

Metaboverse: A new tool for contextualizing chaotic metabolic networks and regulation

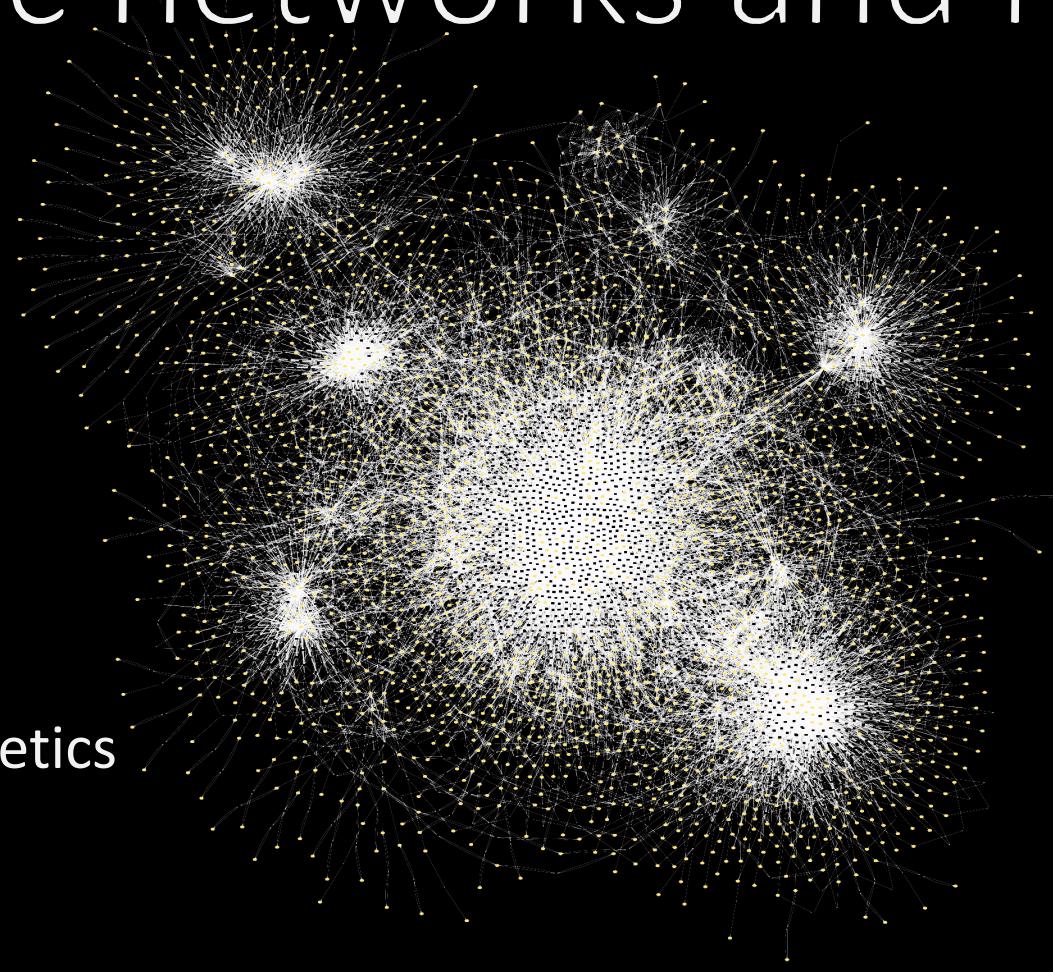
Jordan Berg

Rutter Lab

University of Utah

Metabolism Meets Epigenetics

22 Nov 2019



tweetable



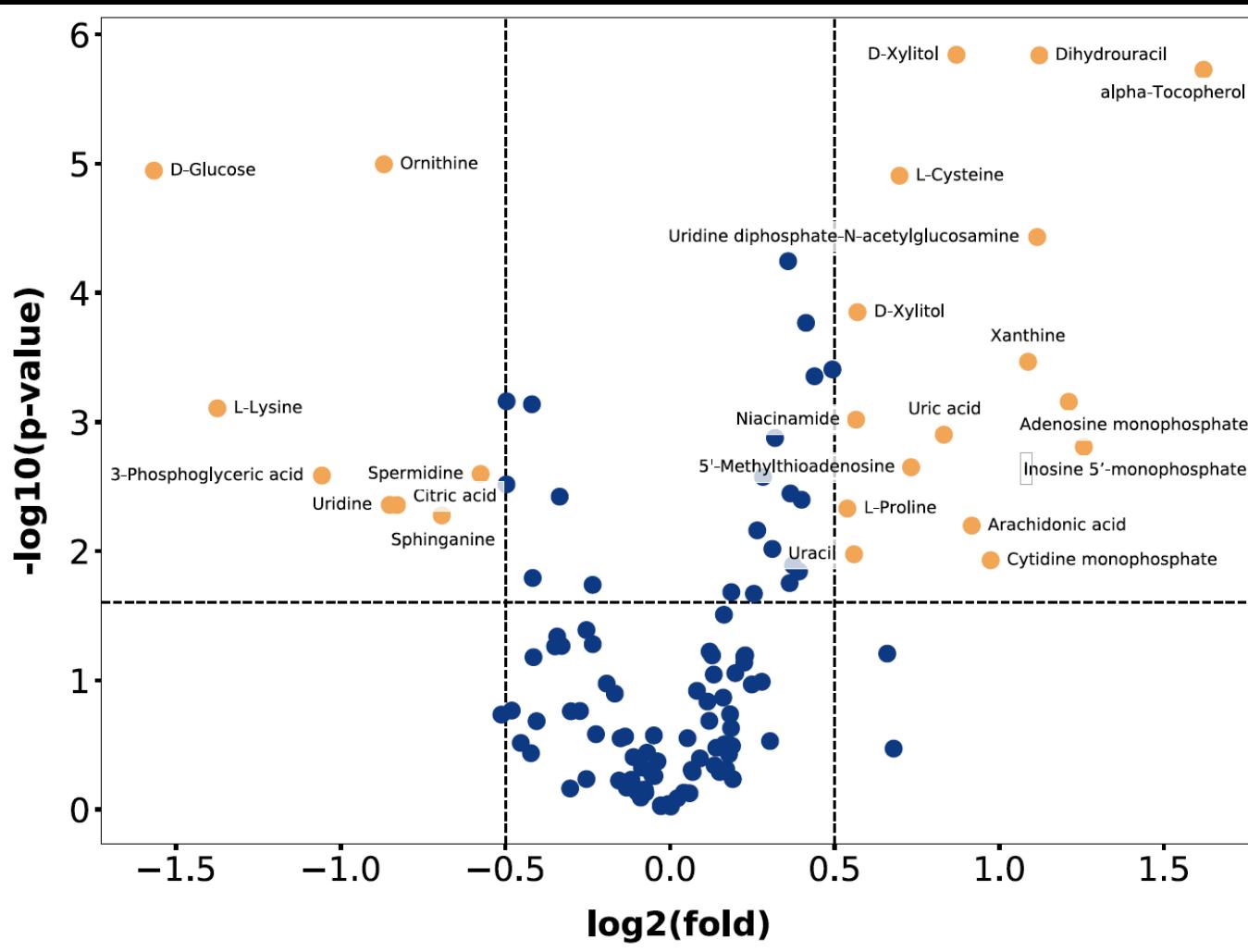
big little Red
gathering mind ate knew Take certain lived grandchild house
Forest running working dared took ill say live got time good
Pull poor fell mother better immediately door going
dated tap roundabout set sawing One seen afterwards far well
still see knocked wood child ran met woodcutters country extremely
butterscotch day called roundabout ran met woodcutters country extremely
pulled voice girl nearby wood creature
upon first dangerous beyond will brought fast pot butter
everybody gently cried beyond will brought fast pot butter
first go mill opened said talk asked path told prettiest
village latch answered taking come run around told great
shortest way another another another telling following
latch eyes answered taking come run around told great

