

# Spectra processing, statistical analysis and functional integration using **MetaboAnalyst 5.0**

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# Acknowledgements



# Your TAs



**Qiang**



**Jessica**



**Yao**

# Schedule

## Part I: 8:15 AM – 10:15 PM

8:15 – 8:30: Opening lecture (Jeff)

8:30 – 8:50: Section 1: LC-MS spectral processing (Qiang)

8:50 – 9:15: Section 1: Hands on

9:20 – 9:45: Section 2: Stats I – simple experimental design (Jessica)

9:45 – 10:15: Section 2 Hands on

## Part II: 10:30 AM – 12:30 PM

10:30 – 10:50: Section 3: Functional analysis (Yao)

10:50 – 11:10: Section 3: Hands on

11:15 – 11:40: Section 4: Stats II - complex experimental design (Jessica)

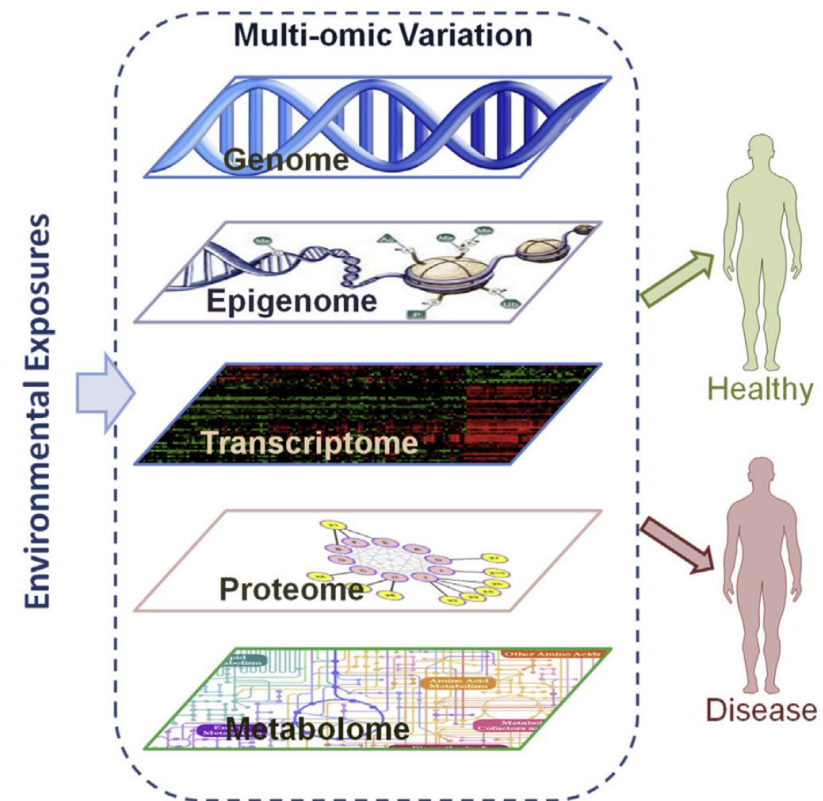
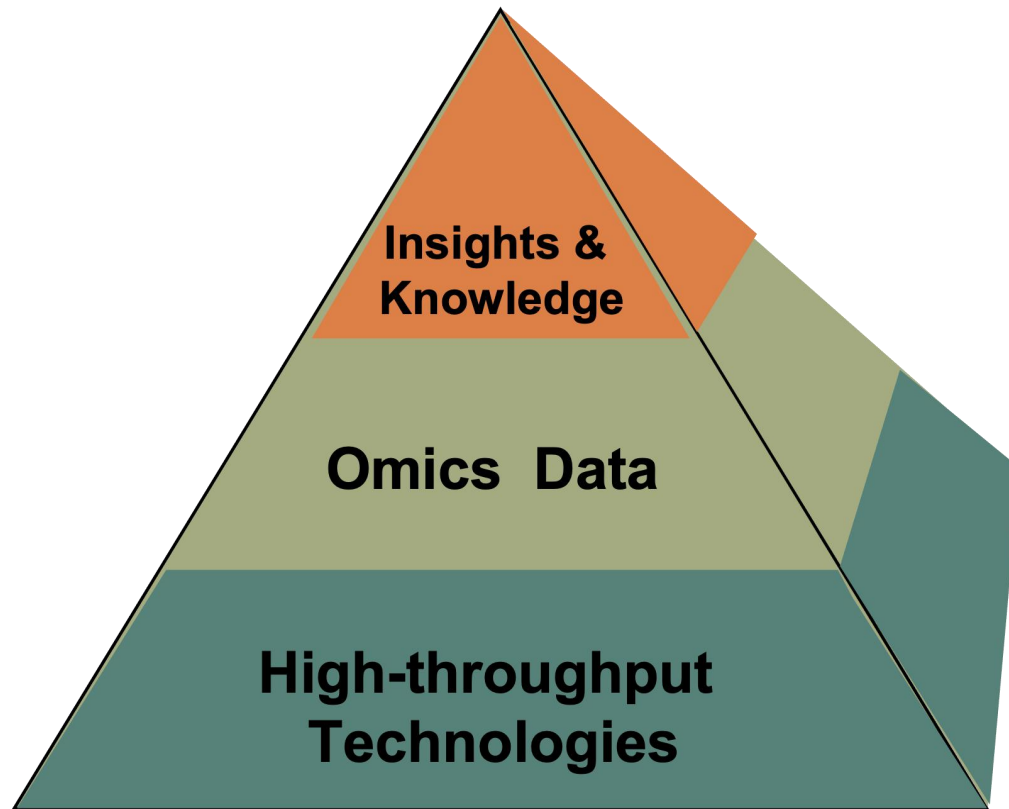
11:40 – 12:15: Section 4: Hands on

