

SBGN-ED – working with the Systems Biology Graphical Notation

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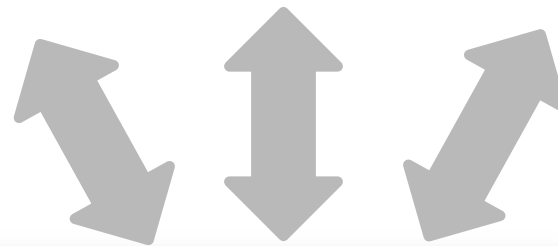


Working with SBGN

Creating
Editing
Translating
Validating

Exploring
Navigating

Data
integrating
Analysing



SBGN-ED

www.sbgn-ed.org

GML
GraphML
SBGN-ML(M1)
Import

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

Creating and Editing SBGN Maps

The image displays the VANTED V2.0 software interface, showing a SBGN map of neuronal muscle signalling and its editing tools.

neuronal_muscle_signalling.graphml - view 1

The map is divided into two main compartments: **synaptic button** and **muscle cytosol**.

synaptic button: Contains nodes for **actin**, **Ca²⁺**, **ChAT**, **vAChT**, **choline**, **ACh**, **synaptic vesicle**, **SNARE**, and **synaptic cleft**. Arcs show the release of ACh from the vesicle into the cleft.

muscle cytosol: Contains nodes for **nAChR** (closed/open), **Ca²⁺**, **ER**, **ATP**, **ADP**, **P_i**, **actin**, **myosin**, and **muscle contraction**. Arcs show the binding of ACh to nAChR, leading to channel opening, Ca²⁺ release from the ER, and subsequent actin-myosin interaction for contraction.

Editing Tools (Right Panel):

- Entity Relationship:** Apply Changes, Clear Glyph Labels, Clear Arc Labels.
- Entity Pool Nodes:** Select from various shapes (circle, rectangle, oval, etc.).
- Auxiliary Units:** Units of Information, State Variables, Clone Marker.
- Container Nodes:** Select from various shapes (rectangle, oval, etc.).
- Reference Nodes:** Select from various shapes (rectangle, oval, etc.).
- Process Nodes:** Select from various shapes (square, circle, hexagon, etc.).
- Connecting Arcs:** Select from various shapes (straight line, arrow, etc.).
- Logical Operators:** AND, OR, NOT.
- Statements:** Select from various shapes (rectangle, oval, etc.).
- Influences:** Select from various shapes (rectangle, oval, etc.).
- Reference Nodes:** Select from various shapes (rectangle, oval, etc.).

Bottom Status Bar:

- 48 nodes, 38 edges, 46 MB
- 21 nodes, 28 edges, 40 MB
- 7 nodes, 7 edges, 38 MB

Translating SBGN Maps from KEGG

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 6-phosphate

beta-D-Fructose 6-phosphate

Peritrate phosphate pathway

Carbon fixation in photosynthetic organisms

Citrate cycle (TCA cycle)

Pyruvate metabolism

Propanoate metabolism

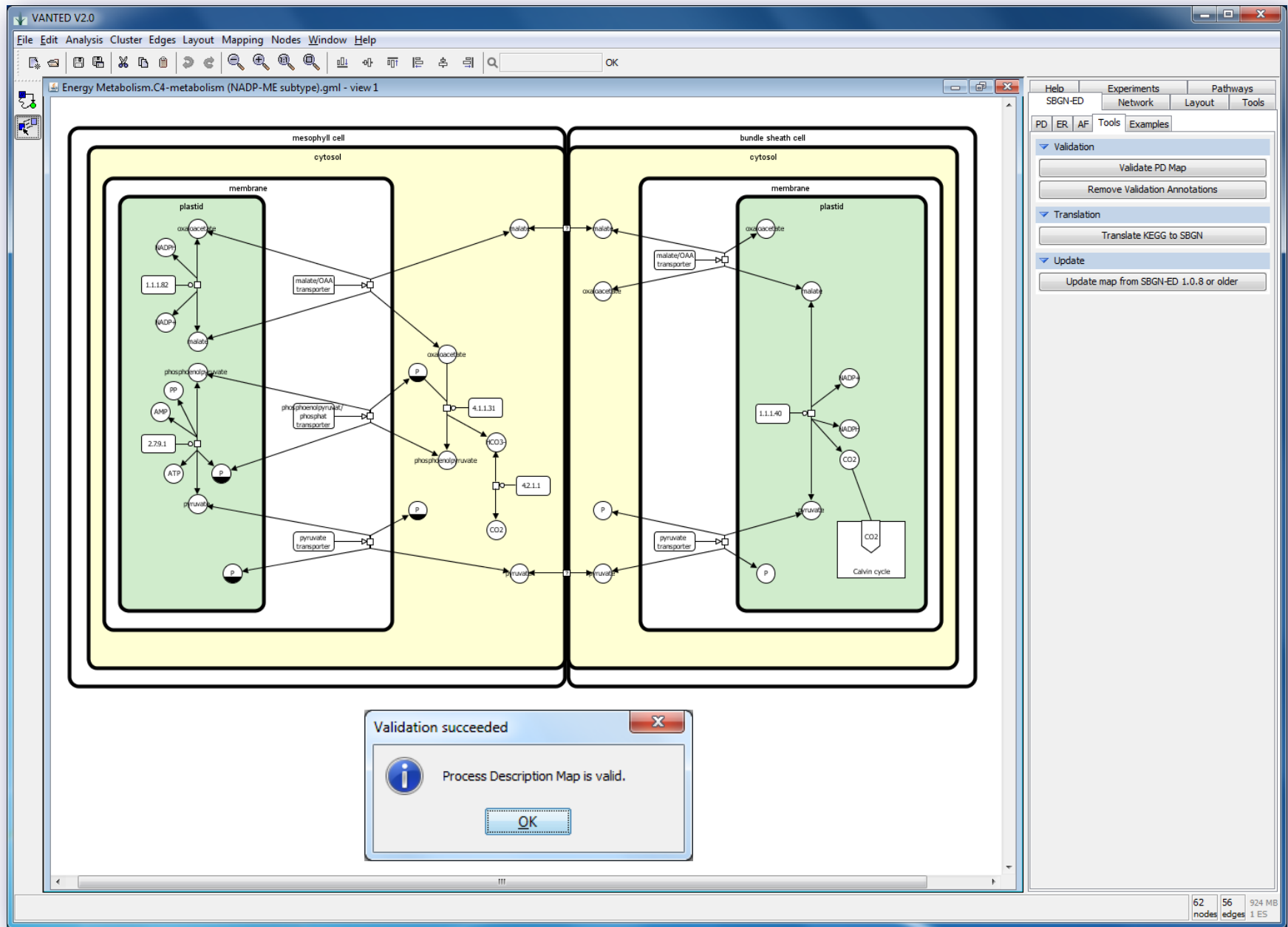
95 nodes 129 edges 1071 MB 2 ES

Validation

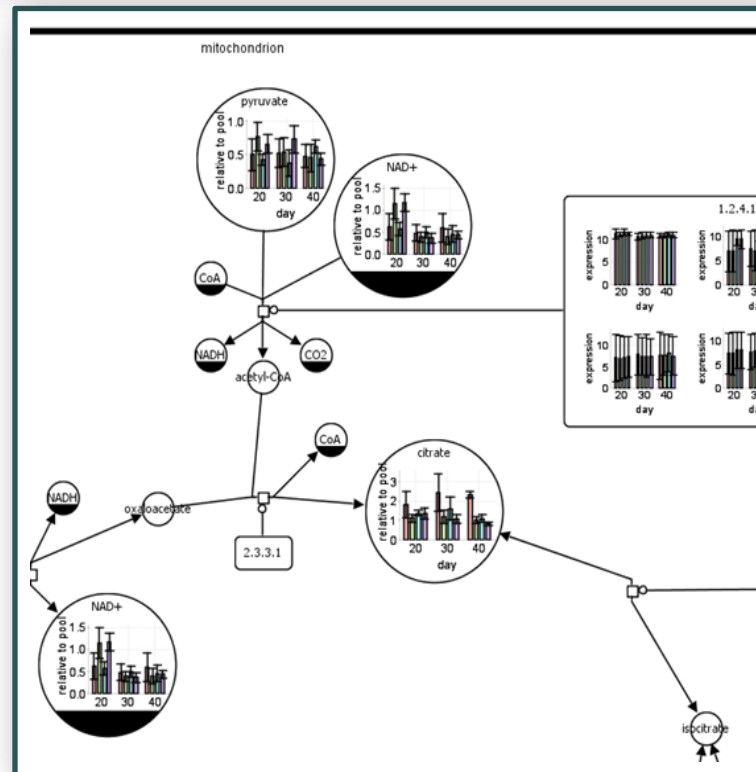
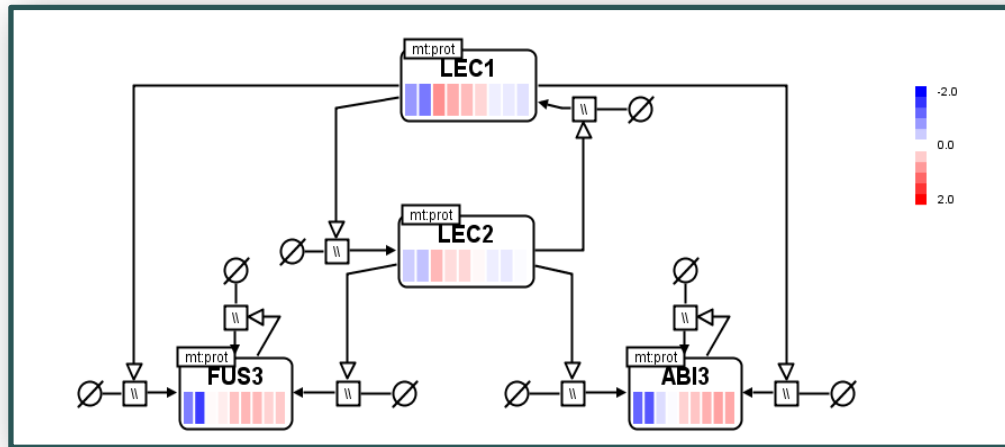
Translate KEGG to SBGN

