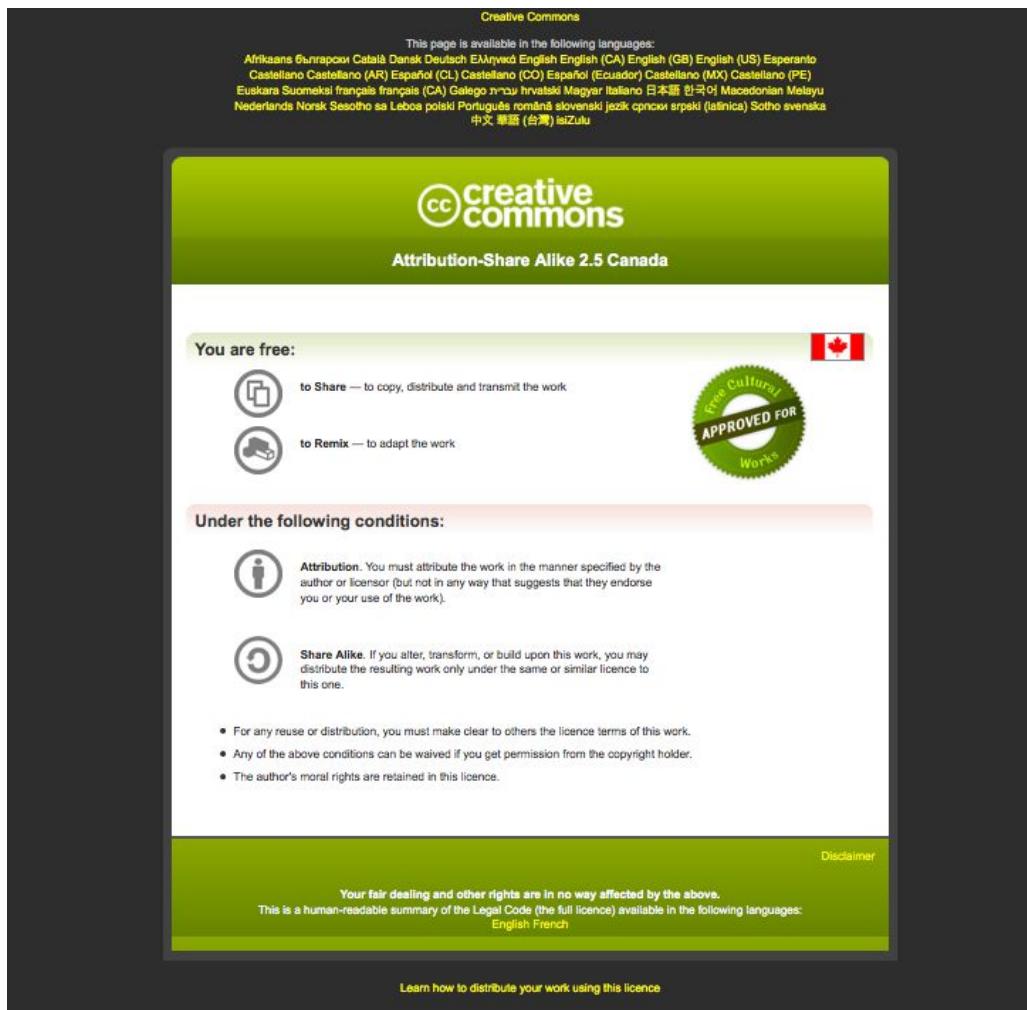




# Canadian Bioinformatics Workshops

[www.bioinformatics.ca](http://www.bioinformatics.ca)

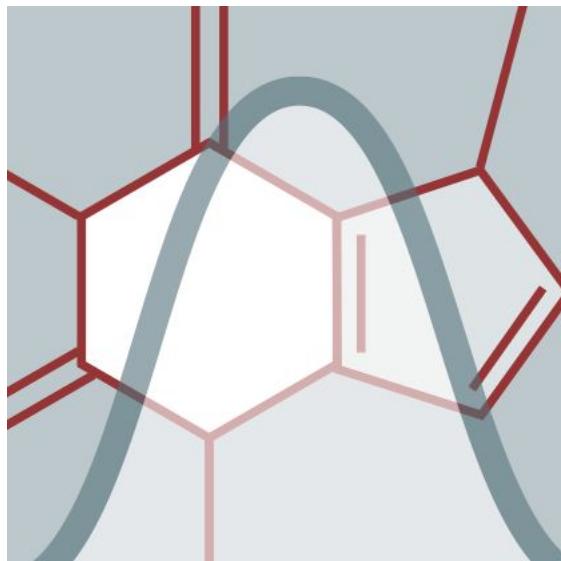
[bioinformaticsdotca.github.io](https://bioinformaticsdotca.github.io)



# Integrating Metabolomics with other Omics



Jianguo (Jeff) Xia  
Metabolomics Analysis  
July 6-7, 2023



**McGill**

# Learning Objectives

1. To understand common multi-omics study designs involving metabolomics
2. To become familiar with the common strategies in multi-omics integration
3. To learn how to use several web-based tools to perform common multi-omics integration

# *Beyond metabolomics*

Genomics

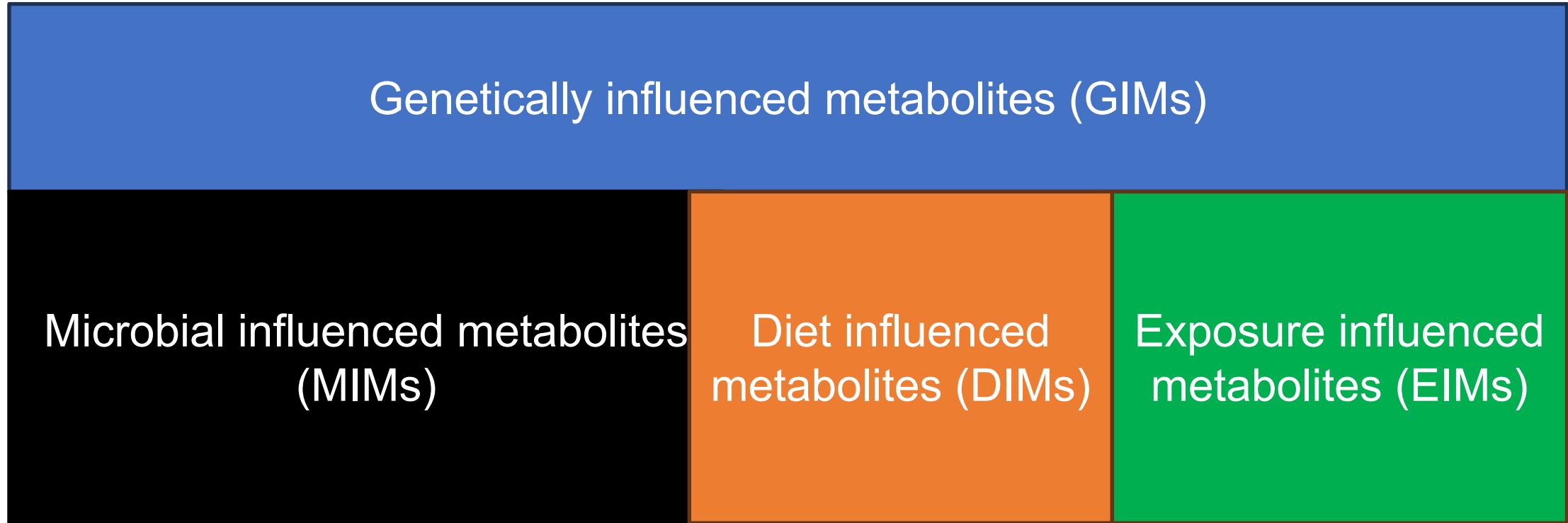
Microbiomics

Metabolomics

Foodomics

Exposomics

# Dissecting the metabolome



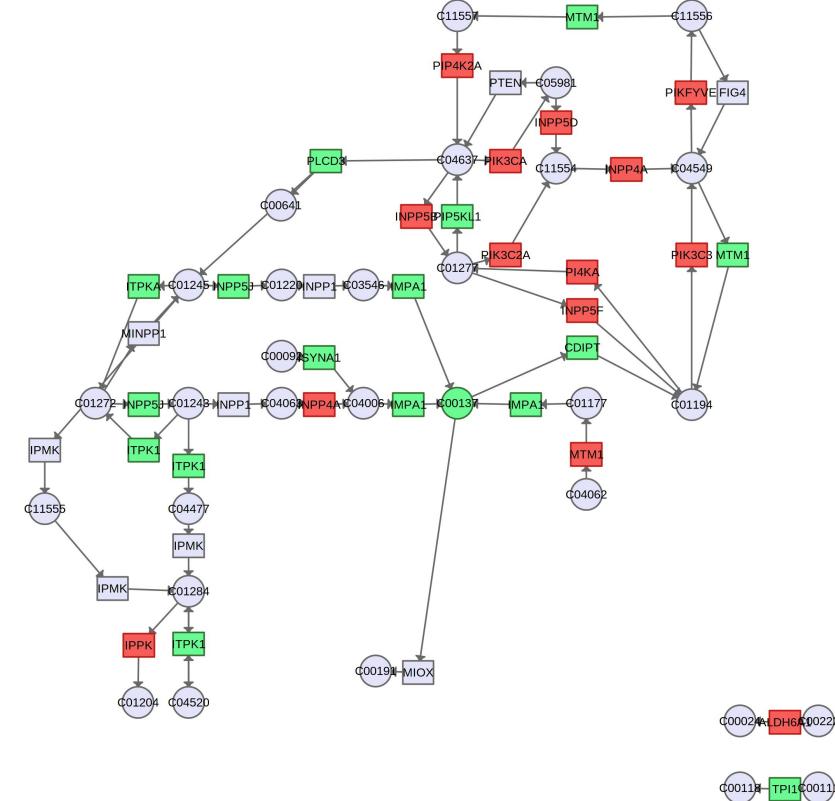
# Joint-pathway analysis

Input Data Type	Available Modules (click on a module to proceed, or scroll down for more details)						
Raw Spectra (mzML, mzXML or mzData)					LC-MS Spectral Processing		
MS Peaks (peak list or intensity table)			Functional Analysis	Functional Meta-analysis			
Annotated Features (compound list or table)		Enrichment Analysis	Pathway Analysis	Joint-Pathway Analysis	Network Analysis		
Generic Format (.csv or .txt table files)	Statistical Analysis	Biomarker Analysis	Time-series/Two-factor Analysis	Statistical Meta-analysis	Power Analysis	Other Utilities	

Integrating metabolomics (**peaks/compounds**) and transcriptomics (**genes**) are only supported by **Joint-pathway analysis**

# Joint pathway analysis

- Multi-omics input
  - Gene list
  - Compound / peak list
- When to integrate?
  - **Early integration (feature-level)**: merge the input lists and perform enrichment analysis
  - **Late integration (pathway-level)**: perform enrichment analysis separately and merge pathway p-values



# Early vs. late integration

- Early (feature-level) integration
  - Often dominated by the “big” omics
    - ~10s DE compounds combined with ~100s of DE genes
  - Not clear how to merge peaks with genes
- Late (pathway-level) integration
  - Flexible integration of different evidence based on p values
    - Fisher’s method: emphasize small p values
    - Stouffer’s method: p values are treated equally
  - Can be used to integrate peaks and genes

# Towards unified framework for individual omics data analysis

 MetaboAnalyst 5.0 - user-friendly, streamlined metabolomics data analysis

News & Updates

- MetaboAnalyst 5.0 is launched! [View](#)
- Fixed the issue with synchronized 3D scatter plots for scores and loadings (04/12/2021); [View](#)
- Upgraded to PrimeFaces 10 and fixed the issue for multi-group figure legend (04/08/2021); [View](#)
- Added support for merging technical replicates with different mathematical models and QC measures (02/18/2021); [View](#)
- Updated KEGG IDs in internal compound databases (02/09/2021); [View](#)
- Enhanced name handling to better accommodate special characters in compound/lipid names (02/09/2021); [View](#)
- Added [server tutorials](#) introducing new features in MetaboAnalyst 5.0 (01/15/2021); [View](#)
- Users can perform meta-analysis of global metabolomics data using [Functional Meta-analysis](#) module as illustrated in our [COVID-19 paper](#) (01/09/2021); [View](#)
- Updated the KEGG global metabolite map for better metabolome coverage (01/08/2021); [View](#)

Home  
Data Formats  
Tutorials  
FAQs  
APIs  
Update History  
MetaboAnalystR  
Contact  
User Stats  
Publications  
About  
  


 PROTOCOL EXTENSION  
<https://doi.org/10.1038/s41596-022-00710-w>  


## Using MetaboAnalyst 5.0 for LC-HRMS spectra processing, multi-omics integration and covariate adjustment of global metabolomics data

 Article  
<https://doi.org/10.1038/s41467-023-38785-y>  


## ExpressAnalyst: A unified platform for RNA-seq analysis in non-model species

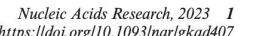
 MicrobiomeAnalyst -- comprehensive statistical, functional and integrative analysis of microbiome data

Please choose a module based on your data

Marker Data Profiling Analyze marker gene counts data	Shotgun Data Profiling Analyze shotgun metagenomics data	Taxon Set Analysis Discover enriched microbial signatures
Microbial Metabolomics Co-analyze microbiome & metabolomics data	Statistical Meta-analysis Integrate multiple marker gene data	Raw Data Processing Convert 16S/18S/ITS reads to ASV table

Please use [OmicsForum](#) for support & troubleshooting request

Publications

 Nucleic Acids Research, 2023 |  
<https://doi.org/10.1093/nar/gkad407>

## MicrobiomeAnalyst 2.0: comprehensive statistical, functional and integrative analysis of microbiome data

Yao Lu<sup>1</sup>, Guangyan Zhou<sup>2</sup>, Jessica Ewald<sup>2</sup>, Zhiqiang Pang<sup>2</sup>, Tanisha Shiri<sup>2</sup> and Jianguo Xia<sup>1,2,3,\*</sup>

<sup>1</sup>Department of Microbiology and Immunology, McGill University, Quebec, Canada, <sup>2</sup>Institute of Parasitology, McGill University, Quebec, Canada and <sup>3</sup>Department of Animal Science, McGill University, Quebec, Canada

Received February 28, 2023; Revised April 17, 2023; Editorial Decision May 02, 2023; Accepted May 03, 2023

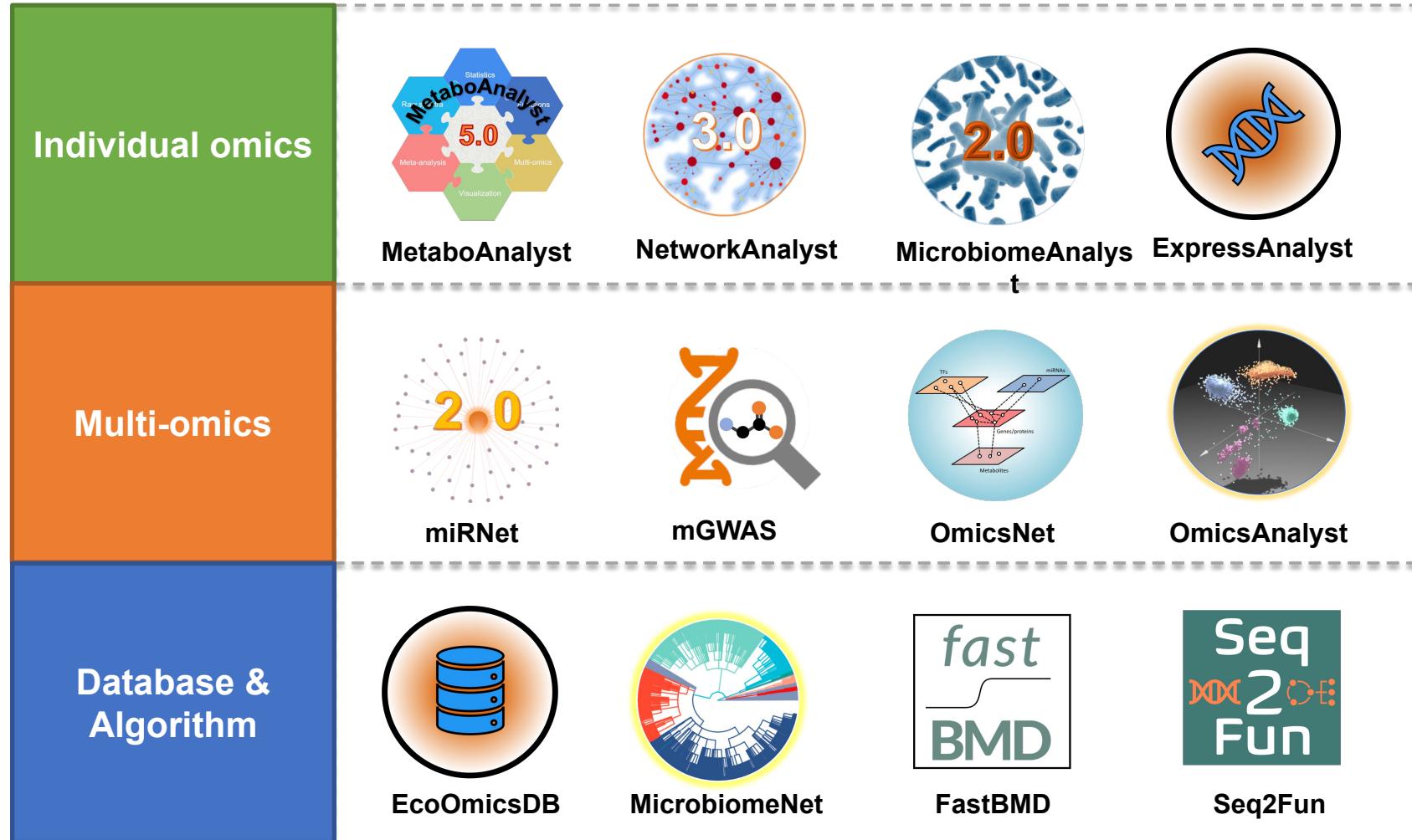
### ABSTRACT

Microbiome studies have become routine in biomedical, agricultural and environmental sciences with diverse aims, including diversity profiling, functional characterization, and translational applications. The resulting complex, often multi-omics datasets demand powerful, yet user-friendly bioinformatics tools

