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Tropical Fruit Flavour: Identifying Key Aroma Compounds that Underpin Sensory Quality Traits

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Abstract

Pineapple (*Ananas comosus* var. *comosus*), with its unique sweet flavour, is one of the most popular tropical, non-climacteric fruits consumed worldwide. It is also the third most important tropical fruit in global production. In Australia, all pineapple production is centred in Queensland due to favourable climatic conditions. Although numerous pineapple varieties are cultivated globally, only a few leading types are sold commercially. This flavourful fruit is known to contain a significant number of volatile organic compounds (VOCs) at varying concentrations, which greatly contribute to its flavour quality by providing distinct sensory aromas that are sweet, fruity, tropical, pineapple-like, caramel-like, and coconut-like notes. The aroma of pineapple is a key factor in attracting consumers and reinforcing its presence in the marketplace. This thesis explores the intricate relationships among pineapple aroma chemistry, sensory attributes, and genetic composition across six research chapters. Chapter one introduces the research hypothesis and objectives, offering a comprehensive framework for the study.

The second chapter presents a comprehensive literature review, which was undertaken to provide an overview of the volatile composition of pineapple varieties grown worldwide, with a focus on GC-MS-based analysis of key aroma compounds. The review revealed approximately 480 reported VOCs, along with around 40 key aroma compounds contributing to the unique flavour of pineapple. This chapter was published as 'Review of the Aroma Chemistry of Pineapple' in *Journal of Agriculture and Food Chemistry*, 2023.

Chapter three details a high-throughput analytical method developed to measure targeted key aroma compounds in different Australian pineapple cultivars. This method incorporated a matrix-matched stable isotope dilution assay (SIDA) with headspace (HS) solid-phase microextraction (SPME) and gas chromatography-mass spectrometry (GC-MS), and was validated using several commercial cultivars of Australian-grown pineapples. This chapter was published as 'Stable isotope dilution assay and HS-SPME-GC-MS quantification of key aroma volatiles of Australian pineapple (*Ananas comosus*) cultivars' in *Food Chemistry*, 2024. This publication received the esteemed 'Original Research Publication Award' (national level) from the 'Analytical and Environmental Chemistry Division of the Royal Australian Chemical Institute (RACI)' in 2024.

Chapter four presents an investigation of the sensory properties and composition of Australian-grown commercial pineapple cultivars. Sensory and consumer studies were conducted at the Queensland Department of Agriculture and Fisheries (QDAF), now known as the Queensland Department of Primary Industries (DPI), using commercial cultivars. A subset of fruit samples were analysed compositionally for non-volatile and volatile components. The study examined the relationship between chemical composition and sensory attributes using multivariate statistical analysis. Results

indicated that high hedonic ratings are partially attributed to distinct flavour profiles such as *tropical fruit*, *sweetness*, *coconut*, *floral aroma*, and textural qualities like *juiciness* and *fibrousness*. Aroma is a crucial criterion for flavour assessment, with positive sensory experiences associated with volatile compounds, including several methyl and ethyl esters, and terpenoid-like substances such as alpha-terpineol, limonene, and damascenone. A high °Brix to % titratable acidity ratio further enhances overall appeal. Conversely, green and acidic flavours correlate with lower hedonic ratings and higher acidity levels. The findings highlight the complex interplay among chemical components within pineapple cultivars, offering valuable insights for selecting and developing improved varieties. This chapter was published as 'Relationship between key aroma compounds and sensory attributes of Australian-grown commercial pineapple cultivars' in *Journal of Agriculture and Food Chemistry*, 2025.

Chapter five details a genetic analysis of pineapple populations from the Maroochy Research Facility's (DPI) breeding programme, exploring compositional and sensory traits across multiple genetic lines. Two large-scale experiments conducted between 2022 and 2024 analysed about 400 pineapple samples for volatile and non-volatile compounds. Measurements included colour parameters, °Brix, pH, titratable acidity (as citric acid equivalents), organic acids, sugars, and key aroma compounds. Sensory studies complemented these analyses, revealing varietal differences and phenotypic markers through genome-wide association studies (GWAS). This study explored genetic factors influencing VOCs synthesis, aiming to correlate the profile of key aroma compounds with traits that enhance consumer preference. The findings contributed to marker-assisted breeding strategies for improving pineapple flavour and quality, and deepened understanding of genetic pathways linked to flavour.

Chapter six provides a summary and conclusion to the thesis that highlights the limitations of analytical and sensory evaluations, while outlining future research directions. Recommendations included expanding aroma profiling with additional key compounds, conducting aroma omission and reconstitution studies, extending sensory analysis to more cultivars, and refining genetic linkage methods to discover new molecular markers for flavour enhancement. The thesis provides a solid foundation for genomics-assisted breeding of superior pineapple varieties, with future efforts focused on identifying causal variants through whole-genome sequencing and advancing molecular breeding techniques to optimise flavour and consumer appeal.

Declaration by Author

This thesis is composed of my original work, and contains no material previously published, written by another person, or generated by artificial intelligence (AI), except where clearly referenced and acknowledged either in the main text or the preliminary pages of this thesis. I have clearly stated the contribution of others to jointly authored works that I have included in my thesis.

I have clearly stated the contribution of others to my thesis as a whole, including statistical assistance, survey design, data analysis, significant technical procedures, professional editorial advice, use of AI tools, financial support and any other original research work used or reported in my thesis. The content of my thesis is the result of work I have carried out since the commencement of my higher degree by research candidature and does not include a substantial part of work that has been submitted to qualify for the award of any other degree or diploma in any university or other tertiary institution. I have clearly stated which parts of my thesis, if any, have been submitted to qualify for another award.

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Publications Included in this Thesis

1. Review of the Aroma Chemistry of Pineapple (Ananas comosus); **Jenson George**, Thoa Nguyen, David Williams, Craig Hardner, Garth Sanewski, and Heather Eunice Smyth; J. Agric. Food Chem. 2023, 71, 9, 4069–4082; https://doi.org/10.1021/acs.jafc.2c08546. This publication was included in Chapter 2.
2. Stable Isotope Dilution Assay and HS-SPME-GC-MS Quantification of Key Aroma Volatiles of Australian Pineapple (Ananas Comosus) Cultivars; **Jenson George**, Thoa Nguyen, Craig Hardner, Garth Sanewski, and Heather Eunice Smyth; https://doi.org/10.1016/j.foodchem.2024.139956. This publication was included in Chapter 3.
3. Relationship between Key Aroma Compounds and Sensory Attributes of Australian Grown Commercial Pineapple Cultivars; **Jenson George,** Ishita Pramanik, Garth Sanewski, Thoa Nguyen, Sharon Pun, David Edwards, Margaret Currie, Simoné Møller, Craig Hardner, Philippa Lyons, and Heather Eunice Smyth; Journal of Agricultural and Food Chemistry 2025 73 (10), 5839-5849; https://doi.org/10.1021/acs.jafc.4c12482.
   This publication was included in Chapter 4.

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Other Publications During Candidature

Conference abstracts and presentations

1. **George J.** Key Aroma Compounds as Predictors of Pineapple Sensory Quality. Crop to Kitchen Symposium, organised by QHealth, 24 June 2025 (*oral presentation*).
2. **George J.** Key Aroma Compounds as Predictors of Pineapple Sensory Quality. QAAFI Research Meeting, 19 March 2025 (*oral presentation*).
3. **George J.** Key Aroma Compounds as Predictors of Pineapple Sensory Quality. 19th NZOZ Sensory Symposium - Expanding Horizons, 19 - 21 Feb 2025, Palmerston North, New Zealand (*oral presentation*).
4. **George J.** Key Aroma Compounds as Predictors of Pineapple Sensory Quality. Global Food Systems Leadership Program (GFSLP) - Visit of Malaysian Government Officials, 14 Jan 2025 (*oral presentation*).
5. **George J.** Key Aroma Compounds as Predictors of Pineapple Sensory Quality. 2024 RACI R&D Topics Conference in Analytical and Environmental Chemistry (AND1657), 2 - 4 Dec 2024, University of Tasmania, Hobart (*plenary lecture*).
6. **George, J.**, Pramanik, I., Sanewski, G., Nguyen, T., Pun, S., Edwards, D., Currie, M., Møller, S., Hardner, C., Lyons, P., & Smyth, H. E., Key Aroma Compounds as Predictors of Pineapple Sensory Quality. 17th Weurman Flavour Research Symposium, 24 - 27 Sep 2024, Wageningen, The Netherlands (*oral presentation and conference proceedings*).
7. **George, J.**, Stable isotope dilution assay and HS-SPME-GC-MS quantification of key aroma volatiles of Australian pineapple (Ananas comosus) cultivars. QAAFI, UQ, All Staff and Student Workshop, 12 Jun 2024 (*oral presentation*).
8. **George, J.**, Tropical Fruit Flavour - Identifying key Aroma Compounds that underpin sensory quality traits. 'AS19003 – genetics of fruit sensory preferences', Hort Innovation- Department of Primary Industries (DPI) - Queensland Alliance for Agriculture and Food Innovation (QAAFI) – Griffith University (GU) – joint project workshop series, 10 Oct 2024, 17 Oct 2023, 03 May 2023, 20 Oct 2022 (*multiple oral presentations*).
9. **George, J.**, Key Aroma Compounds as Predictors of Pineapple Sensory Quality. 3MT QAAFI, 24 May 2023 (*oral presentation*).
10. **George, J.**, Sanewski, G., Nguyen, & Smyth, H. E., 'Smarter selections for tropical fruit - Using key Aroma Components as predictors of sensory quality'. International Tropical Agriculture Conference (TropAg 2022), 31 Oct - 2 Nov 2022, Brisbane, Australia. (*oral presentation and conference proceedings*).

