MASS SPECTROMETRY
METABOLOMICS SERVICE OVERVIEW

Service Description

Metabolomics is the scientific study of chemical processes involving metabolites, the small molecule substrates, intermediates and products of metabolism that occur within cells, biofluids, tissues or organisms. Collectively, these small molecules and their interactions within a biological system are known as the metabolome.

Metabolites and their concentrations directly reflect the underlying biochemical activity and state of cells and tissues. BGI Genomics metabolomic solutions therefore provide researchers a way to study the 'unique chemical fingerprint that specific cellular processes leave behind'.[1]

BGI Genomics has extensive experience in the field of metabolomics and offers a wide range of services including overall metabolite profiles as well as targeted small molecule analysis services.

By applying cutting-edge LC-MS/MS systems and techniques, BGI Genomics offers validated metabolomics workflows including:

- Untargeted metabolomics (water/lipid-soluble)
- Lipidomics profiling (FA, GL, GP, SP, ST, PR, SL, and PK)
- Targeted metabolomics (High-throughput panels HM Pro2300 , vitamins, amino acids, hormones, bile acids, TMAO, SCFA etc.)

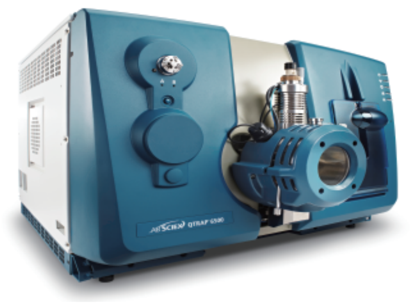
Turnaround Time

Typical 4-6 weeks for Metabolomics products

Instrumentation

Liquid chromatography column: Waters C18, HILIC
Orbitrap: Thermo Q Exactive HFX, Thermo Q Exactive HF, Q Exactive...
Triple quadrupole: QTRAP 6500+

Q Exactive HF-X



QTRAP 6500+

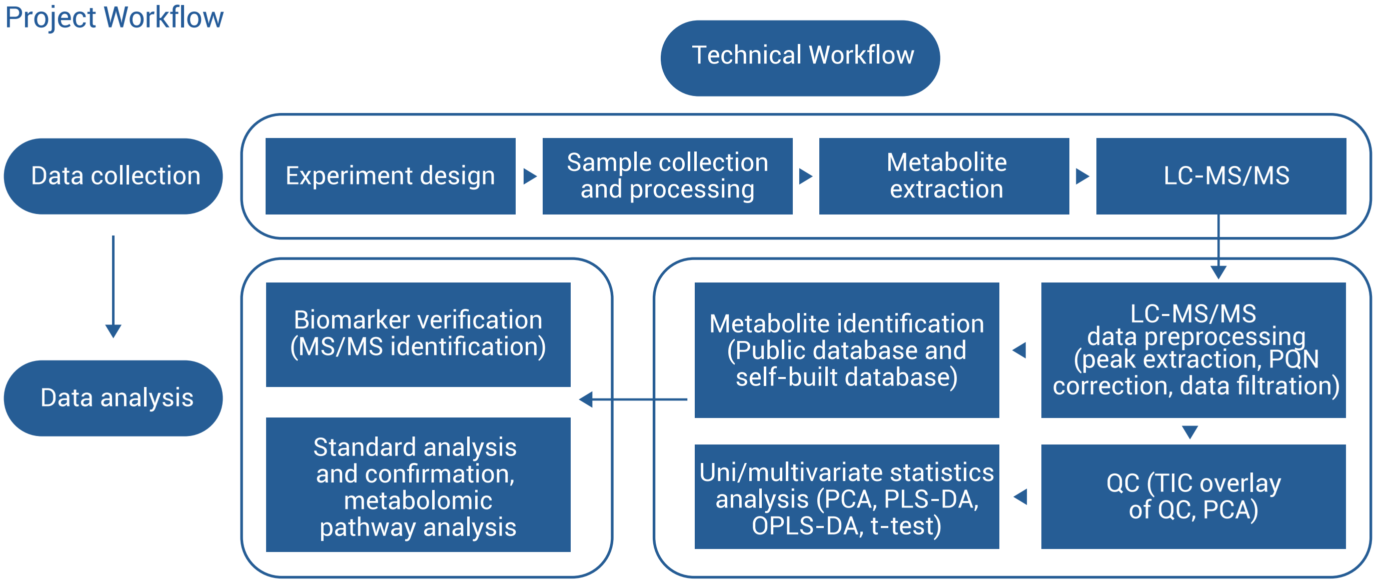
Quality Data Fast TAT Cost Effective

Untargeted Metabolomics Solutions

BGI Genomics provide LC-MS/MS untargeted metabolomics services to support biomedical and biotechnology applications. Our untargeted metabolomics services are designed to obtain a metabolite profile and screen for differentially-expressed molecules in the sample.

