Lc-ms targeted polar metabolome analysis methods.

Mahammad Ali*

Department of Postharvest Science of Fresh Produce, Agricultural Research Organization, Volcani Center, Rishon LeZion 7505101, Israel

Abstract

A new and quickly expanding field called "metabolomics" is dedicated to the thorough examination of biological things' metabolites. Metabolites have a variety of physical and chemical characteristics that can be examined using analytical chemistry techniques that are specific to particular chemical component groups. Identification and measurement of tiny molecules involved in metabolic processes are the goals of metabolomics. Due to its high throughput, gentle ionisation, and adequate metabolite coverage, LC-MS has gained favour as a platform for metabolomic investigations. Metabolomics is being utilised more frequently as a method to distinguish between how an organism reacts to different stimuli or medications as a result of considerable advancements in LC-MS technology. The workflow of a typical LC-MS-based metabolomic investigation is presented in this review with the purpose of identifying and quantifying metabolites that are indicative of biological or environmental disturbances. For toxicological applications in the clinical laboratory, LC-MS is a potent tool. An LC-MS is mostly used in toxicology laboratories for broad spectrum drug screening and drug confirmation testing after an immunoassay screen. Toxicology testing has used a variety of LC-MS technologies, including LC-MS, LC-MS/MS, LC-TOF, LC-QTOF, and LC-Orbitrap. Additionally, a variety of other data acquisition strategies have been reported, including targeted and untargeted data acquisition techniques, as well as capture of product ion spectra with and without data dependence (DDA or DIA). The two LC-MS applications in this chapter opioid confirmation testing and broad spectrum drug screening as well as one laboratory's technique development, validation, and application experience are highlighted. Toxicology laboratories thinking about using LC-MS might use the literature's descriptions of several methods for each of these applications, which are referenced in this chapter.

Keywords: Metabolomics, Metabolites, lc-ms, Analytical chemistry.

Introduction

Utilizing a variety of technical platforms to describe a biological object's features at the genome, transcriptome, proteome, and metabolome levels defines current biology studies. Combining these platforms allows for systemic analyses of various biological processes, including the sequential "flow" of information from genes to phenotypes of specific biological objects [1].

Because a metabolite profile is one of the most instructive aspects of the phenotype, metabolomics represents the logical conclusion. Global molecular profiling technologies have significantly advanced genomic and transcriptome research over the past few years, while the rapid expansion of proteomic and metabolomic research has been fuelled by enhanced mass spectrometers and more sensitive and selective mass spectrometers. This led, for instance, to the relatively quick whole genome sequencing of a wide range of pathogens, including Plasmodium, Leishmania, Trypanosoma, and Schistosoma, and the subsequent use of metabolic fingerprints for the detection of biomarkers in parasitic infection in parasitology. Metabolomics may examine the final expression of the genotype and is therefore the profiling method that works most closely with the final phenotype, whereas genomics and transcriptomics research the beginning of the molecular cascade leading to a chosen phenotype [2]. Additionally, while the metabolome consists of relatively few low relative molecular mass molecules, known as metabolites, many of which are key actors of cellular processes that are universal across organisms, like energy metabolism, genome and proteome studies frequently struggle with functional annotation of identified sequences. As our favourite model organisms, the unicellular trypanosomatid parasites, including pathogens like Trypanosome and Leishmania, are almost exclusively regulated at the posttranscriptional level; genome and transcriptome studies may need to be restricted, especially when studying the rapid effects of drug treatment or the mechanisms of drug resistance. This is where metabolomics comes into play [3].

***Correspondence to:** Mahammad Ali, Department of Postharvest Science of Fresh Produce, Agricultural Research Organization, Volcani Center, Rishon LeZion 7505101, Israel, Email: mahammad@ali.ir

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The initial stage is sample collection, and stabilisers and/or standardised collectors are used less frequently in urine sampling. As a result, even though sterile collectors constructed of nonadsorbing material are typically used in metabolomic experiments, using regular transparent tubes can frequently modify some light-sensitive analytes. The use of preservatives may be beneficial for the preservation of specific analytes. For example, it has been discovered that adding hcl to the sample is suitable for the preservation of specific urine metabolites, such as acid [4,5].

Conclusion

In this review, we've discussed the key points to keep in mind when conducting targeted metabolomics investigations of human urine by LC-MS/MS. In the not-too-distant future, LC- MS/MS will continue to be the preferred analytical method to assess the metabolome in any biological samples, but particularly in urine. It will be crucial in this field, whether used independently or in conjunction with other types of equipment. As a result, it is projected that the research of metabolomics will adopt tailored LC-MS/MS methods more frequently. The data will be used in a variety of sectors, including doping control analyses, clinical diagnosis, and personalised medicine.

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