mMAP: mouse Metabolomics Analysis Platform

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The Jackson Laboratory
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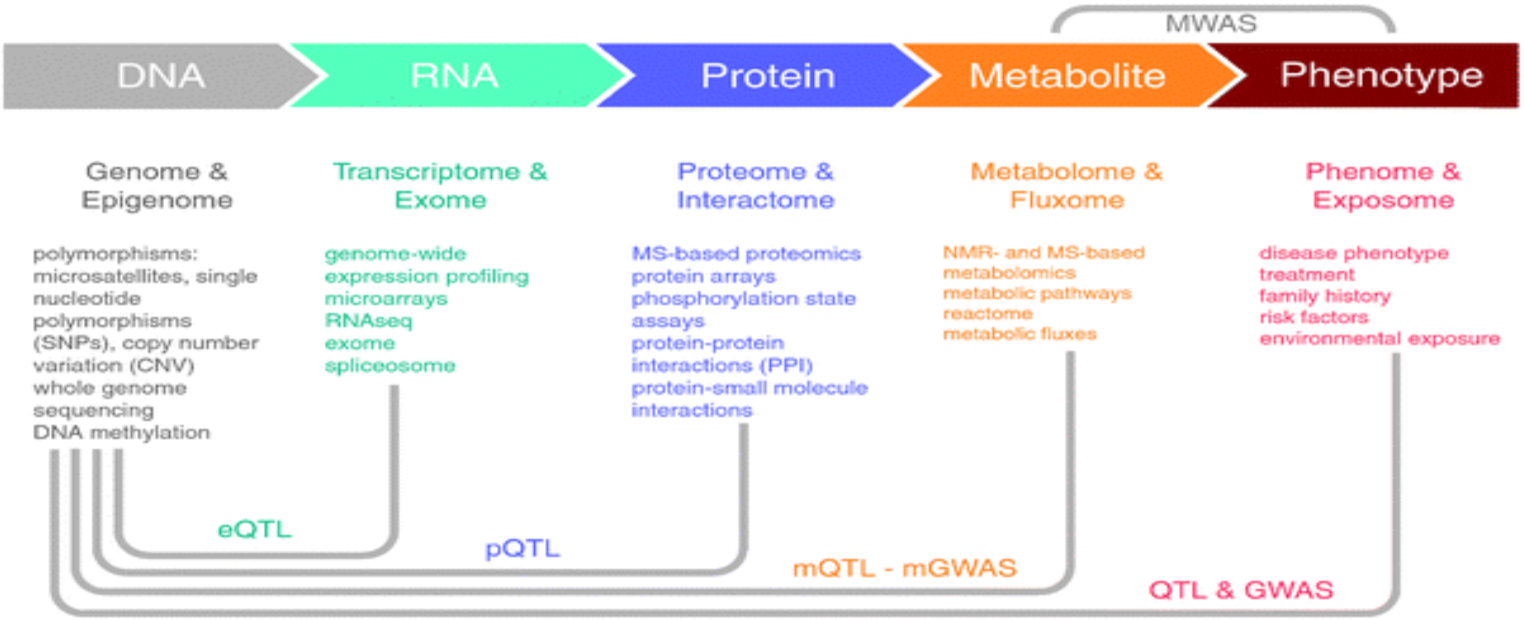
Outline

1. **Introduction:** What is Metabolomics ?
2. **Problem:** Need for Bioinformatics Infrastructure
3. **Solution:** mMap Database and Pipeline

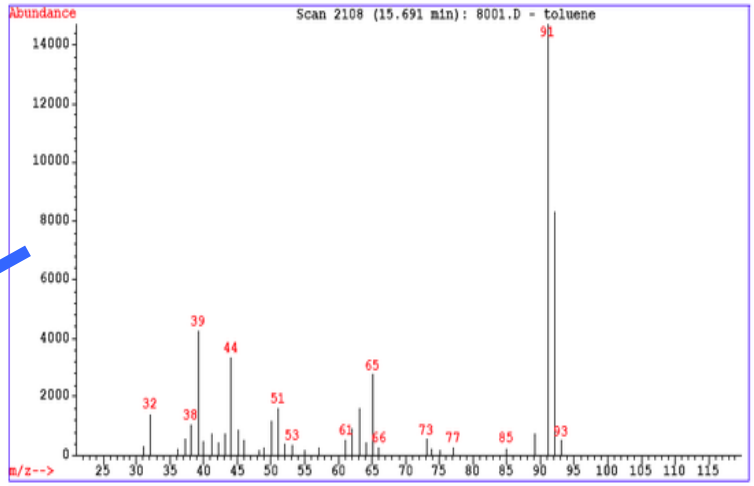
What is Metabolomics?