WOLF Red Riding Hood
little cake made said

Challenges in data contextualization



Current conventions in metabolomics analysis



MetaboAnalyst

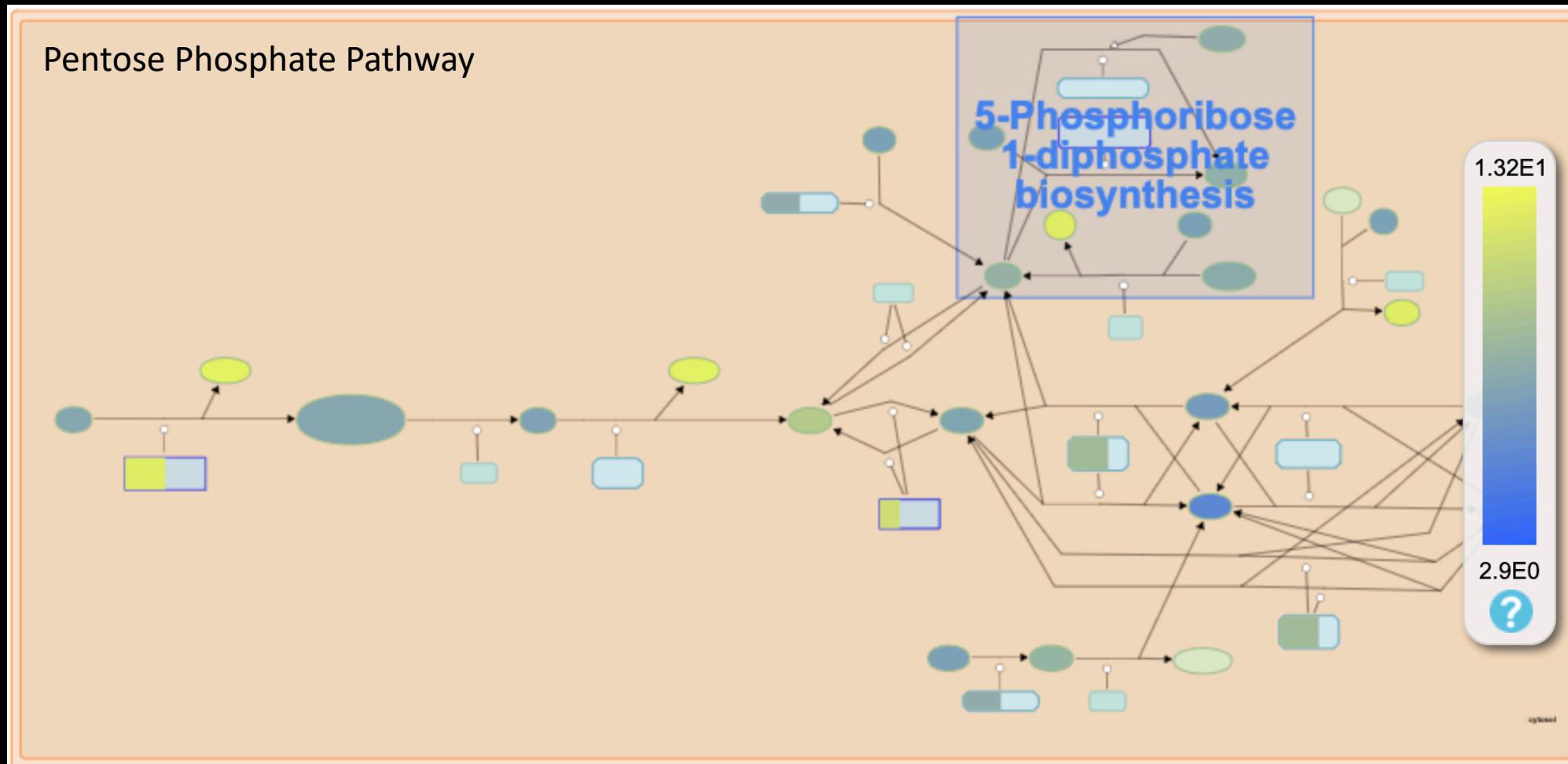
MetaboAnalyst - statistical, functional and integrative analysis of metabolomics data

