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Edited by Sreeraj Gopi, Nimisha Pulikkal Sukumaran, Joby Jacob, and Sabu Thomas

Natural Flavours, Fragrances, and Perfumes

Chemistry, Production, and Sensory Approach

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Preface

It has been a while since a book was put together to address the natural flavors in industrial formulations, including concise treatments of the relation between sophisticated methods and better comprehension of consumer perception and behavior using a multidisciplinary metabolic engineering methodology by connecting with fields. It appears, however, that a gap has arisen between the new advances in basic information and the direct application to product situations, with a critical requirement for scientific data. Besides, flavor innovation is a developing powerful field, which keeps on expanding its applications from its foundations in food and beverage to incorporate categories as different as personal care products and household products. But, consumer perceptions of naturalness and perceived healthiness influence their product choices and increase the preference for products labeled as natural. Consequently, keeping in mind the negative health perceptions brought about by many factors, including artificial flavors, ingredient unfamiliarity, advancements in processing, and so on, researchers all over the world have recently focused on flavors from natural resources with much success.

The idea of compiling the book *Natural Flavors, Fragrances, and Perfumes: Chemistry, Production, and Sensory Approach* took seed in mid-2018. The urge to foster such a book originated from the perspective of growing in this area, giving special emphasis on fundamental and applied research findings, and more persuasively in a food manufacturing business, to enhance product quality, and extend the shelf life of the products and improve process efficiency. This book is a systematic, complete, sequential compilation of information about the engineering of flavors and flavor products in the area of its application to provide insights to help guide development and in commercial strategy. Indeed, the goal of this book is to bring together some of the core knowledge in the field to provide a practical and wide-ranging guide for molecular biologists, new product researchers, and scientists involved in the commercial development of natural flavors and flavor-related compounds, and their use in applications as varied as pharmaceuticals, nutraceuticals, or fragrances.

This book is divided into 5 parts, including 13 chapters encompassing from natural product diversity and synthesis of flavor compounds to all different kinds of applications in the food and fragrance industries. It begins with a part devoted to the natural product diversity and its biomolecular aspects. Chapters 2 and 3 present advances in the strategies of metabolic pathway engineering and the biogenesis of plant-derived aroma compounds. The next part of the book (Chapters 4–6) focuses on flavor technology and the different kinds of flavor-delivering systems, signatures, and biochemistry of beverages. Chapters 7 and 8 are oriented to specific examples and applications of seasonings, herbs, spices, and resinoids to get a better understanding of their chemistry and uses. The last chapters are focused on regulatory aspects, sensory science and its challenges, advances in *in silico* approaches, and sensory perceptions.

A book like this is impossible without the support and effort of the contributors who have taken the time to submit their manuscripts during the pandemic period. Our editors wish to thank the authors who have generously contributed material to this book. They are experts in their fields and have provided valuable information and insights into the naturally derived flavors. The contributors include Valsaraj T.V.; Akhila Nair; Józef T. Haponiuk; Sumith K.; Anjali Anil;

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Part I
Biodiversity

1
Natural Product Diversity and its Biomolecular Aspects in Flavors and Fragrances

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1.1 Introduction

In pharmaceutical, food, cosmetic, and nutraceutical industries, flavors and fragrances play a vital role. The natural selection method or processes facilitate unique as well as wide chemical diversity with optimal interactions with other biological macromolecules. Moreover, since a millennium, it is observed that the introduction of continental and conventional selective breeding efforts has resulted in land race, elite cultivars that could not only adapt to globally diverse habitats but also ensure vivid quality and productivity in flavors and fragrances worldwide. However, unraveling the genomic basis of these vivid adaptations remains indecipherable. For example, the world's oldest and most popular caffeine-containing beverage, the tea, comes along with immense medicinal, economic, and cultural virtues. Constant research will definitely pave way for a diverse metabolic, functional, and genomic refinement for the evaluation of their biosynthetic pathways [1]. Although it is well recognized that the differential accumulation of the three major characteristic constituents in tea tree leaves largely determines the quality of tea, little genomic information is currently available. Sequencing of the tea tree genome would facilitate to uncover the molecular mechanisms underlying secondary metabolic biosynthesis with the promise to improve breeding efficiency and thus develop better tea cultivars with even higher quality. The development of tea clones with more desirable quality traits and enhanced stress resistance becomes a necessity. Strategizing such crop improvement procedures based on miRNAs requires a detailed understanding of the miRNA–mRNA modules associated with stress tolerance and quality in tea plants [2].

