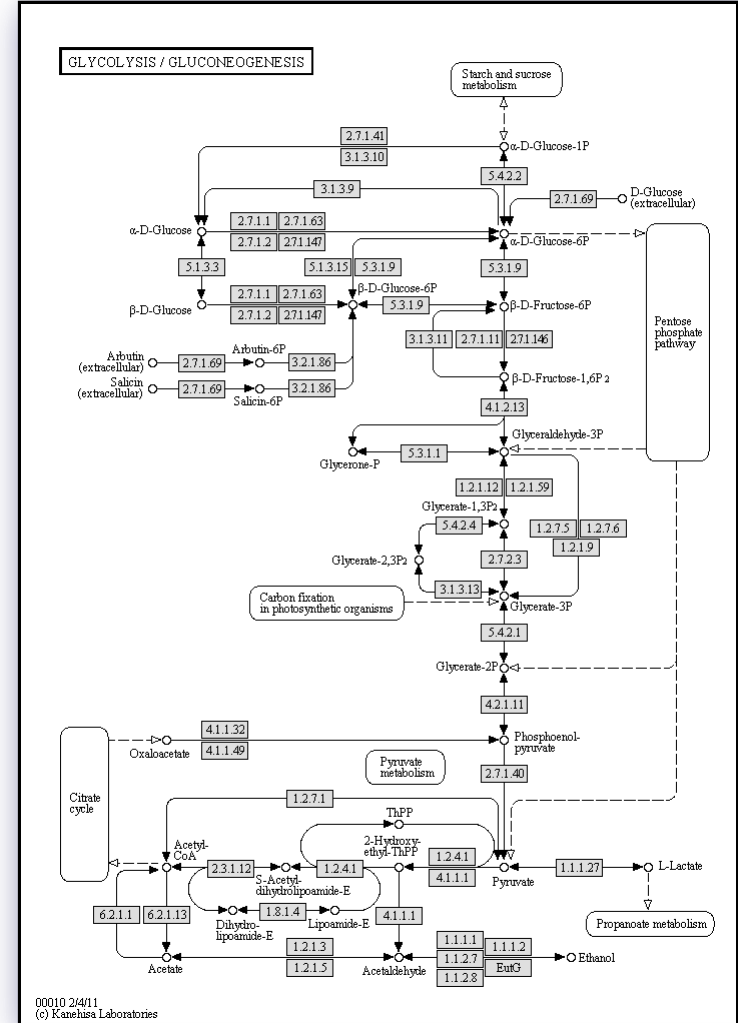
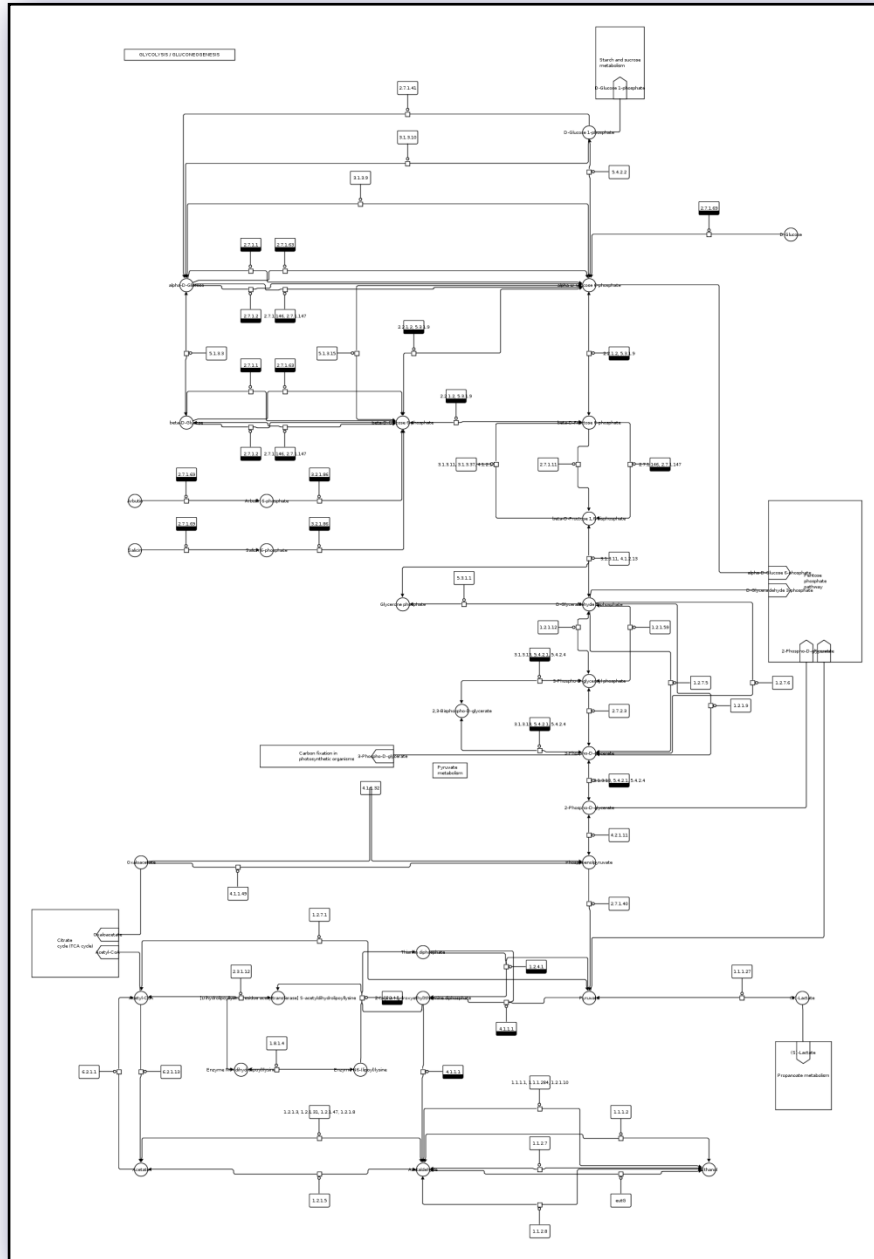
The screenshot displays the VANTED V2.0 software interface. The main window shows a metabolic pathway network titled "GLYCOLYSIS / GLUCONEOGENESIS". The network is a complex graph of nodes and edges, with nodes labeled with enzyme EC numbers and metabolite names. Key metabolites include Starch and sucrose, D-Glucose 1-phosphate, D-Glucose, alpha-D-Glucose 6-phosphate, beta-D-Fructose 6-phosphate, beta-D-Glucose, Arabinose, Arabinose 5-phosphate, Salicin, Salicin 6-phosphate, Glycerone phosphate, D-Glyceraldehyde 3-phosphate, 2,3-Bisphosphoglycerate, 3-Phosphoglycerate, 2-Phosphoglycerate, Phosphoenolpyruvate, Pyruvate, (S)-Lactate, Ethanol, Acetaldehyde, and Acetate. The network is organized into several functional modules, such as "Starch and sucrose metabolism", "Carbon fixation in photosynthetic organisms", and "Citrate cycle (TCA cycle)". A zoomed-in view of a specific section of the network is shown in the foreground, highlighting the central part of the glycolysis pathway. The software interface includes a menu bar (File, Edit, Analysis, Cluster, Edges, Layout, Mapping, Nodes, Window, Help), a toolbar with various icons, and a right-hand panel with tabs for "Help", "Experiments", and "Pathways". The right-hand panel also contains a "Validation" section with a "Validate" button and a "Remove Validation Annotations" button. The bottom right corner of the window displays the following statistics: 95 nodes, 129 edges, 1071 MB, and 2 ES.