### GRAPHICAL ABSTRACT



# An ecosystem for omics data analytics



# # 1. Linking metabolomics to genomics

- **mGWAS**
- **mGWAS-explorer**

# Metabolite Genome-Wide Association Study (mGWAS)

Linking the genomics with metabolomics to identify genetic variants affecting metabolite levels

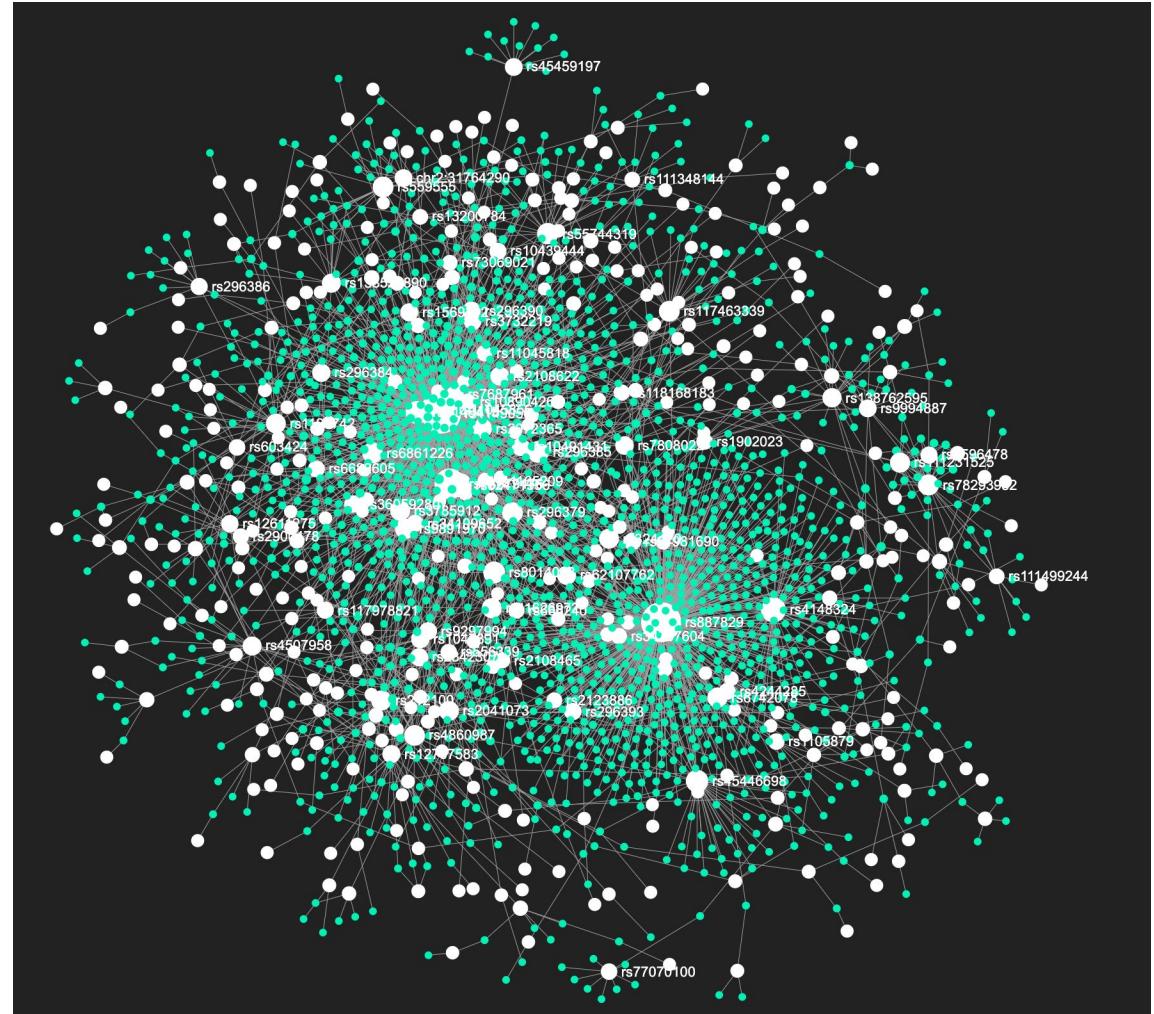
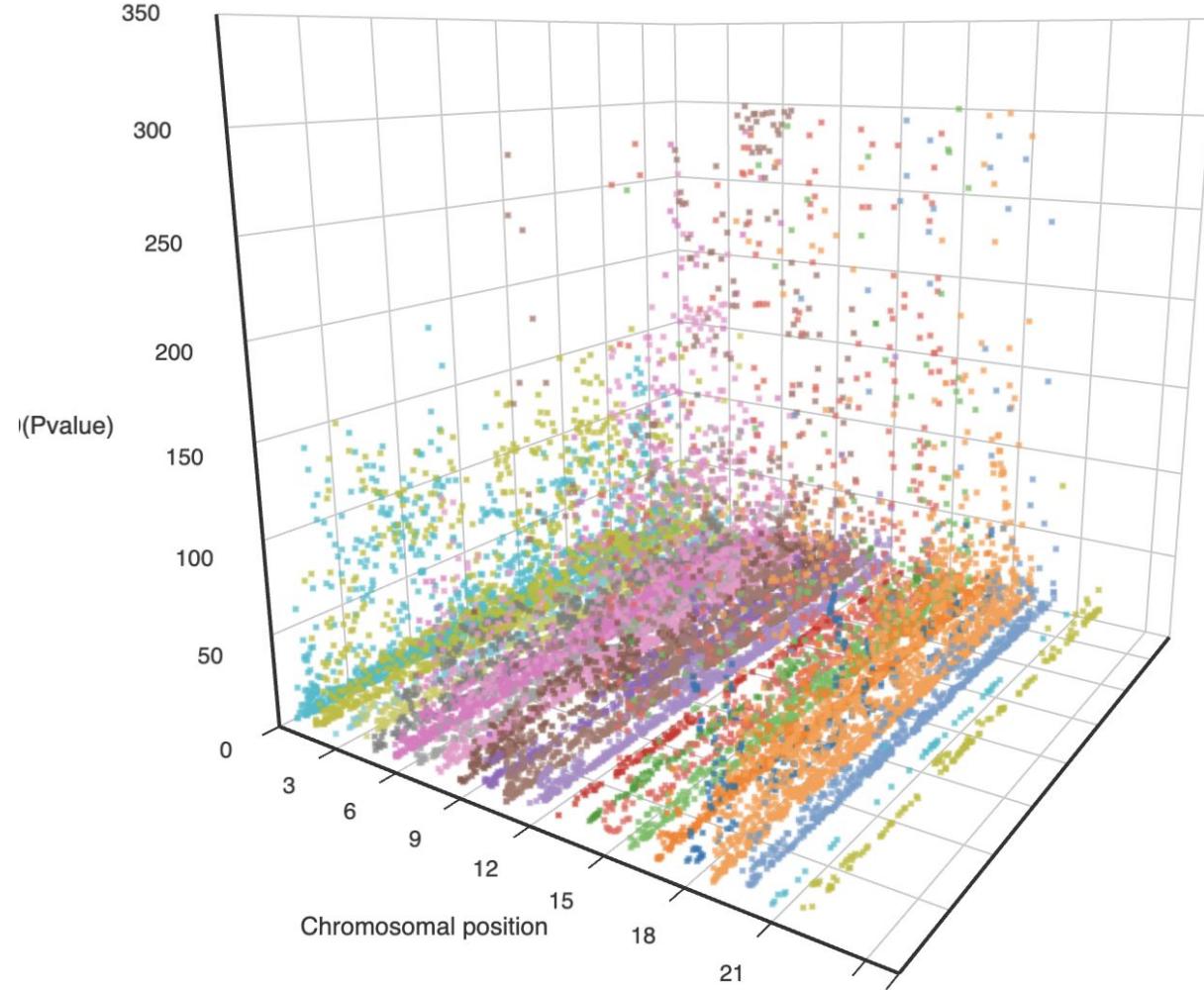
Sample Type	Study #	* Metabolite #	** Metabolite Ratio #	SNP #	SNP-Metabolite Associations #
Blood	57	3992	1265	67,570	30,3090
Urine	5	271	1123	6877	9647
Saliva	1	14	0	1364	1454
Cerebrospinal fluid (CSF)	1	15	0	1178	1182
Mitochondria	1	0	390	194	404
Sum (unique)	65	4147	2388	73,737	313,720

Chang et al. *Metabolites* 2022, 12(6), 526

# Browse mGWAS studies

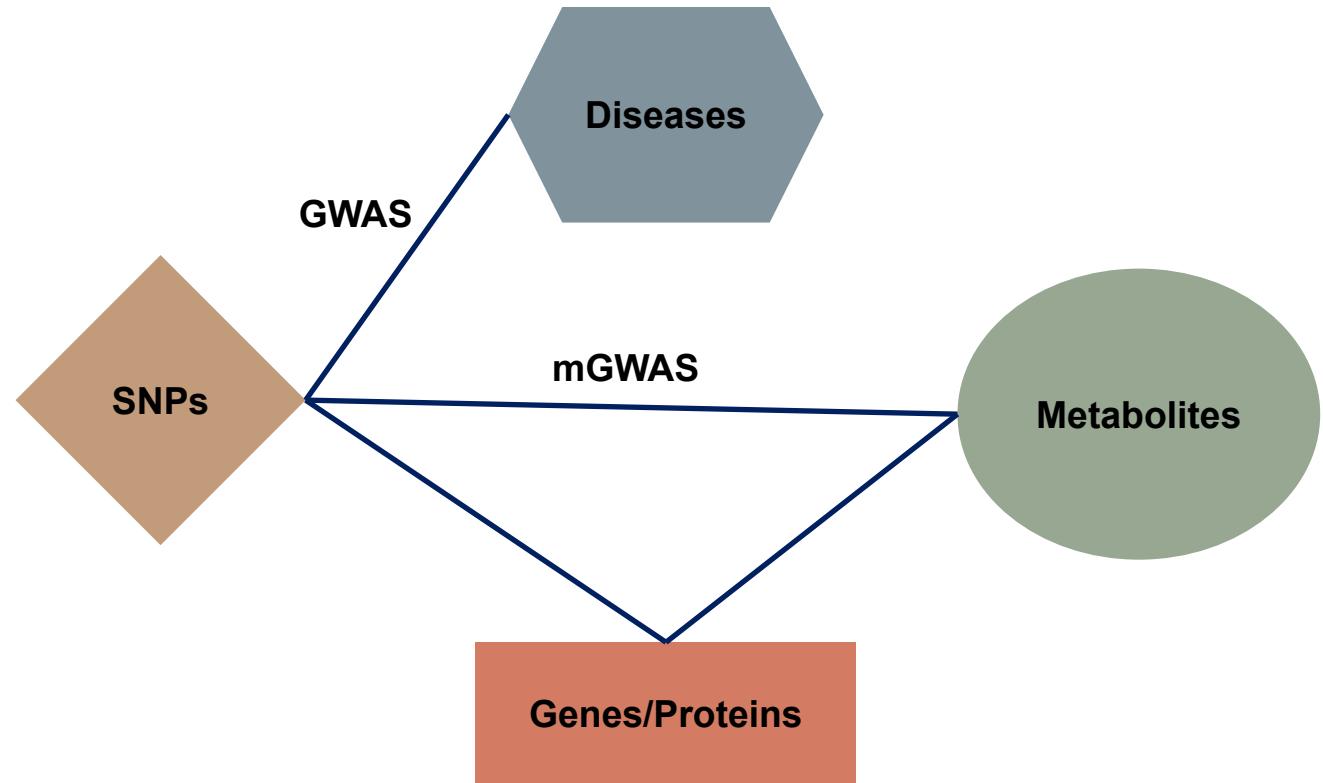
ID	Biofluid	Study	Publication	Sample Size	Population	Genotyping Platform	Metabolomics Platform	Cutoff Threshold	Browse
65b	Blood	Viñuela_medRxiv_2021_targeted	<a href="#">Genetic analysis of blood molecular phenotypes reveals regulatory networks affecting complex traits: a DIRECT study</a>	3029	European	Illumina HumanCore array (HCE24 v1.0)	BIOCRAVES (AbsoluteIDQ™ p150 kit)	5e-08	 View
65a	Blood	Viñuela_medRxiv_2021_untargeted	<a href="#">Genetic analysis of blood molecular phenotypes reveals regulatory networks affecting complex traits: a DIRECT study</a>	3029	European	Illumina HumanCore array (HCE24 v1.0)	Metabolon (LC-MS/MS)	5e-08	 View
64	Blood	Qin_medRxiv_2020	<a href="#">Genome-wide association and Mendelian randomization analysis prioritizes bioactive metabolites with putative causal effects on common diseases</a>	8738	European	Illumina genome-wide SNP arrays (HumanCoreExome BeadChip, Human610-Quad BeadChip and HumanOmniExpress)	Thermo Q Exactive Orbitrap	4.5e-12	 View
63	Blood	Borges_UKBB_2020	<a href="#">Metabolic biomarkers in the UK Biobank measured by Nightingale Health 2020</a>	500000	European	Affymetrix genome-wide genotyping array	Nightingale NMR	5e-08	 View
62	Blood	Montasser_bioRxiv_2021	<a href="#">Leveraging a founder population to identify novel rare-population genetic determinants of lipidome</a>	650	Old Order Amish founder population	Affymetrix 500K array	Agilent (6550 Q-TOF LC/MS)	5e-08	 View
61	Mitochondria	Aboulmaouahib_HMG_2021	<a href="#">First mitochondrial genome wide association study with metabolomics</a>	2718	European	Illumina MiSeq	BIOCRAVES (AbsoluteIDQ™ p150 kit)	1e-05	 View
60	Blood	Harshfield_BM_2021	<a href="#">Genome-wide analysis of blood lipid metabolites in over 5000 South Asians reveals biological insights at cardiometabolic disease loci</a>	13814+5662	European+South Asian	Illumina 660-Quad, Illumina HumanOmniExpress, Affymetrix	Thermo Q Exactive Orbitrap	8.9e-10	 View

# Associations between SNPs and compounds/peaks

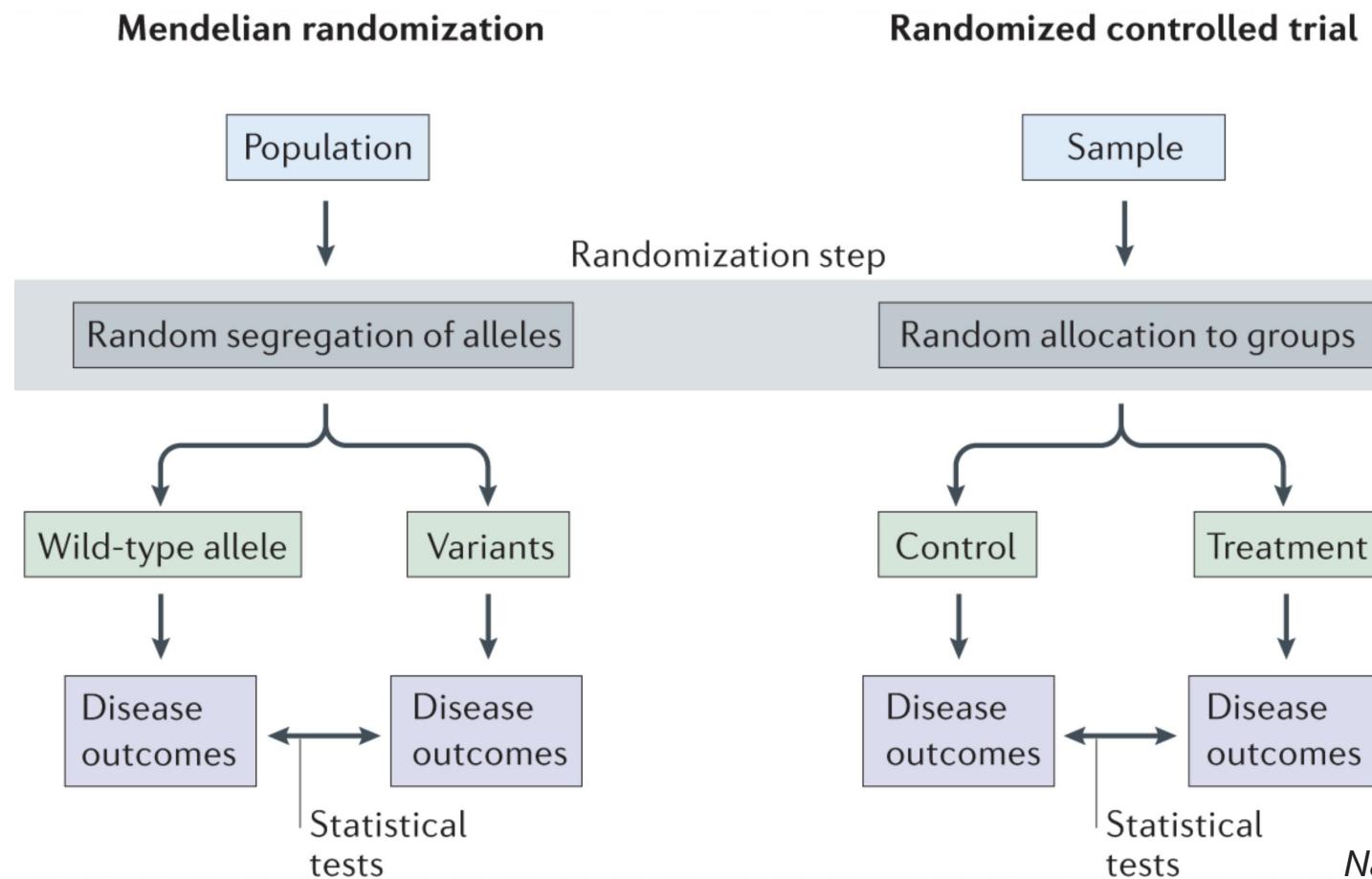


# Understanding genetic influenced metabolome

- SNP to gene mapping
  - Positions
  - LD proxy
  - QTLs: eQTLs, pQTLs
- SNP-disease mapping
  - GWAS
- Proteins
  - Enzymes, transporters
  - Protein-protein interactions



