Methods and Protocols in Food Science

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Sastia Prama Putri *Editor*

Gas Chromatography-Mass Spectrometry

Based Metabolomics in Food Science

Methods and Protocols in Food Science

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Gas Chromatography-Mass Spectrometry

Based Metabolomics in Food Science

Edited by

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Dedication

This book is dedicated to

Professor Eiichiro Fukusaki

in sincere gratitude for his guidance and unwavering support

福﨑先生に心より感謝を込めて

Foreword

The application of metabolomics has expanded rapidly in recent years, encompassing a wide range of disciplines, including food science. In this field, metabolomics has emerged as a powerful tool for quantifying constituent compounds in food samples and elucidating their relationships to phenotypic traits. Owing to its comprehensive analytical capabilities, metabolomics is now widely employed in food science for various purposes, such as authenticating geographic origin, enhancing sensory quality, evaluating nutritional value, and ensuring food safety.

Among the analytical platforms available, gas chromatography–mass spectrometry (GC-MS) stands as a cornerstone of food metabolomics. Its relatively low operational cost, high batch-to-batch reproducibility, and broad coverage of bioactive metabolites make GC-MS particularly attractive for many applications. Nevertheless, the methodologies required for GC-MS analysis can vary significantly depending on the nature of the sample, the range of metabolites targeted, and the specific research objectives. As such, a thorough understanding of the nuances in sample preparation and method selection is critical for obtaining reliable and meaningful results. A deep understanding of sample preparation and methodological optimization is therefore essential to ensure accuracy, reproducibility, and meaningful interpretation of results.

This book is designed to serve as a comprehensive reference for researchers and professionals working in food metabolomics. It provides detailed, step-by-step guidance on GC-MS analysis procedures across the major stages of sample preparation, including extraction and derivatization techniques tailored to different types of food matrices. Each chapter focuses on specific applications and potential metabolite coverage, offering insights into alternative strategies that may be adopted to meet diverse analytical needs.

By bringing together contributions from experts with extensive experience in GC-MS-based food metabolomics, this book aims to support the advancement of knowledge and practical skills in the field. It is my sincere hope that the chapters herein will assist researchers, students, and industry professionals in refining their analytical approaches and accelerating the integration of GC-MS into innovative and impactful food science research.

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Preface to the Series

The Methods and Protocols in Food Science series is devoted to the publication of research protocols and methodologies in all fields of food science. The series is unique as it includes protocols developed, validated, and used by food and related scientists as well as provides theoretical basis for each protocol. Aspects related to improvements in the protocols and adaptations and further developments in the protocols may also be approached.

The Methods and Protocols in Food Science series aims to bring the most recent developments in research protocols in the field as well as very well-established methods. As such the series targets undergraduates, graduates, and researchers in the field of food science and correlated areas. The protocols documented in the series will be highly useful for scientific inquiries in the field of food sciences and are presented in such a way that the readers will be able to reproduce the experiments in a step-by-step style.

Each protocol will be characterized by a brief introductory section, followed by a short aims section, in which the precise purpose of the protocol is clarified. Then, an in-depth list of materials and reagents required for employing the protocol is presented, followed by comprehensive and step-by-step procedures on how to perform that experiment. The next section brings the dos and don'ts when carrying out the protocol, followed by the main pitfalls faced and how to troubleshoot them. Finally, template results will be presented and their meaning/conclusions addressed.

The Methods and Protocols in Food Science series will fill an important gap, addressing a common complaint of food scientists, regarding the difficulties in repeating experiments detailed in scientific papers. With this, the series has a potential to become a reference material in food science laboratories of research centers and universities throughout the world.

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Anderson S. Sant'Ana

Preface

Gas chromatography–mass spectrometry (GC-MS) has become one of the most widely used techniques in metabolomic analysis, particularly in food science, due to its affordability, robustness, and consistent performance. Compared to other analytical platforms such as liquid chromatography–mass spectrometry (LC-MS) and nuclear magnetic resonance (NMR), GC-MS offers practical advantages, including higher reproducibility, analytical stability, and streamlined data processing.

