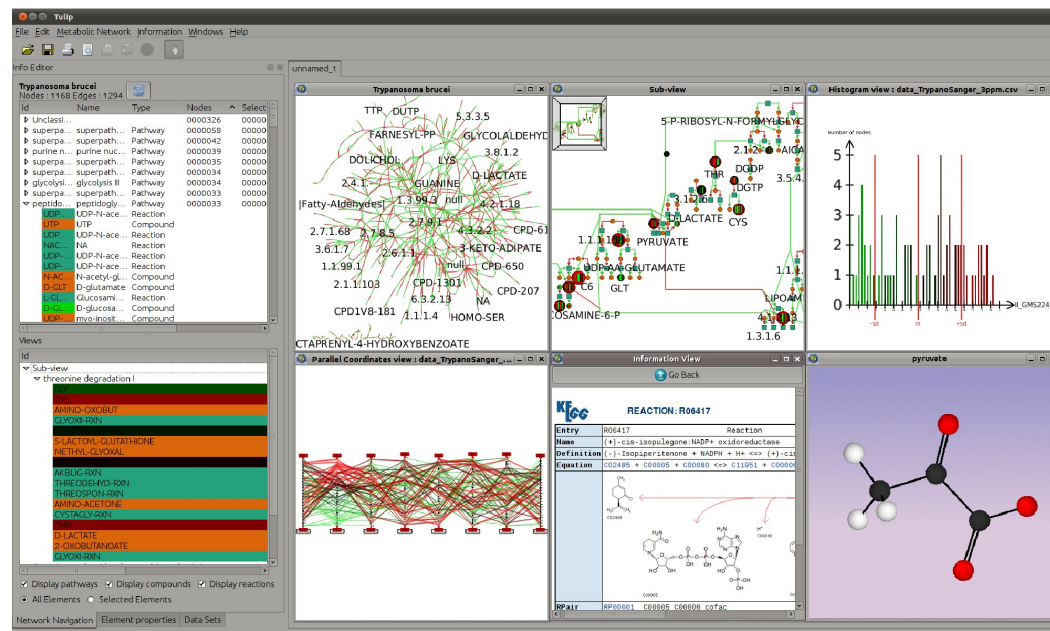


Systrip

A visual environment dedicated to metabolic network analysis

Jonathan Dubois, Romain Bourqui



Objectives

Give tools to help user during metabolic network analysis

- Visualization of metabolic networks and time-series data
- Network and data manipulation
- Combination of network and bioinformatics related algorithms

Existing software

- **Vanted** <http://vanted.ipk-gatersleben.de/>
- **Cytoscape** <http://www.cytoscape.org/>
- **PathwayExplorer**
<https://pathwayexplorer.genome.tugraz.at/>