Media release

1. **George, J.**, Sanewski, G., Nguyen, & Smyth, H. E., ‘Unveiling the aromatic secrets of Australian pineapple’. *Food Australia* Journal, Vol. 76 (4), Oct–Dec 2024 (AIFST).
2. **George, J.**, Sanewski, G., Nguyen, & Smyth, H. E., ‘Unlocking the Aromatic Secrets of Australian Pineapple: Innovative Research Reveals Key Aroma Compounds’. Press release for pineapple growers' field day, 2024.

Contributions by Others to this Thesis

For all chapters, the candidate's supervisors, Professor Heather Smyth, Dr. Garth Sanewski, and A/Prof. Craig Hardner, Dr. Thoa Nguyen, and the PhD review committee, Dr. Michael Netzel, Professor Craig Williams, and Dr. Bernadine Flanagan provided editorial suggestions.

Dr. Thoa Nguyen assisted in the development of the HS-GC-MS method in Chapter 3.

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Dr Natalie Dillon, Senior Biotechnologist, Genetic Improvement, DPI, The fruit genetic project co-ordinator, editorial suggestions for chapter 4 and publications.

Anne Hasted, Director and Senior Statistician, Qi Statistics Ltd, UK, inputs to statistical analysis for Chapters 4 and 5.

Use of Artificial Intelligence

Grammarly (free version): Used to check spelling and grammar and edit my final document (entire work), to enhance my text, and to improve clarity and expression (as a prompt), during the period May-July 2025 (grammarly, 2025).

Microsoft Copilot: Used to modify the written tone/style (across the document), with a prompt# rewrite this paragraph with clarity so that the tone is appropriate for a university assignment, during the period May-July 2025 (Microsoft, 2025)

Artificial Intelligence (AI) Declaration Table:

AI Tool	**Purpose of Use**	**Prompts Used**	**Thesis Section**
Grammarly	To check spelling and grammar, and edit my final document	Enhance text, and improve clarity and expression	Entire work
Microsoft Copilot	To modify the written tone/style	Rewrite the paragraph with clarity so that the tone is appropriate for a university assignment	Across the entire document

Editorial Assistance

No editorial assistance

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Inclusion of Work Submitted for Another Degree

No works submitted towards another degree or diploma have been included in this thesis.

Research Involving Human or Animal Subjects

Consumer and sensory assessments in Chapter 4 were conducted in line with the Professional Food Sensory Group of the Institute for Food Science and Technology (IFST) guidelines for ethical and professional practices for the sensory analysis of food. Informed consent was collected from all assessors (trained panel and naïve consumers) before the study commenced.

Sensory evaluation in Chapter 5 was approved by the Human Ethics Committee of the University of Queensland and the Australian National Statement of Ethical Conduct in Human Research (approval number: 2019002607).

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On a personal note, I am eternally grateful to my family. To my parents, whose sacrifices lit the path for my education like candles burning in the dark; to my sisters, for their unwavering support and encouragement; and to my extended family and well-wishers, thank you for your love and prayers.

To my beloved wife, my son, and my daughter, thank you for your patience, love, and belief in me, even during the most challenging times. Your presence has been my greatest source of strength.

Dedications

With deepest gratitude and reverence, I dedicate this thesis to God Almighty, whose guidance and blessings have been my constant source of strength.

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Table of Contents

List of Tables

List of Figures

List of Abbreviations

ACSs	acyl-CoA synthetases
AAT	alcohol acyl transferase
ADHs	alcohol dehydrogenases
AKR	aldo-keto reductase
AECA	aroma extract concentration analysis
AEDA	aroma extract dilution analysis
BEBT	benzyl alcohol O-benzoyltransferase
CRISPR	Clustered Regularly Interspaced Short Palindromic Repeats
DPI	Queensland Department of Primary Industries
DAF	Queensland Department of Agriculture and Fisheries
FID	flame ionisation detector
FR	fully ripe
GDSL	Gly-Asp-Ser-Leu esterase/lipase
GWAS	genome-wide association studies
GC	gas chromatography
GC-MS	gas chromatography–mass spectrometry
GCxGC	two-dimensional gas chromatography
LRI	linear retention index
LLE	liquid−liquid-extraction
LD	linkage disequilibrium
MAS	marker-assisted selection

MLM	mixed linear model
MS	mass spectrometry
OT	odour threshold
OAV	odour activity value
PTR ToF MS	Proton Transfer Reaction Time-of-Flight Mass Spectrometry
RNA	ribonucleic acid
SIDA	Stable Isotope Dilution Assay
SNP	single-nucleotide polymorphism
SPME	solid phase microextraction
SAFE	solvent-assisted flavour evaporation
TASSEL	Trait Analysis by aSSociation, Evolution and Linkage
TPS	terpene synthases
VOC/s	volatile organic compound/s

Chapter 1

1.1 Introduction

Tropical fruits play a vital role in global agriculture, not only for their economic value but also for their unique sensory appeal. Among these, pineapple (*Ananas comosus* var. *comosus*), a member of the Bromeliaceae family, stands out as one of the most widely consumed non-climacteric fruits, ranking third in global tropical fruit production with over 32 million metric tons harvested annually (*FAO. 2023. Major Tropical Fruits Market Review – Preliminary results 2022. Rome.*, 2023; *FAO. 2024. Major Tropical Fruits Market Review – Preliminary results 2023. Rome.*, 2024). Its popularity is largely driven by its distinctive flavour, which is a complex interplay of sweetness, acidity, and a rich aromatic profile.

The sensory characteristics of pineapple are primarily shaped by volatile organic compounds (VOCs), which include esters, terpenoids, aldehydes, ketones, and alcohols. These compounds contribute to the fruit's signature tropical, floral, and fruity notes. Though hundreds of VOCs have been identified in pineapple, only a few of them are considered aroma-active and significantly influence consumer perception. The composition and concentration of these VOCs are influenced by factors such as cultivar genetics, ripeness, postharvest handling, and environmental conditions.

Advancements in analytical chemistry have enabled more precise profiling of these aroma-active VOCs. Techniques such as gas chromatography-mass spectrometry (GC-MS), gas chromatography-olfactometry (GC-O), and stable isotope dilution analysis (SIDA) have become standard tools in flavour research. Studies have highlighted the importance of refining these methods to detect low-abundance volatiles and avoid analytical artifacts. It is essential to have a suitable, validated method tailored to Australian-grown pineapple cultivars, addressing existing challenges in accurately and efficiently quantifying volatile organic compounds (VOCs). Such a method supports a deeper understanding of the link between aroma compounds, sensory attributes, and consumer preferences, and contributes to breeding strategies aimed at improving fruit quality.

While extensive chemical profiling of pineapple cultivars has been conducted, the translation of these chemical attributes into consumer sensory preferences remains insufficiently understood, particularly for region-specific varieties. Recent advances in sensory evaluation, including preference mapping and multivariate statistical analysis, have begun to clarify the relationships between chemical composition and hedonic responses. In Australia, pineapple production is mainly located in Queensland, where climatic conditions support the cultivation of several commercial cultivars.

Despite the global diversity of pineapple varieties, only a limited number dominate the commercial market, often chosen based on agronomic traits rather than flavour quality. This context highlights the need for targeted research into the sensory and chemical profiles of Australian-grown cultivars. Addressing this gap requires an integrated approach combining sensory evaluation, quantitative analysis of VOCs, and advanced statistical modelling to link consumer preferences to specific sensory attributes, thereby providing valuable insights to inform breeding programmes aimed at improving flavour and consumer satisfaction in Australian pineapples.

In recent years, the focus of fruit breeding programs has shifted from yield and disease resistance to consumer-centric traits such as flavour and aroma. This transition has been supported by integrative approaches combining metabolomics, sensory science, and genomics. Marker-assisted selection (MAS) and genome-wide association studies (GWAS) have emerged as powerful tools for identifying genetic loci associated with desirable flavour traits. For example, the alcohol acyltransferase gene (AAT1) has been linked to ester biosynthesis, a key determinant of pineapple aroma.

This thesis builds upon these foundations by exploring the aroma chemistry, sensory attributes, and genetic determinants of pineapple flavour. It aims to develop robust analytical methods, identify key aroma compounds, and integrate sensory and genomic data to support the breeding of superior pineapple cultivars. The findings contribute to a growing body of literature that underscores the importance of flavour in driving consumer acceptance and guiding future breeding strategies.

1.2 Hypothesis, research aims and objectives

1.2.1 Hypothesis

- The key aroma compounds in pineapple are variety-specific and contribute to the sensory properties and consumer acceptability of pineapple.
- The unique profile of volatile aroma compounds can be linked to the genetics of the fruit.

1.2.2 Aims

- Identification and characterisation of key quality-determining flavour compounds present in pineapple cultivars across the world.
- Development of high-throughput analytical methods to measure those key components accurately and precisely.
- Application of these methods to study the compositional profile of pineapple varieties from the DPI breeding program and commercial growers to profile key parent and progeny lines to support identification of molecular markers and support marker-assisted breeding.

1.2.3 Specific Objectives

Specific objectives of the thesis are given in **Table 1.1** below.