Mol. BioSyst., 2012,**8**, 2494-2502

Metabolomics Workflow

	Methionine	Serine	Glu	Metabolite 10	Metabolite 11	Metabolite 12	Metabolite 13
MT1	1.0	23.3	2000				..
MT2	1.5	23	2200				..
MT3	1.3	22	2300				..
WT1	100.2	22	2500				..
WT2	111.1	22	2500				..
WT3	100	22.1	2200				..



Project Goals

- To identify metabolic pathways related to pathogenesis in mouse models of 3 neuromuscular degeneration mutants
- To develop informatics tools to assign metabolomics data to curated biochemical pathways and functional annotations for mouse genes and proteins

Data Generation -> Data Analysis -> Data Interpretation

Metabolites->Biochemical Pathways->Genes->Annotations

Bioinformatics infrastructure is lacking for metabolomics data analysis and interpretation

- Metabolite names are variable and are used inconsistently (e.g. B-Alanine, Beta-Alanine)
- Very few metabolomics data analysis pipelines are designed for the biologists (e.g HMDB, plantmetabolomics.org)
- Need to combine the metabolomics data with genomics data and biological annotations for interpretation

mMAP Features: Data Base and Data Analysis Pipeline

Vs

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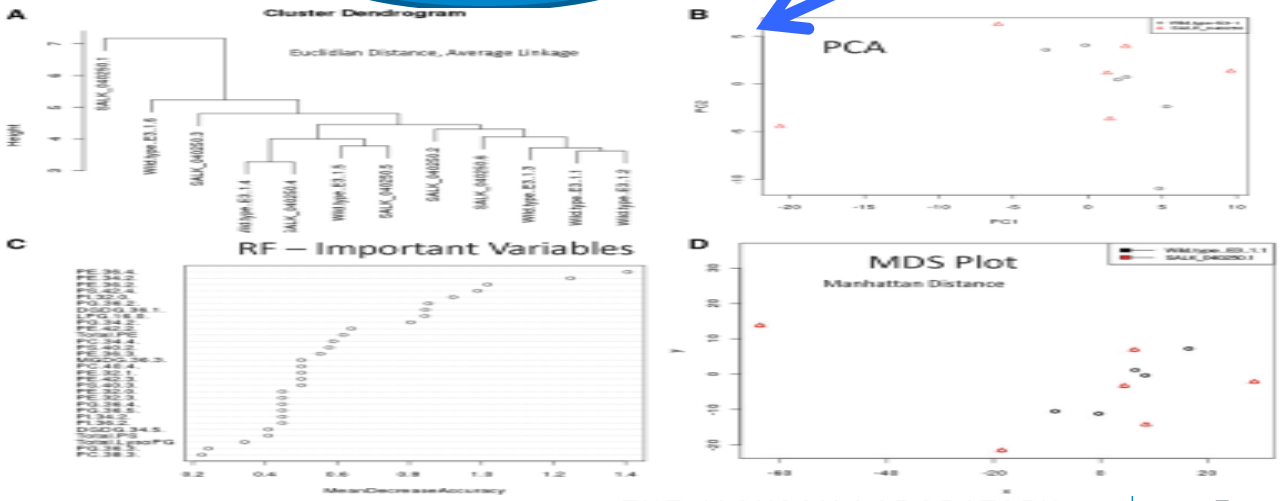
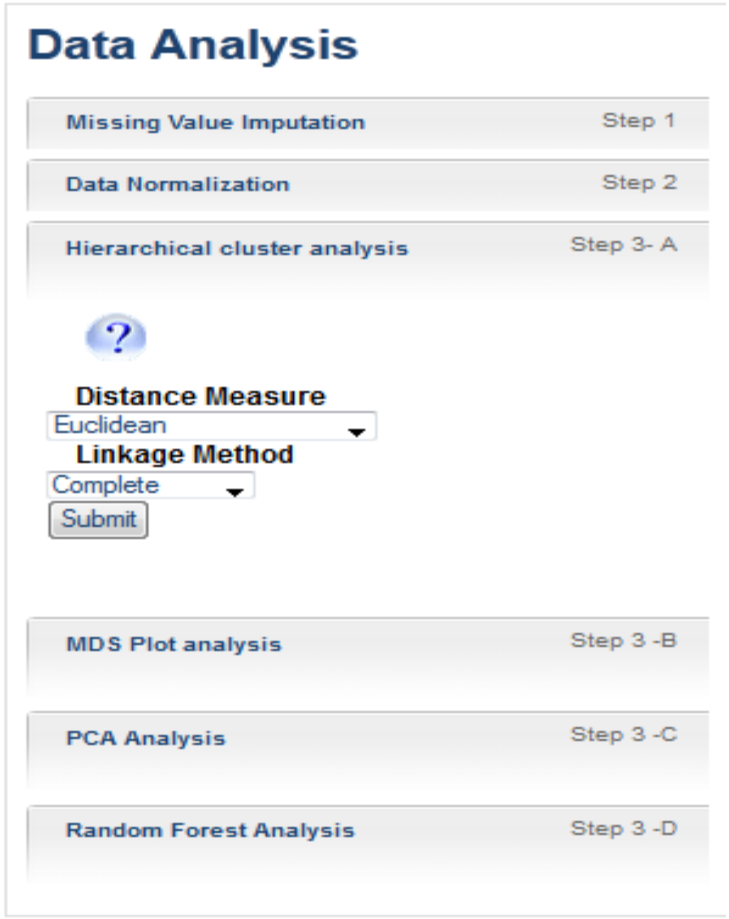
Metabolomics Data Reporting Standards