Dealing with networks

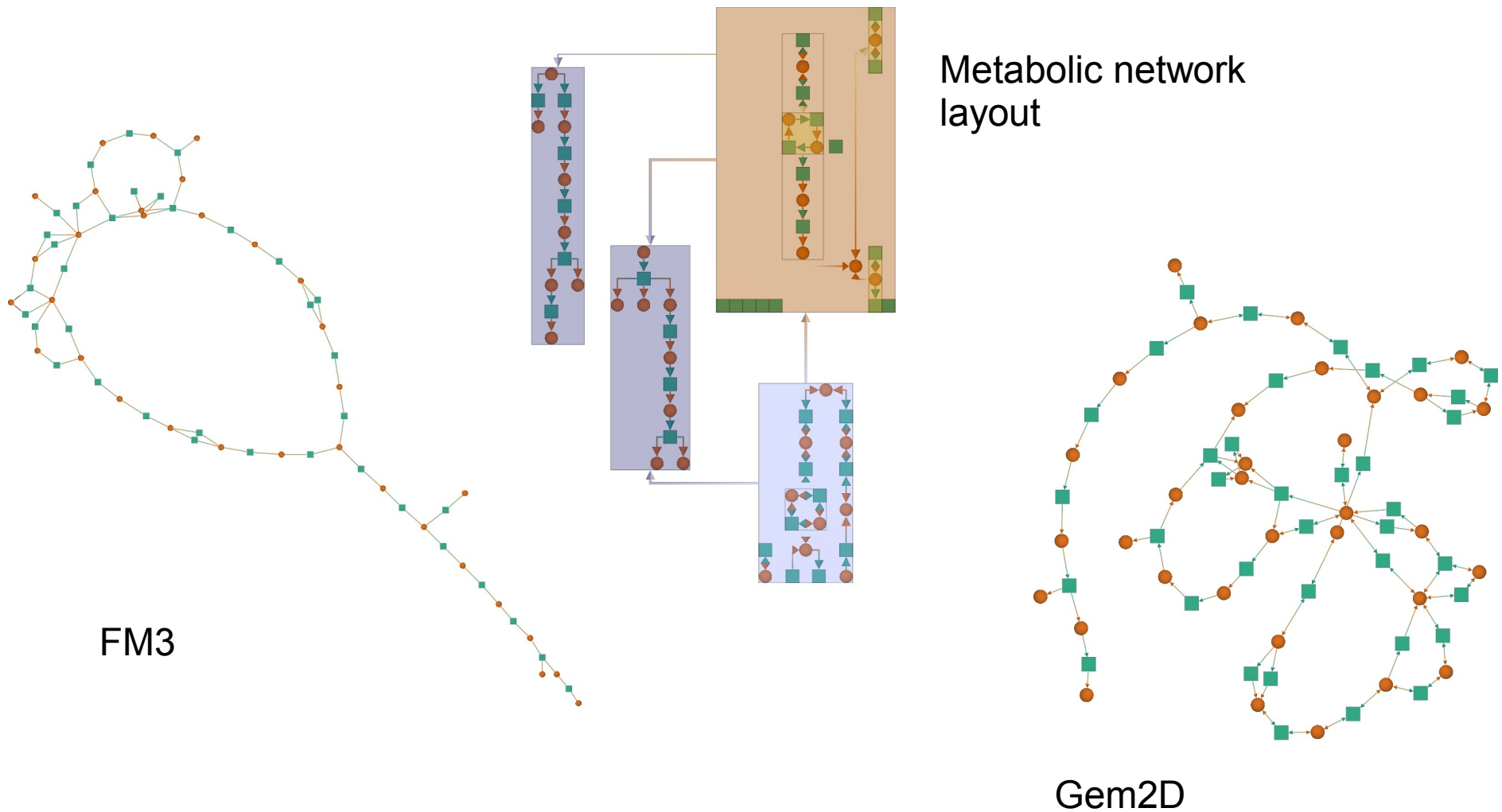
- Import a network from a SBML file
- Drawing the network
- Customize visual parameters
- Interact with the network
- Modify the network structure

Drawing networks

Can use both **Tulip** and **Systrip** drawing algorithms

- Biological convention preserving
- Force directed (2D and 3D)
- Hierarchical (or layered)
- Circular
- All the other Tulip drawing algorithms

Drawing networks (2)