Update map from SBGN-ED 1.0.8 or older

Validating SBGN Maps



Data Integrating and Analysing in SBGN Maps



What's New

Current version (see www.sbgn-ed.org)

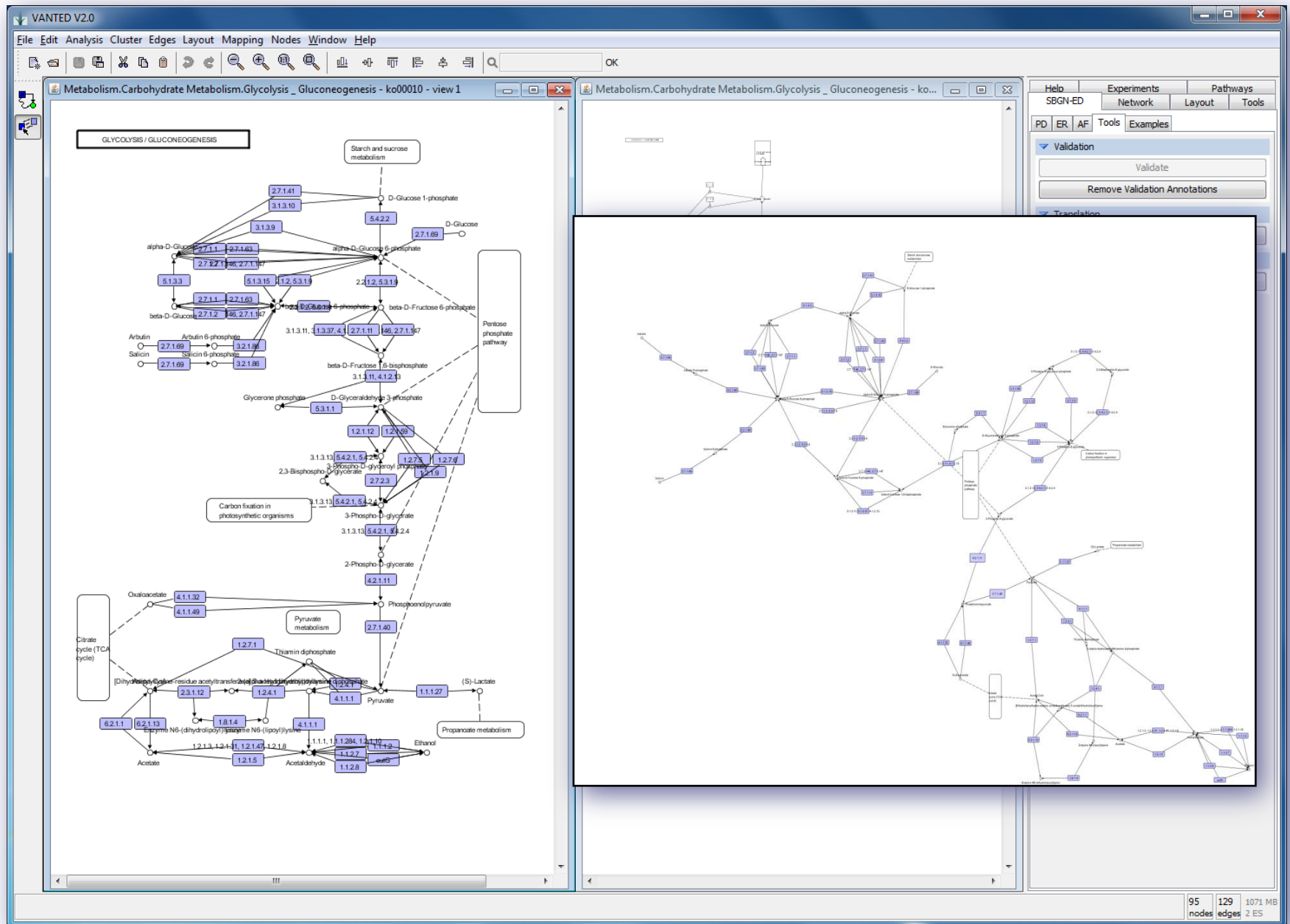
- ▶ Improved user interaction
- ▶ More export possibilities
 - ▶ Powerpoint
 - ▶ Webpages
 - ▶ SBGN-ML(M1)

Next version (under development)

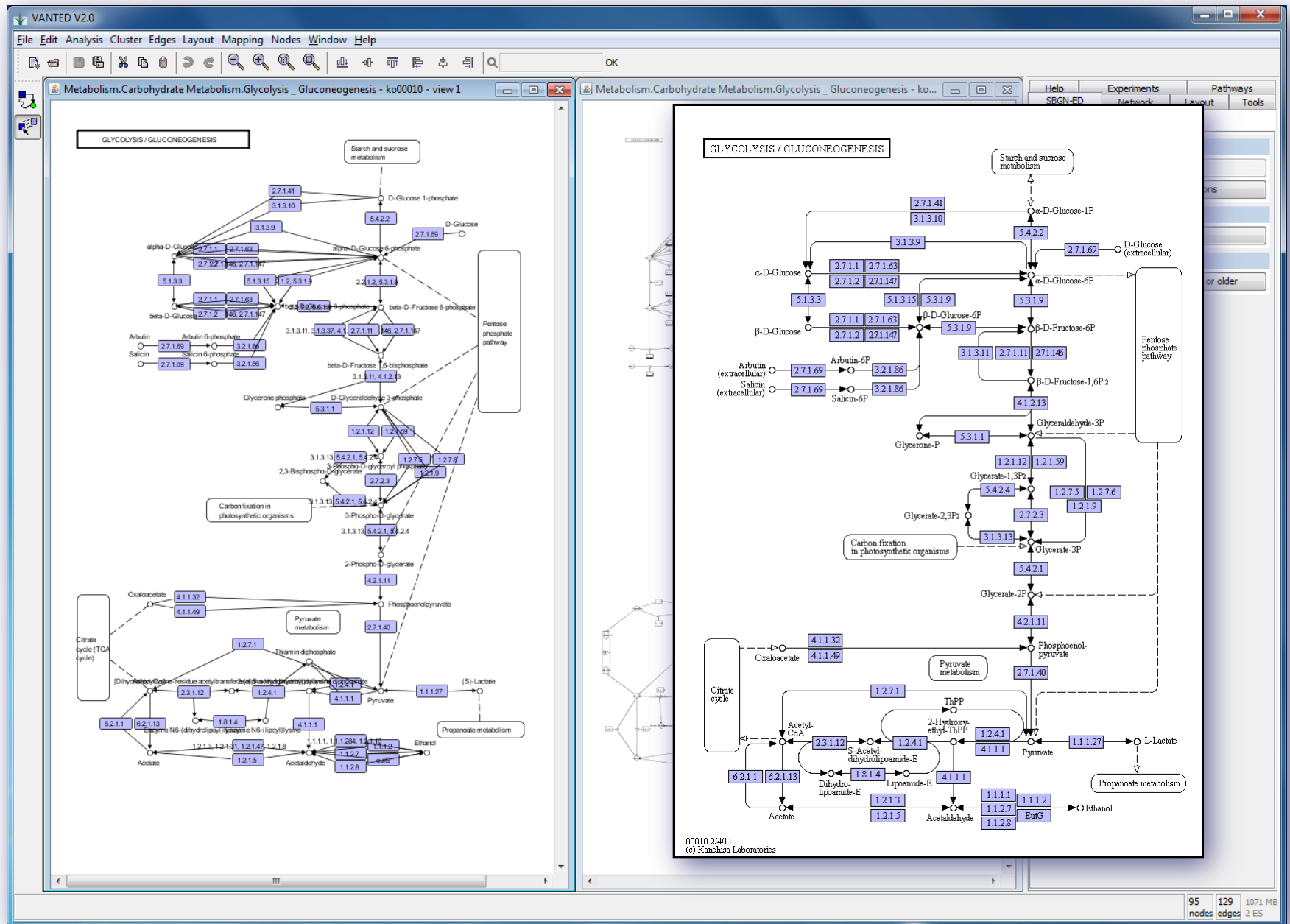
- ▶ More importers
 - ▶ SBML (all up to L3V1) (JSBML)
 - ▶ BioPAX (L2,L3) (Paxtools V4)
- ▶ Automatic layout
- ▶ More interaction possibilities