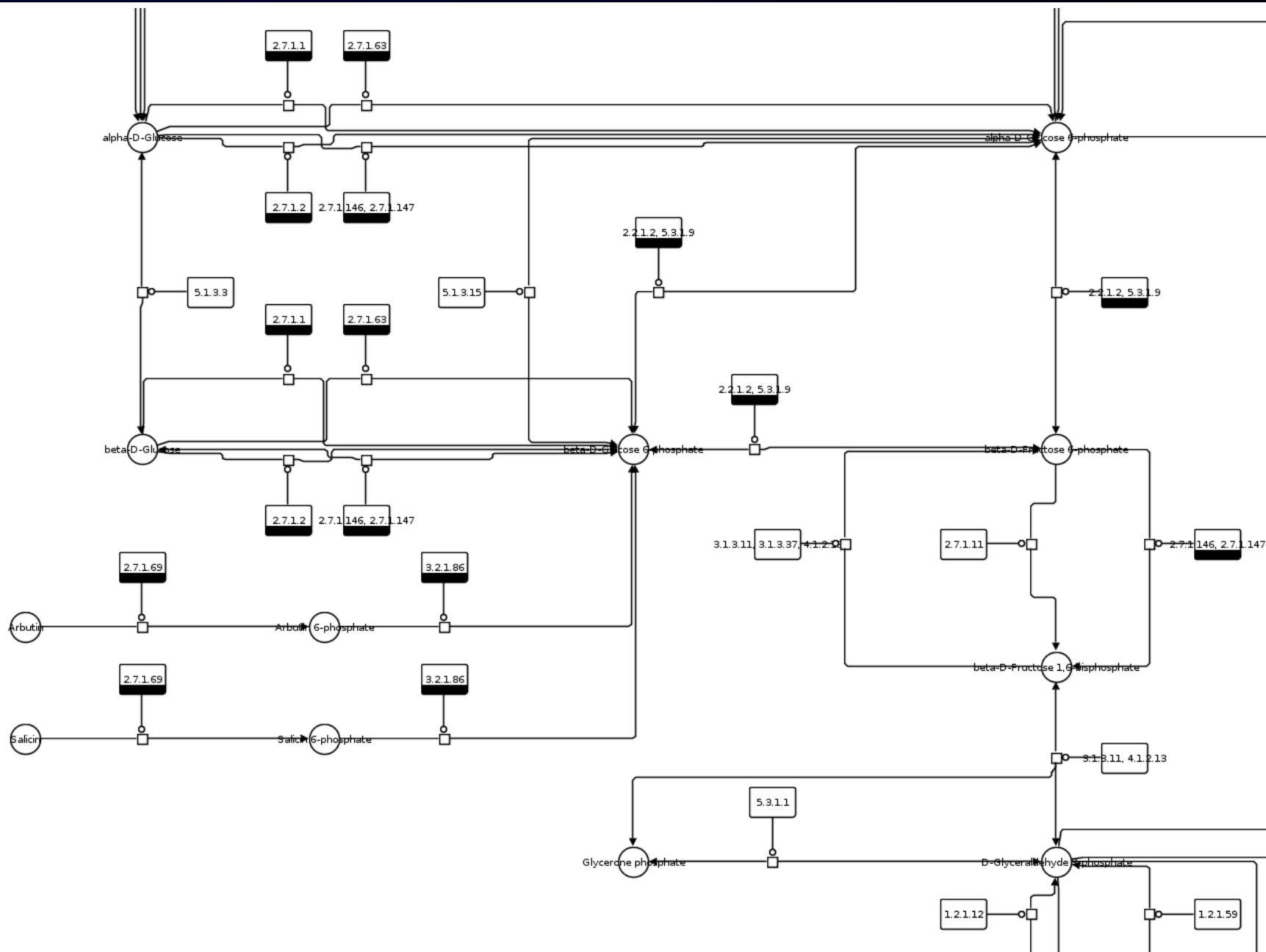
# Constrained KEGG Layout

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011



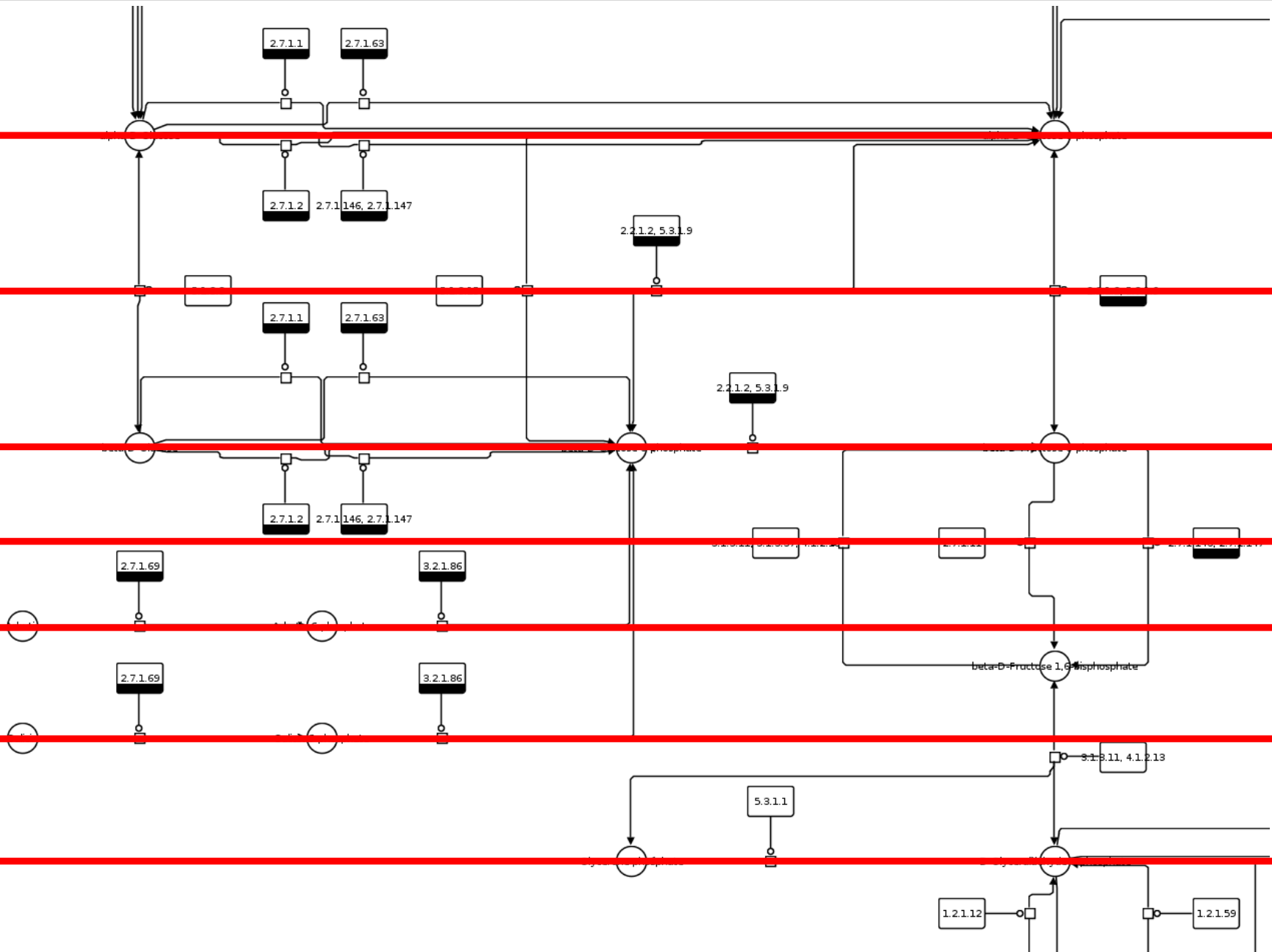
# Constrained KEGG Layout

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011



