

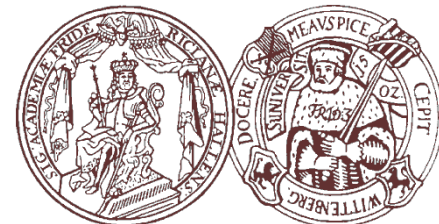
# SBGN-ED – working with the Systems Biology Graphical Notation

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# Overview

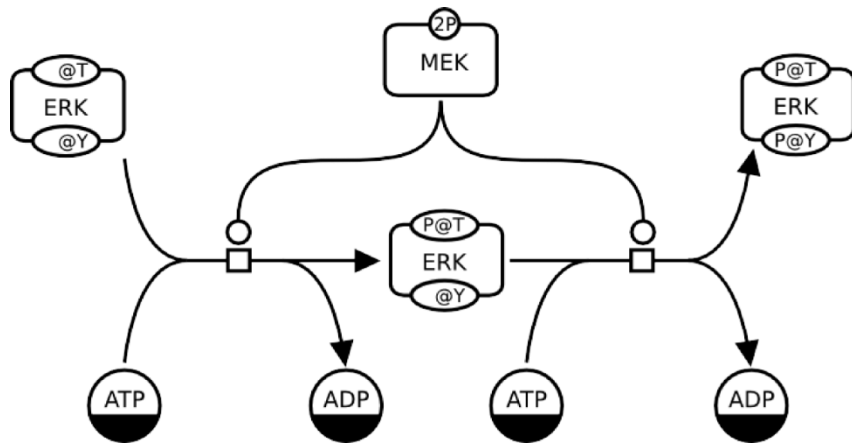
- ▶ SBGN
- ▶ SBGN-ED and VANTED
- ▶ Working with SBGN-ED
  - ▶ Installation
  - ▶ Editing
  - ▶ Validation
  - ▶ Import / Export
  - ▶ Translation
  - ▶ Additional features from VANTED
- ▶ Outlook
- ▶ Hands on

# What is SBGN

- ▶ Visualisation of biological information
- ▶ A way to unambiguously describe biochemical and cellular events in graphs
- ▶ Can graphically represent quantitative models, biochemical pathways, at different levels of granularity
- ▶ Developed over six years by a growing community
- ▶ Limited amount of symbols (32) → Smooth learning curve
- ▶ Three languages
  - ▶ Process Descriptions → one state = one glyph
  - ▶ Entity Relationships → one entity = one glyph
  - ▶ Activity Flow → conceptual level

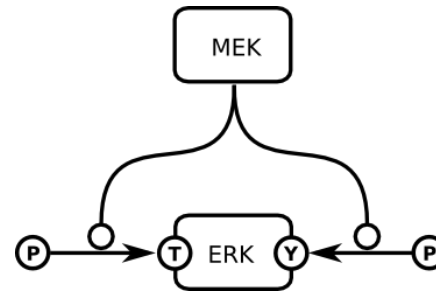
# Graph Trinity: Three Languages in One

## Process Description maps



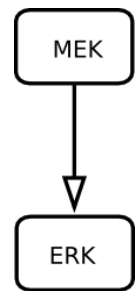
- ▶ Unambiguous
- ▶ Mechanistic
- ▶ Sequential
- ▶ Combinatorial explosion

## Entity Relationships maps



- ▶ Unambiguous
- ▶ Mechanistic
- ▶ Non-Sequential

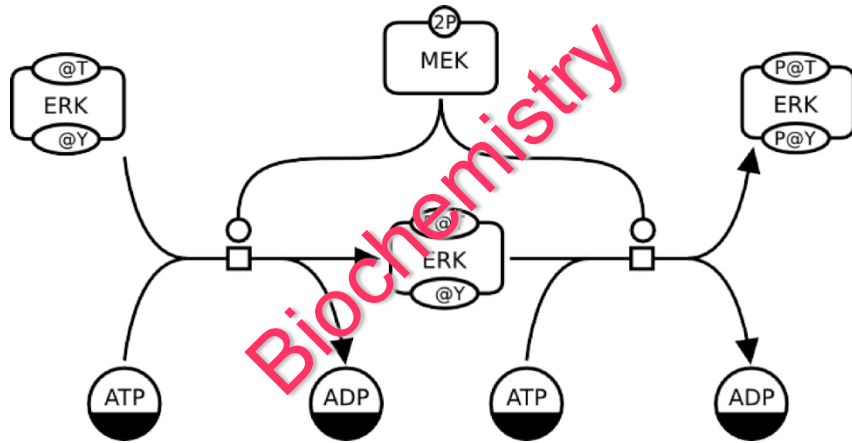
## Activity Flow maps



- ▶ Ambiguous
- ▶ Conceptual
- ▶ Sequential

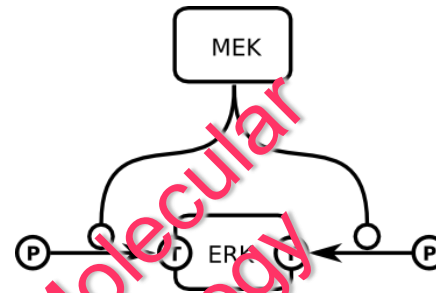
# Graph Trinity: Three Languages in One

## Process Description maps



- ▶ Unambiguous
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## Entity Relationships maps



- ▶ Unambiguous
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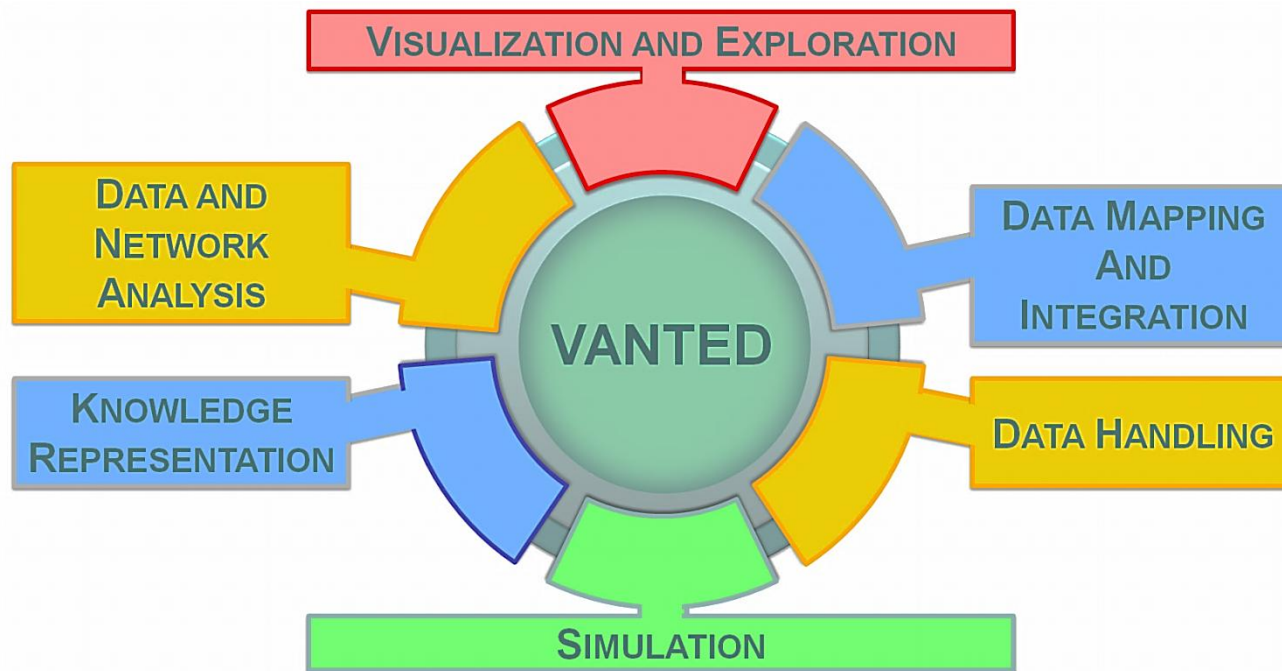
## Activity Flow maps



- ▶ Ambiguous
- ▶ Conceptual
- ▶ Sequential

# VANTED and SBGN-ED

- ▶ SBGN-ED is an add-on (extension) of VANTED
- ▶ VANTED framework
  - ▶ Integration, analysis and visual exploration of experimental data in the context of biological networks
  - ▶ Main functions