# Correlation vs causal relationship?

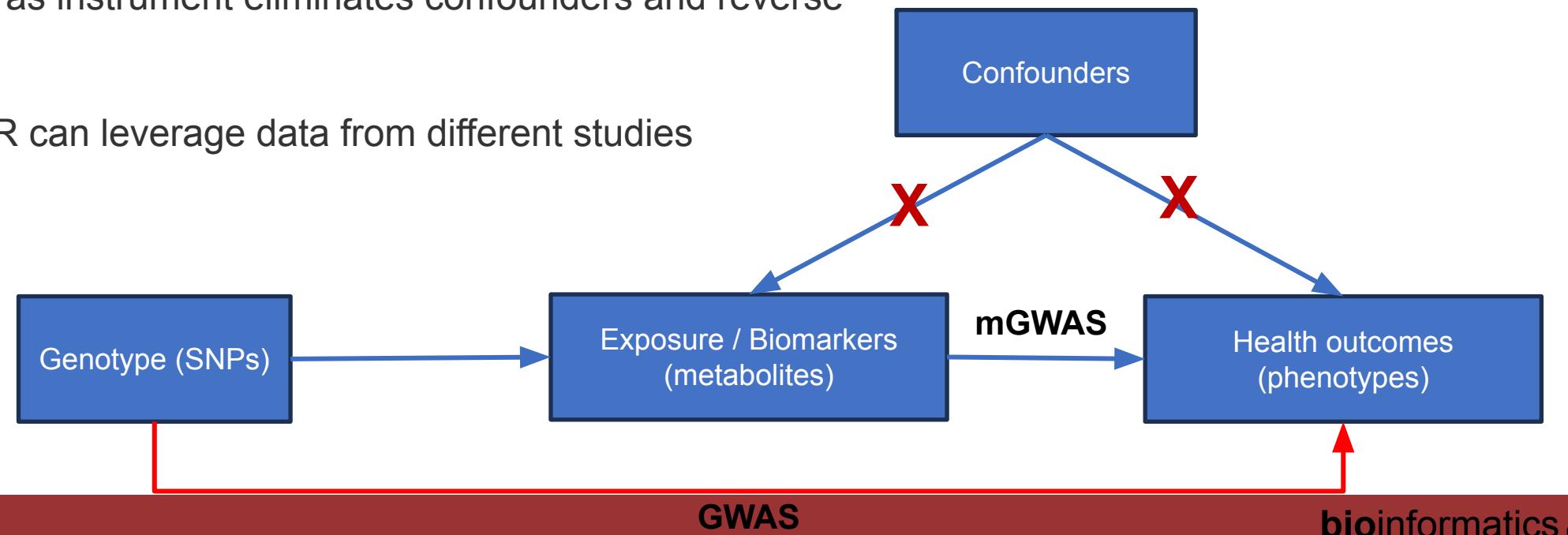


*Nat Rev Methods Primers* 2, 6 (2022)

**Mendelian randomization (MR) analysis:** nature's randomized controlled trials

# Mendelian randomization analysis

- Based on Mendel's laws of inheritance and instrumental variable estimation methods
- If an exposure / biomarker is causal for a disease, then genetic variants which influence the levels of the biomarker should result in a higher risk of the disease.
- Using genetics as instrument eliminates confounders and reverse causality
- Two sample MR can leverage data from different studies



# Linking metabolites with SNPs and phenotypes

The screenshot shows the homepage of the mGWAS-Explorer website. At the top is a blue header bar with the logo "mGWAS-Explorer" and navigation links for Home, Tutorials, Forum, mGWASR, and Updates. Below the header is a grid of eight colored boxes arranged in two rows of four. The top row contains "Start with Metabolites" (blue), "Start with SNPs" (green), "Start with Genes" (purple), and "Integrated Search" (light gray). The bottom row contains "MR Analysis" (dark purple), "Browse mPheWAS" (yellow), "Browse mGWAS" (light blue), and "mGWASR Package" (orange). Each box has a brief description below it. Below the grid is a note to use the OmicsForum for support. A red-bordered box in the center contains the website URL "www.mgwas.ca". At the bottom are three columns: "Comprehensive Libraries", "Causal Analysis", and "Functional Insights", each with a detailed description.

**mGWAS-Explorer**

Home Tutorials Forum mGWASR Updates

Start with Metabolites Connect metabolites to SNPs, genes or diseases	Start with SNPs Connect SNPs to genes, metabolites or diseases	Start with Genes Connect genes to SNPs, metabolites or diseases	Integrated Search Joint search of individual SNP and/or metabolite
MR Analysis Perform Mendelian randomization analysis	Browse mPheWAS Browse phenome-wide MR of metabolome	Browse mGWAS Browse 65 manually curated mGWAS studies	mGWASR Package Use R package for batch processing or extension

Please use [OmicsForum](#) for support & troubleshooting request

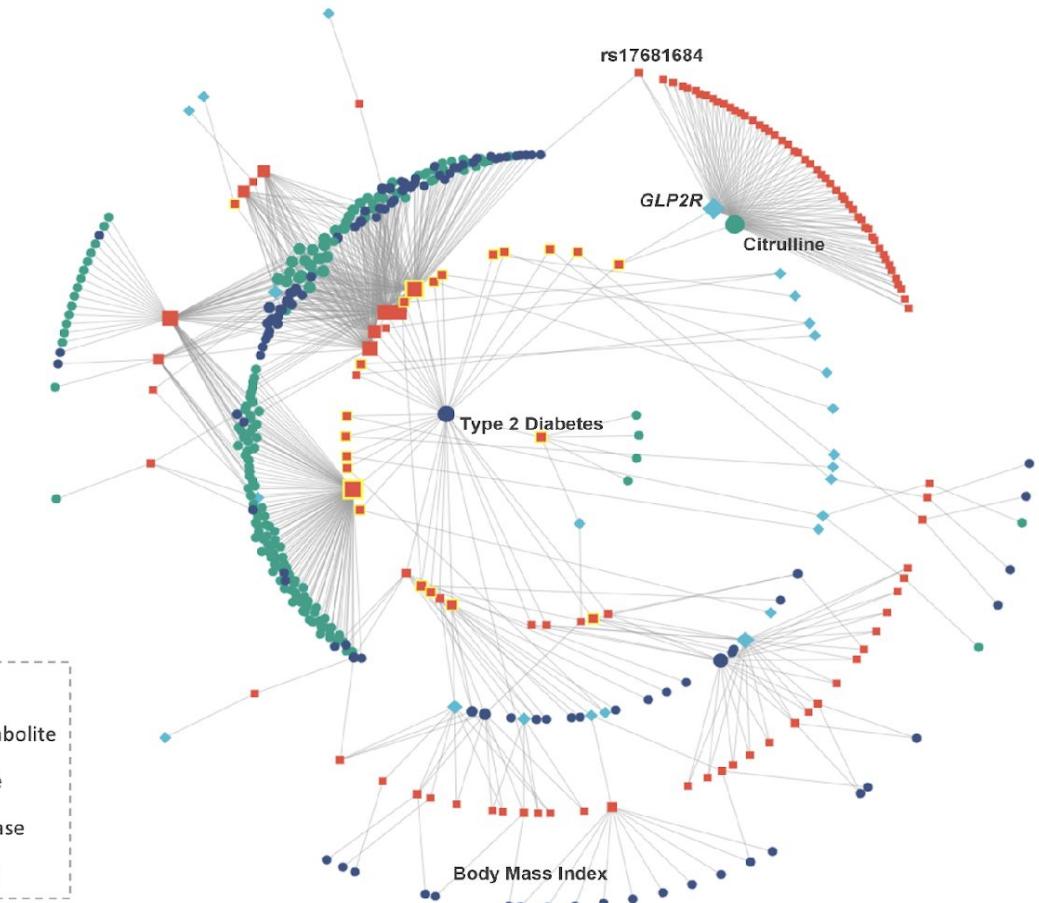
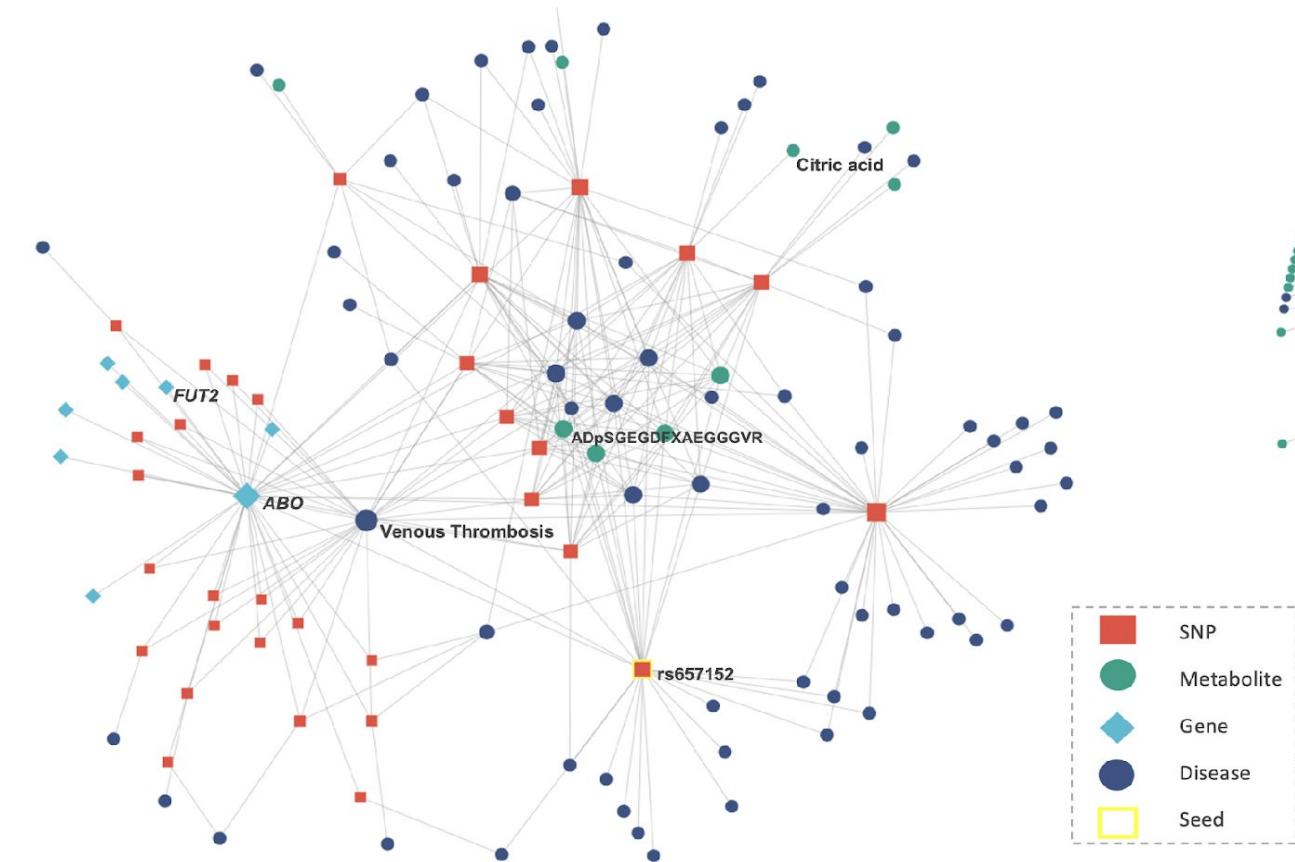
**www.mgwas.ca**

**Comprehensive Libraries**  
Comprehensive collection and deep annotation of results from [65 mGWAS publications](#). Integrated with HaploReg, VEP, KEGG, Transporter Classification Database (TCDB), Recon3D, as well as common PPI databases.

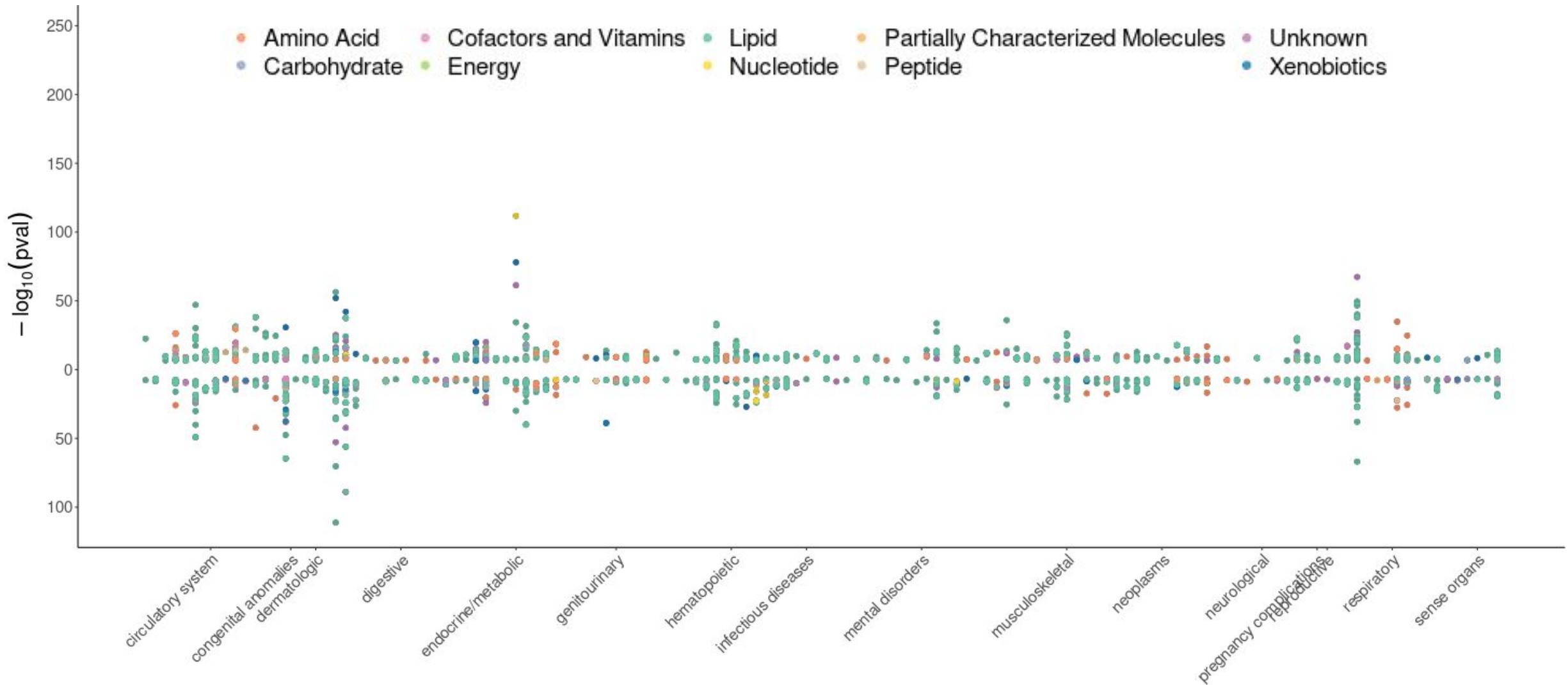
**Causal Analysis**  
Leverage known diseases associated with SNPs, genes or metabolites to perform causal analysis causal analysis between >4000 metabolites and various disease phenotypes based on two sample Mendelian randomization, with comprehensive support for data harmonization

**Functional Insights**  
Create and visually explore SNP, gene, metabolite, eQTL, pQTL, or disease networks, coupled with enrichment analysis; Or perform semantic triples analysis for triangulation of evidence based on literature mining.