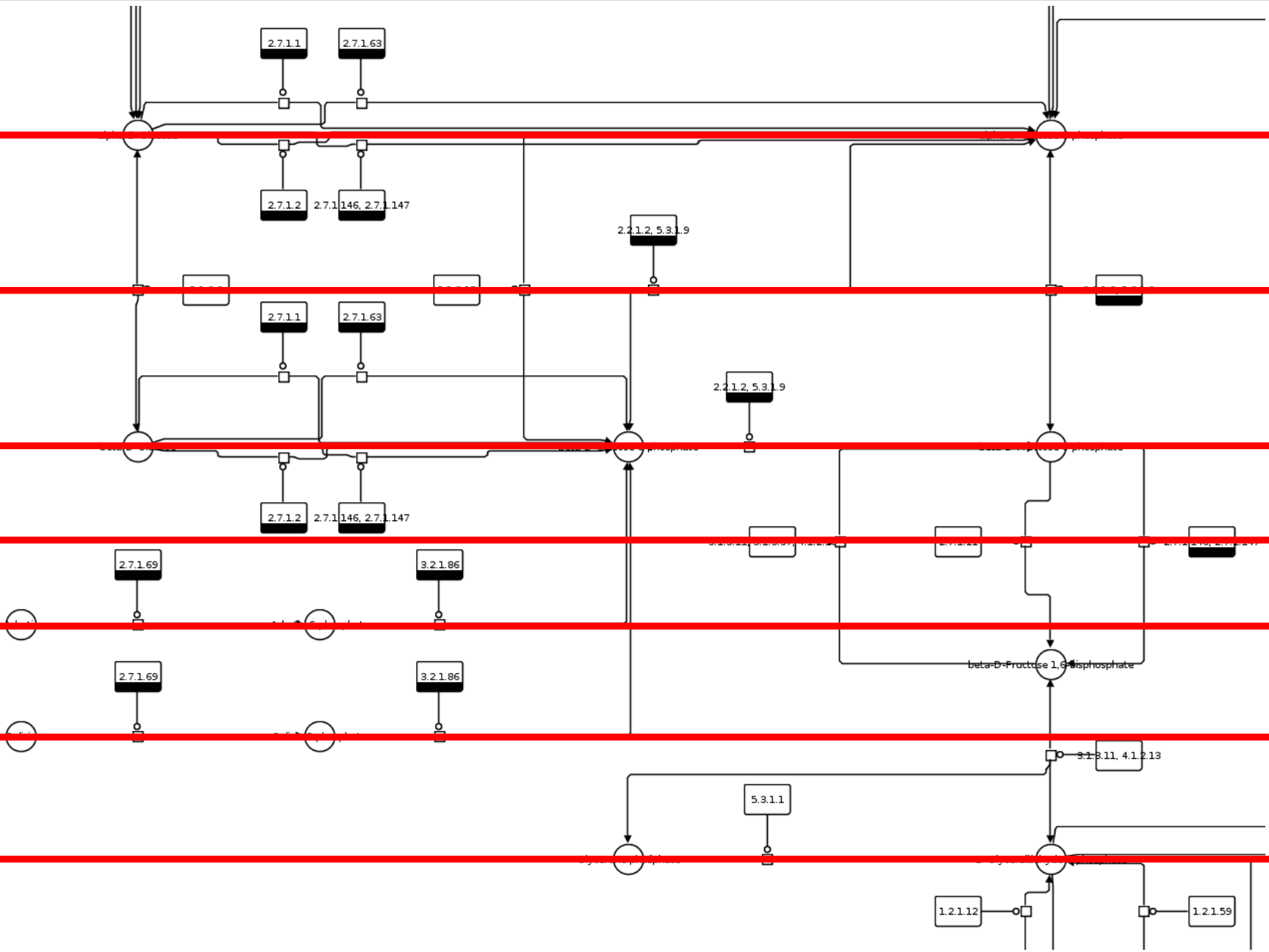
# Constrained KEGG Layout

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011



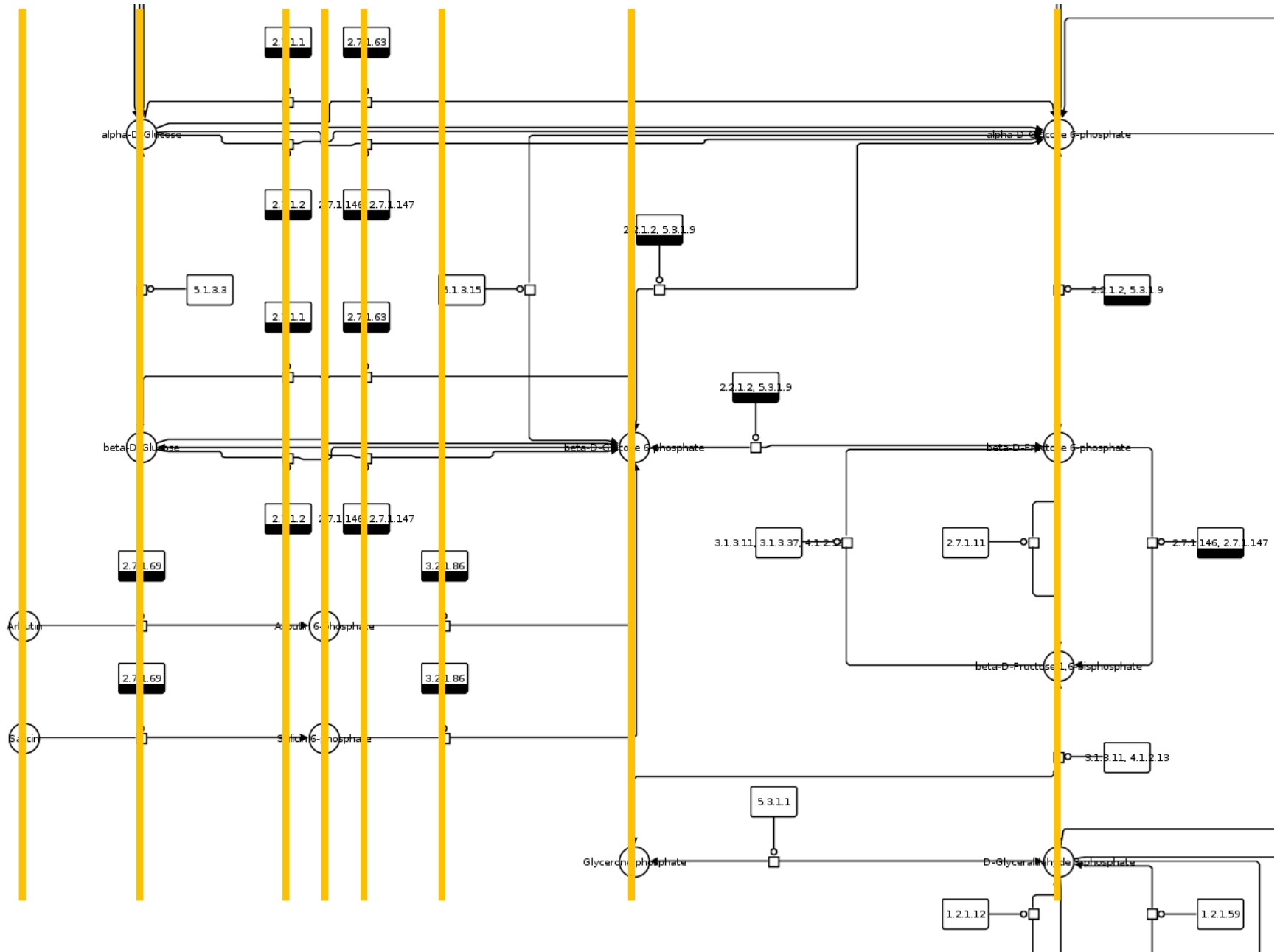
# Constrained KEGG Layout

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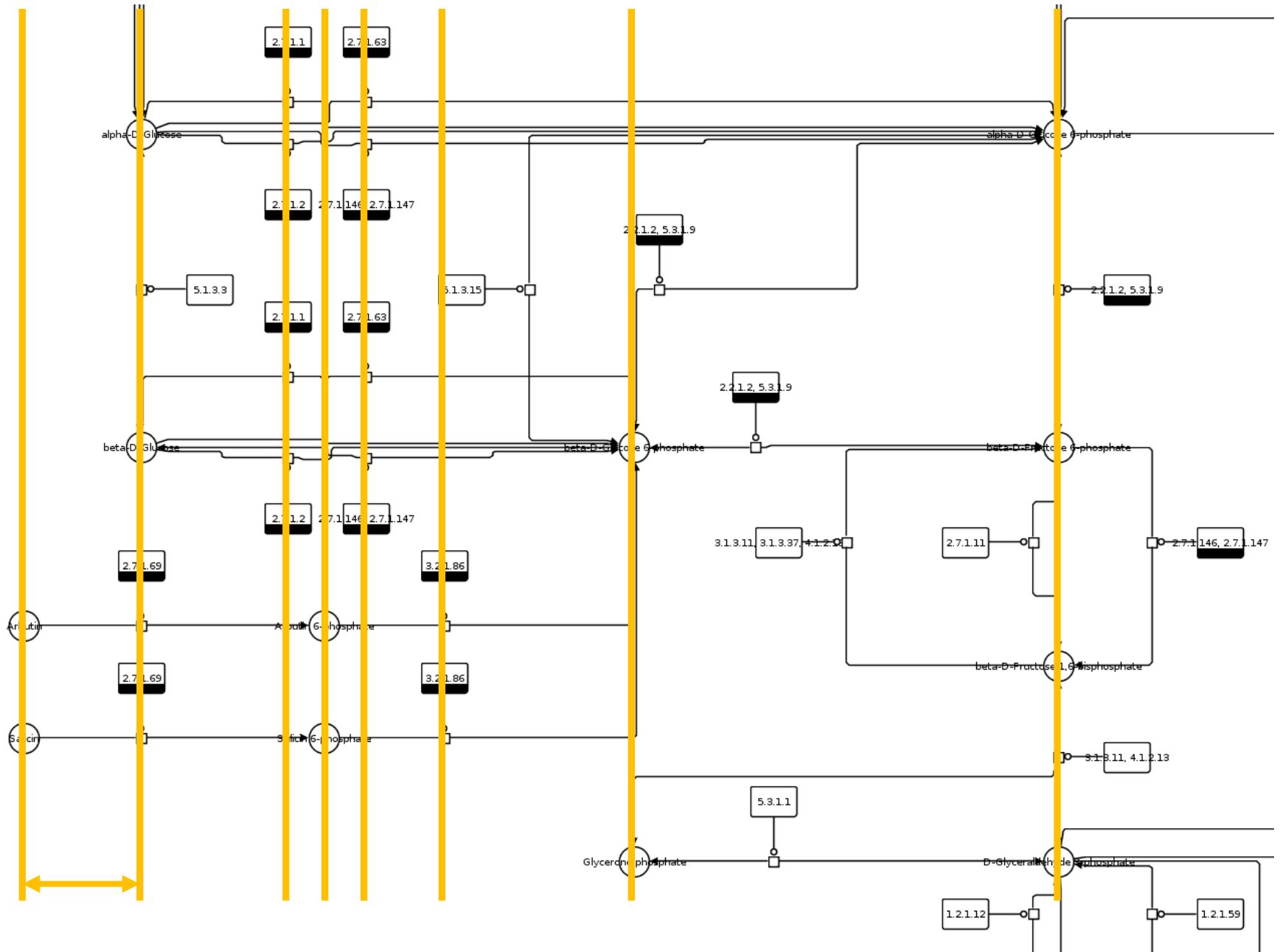