Select an analysis path to explore :

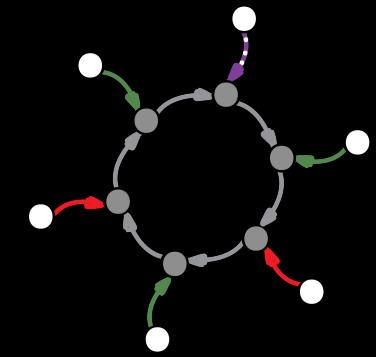
- Univariate Analysis**
 - Fold Change Analysis T-tests Volcano plot
 - One-way Analysis of Variance (ANOVA)
 - Correlation Analysis Pattern Searching
- Chemometrics Analysis**
 - Principal Component Analysis (PCA)
 - Partial Least Squares - Discriminant Analysis (PLS-DA)
 - Sparse Partial Least Squares - Discriminant Analysis (sPLS-DA)
 - Orthogonal Partial Least Squares - Discriminant Analysis (orthoPLS-DA)
- Feature Identification**
 - Significance Analysis of Microarray (and Metabolites) (SAM)
 - Empirical Bayesian Analysis of Microarray (and Metabolites) (EBAM)
- Cluster Analysis**
 - Hierarchical Clustering: Dendrogram Heatmaps
 - Partitional Clustering: K-means Self Organizing Map (SOM)
- Classification & Feature Selection**
 - Random Forest
 - Support Vector Machine (SVM)

Xia Lab @ McGill (last updated 2018-11-15)

Limited options for network perspectives

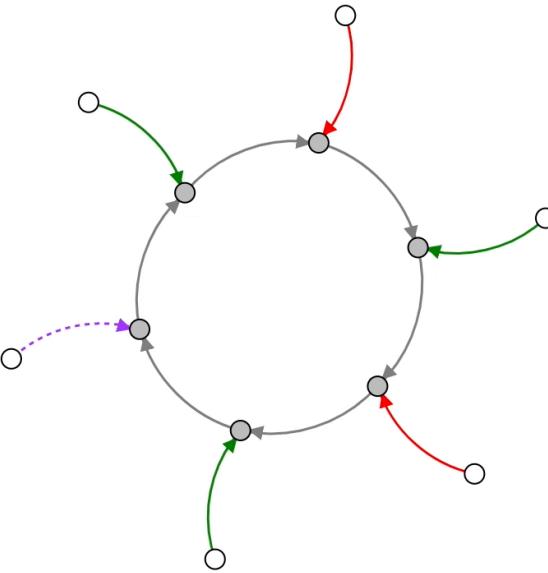


Metaboverse



- Computational framework built to be user friendly and near instantaneous in processing
- Low memory footprint – don't need a special computer to run
- Curated networks for all model organisms and more
- Integration of multi-omic data
 - RNA-Seq
 - Ribo-Seq
 - Proteomics
 - Metabolomics
 - Isotope tracing
 - etc





