



Original Research Article

Application of Metabolomics for Species Differentiation

Article History:

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Received: 04-11-2025

Revised: 19-11-2025

Accepted: 05-11-2025

Published: 20-12-2025

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Abstract: Interactions between species are a frequent occurrence in the natural world. Genomic, transcriptomic, proteomic, and metabolomic methods are primarily used to study the mechanisms of interaction between various species. Precision instrument analysis is the foundation of metabolomics, an essential component of system biology. The new field of metabolomics has drawn a lot of attention in the past ten years. The technology for the thorough examination of metabolites and low-molecular-weight substances in a biological system, such as cells or tissues, is known as metabolomics. Through their direct involvement in the control of physiological processes, such as preserving cell homeostasis or signal transmission via protein-protein interactions, metabolites play a significant role in biological events. A crucial first step in enhancing additional phenotypic evidence to clarify the extent of environmental effects for genomic variations linked to metabolic processes is the integration of metabolomics data with sequencing data. Additionally, in order to create a system for data extraction, selection, and metabolomic data analysis for the interpretation of biological consequences of biotechnology developments, information analysis technologies like big data, machine learning, and IT investment must be implemented. In this paper we will discuss. Application of metabolomics for species differentiation.

Keywords: Metabolomics, Species Differentiation, Genomic, Biological System, Organisms, Biotic and Abiotic, Low-Molecular-Weight Substances, Mass Spectrometry, Pathogenic Organisms.

INTRODUCTION

The technology for the thorough examination of metabolites and low-molecular-weight substances in a biological system, such as cells or tissues, is known as metabolomics. By systematically identifying and measuring these tiny molecules involved in organisms' biochemical interactions, metabolomics helps to clarify intricate biological interactions, reactions, and functions. Because the functional expression of the genes involved

is connected to metabolomes through transcriptome and proteome control, organisms developed and engineered through biotechnology (synthetic biology) exhibit new biological functionalities. [1]

The term "metabolome" refers to the metabolic end products, which can range from hundreds to thousands of metabolites, depending on the size of the organism or biological system in question. This is comparable to

genomics, which refers to all the genetic information in an organism. In order to gain a thorough grasp of the intricate physiology and biochemistry of organisms, it is possible to validate the qualitative or quantitative changes of metabolites in living things through a variety of instrumental analyses. These analyses can be used to interpret different physiological phenomena or mechanisms of cells or organisms. [2]

In addition to offering a comprehensive understanding of metabolic pathways, the use of metabolomics in the analysis of interactions between various species clarifies the mechanisms behind microbial and host interactions A. A thorough examination of relationships based on metabolomics can successfully determine the roles of the genes engaged in defensive mechanisms. In practice, metabolomics can be used in conjunction with genetic methods to search for resistant types and supplemental breeding. In this study, we primarily review the benefits and drawbacks of each metabolomics analysis platform and its use in interspecies interactions. This should aid in the advancement of biotechnology, particularly metabolomics techniques, in addition to helping to clarify the use of metabolomics in pathogenic and defense systems. [3]

Review of Literature:

Peptides, amino acids, nucleic acids, lipids, carbohydrates, organic acids, vitamins, polyphenols, alkaloids, minerals, and chemical compounds absorbed and synthesized by cells or organisms are examples of metabolites that are created and altered by the metabolism of biological systems (such as cells, tissues, or organisms). Different environmental stimuli (biotic and abiotic) cause these compounds to undergo changes in metabolic levels. By examining these environmental factors, the organism can be characterized and metabolomic responses by particular factors can be predicted in relation to the mechanism of metabolic pathways (Poltronieri et al., 2013). [4]

Low-molecular-weight substances found in plants include polar molecules from hydrophilic portions of the cell membrane, lipophilic compounds found in the plant cell wall, acidic and basic ions, and stable and oxidized structures. Both endogenous (homeostatic, illnesses, growth, and senescence) and exogenous (environmental stressors, such as drought, high temperature, circadian, etc.) factors can alter metabolite levels. This is due to the fact that the proteome (protein products) and the genome, which contains the genetic code of metabolites, are connected to the metabolome (metabolites), the form of end products that govern a cell's activity (Sharma et al., 2018). Therefore, integrating metabolomic data with genomic and proteomic data will be helpful for

obtaining results with more relevant consequences and meanings in order to investigate particular responses in plants created by mutations or engineered through biotechnology. [5]