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Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011



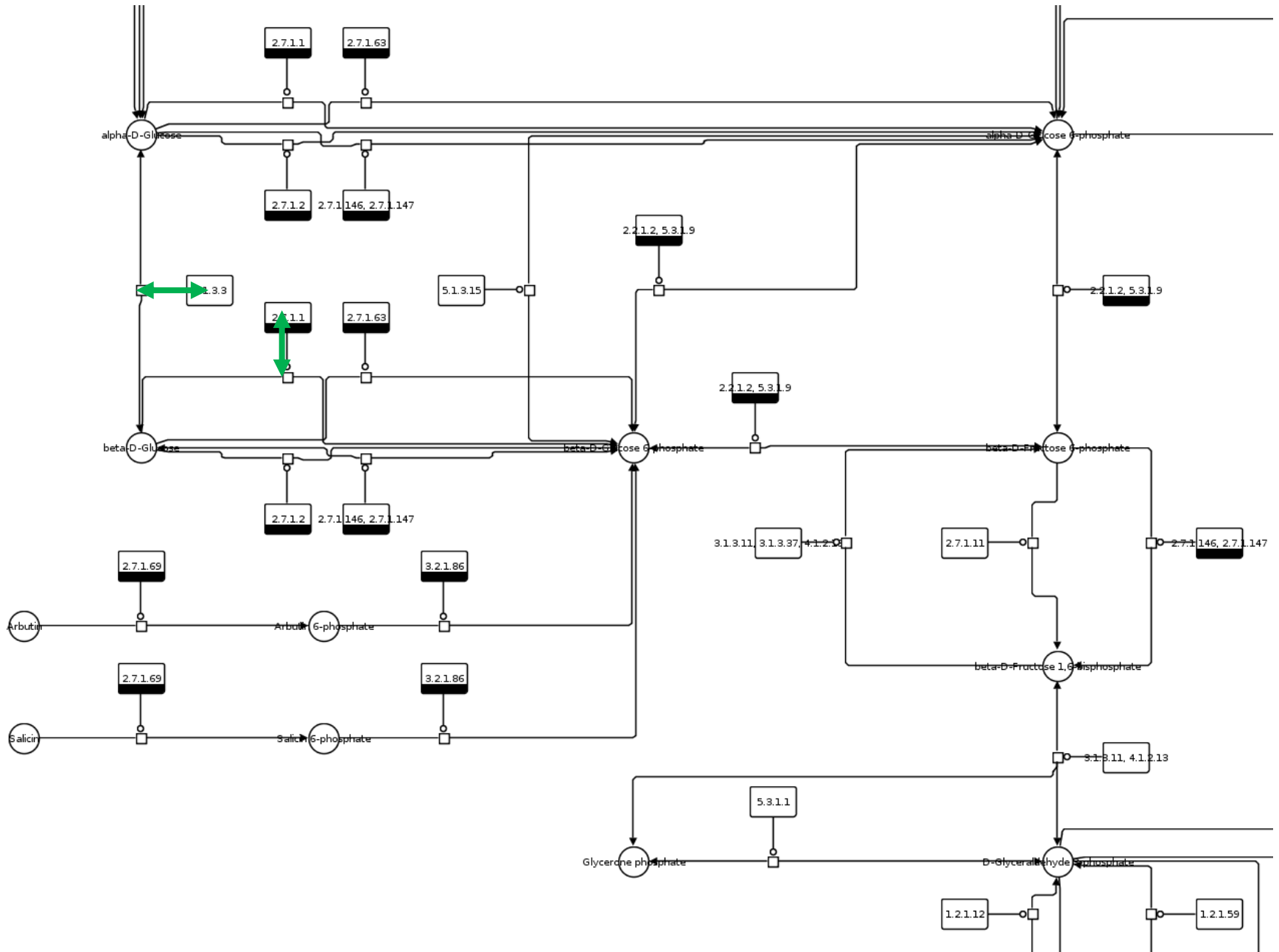
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# Constrained KEGG Layout