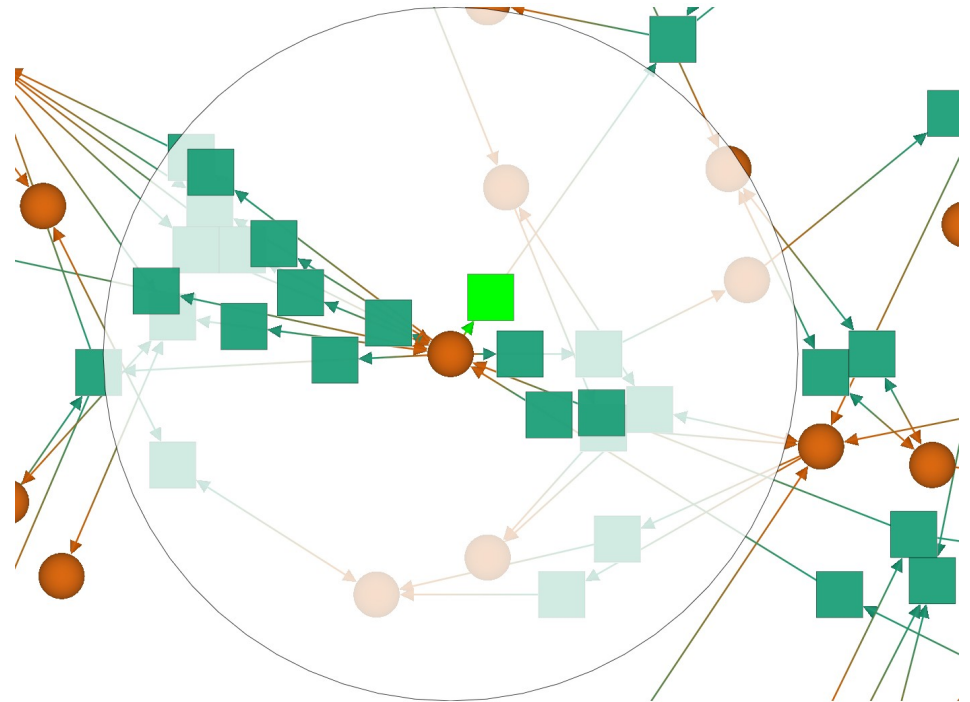
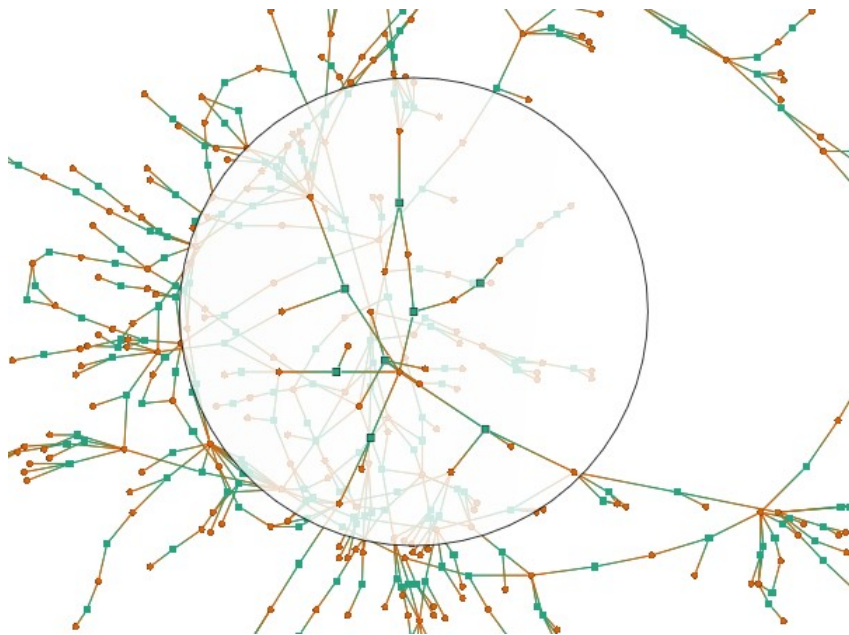
Visual parameters

- Display / hide labels
- Elements colour (nodes and edges)
- Background colour
- Elements sizes
- Elements shapes
- Orientation of reactions

Visual interaction

- Classical *zoom and pan* interaction tools
- Element(s) *selection*
- Drawing modification : element(s) position (*Drag and Drop*), edge shape (bends edition)
- Neighbourhood navigation

Visual interaction (2)



