

Improving metabolite evaluation in integrated pathway analysis

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Introduction

PathVisio is an open source platform for displaying and editing pathways. It is also used to visualize and analyze the experimental data on the pathways. The modular structure allows us to extend the tool with added functionality by implementing plugins.

In the initial stage of this project we will follow two approaches. Firstly, connect pathway analysis to different quantitative methods which are actively used for metabolic network modeling, such as flux balance analysis and dynamic simulation.

Secondly, we will integrate GO analysis into PathVisio to be able to categorize pathways and metabolites based on Go terms.

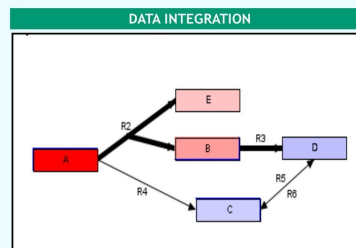
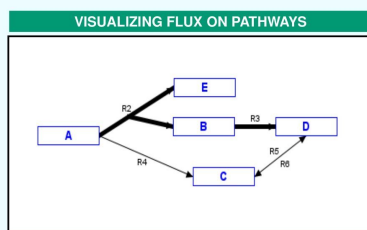
Objective

To improve the depth and quantitative potential for pathway analysis. The model visualization work will build a bridge between biologists and metabolic modellers, enabling both communities to better leverage each other's insights. The metabolite ontology work will enrich integrated approaches by extending resources to metabolite analysis that were previously only available for genes.

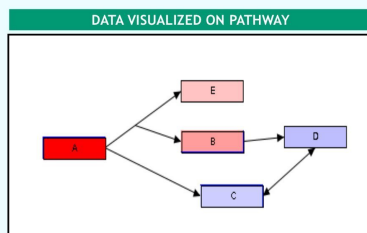
Project 1: Visualization Of Flux Balance Analysis in Pathways

- ❖ Model Experimental flux data to a specific Pathway
- ❖ Create BridgeDb database of reaction Identifiers
- ❖ Create PathVisio Plugin to visualize the metabolic fluxes on Pathways
- ❖ Integration of visual Modeling standards (SBGN and MIM)

FLUX DATA		
Model	Reactions	Metabolite
R1:	==> 1 A	A:6
R2:	1 A ==> 1 B +1 E	B:3
R3:	2 B ==> 1 D	C:6
R4:	1 A <==> 1 C	D:6
R5:	1 C ==> 1 D	E:3
R6:	1 C <==> 1 D	



METABOLITE DATA			
ID	system co	log2FC	pvalue
C00127	Ck	1.3	0.027317
C00135	Ck	0.387564	0.528715
C00148	Ck	-0.19343	0.044972
C00152	Ck	-0.25404	0.169222
C00183	Ck	0.231627	0.144458



Project 2: GO Analysis Integration

- ❖ Categorization of pathways according to Gene Ontology terms
- ❖ Assignment of automatically inferred GO categories to all metabolites.
- ❖ GO visualization plugin to show gene categories (eg:cellular locations) on Pathways
- ❖ Building Metabolite Ontology(MO) based on GO.

GO:0005813 Centrosome	GO:0005737 Cytoplasm	GO:0005634 :Cell Nucleus
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