# Metabolites, genes, SNPs and diseases



# 825 metabolites on 236 disease phenotypes



# Potential causal associations between >800 metabolites and >200 diseases

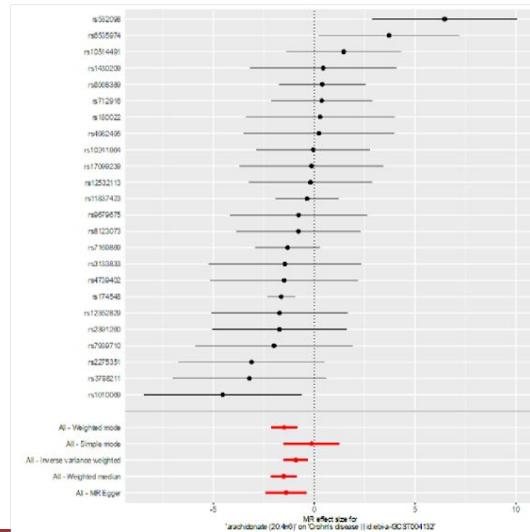
			SNP		Pval
Atherosclerotic heart disease	serine		5	-0.0279495	0.00203363 5.5606E-43
	sm c24:0		5	0.02832925	0.00217185 6.8912E-39
	sm (oh) c22:2		5	0.02907336	0.0022289 6.8912E-39
Inflammatory bowel disease	x-11381		3	-0.8251061	0.04109667 1.1679E-89
	nervonoylcarnitine (c24:1)*		3	-0.9093196	0.04529115 1.1679E-89
	margaroylcarnitine (c17)*		2	-1.0991236	0.06922023 8.9079E-57
	linoleoylcarnitine (c18:2)*		2	-0.8909735	0.05611142 8.9079E-57
	x-24241		1	-1.2770696	0.09285142 4.8253E-43
	histidine betaine (hercynine)*		1	1.24068493	0.09046718 8.3483E-43
	pc aa c32:2		5	0.46386518	0.03590836 3.5615E-38
	pc ae c34:2		5	0.4087556	0.03164226 3.5615E-38
	1-oleoyl-2-eicosapentaenoyl-gpc (18:1/20:5)		4	-0.2323055	0.0195418 1.3726E-32
	arachidoylcarnitine (c20)*		1	-0.9189255	0.07831706 8.5934E-32
Asthma	nisinate (24:6n3)		4	-0.3856061	0.03335131 6.4236E-31
	x-11381		3	0.04781557	0.0027428 4.6252E-68
	pc ae c36:3		8	-0.021023	0.00120984 1.2411E-67
	1-oleoyl-2-eicosapentaenoyl-gpc (18:1/20:5)		4	0.02003149	0.00134398 3.0763E-50
	linoleoylcarnitine (c18:2)*		2	0.05415016	0.00374454 2.1338E-47
	docosatrienoate (22:3n6)*		3	0.0276776	0.00206776 7.3688E-41
	1-eicosapentaenoyl-gpc (20:5)		3	0.02112966	0.00162433 1.0981E-38
	1-palmitoyl-2-eicosapentaenoyl-gpc (16:0/20:5)		3	0.02159433	0.00166005 1.0981E-38
	1-dihomo-linolenoyl gpe (20:3n3 or 6)		3	-0.016672	0.00128165 1.0981E-38

# Explore causally links and evidences

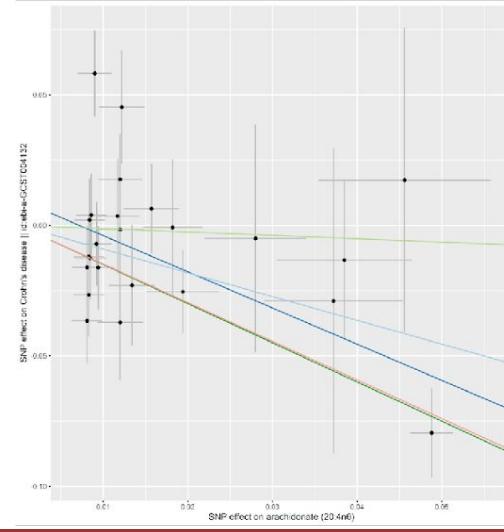
(a)

Methods	MR Results				Heterogeneity Tests			Horizontal Pleiotropy		
	Number of SNPs	Beta	SE	P value	Q	Q_df	Q_pval	Egger intercept	SE	P value
Inverse variance weighted	24	-0.91	0.313	0.0036	42.1	23	0.00893	-	-	-
MR Egger	24	-1.39	0.523	0.0146	39.7	22	0.0116	0.00993	0.00877	0.27
Simple mode	24	-0.128	0.711	0.858	-	-	-	-	-	-
Weighted median	24	-1.5	0.323	3.46e-06	-	-	-	-	-	-
Weighted mode	24	-1.48	0.315	9.73e-05	-	-	-	-	-	-

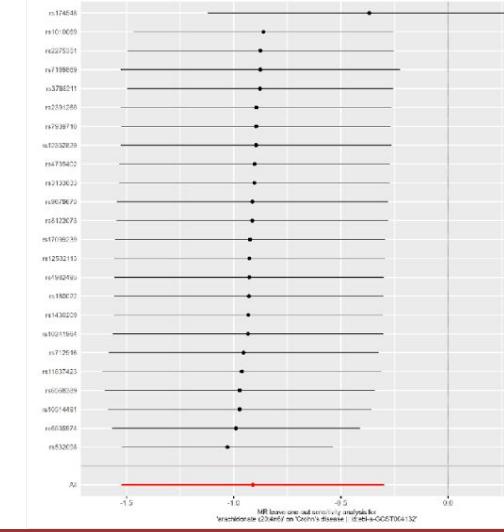
(b)



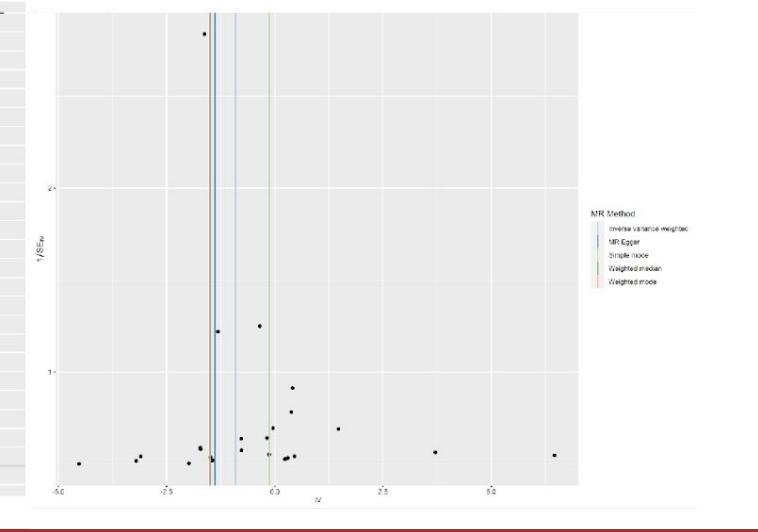
(c)



(d)



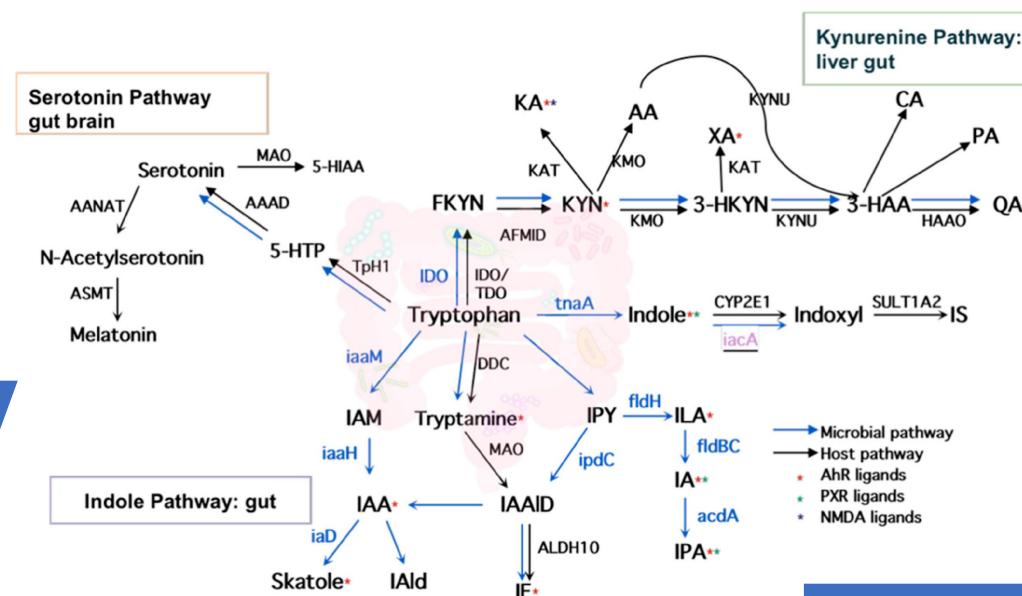
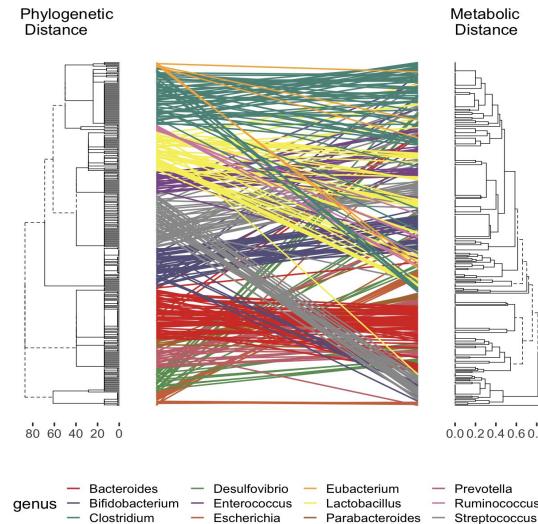
(e)



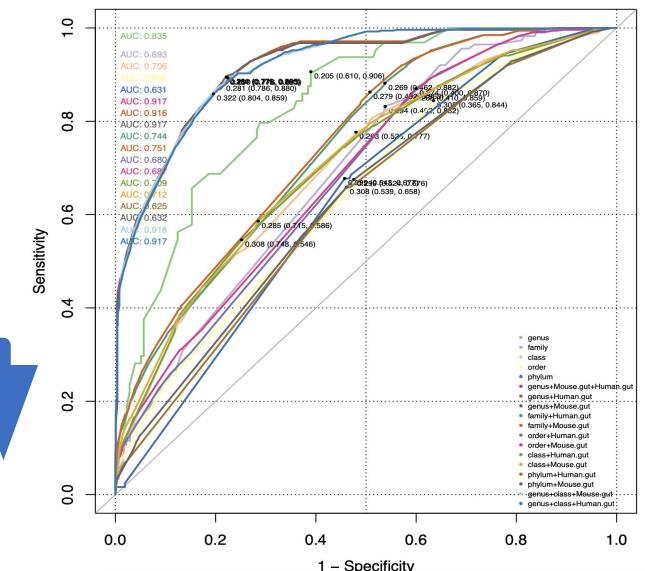
## # 2. Linking metabolomics to microbiomics

- Leveraging GEMs
- Predictive modeling
- Contextualized network analysis

# Predicting metabolome based on taxonomy profiles

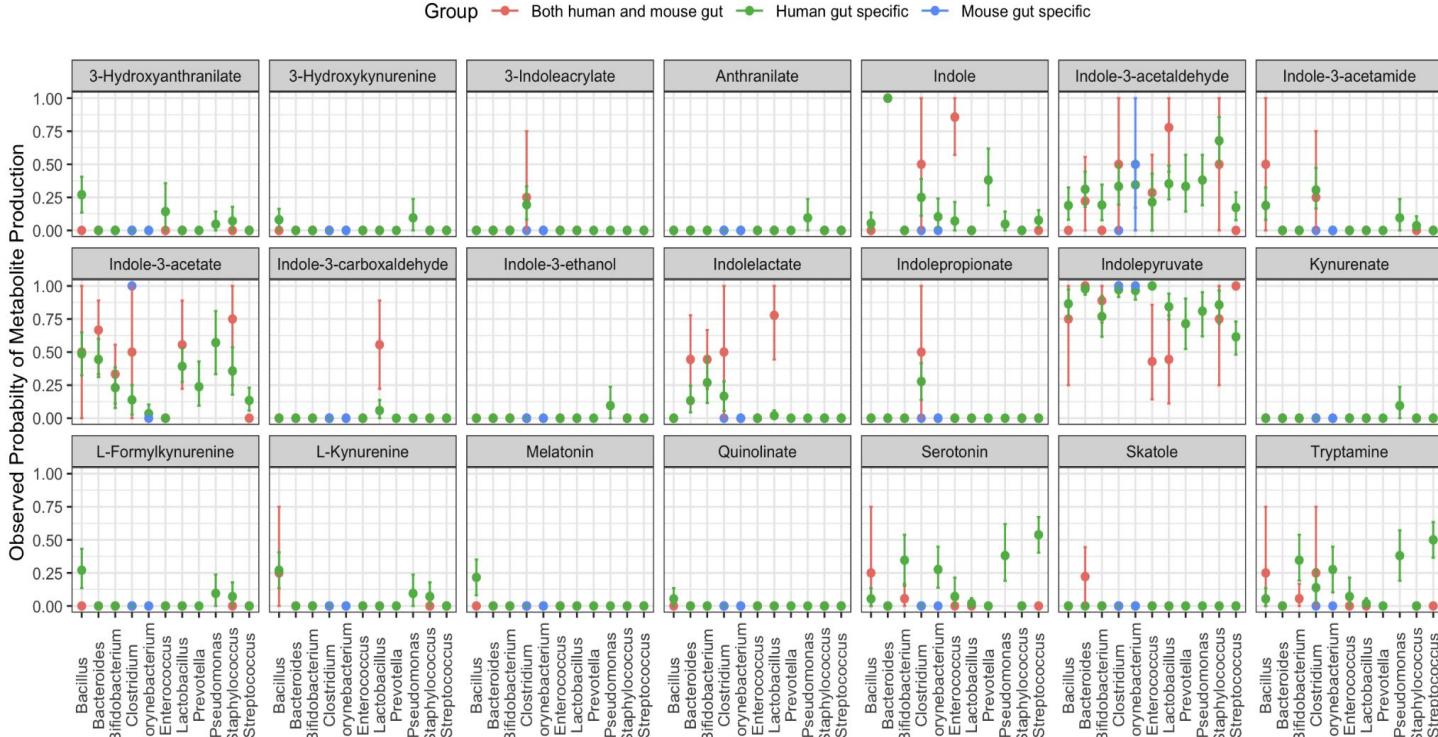


Predict tryptophan metabolites from 16S rRNA abundance information using  
Bayesian logistic regression models

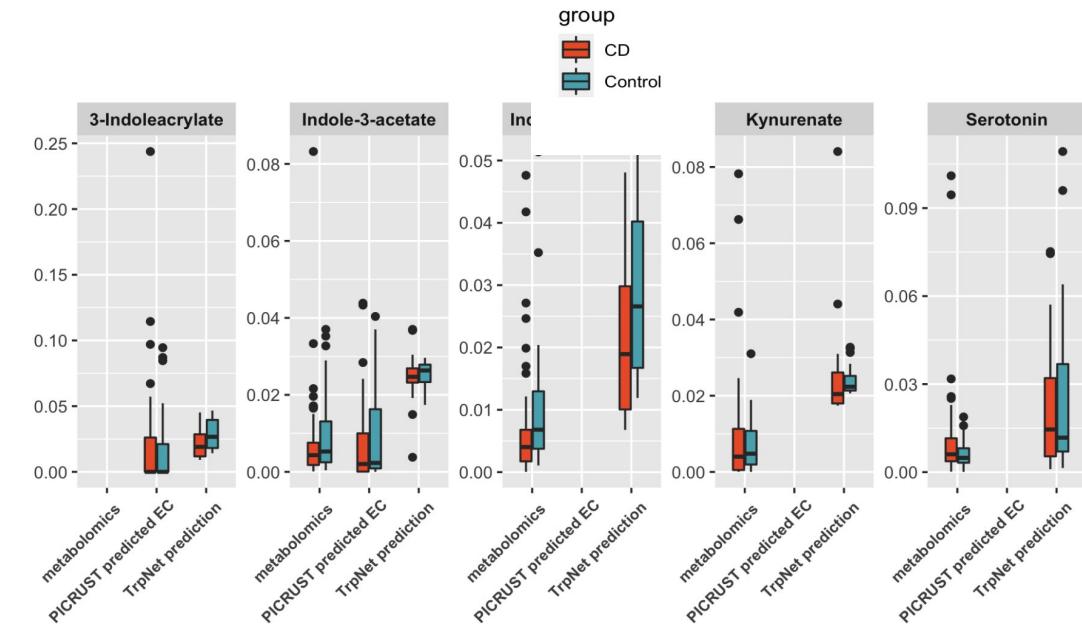


Lu, et al, Metabolites 2022, 12(1), 10

# Performance varies – taxa, metabolites and hosts



Lu, et al, *Metabolites* 2022, 12(1), 10



# A unified platform for microbiomics

The screenshot shows the MicrobiomeAnalyst 2.0 homepage. At the top left is a circular logo with '2.0' in the center. To its right is the header: 'MicrobiomeAnalyst -- comprehensive statistical, functional and integrative analysis of microbiome data'. Below the header are navigation links: Home, Formats, Forum, Updates, Resources, and Contact. The main content area has a heading 'Please choose a module based on your data' followed by six colored boxes arranged in a 2x3 grid:

Marker Data Profiling	Shotgun Data Profiling	Taxon Set Analysis
Analyze marker gene counts data	Analyze shotgun metagenomics data	Discover enriched microbial signatures
Microbial Metabolomics	Statistical Meta-analysis	Raw Data Processing
Co-analyze microbiome & metabolomics data	Integrate multiple marker gene data	Convert 16S/18S/ITS reads to ASV table

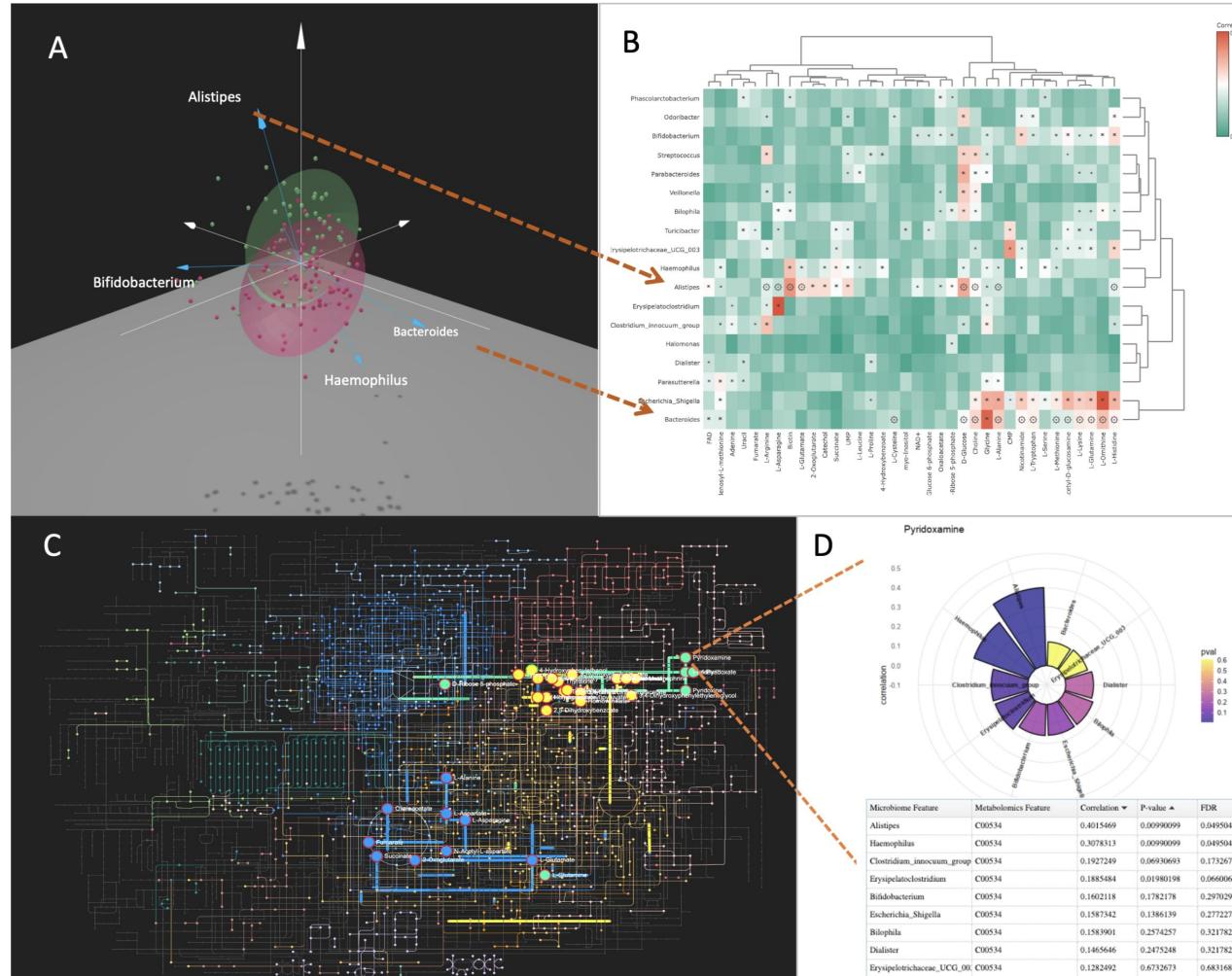
Below the grid, a note says 'Please use [OmicsForum](#) for support & troubleshooting request'. A section titled 'Publications' lists two papers:

- Chong, J., Liu, P., Zhou, G., and Xia, J. (2020) "Using MicrobiomeAnalyst for comprehensive statistical, functional, and meta-analysis of microbiome data" *Nature Protocols* 15, 799–821 (DOI: [10.1038/s41596-019-0264-1](https://doi.org/10.1038/s41596-019-0264-1))
- Dhariwal, A., Chong, J., Habib, S., King, I., Agellon, L.B., and Xia, J. (2017) "MicrobiomeAnalyst - a web-based tool for comprehensive statistical, visual and meta-analysis of microbiome data" *Nucleic Acids Research* 45, W180-188 (DOI: [10.1093/nar/gkx295](https://doi.org/10.1093/nar/gkx295))

<https://www.microbiomeanalyst.ca>

# Integrating compositional information for better functional analysis

Understand metabolic potential of key taxa

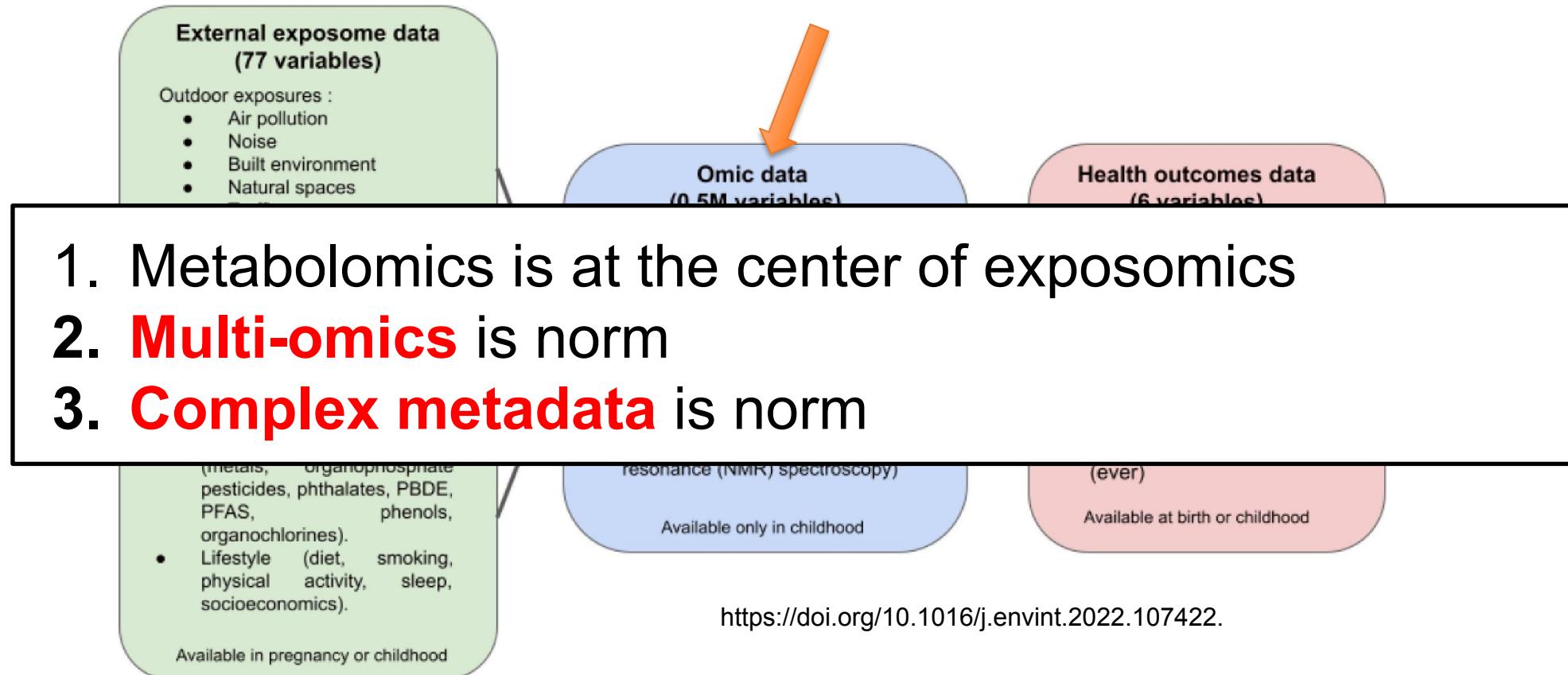


Refine background pathways based on composition

## # 3. Linking metabolomics to exposomics

- Metadata and covariate
- OmicsNet & OmicsAnalyst

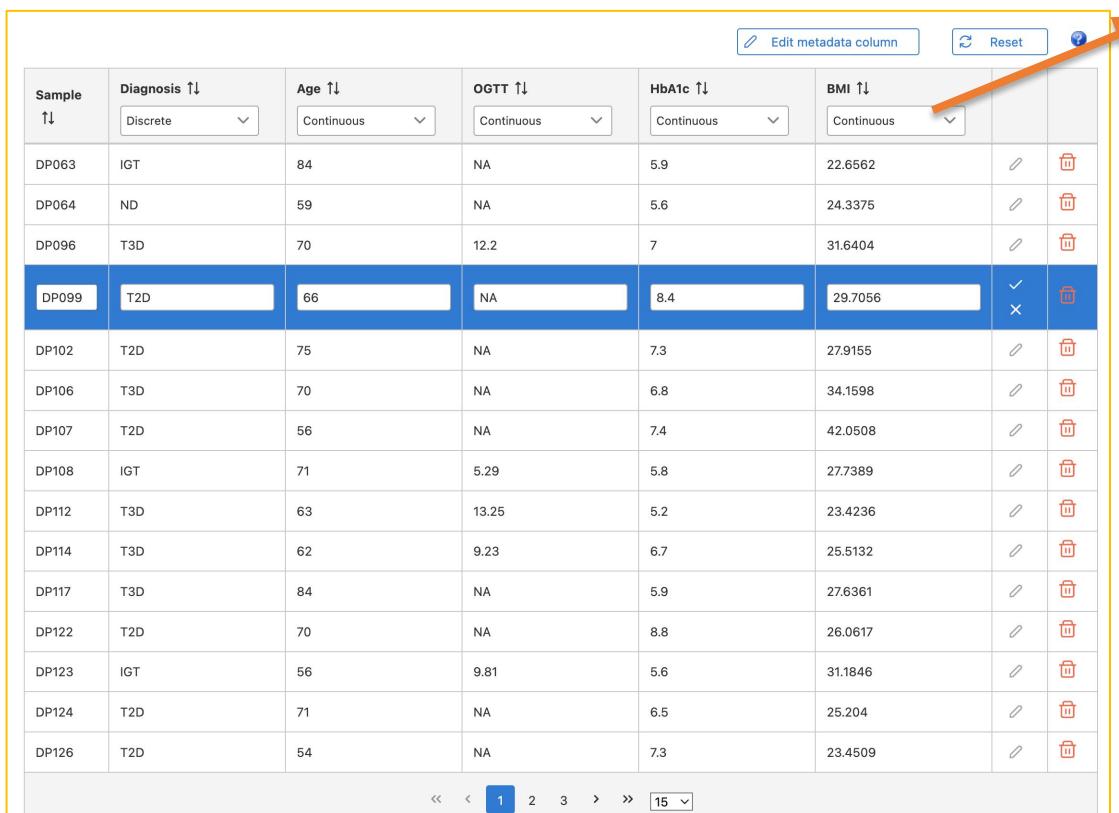
# What does exposomics data look like?



The data were based on the **HELIX project** which collected exposome, omics and health data from six mother-child cohorts across Europe in 1301 participants

# Metadata are critical for exposomics data analysis

Edit



Sample ↑	Diagnosis ↑	Age ↑	OGTT ↑	HbA1c ↑	BMI ↑	
DP063	IGT	84	NA	5.9	22.6562	
DP064	ND	59	NA	5.6	24.3375	
DP096	T3D	70	12.2	7	31.6404	
DP099	T2D	66	NA	8.4	29.7056	
DP102	T2D	75	NA	7.3	27.9155	
DP106	T3D	70	NA	6.8	34.1598	
DP107	T2D	56	NA	7.4	42.0508	
DP108	IGT	71	5.29	5.8	27.7389	
DP112	T3D	63	13.25	5.2	23.4236	
DP114	T3D	62	9.23	6.7	25.5132	
DP117	T3D	84	NA	5.9	27.6361	
DP122	T2D	70	NA	8.8	26.0617	
DP123	IGT	56	9.81	5.6	31.1846	
DP124	T2D	71	NA	6.5	25.204	
DP126	T2D	54	NA	7.3	23.4509	

<< < 1 2 3 > >> [15]

Edit metadata columns:

Include/Exclude Primary metadata Order (factor-level)

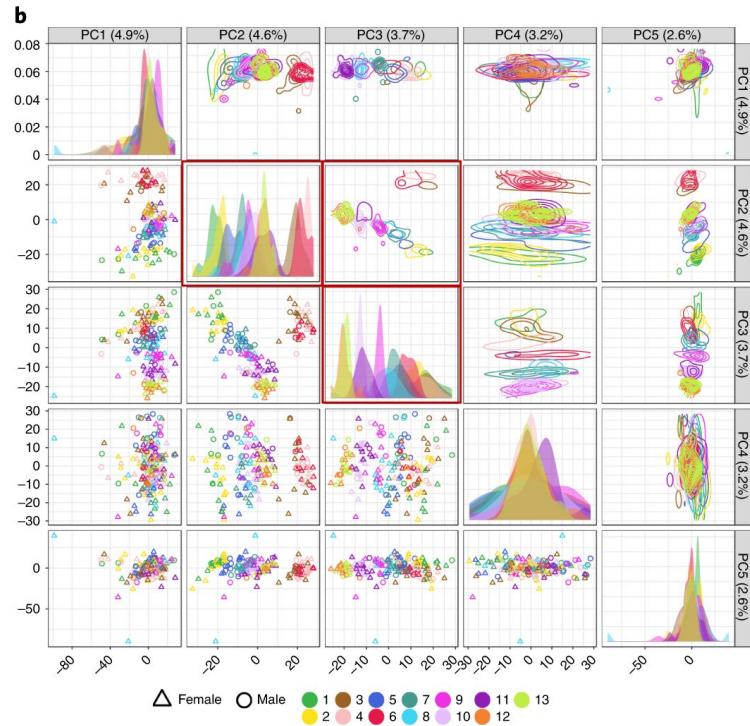
Only applicable to categorical metadata.

Select metadata: Diagnosis

T2D  
T2D  
IGT  
ND

Update Cancel

View

# Using linear models for complex design

Simple Metadata    **Complex Metadata**

Primary metadata: Diagnosis

Reference group: T3D

Contrast: All contrasts (ANOVA-style)

Covariates (control for):

Blocking factor:

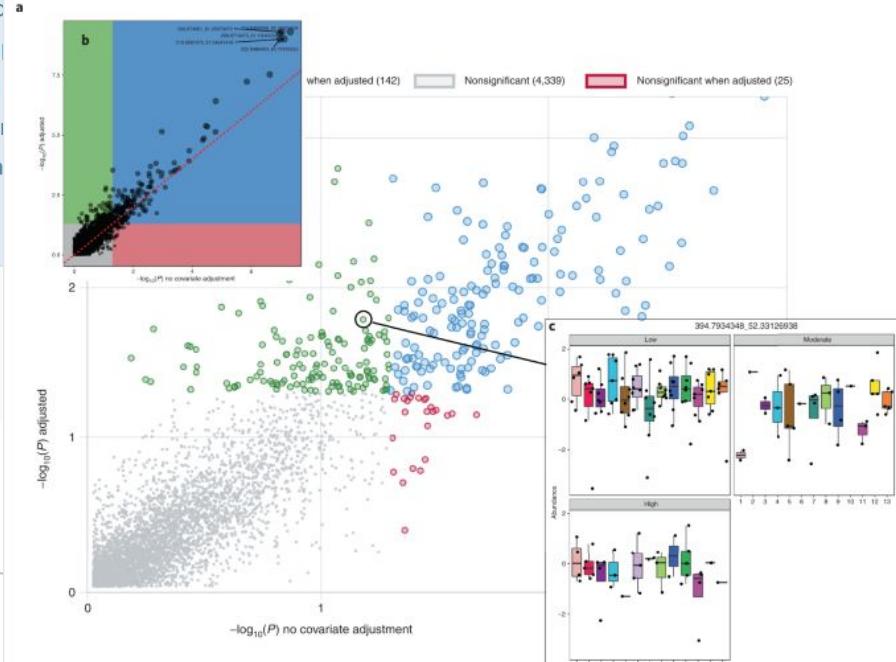
Adjust using robust trend

--- Not Available ---  
 Diagnosis  
 Age  
 OGTT  
 HbA1c  
 BMI

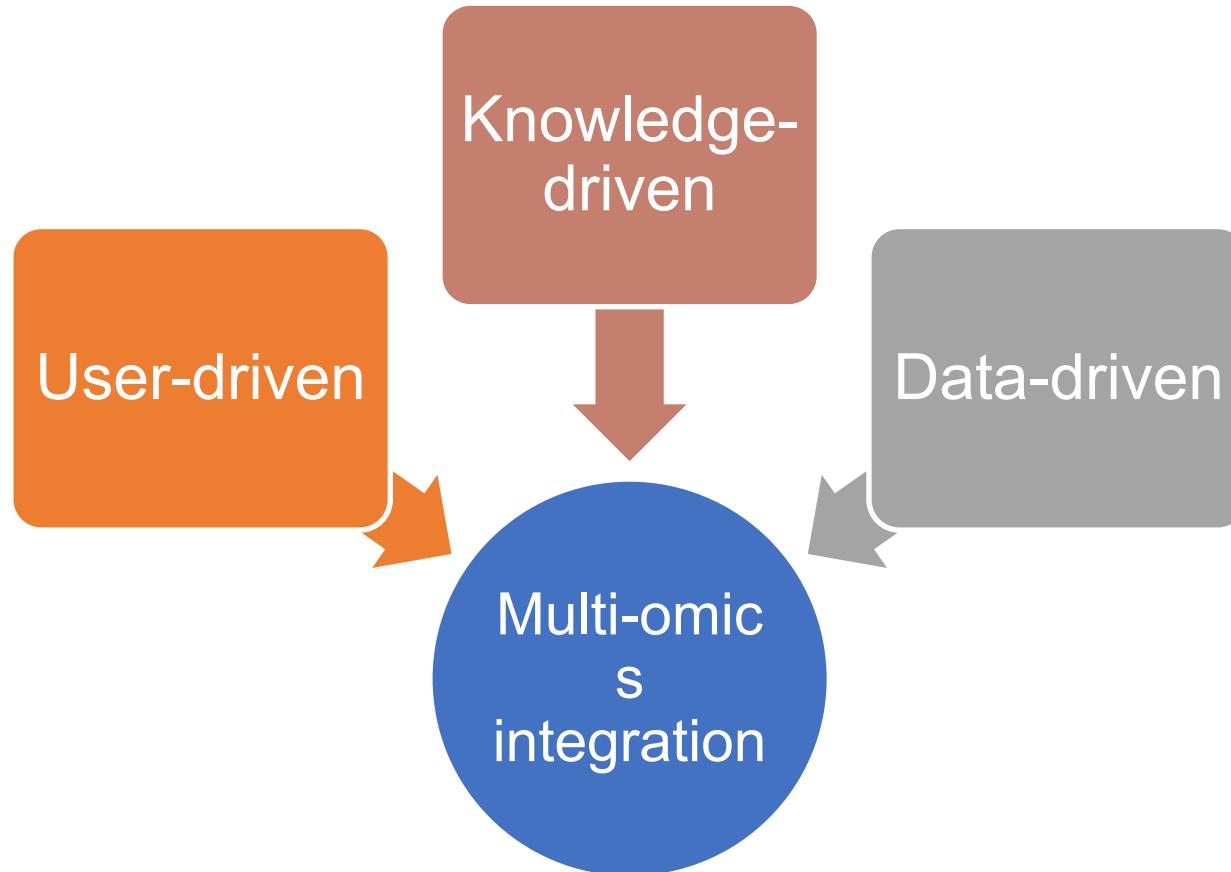
Submit

**Did you know?**

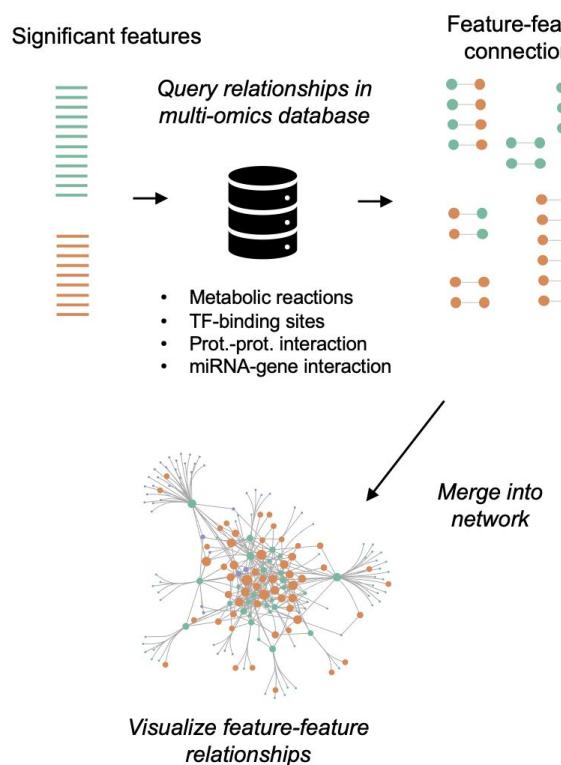
To perform multi-factor comparison analysis for complex metadata, we leverage the linear models with covariate adjustments of [limma](#) for its high-performance implementation. Some data may include some form of blocking in the study design to control for confounding effects. Please note that although you can specify covariates to control for confounding effects, we in general recommend **keeping them in the model**. A covariate adjustment effect model not only is computationally more efficient than a full factorial model, but also is more consistent with the interpretation of different factors. [\(2009\)](#) for more technical discussions.