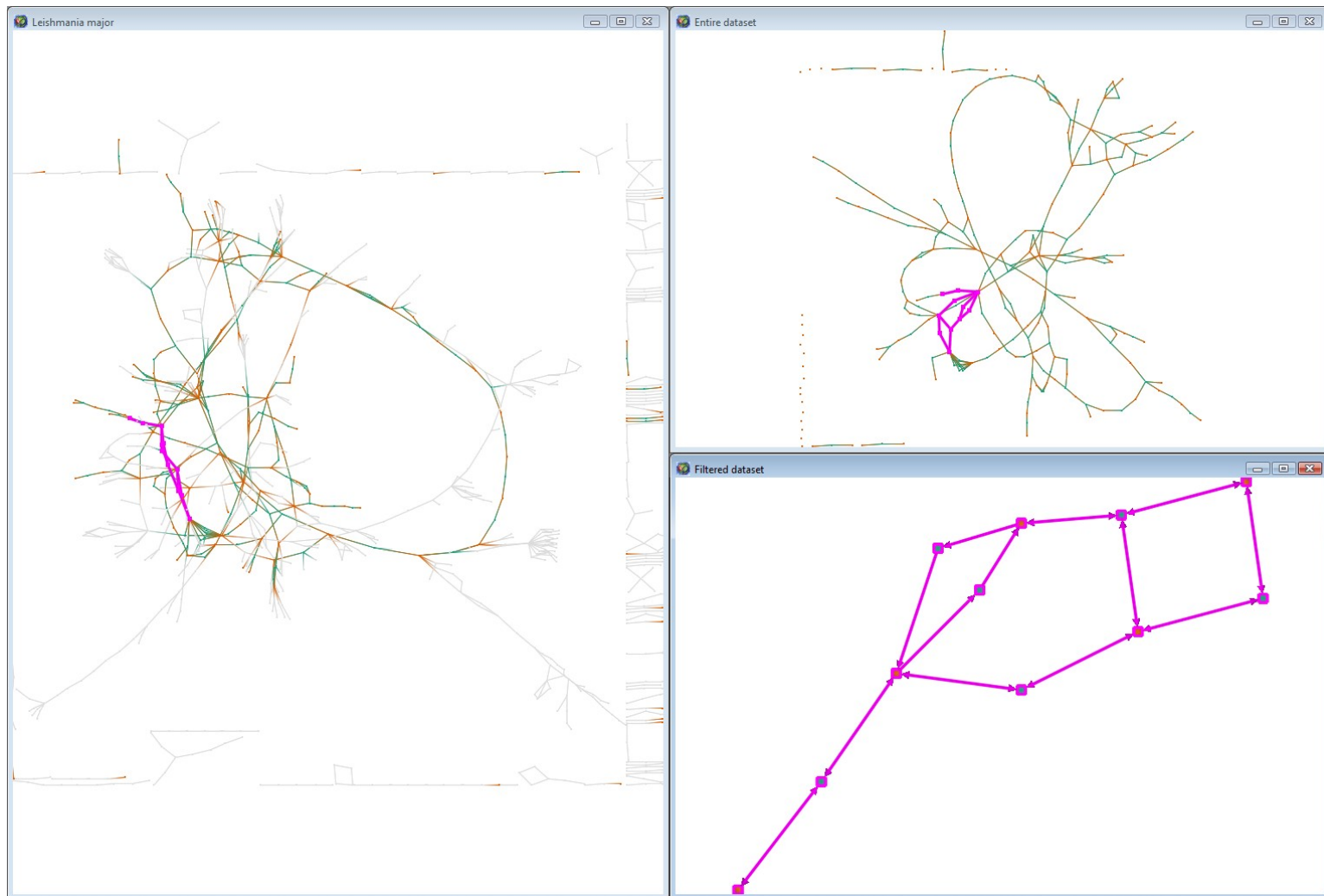
Network structure manipulation

- Pathways creation and removal
- Element removal, selection
- Export to SBML file
- Import data from CSV file
- Sub-network creation and manipulation

Sub-networks

- Help user to focus on a small part of the network
- Original data and sub-networks share visual properties
- Sub-networks structures are disconnected from original structure