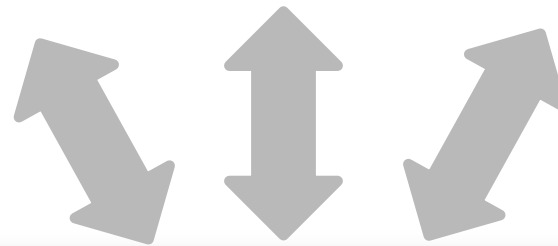
- ▶ [www.vanted.org](http://www.vanted.org)
- ▶ Open source (sourceforge)

# VANTED and SBGN-ED

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

**Exploring**  
**Navigating**

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



GML  
GraphML  
SBGN-ML



**Import**

**SBGN-ED**

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



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

**Export**

# Installation

## 1. Install VANTED

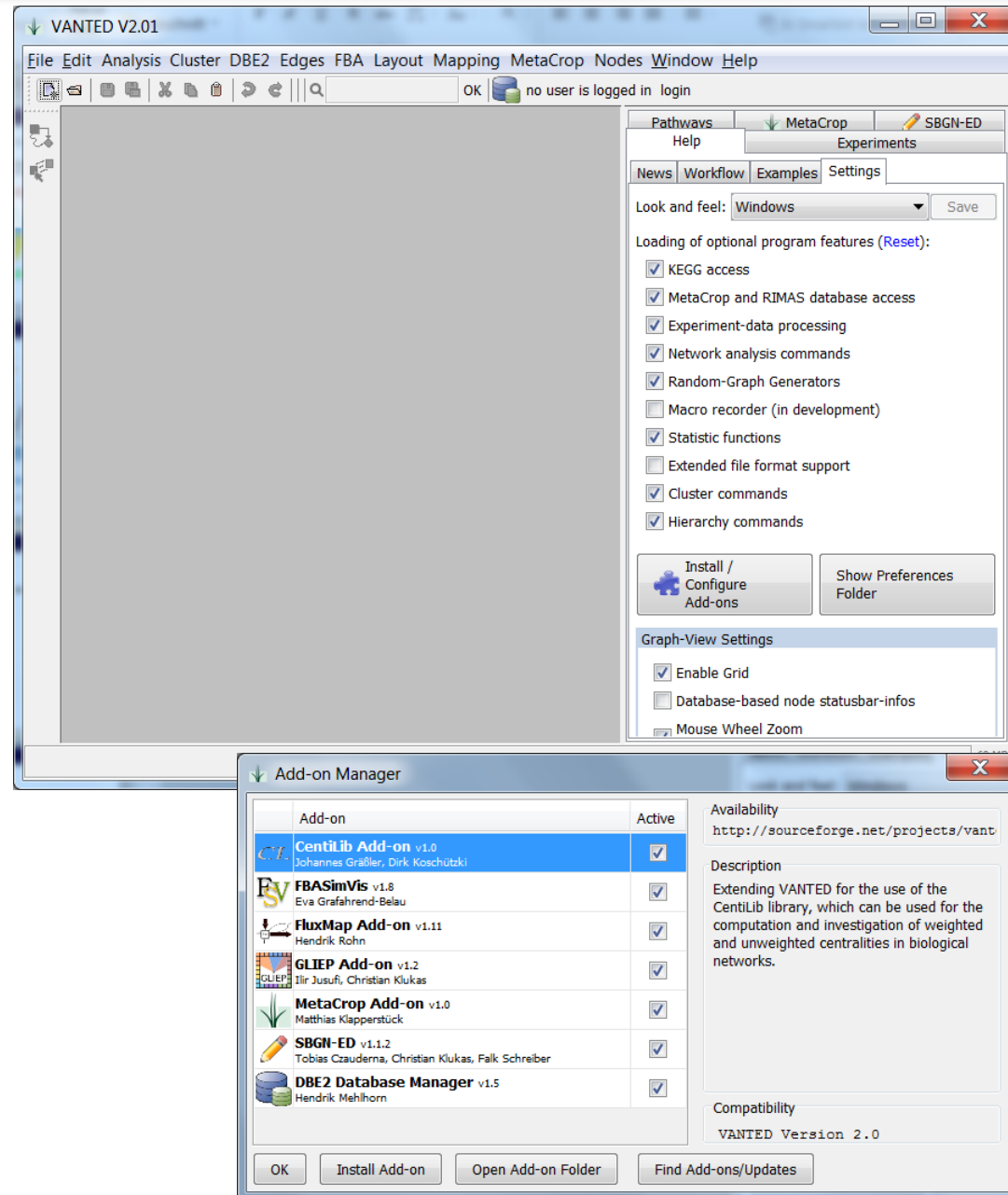
1. [www.vanted.org](http://www.vanted.org)
2. Webstart version or stand alone version (download)

## 2. Download SBGN-ED

1. [www.sbgn-ed.org](http://www.sbgn-ed.org)
2. Put it into arbitrary directory

## 3. Help (tab) → Settings (subtab) → Install / Configure Add-ons

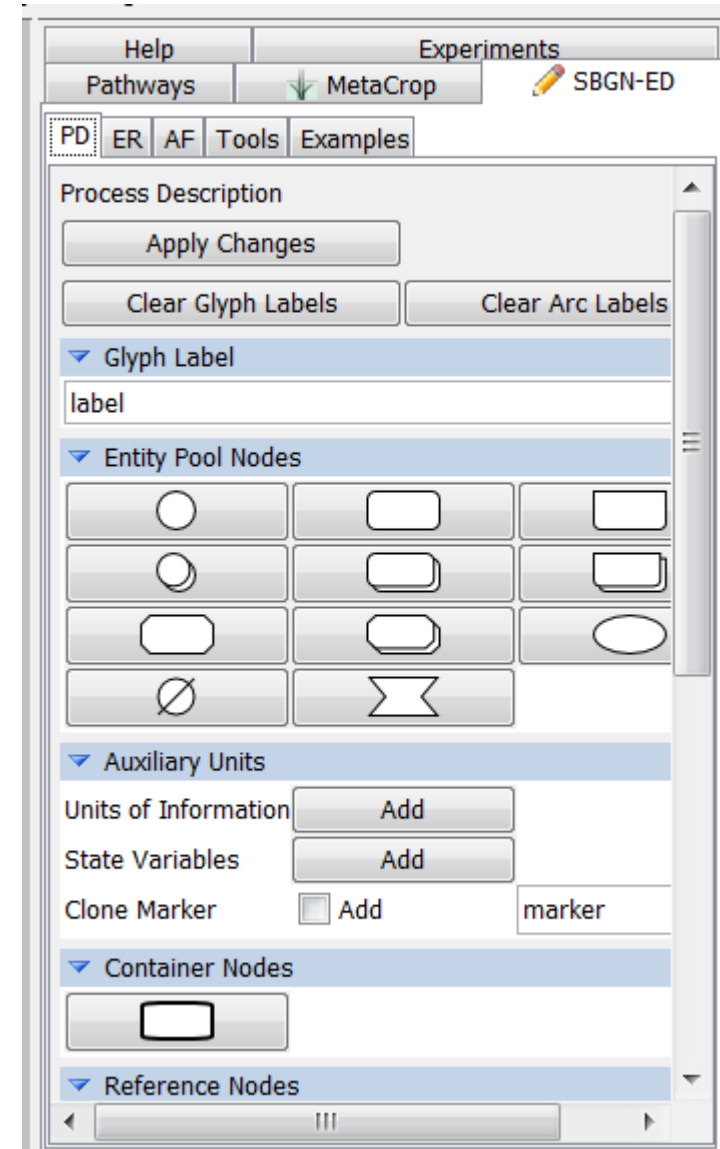
1. Install from directory





# SBGN-ED Tabs

- ▶ Three languages
  - ▶ Process Description (PD)
  - ▶ Entity Relationship (ER)
  - ▶ Activity Flow (AF)
- ▶ Tools
  - ▶ Validate
  - ▶ Translate
- ▶ Examples
- ▶ Other functionalities such as Import, Export, Layout, Data Mapping, Network Analysis etc are part of the underlying VANTED system and part of VANTEDs menus



# Import

- ▶ Files
  - ▶ File (menu) → Open
    - ▶ File formats: GML, GraphML, SBGN-ML, KGML
- ▶ Pathway database (Pathway tab)
  - ▶ MetaCrop
  - ▶ Choose pathway
- ▶ Examples
  - ▶ SBGN-ED → Examples (tab)
  - ▶ Choose example

# 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**, **ChAT**, **vAChT**, **choline**, **ACh**, **synaptic vesicle**, **SNARE**, and **synaptic cleft**. Arcs show the synthesis and release of ACh.