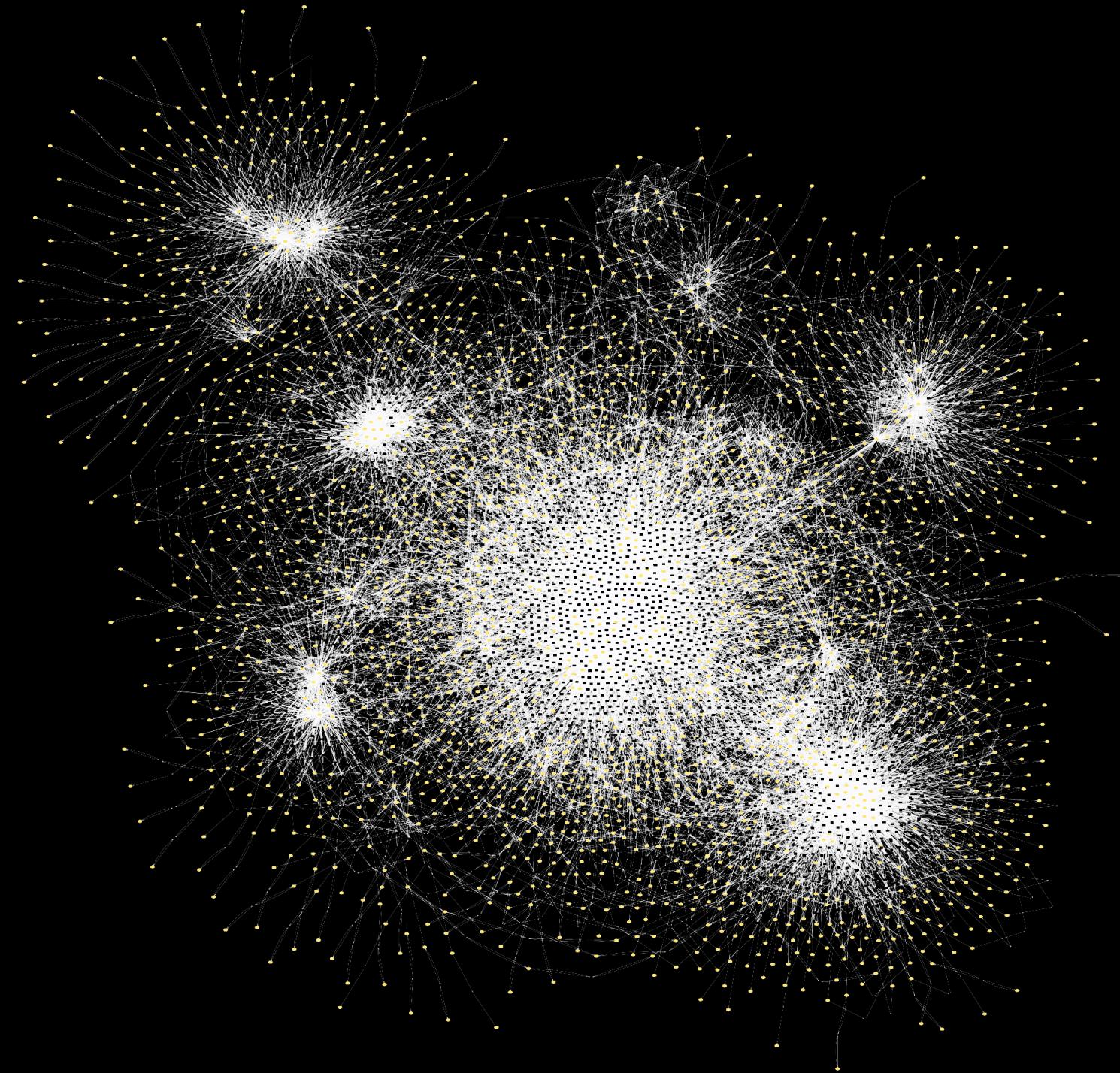
Metaboverse

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Welcome to Metaboverse. Let's get started...