# General strategies for multi-omics integration



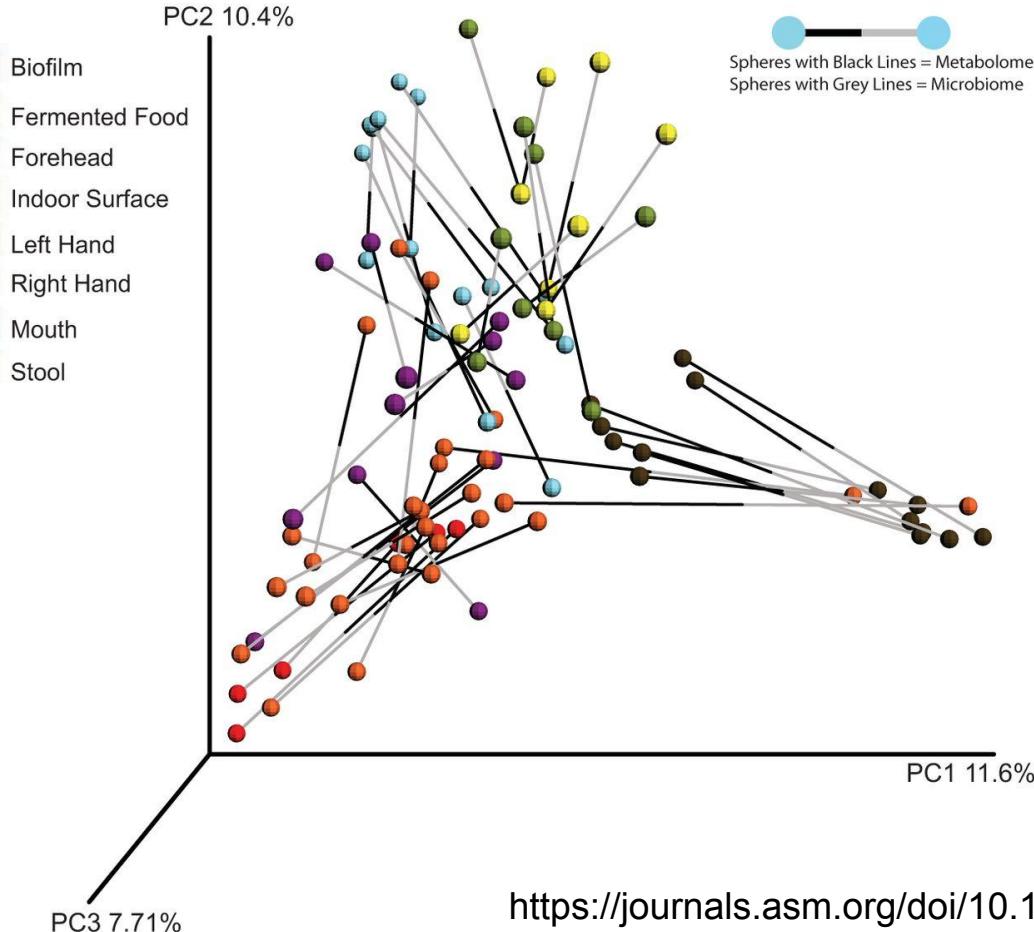
# Knowledge-driven integration (“connect the dots”)



1. Perform comprehensive analysis on individual omics data
2. Connect the signatures from each omics layer through a knowledge framework (knowledge graph)
  - *Don't connect at raw omics layers*
3. Apply different algorithms for network analysis
  - *Enrichment analysis, topology analysis, etc*
4. Engage user (expert knowledge) to interpret the pattern

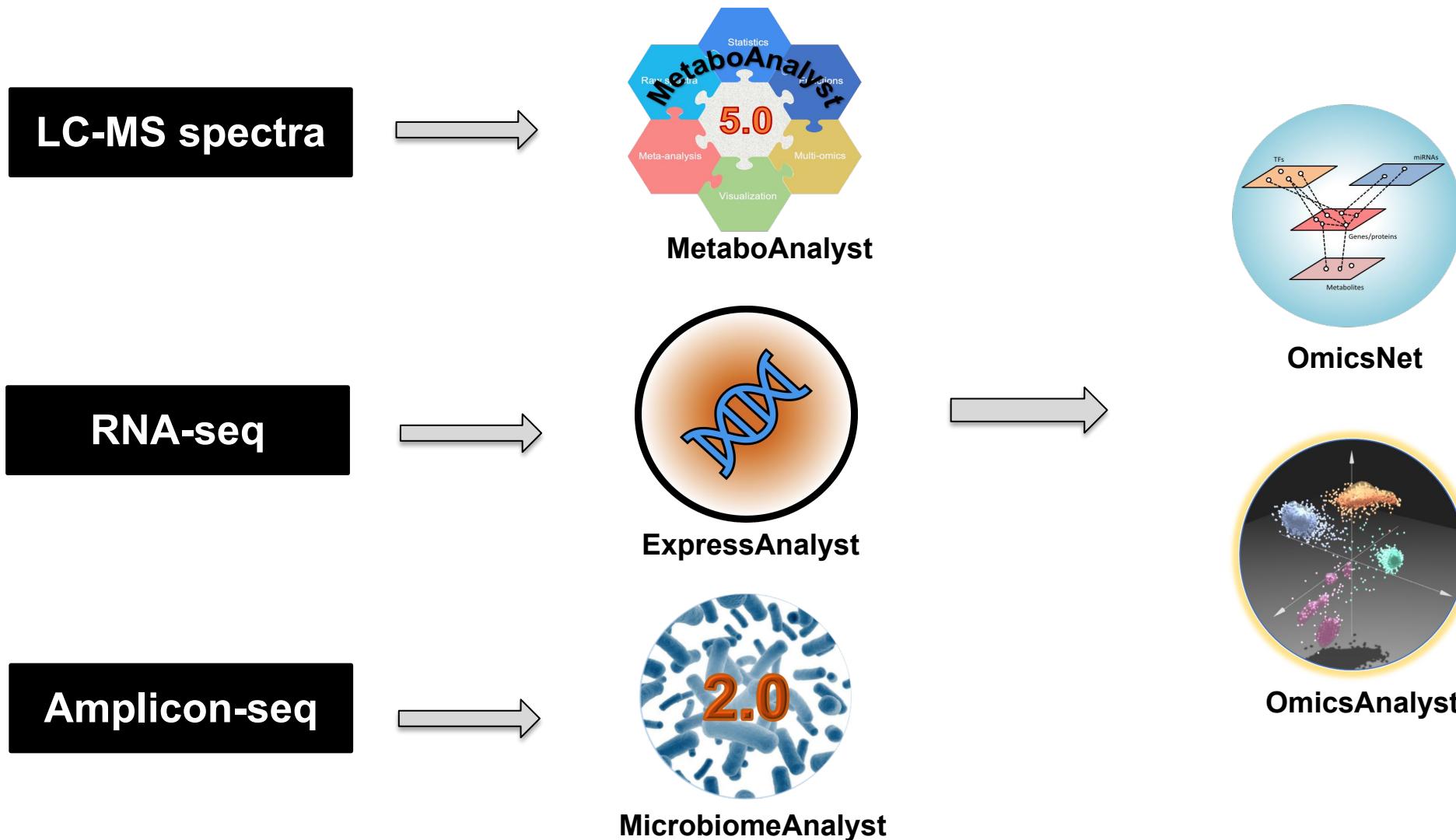
# Data/model-driven integration (“shared patterns”)

Mainly clustering & dimensionality reduction methods



<https://journals.asm.org/doi/10.1128/mSystems.00038-16>

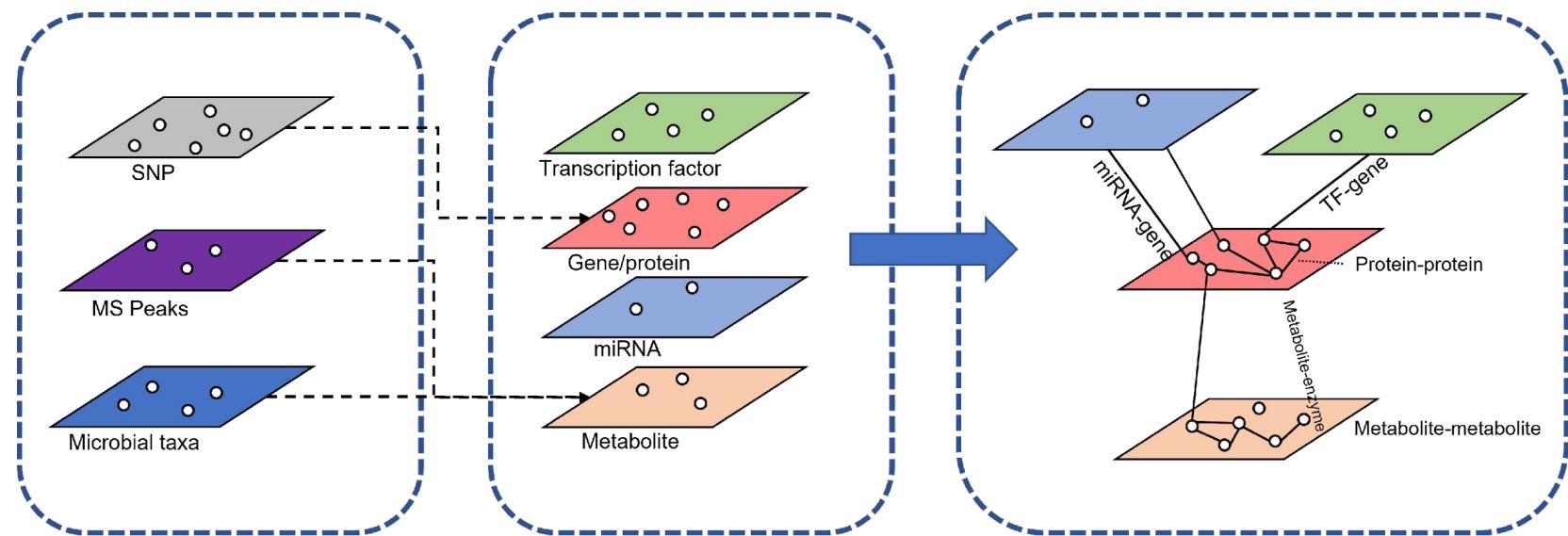
# From raw data to multi-omics



# Knowledge-driven multi-omics: OmicsNet

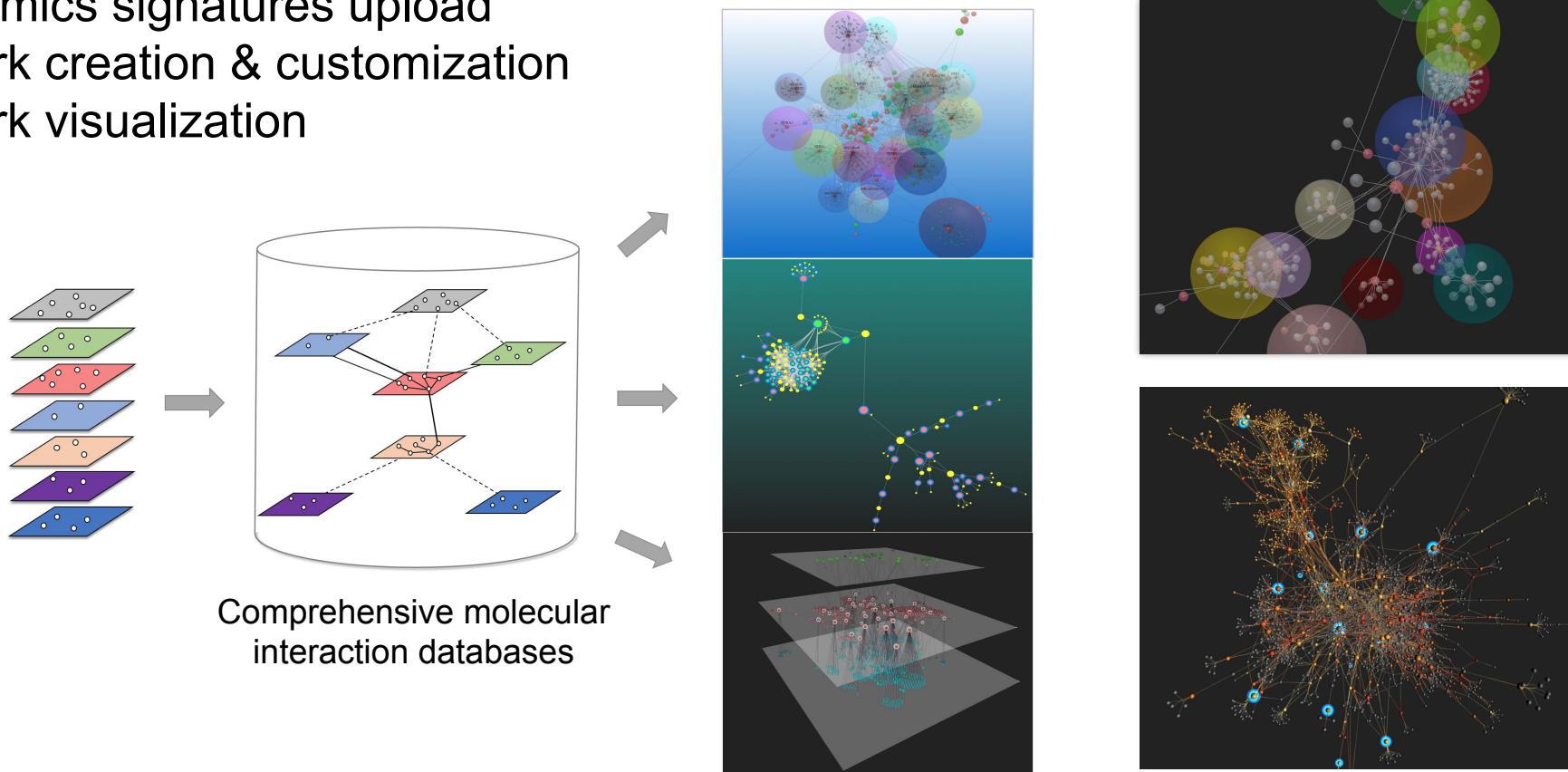
Motivation: to connect multi-omics molecular signatures via a knowledge-based network

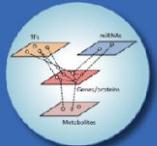
- Molecule types:
  - SNPs
  - Genes
  - Proteins
  - Metabolites
    - LC-MS peaks
  - miRNAs
  - TFs
  - Microbes



# The overall design (three steps)

1. Multi-omics signatures upload
2. Network creation & customization
3. Network visualization





Please upload omics signatures using their corresponding buttons below

A Graph File				
SNPs	Microbial Taxa	LC-MS Peaks		
Genes/mRNAs	Proteins	Transcription Factors	miRNAs	Metabolites

Proceed

Reset

For troubleshooting & support, please use [OmicsForum](#)

# Integrating multi-omics signatures via networks

Seeds =>  
interactors /  
neighbors

Connection  
based on  
shared nodes  
& edges

**Input list(s) (?)**

Gene (51)
Protein (28)
Transcription factor (6)
miRNA (6)
Metabolite (33)

**Database Selection**

Databases are organized under different tabs. Please choose proper database(s) for network creation based on your analysis objectives. Multiple types of networks will be merged (based on shared nodes) and customized in the next page

**Protein-protein   miRNA-gene   Metabolite-protein   TF-gene**

[InnateDB](#) Manually curated comprehensive PPI (human/mouse) (updated on 01/04/2022)  
 [STRING](#) Comprehensive PPI containing both known and predicted PPI (updated on 01/04/2022) [\(parameters\)](#)  
 [IntAct](#) Manually curated experimentally validated PPI (updated on 01/04/2022)  
 [HuRI](#) Reference interactome map of human binary protein interactions (updated on 01/04/2022)

Add edges only  
Do not introduce new nodes.  
Only identify connections within current nodes.

**Submit**

**Individual Omics Networks**

Each network is created independently by searching input list against a selected database. The network usually contains several disconnected subnetworks.