**muscle cytosol:** Contains nodes for **nAChR** (closed/open), **Ca2+**, **ER**, **ATP**, **ADP**, **Pi**, **actin**, **myosin**, and **muscle contraction**. Arcs show the activation of nAChR, calcium release from the ER, and the resulting muscle contraction cycle.

**Editing Tools (Right Panel):**

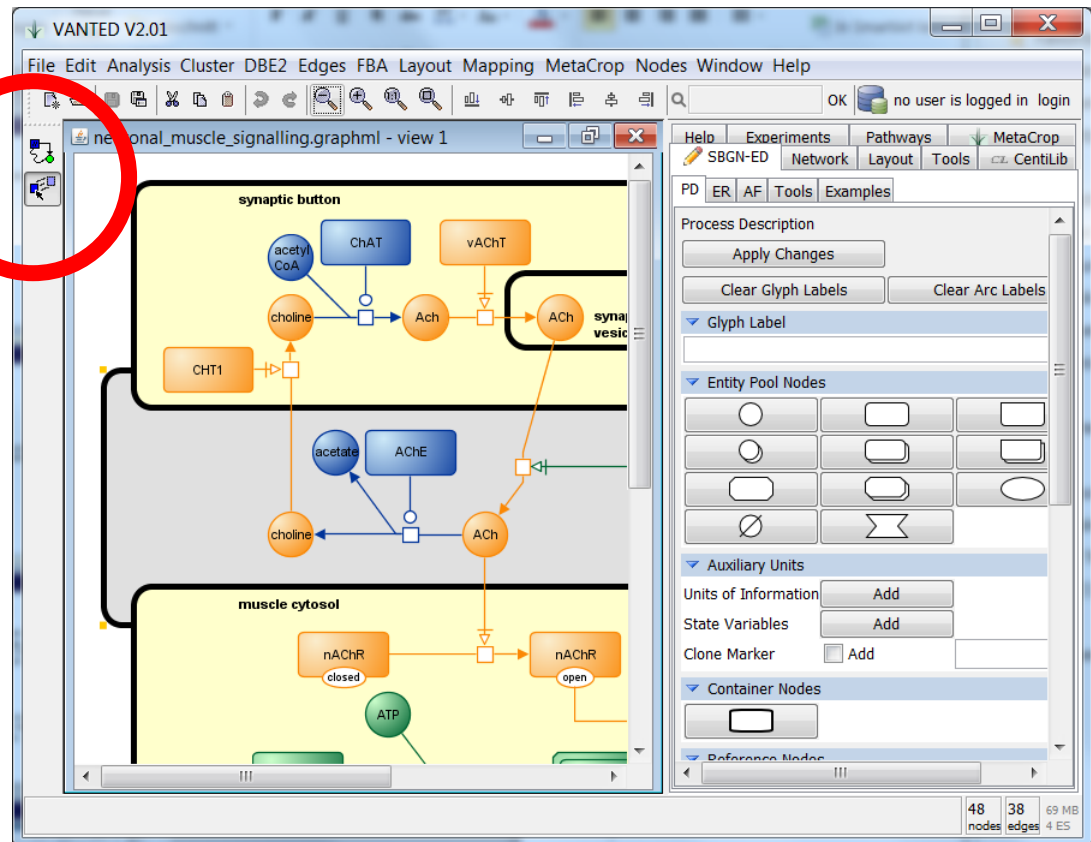
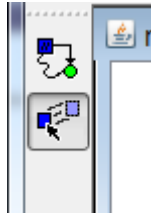
- Entity Relationship:** Apply Changes, Clear Glyph Labels, Clear Arc Labels.
- Entity Pool Nodes:** Select from various shapes (circle, rectangle, oval, etc.).
- Auxiliary Units:** Add Units of Information, State Variables, Clone Marker.
- Container Nodes:** Select from various container shapes.
- Reference Nodes:** Select from various reference shapes.
- Process Nodes:** Select from various process shapes (square, circle, hexagon, etc.).
- Connecting Arcs:** Select from various arc types (straight, curved, T-junction, etc.).
- Logical Operators:** AND, OR, NOT.
- Statements:** Select from various statement shapes.
- Influences:** Select from various influence shapes.
- Reference Nodes:** Select from various reference shapes.

**Bottom Status Bar:**

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

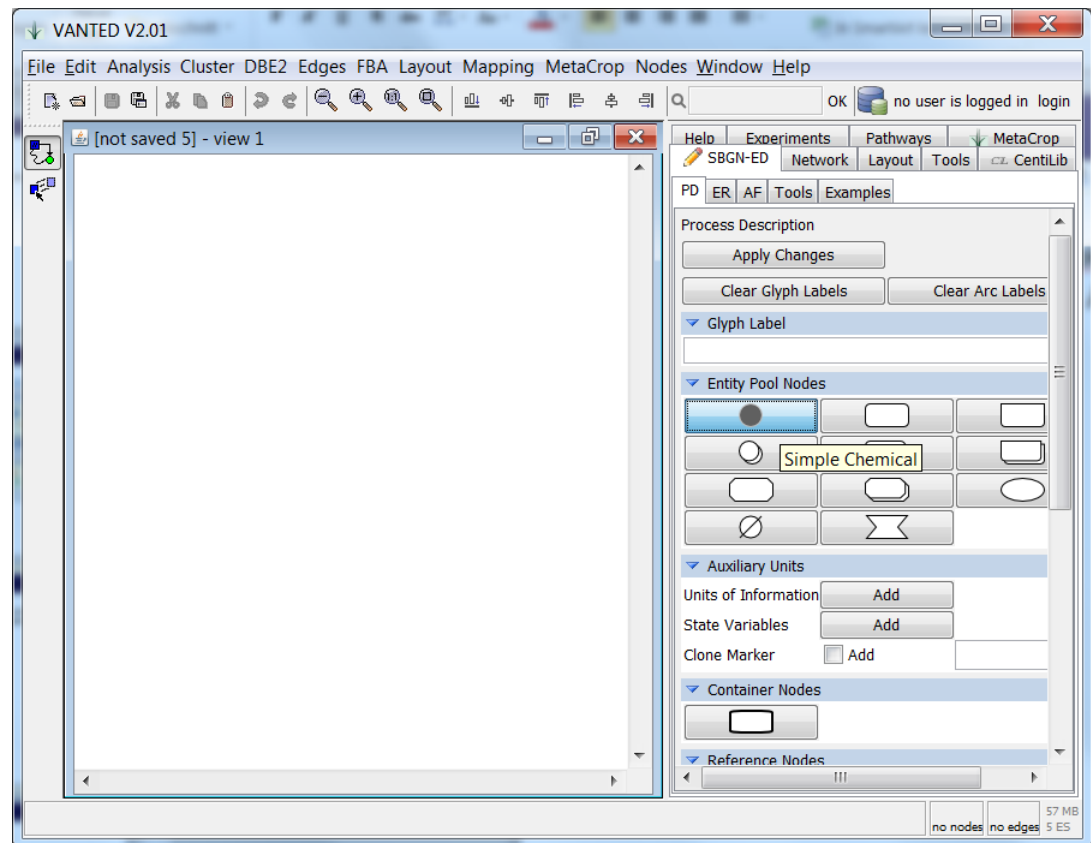
# Editing or Creating Maps

- ▶ PD maps (ER and AF works similarly)
- ▶ Two modes
  - ▶ Create
  - ▶ Move/edit
- ▶ Always check in which mode you are



