MASS SPECTROMETRY
## METABOLOMICS SERVICE OVERVIEW

BGI

Service Description

Metabolomics is the scientific study of chemical processes involving metabolites, the small molecule substrates, inter-mediates 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's metabolomic solutions therefore provide researchers a way to study the 'unique chemical fingerprint that specific cellular processes leave behind'.[1]

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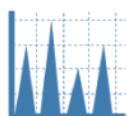
- Untargeted metabolomics (water/lipid-soluble)
- Lipidomics profiling (FA, GL, GP, SP, ST, PR, SL, and PK)
- Targeted metabolomics (High-throughput panels HM Pro2300 , vitamins, amino acids, hormones, bile acids, TMAO, SCFA etc.)

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+

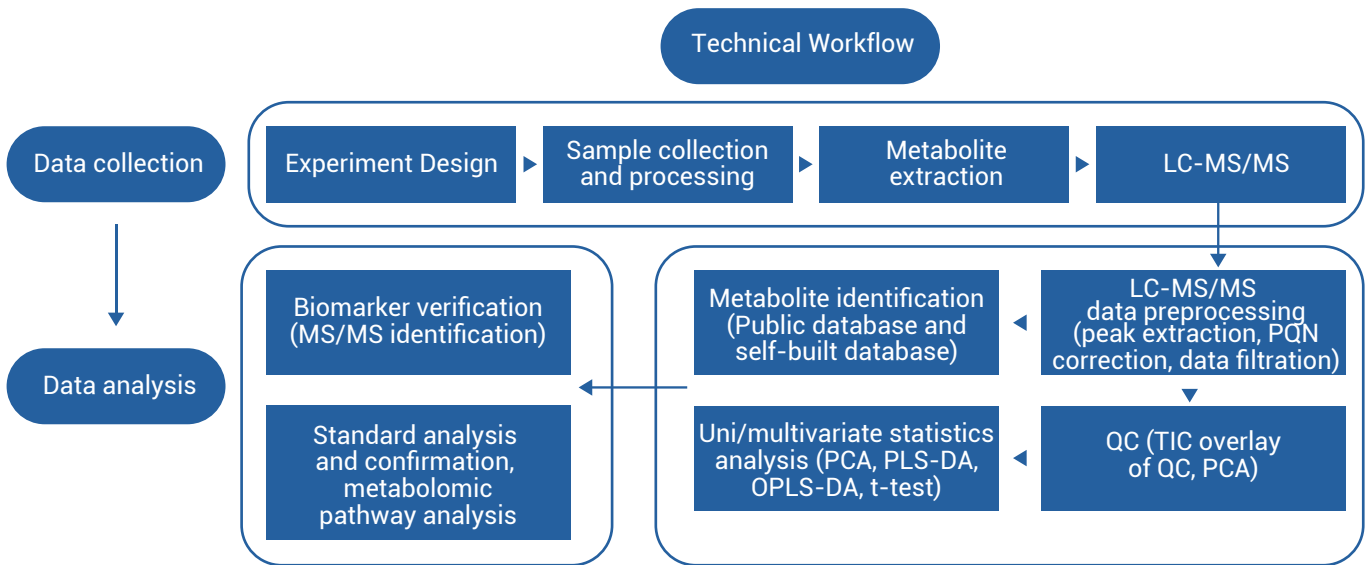Quality Data   Fast TAT   Cost Effective

Untargeted Metabolomics Solutions

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

Metabolites are identified using self-built metabolite standard database (3,000+) and Thermo mzCloud standard database. mzCloud is an online standard database of over 20,000 compounds containing both MS1 and MS2 spectra information.

Project Workflow

Technical Workflow

Data collection

Experiment Design ▸ Sample collection and processing ▸ Metabolite extraction ▸ LC-MS/MS

Data analysis

Biomarker verification (MS/MS identification)