Table 1.1 Specific objectives of the thesis

Objective	Description	Purpose
1. Target aroma compound List	Develop a list of key aroma compounds relevant to pineapple	Focus on compounds that define pineapple aroma.
2. Analytical method development	Create a high-throughput, matrix-matched SIDA-HS-SPME-GC-MS method.	Ensure accurate and precise quantification across different pineapple samples.
3. Application of method – Commercial Cultivars (2023)	Analyse compositional and sensory profiles of 5 Australian-grown pineapple cultivars.	Explore links between composition and consumer-perceived flavour.
4. Application of Method – genetic population samples (MRF, 2022)	Assess 196 fruits from MRF for compositional and flavour attributes.	data to find connections between aroma compounds, sensory attributes, and genetics.
5. Evaluation of genetic population samples (MRF, 2024)	Evaluate 154 pineapple samples from MRF for composition and sensory attributes.	data to find connections between aroma compounds, sensory attributes, and genetics.
6. GWAS and linkage analysis	Analyse compositional data to find connections between aroma compounds, sensory attributes, and underlying genetics.	Support selection and marker-assisted breeding for improved flavour.

1.3 Expected Outcomes

This study will provide

- a targeted list of key aroma compounds important to pineapple flavour.
- robust SIDA-HS-SPME-GC-MS method/s to monitor the volatiles in pineapples/other selected tropical fruit.
- a platform where the volatiles can be assigned to their sensory information and genetic origin.
- data, to develop tools that support the active pineapple/other selected tropical fruit breeding program, allowing the co-development of superior varieties.

Chapter 2 Literature Review: A review of the Aroma Chemistry of Pineapple (*Ananas comosus* var. *comosus*)

Pineapple (*Ananas comosus* var. *comosus*), often referred to as 'the king of fruit,' is one of the most flavourful and widely consumed tropical fruits globally. Its unique aroma and flavour are attributed to a complex blend of volatile and non-volatile compounds, with volatile organic compounds (VOCs) playing a central role in defining its sensory appeal. Despite nearly 480 VOCs being identified in pineapple over the past seven decades, only around 40 have been consistently reported as key aroma compounds contributing to its characteristic sweet, fruity, tropical, and coconut-like notes.

This chapter presents a comprehensive review of the published literature on volatile composition of pineapple varieties grown worldwide, with a particular focus on gas chromatography-mass spectrometry (GC-MS)-based analysis of flavour-contributing VOCs. Drawing from 58 studies spanning 77 years, the review consolidates data on analytical methodologies, VOCs profiles across different cultivars and maturity stages, and the factors influencing aroma compound identification and quantification, including geographical origin, seasonal variation, fruit development, postharvest handling, and tissue-specific differences. The absence of a consolidated database of pineapple VOCs has posed challenges for research in fruit genetics and breeding. By synthesising existing literature, this review identifies a subset of key aroma volatiles that can be targeted in future analytical method development and varietal improvement programs. The findings provide a valuable resource for researchers and breeders seeking to improve pineapple flavour through more precise chemical profiling and genetic selection. This chapter was published as 'Review of the Aroma Chemistry of Pineapple' in *Journal of Agriculture and Food Chemistry* (George et al., 2023).

Author contributions for this chapter are summarised in **Table 2.1** below.

Table 2.1 Author contributions in Chapter 2

	Jenson George	Garth Sanewski	Thoa Nguyen	Craig Hardner	David Williams	Heather E. Smyth
Conceptualization	x					x
Methodology	x					x
Software	x		x			x
Validation	x					
Formal analysis	x					
Investigation	x		x			x
Resources	x	x	x		x	x
Data curation	x	x				x
Writing - original draft	x					
Writing - review & editing	x	x	x	x	x	x
Visualization	x	x	x	x		x
Supervision		x	x	x		x

2.1 Introduction

Pineapple (*Ananas comosus*) is a tropical plant with an edible fruit and is the most economically significant plant in the family *Bromeliaceae* (G. M. Sanewski et al., 2018). The so called 'the king of fruit', named because of its crown of leaves (Wei, Liu, Liu, Lv, et al., 2011), is mainly cultivated in the tropical and sub-tropical regions due to the favourable climate and rainfall distribution. In 2020, the worldwide pineapple production was 27.8 million metric tons (FAOSTAT 2021). In Australia, 99% of the pineapple productions is in the state of Queensland, at around 71084 tonnes valued at AU$47 million in 2021 (Australian Horticulture Statistics Handbook 2020/21). Many cultivars of pineapples are known representing variation in colour, shape, size, odour, and flavour sensory characteristics like sweetness, acidity balance and juiciness (Lukás et al., 2013) but most are only grown for local markets. The 'Smooth Cayenne' cultivar is one of the most significant in terms of production worldwide (Garth M. Sanewski et al., 2018) and produces the flavour most people associate with pineapple. It is grown for processing and fresh consumption. Since the mid-1990's, the 'hybrid' fresh market cultivar, "MD-2" has become very popular due to its yellow flesh, good storage characteristics and improved aromatic flavour profile.

The exotic aroma and flavour of pineapple fruit which is widely appreciated by consumers (Steingass, Langen, et al., 2015; Turazzi et al., 2017) is a blend of several volatile and non-volatile compounds that are present in small amounts and in complex mixtures as well as the sugar: acid balance and textural characteristics. The volatile organic compounds (VOCs) which play an important role in the aroma component of fruit flavour and are important components of fresh and processed fruit (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010). The VOCs, that produce the characteristic aroma of pineapple are formed through various biosynthetic pathways and are organic compounds with defined chemical structures. The VOCs profile depends on the pineapple variety, geographical production location (Teai et al., 2001), seasonality (Liu et al., 2011), stage of fruit maturity (Elss et al., 2005; Umano et al., 1992), development of the fruit, postharvest storage conditions (Kaewtathip & Charoenrein, 2012; Turazzi et al., 2017; Wei, Liu, Liu, Zang, et al., 2011) and tissue type (top, middle, and bottom cross-sections along the central axis of the fruit) (Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012).

Fresh pineapples are characterised by a complex profile of VOCs (Elss et al., 2005; Steingass et al., 2014; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992), however, only a few key aroma compounds evoke their typical odour and play a significant role in the sensory notes of pineapple flavour (Mohd Ali et al., 2020; Vollmer et al., 2021). The volatiles of pineapple have been

the subject of extensive studies over several decades, mainly using gas chromatography (GC), and/or combined with olfactometry (GC-O), and mass spectrometry (GC-MS) (Kaewtathip & Charoenrein, 2012; Wei, Liu, Liu, Lv, et al., 2011). The earliest work on pineapple volatiles was reported by Haagen-Smit et al. in 1945 (Haagen-Smit et al., 1945). A few reviews on pineapple flavour and volatile profile have been published (Berger, 1991; Engel et al., 1990; F.P Mehrlich & Felton, 1971; Flath & Forrey, 1970; Hodgson & Hodgson, 1993; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Paull & Chen, 2003; Po & Po, 2012) and nearly 480 VOCs in pineapple have been reported including alcohols, esters, aldehydes, ketones, and terpenoids (Brat et al., 2004; Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Tokitomo et al., 2005; Umano et al., 1992; Wei, Liu, Liu, Lv, et al., 2011). However, a full structure elucidation and identification is not possible for all these compounds. MS fragmentation permits a tentative assignment of the volatiles, when additionally considering GC retention indices. To date, only around 40 compounds have been identified as characteristic key aroma compounds that significantly contribute to the distinct pineapple aroma (Lukás et al., 2013; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021).

Though there are limited reviews to consolidate a comprehensive inventory of VOCs important to pineapple flavour and the factors influencing the qualitative and quantitative profile of VOCs in pineapple, the lack of reliable data is an obstacle for research in pineapple plant genetics and breeding. Accurate quantification of the aroma of any fruit is important task and robust chemical analysis based on reliable databases of key aroma compounds are essential for the ongoing breeding strategies. Thus, this review provides a comprehensive overview of the volatile composition of pineapple varieties grown worldwide with a focus on GC-MS based analysis of key flavour contributing VOCs. About 58 studies of pineapple VOCs from the past 77 years have been reviewed herein, including a discussion of factors influencing the identification and quantification of VOCs with regard to the sample collection, preparation and analysis.

2.2 Methods

From 1945 to 2022 more than 200 papers were published concerning pineapple and more than 100 papers focusing on the pineapple flavour (Scopus search with descriptor pineapple AND (aroma OR volatiles)). Of the published literature, manuscripts from the last 32 years were chosen for evaluation (**Figure 2.1** on page 7) based on a) time of publication, b) significance of the VOCs analyses reported, c) reports of pineapple involving VOCs identification. This approach ensured that studies with comparable objectives were included and that the research focused on the analysis of the pineapple VOCs.

As the evaluated literature covered only the past 32 years, a general overview of the pineapple VOCs prior to 1990 is also included.

Most published literatures listed VOCs by their chemical name. Internationally accepted common chemical abstract service (CAS) registry numbers and International Union of Pure and Applied Chemistry (IUPAC) names were manually assigned to overcome any existing inconsistencies in reporting. Online open databases (PubChem: pubchem.ncbi.nlm.nih.gov; Merck Index: www.rsc.org/merck-index) were searched for the CAS numbers and the obvious literal errors in the names were corrected. For substances with stereoisomers, the unspecified substance name was listed if no reliable isomer determination was possible to avoid ambiguities.

