

Application of Metabolomics to Reveal the Biological Mechanism of Toxicological Research

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Abstract

Metabolomics can illustrate microscopic changes in the metabolic mechanisms of toxicity caused by frequent exposure to drugs, herbs, and environmental pollutants, and recent reports have supported the great potential and value of metabolomics in reducing the occurrence of injury reactions.

Keywords: Metabolomics; Toxicology; Biomarkers; Metabolic pathways; Mechanisms

Abbreviations:GC: Gas Chromatography; LC:Liquid Chromatography; MS: Mass Spectrometry; NMR:Nuclear Magnetic Resonance

Introduction

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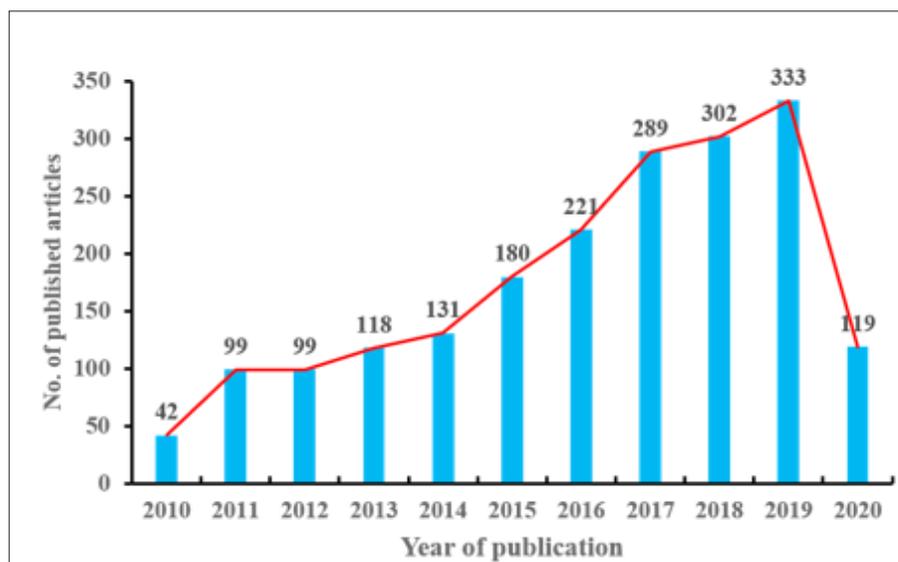


Figure 1: Histogram of metabolomics in the toxicity study manuscript, with “metabolomics, toxicity” as the key word, in their all fields were extracted from PubMed from January 2010 to September 2020. No. of publications of related articles is increasing.

Humans are often exposed to exogenous substances such as drugs, herbs, and environmental pollutants, which can harm health to varying degrees, and traditional toxicology regulates them more in dose and time than in mechanisms and solutions. Metabolomics practice high throughput sensitive analytical instruments to monitor metabolites with a molecular weight of less than 1000 in the organism, and mathematical models of multivariate statistical analysis find changes in metabolic contours after stimulation of organisms, verify biomarkers and metabolic mechanisms, and then take preventive, therapeutic and rehabilitation measures to

reduce harmful effects [1,2]. Metabolomics is widely employed in toxicology studies presently (Figure 1). Their specific studies include the utilization of metabolomic methods to clarify the avoidance of biomarkers under sub-accumulation of environmental pollution, the discovery of damage metabolism mechanisms for herbal toxic target organs, in addition, regulatory drug abuse finds stable and reliable markers, including drug metabolites and biomarkers in the body, because of the transient detection of addictive drugs, which is a challenge for regulators [3-5]. In short, the future research of metabolomics in toxicology will be gradually standardized, with a wide range of applications.

High-throughput Analytical Platforms and Abundant Databases Contribute to the Study of Toxicology Mechanisms

The data matrix collected by high-throughput and high-sensitivity instruments is multidimensional and detailed, in which gas chromatography (GC), liquid chromatography (LC), mass spectrometry (MS) and nuclear magnetic resonance (NMR) are the main tools of metabolomic workflow, and their respective advantages make the results of experiments complement each other in favor of the thorough clarification of the mechanism [6]. The inherent limitation of GC-MS is that it detects only volatile compounds or compounds that can be derived into volatile compounds. The high repeatability, non-destructive and non-invasive of NMR is the most important advantages of NMR in metabolomics research, NMR is mainly used for chemical identification and quantification of chemical composition of a given sample. It not limited to liquid samples, but also for solid, gas phase and tissue samples. The evolving MS technique provides a highly specific analytical tool that provides chemical information such as the exact mass of element formulas, isotope distribution patterns, structural analysis of the properties of parent and fragment ions, identification of real compound data using spectral matching, and comparison of concentration levels of different chemicals in mixed samples. MS has the advantage of analyzing secondary metabolites compared to NMR. In addition, different ion source technology may increase the number of metabolite detections. It is worth noting that there is no single analytical platform capable of fully quantifying and identifying all molecules in the sample. Therefore, in addition to 1D and 2D NMR experiments, different ionizing methods, LC-MS and GC-MS and other tandem technologies are needed to maximize the identification of different metabolites in complex samples. The electronic database contains a wealth of information on the chemical composition and biological function of the metabolites of organisms, which is conducive to accurately interpreting the activities and effects of biomarkers in metabolomics, thereby clarifying the mechanism, and performing subsequent verification [7]. It is noteworthy that the online and offline databases target pre-existing metabolite information but supplementing and perfecting the database data is an important part of metabolomic progress, and it is suggested researchers should take the discovery of new bioactive compounds a major direction for metabolomic research.

Application of Metabolomics Strategy to Clarify Connotation of Toxic Effects

The ideal goal of metabolomics in the research of the mechanism of toxic substances is to take targeted measures to prevent and reduce health damage. Metabolomic plans have considerable application prospects in clarifying the mechanism of biomarkers and solving the transient and difficult to detect drug abuse of new psychoactive substances, the complex composition of herbs and the unclear effective and toxic substances, and the accumulation damage of industrial chemically contaminated organisms [8-10]. The adverse effects they cause involve a variety of metabolic mechanisms, such as lipid metabolism affecting the cell's biofilm transport and signal recognition function, citric acid circulation interfering with normal energy metabolism and oxidative stress, and amino acid metabolism disorders causing abnormal synthesis of functional proteins. Combined with general physiological and biochemical examination, the metabolic mechanism of biomarkers can be accurately identified, and corresponding preventive, therapeutic, diagnostic and aftercare measurements can be taken to reduce the occurrence of injury response and economic loss.

Discussion and Conclusion

The application potential and value of metabolomics in toxicological research are worth developing, while challenges were still existed. Unified analytical standards and principles are the main directions for the future supplement and update of metabolomics. In addition, the results of metabolomics studies are expressed in the form of biomarkers and metabolic pathways. It is necessary to identify and clarify the metabolic changes of adverse reactions caused by herbal medicine and chemicals. It is important to establish the correlation between exogenous substances and biomarkers, which makes the corresponding preventive measures more specific and targeted [11-12]. In short, maintaining the biological sample activity of metabolomics analysis, perfecting the database, using a variety of analytical instruments, standardizing the operation process thus, to obtain a stable, reliable and reproducible result. In addition, it is believed the combination of metabolomics and other advanced omics techniques can effectively improve the quality of toxicology research in the future.

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