Standard analysis and confirmation, metabolomic pathway analysis

Metabolite identification (Public database and self-built database) ◂

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

LC-MS/MS data preprocessing (peak extraction, PQN correction, data filtration)
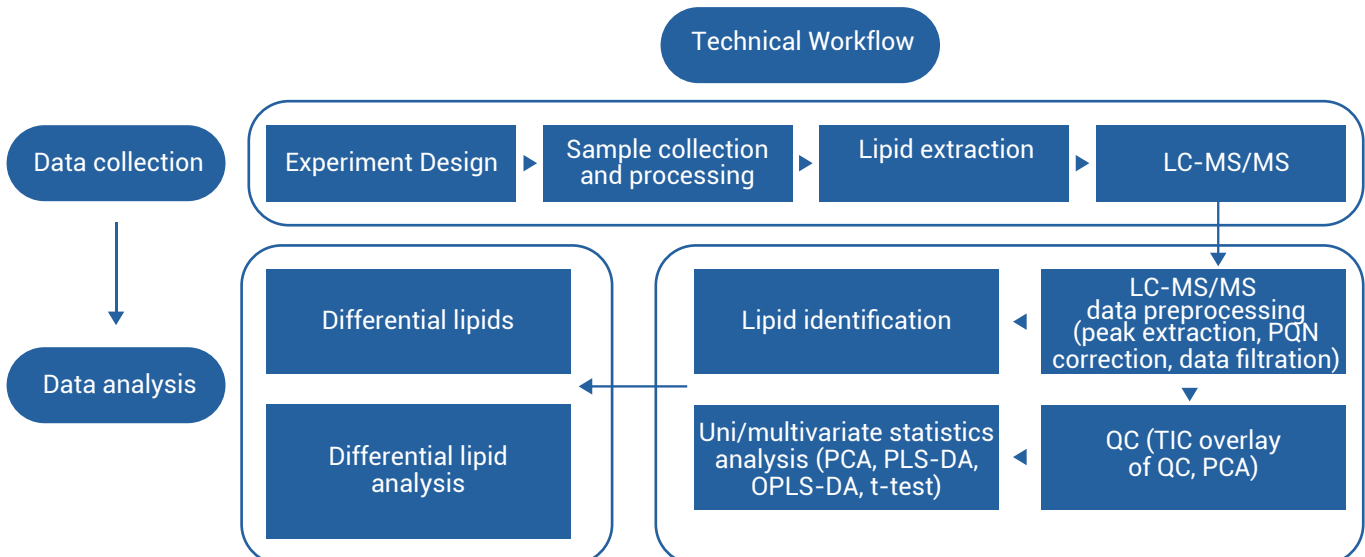
QC (TIC overlay of QC, PCA)

Lipidomics Profiling Solutions

BGI lipidomics services are designed to obtain a lipid profile and screen for deferentially-expressed lipids in the sample. BGI's 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.

LipidSearch is equipped with 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

Technical Workflow

Data collection

Experiment Design ▸ Sample collection and processing ▸ Lipid extraction ▸ LC-MS/MS

Data analysis

Differential lipids

Differential lipid analysis

Lipid identification ◂

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

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

QC (TIC overlay of QC, PCA)

Targeted Metabolomics Solutions

HM Pro2300

BGI 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	13
Bile acid	15/45
Trimethyamine oxide	6
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 use the commercial software CD (version 3.2) and LipidSearch (version 4.1) and 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.
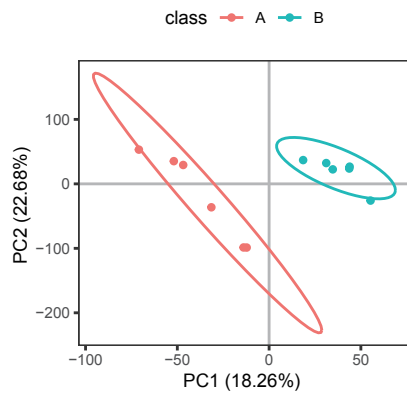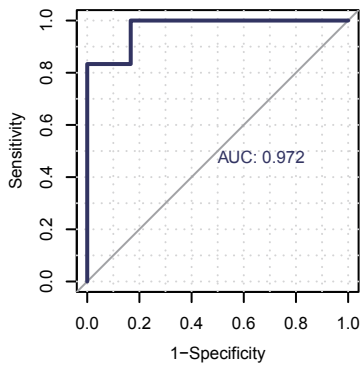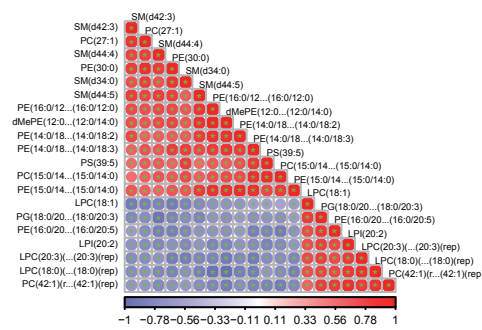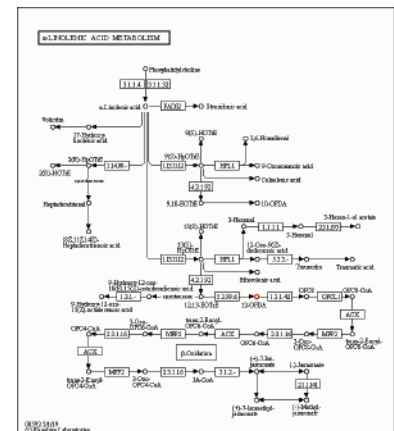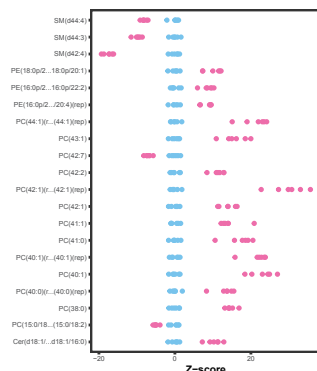

