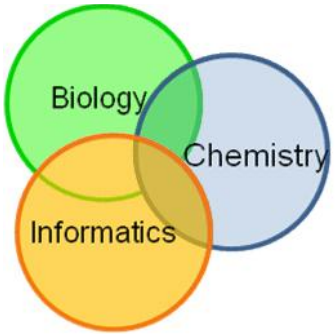


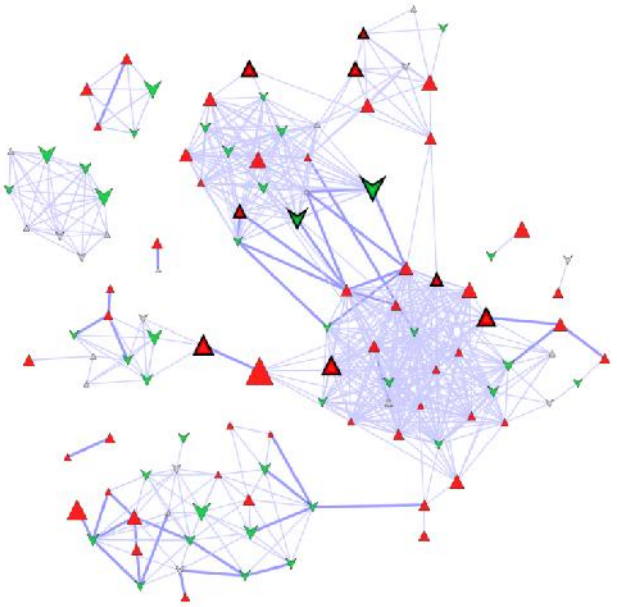
Biochemical and Structural Similarity Network Mapping

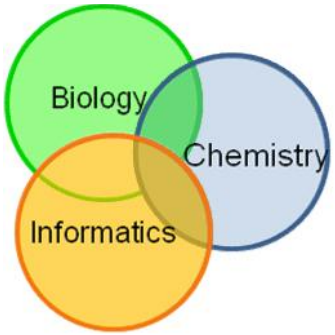
Network Mapping

Goal: Generate a mapped biochemical product/substrate and chemical similarity network

Topics:

1. Edge list generation
2. Node attributes generation
3. Network Mapping





Biochemical and Structural Similarity Network Mapping

Network Mapping

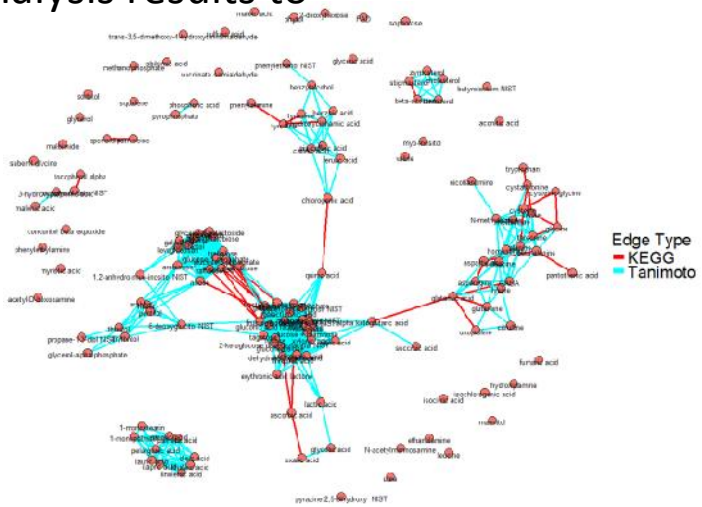
Data: Pumpkin and Tomatillo data for network.csv

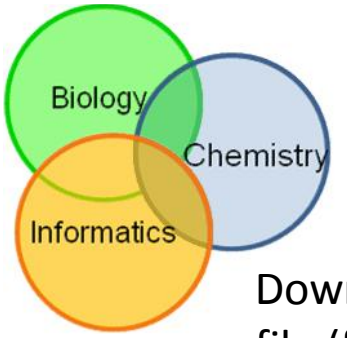
Steps

Use **MetaMapR** (see startup.R to launch):