There are two main standard databases available for untargeted metabolomics analysis: BGI Genomics self-build standard database and Thermo mzCloud standard database. BGI Genomics self-build standard database is divided into plant and medical databases. The medical database contains more than 2,000 metabolites, while the plant database contains more than 2,500 metabolites. The mzCloud standard database provides information on over 30,000 metabolites.

Project Workflow



Technical Workflow

Data collection

Experiment design

Sample collection and processing

Metabolite extraction

LC-MS/MS

Data analysis

LC-MS/MS data preprocessing (peak extraction, PQN correction, data filtration)

Metabolite identification (Public database and self-built database)

QC (TIC overlay of QC, PCA)

Uni/multivariate statistics analysis (PCA, PLS-DA, OPLS-DA, t-test)

Biomarker verification (MS/MS identification)

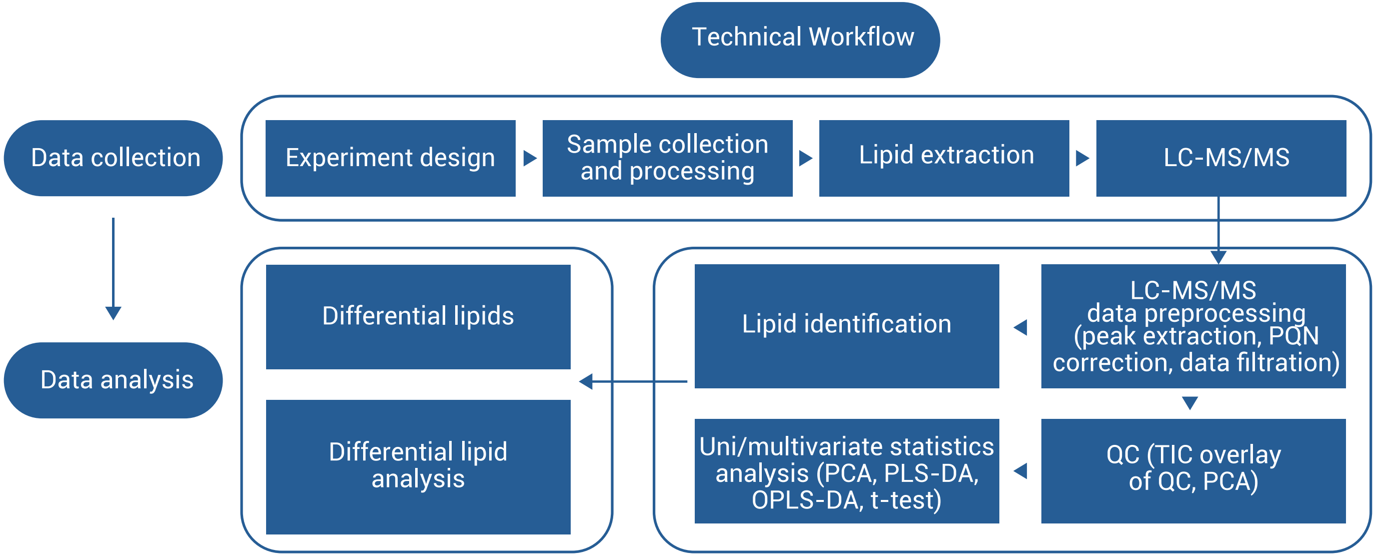
Standard analysis and confirmation, metabolomic pathway analysis

Lipidomics Profiling Solutions

BGI Genomics lipidomics services are designed to obtain a lipid profile and screen for deferentially-expressed lipids in the sample. BGI Genomics lipidomics service enables confirmation of lipid structure characteristics such as lipid molecule head structure, fatty acid branch chain length and unsaturated double bond number by comparing the characteristic signals of precursor ions, MS2 fragments and neutral loss.