Score graph of PLS-DA
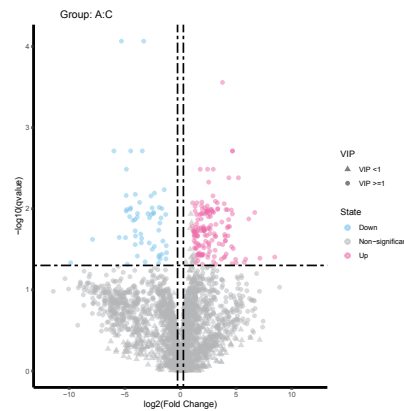
Volcano plot
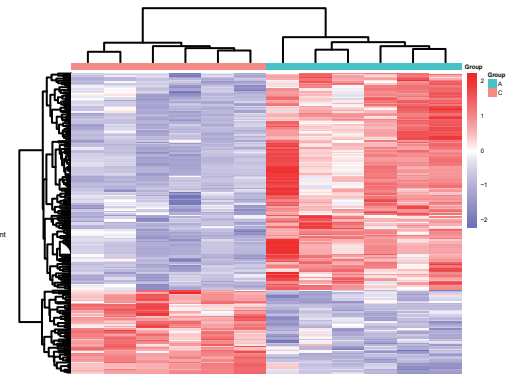
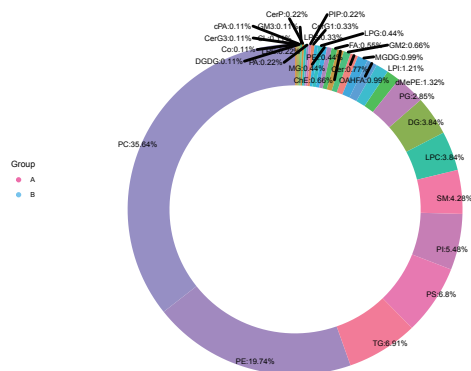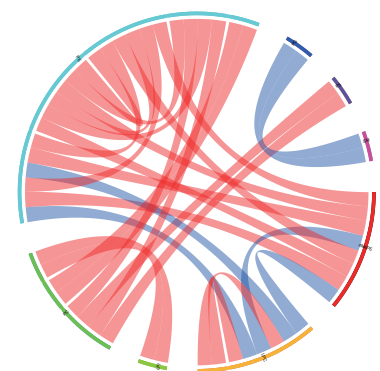Cluster analysis

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
2022	Nature Genetics	41.31	Mendelian randomization analyses support causal relationships between blood metabolites and the gut microbiome
2022	European Respiratory Journal	16.67	Metabolomic analyses reveals new stage-specific features of the COVID-19
2021	Gut	19.82	Alterations in the human oral and gut microbiomes and lipidomics in COVID-19
2021	Nature Ecology and Evolution	15.40	Molecular mechanisms of mutualistic and antagonistic interactions in a plant–pollinator association
2021	Theranostics	11.56	Metabolomic profiling reveals amino acid and carnitine alterations as metabolic signatures in psoriasis
2021	Nature Communicantions	12.12	The trans-omics landscape of COVID-19

References

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

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

Request Information or Quotation

Contact your BGI account representative for the most affordable rates in the industry and to discuss how we can meet your specific project requirements or for expert advice on experiment design, from sample to bioinformatics.

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We Sequence, You Discover