12:15 – 12:30: Summary (Jeff)



# A Gentle Introduction to Key Concepts in 'Omics Data Analysis

# Omics & multi-omics era



# Two distinct challenges

## Size challenge (raw data)

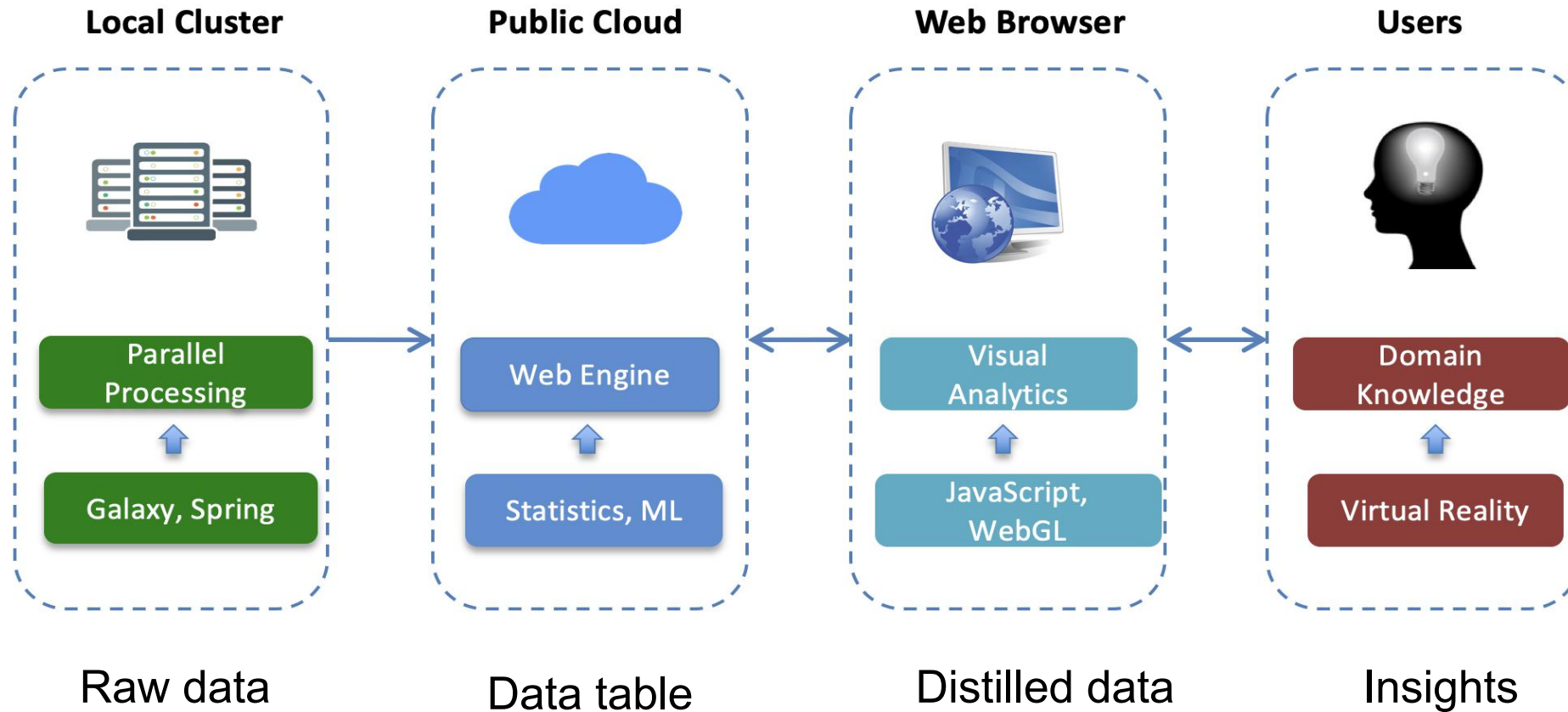
- Raw reads, spectra, images
- Large (GB ~TB)
- Large storage and computing resources



