

# Towards a Comprehensive Analysis of Metabolome

Guowang Xu\*

CAS Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 116023, Dalian, China. \*e-mail: xugw@dicp.ac.cn

## Gold statement

- New analytical strategy of metabolome
- New identification method for metabolites
- New applications of metabolomics

## Introduction

Metabolomics is a science to study whole metabolome change caused by genetic, pathological or environmental perturbations in a biosystem. Therefore, a comprehensive analysis of the endogenous metabolites is the basis of metabolomics study. Because of metabolome complexity, one single analysis to acquire the information of whole metabolome is not possible, several analytical methods or platforms usually are needed. Mass spectrometry (MS) coupled with different chromatographic techniques including capillary electrophoresis is one of the most important analytical tools for metabolomics.

## Body

In our laboratory, we have established a very good analytical platform for metabolomics by using GC-MS, LC-MS and CE-MS. Besides the traditional targeted and nontargeted methods, following work has been performed to achieve comprehensive metabolome information,

1. Two-dimensional LC-MS methods based on the stop-flow technique to improve the peak capacity of analytical systems [1];
2. Pseudotargeted metabolomics and lipidomics methods to improve the data quality with a good analytical coverage [2].
3. Nanoparticle-assisted and/or derivatization methods to improve the detection of trace metabolites;
4. Stable isotope labeling to obtain dynamic lipidomics and metabolomics information;
5. A “live” LC-MS database for the identification of metabolites based on the retention times, MS and MS/MS of standard samples. In the meantime, structure-retention relationship was used to predict and extend the metabolite information. In total, about 7000 metabolites have been included in home-made database.

## Conclusion

By using above described methods, we can semi-quantitatively analyze almost 2000 metabolites in an analysis [1]. This lecture will report our newest results on the method development and their applications in disease studies, especially in helping the treatment of acute-on-chronic liver failure (ACLF) [3].

## References

- [1] W. Lv, et al. *Anal. Chem.*, **92**(2020)6043-6050
- [2] F. Zheng, et al. *Nature Protocols*, **15**(2020)2519-2537
- [3] Z. Yu, et al. *Advanced Science*, **7**(2020) 1902996.