Originally, GC-MS was primarily employed for the analysis of volatile compounds, as it is well-suited for detecting substances in the gas phase. However, significant advances in derivatization techniques have extended the capabilities of GC-MS to include the analysis of a broad range of low-molecular-weight, nonvolatile metabolites. This advancement has significantly expanded its applicability in metabolomic research.

GC-MS is particularly valued for its consistent retention times and reliable mass spectral data. Retention time reproducibility is further enhanced through the use of retention indices, calculated with reference compounds such as n-alkanes or fatty acid methyl esters, and compared against established databases including the Fiehn Library, Golm Metabolome Database, MassBank, Wiley Database, and the NIST Library. Additionally, the standardized use of electron ionization at 70 eV allows for consistent spectral matching across laboratories using shared reference libraries.

The combination of robust derivatization techniques and the inherent strengths of GC-MS as a reliable analytical platform has made it an increasingly preferred tool among researchers. As the role of GC-MS continues to expand in food metabolomics, a solid understanding of sample preparation strategies becomes critical to ensuring accurate and comprehensive metabolite profiling.

This chapter aims to provide foundational insights into sample preparation for GC-MS-based metabolomics, with a particular focus on food science applications. It serves as a practical guide to navigating the complexities of preparing diverse food matrices for effective GC-MS analysis. This volume presents standardized protocols for sample preparation in GC-MS-based metabolomics, covering 18 different types of food samples along with detailed handling instructions. The opening chapter discusses the general applications of GC-MS in food metabolomics and highlights how this approach supports robust and meaningful advances in the field.

We would like to express our sincere appreciation to all contributing authors for accepting our invitation and sharing their valuable expertise, which has been essential to

the timely and successful completion of this volume. We hope that the chapters provide useful guidance on sample preparation protocols for GC-MS-based metabolomics in food science and serve as a practical reference for researchers working with similar sample types. Finally, we extend our gratitude to Springer Nature for the opportunity to contribute to this important publication.

Suita, Osaka, Japan — ***Sastia Prama Putri***
Suita, Osaka, Japan — ***Enik Nurlaili Afifah***
Suita, Osaka, Japan — ***Rafidha Irdiani***
R. R. C. Voluntad

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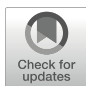
Part I

General Introduction



Chapter 1

General Considerations for Method Development in GC/MS Analysis

Sastia Prama Putri, Rafidha Irdiani, Rifqi Ahmad Riyanto, and Takeshi Bamba

Abstract

Gas chromatography/mass spectrometry (GC/MS) is a powerful analytical technique that is widely used to detect and characterize low molecular weight compounds across diverse research fields, including food science. By combining the separation ability of a gas chromatograph with the identification capability of a mass spectrometer, GC/MS analysis allows the identification of a wide range of compounds. This technique offers several advantages, including fast, able to provide high resolution results, sensitive, inexpensive, and reliable when appropriate methods and components are applied. The selection of appropriate methods, instrument components, and analysis modes is critical to ensure that analysis objectives are met. Careful selection can significantly influence the accuracy and reliability of the results. Therefore, this chapter provides an overview of general considerations for method development in GC/MS analysis, highlighting the characteristics and roles of major components in analytical performance.

Key words Gas chromatography, Mass spectrometry, Materials, Methods, Parameters

1 Introduction

Chromatography is an analytical method used to separate compounds based on their interactions with a stationary phase, over which a mobile phase flows to transport compounds. In the case of gas chromatography, gas is used as the mobile phase, carrying vaporized samples. Separation in gas chromatography occurs due to different chemical characteristics of each compound, leading to specific interactions with the chromatographic column as the stationary phase. Factors influencing separation include molecular size, polarity, affinity, charge, and hydrophobicity [1]. Compounds with higher affinity for the stationary phase are retained and eluted later, while those with lower affinity pass through more quickly and reach the detector earlier. The time required for a compound to elute is referred to as its retention time [2].