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

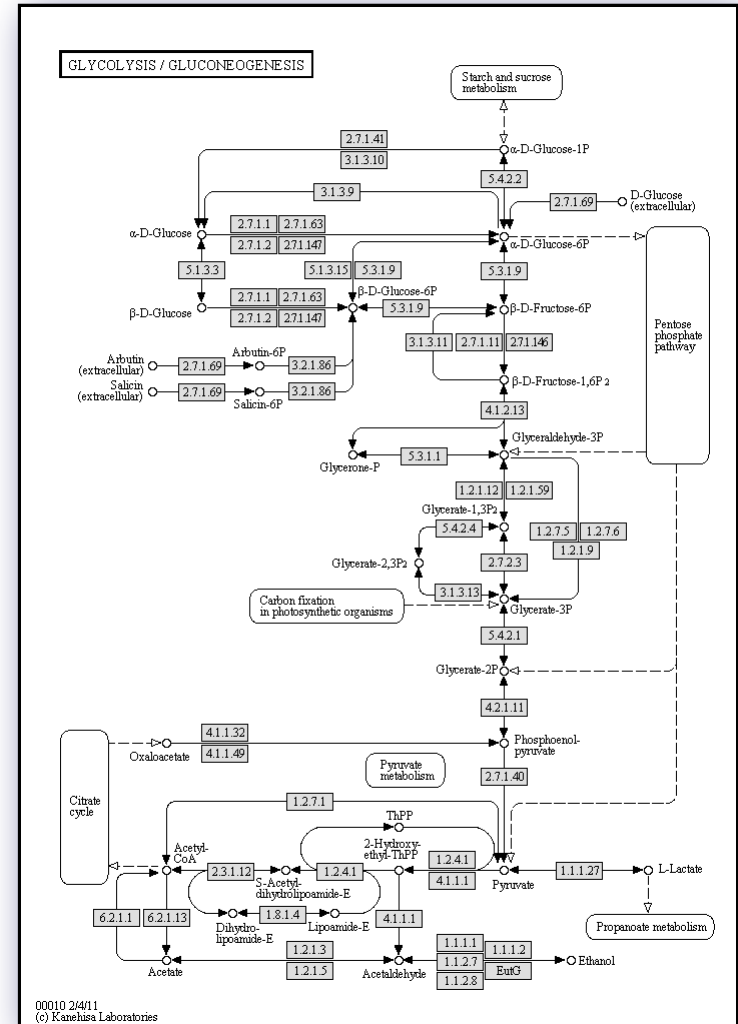
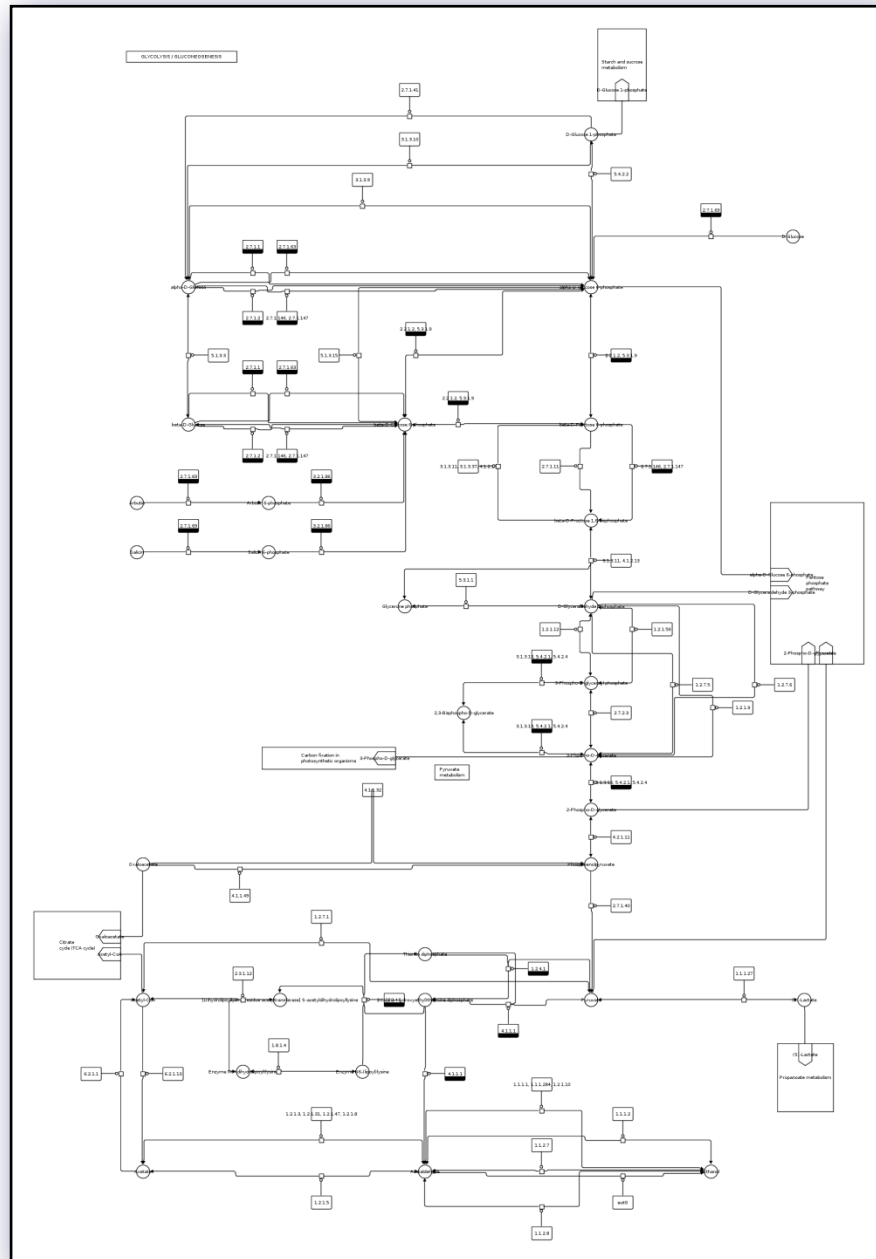
Layout