The field is developing quickly. Since the early years of the twenty-first century, metabolomics has been recognized as a separate field. The endeavor to concurrently detect and quantify as many metabolites as possible as part of what is known as the "global approach" is one feature of metabolomics that sets it apart from earlier metabolically based investigations, even though the notion of metabolic analysis is not new. Studies of cancer, heart disease, medication toxicity and gene function, microbiology, nutrition, plant sciences, ecotoxicology, and veterinary medicine are just a few of the many fields in which metabolomics has been successfully applied due to its adaptability. However, it has not yet reached its full potential in the realm of ecology. This is unexpected because metabolomics has enormous promise for examining the biochemical consequences of a variety of ecologically significant phenomena, including the effects of sickness, food restriction, infection, parasite load, and climate change (Veldhoen et al. 2012). Through their impact on stress tolerance, inter-organismal interactions, color, flavor, nutritional value, and shelf life, the metabolites of horticultural and agricultural crops directly affect their phenotypes. [6]

In general, metabolites can be separated into two categories: primary metabolites, which are necessary to sustain the organism's basic life activities, and secondary (specialized) metabolites, which support processes unique to each organism. The metabolome, which is made up of the primary and secondary metabolites, is thought to be the biological "ome" that most accurately reflects the phenotype, along with the genome, transcriptome, and proteome (Guijas et al. 2018, Patti et al. 2012). [7]

Objectives:

- To study the Application of Metabolomics for Species Differentiation
- To Study the metabolomics in the Interactions between Different Species

Research Methodology:

The study is exploratory in nature. The data used for preparing this paper are secondary in nature which is collected from the various published resources. The data derived for preparing this research paper has been extracted from various elite journals and relevant websites.

RESULTS AND DISCUSSION

It was suggested to use the notion of omics from a holistic perspective since, as science and technology have advanced, scientists have discovered that merely researching a certain path cannot explain all health problems. A new method for investigating the pathophysiology of human disease has been made possible by the development of genomes, metabolomics, proteomics, lipidomics, and transcriptomics. The most recent advancements in science and technology are intimately linked to the use of metabolomics as a crucial technique for researching contemporary life sciences (Fig. 1). As a crucial component of systems biology, metabolomics primarily examines materials including blood, urine, and feces before researching small molecule metabolites of different metabolic pathway matrices and products. [8]

Nuclear magnetic resonance, mass spectrometry (MS), and chromatography are technologies used in metabolomics. Clinical research, illness therapy, medication characterization, animal and plant research, agricultural research, and nutrition all benefit from mass spectrometry-based metabolomics. Two Many academics, both domestic and international, have focused on metabolomics research in recent years. Because of their significant role in the scientific community, metabolomics methodologies and procedures have been refined. Further research on metabolomics and the development of metabolic pathways will be made possible by an understanding of the research status, accomplishments, and shortcomings of many academics in this subject. We shall talk about this from the viewpoints of MS application and metabolomics research.