Sub-networks



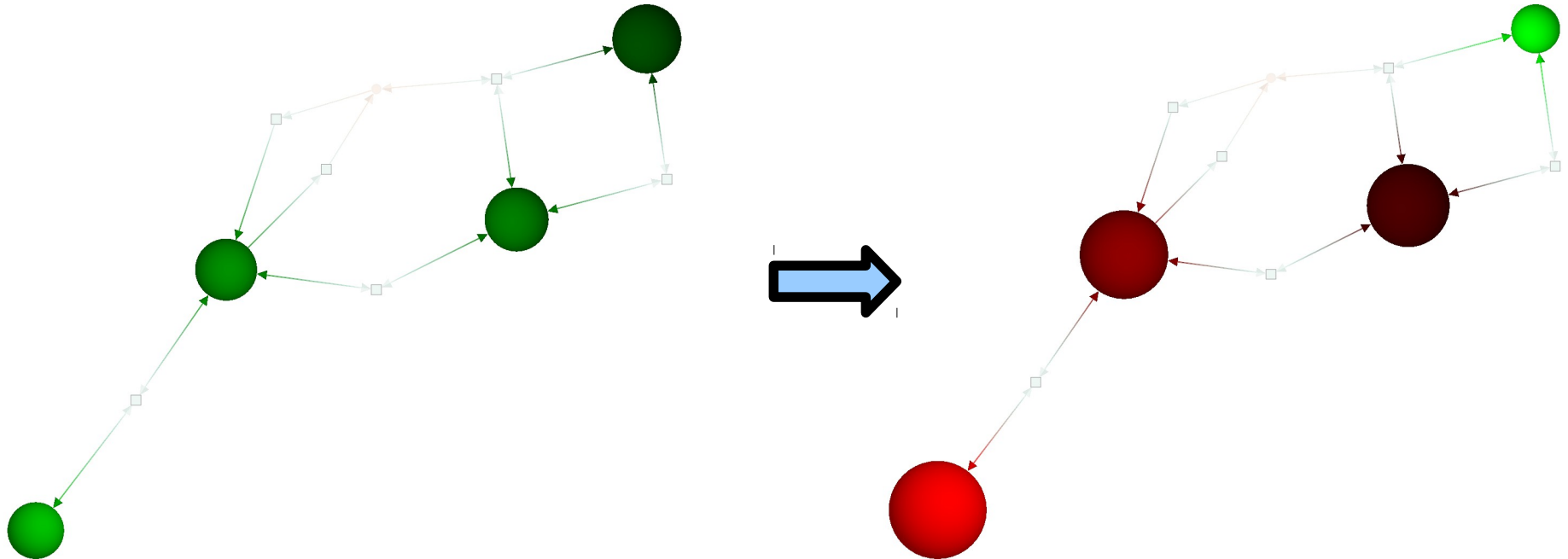
Working with time-series data

- Import data from CSV files
- Visualize and animate time-series data
- Display data on elements (augmented display)
- Views dedicated to data analysis

Visualize and animate time-series data

- Mapping of data values on visual parameters (colour and/or size)
- Can combine 2 kind of animations :
 - On Colour
 - On Size
- Animate on all displayed views

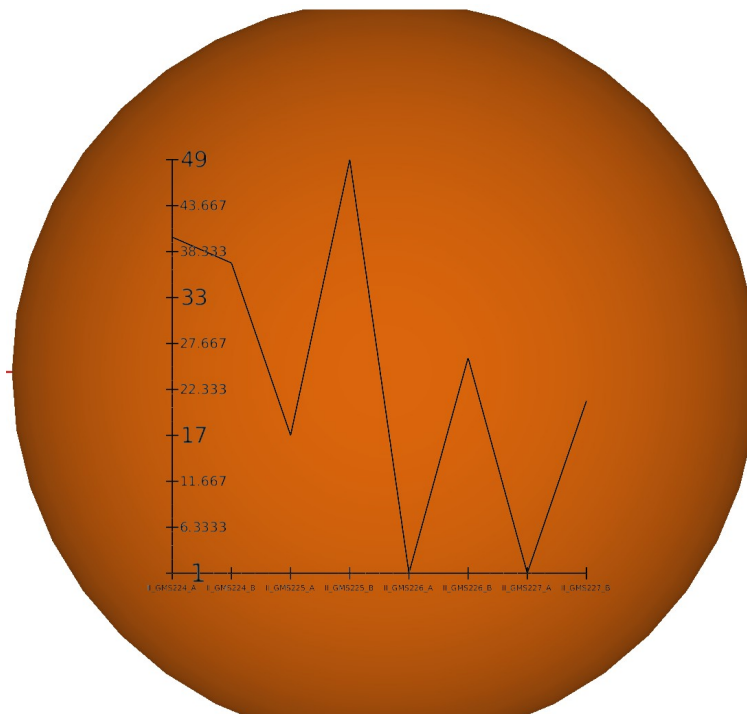
Visualize and animate time-series data (2)