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Gas chromatography is classified into two types—gas-liquid chromatography (GLC) and gas-solid chromatography (GSC). In GSC, the stationary phase consists of solid material, including alumina, silica, or carbon, whereas in GLC, the stationary phase is liquid adsorbed onto a solid inert packing on the capillary tubing walls [3, 4]. In GSC, polar molecules tend to interact strongly with the solid stationary phase, resulting in prolonged retention and severe peak tailing in the chromatograms [5]. These limitations have led to a more widespread use of GLC across most fields of science. At present, the term "GC" is generally used to refer to GLC [6].

The mass spectrometer (MS) is an instrument used to detect and identify compounds within a sample mixture. When coupled with gas chromatography (GC), the MS consists of several key components, including a vacuum pump, sample introduction unit, ionization chamber, mass analyzer, and detector. In the sample injection unit, compounds that have been separated by GC enter the MS. These compounds are then ionized in the ionization chamber. For GC/MS analysis, the most commonly employed ionization method is electron ionization (EI), also referred to as hard ionization. In EI, a heated filament generates electrons, which bombard the incoming molecules, producing molecular ions. This process typically causes fragmentation, in which molecules are broken down into a fragment ion and a neutral fragment. The resulting fragmentation patterns are highly reproducible and unique to each compound, serving as a "fingerprint" for annotation. After ionization, the fragment ions go into the mass analyzer and are subsequently detected by the detector [7].

When combined, gas chromatography/mass spectrometry (GC/MS) is a powerful analytical technique that is widely used to analyze biological samples. The combination of gas chromatography and mass spectrometry enables both qualitative and quantitative evaluations of the chemical constituents in a sample. In GC/MS, compounds are first separated by the gas chromatograph, while the mass spectrometer detects and characterizes each compound based on its mass-to-charge ratios [8].

GC/MS offers several advantages, including fast, able to provide high resolution results, sensitive, inexpensive, and reliable [7]. However, the quality and the reliability of the data are dependent on parameter selection. Careful selection and consideration are necessary to improve analytical performance. Therefore, in this chapter, the principles and key components of GC/MS will be discussed briefly, aiming to provide readers with fundamental information and general considerations in conducting GC/MS analysis.

2 Materials Selection

GC-MS instruments consist of several components that work together to detect and characterize compounds. Key elements, including carrier gas, columns, and mass analyzers, offer multiple options that can be applied depending on the analysis objectives and practical considerations. This section discusses the characteristics and roles of these components.

2.1 Carrier Gas Selection

In gas chromatography, the mobile phase is also known as *carrier gas*. Carrier gas must have a high purity in order to provide good chromatograms with minimum baseline noise and to maintain column performance. In addition, the gas used must meet several criteria, such as being inert, having no interaction with the target compounds and the stationary phase, being compatible with the detection method, and being able to diffuse quickly across the column to promote high separation [2, 9].

Several gases are commonly used as carrier gas, including helium, hydrogen, nitrogen, and argon. Of these, helium and hydrogen are the most widely used, with helium being the predominant choice in many laboratories. Some advantages and disadvantages of each carrier gas are summarized in Table 1.

Other than the type of carrier gas, several parameters including temperature and carrier gas flow are also necessary to be

Table 1
Advantages and disadvantages of each carrier gas

Gas	Advantages	Disadvantages	References
Helium	Easy to handle Nonflammable Wide flow range Compatible with almost all types of detectors	High cost Limited and nonrenewable	[10]
Hydrogen	Great separation efficiency Faster analysis Improved resolution Relatively affordable Stable supply	Flammable Rapid expansion at high pressure Corrosive potential to the ion source More background noise	[11]
Nitrogen	Stable supply Higher separation efficiency than helium and hydrogen at its optimum linear velocity Greater vacuum pump efficiency Relatively affordable	Low sensitivity Longer analysis time is necessary	[10, 12]
Argon	Greater vacuum pump efficiency Less expensive than helium	More expensive than nitrogen	[13]

considered. Temperature affects the ratio of the viscosity to diffusion coefficient. The diffusion coefficient describes how quickly molecules (the carrier gas or analytes within it) spread out due to random molecular motion inside the column. Low viscosity combined with a high diffusion coefficient is preferred as this promotes high separation efficiency [14].