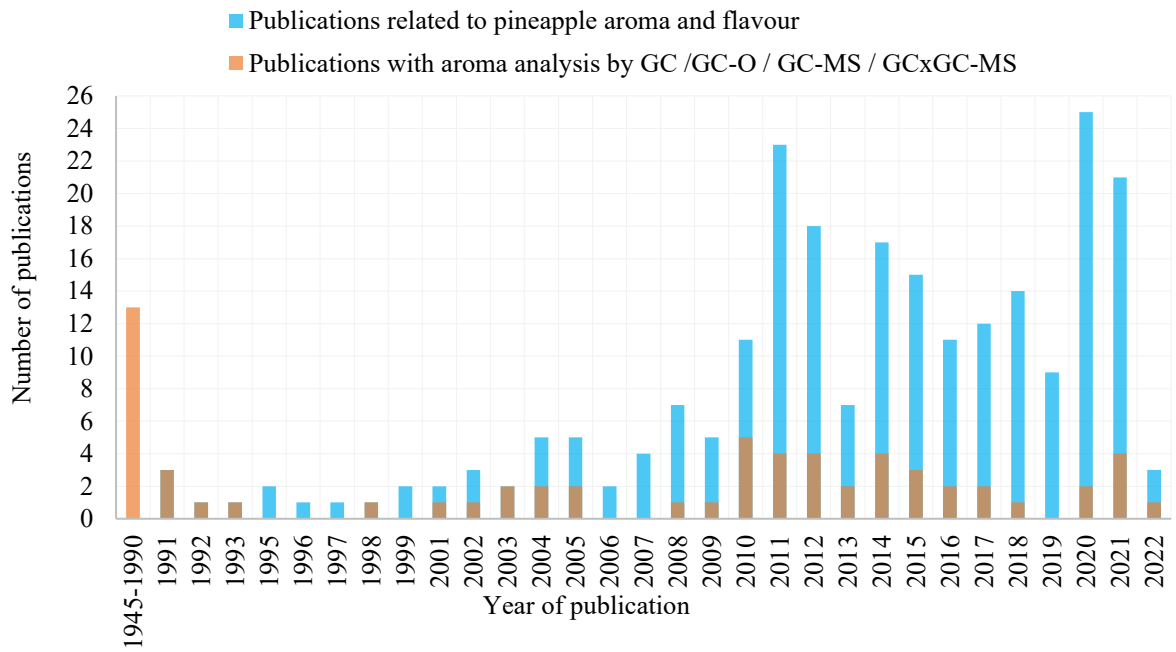


Figure 2.1 Summary of publications in pineapple relevant to pineapple aroma and relevant to VOC analysis (as at the time of this review 2022)

According to the guidelines from Molyneux, R.J. and P. Schieberle, 2007 (Molyneux & Schieberle, 2007), VOCs identification based on a simple search in mass spectrometric libraries cannot be considered sufficient. The guidelines recommend, (a) mass spectrometric fragmentation and retention indices must be determined on at least two separation columns of different polarity and (b) comparison of the mass spectra and retention indices (RI) with those of authentic reference substances as a so-called coelution must be made for the accurate identification of volatile compounds. A high level of confidence of VOCs identification and quantitation exists only when the criteria (calculation of RI using GC columns of different polarities, MS fragmentation pattern, co-elution with reference materials, use of external and internal reference standard materials, and additional confirmation using

GC-O) meet the guidelines. If the identification was made without meeting these criteria, VOCs are considered herein as 'tentatively identified'.

For volatile compound quantitation (though it is not the focus of this review), the published studies were also inconsistent. Using gas chromatography−flame ionization detector (GC-FID) or gas chromatography-mass spectrometry (GC-MS), the term "quantitation" could be used when accompanied by a stable isotope dilution analysis (SIDA) or by another standard addition quantification method. In other cases, the terms 'semi-quantitation' or 'semi-quantified' are considered as acceptable.

2.3 The body of literature on pineapple flavours and VOCs analysis

Early research on pineapple flavour was discussed by Flath, R.A. and R.R. Forrey in 1970 (Flath & Forrey, 1970) and Tressler, D.K. and M.A. Joslyn in 1971 (F.P Mehrlich & Felton, 1971), and summarised the available literature information till that time by reporting 45 VOCs which were previously identified. Another compilation work by Berger, R. G.,1991, summarised publications till 1988 (Berger, 1991), covering the previously published summary by Flath R.A., 1980 (R.A., 1980), reporting 117 compounds. In 1990, Engel, K.-H., J. Heidlas, and R. Tressl (Engel et al., 1990), discussed data till 1989 and reported ester compounds as the major class of compounds in pineapple. The importance of individual constituents to the aroma of pineapple was also reported and compiled the odour threshold values of several compounds. The reported 197 pineapple volatiles till 1989 in pineapple were summarised by Hodgson, A.S. and L.A. Hodgson, 1993 (Hodgson & Hodgson, 1993) and classified them as esters, acids, alcohols, aldehydes, ketones, lactones, and other miscellaneous compounds. However, a major work done by Umano, K., et al. 1992 (Umano et al., 1992) with the identification of several new compounds was not covered in the review by Hodgson, A.S. and L.A. Hodgson, 1993. In a comprehensive review by Montero-Calderón, M., M.A. Rojas-Graü, and O. Martín-Belloso, 2010 (Marta Montero-Calderón et al., 2010), reported the recognition of nearly 380 VOCs, summarised 338 compounds (based on the data till 2005) to different classes, and provided the OT of 34 compounds and odour description of nearly 100 VOCs. Smooth Cayenne was the leading variety at the time of this review (Marta Montero-Calderón et al., 2010), and the authors indicated the requirements to identify the VOCs profile of the MD2 variety that was substituting a large portion of the pineapple world market. Another review by Po, L.O. and E.C. Po, 2012 (Po & Po, 2012) briefly summarised the findings of published data till 2010 but did not cover the review by Montero-Calderón, M., M.A. Rojas-Graü, and O. Martín-Belloso, 2010. A recent review by Mohd Ali, M., et al.,2020 (Mohd Ali et al., 2020) reported the presence of hundreds of volatiles in pineapples (details were not included) but noted that only several of the aroma-active compounds are responsible for the

characteristic aroma of pineapples. Though the volatile profile of pineapples from published literature has been reviewed, a detailed examination with a focus on accurate qualitative and quantitative analysis is missing.

The published literature on pineapple VOCs analyses selected herein can be grouped into several categories based on the main objective of the study, such as works focused on:

- Review of published information (Berger, 1991; Engel et al., 1990; F.P Mehrlich & Felton, 1971; Flath & Forrey, 1970; Hodgson & Hodgson, 1993; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Paull & Chen, 2003; Po & Po, 2012)
- Identification of VOCs using instrumental analysis (Berger et al., 1985; Connell, 1964; Haagen-Smit et al., 1945; Pedroso et al., 2011; Rodin et al., 1966; Rodin et al., 1965; Silverstein et al., 1965; Steingass, Carle, et al., 2015; Takeoka et al., 1991; Wu et al., 1991)
- Odour threshold (OT), Odour activity value (OAV) calculation and odour description (Pino, 2013; Takeoka et al., 1989; Tokitomo et al., 2005; Wei et al., 2014)
- Effect of ripeness and maturity (Steingass et al., 2016; Steingass et al., 2014; Steingass, Langen, et al., 2015; Umano et al., 1992)
- Effect of post-harvest storage and logistics (Lamikanra & Richard, 2004; Spanier et al., 1998; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass, Jutzi, et al., 2015; Turazzi et al., 2017; Wei, Liu, Liu, Lv, et al., 2011)
- Influence of VOCs isolation- extraction techniques (Akioka & Umano, 2008; Kaewtathip & Charoenrein, 2012; Lukás et al., 2013; Pino, 2013; Teai et al., 2001; Wei et al., 2014)
- Varieties and geographical locations (Asikin et al., 2022; Brat et al., 2004; Kaewtathip & Charoenrein, 2012; Lasekan & Hussein, 2018; Xiao et al., 2021; Zainuddin et al., 2021; Zheng et al., 2012)
- Seasons and environmental factors (Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Liu & Liu, 2014; Liu et al., 2011; Preston et al., 2003)
- Effect of processing and handling (Braga et al., 2009; Braga et al., 2010; Kaewtathip & Charoenrein, 2012; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Orellana-Palma et al., 2020; Vollmer et al., 2021; Zhang et al., 2012)
- Sampling uniformity/tissue type (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Wei, Liu, Liu, Lv, et al., 2011)
- Self-interaction of VOCs within the fruit matrix (Teai et al., 2001; Xiao et al., 2021)