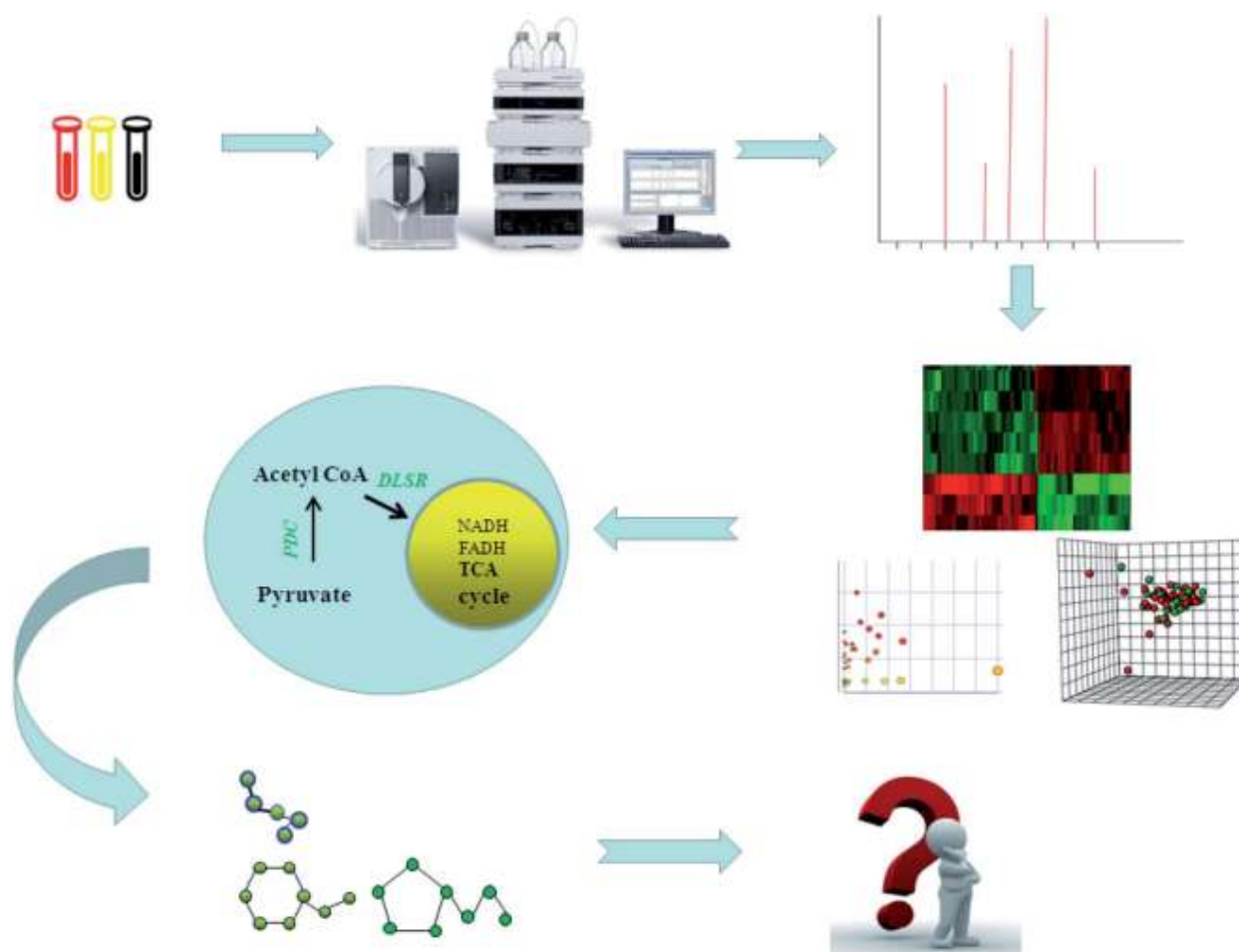


Figure 1: A flow chart of metabolomics analysis technology

The Application of Metabolomics in the Interactions between Different Species:

Plants and Pathogenic Organisms: Their Interaction Invasive microorganisms including bacteria, fungi, and invertebrates can harm plants. Plants can undergo a number of metabolic and phenotypic changes when they interact with pathogens. Different metabolic and genetic reactions, such as the production of disease-resistant stimulus metabolites or the identification of a pathogen-associated molecular pattern, are developed by plants and trigger autoimmune reactions.

The genus *Fusarium* is well-known for its active and rather broad secondary metabolism, which produces mycotoxins that kill the host before proliferating and growing. After describing the various metabolomic fingerprints of infected and control barley samples using the LC-MS technology, Cajka discovered that the mycotoxin deoxynivalenol (Figure

2) and its low-toxicity glycosylated complex, deoxynivalenol-3-glucoside, can serve as biomarkers for identifying genotypes of resistant barley. [9-10]