Input Type	Network Type	Sizes (node# - edge# - seed#)	Browse	Download	Delete
Gene	PPI	449 - 489 - 46	<a href="#">Browse</a>	<a href="#">Download</a>	<a href="#">Delete</a>
Protein	PPI	210 - 223 - 26	<a href="#">Browse</a>	<a href="#">Download</a>	<a href="#">Delete</a>
Transcription factor	TF-gene	487 - 501 - 8	<a href="#">Browse</a>	<a href="#">Download</a>	<a href="#">Delete</a>
miRNA	miRNA-gene	997 - 1051 - 10	<a href="#">Browse</a>	<a href="#">Download</a>	<a href="#">Delete</a>
Metabolite	Metabolite-protein	373 - 417 - 32	<a href="#">Browse</a>	<a href="#">Download</a>	<a href="#">Delete</a>

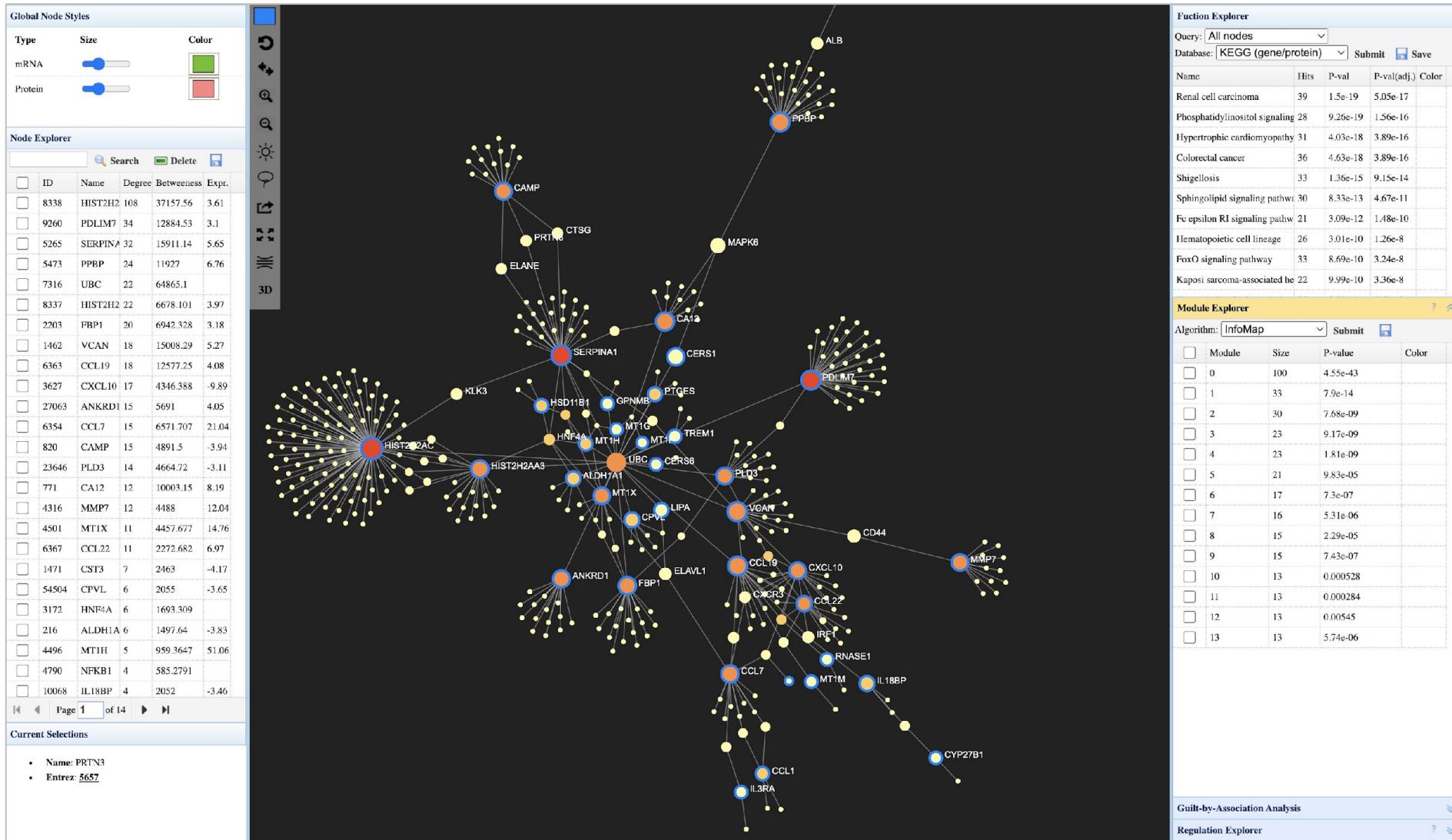
# Intuitive network creation & customization

The screenshot shows the OmicsNetR Network Builder interface. At the top, there's a navigation bar with 'Database Selection' and 'Network Builder'. On the right, there's a 'Navigate to:' dropdown. Below the navigation is a sidebar titled 'Network Tools' with a question mark icon. It contains ten buttons: 'Degree Filter', 'Betweenness Filter', 'Minimum Network', 'Steiner Forest (PCSF)', 'Tissue Filter', 'P-value Filter', 'Zero-order Network', 'Reset to Default', and 'Save Network (.json)'. The main content area is titled 'Multi-omics Network Building'. It contains a text block explaining how shared nodes from multiple networks are merged into a multi-omics network, which can then be decomposed into subnetworks for analysis. It also mentions that subnetworks can be trimmed if they are too large. A table lists six subnetworks with their details: subnetwork1 (TF: 4; Gene/protein: 42), subnetwork2 (Gene/protein: 1), subnetwork3 (Gene/protein: 1), subnetwork4 (TF: 1), subnetwork5 (Gene/protein: 1), and subnetwork6 (Gene/protein: 1). Each row includes 'View' and 'Download' buttons. At the bottom of the table is a page navigation bar with '<<', '<', '1', '>', and '>>'. To the right of the main content is an 'R Command History' section with a 'Save' button. It lists seven R commands:

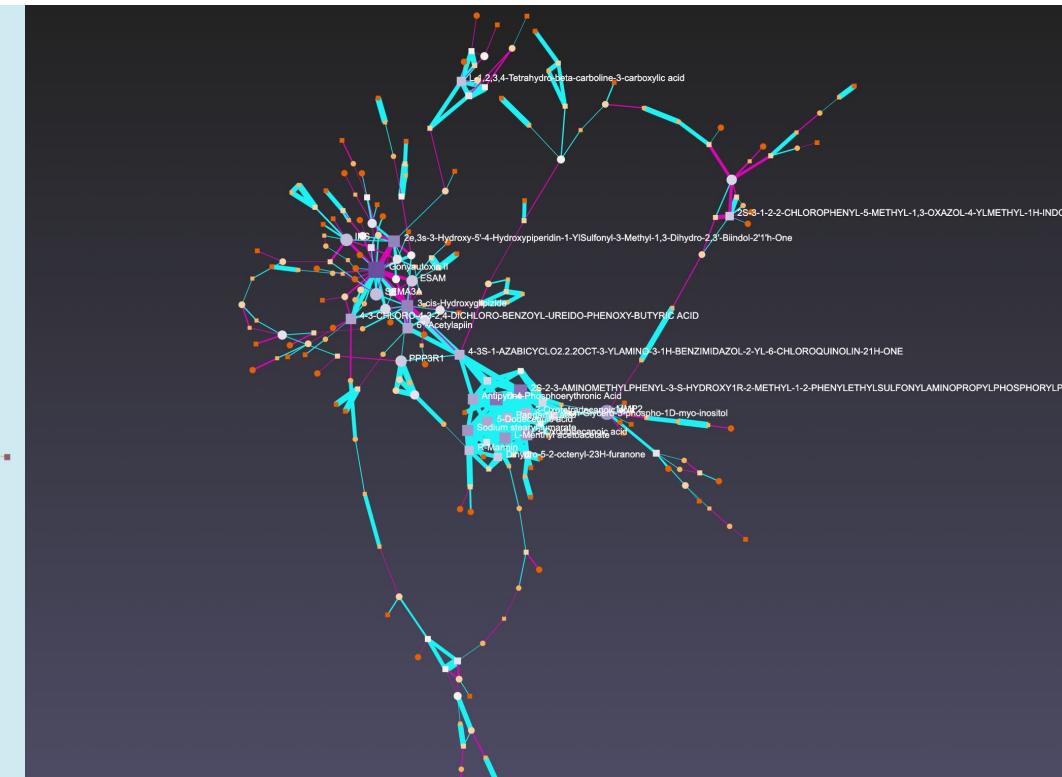
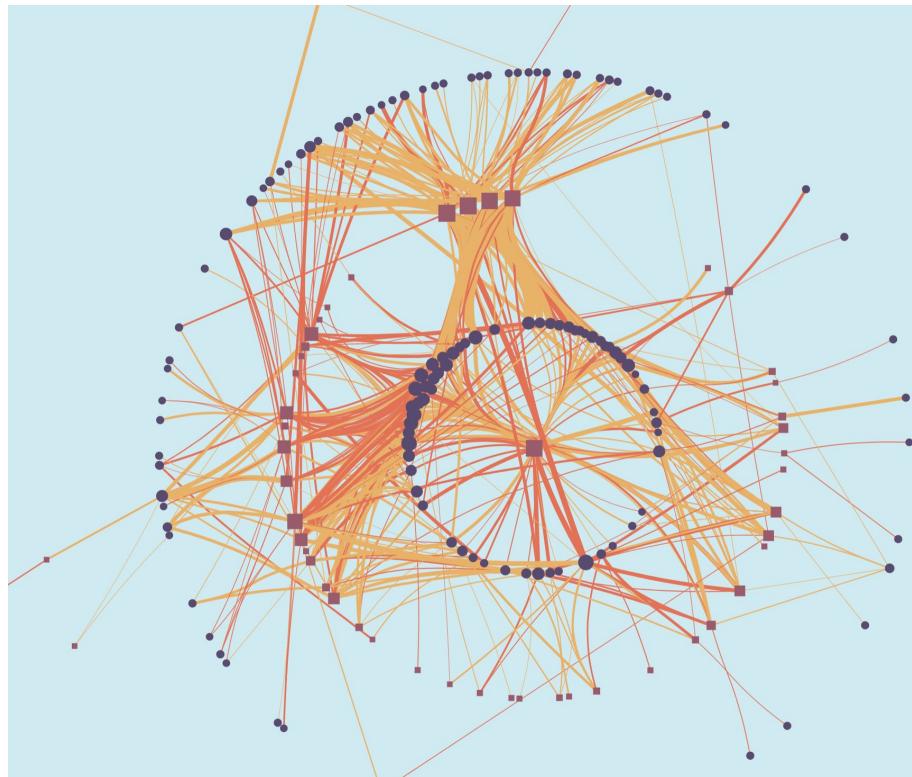
1. dataSet<-Init.Data()
2. dataSet<-PrepareInputList(dataSet,"Your input list", "hsa", "gene", "entrez");
3. dataSet<-PrepareInputList(dataSet,"Your input list", "hsa", "tf", "symbol");
4. SetPpiZero(FALSE)
5. dataSet<-QueryNet(dataSet, "gene", "innate", "gene" )
6. dataSet<-QueryNet(dataSet, "tf", "trrtrust", "tf" )
7. dataSet<-CreateGraph(dataSet)

Transparent & reproducible: <https://github.com/xia-lab/OmicsNetR>

# Network visual analytics



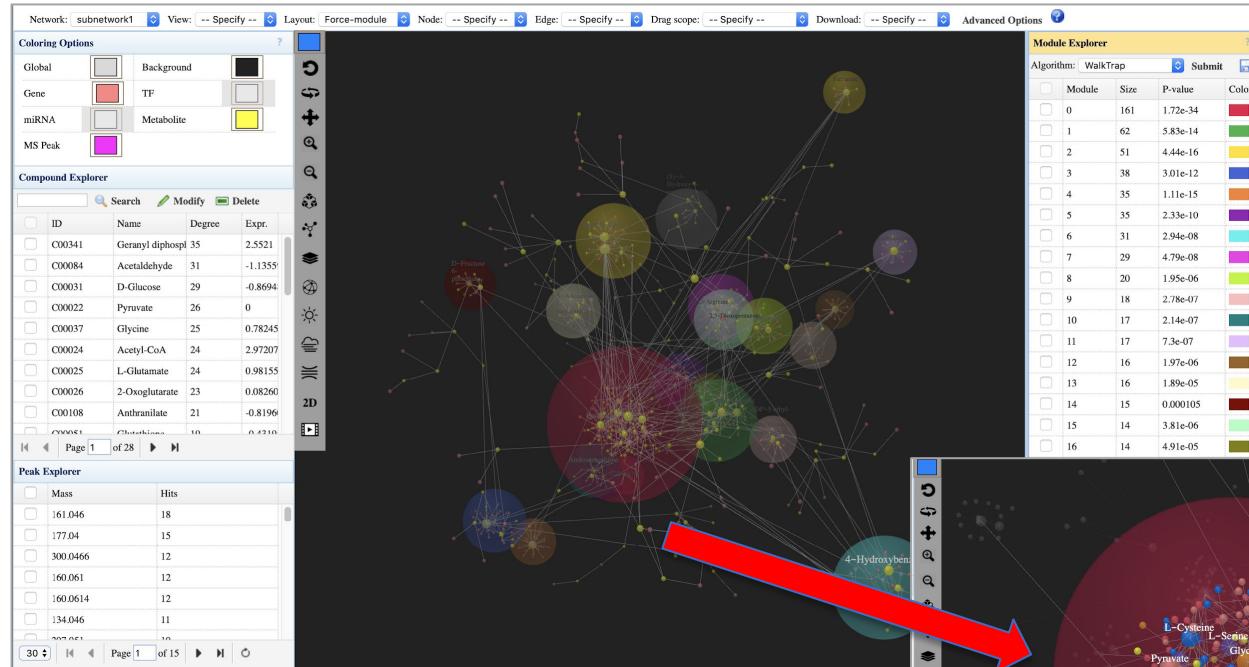
# Diverse options for network styles



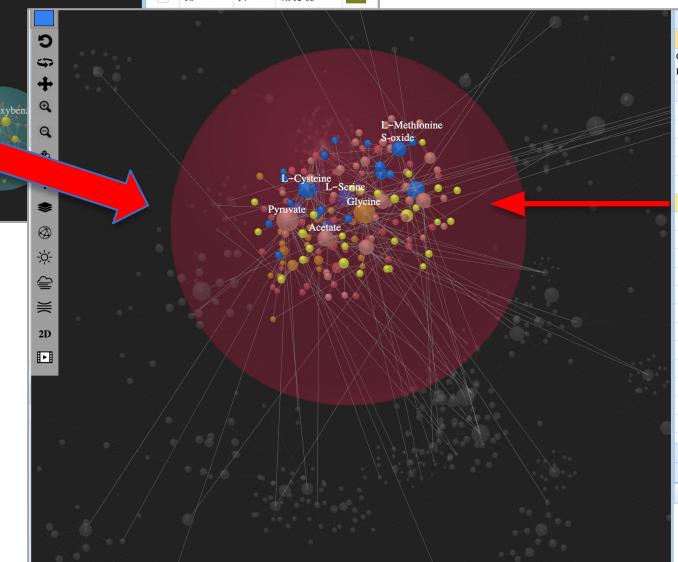
Some 2D networks generated by OmicsNet

# From network to modules to insights

## 1. Module detection



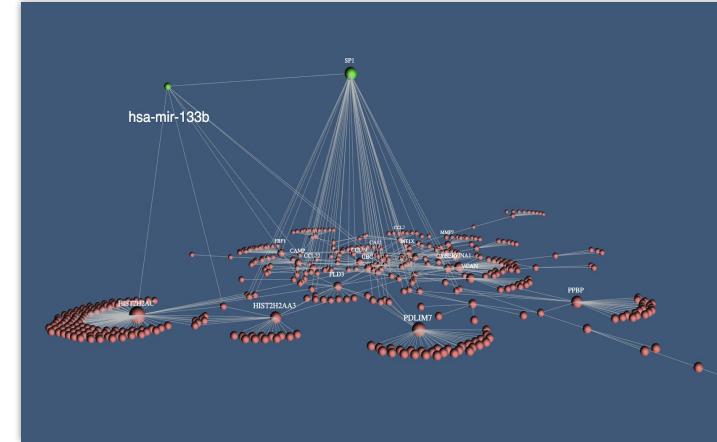
## 2. Select a module of interest



## 3. Enrichment analysis

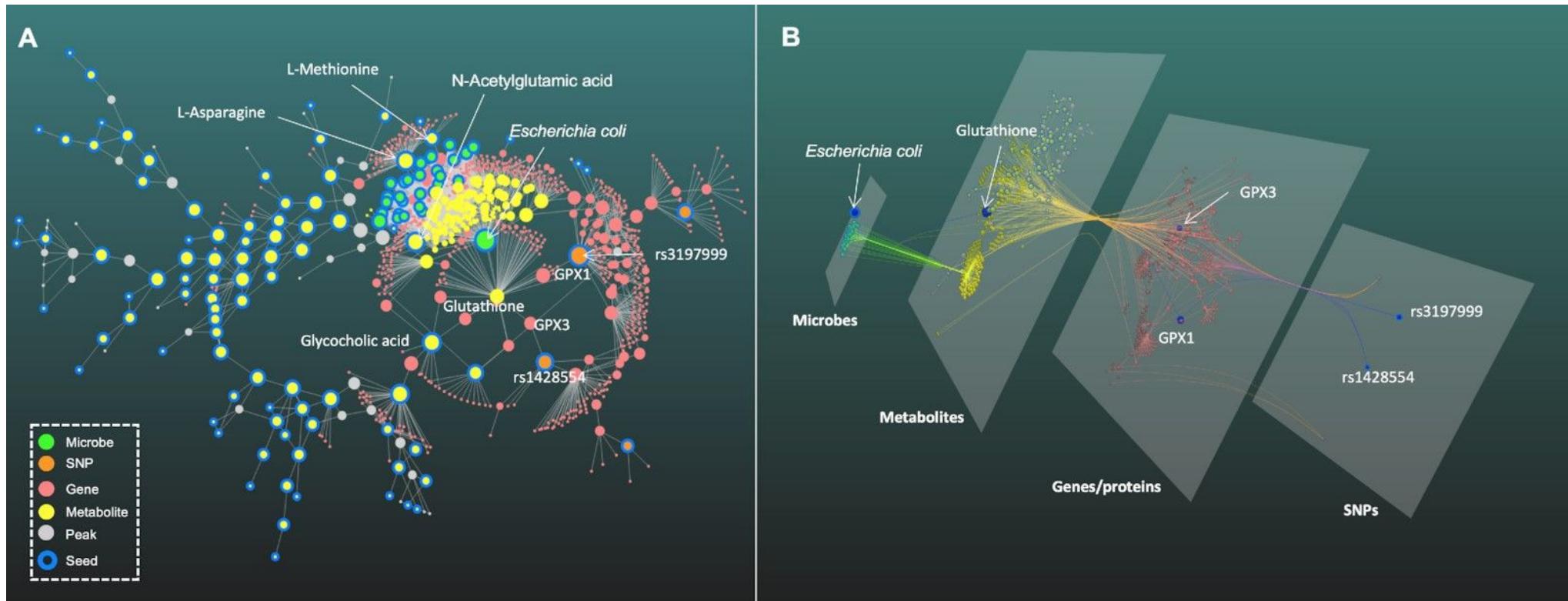
Name	Hits	P-value	Color
Arginine and proline metabolism	6	0.080564	Grey
Glyoxylate and dicarboxylic acid metabolism	15	0.080575	Grey
Phenylalanine metabolism	1	0.080651	Grey
Alanine, aspartate and glutamate metabolism	10	0.080691	Grey
Tryptophan metabolism	3	0.080697	Grey
<b>Cysteine and methionine metabolism</b>	<b>22</b>	<b>0.080745</b>	<b>Yellow</b>
Aminoacyl-tRNA biosynthesis	11	0.080755	Grey
Propanoate metabolism	4	0.080844	Grey
Valine, leucine and isoleucine biosynthesis	2	0.080976	Grey
Lysine degradation	2	0.081425	Grey
Phenylalanine, tyrosine and tryptophan metabolism	1	0.081444	Grey
Vitamin B6 metabolism	4	0.081444	Grey
Nicotinamide and nucleotide biosynthesis	2	0.081722	Grey
Glycine, serine and threonine metabolism	11	0.082608	Grey
Valine, leucine and isoleucine biosynthesis	1	0.082655	Grey
Ascorbate and aldarate metabolism	1	0.084104	Grey
pentose and glucuronate interconversion	1	0.084471	Grey
Nitrogen metabolism	6	0.084471	Grey
Sulfur metabolism	0	n.missing	Grey