Early works in the period 1945-1989 were mainly focused broadly on the identification of VOCs of pineapple, and their structural elucidations. During this period, nearly 180 VOCs, including esters, sulphur-containing compounds, aldehydes, and terpenoid compounds, were identified and reported (Berger et al., 1985; Connell, 1964; Haagen-Smit et al., 1945; Rodin et al., 1966; Rodin et al., 1965; Silverstein et al., 1965). In one of the earlier works by Takeoka, G., et al., 1989 (Takeoka et al., 1989), 183 volatile compounds were identified in Smooth Cayenne pineapple. In one of the recent major studies, using comprehensive two-dimensional GC-MS (HS-SPME-GCxGC-MS) Steingass, C.B., R. Carle, and H.G. Schmarr, 2015 (Steingass, Carle, et al., 2015), reported the separation of 372 VOCs and identified 290 compounds in MD2 pineapple. Esters were the main class of compounds in most of these earlier and later works, comprising about 50% of the total VOCs of pineapple. Several new VOCs (mainly alkane and terpene class of compounds) were reported for the first time in processed pineapple waste (but not included in this review) by C. Ravichandran et al., 2020 (Ravichandran et al., 2020) (fruit pomace after juice removal) of Queen and King cultivars grown in India, and by A.S. Sengar et al., 2022 (Sengar et al., 2022). At the time of this review, more than 480 different volatiles were identified in total in different pineapple varieties. The most frequently found VOCs in pineapple are methyl and ethyl esters of butanoic, propanoic, hexanoic and octanoic acids. Ethyl and methyl thio esters of propanoic acids, several aldehydes, lactones, ketones, 4-hydroxy-2,5-dimethylfuran-3-one (DHMF), 4-methoxy-2,5-dimethylfuran-3-one (DMMF) and other terpenoid compounds are also found frequently in pineapples. A combined list of all the VOCs reported to date is given in Appendix 1, **Table A1.**

Though several VOCs were identified by various researchers, relatively little attention was paid to their aroma properties and sensory significance. Out of the hundreds of VOCs identified in various pineapple varieties to date, only around 40 compounds were considered as key characteristic aroma compounds. Only a few of the studies focused on the calculation of OAVs from the OT values and or in combination with aroma extract dilution analysis (AEDA), Gas chromatography-olfactometry (GC-O) techniques to identify key aroma compounds and provide odour description (Akioka & Umano, 2008; Berger et al., 1985; Pino, 2013; Spanier et al., 1998; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Wei et al., 2014). A detailed discussion of the key aroma compounds is provided below under the section titled as ‘key aroma compounds identified in pineapple’.

Influence of self-interaction of sulphur compounds, esters, lactones and furanoid compounds within the fruit towards the aroma of pineapple was explored and reported in one of the early and later works (Teai et al., 2001; Xiao et al., 2021). Effect of fruit maturity at the time of harvest and the influence of post-harvest storage on the volatiles of pineapples were the focus of many published works.

Successful attempts were made to make of volatile profile to confirm the authenticity and storage life of plant and stored fruits (Lamikanra & Richard, 2004; Spanier et al., 1998; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Steingass, Langen, et al., 2015; Turazzi et al., 2017; Umano et al., 1992; Wei, Liu, Liu, Lv, et al., 2011). Effect of environmental factors (Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Liu & Liu, 2014; Liu et al., 2011; Preston et al., 2003), and the contribution of analytical methods were also the objectives of many researchers (Akioka & Umano, 2008; Lukás et al., 2013; Pino, 2013; Teai et al., 2001; Wei et al., 2014).

Appendix 1, **Table A2** summarises the scientific aims of pineapple VOCs measurements in detail. It must be understood from the outset that the authors focusing on different objectives may not have invested more in the accuracy of the analytical methods employed for analysis and reported VOCs as 'tentatively identified' or 'assigned', wherever the criteria specified by Molyneux, R.J. and P. Schieberle, 2007 (Molyneux & Schieberle, 2007) did not match.

2.4 Key aroma compounds identified in pineapple

Though more than 480 volatile compounds have been identified in pineapple to date, only around 40 aroma-active compounds are associated with contributing to the distinct pineapple flavour (Lukás et al., 2013; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021) we have come to know from the varieties 'Smooth Cayenne' (before 1990) and MD-2. The aroma value concept, including the determination of OAV and OT values as well as the GC-O approach using aroma extract dilution analysis (AEDA) and aroma extract concentration analysis (AECA), are the practical tools applied to identify the most odour active compounds among the volatiles (Spanier et al., 1998; Tokitomo et al., 2005). CHARM analysis, founded in the measurement of the relative gas phase detection thresholds of individual chemicals, was introduced by T. E. Acree et al., 1984 (Acree et al., 1984) but, not reported in pineapple VOCs analysis. For the first time in pineapple aroma analysis, Tokitomo, Y., et al., 2005 (Tokitomo et al., 2005), used SIDA to accurately identify and quantify 29 VOCs by GC-MS. The authors performed AEDA using the isolated pineapple volatiles prepared by solvent-assisted flavour evaporation (SAFE) of the pineapple extract, calculated OAVs of 12 selected odorants and identified them as the key aroma compounds in fresh 'supersweet' pineapples (*syn*. MD-2). Additional sensory evaluations were also performed using fresh pineapple juice and pineapple flavour reconstituted model mixture and using trained panellists to determine the flavour (Tokitomo et al., 2005). Substances with high OAV (>1) are generally considered as compounds responsible for a particular aroma (Zheng et al., 2012). Out of 58 published literatures considered for this review, only a few studies (Akioka & Umano, 2008; Berger et al., 1985; Pino, 2013; Spanier et al., 1998; Takeoka

et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Wei et al., 2014) focused on identifying the characteristic aroma compounds of pineapple. One of the studies (Xiao et al., 2021) used the OAV values to study the interaction of sulphur and ester compounds in pineapple. Though substances with high OAV (>1) are generally considered as compounds responsible for characteristic aroma, the contribution of other VOCs and interaction (masking, additive and synergistic effects) of the VOCs also play an important role (Gonçalves, 2018; Teai et al., 2001; Xiao et al., 2021) towards the aroma of pineapples. Diastereomers of the same VOCs were separated and reported after the introduction of chiral columns (Umano et al., 1992). However, in most cases, a particular isomer over the other forms possesses different characteristic aroma properties (Pickenhagen, 1989). Ethyl (Z)-3- hexenoate is reported to have characteristic green-pineapple, fruity, pineapple-like, tropical, wine-like aroma (in stored fruit) with an OT of 1-2µg/kg, while the ethyl (E)-3- 3-hexenoate is reported to contribute a pungent, pineapple peel-like aroma with an OT of 25-50µg/kg (Berger et al., 1985; Marta Montero-Calderón et al., 2010).

Table 2.2 on page 13 summarises the frequently reported key aroma compounds reported in the literature with their OT values, FD factor. CAS number, odour description and their reported concentration. VOCs with less frequency but relevant due to their FD factor and/or OT values are also included.

Table 2.2 Most frequently identified Key VOCs in pineapples, reported FD factors, OT values and concentrations

VOCs ***CAS No.*** ***Classification*** ***(Odour description)***	**LRI** [ref] **Wax**	 **DB1**	 **5MS**	**Entries**	**FD factor [ref]**	**Odour threshold (µg/kg) [ref]**	**Reported Concentration (µg/Kg)** [ref] **Conc. µg/Kg; *variety**; [ref]****
methyl hexanoate *106-70-7* *ester* *(pineapple, fruity)*	1190[a] 1195[b] 1185[c] 1200[d]	915[g] 908[h]	925[a] 923[c] 922[d]	34	128 (Pino, 2013) 8 (Akioka & Umano, 2008) 16, 32, 64 (Lasekan & Hussein, 2018)	70 (Pino, 2013; Sun et al., 2016; Takeoka et al., 1989; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012) 77 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010)	27.0-152.9 (Lukás et al., 2013); 2330 (Vollmer et al., 2021); 1550-4810 (Steingass et al., 2021); 44 (Lasekan & Hussein, 2018) *MD2* 67.75 (Zheng et al., 2012) *Tainung No.4,* 4.71 (Zheng et al., 2012) *Tainung No.6,* 1628.62 (Sun et al., 2016) *Tainung17*, 211.62 (Sun et al., 2016) *Tainung17* 24.96 (Wei, Liu, Liu, Lv, et al., 2011); 27-39 (Kaewtathip & Charoenrein, 2012); 20 (Mohd Ali et al., 2020); 3442 (Takeoka et al., 1989) *Smooth Cayenne* 143.04 (Sun et al., 2016) *Queens-land Cayenne* 99.54 (Wei et al., 2014); 100 (Mohd Ali et al., 2020); 332.55 (Sun et al., 2016) *Shenwan* 1083-1248 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 1163-1204 (Mohd Ali et al., 2020); 286-1452 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* 397 *Morris* (Lasekan & Hussein, 2018); 19 *N36* (Lasekan & Hussein, 2018); 32 *Sarawak* (Lasekan & Hussein, 2018) 1101 (Teai et al., 2001) *NA;* 623.86 (Sun et al., 2016) *New Phuket* 188.4 (Asikin et al., 2022) *N67-10*; 114.0 (Asikin et al., 2022) *Yugafu*; 2639.1 (Asikin et al., 2022) *Yonekura*
ethyl hexanoate *123-66-0* *ester* *(pineapple, banana, fruity)*	1231[a] 1239[b] 1233[c] 1241[d]	984[g] 980[h]	999[abc]	33	4 (Tokitomo et al., 2005) 256 (Pino, 2013)	0.76 (Sun et al., 2016; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012) 1 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pino, 2013)	1233 (Mohd Ali et al., 2020); 4150[i] (Vollmer et al., 2021); 217-7650[i] (Steingass et al., 2021) *MD2* 8.35 (Zheng et al., 2012) *Tainung No. 6;* 1080.39 (Sun et al., 2016) *Tainung17;* 8.75 (Sun et al., 2016) *Tainung17* 106 (Mohd Ali et al., 2020); 20 (Kaewtathip & Charoenrein, 2012); 106.21 (Wei, Liu, Liu, Lv, et al., 2011) *Smooth Cayenne* 101-623 (Mohd Ali et al., 2020); 52-357 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010) *Gold* 13 *Morris* (Lasekan & Hussein, 2018) ; 1 *Sarawak* (Lasekan & Hussein, 2018) 40 (Teai et al., 2001) *NA;* 36.26 (Sun et al., 2016) *New Phuket* 1.5 (Asikin et al., 2022) *N67-10*; 101.3 (Asikin et al., 2022) *Yugafu;* 15.0 (Asikin et al., 2022) *Yonekura*
methyl 2-methylbutyrate *868-57-5* *ester* *(pungent, fruity)*	1013[a] 1011[b] 1010[c] 1019[d]	738[g] 764[h]	772[ad] 774[c]	32	1024 (Pino, 2013) 2048 (Tokitomo et al., 2005) 128(Akioka & Umano, 2008)	0.25 (Takeoka et al., 1989; Wei, Liu, Liu, Lv, et al., 2011) 1, 2 (Pino, 2013; Tokitomo et al., 2005) 0.1 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010)	31.7-253.3 (Lukás et al., 2013); 465 (Vollmer et al., 2021); 496-782 (Steingass et al., 2021) *MD2* 19.48 (Zheng et al., 2012) *Tainung No.4* 2079 (Takeoka et al., 1989) *Smooth Cayenne* 1966-3263 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 2105-2427 (Mohd Ali et al., 2020); 1034-2646 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* 103 *Morris* (Lasekan & Hussein, 2018; Mohd Ali et al., 2020) 154 (Teai et al., 2001) *NA*