## Complexity challenge (feature table)

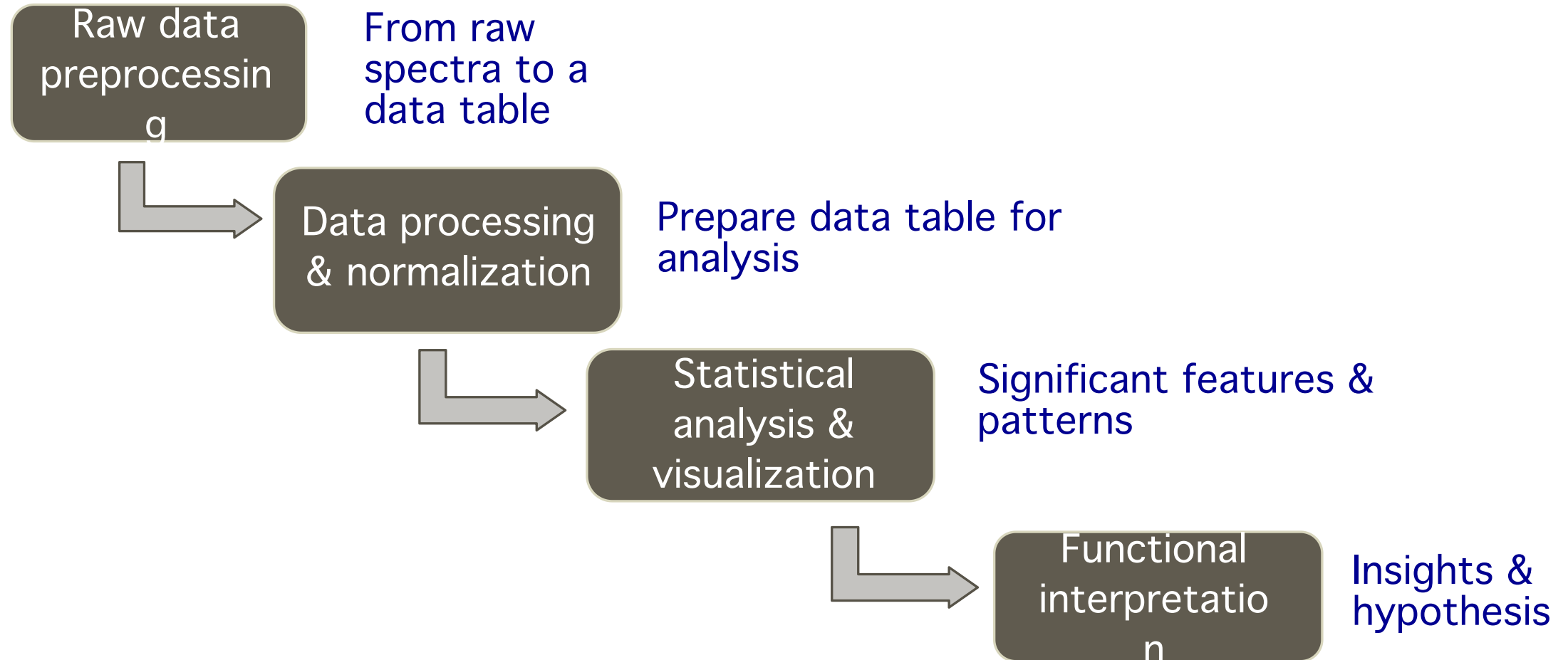
- Feature table (abundance, intensities)
- Small (100s KB ~ MB)
- High-dimensional, missing values
- Data analysis starts here