Metabolomics Data Base

Data Mining Pipeline

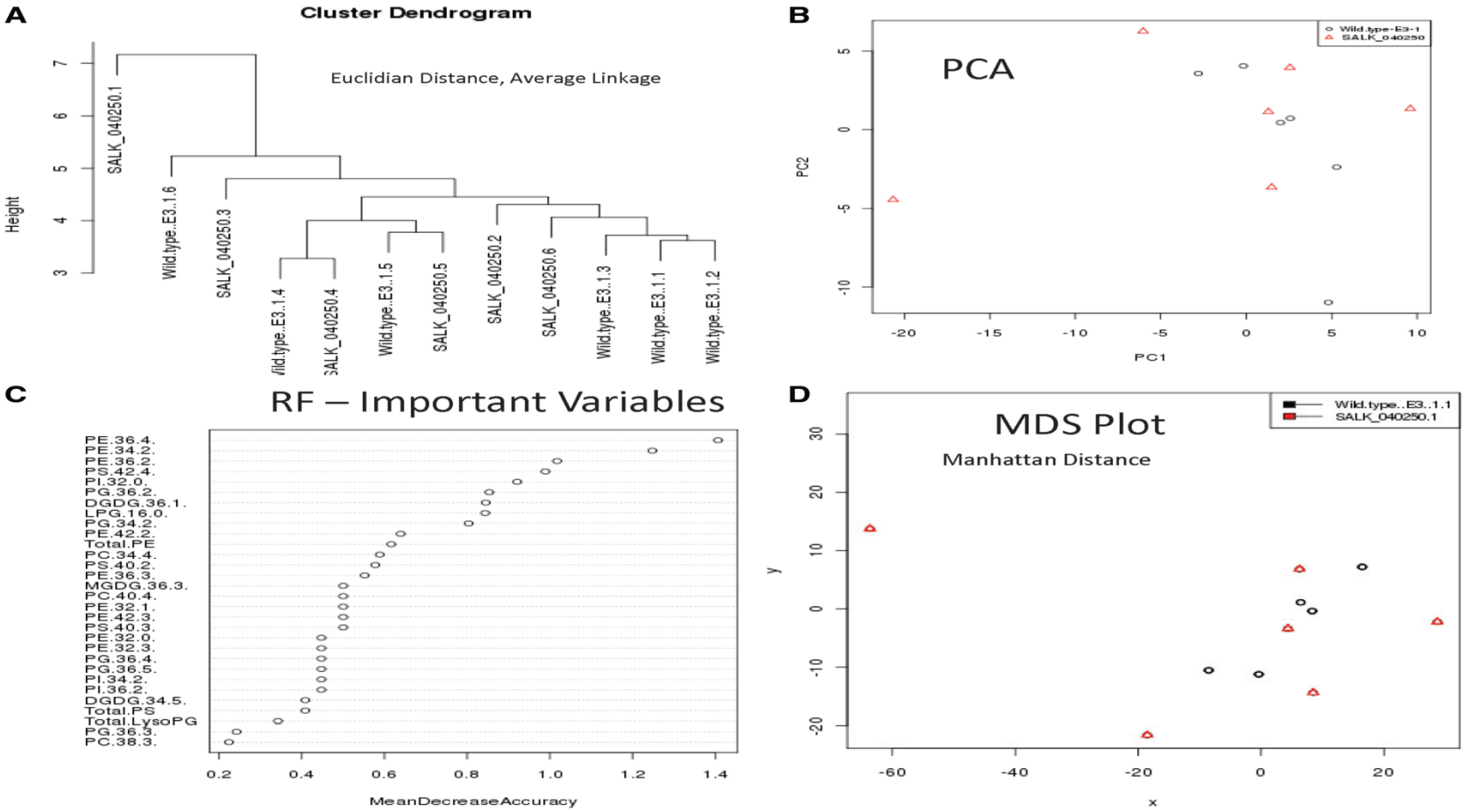


mMap Features: Advanced Data Analysis Tools

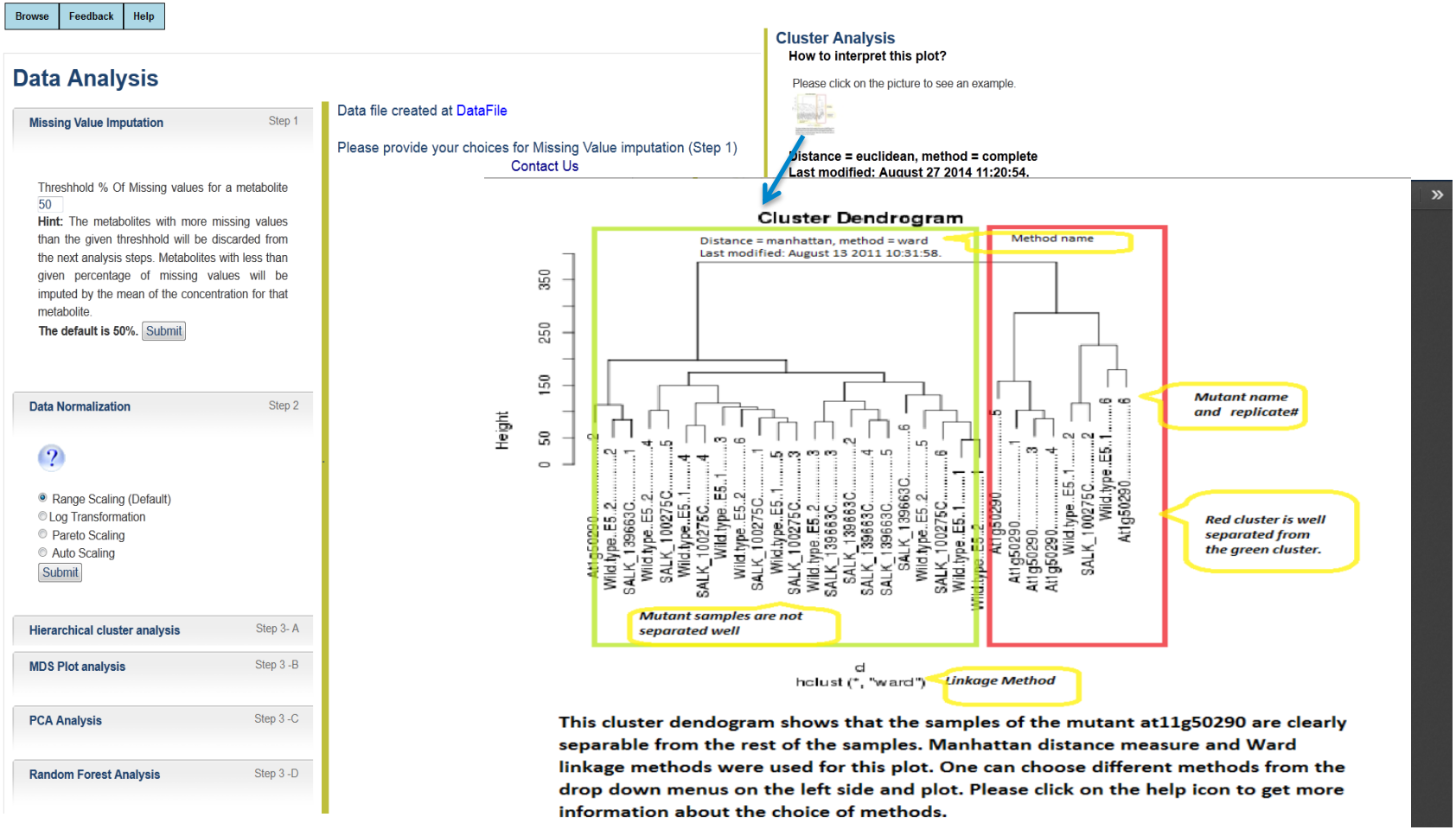


- Menu Driven automated data analysis pipeline
- Best practices in metabolomics data analysis
- Connected to genomics information
- Interactive plots : Download/Print
- Flexible pipeline
- Help in interpretation of plots with examples