VOCs ***CAS No.*** ***Classification*** ***(Odour description)***	**LRI** [ref] **Wax**	**DB1**	**5MS**	**Entries**	**FD factor [ref]**	**Odour threshold (µg/kg) [ref]**	**Reported Concentration (µg/Kg)** [ref] **Conc. µg/Kg; *variety**; [ref]****
methyl 3-(methylthio) propionate *13532-18-8* *sulphur containing, ester* *(meaty, onion like)*	1518[a] 1533[b] 1517[c] 1540[d]	1001[h]	1024[a] 1026[c] 1023[d]	32	32 (Pino, 2013)	180 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pino, 2013; Takeoka et al., 1989; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012)	17.9-110.4 (Lukás et al., 2013); 880-894 (Vollmer et al., 2021); 1020-2400 (Steingass et al., 2021); 28.7 (Lasekan & Hussein, 2018) *MD2* 622.49 (Zheng et al., 2012) *Tainong No.4 and* 32.94 (Mohd Ali et al., 2020; Zheng et al., 2012) *Tainong No 6* 27.38 (Mohd Ali et al., 2020; Wei, Liu, Liu, Lv, et al., 2011); 102-127 (Kaewtathip & Charoenrein, 2012); *Smooth Cayenne* 19.43 *Shenwan* (Wei et al., 2014) 507-682 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010) ; 241-644(M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* 180 *Red Spanish* (Mohd Ali et al., 2020) ;307 *Morris* (Lasekan & Hussein, 2018) ;17 *Sarawak* (Lasekan & Hussein, 2018) 1140 (Teai et al., 2001) *NA* 186.7 (Asikin et al., 2022) *N67-10*; 22.0 (Asikin et al., 2022) *Yugafu;* 1284.9 (Asikin et al., 2022) *Yonekura*
methyl octanoate *111-11-5* *ester* *(fruity)*	1390[a] 1392[b] 1387[c] 1396[d]	1018[g] 1107[h]	1125[ac] 1112[d]	32	_	200 (Takeoka et al., 1989; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012)	23.9-34.3 (Lukás et al., 2013); 29.6[i] (Vollmer et al., 2021); 66.4-496[i] (Steingass et al., 2021); 3.0 (Lasekan & Hussein, 2018) *MD2* 142.25 (Zheng et al., 2012) *Tainung No.4,* 20.52 (Mohd Ali et al., 2020; Zheng et al., 2012) *Tainung No.6 and* 14.0 (Mohd Ali et al., 2020) *Tainung No.17* 8.39 (Wei, Liu, Liu, Lv, et al., 2011); 64 (Kaewtathip & Charoenrein, 2012; Mohd Ali et al., 2020); 1451 (Takeoka et al., 1989) *Smooth Cayenne* 326.97 (Mohd Ali et al., 2020; Wei et al., 2014) *Shenwan* 43- 49.6 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 13.9-100.4(M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* 101 *Morris* (Lasekan & Hussein, 2018) ;4 *Sarawak* (Lasekan & Hussein, 2018) ;1496 (Teai et al., 2001) *NA* 8.4 (Asikin et al., 2022) *N67-10*; 1.9 (Asikin et al., 2022) *Yugafu;* 102.8 (Asikin et al., 2022) *Yonekura*
ethyl 2-methylbutyrate *7452-79-1* *ester* *(apple, Pineapple, fruity)*	1050[a] 1054[b] 1048[c] 1060[d]	835[g] 764[h]	846[acd]	28	1024 (Pino, 2013) 4096 (Tokitomo et al., 2005) 128 (Akioka & Umano, 2008)	0.006 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012) 0.15 (Pino, 2013; Tokitomo et al., 2005) 0.3 (Takeoka et al., 1989)	951 (Vollmer et al., 2021); 12.9-263 (Steingass et al., 2021) *MD2* 22.24 (Zheng et al., 2012) *Tainung No.6* 1693.33 (Wei, Liu, Liu, Lv, et al., 2011); 66 (Takeoka et al., 1989) *Smooth Cayenne* 23.5 - 49.4 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 12.5-222.7 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* ;224 (Teai et al., 2001) *NA* 114.8 (Asikin et al., 2022) *Yugafu;* 2.8 (Asikin et al., 2022) *Yonekura*

VOCs ***CAS No.*** ***Classification*** ***(Odour description)***	**LRI** [ref] **Wax**	**DB1**	**5MS**	**Entries**	**FD factor [ref]**	**Odour threshold (µg/kg) [ref]**	**Reported Concentration (µg/Kg)** [ref] **Conc. µg/Kg; *variety**; [ref]****
methyl butyrate *623-42-7* *ester* *(fruity, sweet)*	990[a] 996[b] 986[c] 995[d]	715[g] 705[h]	719[a] 718[c] 717[d]	27	64 (Pino, 2013)	59 (Pino, 2013; Sun et al., 2016) 72 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010)	990 (Mohd Ali et al., 2020); 138 (Vollmer et al., 2021); 212-342[i] (Steingass et al., 2021) *MD2* 2026 (Takeoka et al., 1989) *Smooth Cayenne* 2531-3597 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 1250-3559 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* ; 83 (Teai et al., 2001) *NA* 44.2 (Asikin et al., 2022) *N67-10*; 14.6 (Asikin et al., 2022) *Yugafu;* 234.6 (Asikin et al., 2022) *Yonekura*
ethyl 3-(methylthio) propionate *13327-56-5* *sulphur containing, ester* *(meaty, onion, pineapple)*	1560[a] 1576[b] 1561[c] 1580[d]	1078[h]	1100[a] 1103[c] 1072[d]	24	512 (Pino, 2013)	1 (Pino, 2013) 7 (Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012)	2540[i] (Vollmer et al., 2021); 35.2-3010[i] (Steingass et al., 2021) *MD2* 32.96 (Zheng et al., 2012) *Tainung No.4;* 78.06 (Mohd Ali et al., 2020; Zheng et al., 2012) *Tainung No. 6* 91.21 (Mohd Ali et al., 2020; Wei, Liu, Liu, Lv, et al., 2011); 28 (Kaewtathip & Charoenrein, 2012) *Smooth Cayenne* 5-9.7 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 7.3-97.6 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* ;153 (Teai et al., 2001) *NA* 2.3 (Asikin et al., 2022) *N67-10*; 94.5 (Asikin et al., 2022) *Yugafu;* 9.0 (Asikin et al., 2022) *Yonekura*
ethyl acetate *141-78-6* *ester* *(solvent, fruity)*	890[a] 965[b] 888[c] 897[d]	601[h]	613[a] <700[c] 605[d]	23	2 (Tokitomo et al., 2005) 32 (Pino, 2013)	5000 (Pino, 2013)	546 (Vollmer et al., 2021); 73.5-1400 (Steingass et al., 2021) *MD2* 470 (Wu et al., 1991) 811 (Teai et al., 2001) *NA* 18.2 (Asikin et al., 2022) *N67-10*; 125.8 (Asikin et al., 2022) *Yugafu;* 24.0 (Asikin et al., 2022) *Yonekura*
isobutyl acetate *110-19-0* *ester* *(fermented, ethereal)*	1018[b]	_	_	9	32 (Pino, 2013)	66 (Pino, 2013)	66 (Mohd Ali et al., 2020) *Red Spanish* 41 (Takeoka et al., 1989) *Smooth Cayenne* 1.5 (Asikin et al., 2022) *Yugafu;* 1.6 (Asikin et al., 2022) *Yonekura*
ethyl isobutyrate *97-62-1* *ester* *(fruity, sweet)*	966[a] 989[b] 965[c] 973[d]	_	754[a] 752[c] 751[d]	11	64 (Tokitomo et al., 2005) 1024 (Pino, 2013)	0.02 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pino, 2013; Tokitomo et al., 2005); 0.1 (Takeoka et al., 1989)	114 (Vollmer et al., 2021); 2.2-8.9 (Steingass et al., 2021) *MD2*
2-Methylbutyl acetate *624-41-9* *ester* *(fermented, sweet, balsamic)*	1118[a] 1124[b] 1118[c]	_	874[ac]	10	32 (Pino, 2013)	5 (Pino, 2013)	18.9-1290[i] (Steingass et al., 2021); 48.9[i] (Vollmer et al., 2021) *MD2* 2.1 (Asikin et al., 2022) *Yugafu;* 27.0 (Asikin et al., 2022) *Yonekura*
methyl isovalerate *556-24-1* *ester* *(Fruity, apple like)*	1019[a] 1021[b] 1017[c] 1027[d]	_	776[d]	10	2048 (Tokitomo et al., 2005)	44 (Xiao et al., 2021)	12.0 (Vollmer et al., 2021); 15.9-41.4 (Steingass et al., 2021) *MD2* 2.5-32.7 (Asikin et al., 2022) *Okinawan* 2.9 (Asikin et al., 2022) *N67-10*; 2.5 (Asikin et al., 2022) *Yugafu;* 32.7 (Asikin et al., 2022) *Yonekura*