Biosynthesis of aroma compounds involves metabolic pathways in which the main precursors are fatty acids and amino acids, and the main products are aldehydes, alcohols, and esters. Some enzymes are crucial in the production of volatile compounds, such as lipoxygenase, alcohol dehydrogenase, and alcohol acyltransferase. Composition and concentration of volatiles in apples may be altered by pre- and postharvest factors that cause a decline in apple flavor [3]. Among the volatile aroma compounds produced by ripe apples, esters account for the majority. For example, among the volatile aroma compounds of Golden Delicious and Starking Delicious, esters account for 80% [4]. This chapter discusses the genetic resources and plant breeding, agricultural diversity, conservation of agrobiodiversity, and the economically useful natural products used as flavors and fragrances.

1.2 Genetic Resources and Plant Breeding

From time immemorial, the breeding and domestication of plant varieties and/or species for flavor, aroma, and other characteristics have been a constant and ongoing process. Novel heterogeneity in concentration and combination of secondary metabolites has been a constant source to develop new varieties of flavors and fragrances. These variations in the composition of secondary metabolites are affected by human preferences and domestication in flavors and aromas

[5]. Moreover, the need for a higher nutrition crop or fruit variety in terms of sustainable agriculture has put into limelight the genomic breeding approaches inclusive of marker-assisted selection, backcrossing, haplotype breeding, and genomic prediction methods in synergy with artificial intelligence and machine learning to increase the speed of these breeding approaches. Figure 1.1 depicts an example of the use of an integrated framework of genomic resources [7].

1.3 Agricultural Diversification

Globally, in an agricultural system, aromatic plants are those with aromatic compounds. These aromatic plants synthesize secondary metabolites to produce essential oils, which provide relief from biotic and environmental stress. In addition, these essential oils are used in diverse applications like flavors, perfumes, and fragrance, which will provide economic returns to farmers and manufacturing industries. The increasing interest of research scholars worldwide encourages agricultural activities like proper land utilization as well as focuses on economic returns for aromatic crops. The ecological applications of these aromatic plants in agricultural systems lie in soil erosion control, carbon sequestration, phytoremediation, utilization of low-quality water, pest and disease management, and augmentation of soil properties [8]. The sensory evaluation or validation of spices depends on dominant attributes like color, aroma, and pungency, which is heavily influenced by the varieties, primary processing cultivation, and the processed products.