1. url: https://github.com/dgrapov/MetaMapR
    - Biochemical and structural similarity based edge list for all metabolites with KEGG and PubChem identifiers.
    - Network preview
    - Node attributes

2. Use previously generated Pumpkin/Tomatillo analysis results to generate node attribute mappings
3. Visualize and map network using Cytoscape





MetaMapR: Edge List

Download the generated edge list, overview and save as an .xlsx file (for ease of import).

Network Mapping

MetaMapR Data Network About

Network Options

Biochemical

Database: KEGG

Metabolite index: KEGG

Chemical Similarity

Database: PubChem CID

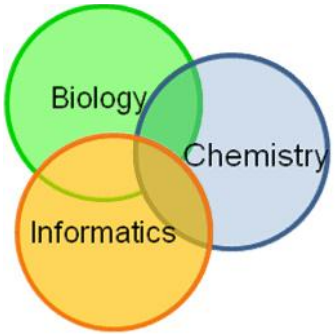
Metabolite index: PubChem

Cutoff: 0.7

Edge List | Node Attributes | Networl

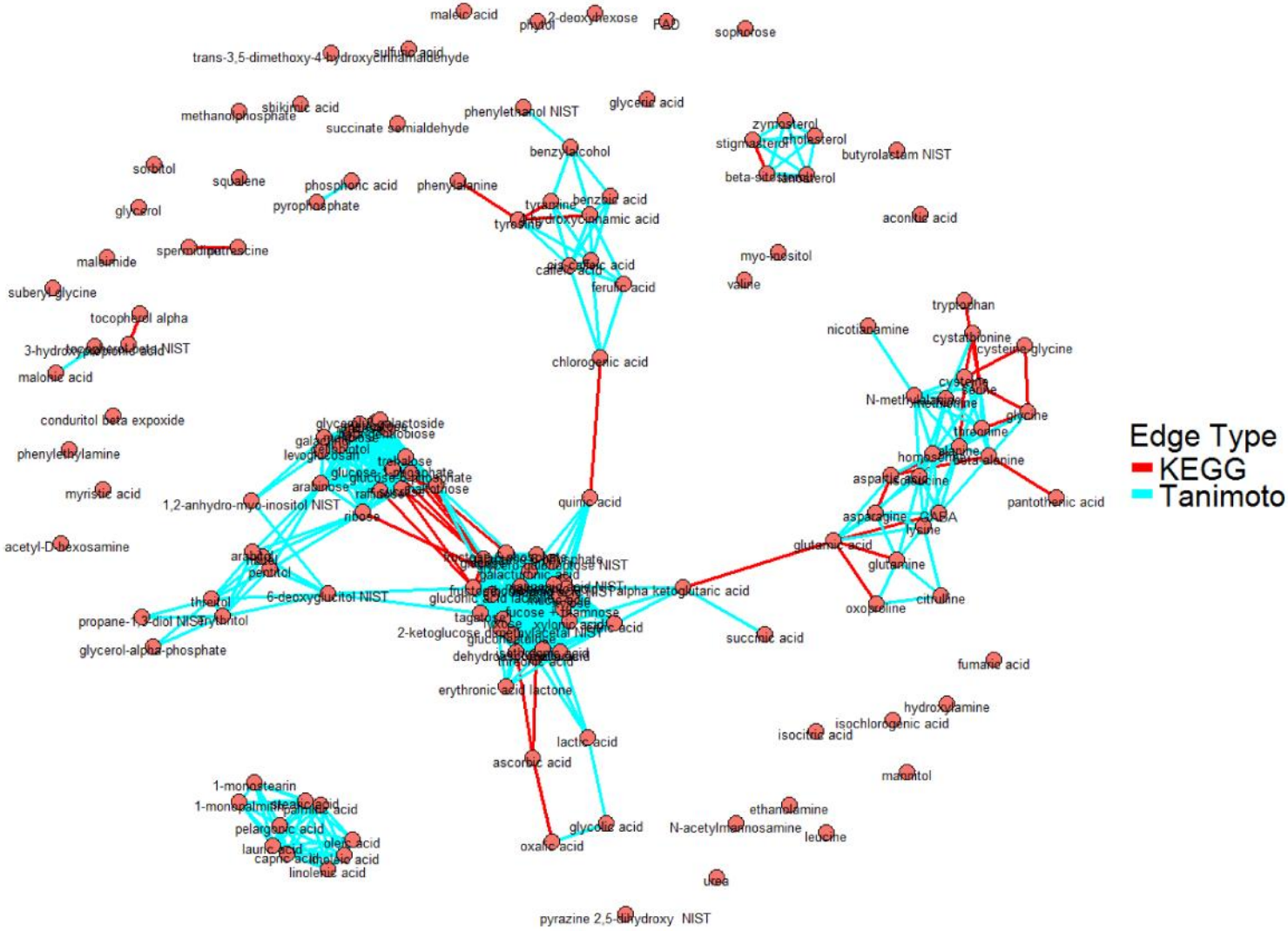
Calculate Connections | Download

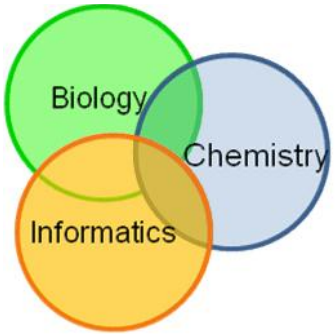
	source	target	type	weight
1	6.00	7.00	KEGG	2.00
2	11.00	12.00	KEGG	2.00
3	8.00	29.00	KEGG	2.00
4	30.00	31.00	KEGG	2.00
5	18.00	33.00	KEGG	2.00
6	25.00	37.00	KEGG	2.00
7	6.00	43.00	KEGG	2.00
8	13.00	88.00	KEGG	2.00