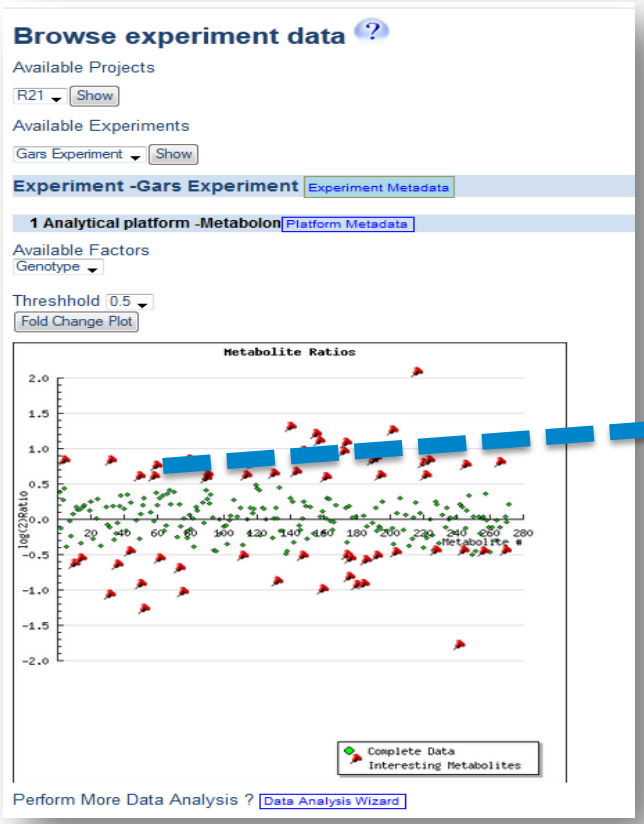
mMap Features: Data Analysis Plots



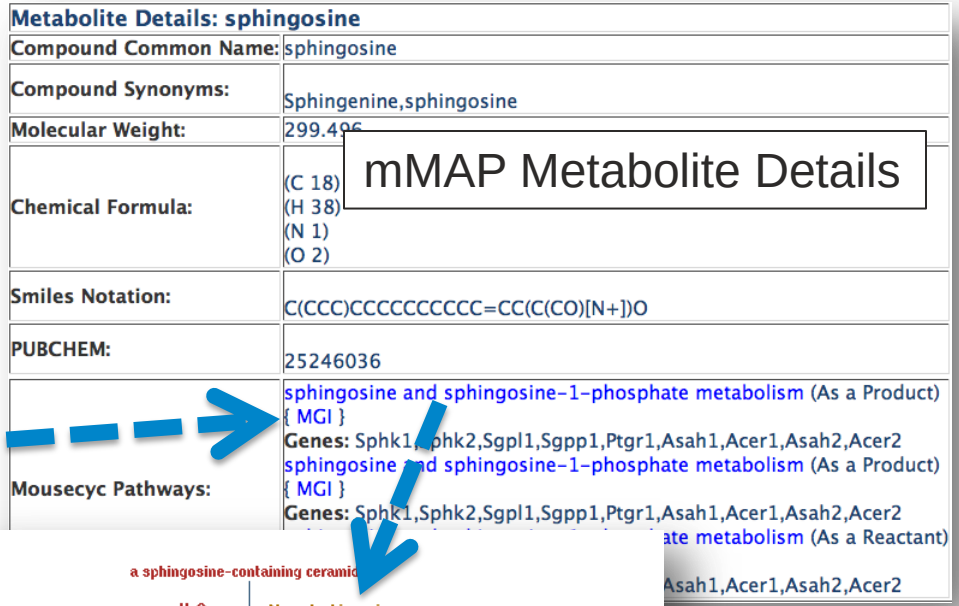
mMap Features : Help in Interpreting the Plots