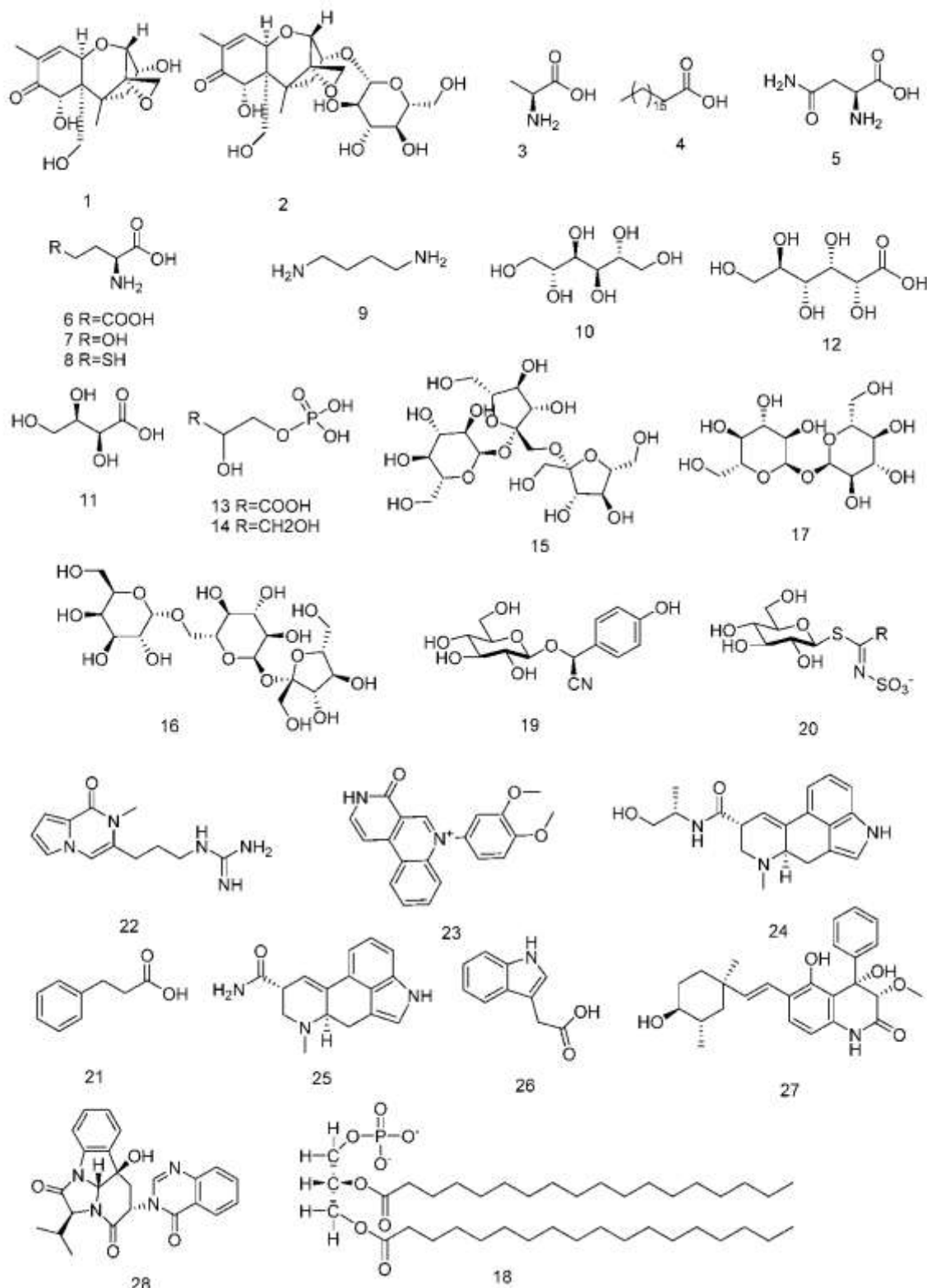


Figure 2. The structures of metabolites 1–28.

The infection of farmed rice (*Oryza sativa*) with the blast pathogen *Magnaporthe grisea* KJ201 (compatible) and *M. grisea* KJ401 (incompatible) was examined using GC/LC-MS and NMR spectroscopy.

Metabolomic Evaluations of Plant-Herbivore Relationships

On the one hand, plants provide the herbivorous insect with a nutrient-rich environment. However, plants also need to obtain helpful compounds from a symbiotic creature and lessen the harm caused by members of other kingdoms, such as nematodes. Metabolomics analysis in ecology has produced new understandings of the mechanisms underlying plant resistance to herbivores.

Metabolomics in the Study of Symbiotic Interactions

The majority of microbial genomes are rich in secondary metabolic synthesis gene clusters at the gene level, although they are largely silent under normal circumstances, as demonstrated by the quick development of sequencing techniques. One popular strategy to deal with variations in culture conditions (temperature, pH, nutritional condition, etc.) is to alter the level of gene expression in order to completely exploit the bioactive components of microorganisms for drug discovery. Additionally, in the presence of numerous strains, microorganisms cause the silence of particular genes as a defensive strategy against external interference, which results in the release of associated model molecules. Co-cultures are a useful tool for promoting microbial contact because they may efficiently increase the expression of secondary metabolites and provide insight into changes in microbial interactions at the substance level.