1. Drag and drop a pre-existing pathway database (optional; file will end in ".json").

No file chosen



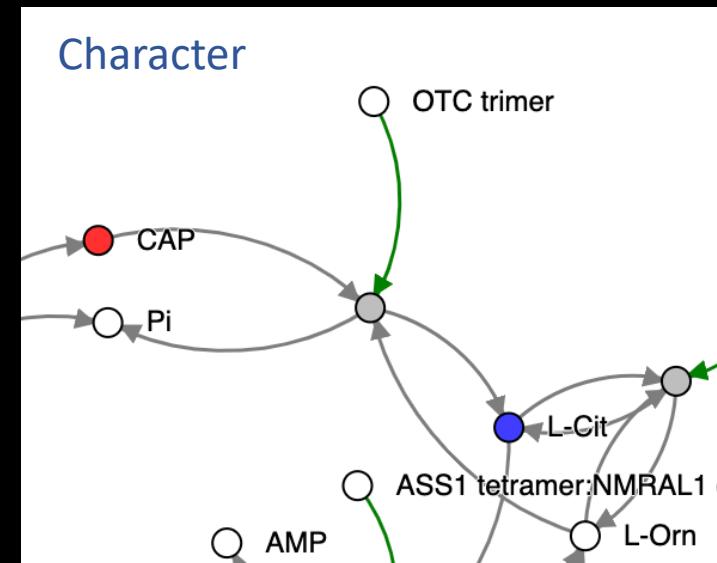
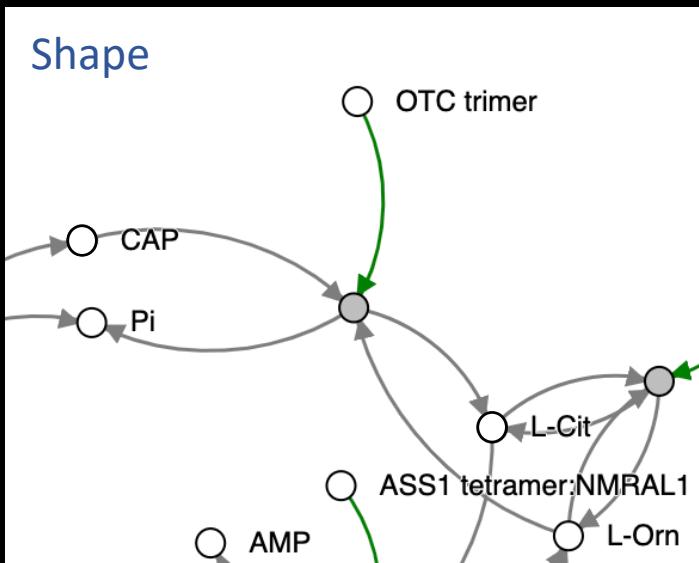
Automating analysis of regulatory events