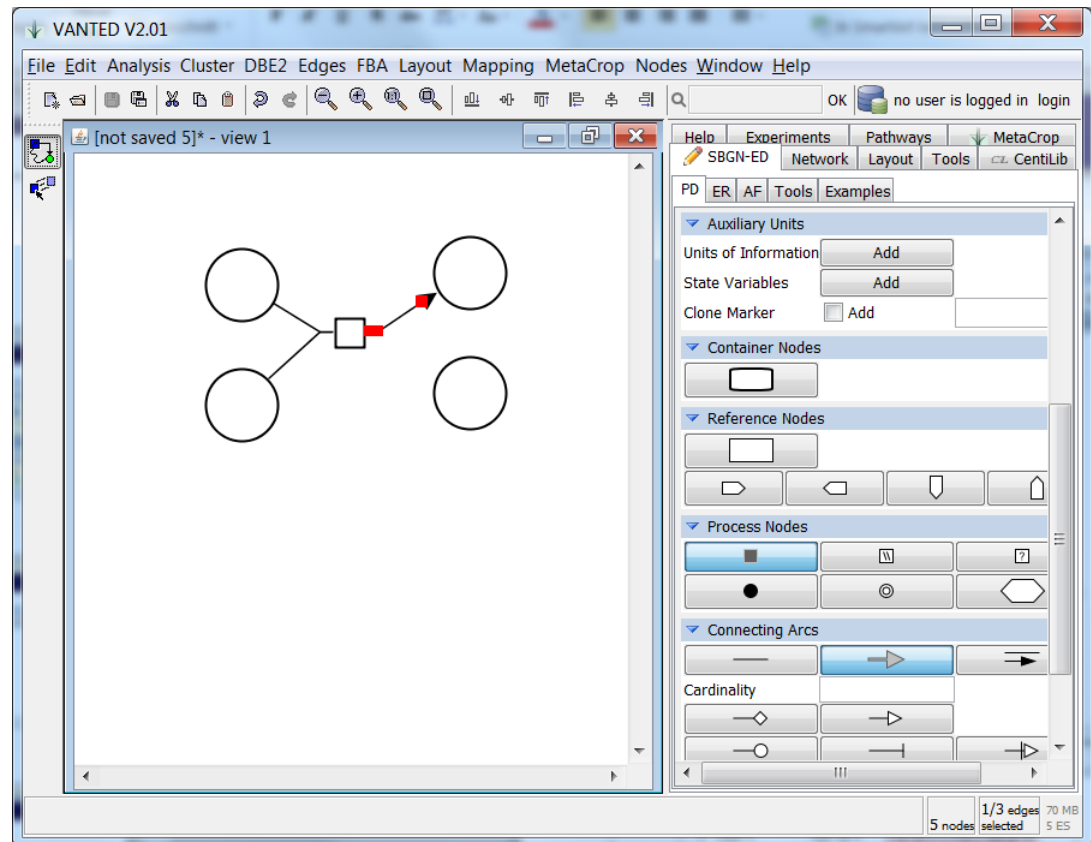
# Editing or Creating Maps

1. Select glyph
2. Click in canvas



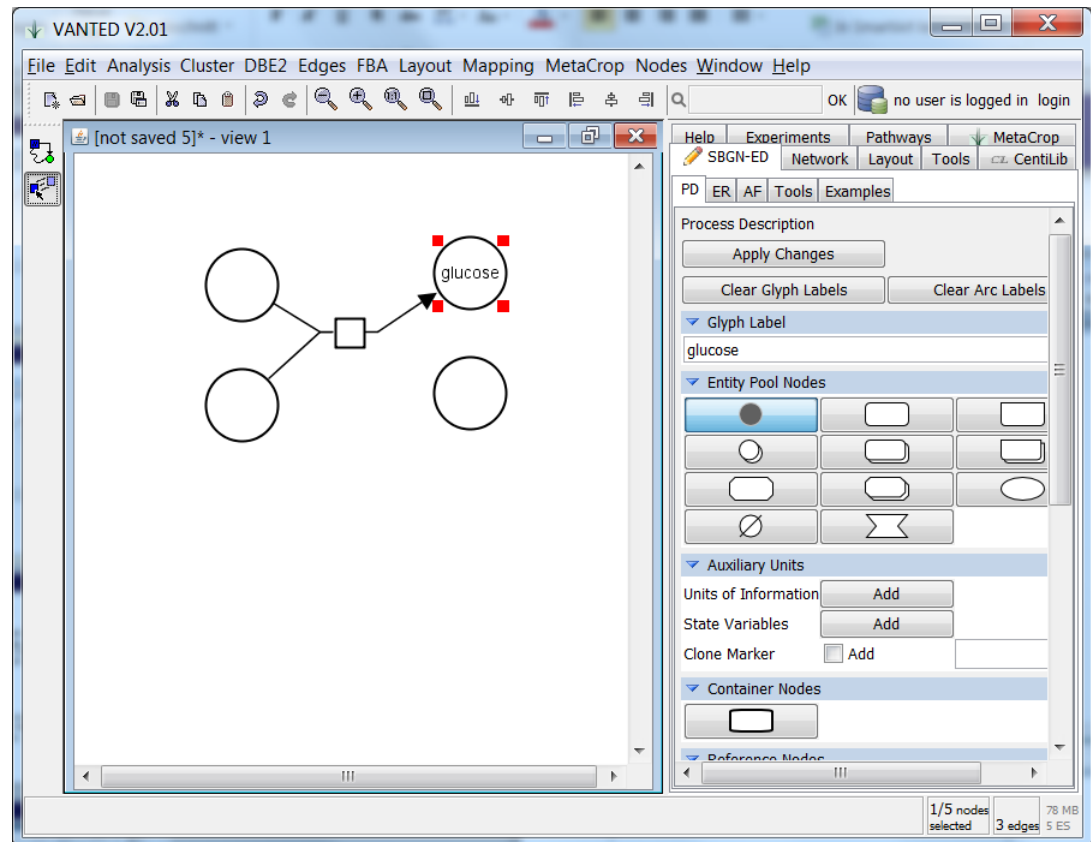
# Editing or Creating Maps

- ▶ Step by step drawing of the map
- ▶ Information can either be added immediately or changed later



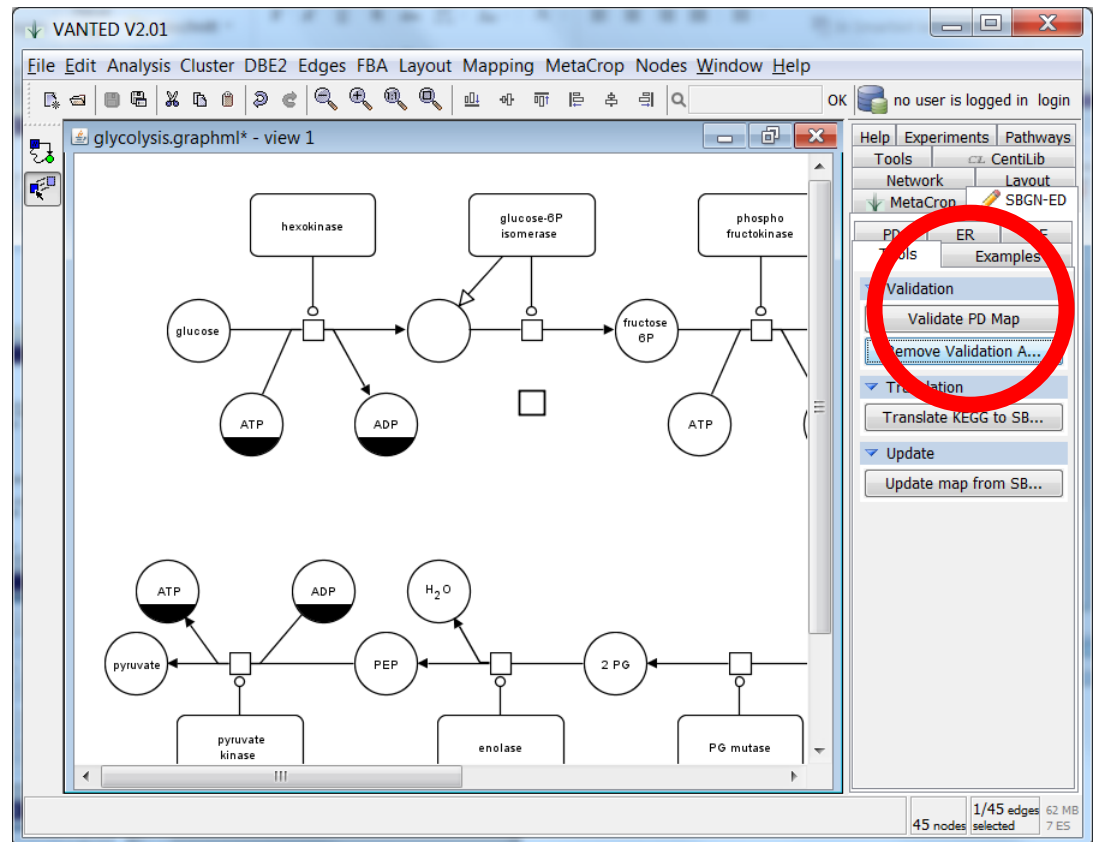
# Editing or Creating Maps

- ▶ Change elements later
  1. Change modulus
  2. Add/change information within tab
  3. Click apply changes