# Omic data analytics framework

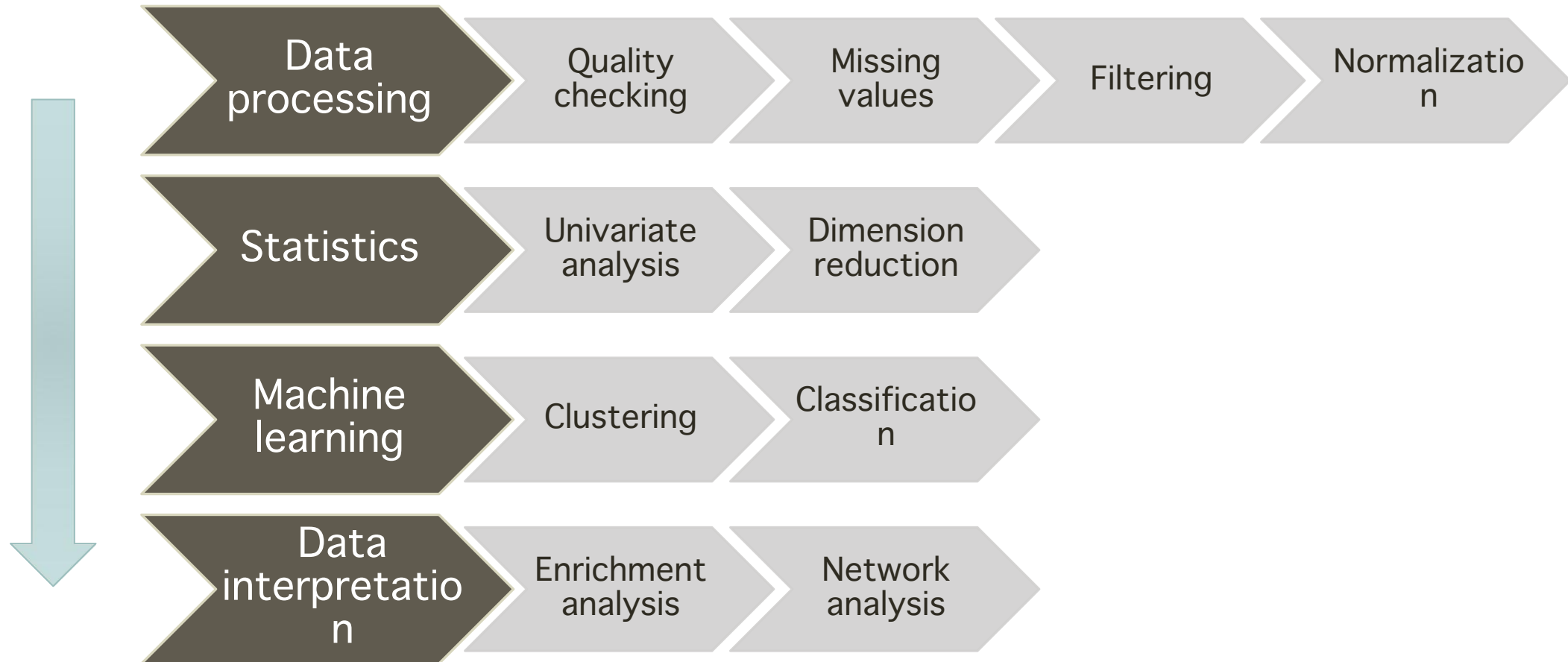