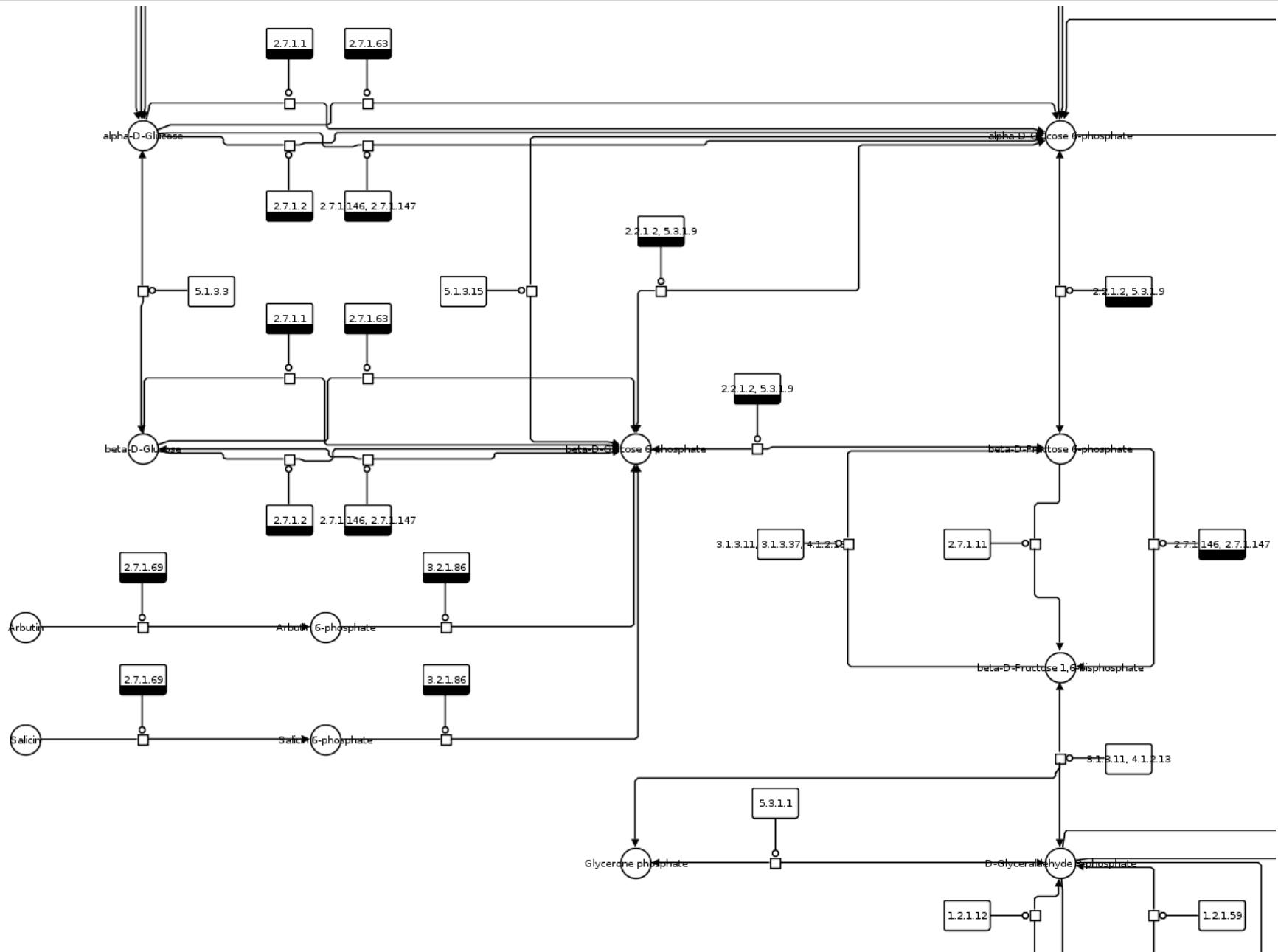
Layout



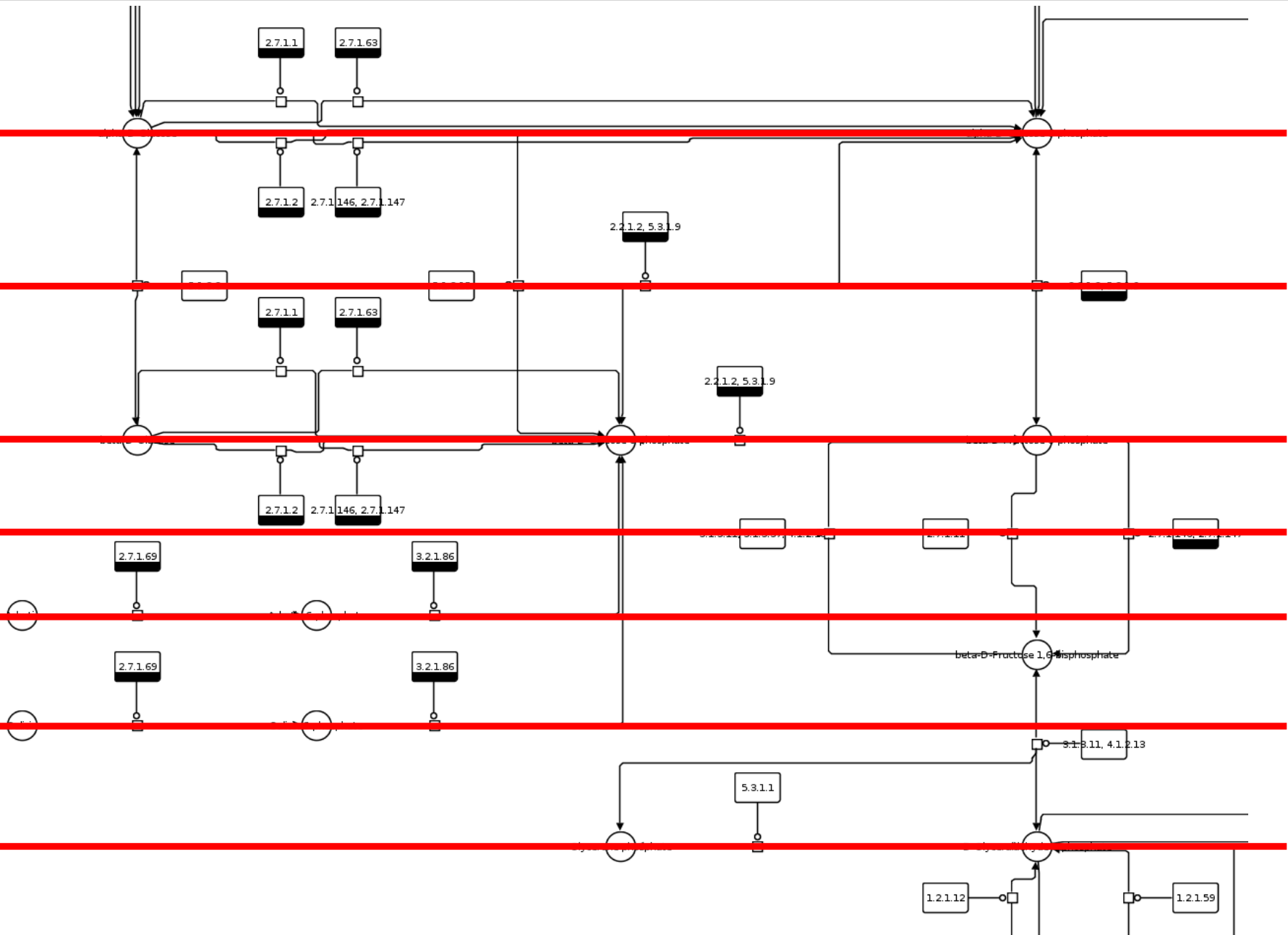
Constrained KEGG Layout



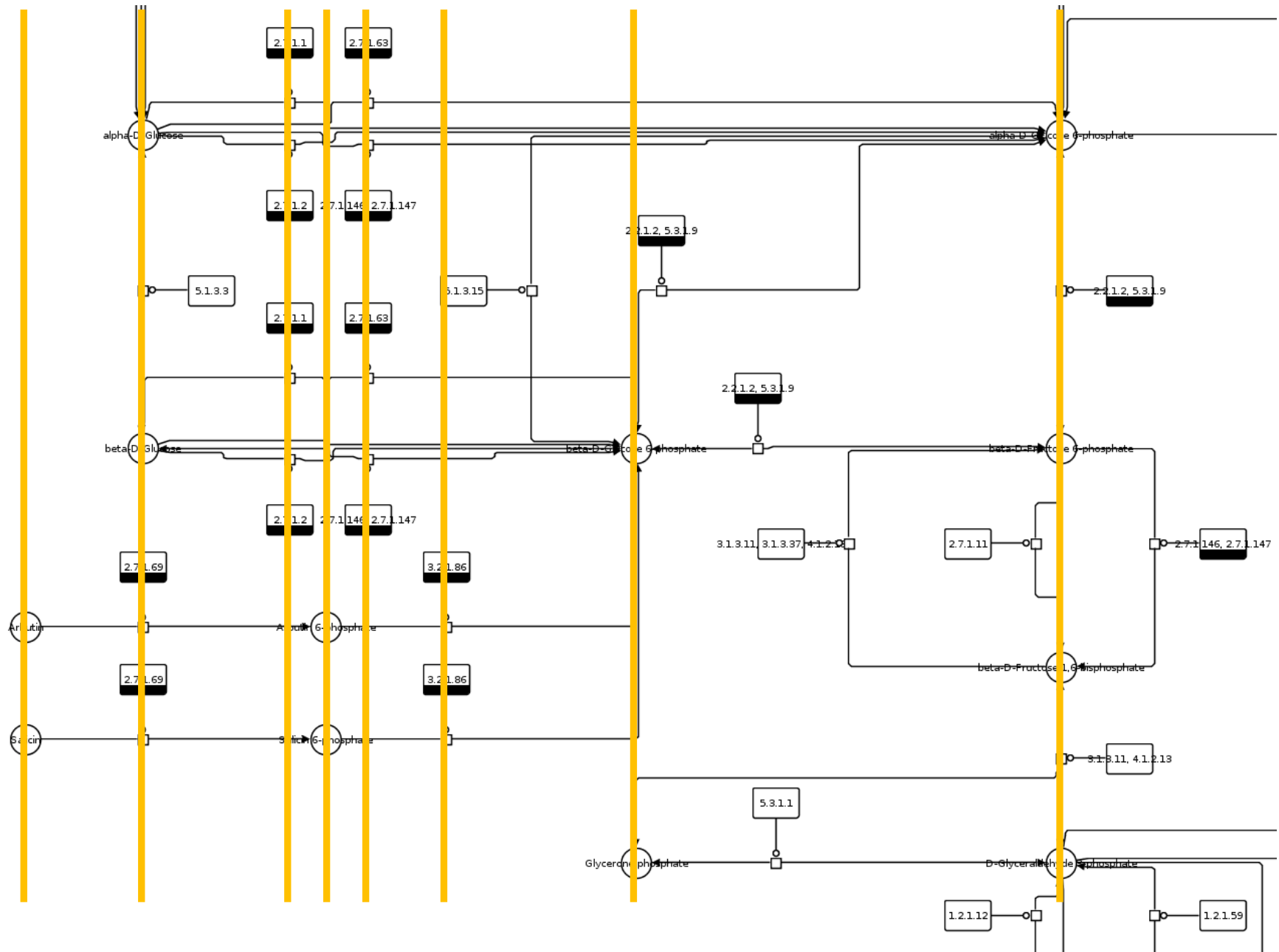
Constrained KEGG Layout



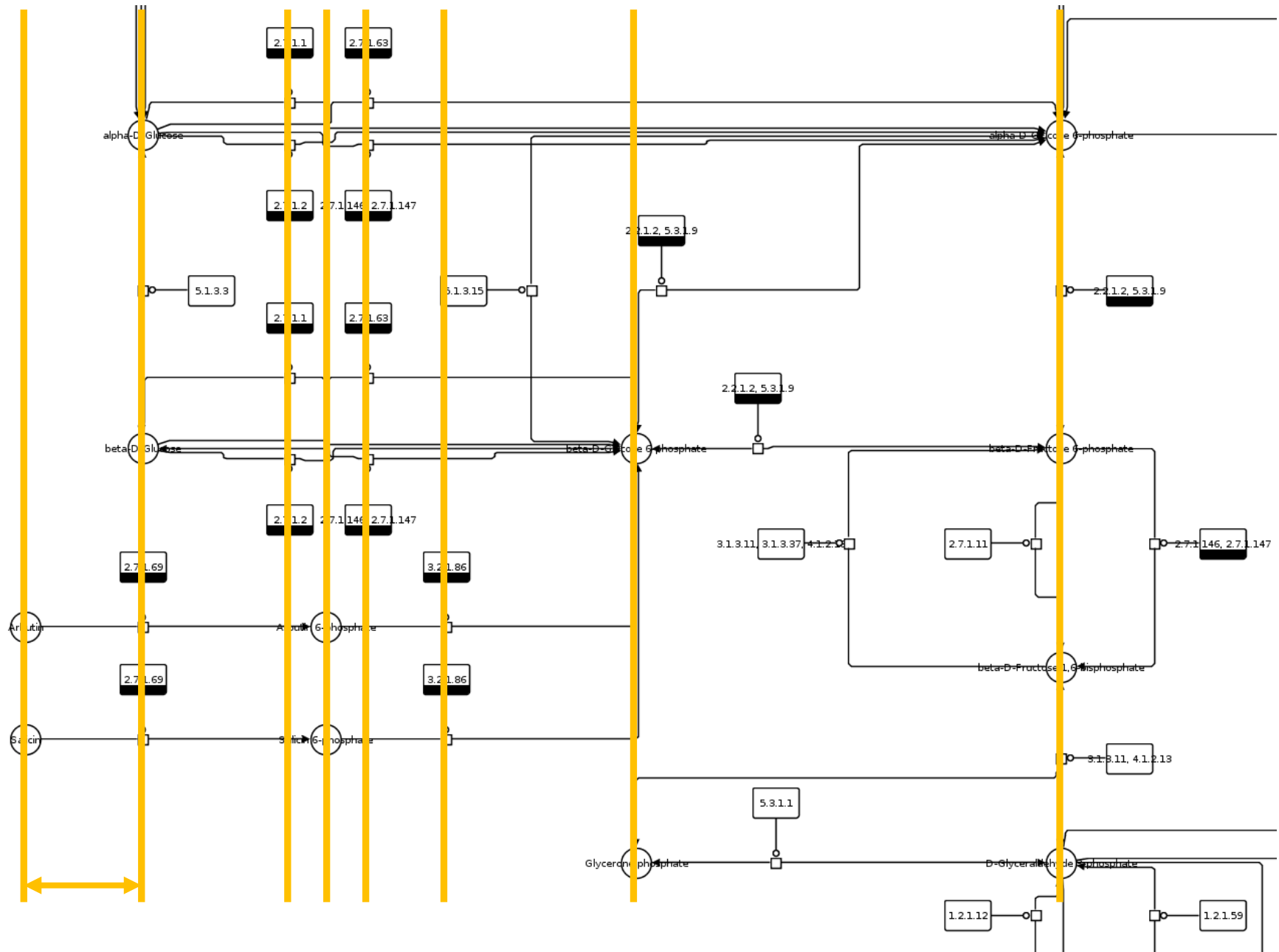
Constrained KEGG Layout



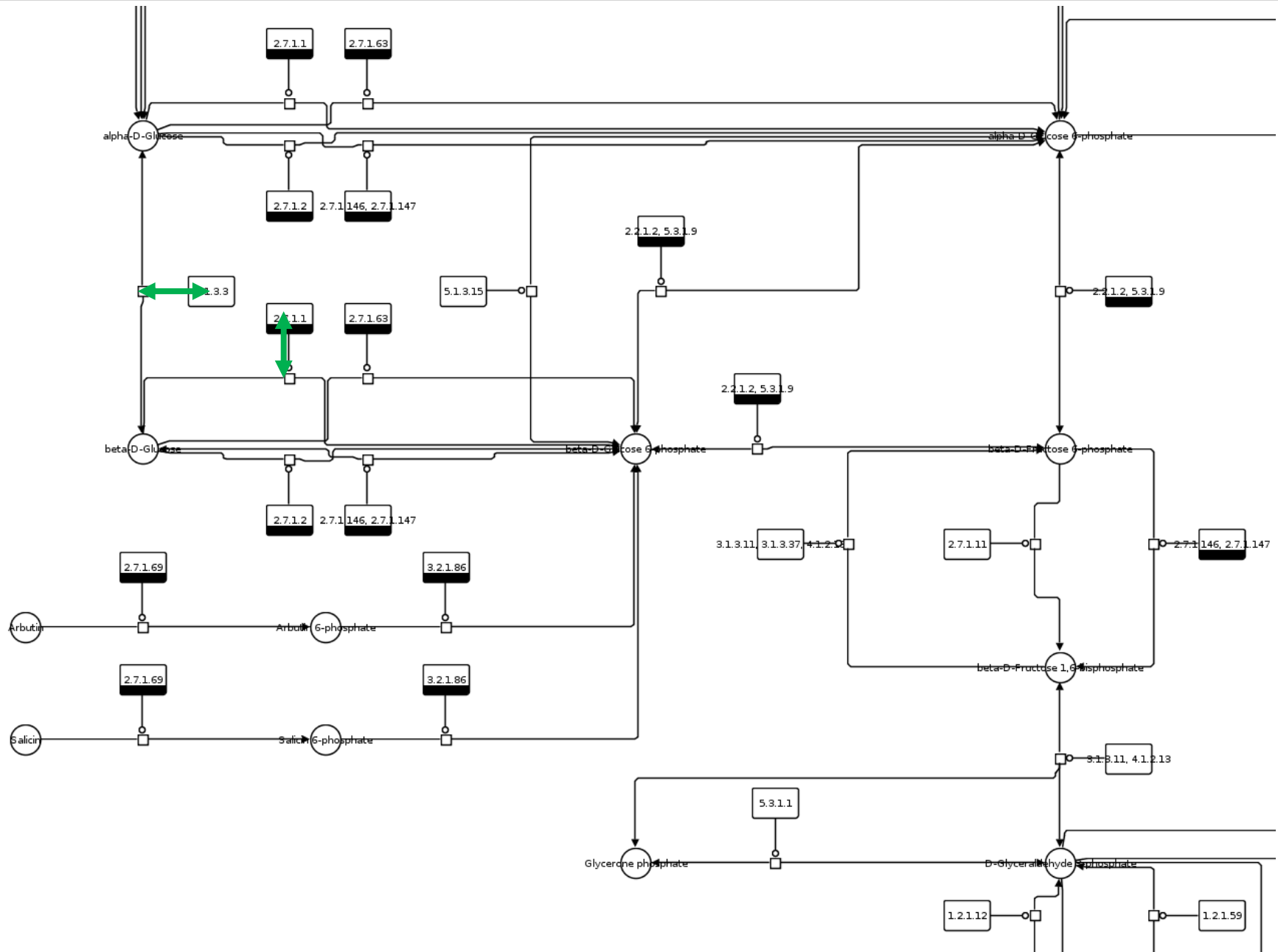
Constrained KEGG Layout



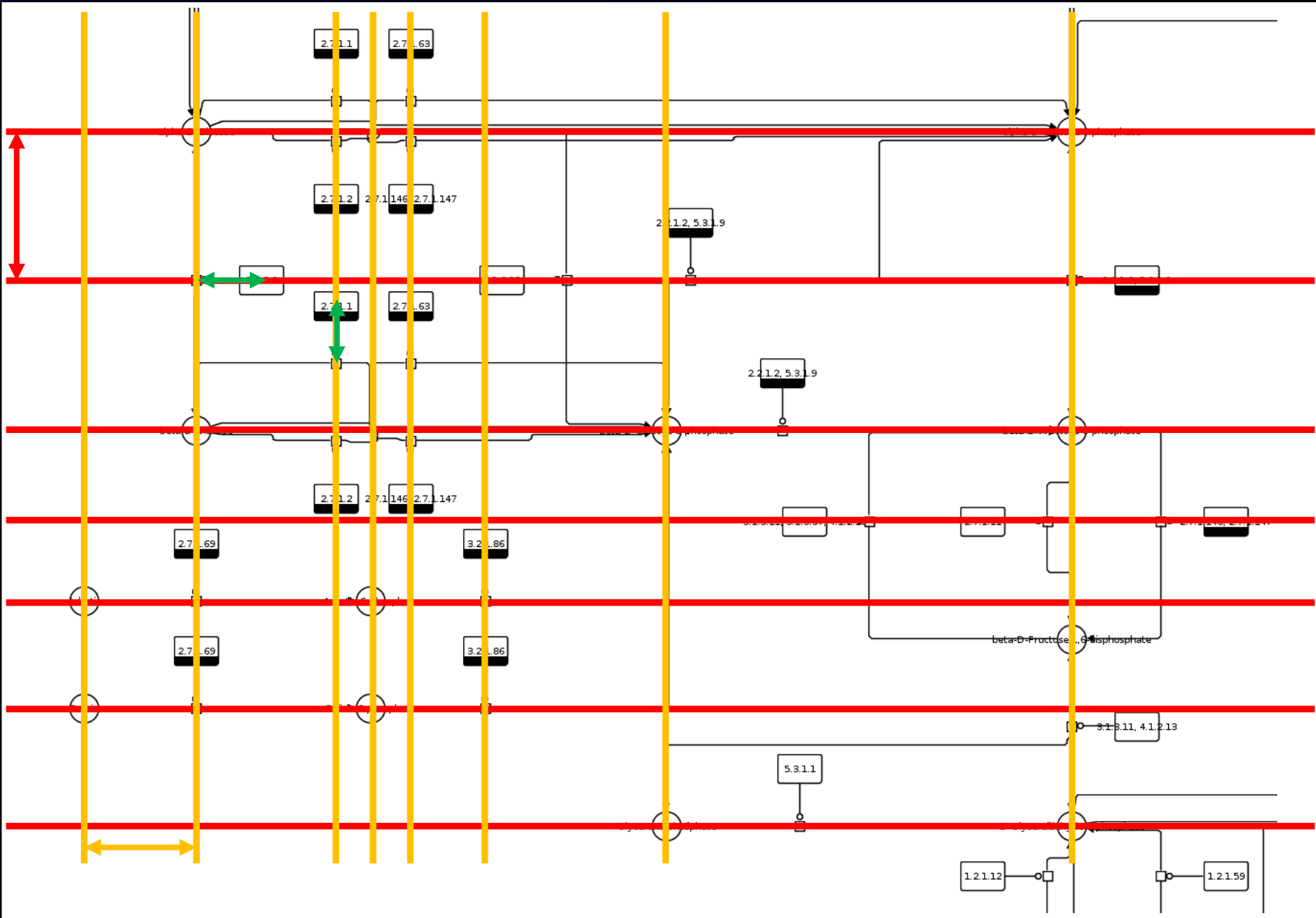
Constrained KEGG Layout



Constrained KEGG Layout

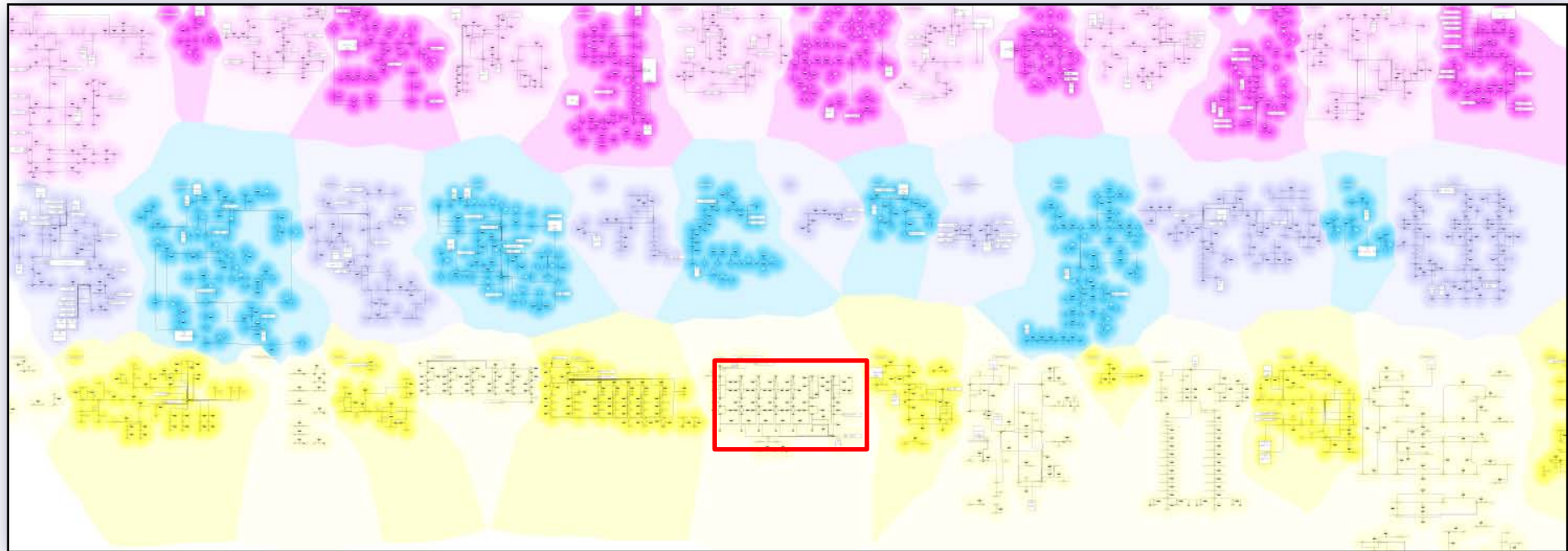


Constrained KEGG Layout



This metabolic map illustrates the pathways of fatty acid metabolism. It begins with **FATTY ACID METABOLISM**, which includes **Fatty acid biosynthesis** (converting Hexanoic acid to Hexadecanoic acid) and **Fatty acid elongation in mitochondria** (converting Hexadecanoic acid to Hexacosanoic acid). **Glycerolipid metabolism** is also shown. The main pathway involves the conversion of long-chain