# Validation

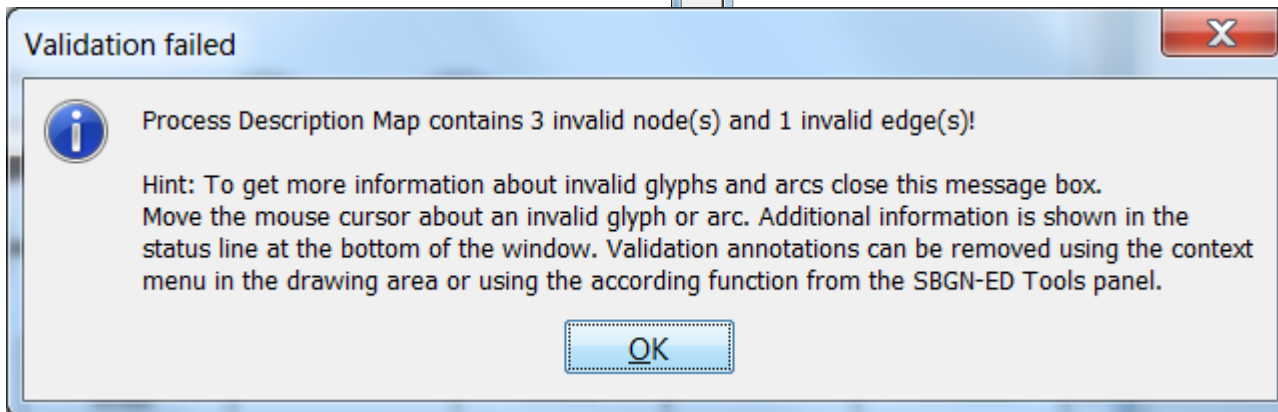
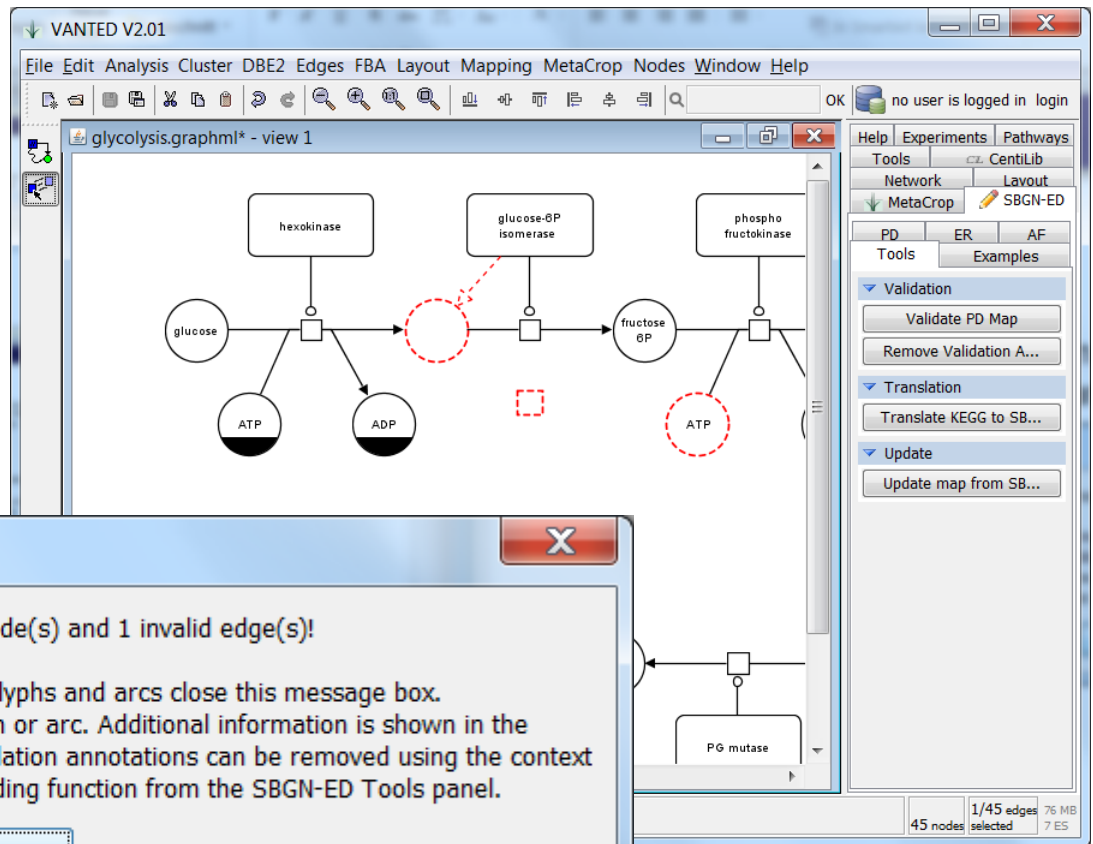
- ▶ In this example
  - ▶ Wrong edge
  - ▶ Missing clone marker
  - ▶ Unconnected node
  - ▶ Missing label