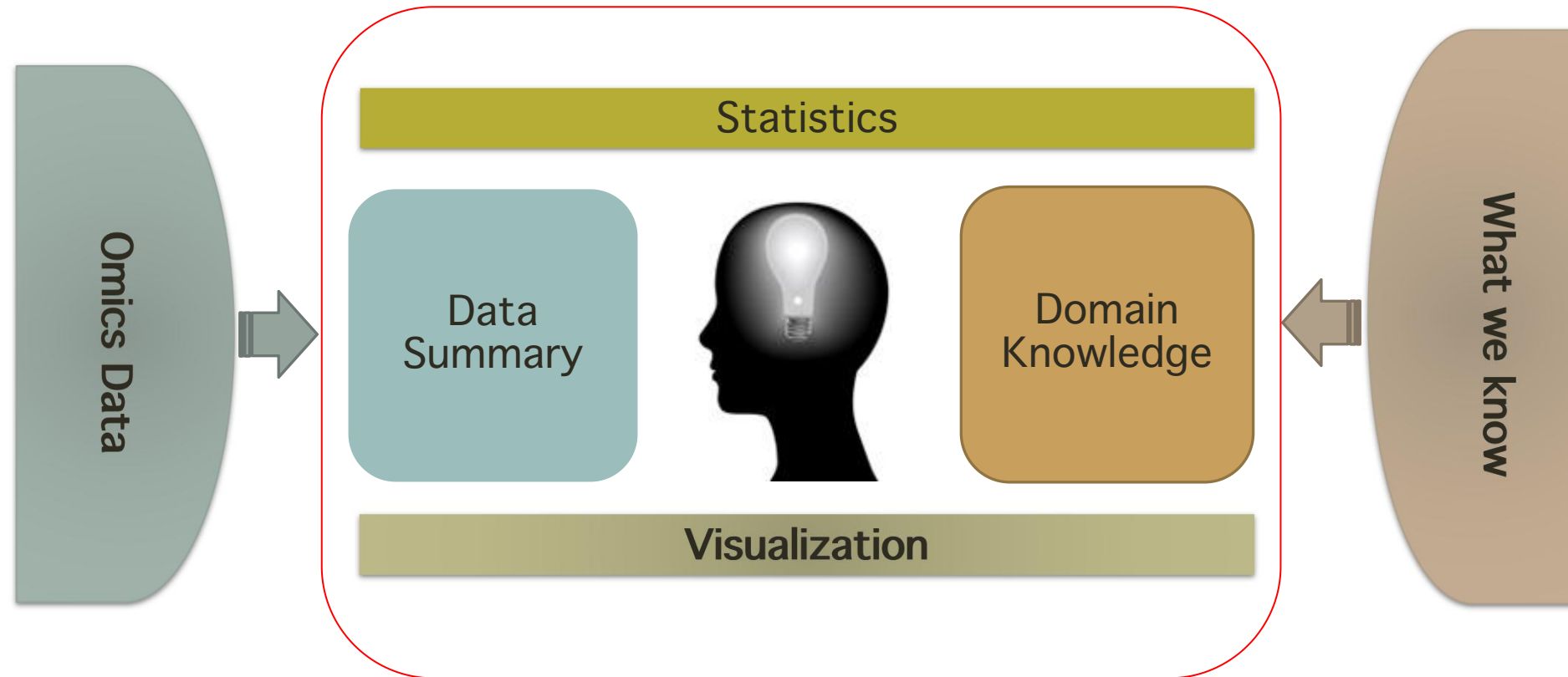
# Omics Data Analysis (in a nutshell)