9	29.00	88.00	KEGG	2.00
10	48.00	95.00	KEGG	2.00
11	94.00	95.00	KEGG	2.00
12	96.00	97.00	KEGG	2.00
13	9.00	98.00	KEGG	2.00
14	18.00	98.00	KEGG	2.00
15	96.00	98.00	KEGG	2.00
16	97.00	98.00	KEGG	2.00



Preview Network

Network Mapping





Node Attributes

Network Mapping

MetaMapR Data Network About

Network Options

Biochemical

Database: KEGG

Metabolite index: KEGG

Chemical Similarity

Database: PubChem CID

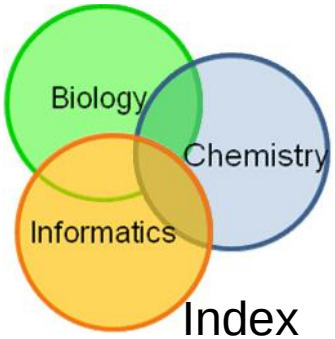
Metabolite index: PubChem

Cutoff: 0.7

Edge List | Node Attributes | Network | Debug

Download

	network.index	biochemical.edge.index	chemical.edge.index
1	1	C05437	92746.00
2	2	C02205	644160.00
3	3	n/a	6602431.00
4	4		
5	5		
6	6	C00082	6057.00
7	7	C00483	5610.00
8	8	C00078	6305.00
9	9	C01083	7427.00
10	10		
11	11	C14152	8989.00
12	12	C02477	14985.00
13	13	C00188	6288.00
14	14	C01620	439535.00
15	15	n/a	169019.00
16	16	D09007	92092.00
17	17	C00059	1118.00



Mapping Analysis results to Node Attributes

Network Mapping

Index matching edge list ID

Labels: metabolite names

Border: O/PLS/-DA selected feature?