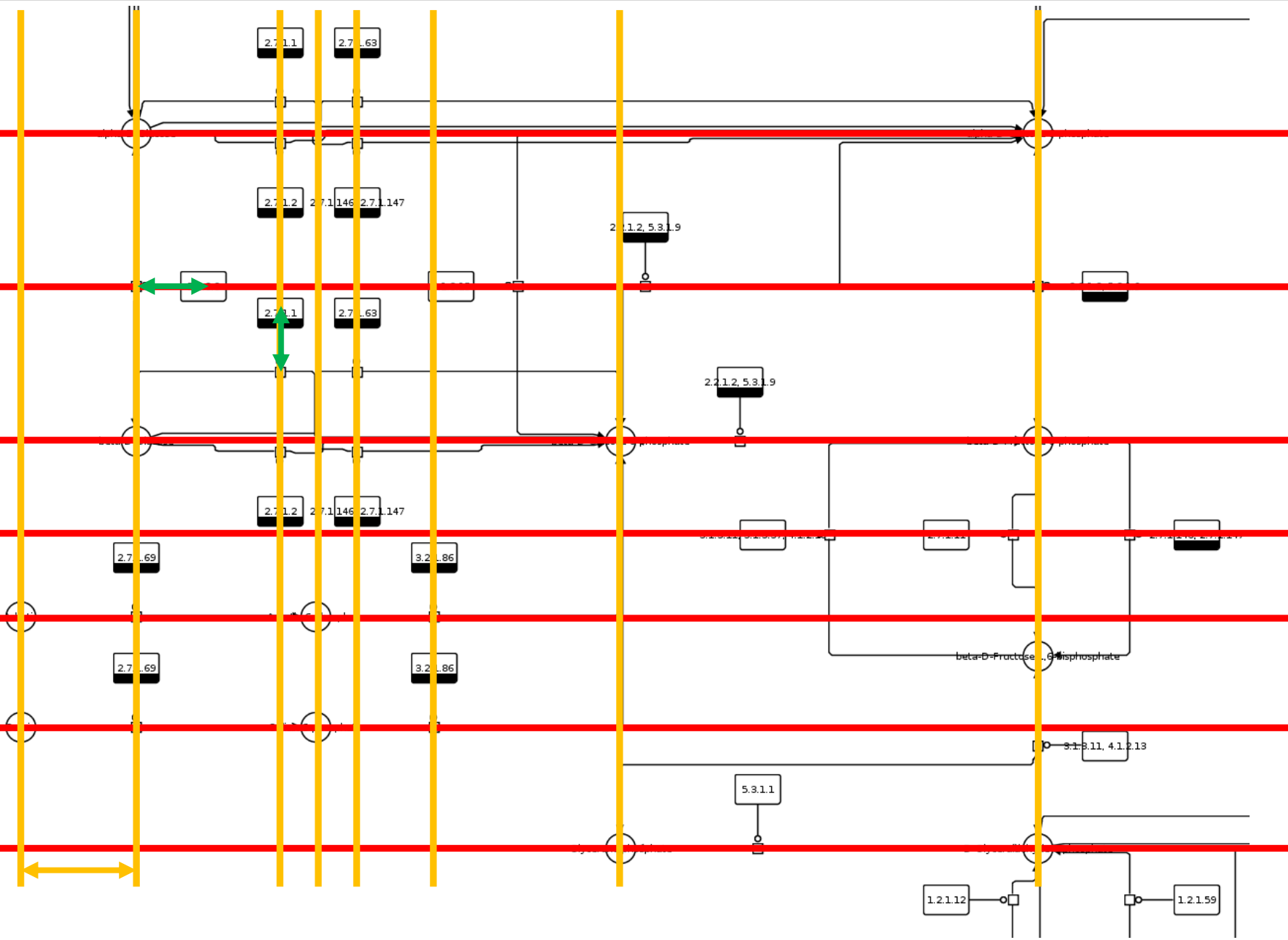
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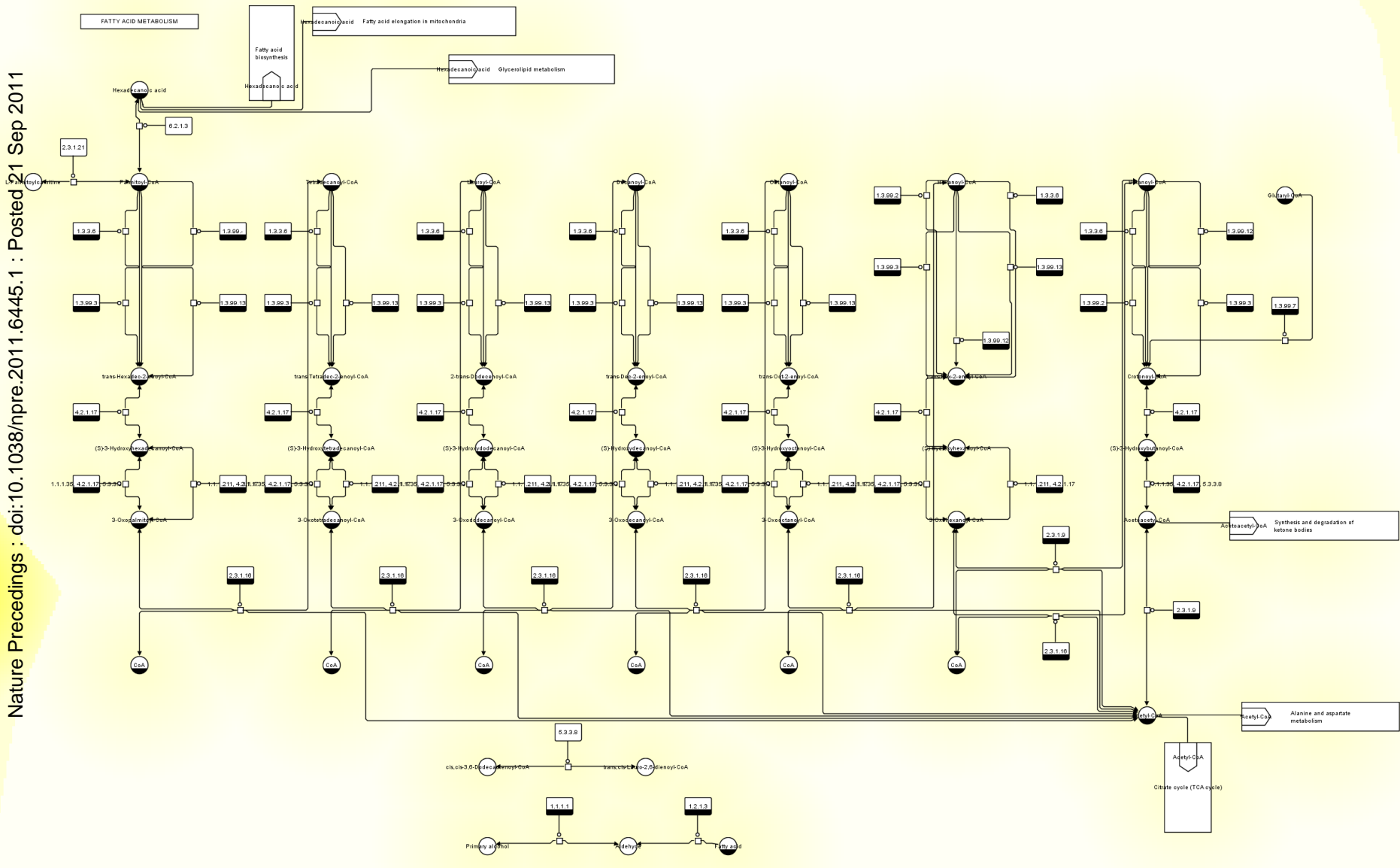
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Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011