Lipid identification utilizes the largest lipids database, covering 8 categories of lipids, 300 lipid subclasses, and containing more than 1.7 million lipid ions and their predictive fragment ions information.

Project Workflow



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Differential lipids

Differential lipid analysis

Targeted Metabolomics Solutions

HM Pro2300

BGI Genomics provides one of the world's most comprehensive panels for targeted metabolomics research. The HM Pro2300 panel uses LC-MS/MS technology for high-throughput targeted metabolomics detection. HM Pro2300 can simultaneously detect more than 2,000 metabolites, including 700 small molecules and more than 1,600 lipids which covers all kinds of important metabolites and core metabolic pathways. We also provide HM700 and HML1600, only detecting small molecules and lipids respectively.

HM700 includes more than 400 metabolites related to intestinal flora, which applies to address key pathophysiological processes relevant in gut microbiota research and cancer research areas. Each metabolite is quantitatively determined using the standard curve. This enables greater in-depth mining of metabolome information, providing accurate quantification, excellent reproducibility and high throughput.

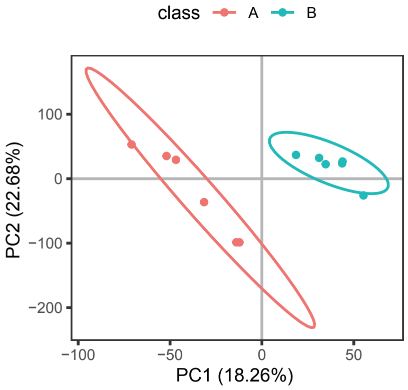
The HML1600 can achieve absolute quantification for more than 1,600 lipids of 12 subclasses by the method of combining standard curves with internal standard, covering all kinds of lipids with important biological functions. HML1600 is used for nervous system disease research, cardiovascular and cerebrovascular disease research, nutritional metabolism research, lipid metabolism research and other fields.

List of targeted metabolomic panels

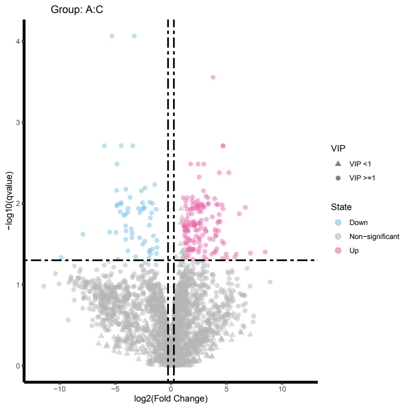
Category of targeted metabolites	Number of metabolites
Amino acid	20
Water-soluble vitamin	5
Fat-soluble vitamin	5
Steroid hormone	12
Bile acid	45
Trimethyamine oxide	4
Short-chain fatty acids	7
Neurotransmitter	39
Trace elements and heavy metals	18
Homocysteine metabolism	9
Plant hormone	32
Tryptophan metabolism	29

Data Analysis

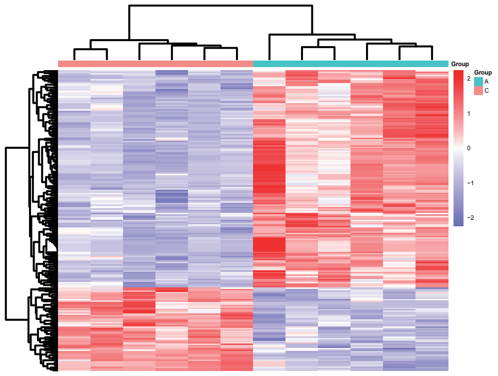
After mass spectrometry data acquisition, we employ commercial software along with the self-developed metabolomics R software package metaX[2] to undertake statistical analysis of mass spectral data, wherein metabolite identification is based on the databases KEGG, HMDB.