# Common steps in omics workflow

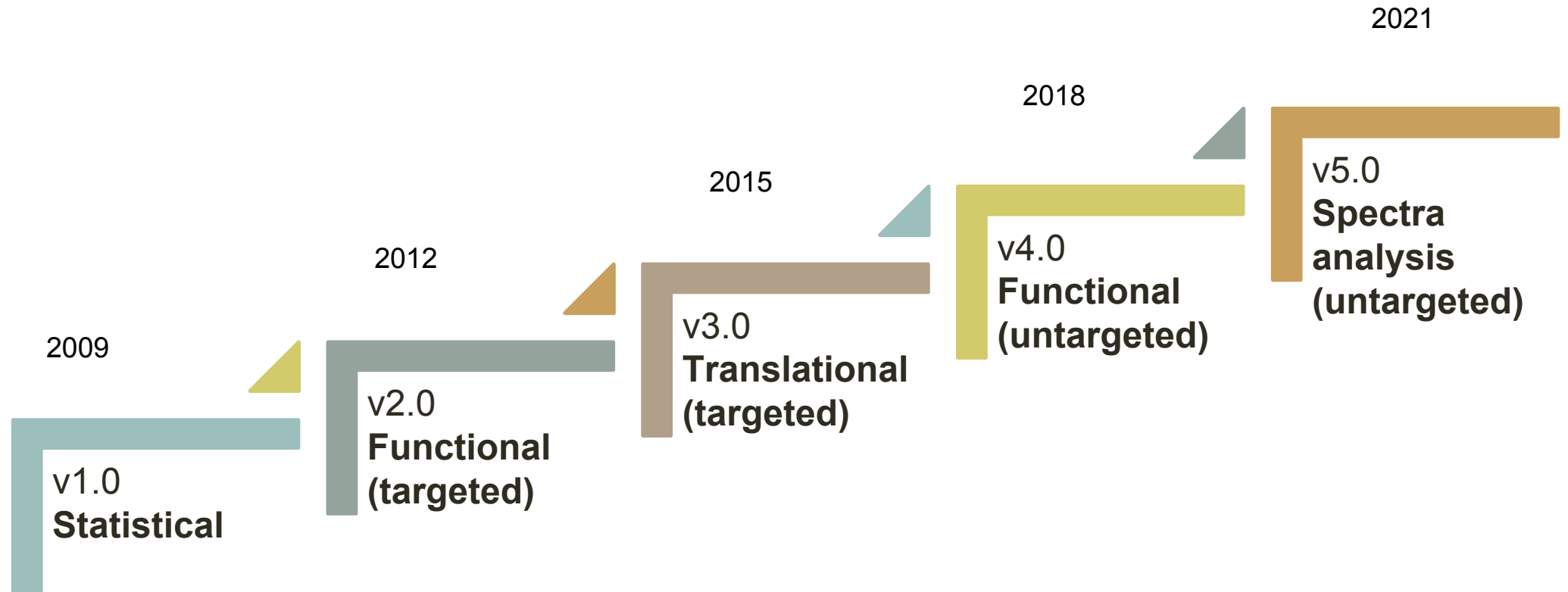


# Don't forget biology & context



Put everything together and write your manuscript

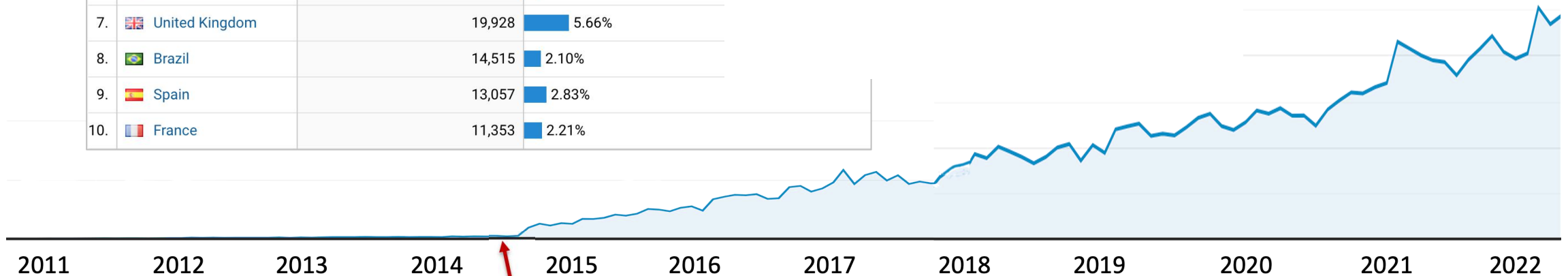
# Journey of MetaboAnalyst



# User Traffic (Google Analytics)

Country	Users	Sessions
	507,732 % of Total: 100.00% (507,732)	13,220,558 % of Total: 100.00% (13,220,558)
1.  China	147,297	20.98%
2.  United States	106,188	27.02%
3.  Germany	22,018	4.23%
4.  Japan	21,376	2.63%
5.  Canada	20,515	3.83%
6.  India	20,434	2.37%
7.  United Kingdom	19,928	5.66%
8.  Brazil	14,515	2.10%
9.  Spain	13,057	2.83%
10.  France	11,353	2.21%

- ~ **2,500** users per day
- Since 2018, >**13 million** data analysis jobs submitted from ~**500, 000** users