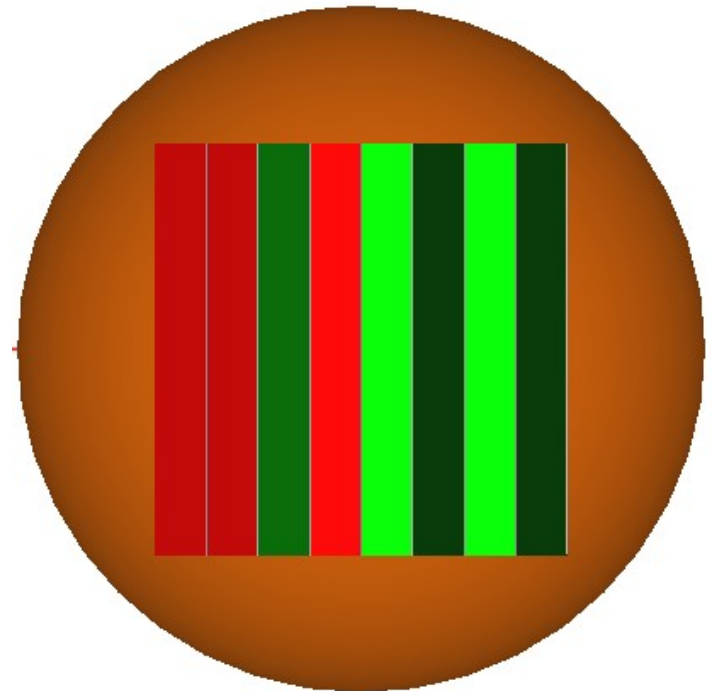
Augmented display

- Display data evolution on elements

Curves



Heat maps



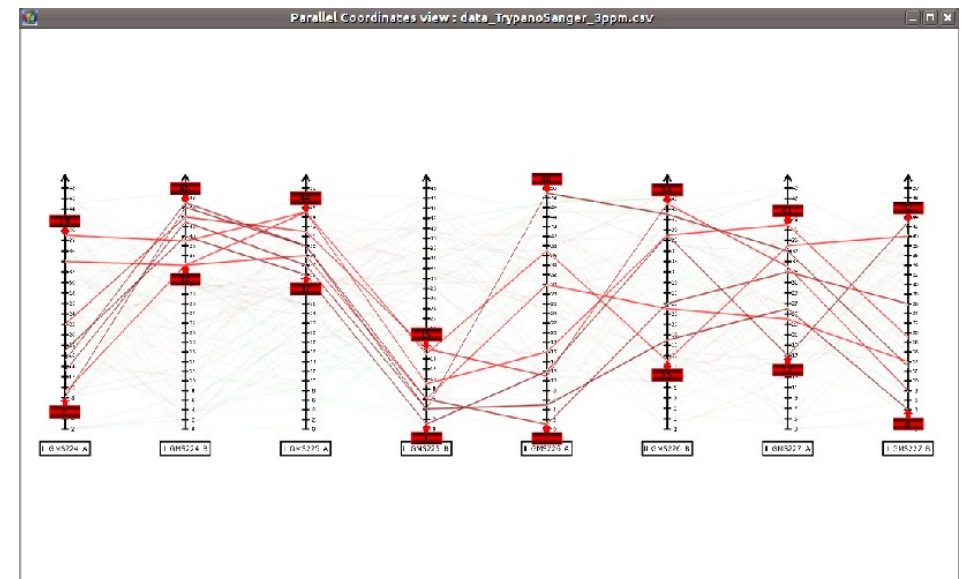
Data analysis views

Table view

Table view: data_TrypanoSanger_3ppm.csv

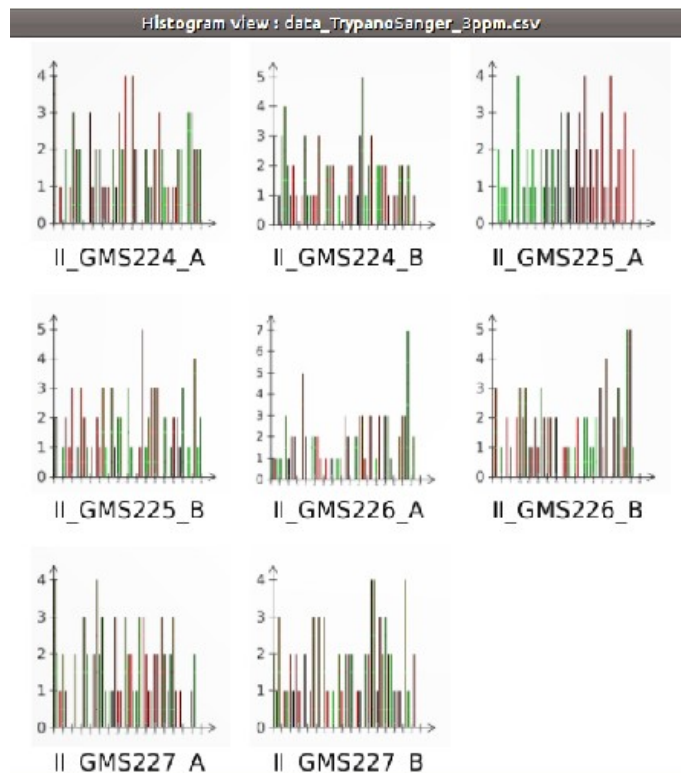
Nodes	Edges									
		ILGMS224_B	ILGMS225_A	ILGMS225_B	ILGMS226_A	ILGMS226_B	ILGMS227_A	ILGMS227_B		metite
46	27	10	46	34	35	12	36	16		L-aspartate
349	36	23	21	42	47	47	31	46		D-glucosamine-5-phospho...
142	35	31	25	31	25	28	42	41		NADP+
23	35	5	23	29	47	22	14	27		L-isoleucine
243	34	34	45	15	37	14	38	40		β-D-glucose-6-phos...
220	34	16	44	32	17	2	10	33		mannose-1-phosphate
571	31	15	24	10	17	16	19	10		L-proline
347	43	31	17	9	30	31	20	34		L-ornithine
454	33	14	38	14	16	5	28	29		hypoxanthine
270	32	21	30	14	39	15	7	44		2-keulo-succinate
552	31	26	24	48	14	38	30	14		glycine
160	30	12	7	3	5	12	19	12		L-glutamate
59	30	26	30	29	11	41	23	8		pyridoxal
27	27	15	31	10	31	15	13	32		L-arginine
133	27	0	19	19	15	36	26	7		N-α-acetylmethine
115	26	42	30	32	25	20	32	0		citruine
450	25	20	41	28	46	11	31	35		deamido-NAD
513	24	8	16	5	19	29	3	2		ribulaviv
0	26	4	9	33	44	17	3	47		β-benzyl-arginine