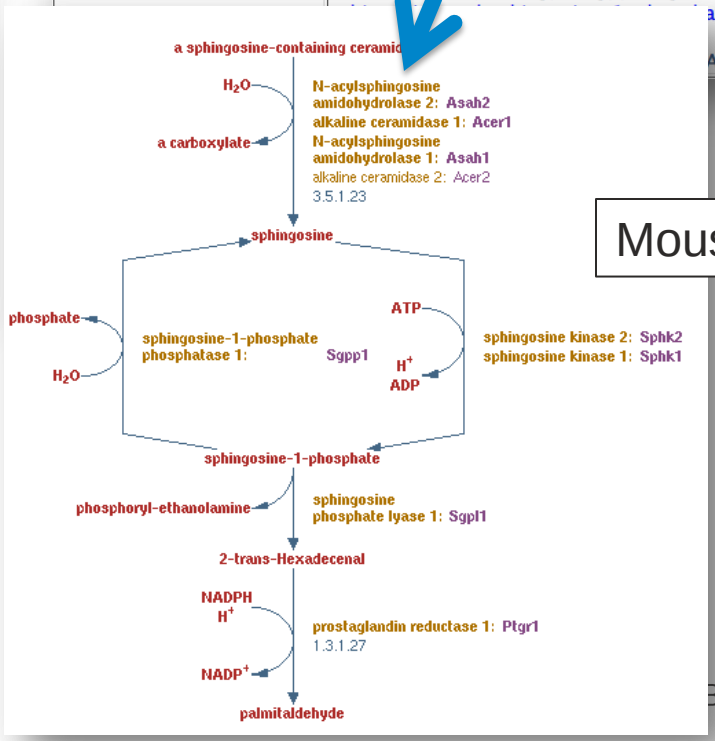
mMAP Features : Interactive Plots



mMAP Data Analysis Results



mMAP Metabolite Details

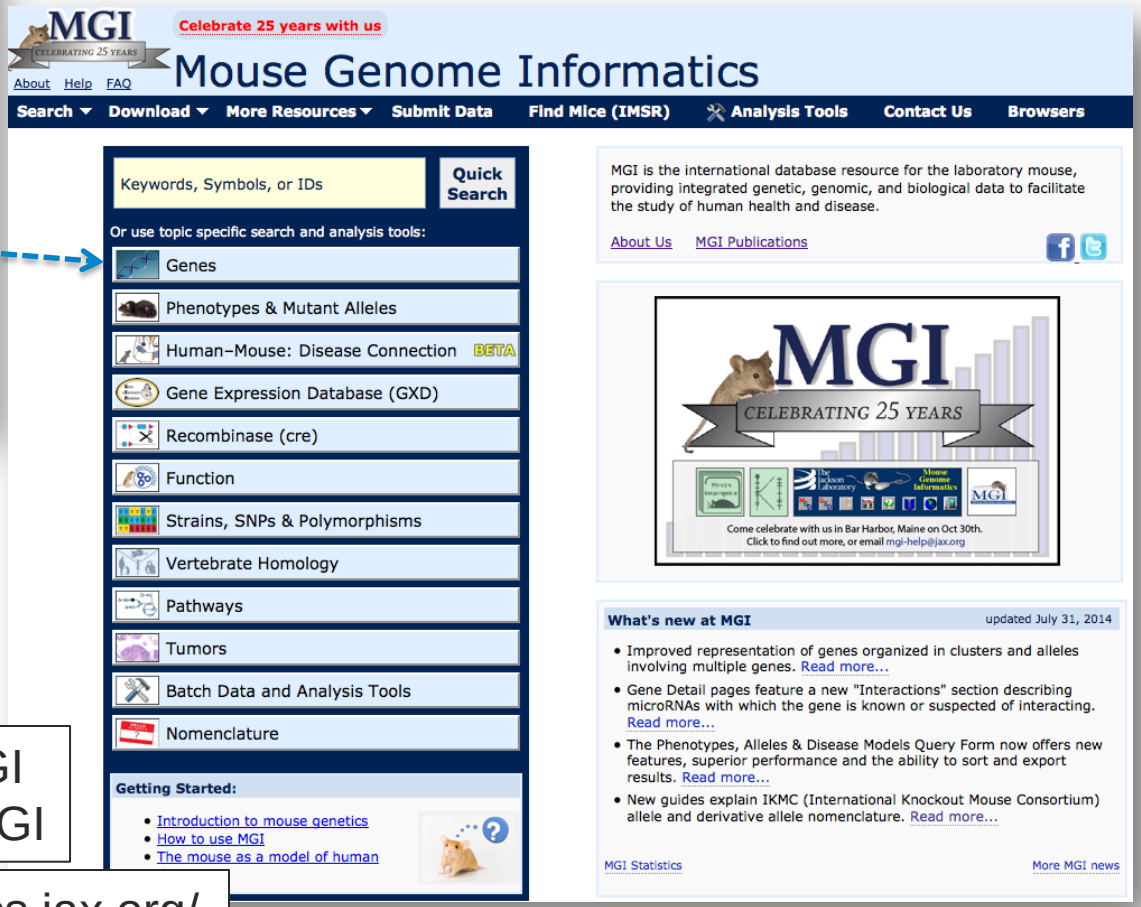


MouseCyc Pathway

mMAP Features: Links to curated pathways, genes, and proteins

Metabolite Details: lanosterol	
Compound Common Name:	lanosterol
Molecular Weight:	426.724
Chemical Formula:	(C 30) (H 50) (O 1)
Smiles Notation:	CC(C)=CCCC(C)C1(CCC2(C)(C3(CCC4(C(C)(C)C(O)CCC(C)(C(CCC(C)12)=3)4))))
CAS:	79-63-0
PUBCHEM:	25200754
Mousecyc Pathways:	lanosterol biosynthesis (As a Product) { MGI } **Genes:** Lss (As a Reactant) { MGI } **Genes:** Sc4mol,Hsd17b7,Ebp,Dhcr7,Sqle,Fdft1,Sc5d,Lss cholesterol biosynthesis I (As a Reactant) { MGI } **Genes:** Cyp51,Sc4mol,Hsd17b7,Ebp,Dhcr24,Dhcr7,Sqle,Fdft1,Tm7sf2,Sc5d,Nsdhl,Lss cholesterol biosynthesis III (via desmosterol) (As a Reactant) { MGI } **Genes:** Cyp51,Sc4mol,Hsd17b7,Ebp,Sc5d,Dhcr7,Sqle,Fdft1,Tm7sf2,Nsdhl,Lss