Meanwhile, the carrier gas flow is important for column efficiency. A stable and reproducible flow rate is essential so that the retention times can be reproduced for reliable compound identification [7]. The carrier gas flow rate (f) can be calculated using Eq. 1, with r represents the radius of the column (mm) and u describes the linear velocity of the carrier gas in cm/s. The linear velocity can be determined by dividing the column length (cm) by the time (s) required for methane, butane, or other compound that is not retained by the column to travel from the point of injection to the detector [9].

$$f = 0.6u\pi r^2 \quad (1)$$

2.2 Column Selection

The column is a critical component of a gas chromatograph, as it plays the main role in separation. There are two types of columns that are mainly used—packed columns and capillary columns.

Packed Columns

Packed columns are the first generation of GC columns. They have an outside diameter of 0.32 or 0.64 cm and are compatible with both GSC and GLC. They can be made of glass, stainless steel, nickel, or teflon. The main characteristic of packed columns is the presence of fillers. The fillers contain some solid adsorbent coated with a solid or liquid stationary phase [3].

Capillary Columns

At present, most GC instruments are compatible with capillary columns. These columns usually have an inner diameter of 0.1–0.5 mm. Unlike packed columns, capillary columns are only compatible with GLC and do not have any fillers. Instead, the inner surface of the column is coated with a thin film of liquid stationary phase. Capillary columns can be divided into three types: porous layer open tubular (PLOT) columns, wall-coated open tubular (WCOT) columns, and support-coated open tubular columns (SCOT). In PLOT columns, the stationary phase is coated on a porous layer of a solid porous layer, while in WCOT, it is directly coated onto the column wall. As for SCOT, the stationary phase is supported by an adsorbed layer of solid particles [3].

The choice of columns depends on the analysis goal. Capillary columns are mainly used for trace analysis in complex mixtures,

whereas packed columns are usually used for analysis of gases, volatile organic compounds (VOCs), and compounds with high molecular weight [15]. Furthermore, the column selection should also consider the polarity of the stationary phase, column length, and column diameter [2]. Longer columns generally provide higher resolution but slower analysis duration. Meanwhile, the column diameter affects the resolution, speed, and capacity of the columns. A smaller diameter typically results in better resolution and faster analysis [3].

2.3 Types of Mass Analyzers

In a mass analyzer, fragment ions generated in the ionization chamber are separated based on their mass-to-charge ratio (m/z). There are several types of mass analyzers. Quadrupole and time-of-flight (TOF) analyzers are the most widely used.

Quadrupole

A quadrupole contains four parallel cylindrical metal rods (electrodes with a hyperboloidal interior surface) inside a vacuum chamber, positioned equidistant from the center axis. Both direct current (DC) and high frequency alternating current or radiofrequency (RF) are applied to the quadrupole, so that only the ions with the target m/z successfully pass through the quadrupole and get to the detector. When a given set of parameters is applied to the poles, certain ions of a specific m/z range maintain a stable oscillation and pass through the quadrupole to reach the detector (resonance ion). The oscillations of ions with other m/z values become unstable, causing them to collide with the poles, go outside of the system, and not be detected (non-resonance ion). The key features of a quadrupole are small and relatively cheap. However, accurate mass cannot be obtained due to low resolution [2].

Time-of-Flight

As for the TOF analyzer, it works based on the measurement of the time needed for the ions to reach the detector from the ionization chamber. The difference in the time needed is due to different m/z results in different velocities. The key features of this analyzer are high sensitivity and better resolution compared to a quadrupole. Despite these advantages, TOF instruments do have certain limitations. Their relatively large size and higher cost make them less practical for routine laboratory use, especially when compared to quadrupole analyzers, which are more compact, cost-effective, and commonly employed in standard GC-MS workflows [2].