fatty acids into CoA derivatives (e.g., Hexadecanoyl-CoA, Octadecanoyl-CoA, Eicosanoyl-CoA, Docosanoyl-CoA, Hexacosanoyl-CoA). These are then processed through a series of steps involving **trans** and **cis** isomers, and **(S)**-hydroxy intermediates, leading to the formation of **3-Oxofattyacyl-CoA** intermediates. These intermediates are then converted to **Acyl-CoA** derivatives (e.g., Hexadecanoyl-CoA, Octadecanoyl-CoA, Eicosanoyl-CoA, Docosanoyl-CoA, Hexacosanoyl-CoA). The **Acyl-CoA** derivatives are then converted to **Acetyl-CoA**, which enters the **Citrate cycle (TCA cycle)**. The map also shows the conversion of **Acetyl-CoA** to **Acetyl-CoA** and **Acetyl-CoA** to **Acetyl-CoA**. The map includes various metabolites and their associated metabolite IDs (e.g., 2.3.121, 1.3.9.5, 1.3.9.3, 4.2.1.17, 1.1.1.3, 2.3.1.10, 5.3.3.8, 1.1.1.1, 1.2.1.3, 1.3.9.2, 1.3.9.3, 1.3.9.12, 1.3.9.13, 1.3.9.14, 1.3.9.15, 1.3.9.16, 1.3.9.17, 1.3.9.18, 1.3.9.19, 1.3.9.20, 1.3.9.21, 1.3.9.22, 1.3.9.23, 1.3.9.24, 1.3.9.25, 1.3.9.26, 1.3.9.27, 1.3.9.28, 1.3.9.29, 1.3.9.30, 1.3.9.31, 1.3.9.32, 1.3.9.33, 1.3.9.34, 1.3.9.35, 1.3.9.36, 1.3.9.37, 1.3.9.38, 1.3.9.39, 1.3.9.40, 1.3.9.41, 1.3.9.42, 1.3.9.43, 1.3.9.44, 1.3.9.45, 1.3.9.46, 1.3.9.47, 1.3.9.48, 1.3.9.49, 1.3.9.50, 1.3.9.51, 1.3.9.52, 1.3.9.53, 1.3.9.54, 1.3.9.55, 1.3.9.56, 1.3.9.57, 1.3.9.58, 1.3.9.59, 1.3.9.60, 1.3.9.61, 1.3.9.62, 1.3.9.63, 1.3.9.64, 1.3.9.65, 1.3.9.66, 1.3.9.67, 1.3.9.68, 1.3.9.69, 1.3.9.70, 1.3.9.71, 1.3.9.72, 1.3.9.73, 1.3.9.74, 1.3.9.75, 1.3.9.76, 1.3.9.77, 1.3.9.78, 1.3.9.79, 1.3.9.80, 1.3.9.81, 1.3.9.82, 1.3.9.83, 1.3.9.84, 1.3.9.85, 1.3.9.86, 1.3.9.87, 1.3.9.88, 1.3.9.89, 1.3.9.90, 1.3.9.91, 1.3.9.92, 1.3.9.93, 1.3.9.94, 1.3.9.95, 1.3.9.96, 1.3.9.97, 1.3.9.98, 1.3.9.99, 1.3.9.100).

