

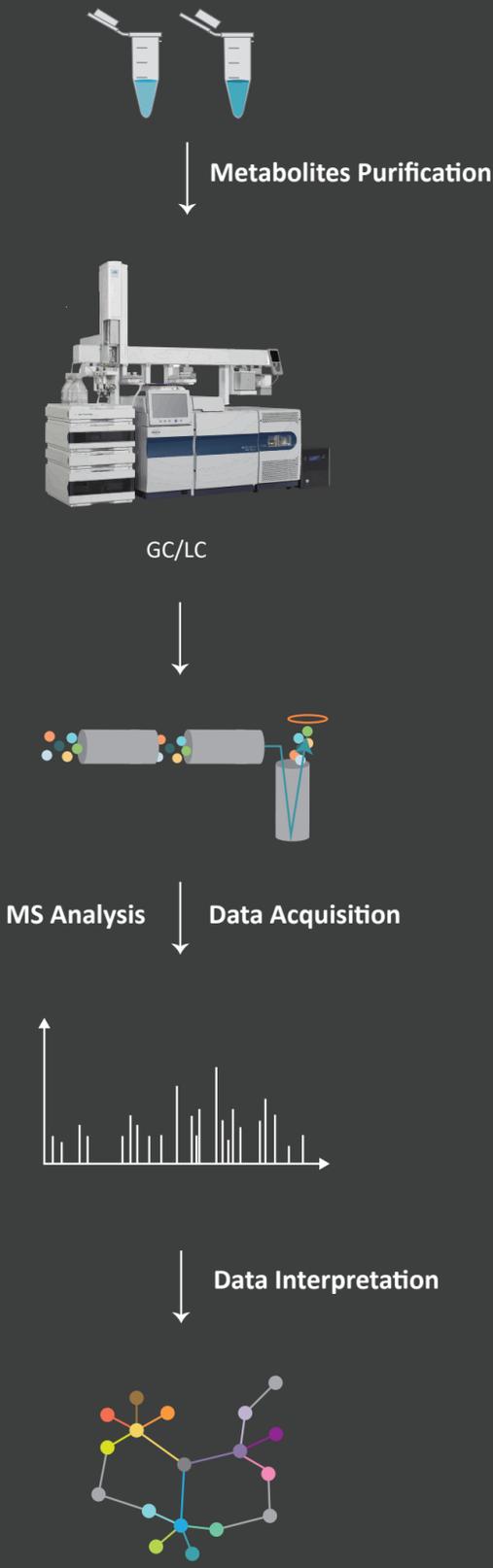
UNTARGETED METABOLOMICS VS TARGETED METABOLOMICS

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



Targeted Metabolomics Strategy



| | Untargeted Metabolomics | Targeted Metabolomics |
|---------------------|--|---|
| Features | <ul style="list-style-type: none"> Discovery Hypothesis generating Globalmetabolomics profiling Metabolomics fingerprinting Metabolomics footprinting Classification/ forming metabolotypes Qualitative identification Relative quantification > 1000s metabolites measured No chemical commercial standartrequired | <ul style="list-style-type: none"> Validation Hypothesis driven Absolute quantification of spesific features Validation of identified feature (Requires commercially available chemicalstandart for validation) Metabolomics ~20 metabolites measured |
| Sample Preparation | <ul style="list-style-type: none"> Global metabolite extraction: <ol style="list-style-type: none"> Hydrophobic fraction: C18 Column Hydrophiic fraction: HILIC Column Derivatization (optional) | <ul style="list-style-type: none"> Extraction procedure for spesific metabo- lites |
| Data Acquisition | <ul style="list-style-type: none"> Chromatographic separation MS ionization (negative and positive modes) (EI, ESI, APCI, MALDI) Mass detection | <ul style="list-style-type: none"> Chromatographic separation MS ionization (negative and positive modes) (EI, ESI, APC, MALDI) Mass detection Multiple Reaction Monitoring (MRM) |
| Data Processing | <ul style="list-style-type: none"> Data preprocessing: noise filtering, reten- tion time correction, peak detecting, chromatogram alignment, unknown features/metabolite identification Data preparation: data integrity checking, data IS normalzasyon, compound name identification Statistical analysis | <ul style="list-style-type: none"> Data preprocessing Statistical analysis Absolute quantitation of metabolite concentrations |
| Data Interpretation | <ul style="list-style-type: none"> Bioinformatics Integrative OMICS Enrichment Analysis Pathway Analysis Metabolic Network | <ul style="list-style-type: none"> Bioinformatics Integrative OMICS Enrichment Analysis Pathway Analysis Metabolic Network |