30,000  
users/month

300 ~ 500 users/month

# MetaboAnalyst 5.0 Modules

Section 1						
Input Data Type	Available Modules (click on a module to proceed, or scroll down for more details)					
Raw Spectra (mzML, mzXML or mzData)	Section 3			LC-MS Spectra 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 [one factor]	Statistical Analysis [metadata table]	Biomarker Analysis	Statistical Meta-analysis	Power Analysis	Other Utilities

Section 2

Section 4

# Detailed protocols



PROTOCOL

## Using MetaboAnalyst 4.0 for Comprehensive and Integrative Metabolomics Data Analysis

Jasmine Chong, David S. Wishart , Jianguo Xia 

First published: 20 September 2019 | <https://doi.org/10.1002/cpbi.86> | Citations: 1,265

[Read the full text >](#)



### Abstract

MetaboAnalyst (<https://www.metaboanalyst.ca>) is an easy-to-use web-based tool suite for comprehensive metabolomic data analysis, interpretation, and integration with other omics data. Since its first release in 2009, MetaboAnalyst has evolved significantly to meet the ever-expanding bioinformatics demands from the rapidly growing



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

Zhiqiang Pang<sup>1</sup>, Guangyan Zhou<sup>1</sup>, Jessica Ewald <sup>2</sup>, Le Chang <sup>3</sup>, Orcun Hacariz<sup>1</sup>, Niladri Basu<sup>2</sup> and Jianguo Xia <sup>1,3</sup> 

Liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) has become a workhorse in global metabolomics studies with growing applications across biomedical and environmental sciences. However, outstanding bioinformatics challenges in terms of data processing, statistical analysis and functional interpretation remain critical barriers to the wider adoption of this technology. To help the user community overcome these barriers, we have made major updates to the well-established MetaboAnalyst platform ([www.metaboanalyst.ca](http://www.metaboanalyst.ca)). This protocol extends the previous 2011 *Nature Protocol* by providing stepwise instructions on how to use MetaboAnalyst 5.0 to: optimize parameters for LC-HRMS spectra processing; obtain functional insights from peak list data; integrate metabolomics data with transcriptomics data or combine multiple metabolomics datasets; conduct exploratory statistical analysis with complex metadata. Parameter optimization may take ~2 h to complete depending on the server load, and the remaining three stages may be executed in ~60 min.

[https://github.com/xia-lab/Metabolomics\\_2023](https://github.com/xia-lab/Metabolomics_2023)



# Logistics



# MetaboAnalyst 5.0 Workshop Checklist

Wifi Account: **Metabolomics 2023**

Code: **Falls2023**

Instructions & Materials:

[https://github.com/xia-lab/Metabolomics\\_2023](https://github.com/xia-lab/Metabolomics_2023)

We have set up multiple servers:

- <https://www.metaboanalyst.ca>
- <https://new.metaboanalyst.ca>
- <https://genap.metaboanalyst.ca>

User Forum:

- <https://omicsforum.ca>

# Cautions & Recommendations

Page display may be slow due to bandwidth limitation in this room

- Be patient
- Do not open multiple tabs to MetaboAnalyst (results will overwrite each other!)
- Form a group and share computers (see next page)

# Group forming

- 2~3 people per group
  - Make new friends
  - Help each other & reduce stress
- Share laptops
  - One for displaying tutorial, and one for using MetaboAnalyst
  - Reduce bandwidth consumption

# https://omicsforum.ca

**OmicsForum** About Rules

**Welcome to the OMICS community**  
Please search before you post, and follow forum rules

Search

To make launching your new site easier, you are in bootstrap mode. All new users will be granted trust level 1 and have daily email summary emails enabled. This will be automatically turned off when 50 users have joined.

**Home > MetaboAnalyst**

MetaboAnalyst ▾ Metabolomics 2022 ▾ all tags ▾ Top New (1) Latest Unseen My Posts Bookmarks + New Topic

Online (2):

≡ Topic Likes Replies Last Post

**Important links for MetaboAnalyst workshop** •

The workshop will use the MetaboAnalyst and OmicsNet software. Different sections will follow different portions of the recent MetaboAnalyst Nature Protocol publication: Section I: Raw spectra data processing (Protoco... read more

jess.ewald 42m 3 42m jess.ewald

- Current topics in MetaboAnalyst: ~700
- Please search topics or open a new topic

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