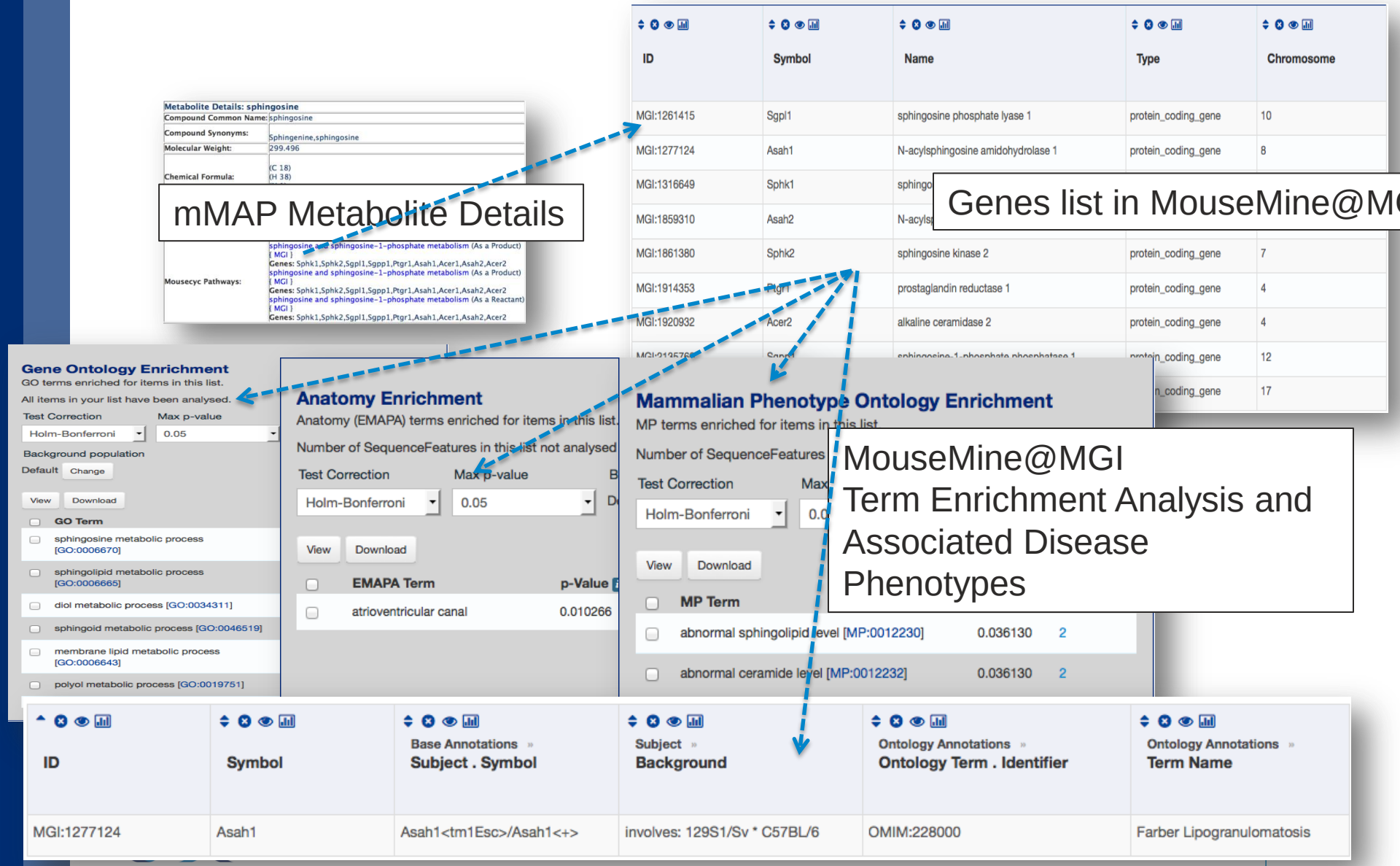
mMAP Metabolite Details



MouseCyc@MGI
MouseMine@MGI

http://www.informatics.jax.org/

mMAP Features: Links to curated pathways, genes, and proteins



Summary and Future Goals

- Provides a computational metabolomics platform for JAX researchers to incorporate metabolomics data in their research. Will be available to the community as well
- The automated pipeline is modular and can easily be extended to experiments to include different factors (e.g. Mutation, Drug, Disease etc.)
- Currently the genomic annotations for mice are available but it can be easily extended to other organisms with Biocyc Pathways (e.g. Worm, Fly, Yeast)

Metabolomics of Peripheral Neuropathy Team

- **PI:** Gregory A. Cox
- **PI:** Robert W. Burgess
- **PI:** Carol J. Bult
- Lauren Kuffler
- Preeti Bais

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