The interaction between three species—the pathogen *Ustilago maydis*, the endophyte *Fusarium verticillioides*, and their common plant host *Zea mays*—suggests that they might interact and evaluates the consequences of the interaction between *F. verticillioides* and *U. maydis*, both of which grow in *Z. mays* [66]. Therefore, depending on the ecological setting, the endophyte *F. verticillioides* may exhibit nutritional modes and act as both a parasite and a protective mutualist. The host plant's basic and secondary metabolisms are both affected by *U. maydis*.

The plant goes through the entire stage of a live nutrition defense response as a result of this significant transformation. Endophytes may also degrade plant chemicals that restrict *U. maydis* growth, benefiting from the pathogen's presence (Figure 3, black). *F. verticillioides* controls *U. maydis* growth, thereby reducing a pathogen's aggressiveness towards the plant (Figure 3, red). Metabolite studies are carried out during the procedure utilizing a UPLC/TOF/MS apparatus. [11]

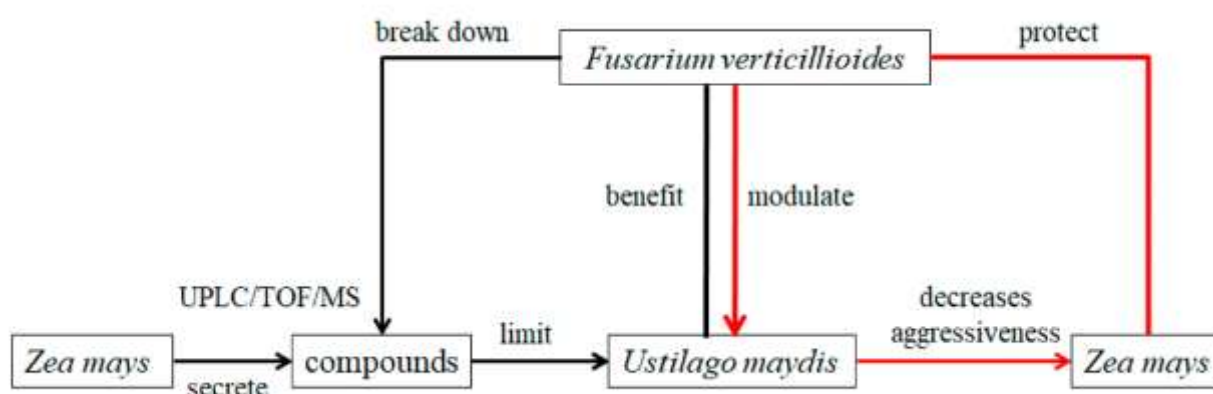


Figure 3. Interactions among *Fusarium verticillioides*, *Ustilago maydis*, and *Zea mays*.

In order to evaluate metabolic activity within biological systems, metabolomics has become a potent method for detecting and measuring the variety of detectable small molecules (the metabolome). The number of publications in this subject has increased over the past 20 years, indicating a steady increase in research interest in metabolomics (Figure 4A). However, whereas plant metabolomics has grown relatively more slowly and subtly, most of those researches have concentrated on human and animal science, especially in relation to human disease and animal health (Figure 4A). The great diversity of phytochemicals and our limited capacity to identify metabolites from liquid chromatography–mass spectrometry (LC–MS) datasets are two of the many factors contributing to this.

