

Vanted & Automatic Layout of SBGN

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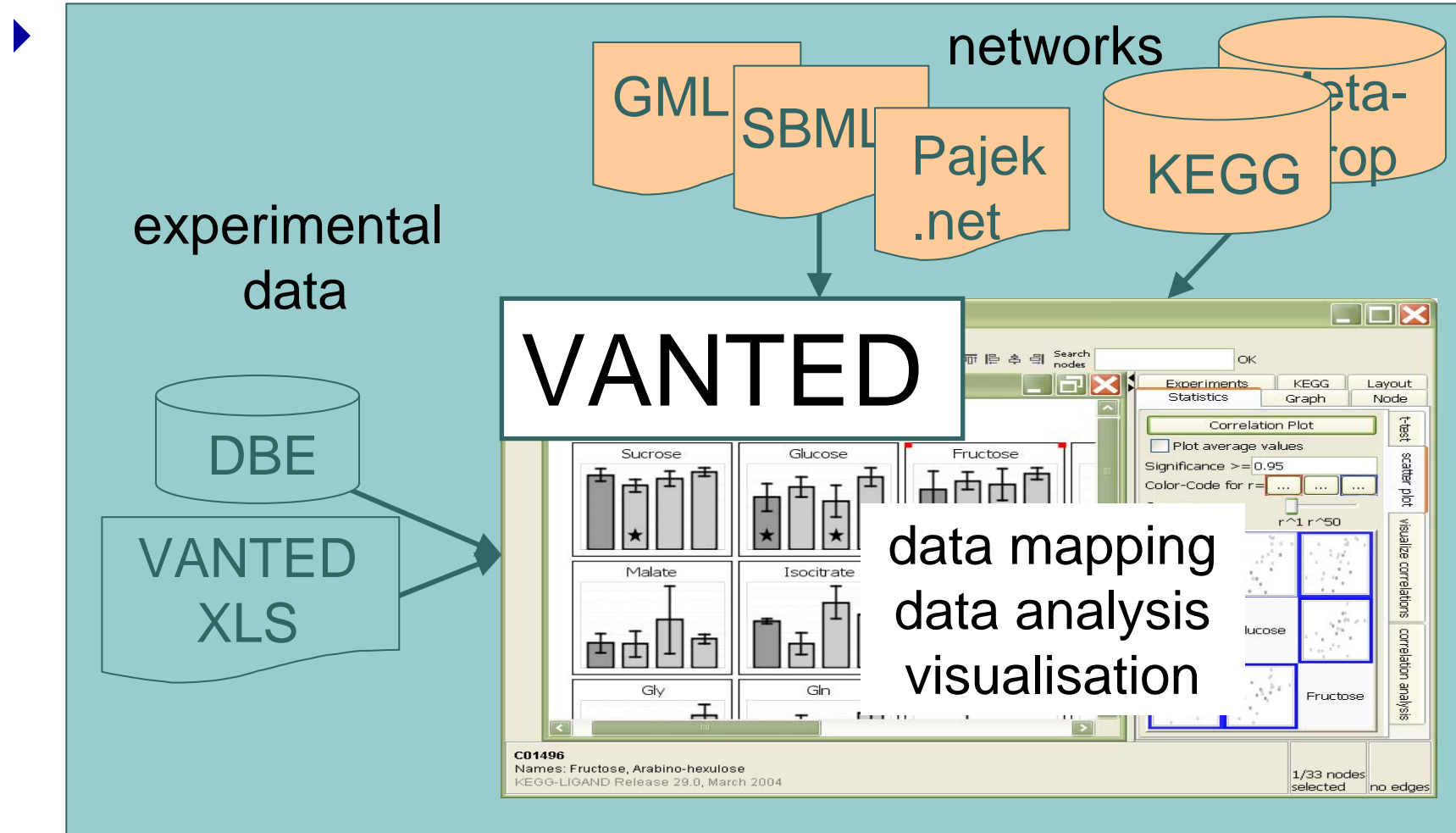