Parallel coordinates

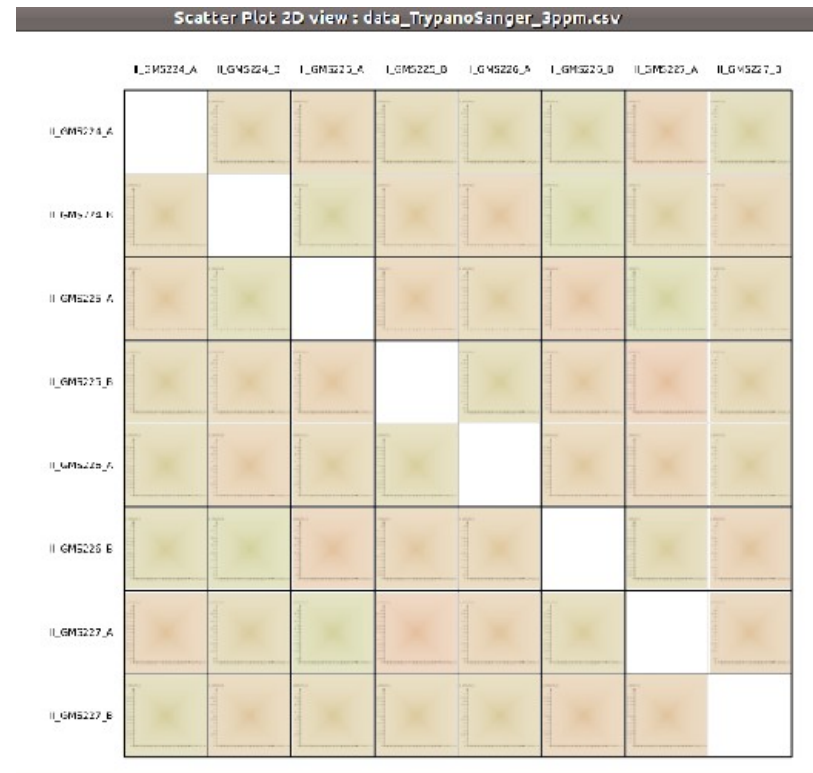


Data analysis views (2)

Histogram



Scatter plot



Analysis tools

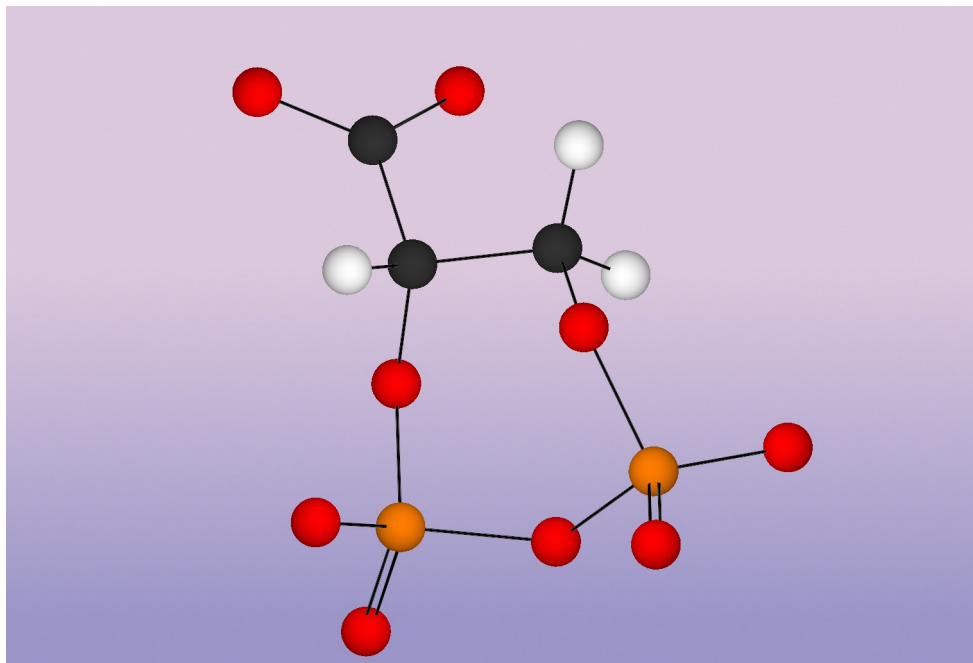
- Tulip graph analysis algorithms:
 - Degree
 - Betweenness centrality
 - Eccentricity
 - ...
- Network analysis algorithms :
 - Choke points
 - Shortest path
(dedicated to metabolic networks)
 - Scope selection