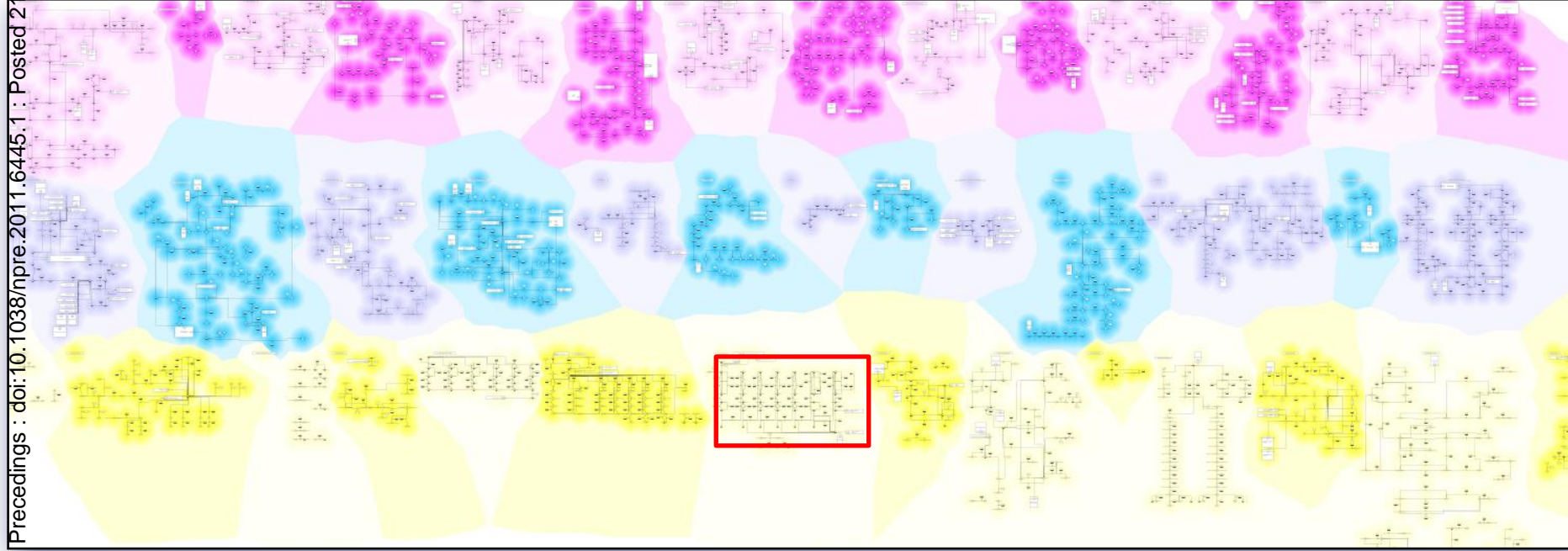
# Constrained KEGG Layout

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011



# Constrained KEGG Layout

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 27 Sep 2011

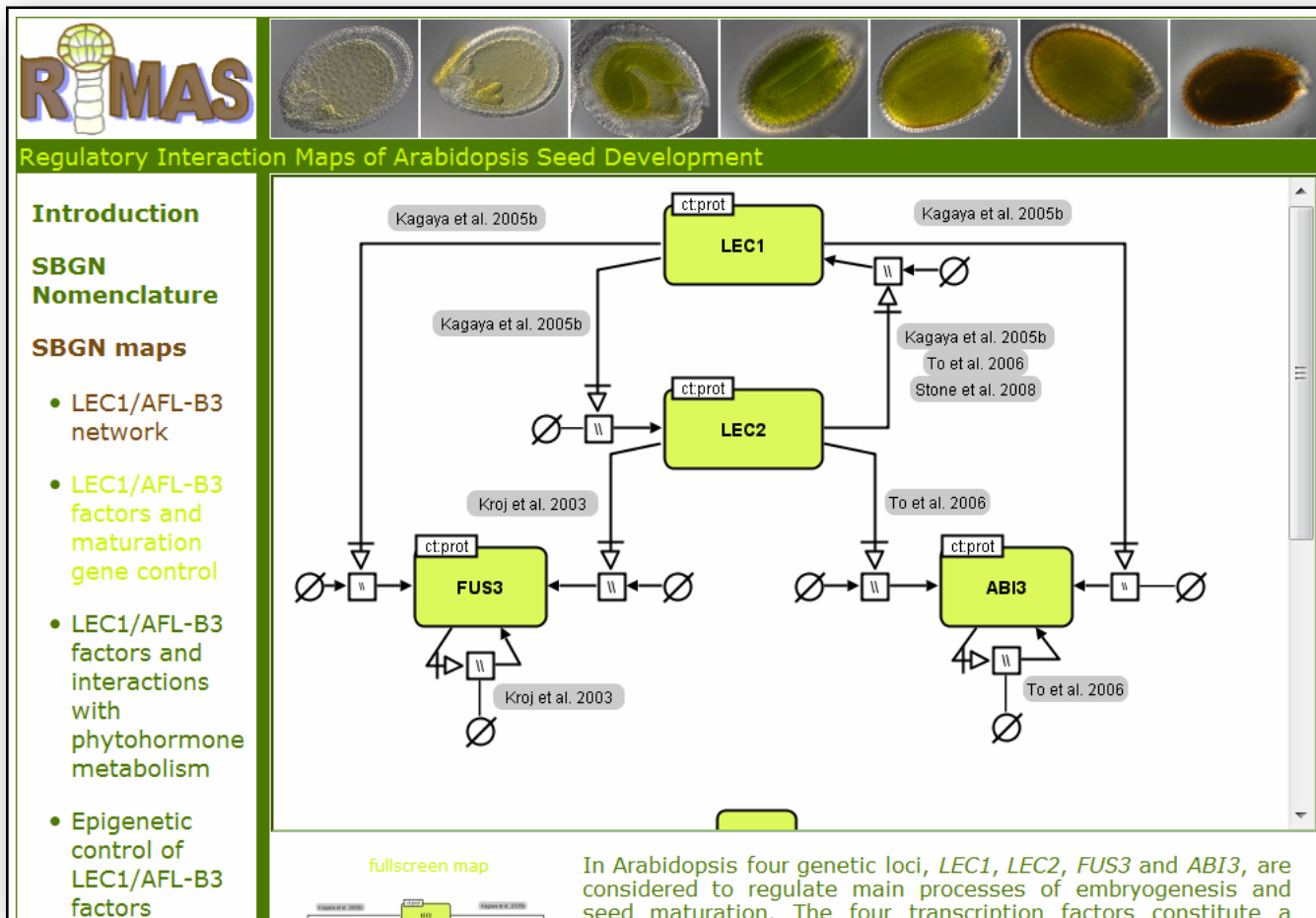


# Automatic Layout of SBGN

- ▶ Network layout algorithms = solve given constraints
  - ▶ Problem: speed
  - ▶ Solution: Solvers for restricted sets of constraints
  - ▶ New method based on stress majorisation
- ▶ Java library for SBGN
- ▶ Joint work with Kim Marriot, Michael Wybrow (both Monash University, Australia) and Tim Dwyer (Microsoft Research)