IPK Gatersleben



Martin-Luther University
Halle-Wittenberg

- ▶ Joint work with *Christian Klukas* (IPK)



- ▶ SBGN support

- ▶ (tool demo – some screenshots on following slide)
- ▶ Full SBGN support (editor)
- ▶ Map and analyse –omics data also in SBGN context
- ▶ Export
 - ▶ Different graph file formats
 - ▶ Images (JPG, PNG/HTML clickable maps, PDF, SVG)

VANTED V1.54

File Edit Analysis Edges Elements Hierarchy Layout Mapping Nodes Window Help

SBGN. Neuro-muscular junction. graphml* - view 1

Help Experiments Pathways Network Layout Tools

KEGG MetaCrop pathways SBGN Template

▼ Auxiliary Units (new node setting)

Label	LABEL	
State variable:	value	
Unit of information:	pre:label	
Add clone marker:	<input type="checkbox"/> Add (text:)	marker

▼ Container Nodes (add node/set style)

Complex, Compartment, Submap

▼ Entity Pool Nodes (add node/set style)

Unspecified entity

Tag

Simple chemical, Source/sink

Macromolecule, Genetic entity

Multimer

Observable, Perturbation

▼ Process Nodes (add node/set style)

Transition

Association, Dissociation

Omitted, Uncertain process

synaptic button

ChAT vChT

cholin

CHT1

synaptic vesicle

ACh SNARE

acetyl CoA AChE

cholin ACh

synaptic cleft

nAChR (closed) nAChR (open)

ER Ca2+

48 nodes 38 edges

The screenshot displays the VANTED V1.54 software interface. The main window shows a metabolic pathway diagram titled "SBGN, Glycolysis.graphml* - view 1". The pathway consists of several steps:

- Glucose is converted to glucose 6P by the enzyme hexokinase, consuming ATP and producing ADP.
- Glucose 6P is converted to fructose 6P by the enzyme glucose-6P isomerase.
- Fructose 6P is converted to fructose 1,6P by the enzyme phospho fructokinase, consuming ATP and producing ADP.
- Fructose 1,6P is converted to 2 PG by the enzyme enolase, producing H₂O.
- 2 PG is converted to PEP by the enzyme pyruvate kinase, producing ATP and consuming ADP.
- PEP is converted to pyruvate.

Each metabolite node (glucose, glucose 6P, fructose 6P, fructose 1,6P, PEP, pyruvate) contains a small line graph showing data trends over time. The enzymes are represented by teal rectangular boxes.

A "Create Image File" dialog box is open in the foreground, prompting the user to "Select the command to be executed:" with the following options:

- Create JPEG image
- Create PNG / HTML
- Create PDF image
- Create SVG image

The right sidebar contains a "Help" menu and a "Load Dataset" section. The "Load Dataset" section shows the file "gerstenentwicklung.xls" loaded. Below this, there are buttons for "Close Tab", "Save Binary", and "Show Input-Form". A "Perform Data Mapping" button is also present. The "Specify Mapping-Data" section shows a list of "Time Points" (day 0, day 2, day 3, day 4, day 5) and "Plants/Genotypes" (Hordeum vulgare (wild type/Tagproben) id=1, Hordeum vulgare (wild type/Nachtproben) id=2).

The bottom right corner of the interface shows the statistics: 44 nodes and 44 edges.

Automatic Layout (of SBGN)

- ▶ Joint work with *Tim Dwyer* (Microsoft Research), *Kim Marriot* and *Michael Wybrow* (Monash University)
- ▶ Network layout algorithms = solve given constraints
 - ▶ Problem: speed
 - ▶ Solution: *Solvers* for restricted sets of constraints, e.g. circular layout, force directed layout, ...
 - ▶ Problem for SBGN: current methods not flexible enough (*wrong* sets of constraints)
- ▶ New method based on stress majorisation (see movie)
- ▶ Java library for SBGN