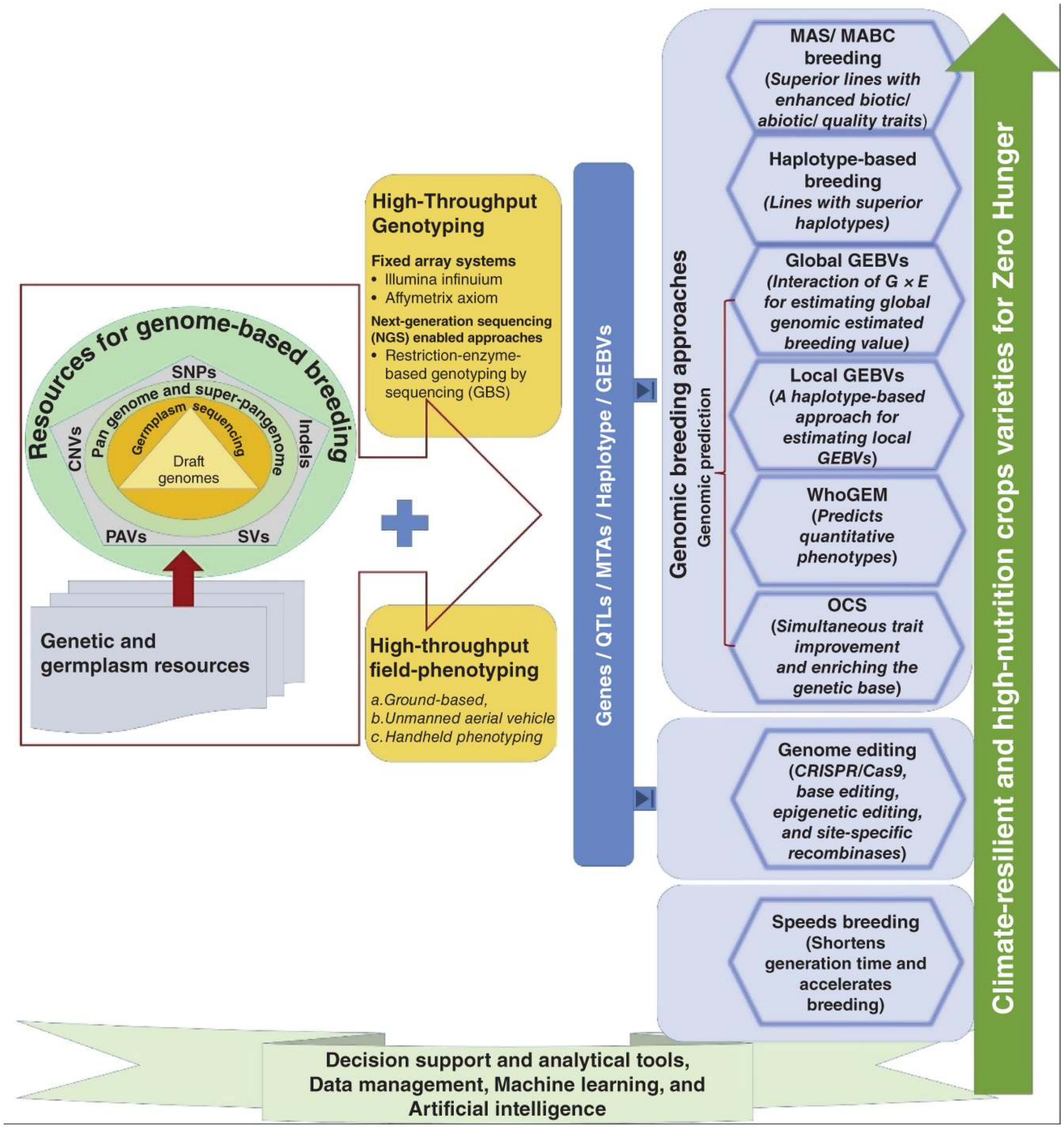

Figure 1.1 A unified framework of using genomic resources for genomic breeding to tailor climate resilient and high nutrition crops.

Source: Adapted from Ashry et al. [6].

1.4 Conservation of Agrobiodiversity

The natural product diversity witness difficulties at economic level due to denial of traditional collective seed ownership, make people helpless to grow, harvest, and channel sufficient surplus food. There are many internationally acclaimed reciprocated responses that work in favor of the intellectual property law of farmers. Furthermore, the United States of America have designed vivid grassroot agricultural and biodiverse conservation projects to regulate the open pollinated seeds within fraternities of similar interest. This project involves exploration of the functions of pollinated seeds and focuses on various other strategies for agricultural biodiversity conservation. There are research projects that collectively disseminate and document open-pollinated seed around Appalachian Mountains and Ozark highlands of southeastern United States. The research methods involve an anthropology team who can conduct ethnographic interviews and make participant observation that cover the growing and sharing of seed varieties with local farmers, seed savers, gardeners, and activists with a definite aim of constructing more integrated, sustainable, and sovereign local food systems.

1.4.1 Strategies for Conservation of Medicinal Plants

The conservation strategies of near-to-extinct species of medicinal and food or aroma importance can be determined through social and scientific actions. The strategies for conservation of medicinal plants to be used for vivid purposes can be classified into (i) the importance of genebanks, (ii) molecular-based phylogenetics, and (iii) chemosystematics [9].