Query biological databases

- Display detailed information as HTML pages.
- Query different databases :
 - KEGG <http://www.genome.jp/kegg/>
 - Public House
<http://biowarehouse.ai.sri.com/PublicHouseOverview.html>

Query biological databases (2)

- Generate and display 3D molecule (OpenBabel library).



KfCC COMPOUND: C00042

Entry	C00042
Name	Succinate; Succinic acid; Butanedioic acid; Ethylenesuccinic acid
Formula	C4H6O4
Mass	118.0266
Structure	 C00042 Mol file KCF file DB search Jmol KegDraw
Reaction	R00402 R00405 R00406 R00407 R00408 R00409 R00410 R00411 R00412 R00432 R00479 R00499 R00713 R00714 R00727 R00999 R01252 R01288 R01412 R01559 R01780 R01879 R02084 R02160 R02164 R02397 R02407 R02444 R02445 R02486 R02508 R02603 R02734 R02956 R02990 R03008 R03009 R03126 R03154 R03218 R03219 R03260 R03376 R03451 R03590 R03640 R03737 R03806 R03809 R03812 R04073 R04276 R04946 R05036 R05037 R05039 R05097 R05228 R05229 R05301 R05302 R05320 R05419 R05466 R05468 R05469 R05588 R05722 R05723 R05857 R06322 R06323 R06335 R06336 R06337 R06338 R06539 R06540 R06551 R06855 R06904 R07184 R07185 R07186 R07187 R07329 R07366 R07367 R07368 R07993 R07996 R07997 R08050 R08081 R08082 R08610 R08611 R08972 R09363
Pathway	ko00020 Citrate cycle (TCA cycle) ko00190 Oxidative phosphorylation ko00250 Alanine, aspartate and glutamate metabolism ko00350 Tyrosine metabolism ko00360 Phenylalanine metabolism ko00361 Chlorocyclohexane and chlorobenzene degradation ko00623 Toluene degradation ko00630 Glyoxylate and dicarboxylate metabolism ko00640 Propanoate metabolism ko00650 Butanoate metabolism ko00720 Carbon fixation pathways in prokaryotes map01060 Biosynthesis of plant secondary metabolites map01061 Biosynthesis of phenylpropanoids map01062 Biosynthesis of terpenoids and steroids map01063 Biosynthesis of alkaloids derived from shikimate pathway map01064 Biosynthesis of alkaloids derived from ornithine, lysine and nicotinic acid map01065 Biosynthesis of alkaloids derived from histidine and purine map01066 Biosynthesis of alkaloids derived from terpenoid and polyketide map01070 Biosynthesis of plant hormones ko01100 Metabolic pathways ko01110 Biosynthesis of secondary metabolites ko01120 Microbial metabolism in diverse environments ko02020 Two-component system

All links

- Pathway (17639)
 - KEGG PATHWAY (17639)
- KEGG MODULE (6)
- Drug (12)
 - KEGG DRUG (4)
 - KEGG EDRUG (8)
- Chemical substance (24)
 - PubChem (1)
 - CHEBI (1)
 - SMET (1)
 - HMDB (1)
 - HSDB (1)
 - PubChem (1)
 - LIPIDMAPS (1)
 - MASSBANK (16)
 - HUGO (1)
- Chemical reaction (175)
 - KEGG ENZYME (58)
 - KEGG REACTION (99)
 - KEGG RXN (18)
- All databases (17850)

Other tools

- Export video / images

Future of Systrip

- Version 2 in development
- Visualized multiple networks at a time
- Can handle new kind of networks (gene/protein – related networks)
- “Cross-network” analysis
- Data clustering
- Clustering comparison