## 4. Refine layout



# A comprehensive case study

- ❖ Integrating SNPs, Taxa, LC-MS peaks to our knowledge framework



\*IBD case study (<https://www.omicsnet.ca/OmicsNet/docs/Tutorial.xhtml>)

# Data-driven multi-omics: OmicsAnalyst

 **OmicsAnalyst**

Home Overview Tutorial OmicsForum Gallery Updates Contact

**Data-driven visual analytics for multi-omics data**

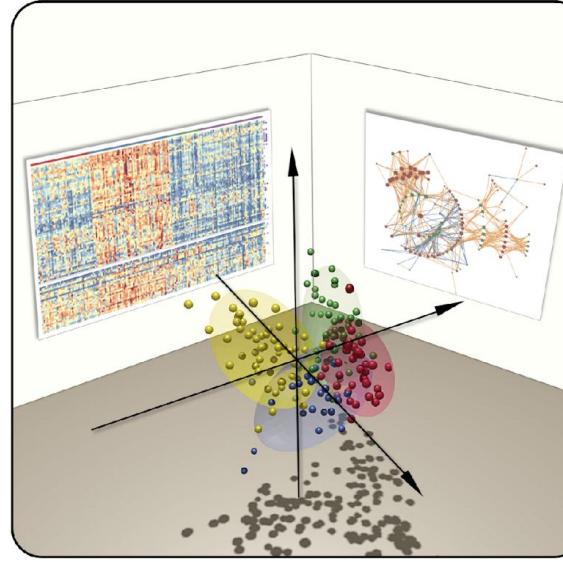
- Joint dimensionality reduction & 3D scatter plots
- Correlation analysis & network visualization
- Multi-view clustering & interactive heatmaps

[GET STARTED](#)

---

**Publication**

Zhou, G., Ewald, J. and Xia, J. (2021) "[OmicsAnalyst: a comprehensive web-based platform for visual analytics of multi-omics data](#)" Nucleic Acids Research 49 W476–W482



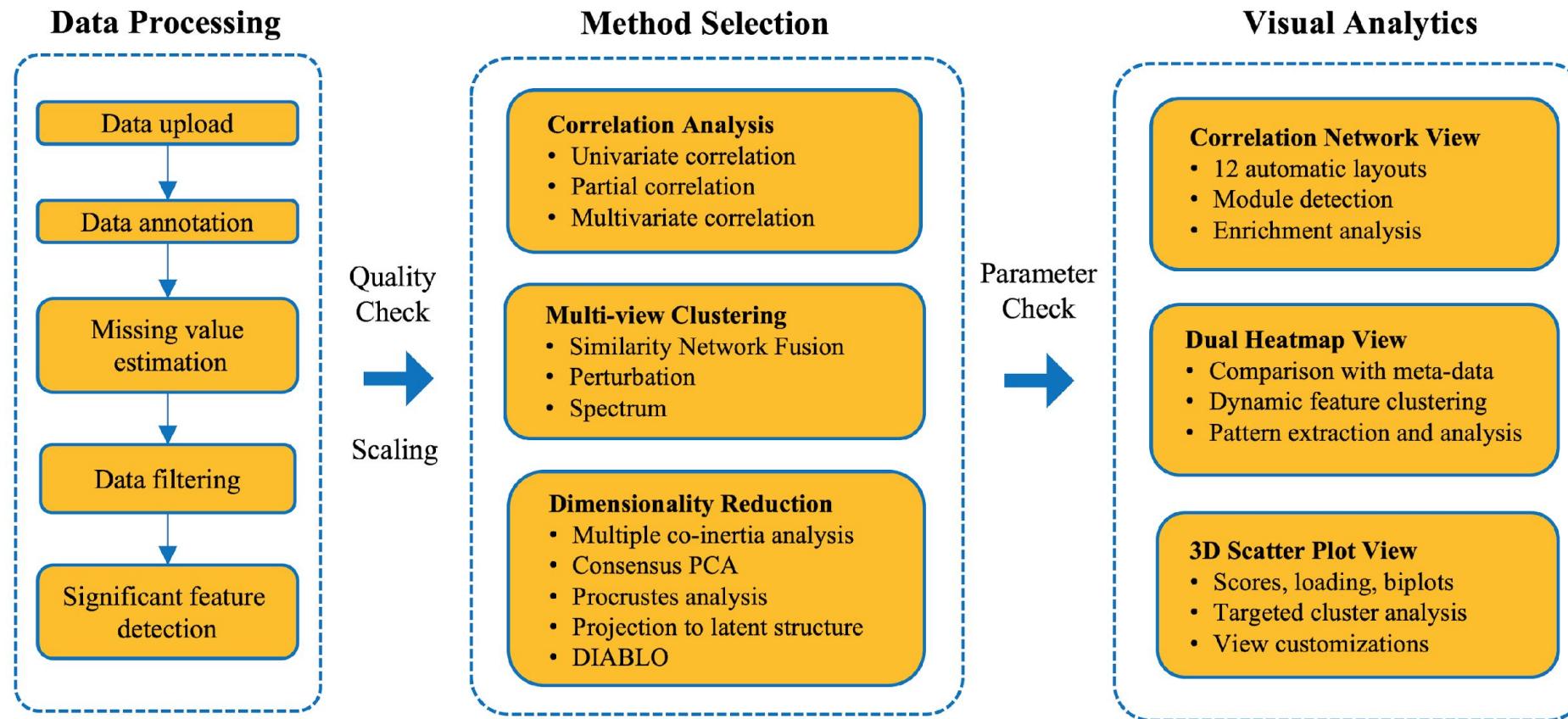
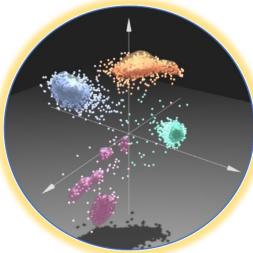
    

[Manage Cookies](#)

[www.omicsanalyst.ca](http://www.omicsanalyst.ca)

[bioinformatics.ca](http://bioinformatics.ca)

# Overall workflow

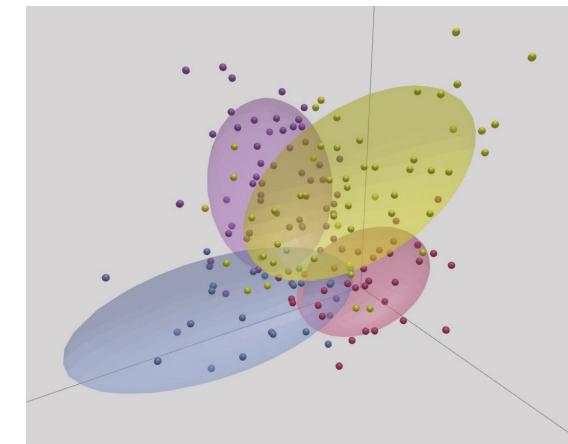
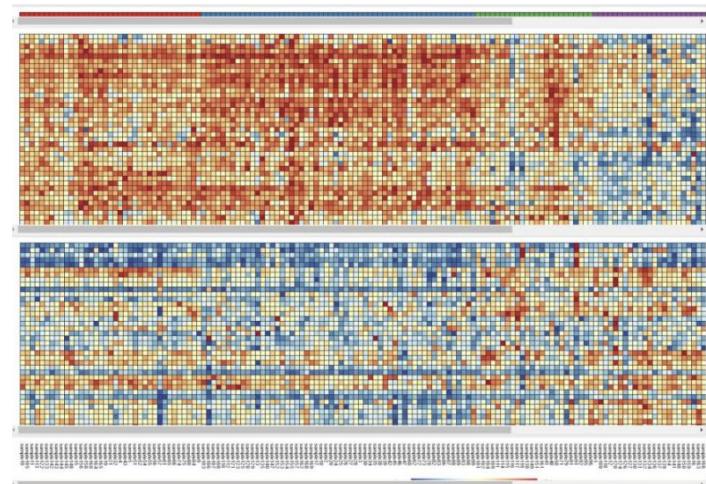


# Data-driven multi-omics: OmicsAnalyst

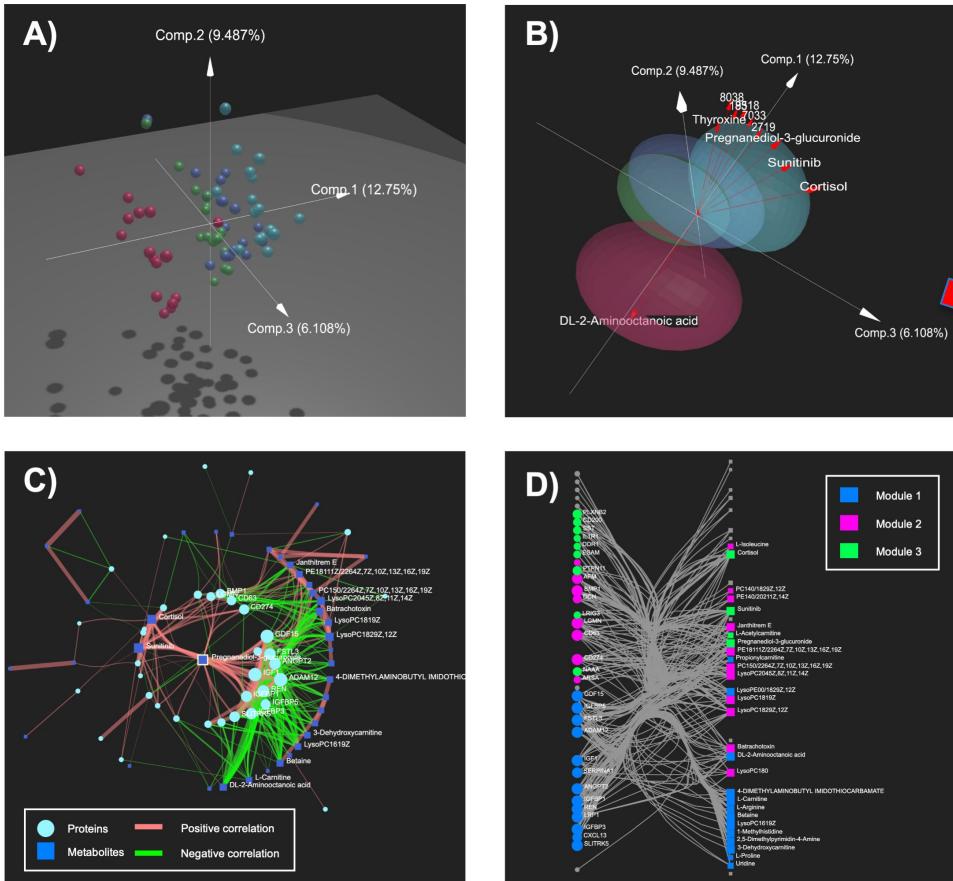
## Upload your multi-omics data

- A single metadata and at least two omics data tables (.csv) are required;
- The metadata table should describe the same sample IDs shared across all omics data; a small percentage of missing values are OK.
- The omics data should already be normalized using methods appropriate for the corresponding omics type; a maximum of 5 omics data types can be uploaded;

Metadata table ✓	normalized_lipids.csv ✓	normalized_rnaseq.csv ✓	OmicsData #3	OmicsData #4	OmicsData #5
---------------------	----------------------------	----------------------------	--------------	--------------	--------------



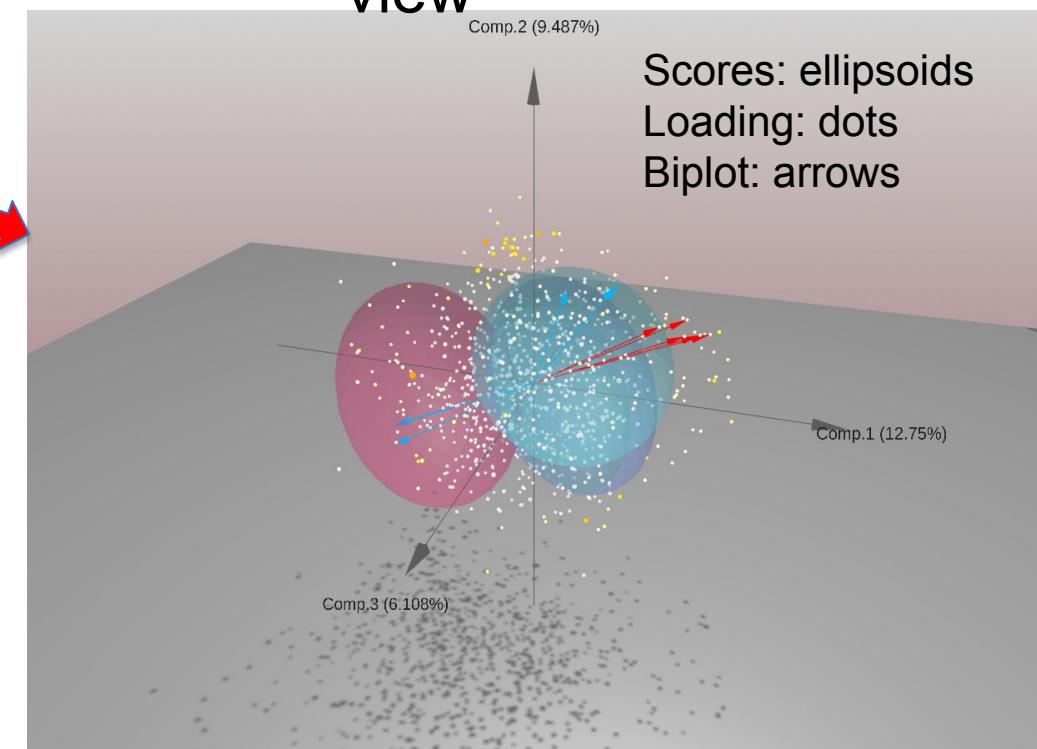
# Powerful visual analytics



“All-in-one”  
view

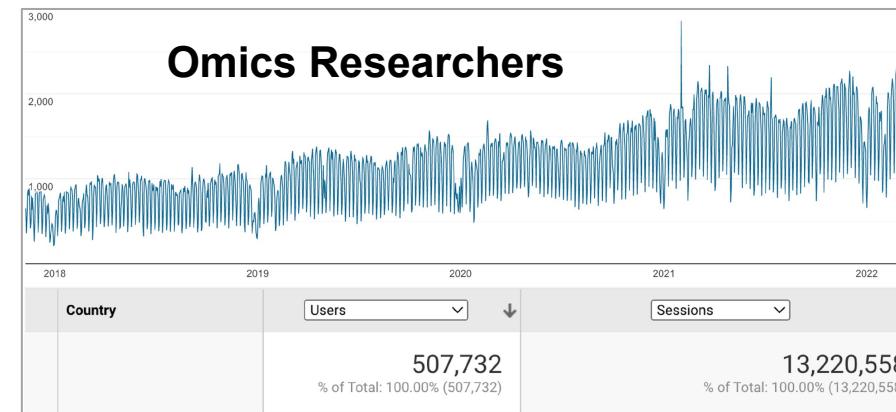
Comp.2 (9.487%)

Scores: ellipsoids  
Loading: dots  
Biplot: arrows



# Future of omics data analytics?

# Democratizing omics data analytics



This screenshot shows the "Partial Least Squares Discriminant Analysis (PLS-DA)" interface. It includes tabs for Overview, 2D Scores Plot, Loadings Plot, Imp. Features, Synchronized 3D Plots, Cross Validation (selected), and Permutation. A sidebar on the right displays a chat interface with messages about related topics and permutation results.

Omics Tools



This screenshot shows the "Welcome to the OMICS community" forum. It features a search bar at the top and a grid of cards for various tools: MetaboAnalyst 5.0, MicrobiomeAnalyst, ExpressAnalyst, OmicsNet, OmicsAnalyst, NetworkAnalyst, miRNet, and mGWAS-explorer. Each card includes a small icon and a brief description.

Omics Forum



# Towards AI-assisted Self-service Omics Data Analytics

Cloud & Edge Computing

Visual Analytics



AI Chatbot

Community Forum &  
Knowledge base

# Thank you!

Workshop Sponsors:



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