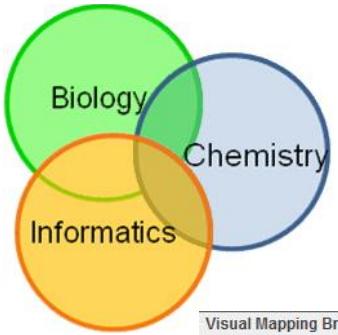
Shape: Direction of change relative to pumpkin

Color: Direction of change for significantly changed species (t-Test)

Index	name	combined.selectio	direction	sig dir	size FC	size log FC	size LV
1	zymosterol	FALSE	increase	increase	6.298	0.86320386	0.07219
2	xylose	FALSE	increase	increase	1.276	0.35717226	0.0864
3	xylonic acid	FALSE	decrease	decrease	2.17391	0.50159502	0.09435
4	valine	FALSE	increase	increase	0.639	0.21457895	0.06987
5	urea	FALSE	increase	increase	0.573	0.19672872	0.05381
6	tyrosine	FALSE	increase	increase	1.956	0.47070443	0.08416
7	tyramine	FALSE	decrease	decrease	1.64474	0.42238247	0.06636
8	tryptophan	FALSE	increase	increase	56.355	1.75857128	0.10076
9	trehalose	TRUE	decrease	decrease	19.6078	1.31403254	0.11088