Constrained KEGG Layout

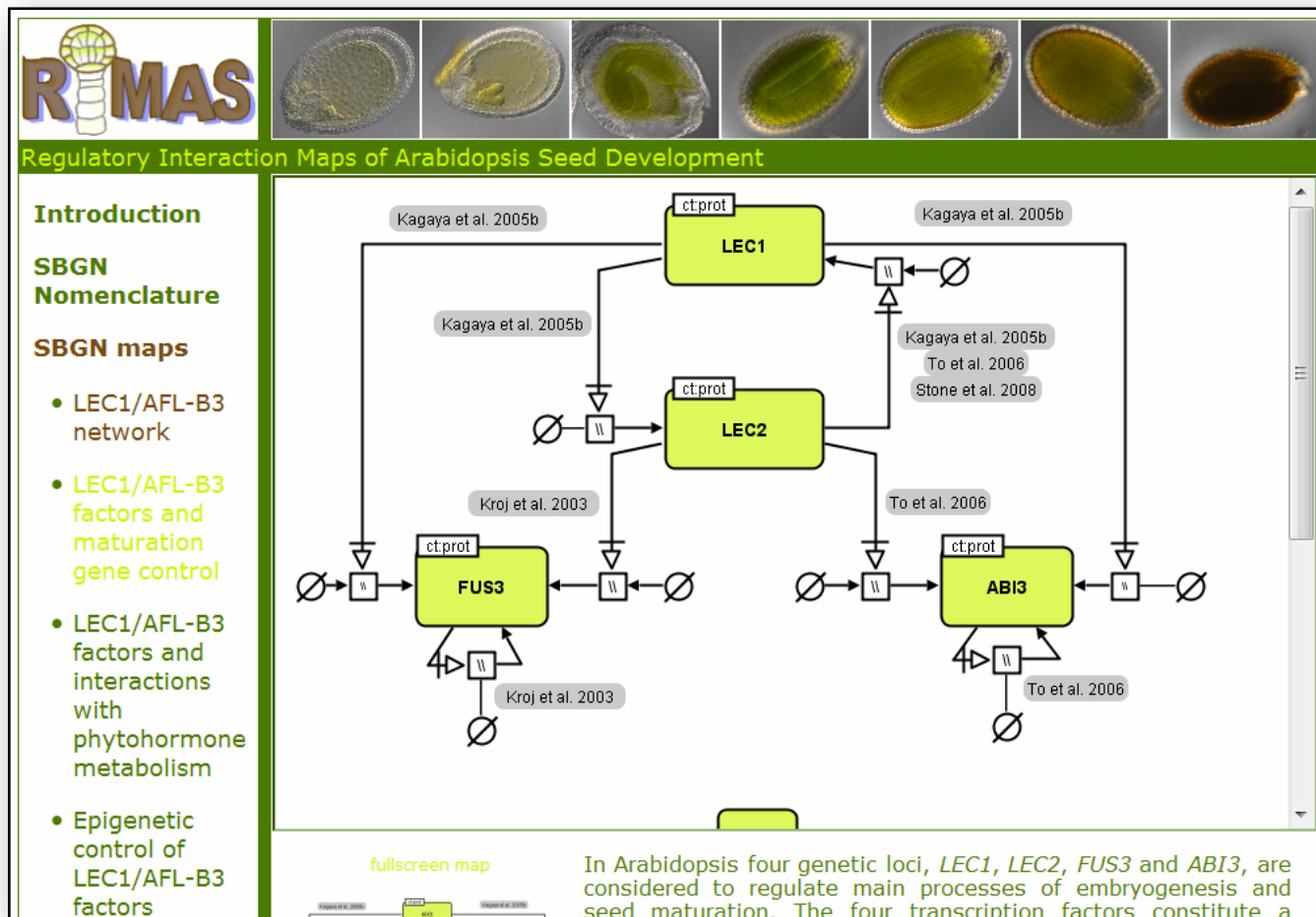


Automatic Layout of SBGN

- ▶ 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) and Tim Dwyer (Microsoft Research)

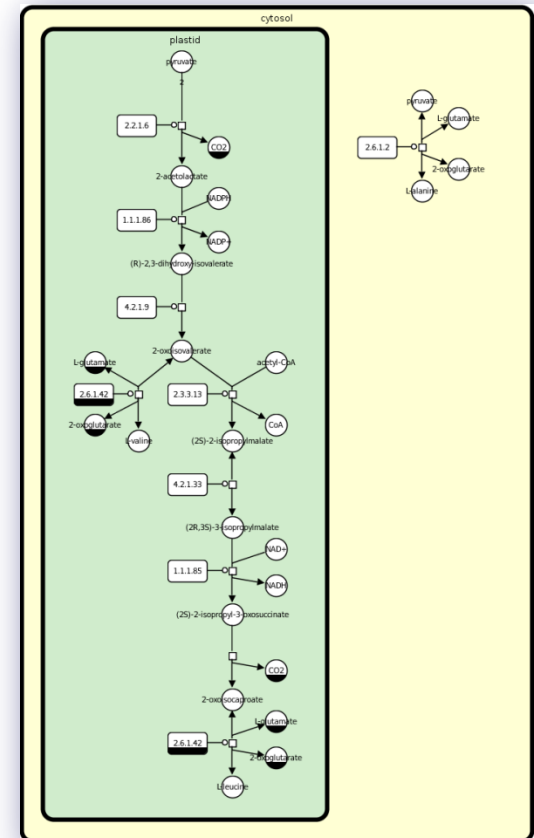
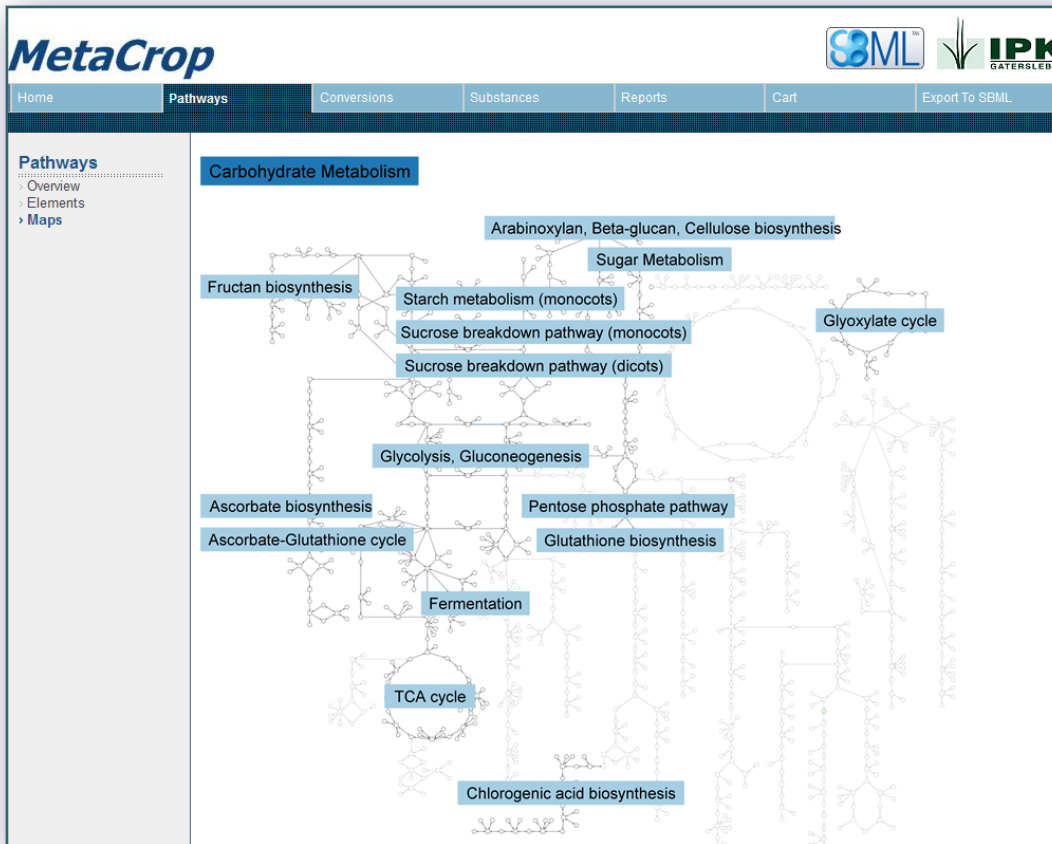
Applications: RIMAS