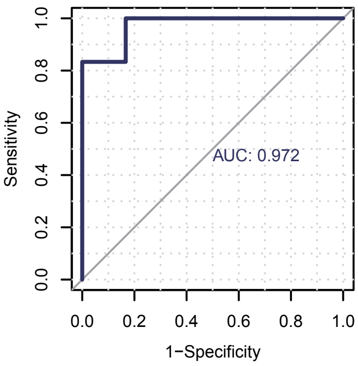
Score graph of PLS-DA



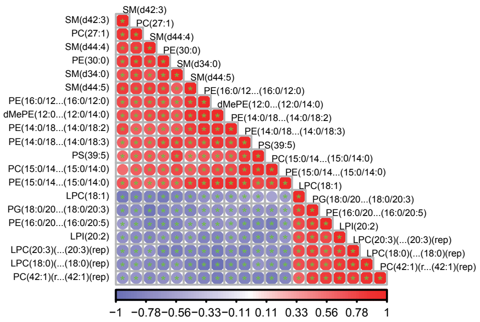
Volcano plot



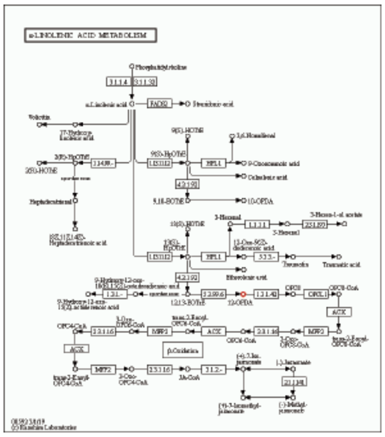
Cluster analysis



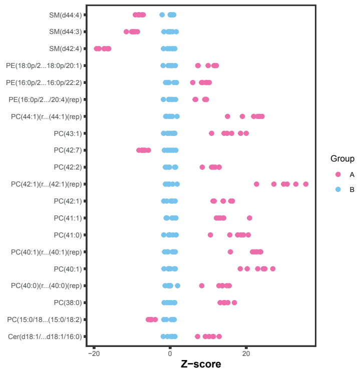
ROC curve



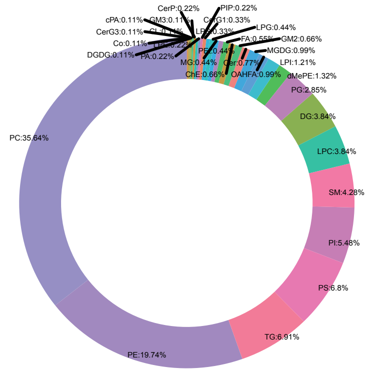
Metabolite correlation analysis



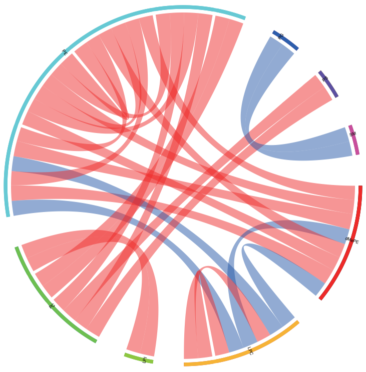
KEGG metabolic pathway



Differential metabolite clusterin



Metabolites donut chart



Correlation chord diagrams
on differential metabolites

Metabolomic Research Applications

Human health

- Metabolome study of physiological change in healthy populations
- Disease biomarker screening and validation
- Clinical sample metabolite detection and analysis
- Drug compound identification, toxicity assessment, drug effect assessment

Plant and animal research

- Important crop traits and improvement
- Animal nutrients and breeding

Microbe research

- Microbial drug tolerance research
- Effect on microbial metabolomic pathways of growth and development by environmental stimulus
- Effect on host metabolism by microbe invasion or inhabitation

Selected Publications

Publication time	Journal	IF	Title
2024	*Gut*	23	Butyrate-producing Faecalibacterium prausnitzii suppresses natural killer/T-cell lymphoma by dampening the JAK-STAT pathway
2024	*Nature Communications*	18	Gut microbiota facilitate chronic spontaneous urticaria
2024	*Advanced Science*	14.3	Multi-Omics Analysis by Machine Learning Identified Lysophosphatidic Acid as a Biomarker and Therapeutic Target for Porcine Reproductive and Respiratory Syndrome
2024	*Molecular Biology and Evolution*	10.7	Multiomics Analyses Provide New Insight into Genetic Variation of Reproductive Adaptability in Tibetan Sheep
2023	*Signal Transduction and Targeted Therapy*	38.1	Baseline gut microbiota and metabolome predict durable immunogenicity to SARS-CoV-2 vaccines

References

[1] "Growing pains for metabolomics". *The Scientist*. 2005.

[2] metaX: a flexible and comprehensive software for processing metabolomics data. *BMC Bioinformatics*. 2017.

Request for Information or Quotation

Contact a BGI Genomics representative to discuss how we can meet your specific needs or for expert advice on experiment design, from sample to bioinformatics.

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