Size(a): log of the magnitude of fold change

Size(b): O/PLS/-DA LV 1 loadings

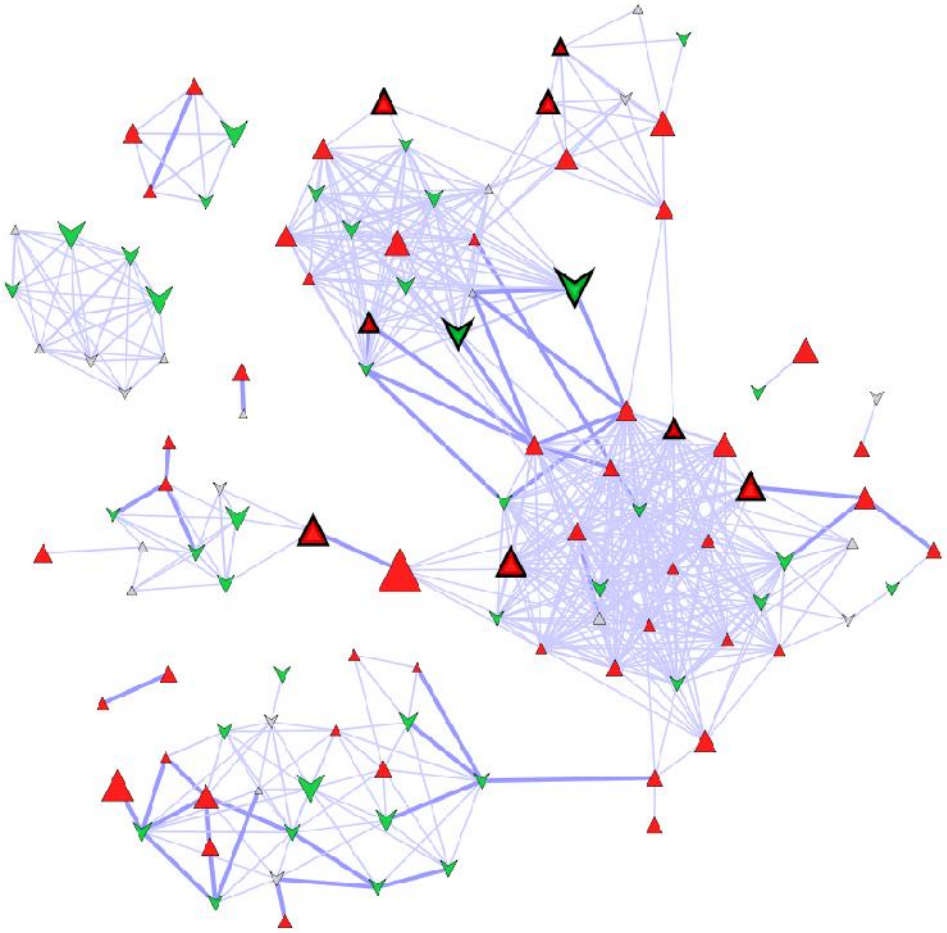


Mapping in cytoscape

Network Mapping

Visual Mapping Browser

Edge Visual Mapping	
Edge Color	type
Mapping Type	Discrete Mapping
KEGG	
Tanimoto	
Edge Line Width	weight
Mapping Type	Continuous Mapping
Graphical View	5.0 / 0.0 / 0.70 / 2.00
Node Visual Mapping	
Node Color	sig dir
Mapping Type	Discrete Mapping
NULL	
decrease	
increase	
Node Font Size	sig dir
Mapping Type	Discrete Mapping
NULL	10.0
decrease	16.0
increase	16.0
Node Label	name
Node Line Width	combined.selection
Mapping Type	Discrete Mapping
false	1.0
true	7.0
Node Shape	direction
Mapping Type	Discrete Mapping
decrease	VEE
increase	TRIANGLE
Node Size	size log FC
Mapping Type	Continuous Mapping
Graphical View	50.0 / 0.0 / 0.00 / 0.11