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

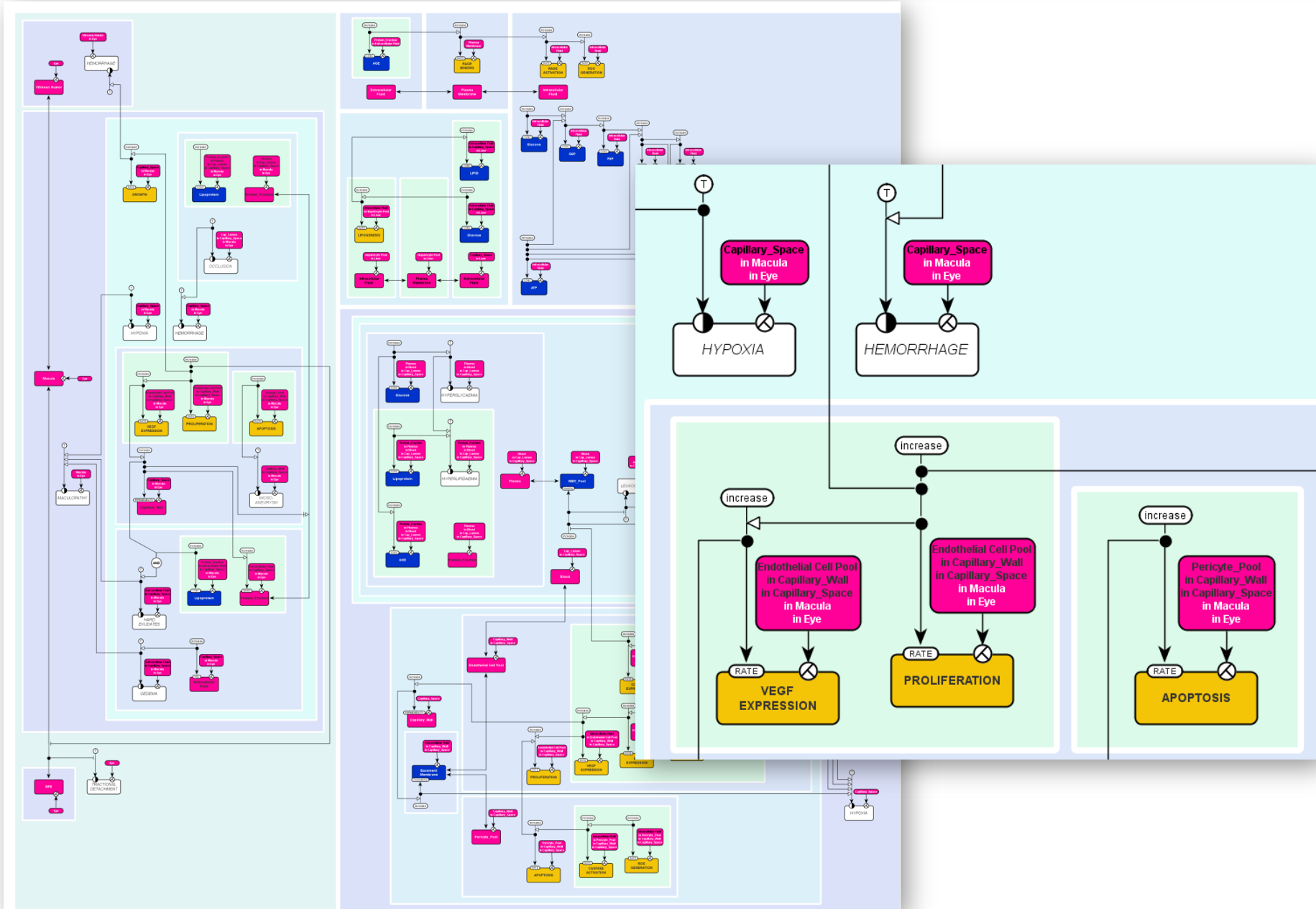


Applications: MetaCrop

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

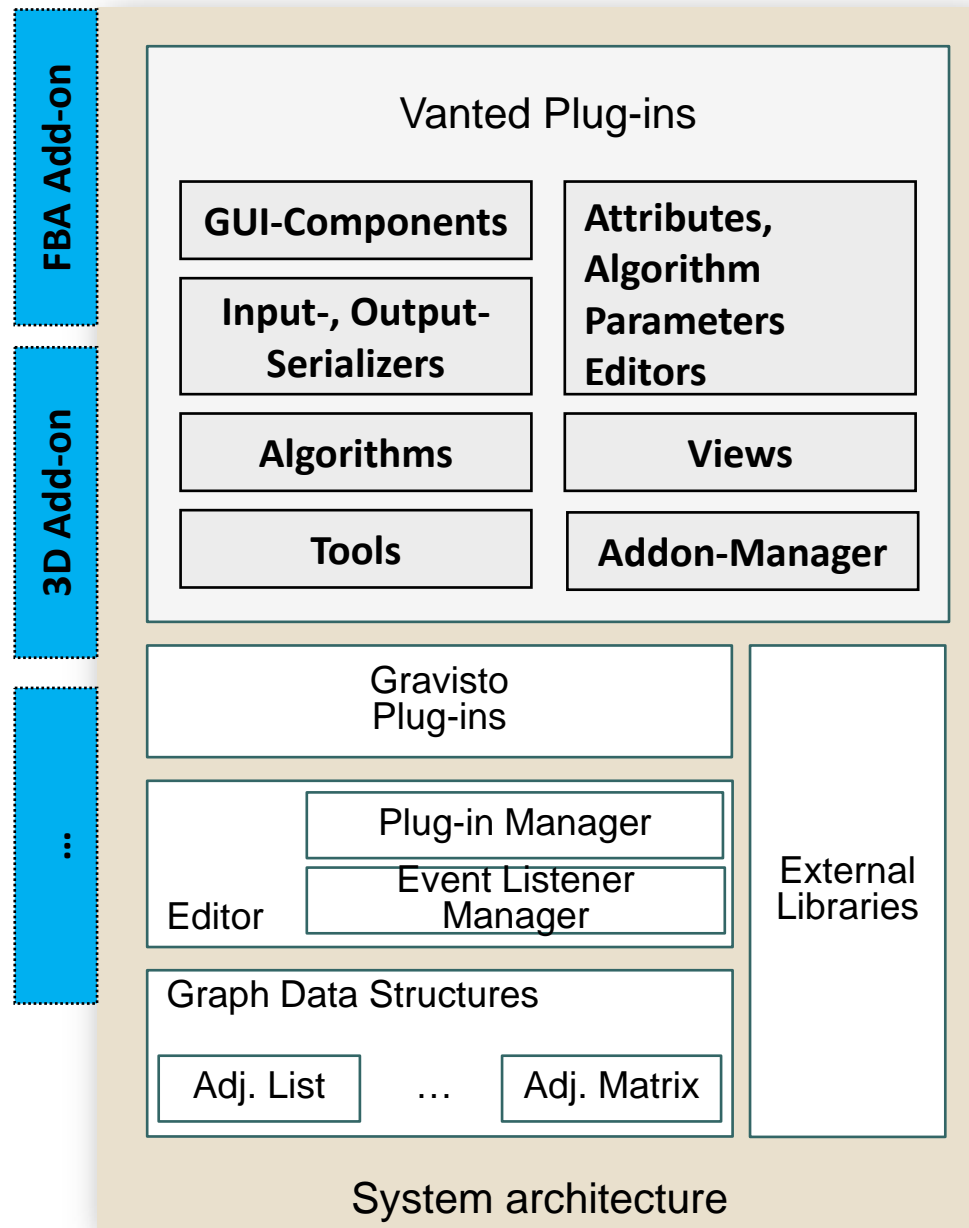


Applications: Maps for Other Groups



Implementation

- ▶ Add-on to Vanted
- ▶ Vanted
 - ▶ Based on extensible, plugin-based graph visualization toolkit Gravisto (Passau University and IPK)
 - ▶ MVC pattern
 - ▶ Event management (observer design pattern)
 - ▶ Java application
 - ▶ External plug-ins ('Add-ons')
 - ▶ www.vanted.org



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

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

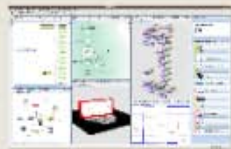
FBA-SimVis is a VANTED Add-on for the constraint-based analysis of metabolic models with special focus on the dynamic and visual exploration of metabolic flux data resulting from model analysis.



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.

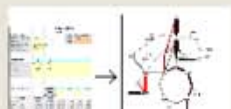
SBGN (Systems Biology Graphical Notation) is an emerging standard for graphical representations of biochemical and cellular processes studied in systems biology.



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
 - ▶ And more
-
- ▶ www.vanted.org (Vanted 2.0)
 - ▶ Open source (GPL)

Acknowledgements

- ▶ Tobias Czauderna
- ▶ Astrid Junker
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- ▶ Eva Grafahrend-Belau
- ▶ Hendrik Rohn
- ▶ Matthias Klapperstück
- ▶ Hendrik Mehlhorn
- ▶ Christian Klukas
- ▶ Kim Marriott (Monash Univ Melbourne)
- ▶ Michael Wybrow (Monash Univ Melbourne)
- ▶ Tim Dwyer (Microsoft)
- ▶ libSBGN community
- ▶ SBGN community

SBGN-ED

www.sbgn-ed.org