Lipidomics Bioinformatics Analysis

Untargeted and targeted lipidomics are two categories of lipidomics that are often used in combination for the discovery and quantification of differential lipid molecules. Untargeted lipidomics uses LC-MS and GC-MS technologies to unbiasedly detect the dynamic changes of all lipid molecules before and after the stimulation or disturbance in cells, tissues, organs, or organisms. Through bioinformatics analysis to screen differential lipid molecules and analyze their pathways, untargeted lipidomics can reveal the physiological mechanism of their changes. Targeted lipidomics is the research and analysis of a specific class of lipids. Obtaining tedious data from this assay is not the end goal. Bioinformatics analysis can organize, mine, and visualize data, and thus extract useful biological information from large amounts of data to help with scientific discovery.

Untargeted Lipidomics Data Analysis

1

Data acquisition

Lipidomics usually requires the use of multiple analytical techniques to meet different experimental needs. Common analytical techniques include liquid chromatography-mass spectrometry (LC-MS), gas chromatography-mass spectrometry (GC-MS), capillary electrophoresis-mass spectrometry (CD-MS), HILIC-MS, etc. The main high-resolution mass spectrometry techniques are TOF-MS, FTICR-MS, Orbitrap-MS, and Sector-MS. The mass spectrometry data obtained by the above techniques are used for subsequent analysis.

2

Data analysis

Data preprocessing

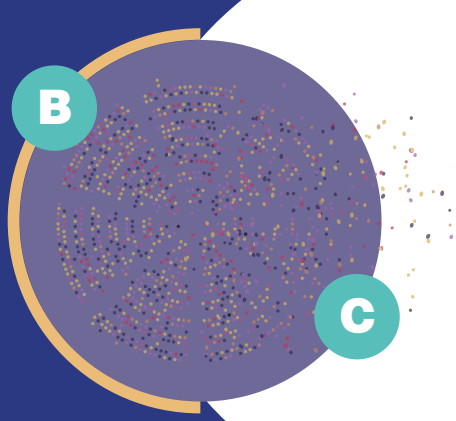
A

Use software such as XCMS, MZmine and MarkerView for raw data processing.

Identify differential lipid molecules

B

Commonly used analysis methods include principal component analysis (PCA), partial least squares discriminant analysis (PLS-DA), orthogonal partial least squares discriminant analysis (OPLS-DA), etc. Data analysis results also need to be screened for differential lipid molecules through t-test and variable importance in projection (VIP) values.



Metabolic pathway analysis

C

Common metabolic pathway databases include LipidMaps, LipidBank, HMDB, KEGG, Reactome, BioCyc, and MetaCyc, which can be used to analyze metabolic pathways and interaction networks.

Multi-omics analysis

D

Available databases and software include IMPaLA, iPEAP, MetaboAnalyst, SAMNetWeb, pwOMICS, MetaMapR, MetScape, Grinn, WGCNA, MixOmic, DiffCorr, qpgraph, huge, etc.

Targeted Lipidomics Data Analysis

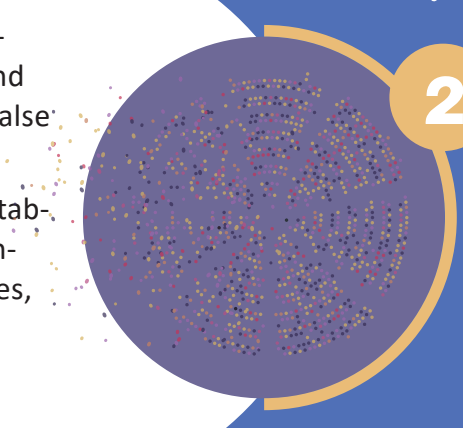
1

Data acquisition

In targeted lipidomics, natural and isotope-labeled standards facilitate the identification and quantification of lipid molecules and reduce false positives.

Quantitative metabolomics can be used to establish baseline levels of lipids in tissues or organisms, for comparison between different studies, or to define normal and "disturbed" states of metabolism.

The use of isotope-labeled internal standards can also help explain the matrix-induced ionization effects that affect the accuracy of the analysis, thereby improving the sensitivity of biological response testing.



2

Data analysis

Since targeted lipidomics focuses on a limited variety of metabolites, data analysis is simpler and more straightforward than untargeted lipidomics.

The methods and databases used are similar to those of untargeted lipidomics, including databases such as LipidMaps and LipidBank.

Creative Proteomics' experts have extensive experience in lipidomics and bioinformatics analysis, assisting you in screening differential metabolites, identifying unknown lipid molecules, and qualitatively and quantitatively analyzing target compounds.

Contact Us

Creative Proteomics