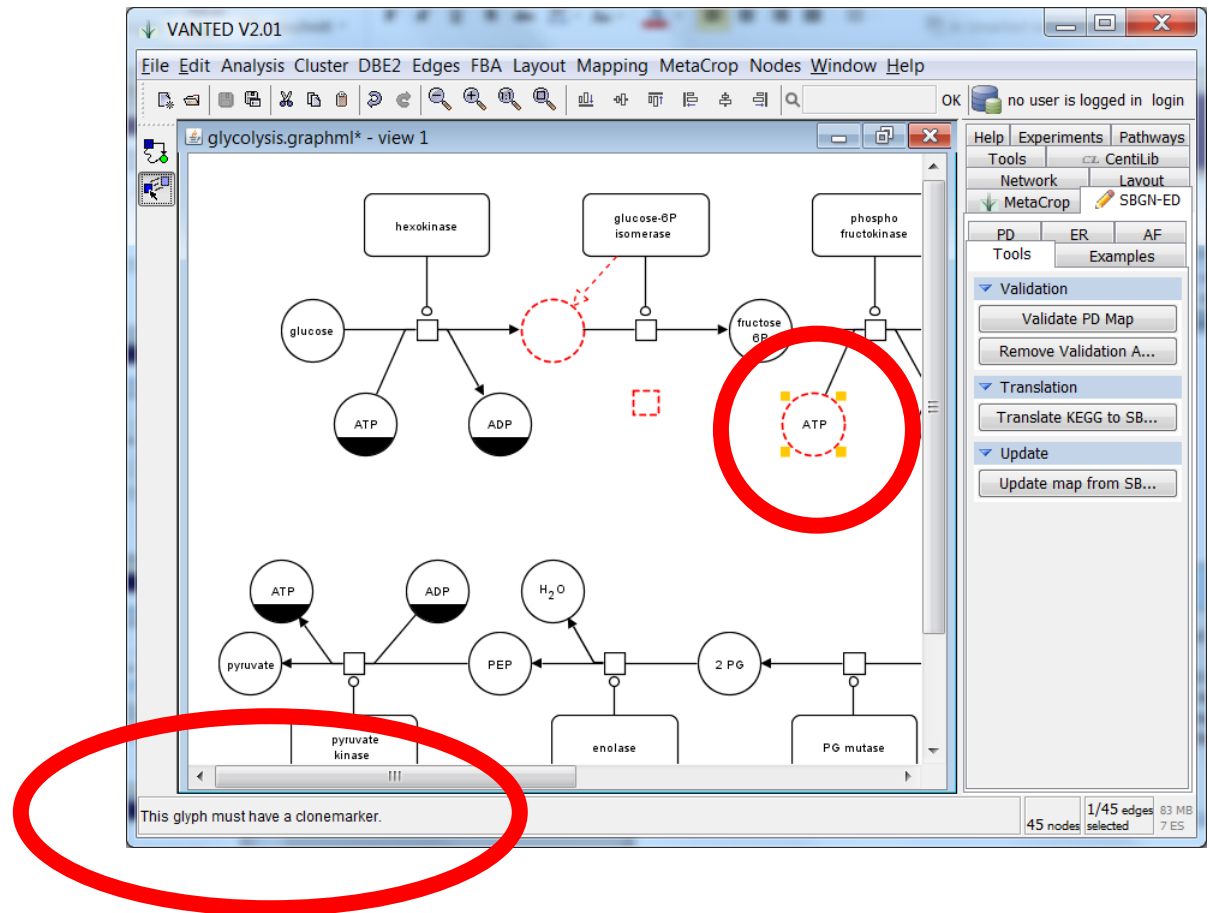
# Validation

- ▶ Click Validate PD Map
  - ▶ Map type is automatically recognised



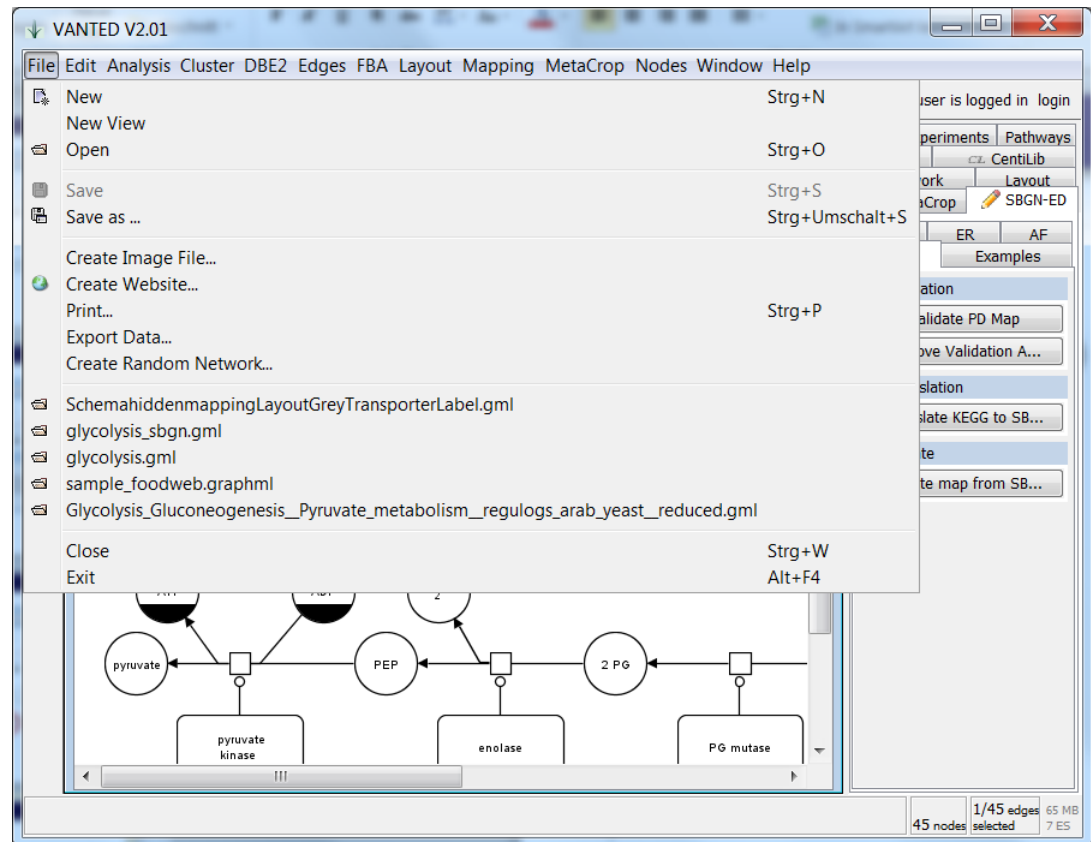
# Validation

- Additional information



# Export

- ▶ File →
  - ▶ Save (as ...)
    - ▶ GML
    - ▶ GraphML
    - ▶ SBGN-ML
  - ▶ Create Image File
    - ▶ JPG
    - ▶ PNG
    - ▶ SVG
    - ▶ PDF
    - ▶ PPT
  - ▶ Create Website ...
    - ▶ HTML



# Website Export

- ▶ Steps with several options for website design
- ▶ Clickable overview and clickable SBGN maps

Step 1/4: Titles

Open a set of networks and choose this command to create a simple website, containing links to graphical representations of the currently opened network files.  
Use the menu command Edit/Add Link... to create links assigned to network nodes, which point to other networks or to websites. This way it is possible to create and publish your own library of interlinked network files, possibly with references to other website resources.

Please specify the title for the whole website and for each loaded network:

Hint: If the network titles contains a dot (.) character, the networks will be put into categories.  
For example the title A.B would place the network into the group 'A' shown with network name 'B'.

Website-Title	<input type="text" value="My Pathway Website"/>
Graph [not saved 5]	<input type="text" value="[not saved 5]"/>
Graph glycolysis.graphml	<input type="text" value="glycolysis"/>
Graph neuronal_muscle_signalling.graphml	<input type="text" value="neuronal_muscle_signalling"/>

OK Cancel

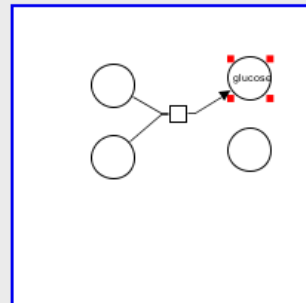
## My Pathway Website

Overview

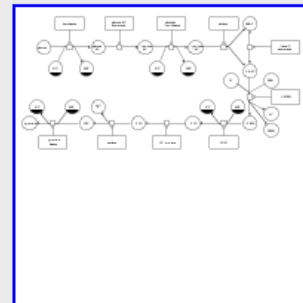
VANTED graph to website export. VANTED is available at <http://vanted.ipk-gatersleben.de>.

[not saved 5]  
glycolysis  
neuronal\_muscle\_signalling

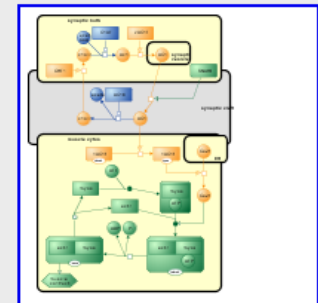
Feedback



[not saved 5]