1.4.1.1 Importance of Genebanks

To compensate the emergent loss of genetic diversity in medicinal crops, the establishment and maintenance of large *ex situ* plant genetic resources (PGRs) was started where systemic breeding was developed by using genetically uniform cultivars to substitute traditional land races around the world. The seeds stocked in genebanks were considered as vital due to the fact it gave an insight of the historical background of the agriculture [10]. To illustrate, *Elettaria cardamomum*, which is an economically important crop, faces limitation in its genomic analysis because of the limitation of inefficient nucleic acid extraction due to its high polysaccharide and polyphenolic content. Therefore, genebanks provide an extraction protocol for nucleic acids that help to develop genetic markers for cardamom, perform gene expression, clone cardamom genes, analyze small RNAs, and clone cardamom-infecting viral genes [11].

1.4.2 Molecule-Based Phylogenetics

Cryptic diversity is often not recognized due to the incapability of recognizing the distinguishable morphological traits and because of inability to quantify the chemical communication systems. For certain plants or animals, species-level taxonomy is obstructed because of its distortion upon preservation and morphological plasticity. The morphological characteristics to differentiate likely related species using these methods become difficult, but recent advances in morphological characteristic-based studies imply several differences in the phenotypes. The revisions in taxonomic as well as molecular-based phylogenetic studies have proved to be promising to garner information related to large species groups with different genera [12].

1.4.3 Metabolomic-Based Phylogeny or Chemosystematics

The initial part of the last century witnessed the evolution of metabolomics-based phylogeny or chemosystematics that eventually gained its popularity in the 1970s [13]. However, these studies centered on the intrafamily classification at the species level as well as the measurement of particular components of single biochemical families, especially alkaloids, in accordance with the technologies of that period. For example, the chemical systematics of the family Rutaceae and the order Rutales received immense research attention. The authenticity of chemosystematic classification was proved by comparison with the phylogeny determined by molecular polymorphism analyses.

1.5 Economically Important Natural Products Used in Flavors and Fragrances

The economically most important plants serving the purpose of flavors and fragrances are cardamom, cinnamon, cocoa, fenugreek, marigold, nutmeg, vanilla, paprika, rosemary, davana oil, olibanum carterii/serrata, lavender, vetiver, and so on (Tables 1.1 and 1.2)

Table 1.1 Economically important plants and their ingredients.

Plant source	Active ingredients	Economic importance
Cardamom [14]	1,8-cineole, α-pinene, α-terpineol, linalool, linalyl acetate and nerolidol, and the ester constituent α-terpinyl acetate	Antioxidant, antimicrobial, antibacterial, anti-inflammatory
Cinnamon [15]	Cinnamaldehyde, trans-cinnamic acid, *o*-methoxycinnamaldehyde, eugenol, and monoterpenoids	Antioxidant, anti-inflammatory, antidiabetic, antimicrobial, anticancer, lipid-lowering, and cardiovascular-disease-lowering compound
Cocoa [16]	Theobromine, serotonin, anandamide, phenylethylamine	Antioxidation, anticancer, anti-microbial, anti-inflammation, anti-diabetes, cardioprotective, physical improvement, antiphotoaging, antidepression, and blood glucose regulation

Plant source	Active ingredients	Economic importance
Fenugreek [17]	Carbohydrates, proteins, lipids, alkaloids, flavonoids, fibers, saponins, steroidal saponins	Hypocholesterolemia, lactation aid, antibacterial, gastric stimulant, for anorexia, antidiabetic agent, galactagogue, hepatoprotective effect, and anticancer
Marigold [18]	Carotenoids, flavonoids, saponins, sterols, phenolic acids	Anti-inflammatory, anti-edematous activity, antioxidant, antibacterial and antifungal activity, immunostimulant activity, genotoxic and antigen-toxic activity, spasmogenic and spasmolytic activity, hepatoprotective activity
Nutmeg [19]	Terpenes (α-pinene, *p*-cymene, sabinene, camphene, myrcene, and γ-terpinene), terpene derivatives (terpinol, geraniol, and linalool), and phenylpropanes	Antioxidant activity, immuno-modulatory and radioprotective activities, anti-carcinogenic and hepatoprotective activity, anti-inflammatory activity, antimicrobial activity

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