

# UNTARGETED **METABOLOMICS**



Metabolomics can be divided into non-targeted and targeted metabolomics. Non-targeted metabolomics can analyze metabolites derived from the organisms comprehensively and systematically. It is an unbiased metabolomics analysis that can discover new biomarkers. Targeted metabolomics is the study and analysis of specific metabolites. Both have their own advantages and disadvantages, and are often used in combination for the discovery and accurate weight determination of differential metabolites, and in-depth research and analysis of subsequent metabolic molecular markers. Targeted and non-targeted metabolomics take parts in food identification, disease research, animal model verification, biomarker discovery, disease diagnosis, drug development, drug screening, drug evaluation, clinical research, plant metabolism research, microbial metabolism research.

### Untargeted **Metabolomics Strategy**



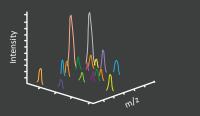


Metabolite Extraction

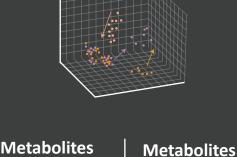
Data Acquisition

**Data Processing** 





**Features Selection** 



Identification

Quantitation





### **Targeted Metabolomics Strategy**

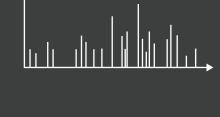


**Metabolites Purification** 



**MS Analysis** 

**Data Acquisition** 



**Data Interpretation** 



## Discovery

**Untargeted Metabolomics** 

Absolute quantification of spesific features

commercially available chemicalstandart

• Extraction procedure for spesific metabo-

Validation of identified feature (Requires

Validation

Hypothesis driven

for validation)

~20 metabolites measured

Chromatographic separation

modes) (EI, ESI, APC, MALDI)

Mass detection

• MS ionization (negative and positive

Metabonomics

**Targeted Metabolomics** 

Sample

**Preparation** 

Data

Acquisition

Features

- Globalmetabolomics profling
- Metabolomics fingerprinting Metabolomics footprinting

Hypothesis generating

- Classification/ forming metabotypes • Qualitative identification • Relative quantification
- > 1000s metabolites measured • No chemical commercial standartrequired
- Global metabolite extraction:
  - a. Hydrophobic fraction: C18 Column
- b. Hydrophiic fraction: HILIC Column Derivatization (optional)
- Chromatographic separation
- MS ionization (negative and positive
- modes) (EI, ESI, APCI, MALDI) Mass detection
- Data preprocessing: noise filtering, reten-
- tion time correction, peak detection,
- chromatogram alignment, unknown
- features/metabolite identification Data preparation: data integrity checking. data IS normalzasyon, compound name
- Multiple Reaction Monitoring (MRM)
  - · Data preprocessing
    - Statistical analysis • Absolute quantitation of metabolite concentrations

Data

Interpretation

Data

**Processing** 

- identification Statistical analysis
- Bioinformatics Integrative OMICS Enrichment Analysis
- Bioinformatics
- Integrative OMICS Enrichment Analysis
- Pathway Analysis Metabolic Network
- Pathway Analysis Metabolic Network



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