VOCs ***CAS No.*** ***Classification*** ***(Odour description)***	**LRI** [ref] **Wax**	**DB1**	**5MS**	**Entries**	**FD factor [ref]**	**Odour threshold (µg/kg) [ref]**	**Reported Concentration (µg/Kg)** [ref] **Conc. µg/Kg; *variety**; [ref]****
ethyl butyrate *105-54-4* *ester* *(fruity)*	1035[a] 1038[b] 1033[c] 1045[d]	794[g]	801[ac] 803[d]	23	4 (Tokitomo et al., 2005) 128 (Pino, 2013)	1 (Pino, 2013; Tokitomo et al., 2005; Wei, Liu, Liu, Lv, et al., 2011)	6.6-247 (Steingass et al., 2021); 418 (Vollmer et al., 2021) *MD2* 6.09 (Wei, Liu, Liu, Lv, et al., 2011); 92 (Takeoka et al., 1989) *Smooth Cayenne* 4.0 (Asikin et al., 2022) *N67-10*; 2.7 (Asikin et al., 2022) *Yugafu;* 3.6 (Asikin et al., 2022) *Yonekura*
methyl isobutyrate 547-63-7 ester *(fruity, sweet)*	924[a] 974[b] 921[c] 931[d]	_	685[a] <700[c] 697[d]	18	8 (Tokitomo et al., 2005) 64 (Pino, 2013)	6,3 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pino, 2013; Tokitomo et al., 2005)	10.7 (Vollmer et al., 2021); 16.9 (Steingass et al., 2021) *MD2* 383-571 (Mohd Ali et al., 2020); 520-860 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010) *Gold*
ethyl octanoate *106-32-1* *ester* *(fruity, winey, sweet)*	1433[ac] 1437[b]	1170[g] 1183[h]	1198[a] 1197[c]	17	32 (Pino, 2013)	192 (Pino, 2013)	6.0 (Vollmer et al., 2021); 16.5-769 (Steingass et al., 2021) *MD2* 46.21 (Zheng et al., 2012) *Tainung No.6* 50 (Kaewtathip & Charoenrein, 2012); 37 (Takeoka et al., 1989) *Smooth Cayenne* 0.7-2.3 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 0.7-43.5 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* ; 197 (Teai et al., 2001) *NA*
methyl 3-acetoxyhexanoate *21188-60-3* *ester* *(fruity green lettuce like)*	1682[a] 1688[b] 1681[c]	1170[g] 1176[h]	1207[a] 1206[c]	15	_	190 (Wei, Liu, Liu, Lv, et al., 2011)	11.5-42.7 (Lukás et al., 2013); 152[i] (Vollmer et al., 2021); 76.1-409 (Steingass et al., 2021) *MD2* 277 (Mohd Ali et al., 2020); 166 (Takeoka et al., 1989) *Smooth Cayenne* ; 61 (Teai et al., 2001) *NA*
ethyl (E)-3-hexenoate *64187-83-3* *ester* *(green, pineapple, tropical)*	1292[a] 1296[b] 1291[c] 1272[d]	_	1006[a] 1005[c] 933[d]	14	_	2 (Wei, Liu, Liu, Lv, et al., 2011)	112 (Vollmer et al., 2021); 1.5-37.7 (Steingass et al., 2021) *MD2* 5.81 (Kaewtathip & Charoenrein, 2012) *Smooth Cayenne*
ethyl decanoate *110-38-3* *ester* *(sweet, fatty, nut like)*	1636[a] 1638[b]	1383[h]	1395[a]	14	_	6300 (Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012)	2.3-69.1 (Steingass et al., 2021) *MD2* 19.96 (Zheng et al., 2012) *Tainung No.6* 3 (Kaewtathip & Charoenrein, 2012); 11.11 (Mohd Ali et al., 2020) *Smooth Cayenne* 1-1.5 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 0.7-46.0 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* ; 114 (Teai et al., 2001) *NA*
ethyl propionate *105-37-3* *ester* *(fruity, sweet)*	956[a] 986[b] 954[c] 966[d]	_	711[a] 708[cd]	14	32 (Pino, 2013)	10 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pino, 2013)	17 (Takeoka et al., 1989) Smooth Cayenne 69.1 (Vollmer et al., 2021); 2.0-20.6 (Steingass et al., 2021) *MD2*
methyl 5-acetoxyhexanoate *35234-22-1* *ester* *(fruity)*	1769[a] 1770[b] 1767[c]	1387[h]	1254[a] 1253[c]	14	_	_	17.1-261 (Steingass et al., 2021); 104 (Vollmer et al., 2021); 30.8-98.3 (Lukás et al., 2013) *MD2* 33 (Takeoka et al., 1989); 64 (Mohd Ali et al., 2020) *Smooth Cayenne* ;145 (Teai et al., 2001) *NA*

VOCs ***CAS No.*** ***Classification*** ***(Odour description)***	**LRI** [ref] **Wax**	**DB1**	**5MS**	**Entries**	**FD factor [ref]**	**Odour threshold (µg/kg) [ref]**	**Reported Concentration (µg/Kg)** [ref] **Conc. µg/Kg; *variety**; [ref]****
isoamyl acetate *123-92-2* *ester* *(fruity-fresh)*	1118[ac] 1124[b] 1127[d]	_	881[a] 876[cd]	14	128 (Pino, 2013)	2 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pino, 2013)	2.9-273.4 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* 48.9[i] (Vollmer et al., 2021); 18.9-1290[i] (Steingass et al., 2021) *MD2*
4-Hydroxy-2,5-dimethyl-3(2H)-furanone *3658-77-3* *furan* *(sweet, cooked pineapple, strawberry)*	2030[a] 2038[b] 2029[c]	1020[g] 1028[h]	1051[ac] 1063[f]	19	1024 (Pino, 2013; Tokitomo et al., 2005) 16 (Lasekan & Hussein, 2018)	0.03 (Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012) 10 (Pino, 2013; Tokitomo et al., 2005)	1.2-31.9 (Steingass et al., 2021); 11.4 (Vollmer et al., 2021) *MD2* 76.47 (Zheng et al., 2012) *Tainung No.4* 3.19 (Wei, Liu, Liu, Lv, et al., 2011) *Smooth Cayenne* 16 (Lasekan & Hussein, 2018) *Morris;* 16 (Lasekan & Hussein, 2018) *Maspine;* 32 (Lasekan & Hussein, 2018) *Josepine* 16 (Lasekan & Hussein, 2018) *Sarawak;* 40 (Teai et al., 2001) *NA* 9.6 (Asikin et al., 2022) *N67-10*; 8.4 (Asikin et al., 2022) *Yugafu;* 18.6 (Asikin et al., 2022) *Yonekura*
4-Methoxy-2,5-dimethyl-3(2H)-furanone *4077-47-8* *furan* *(caramel, roasty, sweet)*	1586[a] 1604[b] 1586[c]	1008[h]	1059[a] 1061[c] 1055[f]	18	8 (Tokitomo et al., 2005)	0.03 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010)	48.6 (Vollmer et al., 2021); 69.5-436 (Steingass et al., 2021); 39.7-48.6 (Lukás et al., 2013) *MD2* 619-934 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 196-487 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold* ;287 (Teai et al., 2001) *NA* 4.6 (Asikin et al., 2022) *N67-10*; 137.2 (Asikin et al., 2022) *Yonekura*
limonene *138-86-3* *terpene* *(citrus)*	1199[a] 1202[b] 1203[d]	1007[g]	1026[a]	13	32 (Pino, 2013)	10 (Pino, 2013)	85.9 (Lukás et al., 2013); 1.4-6.9 (Steingass et al., 2021) *MD2* 3.1-3.9 (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010); 7.6-24.9 (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010) *Gold*
alpha-terpineol *98-55-5* *Terpene* *floral, lilac*	1705[b] 1702[e]	1169[j]	_	10	_	330 (Wei, Liu, Liu, Lv, et al., 2011)	8.6 (Vollmer et al., 2021) *MD2*
acetaldehyde *75-07-0* *aldehyde* *(pungent)*	703[a] 737[d]	_	<500[a] 381[d]	9	32 (Akioka & Umano, 2008; Pino, 2013)	17 (Pino, 2013)	1.2-3.1 (Steingass et al., 2021) *MD2*
octanal *124-13-0* *aldehyde* *(citrus, fatty)*	1293[b] 1285[c]	_	1004[c]	8	2 (Tokitomo et al., 2005)	8 (Tokitomo et al., 2005)	59.7[i] (Vollmer et al., 2021) *MD2*
decanal *112-31-2* *aldehyde* *(waxy, floral, citrus)*	1505[b] 1494[c] 1488[d] 1500[e]	1170[g]	1207[c] 1205[d]	7	_	0.1 (Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012)	6.7-13.4[i] (Steingass et al., 2021); 69.7 (Vollmer et al., 2021) *MD2* 1.61 (Zheng et al., 2012) *Tainung No.6* 8.63 (Wei et al., 2014) *Shenwan*