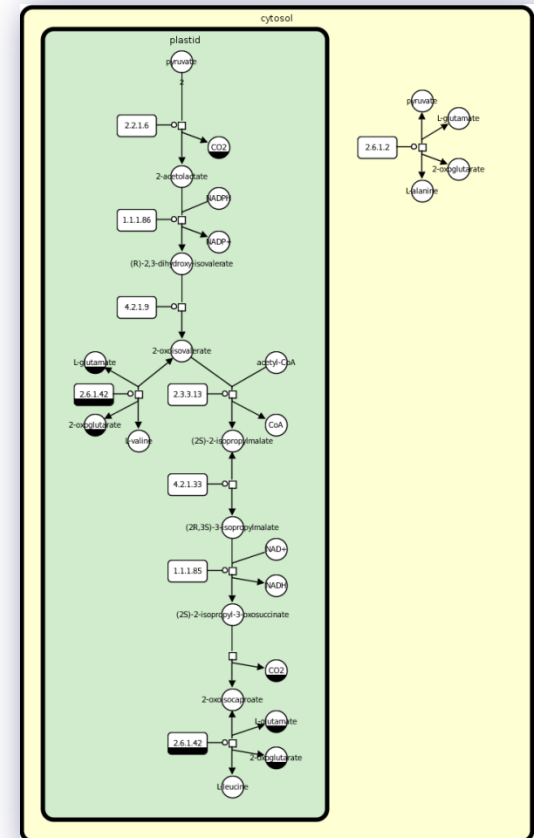
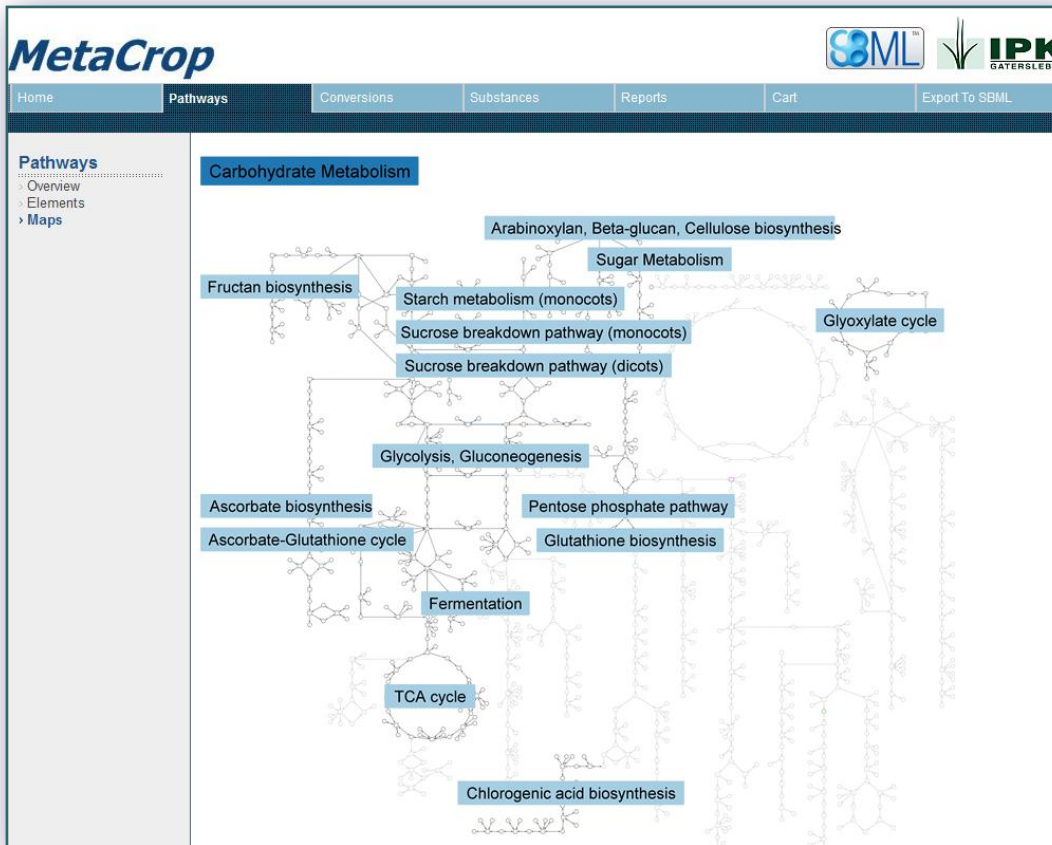
# Applications: RIMAS

- ▶ Regulatory interaction maps of Arabidopsis seed development
- ▶ <http://rimas.ipk-gatersleben.de>



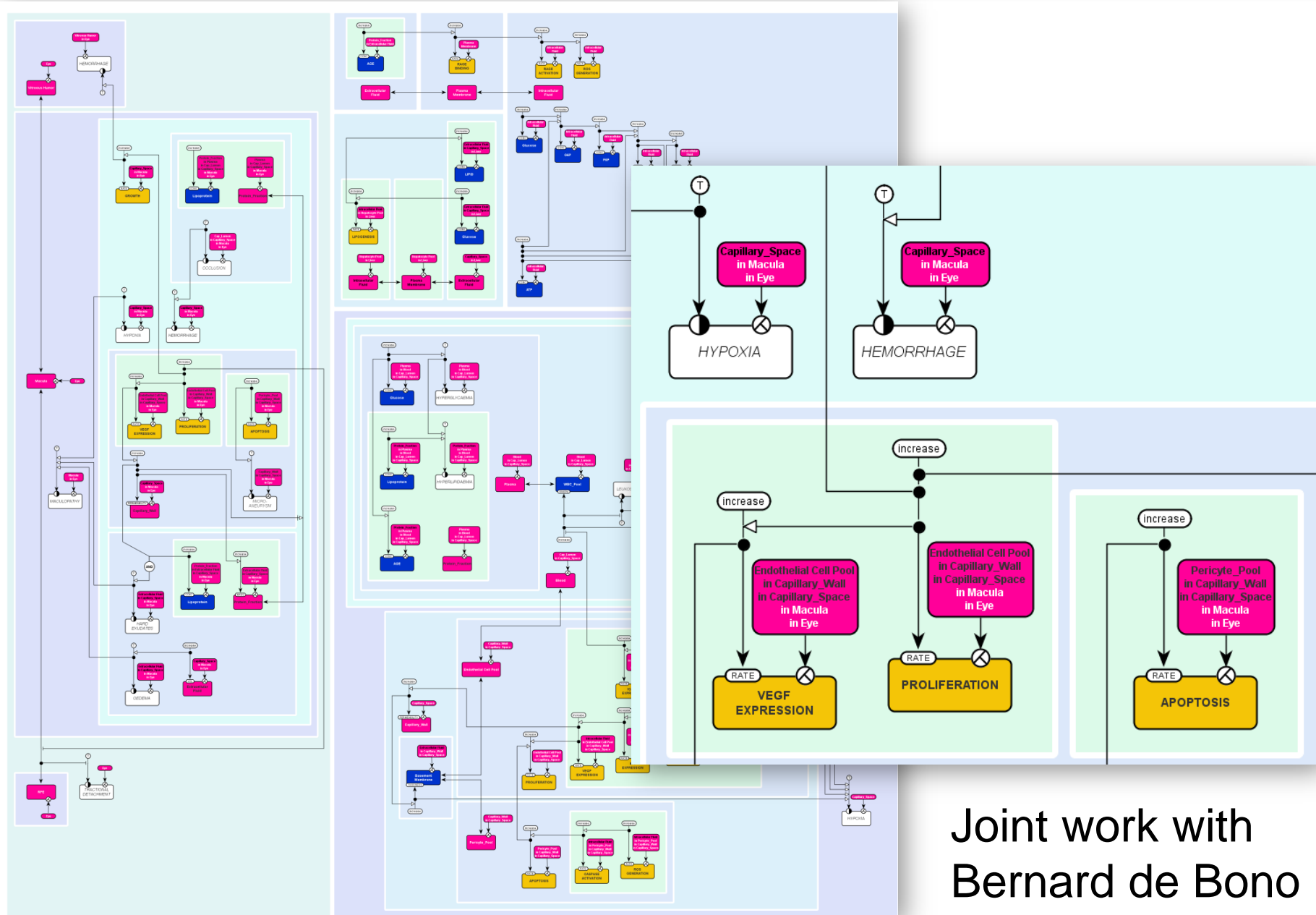
# Applications: MetaCrop

- ▶ Information system for diverse information about metabolic pathways in crop plants
- ▶ Supports creation of detailed metabolic models
- ▶ <http://metacrop.ipk-gatersleben.de>



