Scientists propose a pseudotargeted metabolomics protocol

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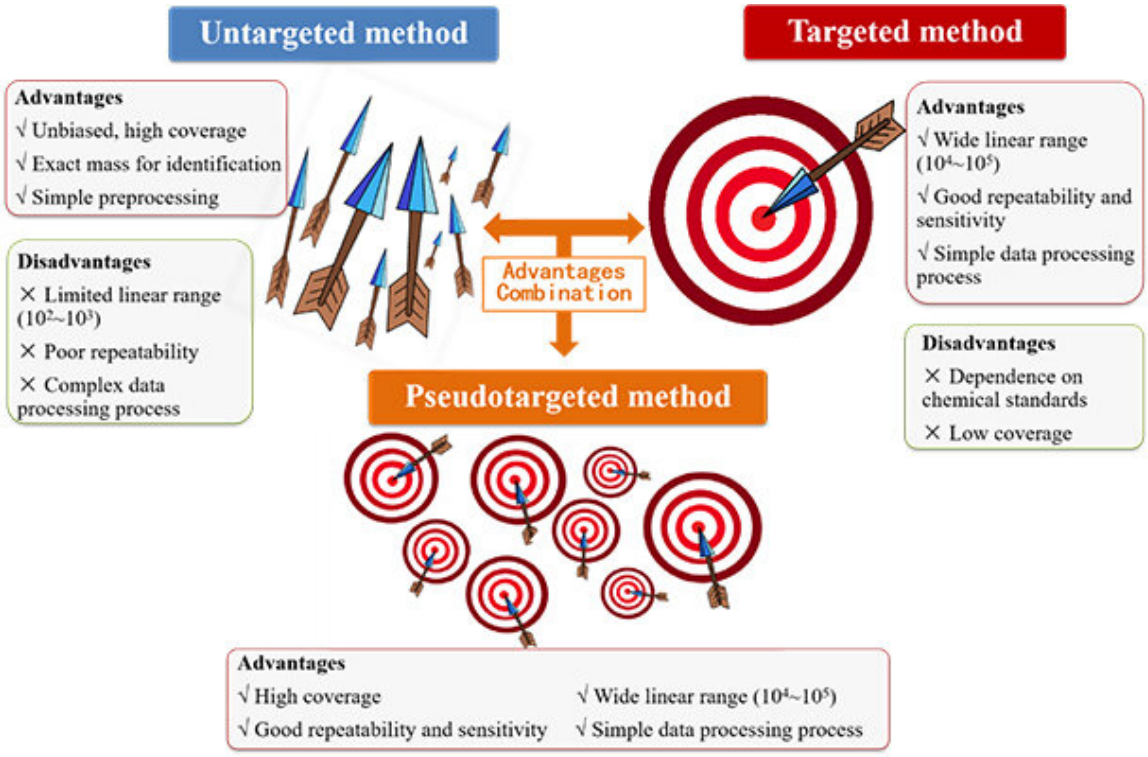

Pseudotargeted metabolomics method is a new method integrating the advantages of untargeted and targeted metabolomics methods. Credit: WANG Ting

A research group led by Prof. Xu Guowang from the Dalian Institute of Chemical Physics of the Chinese Academy of Sciences proposed a protocol by systematically summarizing and upgrading the

pseudotargeted metabolomics method.

The study was published in *Nature Protocols* on June 24.

Metabolomics is the science of studying endogenous metabolites. Ultra-high performance liquid chromatography-mass spectrometry is the most widely used analytical tool.

There are mainly two kinds of analysis strategies: untargeted method and targeted method.

The untargeted method uses high-resolution mass spectrometry to obtain abundant metabolite information, with disadvantages of complex data handling, poor repeatability, and narrow linear range.

The targeted method uses triple quadrupole mass spectrometry. Although data quality is improved, only known metabolites can be detected.

Prof. Xu's group firstly proposed the idea of pseudotargeted metabolomics in 2012. Its innovation lies in a quantitative ions selection algorithm. Both known and unknown metabolites in samples can be measured by using the retention time locking gas chromatography-mass spectrometry- selected ions monitoring. It merges the advantages of untargeted and targeted metabolomics methods.

The idea was extended to liquid chromatography-mass spectrometry in 2013. In the subsequent works, Xu's group further developed software to automatically select ion-pairs to improve the efficiency of method establishment.

On this basis, in order to increase the number of ion-pairs included in the method and improve metabolite coverage, a pseudotargeted

metabolomics method based on the sequential windowed acquisition of all theoretical fragment ion was developed.

In their latest work, in order to further improve the coverage, a pseudotargeted method was developed based on a two-dimensional liquid chromatography-mass spectrometry system with high peak capacity. It can be used to separate and analyze amino acids, bile acids, carnitine, and lysophospholipids, etc.

These methods have played an active role in the studies of malignant tumors, diabetes and other metabolic diseases. The pseudotargeted methods and idea have also been used by other laboratories.

At present, high-coverage quantitative/semiquantitative metabolomics methods are receiving more and more attention in different fields of life sciences, and the pseudotargeted method will play an increasingly important role in the future.

Prof. Xu's group has further optimized the development procedures of pseudotargeted metabolomics, upgraded and provided open-accessed software and tools to allow more colleagues to use the pseudotargeted method.

More information: Fujian Zheng et al. Development of a plasma pseudotargeted metabolomics method based on ultra-high-performance liquid chromatography–mass spectrometry, *Nature Protocols* (2020). DOI: 10.1038/s41596-020-0341-5

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