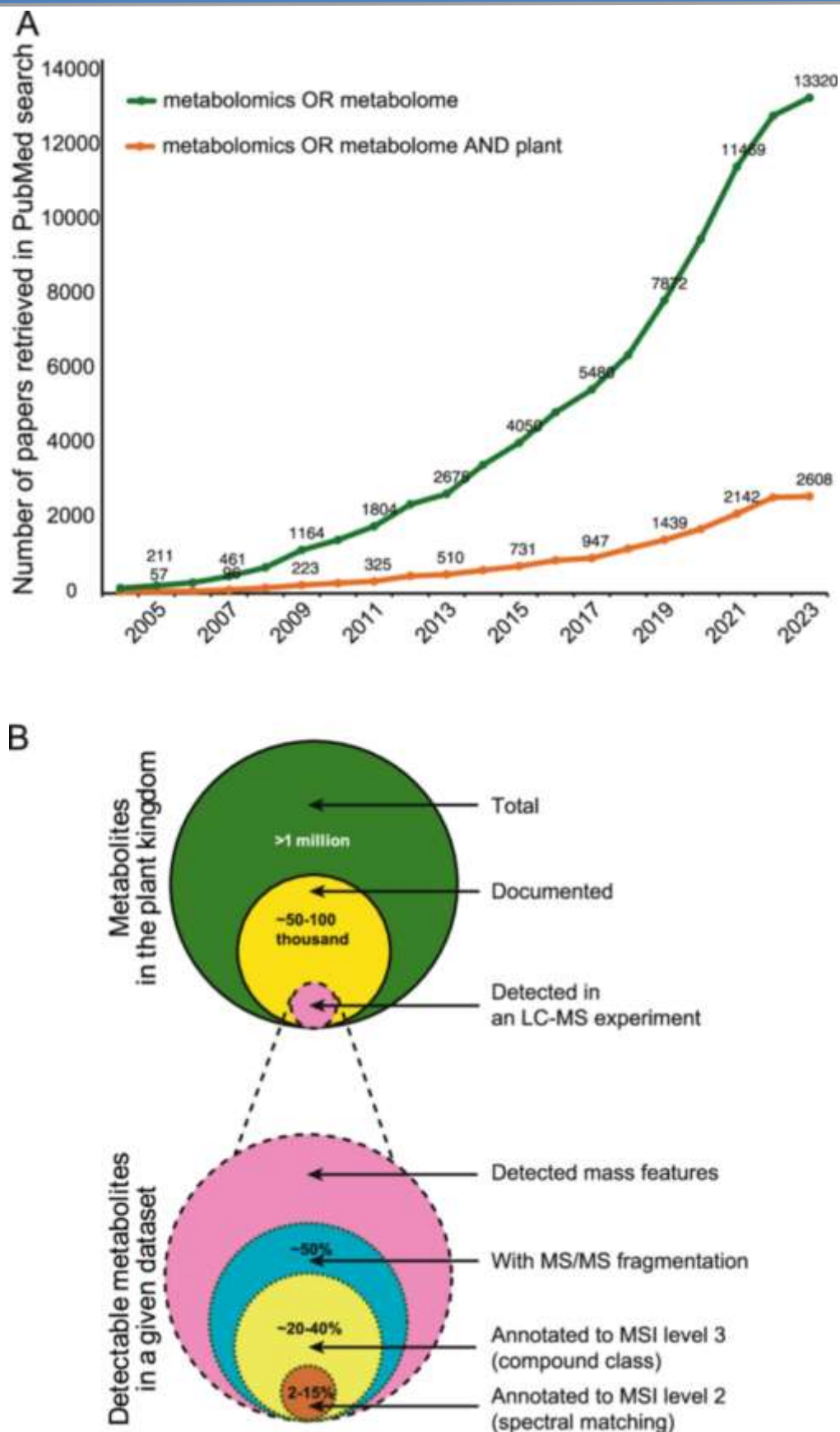


Figure 4: The issue of metabolite identification in plant metabolomics. (A)

The quantity of papers published each year using the specified keywords. (B) The breakdown of detected metabolites in a typical dataset and the predicted total number of metabolites in the kingdom of plants. For the sources of these

figures, please refer to the main text. MSI stands for Metabolomics Standards Initiative, MS/MS for tandem mass spectrometry, and LC-MS for liquid chromatography–mass spectrometry. [12]

CONCLUSION

To ensure the advancement of metabolomics, new cutting-edge technologies will be integrated with metabolomics technology. A scientific foundation for resolving the issue of metabolite research and clarifying metabolic pathways will be provided by various combination techniques, such as LC/MS and GC/MS, which will make metabolomics based on MS more ideal. In the discipline of metabolomics, mass spectrometry is still a key analytical tool. Small molecules called metabolites are created during metabolism and are essential to biological processes because they directly control physiological processes including cell homeostasis and signal transmission via protein–protein interactions.

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