# Applications: Maps for Other Groups

Nature Precedings : doi:10.1038/npre.2011.6445.1 : Posted 21 Sep 2011



Joint work with  
Bernard de Bono

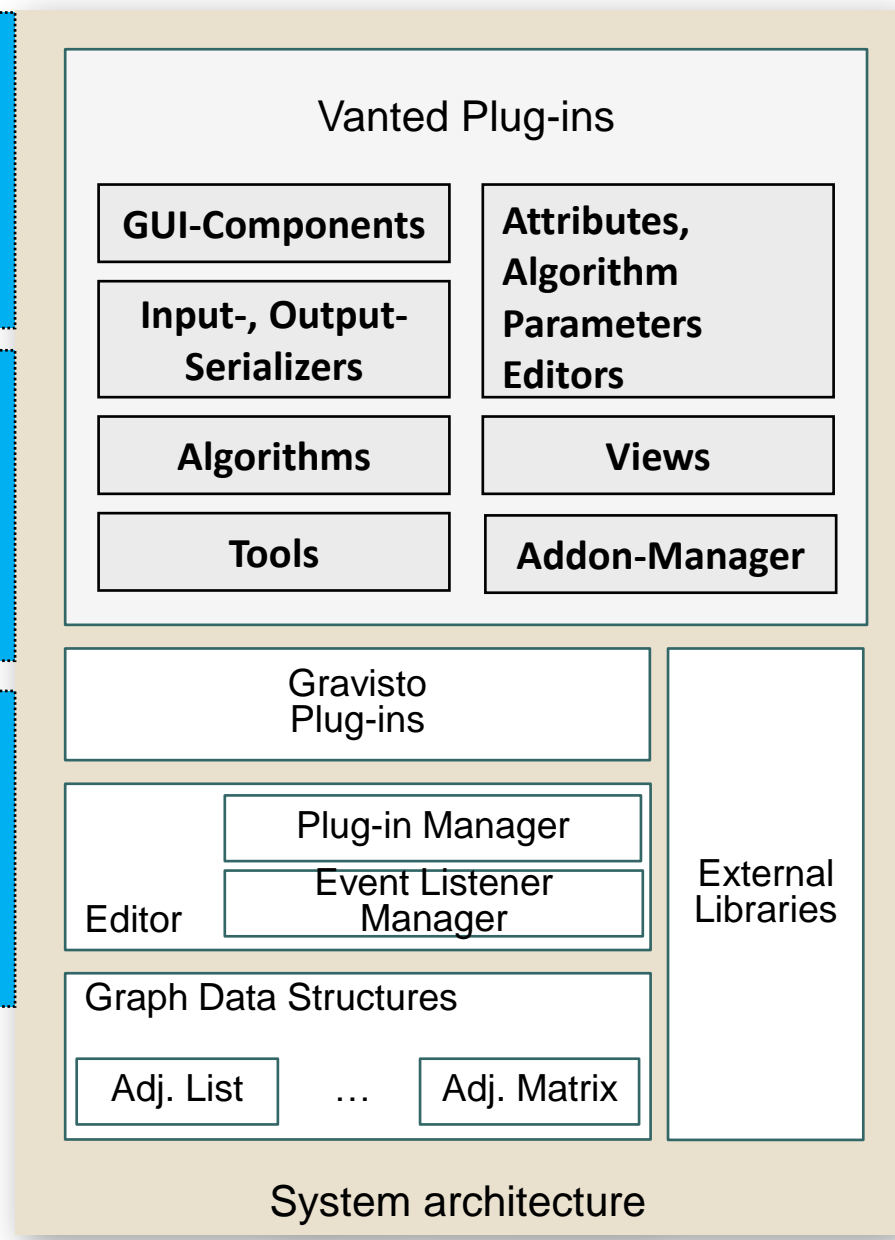
# Implementation

- ▶ Add-on to Vanted
- ▶ Vanted
  - ▶ Based on extensible, plugin-based graph visualization toolkit Gravisto (group of Franz. J. Brandenburg, Passau University)
  - ▶ MVC pattern
  - ▶ Event management (observer design pattern)
  - ▶ Java application
  - ▶ External plug-ins ('Add-ons')
  - ▶ [www.vanted.org](http://www.vanted.org)

FBA Add-on

3D Add-on

...





# Vanted Add-ons - <http://www.vanted.org>

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## VANTED - VISUALIZATION AND ANALYSIS OF NETWORKS CONTAINING EXPERIMENTAL DATA

SOURCEFORCE.NET

VANTED Source Code / Development Add-ons Literature



published, available

Dynamic visualisation of constraint-based metabolic models

FBA-SimVis is a VANTED Add-on for the constraint-based analysis of metabolic models with special focus on the dynamic and visual exploration of metabolic flux data resulting from model analysis.



older publication, available

DBE2 - Database for Biological Experiments

The database system "DBE2", is an extension of the original DBE system, which also supported data presentation in the web ([example](#)). The improved version of this system, DBE2 may now be used to easily store biological experiment data in a central and save place at our institute. It can be accessed directly from within the VANTED tool by installing a VANTED Add-on ([link](#)). Your experiment data can be easily shared and combined with different datasets using the VANTED and DBE2 systems.



outlook presented at OCB'09, available

HIVE - Handy Integration and Visualisation of multimodal Experimental Data

In the frame of the SysSEED project, HIVE combines network-focused Systems Biology approaches with spatio-temporal information. It extends the functionality of VANTED by adding the handling of volumes and images, together with a workspace approach, allowing one to integrate data of different biological data domains. HIVE is written in Java and Java3D and the main tasks are:

- handling of omics data, networks, images and volumes
- integration of different data types using a graph-based workspace
- combining biological data in different ways and
- manifold visualisations of combined data



publication, available

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

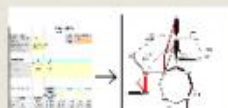
SBGN-ED is a VANTED Add-on which allows to create and edit all three types of SBGN maps, that is Process Description, Entity Relationship and Activity Flow, to validate these maps according to the SBGN specifications, to translate maps from the KEGG and MetaCrap pathway databases into SBGN, and to export SBGN maps into several file and image formats. SBGN (Systems Biology Graphical Notation) is an emerging standard for graphical representations of biochemical and cellular processes studied in systems biology.



available

CentiLib - Computation of network centralities

CentiLib is an Add-on for the computation and investigation of weighted and unweighted centralities in biological networks. Even though CentiLib was developed to integrate the computation of centralities into as many tools for the visualisation and analysis of biological networks as possible, it can be used for other types of networks, too.



FluxMap - visual exploration of flux distributions in biological networks

FluxMap is an easy to use tool for the advanced visualization of simulated or measured flux data in biological networks. Flux data import is achieved via a structured template basing on intuitive reaction equations. Flux data is mapped onto any network and visualized using edge thickness. Various visualization options and interaction possibilities enable comparison and visual analysis of

# Many Additional Functions via Vanted

- ▶ Network analysis and visualisation algorithms
    - ▶ Centralities, motifs, clusters, graph properties
    - ▶ Layout algorithms, graph editing
  - ▶ Data mapping (omics data)
  - ▶ Statistical analysis
  - ▶ Access to databases, importers, exporters
  - ▶ Simulation
  - ▶ 3D visualisation
  - ▶ And more
- 
- ▶ [www.vanted.org](http://www.vanted.org) (Vanted 2.0)
  - ▶ Open source (GPL)

# Acknowledgements

- ▶ Astrid Junker
- ▶ Anja Hartmann
- ▶ Eva Grafahrend-Belau
- ▶ Hendrik Rohn
- ▶ Matthias Klapperstück
- ▶ Hendrik Mehlhorn
- ▶ Christian Klukas
- ▶ Kim Marriott (Monash Univ Melbourne)
- ▶ Michael Wybrow (Monash Univ Melbourne)
- ▶ Tim Dwyer (Microsoft)
- ▶ Franz J. Brandenburg
- ▶ libSBGN community
- ▶ SBGN community

**SBGN-ED**

[www.sbgn-ed.org](http://www.sbgn-ed.org)