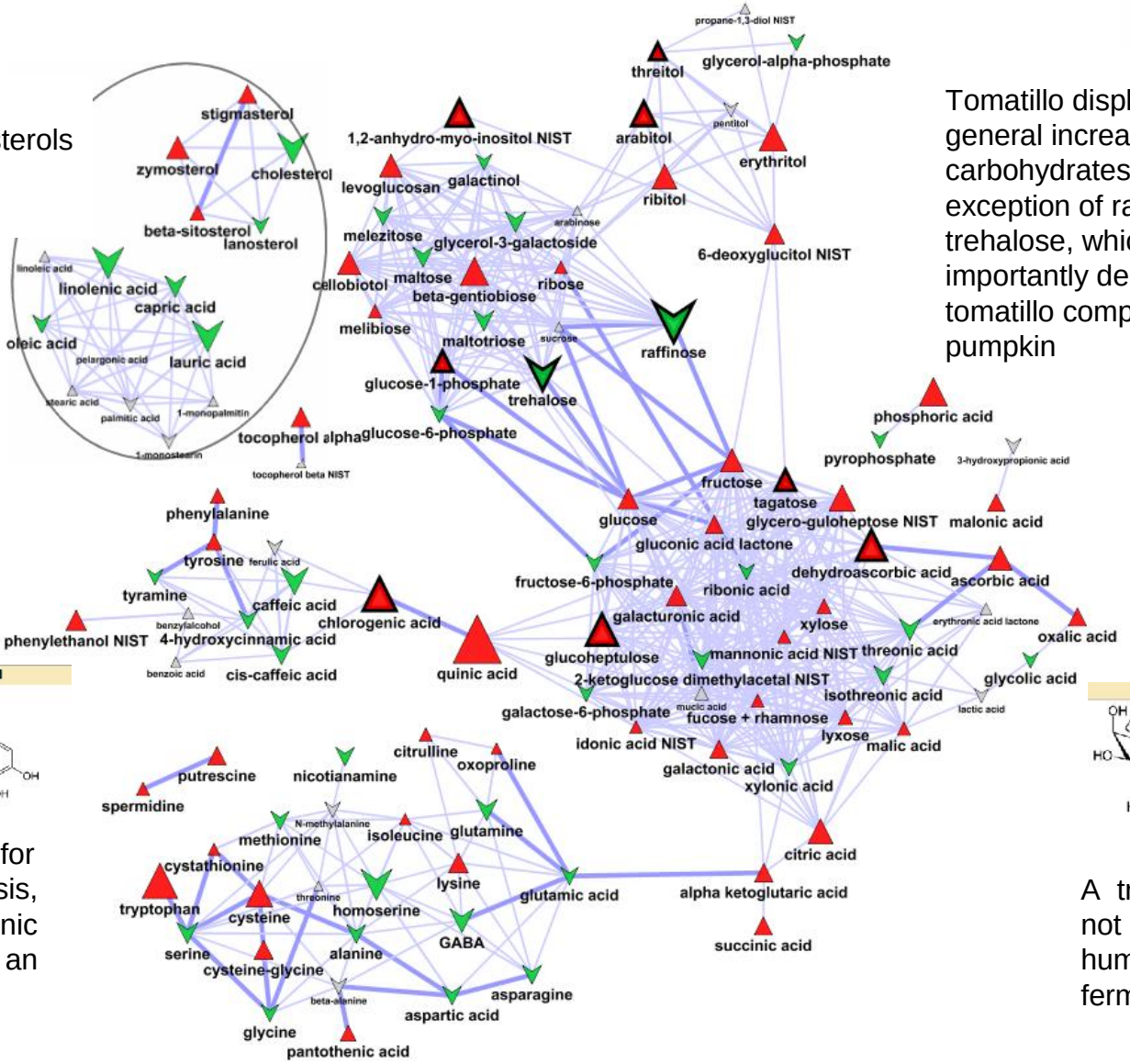


Biochemical and Spectral Similarity Mapped Network for: Differences in Pumpkin and Tomatillo Leaf Primary Metabolites

Biology
Chemistry
Informatics

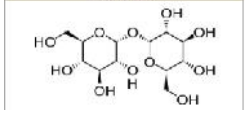
Network Mapping

Leaf fatty acids are decreased and phytosterols increased in tomatillo compared to pumpkin



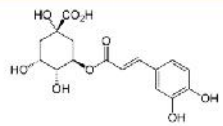
Tomatillo displays a general increases in leaf carbohydrates with the exception of raffinose and trehalose, which are importantly decreased in tomatillo compared to pumpkin

Trehalose



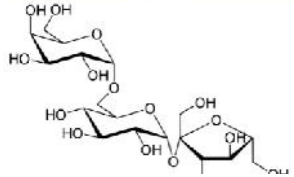
Helps withstand prolonged periods of desiccation

Chlorogenic acid

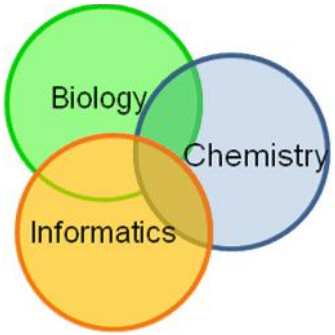


intermediate for lignin synthesis, related to quinic acid which is an astringent

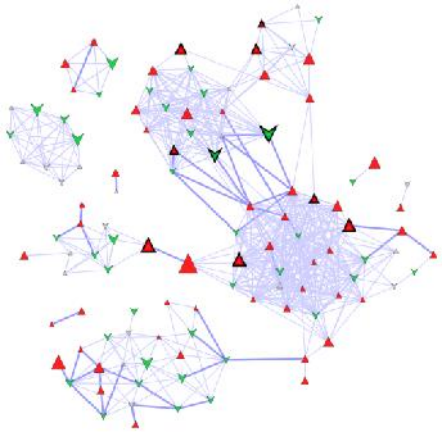
Raffinose



A trisaccharide, can not be digested by humans, but readily fermented by bacteria



Summary



Network Mapping

View all files and mappings used in the network construction in the:

1. Data folder
   - Pumpkin and Tomatillo data for network.csv
2. Network folder
   - Biochemical edge list.xlsx
   - Biochemical node attributes.xlsx
   - Biochemical network.cys (final network)