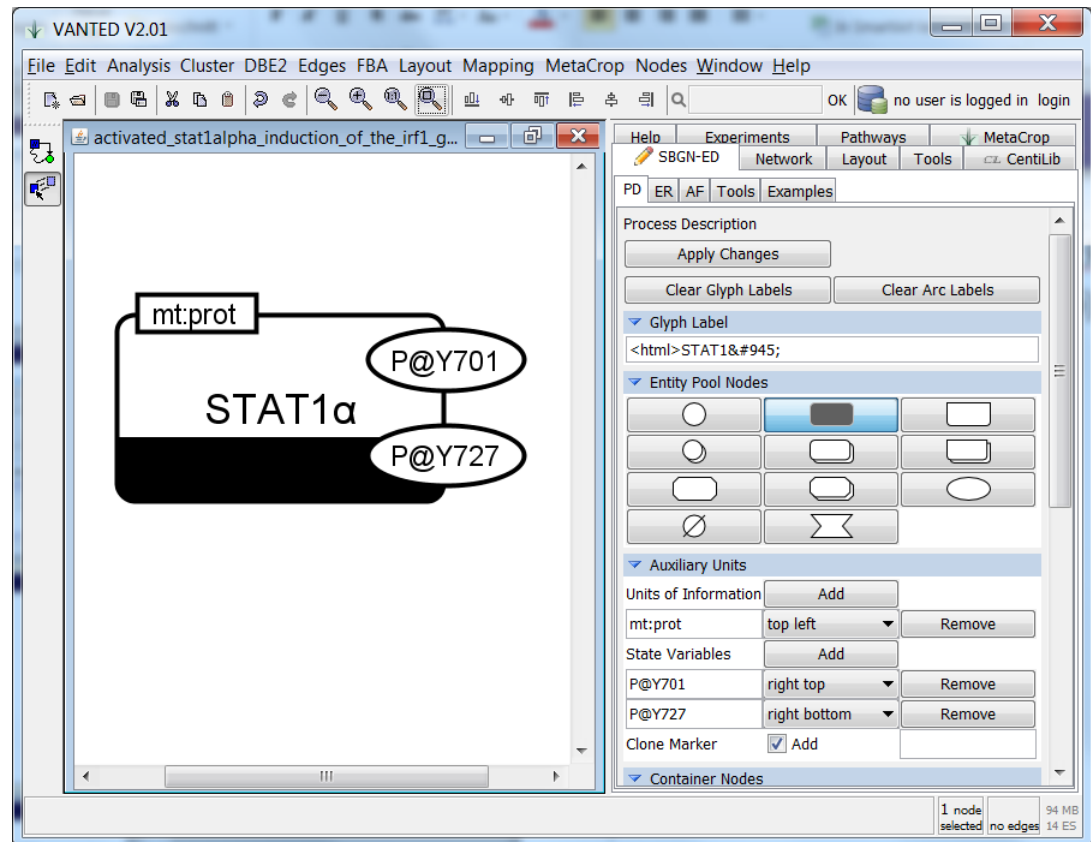
glycolysis



neuronal\_muscle\_signalling

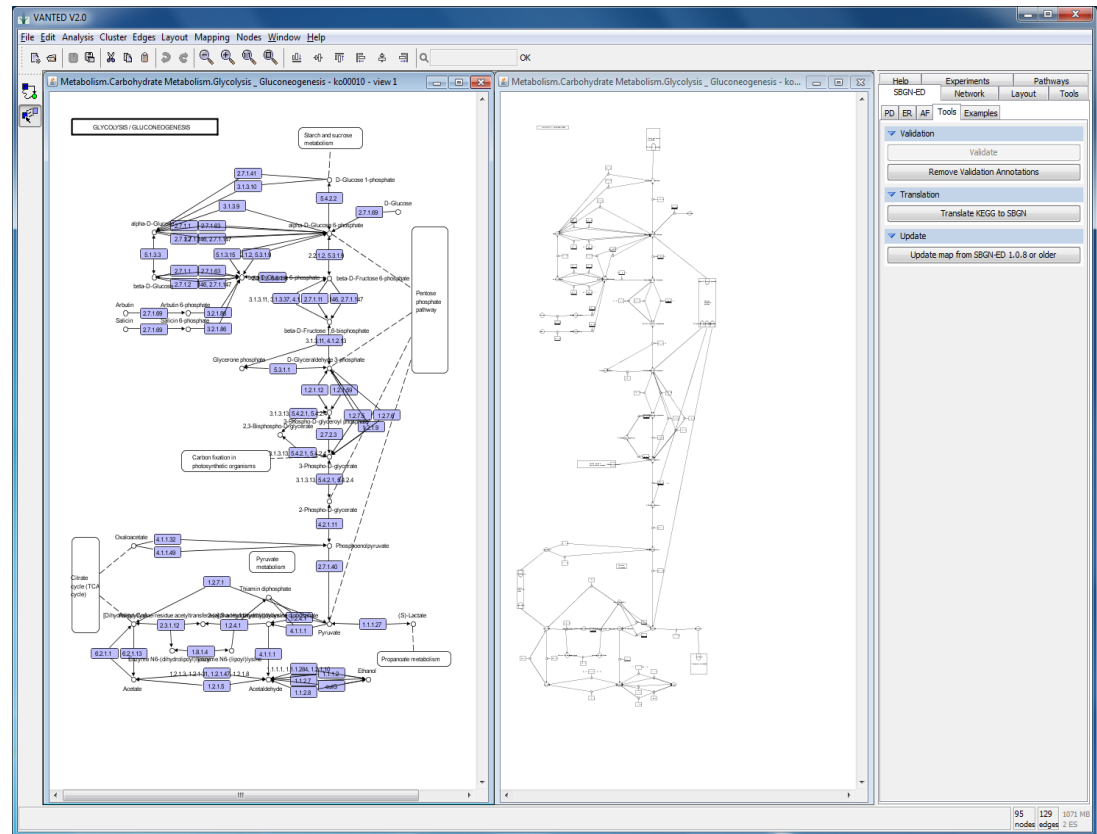
# More Complicated Glyphs

- ▶ With unit of information (mt:prot)
- ▶ With state variable (P@Y701)
- ▶ With Clone markers
- ▶ HTML tags for text
- ▶ And so on



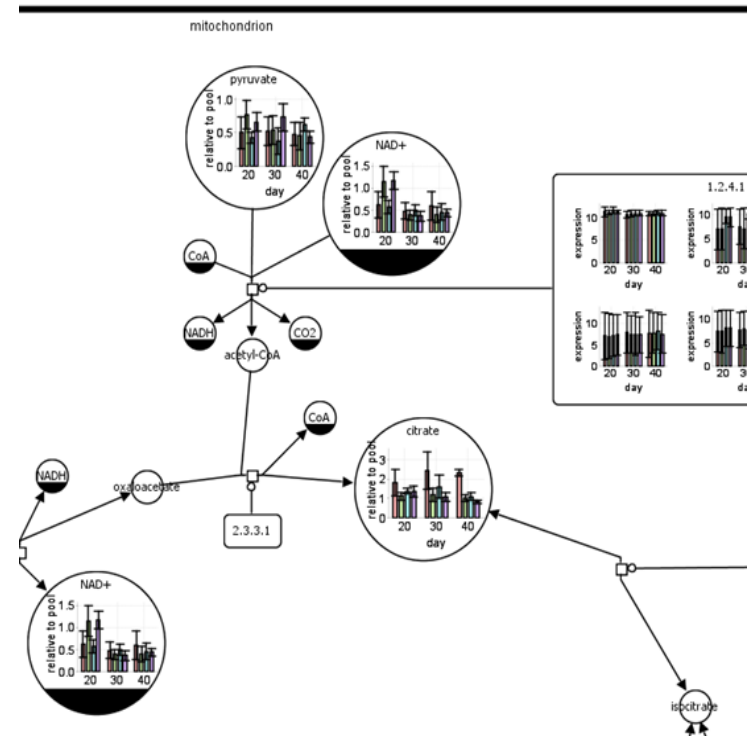
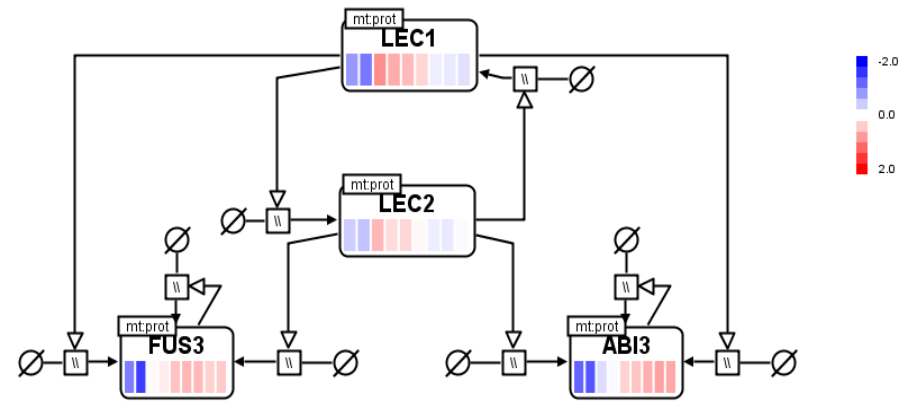
# Translating SBGN Maps from KEGG