Bei Wang



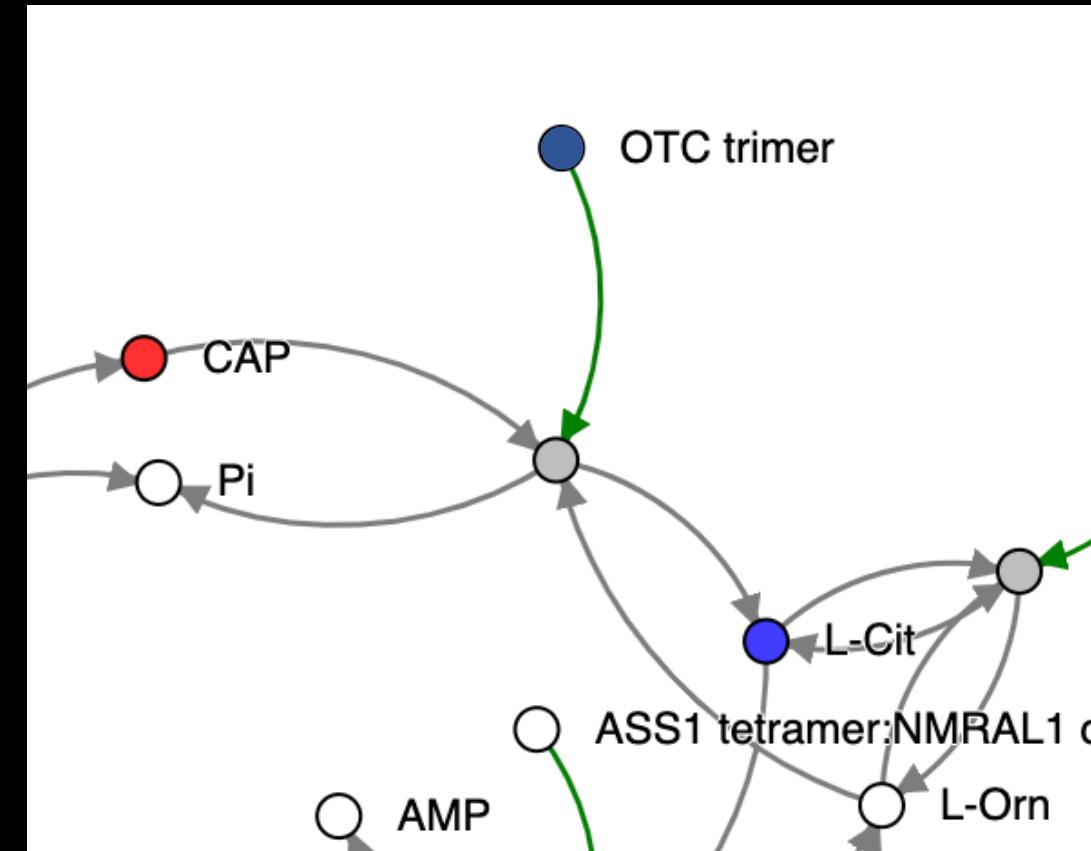
Youjia Zhou



Simulated Data

Inferring mechanism within the network

- Incorporates regulatory information
 - Catalysts
 - Inhibitors
 - Allostery
- Currently runs Reactome
- In future will integrate BRENDA and others



Simulated Data

The Metabolic Search Engine

Metabolic Pathways Visualization

Motif Type	Threshold
Av	1.5
MaxMax	2
MaxMin	2

Stamp View

Pathway View

Motif-Pathway

Youjia Zhou; Simulated Data

Legend:

● Reaction

○ No expression value

● Low expression

● High expression

→ Catalyst

→ Inhibitor

→ Gene Component

- Press Alt to pan and zoom

- Click and drag to pan

- Use mouse wheel to zoom

- Hover to display name

Toggle Feature Labels

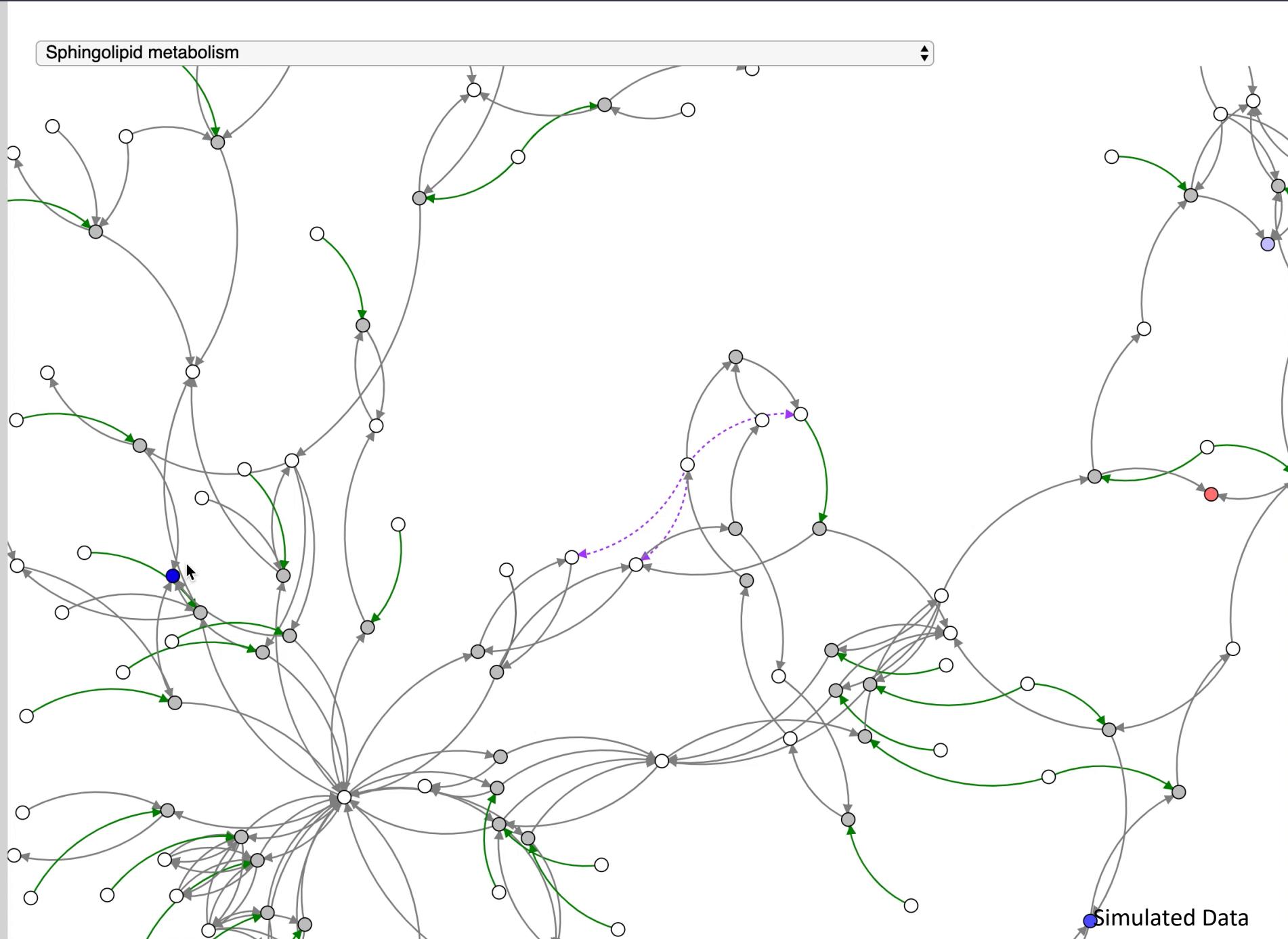
Toggle Reaction Labels

Toggle Expression

Options

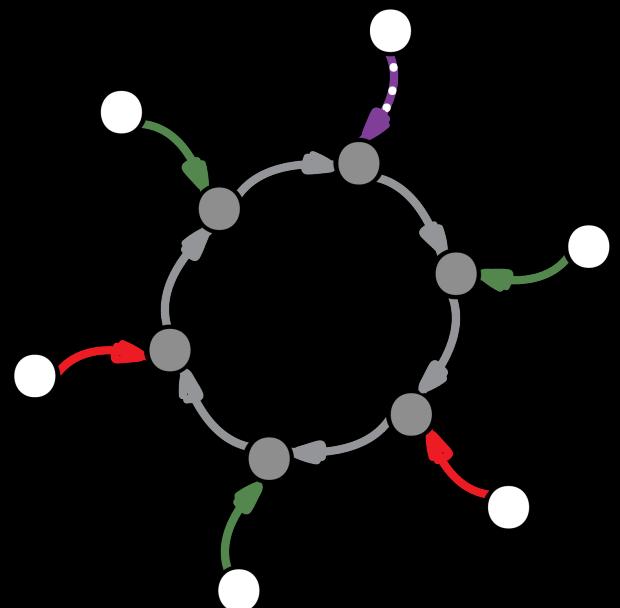
Nearest neighbors:

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Finding meaning in metabolism

- Rapidly identify all regulatory events in global network
- Interactive exploration of flux balance / time-course / other data
- And more planned for the future!



Thanks

- The Organizers
- Jared Rutter
- James Cox
- Bei Wang
- Youjia Zhou
- Cameron Waller
- Ian George
- The Metabolomics and Sensing Rutter Lab Core
- The Rutter Lab



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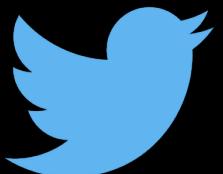
Questions?

- Find the presentation here: <https://github.com/j-berg/presentations>
 - Licensing: CC BY 4.0
- Email me at: [jordan.berg<at>biochem.utah.edu](mailto:jordan.berg@biochem.utah.edu)
- Expected beta release and pre-print:
 - Feb/Mar 2020
- Email: metaboverse@gmail.com
 - Request features
 - Update alerts

Explore the Metaboverse demo



github.com/Metaboverse



@jordanberg0
@RutterLab