- From KGML files due to KEGG restrictions



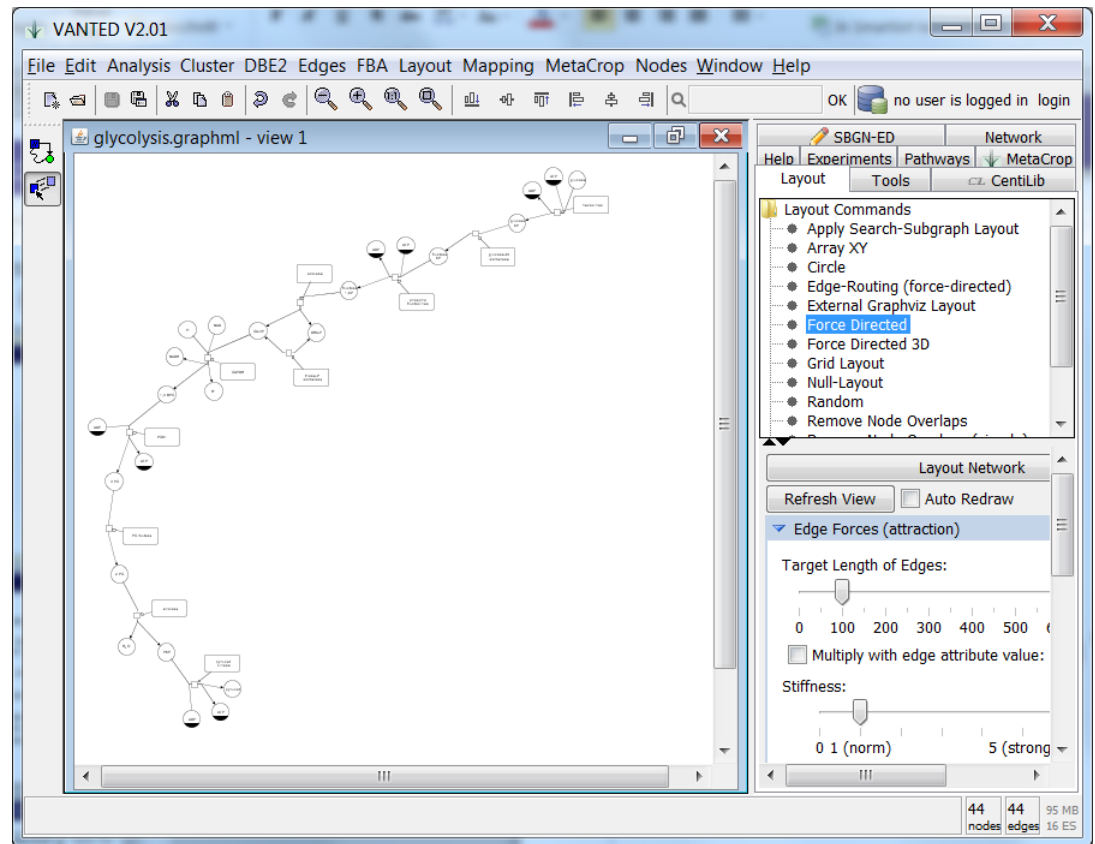
# Data Integrating and Analysing in SBGN Maps

- ▶ VANTED provides many methods for
  - ▶ Data mapping and integration
  - ▶ Data and network analysis
- ▶ Also available in SBGN-ED



# Layout

- ▶ VANTED provides many standard layout algorithm

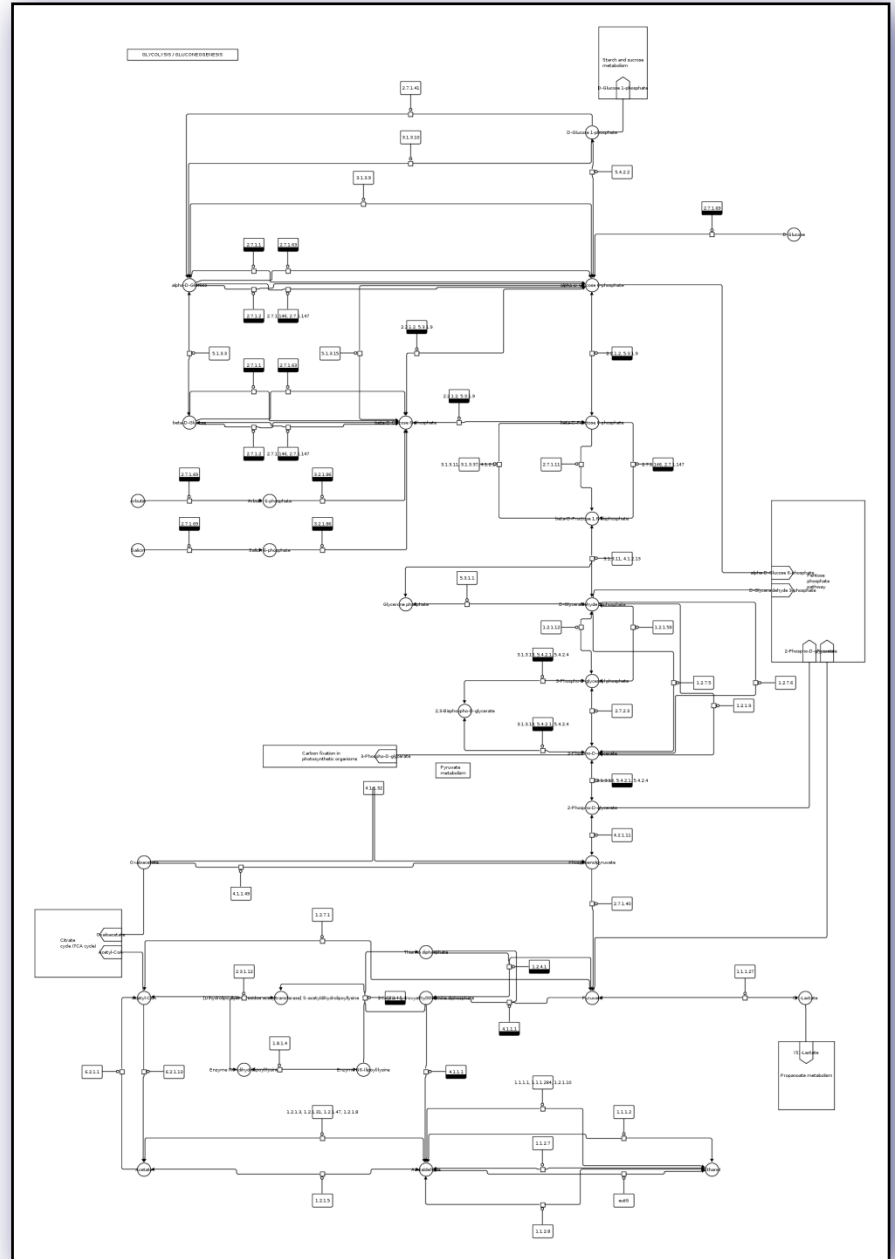
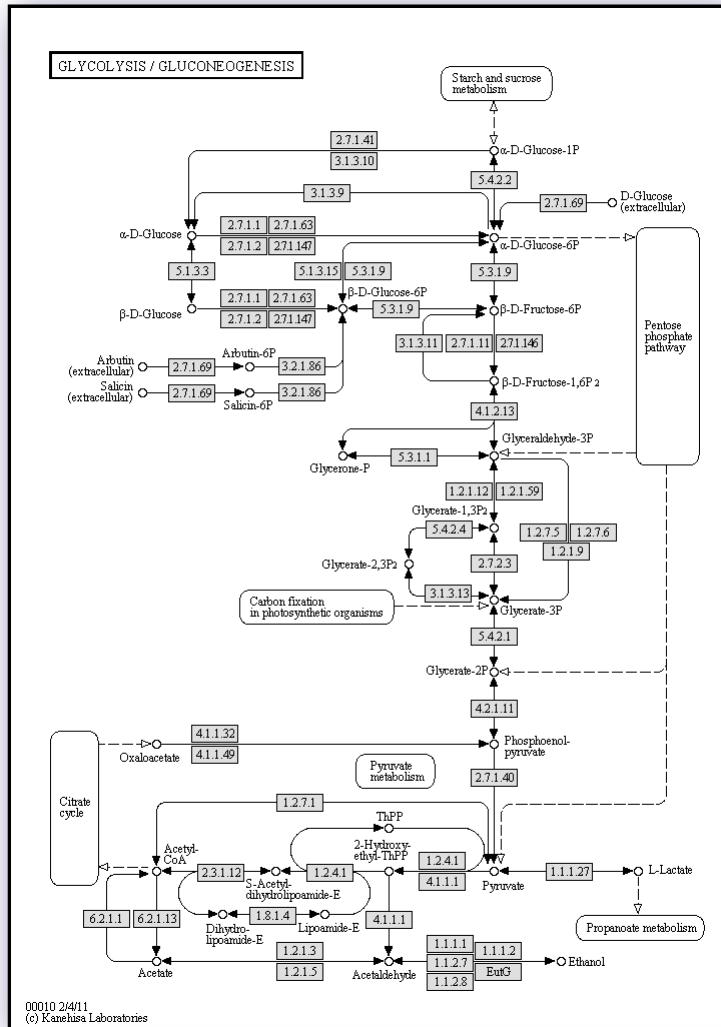




# Outlook

- ▶ Next version (under development)
  - ▶ More importers (in VANTED)
    - ▶ SBML (all up to L3V1) (JSBML)
    - ▶ BioPAX (L2,L3) (Paxtools V4)
  - ▶ More export possibilities (in VANTED) (SBML and BioPAX) planed, but needs validation!
  - ▶ Constraint-based automatic layout
  - ▶ More interaction possibilities
  - ▶ Map translations

## Outlook Screenshots



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