VOCs ***CAS No.*** ***Classification*** ***(Odour description)***	**LRI** [ref] **Wax**	**DB1**	**5MS**	**Entries**	**FD factor [ref]**	**Odour threshold (µg/kg) [ref]**	**Reported Concentration (µg/Kg)** [ref] **Conc. µg/Kg; *variety**; [ref]****
vanillin *121-33-5* *aldehyde* *(vanilla)*	>2200[h]	1368[h]	1408[f]	7	128 (Tokitomo et al., 2005)	25 (Tokitomo et al., 2005)	10.7 (Lukás et al., 2013) *MD2* 35 (Teai et al., 2001) *NA*
isovaleraldehyde *590-86-3* *aldehyde* *(fruity)*	_	_	_	8	64 (Pino, 2013; Tokitomo et al., 2005)	0.5 (Pino, 2013)	1.9 (Lukás et al., 2013) *MD2*
phenylacetaldehyde *122-78-1* *aldehyde* *(floral, sweet)*	_	_	_	5	32 (Pino, 2013)	4 (Pino, 2013)	8.1 (Lukás et al., 2013) *MD2*
2-Methylbutyraldehyde *96-17-3* *aldehyde* *(fruity)*	_	_	_	5	32 (Pino, 2013)	1.5 (Pino, 2013)	NA
1-(E,Z,Z)-3,5,8-undecatetraene *29837-19-2* *hydrocarbon* *(pineapple)*	_	1165[j]	_	5	1024 (Pino, 2013)	0.002 (Pino, 2013) 0.002-0.004 (Marta Montero-Calderón et al., 2010)	5 (Lukás et al., 2013) *MD2* 1 (Berger et al., 1985) *NA*
1-(3E,5Z)-3,5-undecatriene *19883-27-3* *hydrocarbon* *(Pineapple, green)*	1389[e]	1160[h]	1173[a]	12	32 (Akioka & Umano, 2008; Tokitomo et al., 2005) 512 (Pino, 2013)	0.02 (Pino, 2013; Tokitomo et al., 2005) 0.001-0.002 (Marta Montero-Calderón et al., 2010)	29.6[i] (Vollmer et al., 2021) ; 66.4-496[i] (Steingass et al., 2021) *MD2* 1 (Mohd Ali et al., 2020) *Smooth Cayenne* 1 (Berger et al., 1985) *NA*
delta-octalactone *698-76-0* *lactone* *(coconut)*	1949[a] 1984[b] 1944[c]	1250[g]	1290[ac] 1288[f]	18	64 (Pino, 2013)	0.4 (Wei et al., 2014; Zheng et al., 2012) 400 (Tokitomo et al., 2005)	33.3 (Vollmer et al., 2021); 3.5 (Lasekan & Hussein, 2018); 14.7-19.9 (Lukás et al., 2013); 5.8-37.8 (Steingass et al., 2021) *MD2* 63.4 (Zheng et al., 2012) *Tainung No.4;* 48 (Teai et al., 2001) *NA* 12.49 (Wei et al., 2014) *Shenwan* 11 (Lasekan & Hussein, 2018) *Morris;* 3 (Lasekan & Hussein, 2018) *N36;* 11 (Lasekan & Hussein, 2018) *Josepine;* 7 (Lasekan & Hussein, 2018) *Sarawak*
delta-decalactone *705-86-2* *Lactone* *(coconut, sweet)*	2163[a] 2220[b] 2172[c]	_	1502[ac] 1500[f]	10	128 (Tokitomo et al., 2005)	160 (Tokitomo et al., 2005)	1.2-6.7 (Steingass et al., 2021); 6.4 (Vollmer et al., 2021) *MD2*
damascenone *23696-85-7* *ketone* *(fruity, sweet)*	1806[c] 1833[b]	_	1391[c] 1394[f]	5	8 (Tokitomo et al., 2005)	0.00075 (Tokitomo et al., 2005)	0.083 (Tokitomo et al., 2005) *Super Sweet*

VOCs ***CAS No.*** ***Classification*** ***(Odour description)***	**LRI** [ref] **Wax**	**DB1**	**5MS**	**Entries**	**FD factor [ref]**	**Odour threshold (µg/kg) [ref]**	**Reported Concentration (µg/Kg)** [ref] **Conc. µg/Kg; *variety**; [ref]****
isoamyl alcohol *123-51-3* *alcohol* *(pineapple, chocolate)*	1210[a] 1208[b]	_	733[a]	6	32 (Pino, 2013)	300 (Pino, 2013)	2.2-41.9[i] (Steingass et al., 2021) *MD2* 300 (Mohd Ali et al., 2020) *Red Spanish*

** Shenwan and Morris are 'the variety 'Queen'. Gold is MD2. Sarawak is Smooth Cayenne. Tainung 4 and Tainung 6 are a Queen x Smooth Cayenne cross. Josapine is a Ruby x Queen cross. Maspine is 73-50. _/NA – information not available.*

*** Identification criteria is provided in Table 2. 'i' reported along with another compound.*

a (Steingass et al., 2021), b (Steingass, Carle, et al., 2015), c (Vollmer et al., 2021), d (Xiao et al., 2021), e (Akioka & Umano, 2008) , f (Tokitomo et al., 2005), g (Brat et al., 2004), h (Teai et al., 2001), j (Takeoka et al., 1989)

2.5 Factors that impact VOCs in pineapple

The VOCs of pineapple are organic compounds with defined chemical structures, and their basic skeletons are formed through biosynthetic pathways from their primary precursor compounds (fatty acids, lipids, carotenoids, carbohydrates, and amino acids). The quality and quantity of the VOCs depend upon the availability of the precursor compounds, and further diverse VOCs are then formed via additional modification reactions such as acylation, methylation, oxidation/reduction and cyclic ring closure from the basic skeletons (Gonçalves, 2018; Lasekan & Hussein, 2018). The identification of genes responsible for the biosynthesis of VOCs can open new perspectives for the improvement of flavour, by cloning those genes, increasing that specific pathway or silencing the expression of a gene responsible for an undesired compound (Gonçalves, 2018). Several complex factors can affect the composition of VOCs in pineapple, such as varieties and geographical locations (Brat et al., 2004; Kaewtathip & Charoenrein, 2012; Lasekan & Hussein, 2018; Xiao et al., 2021; Zainuddin et al., 2021; Zheng et al., 2012), seasons and environmental factors (Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Liu & Liu, 2014; Liu et al., 2011; Preston et al., 2003), ripeness and maturity (Steingass et al., 2016; Steingass et al., 2014; Steingass, Langen, et al., 2015; Umano et al., 1992).

2.5.1 Storage

Being a non-climacteric fruit, pineapple do not ripen after harvest. However, changes in the volatile profile were observed during post-harvest storage and logistics (Lamikanra & Richard, 2004; Spanier et al., 1998; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass, Jutzi, et al., 2015; Turazzi et al., 2017; Wei, Liu, Liu, Lv, et al., 2011). The volatile profile of pineapple is known to be influenced by post-harvest storage, and clear-cut differences in the volatile profiles of stored pineapples were reported (Berger et al., 1985; Lamikanra & Richard, 2004; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Spanier et al., 1998; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Zang, et al., 2011). In general, elevated concentrations of volatiles were found in fully ripe fresh pineapples, and methyl esters are found at high in fresh fruit compared to ethyl esters in stored pineapples. Additional volatiles, like diverse alcohols and ethyl esters, were generated from fermentative pathways.

Depending on the physiological status of the fruits, different metabolic pathways involved in the biogenesis of pineapple volatiles were hypothesised for the difference in volatile profile of post-harvest maturation of pineapple. Catabolic and fermentative metabolic (Lasekan & Hussein, 2018)

pathways were attributed to post-harvest maturation, and in contrast, anabolic metabolism was attributed to fruits allowed to ripen attached to the plant prior to their harvest (Steingass, Carle, et al., 2015). Chain elongation reactions were attributed to the varying isomeric composition of certain VOCs such as methyl 3-hydroxy hexanoate, methyl 3-acetoxy hexanoate and methyl 5-acetoxy octanoate in fully ripened pineapples. It was also proposed that such reactions may also be involved in the post-harvest biogenesis of chiral-specific lactones using 3-hydroxyoctanoic acid as a precursor (Steingass, Langen, et al., 2015). Ethyl 3-acetoxyoctanoate, a corresponding derivative of this precursor, has previously been identified as a characteristic compound formed during post-harvest maturation of pineapple fruit (Steingass et al., 2014). Several similar independent pathways, such as reactions involving reduction, chain elongation and hydration, were proposed in the post-harvest biogenesis of different VOCs. The majority of the discriminative volatiles (methyl and ethyl esters, lactones and terpenoid compounds) formed during the postharvest period of pineapples harvested at a premature green-ripe stage were attributed to fatty acids, amino acids, and compounds originating from terpene metabolism (Steingass, Jutzi, et al., 2015; Steingass, Langen, et al., 2015).

2.5.2 Varietal differences

All studies that investigated different pineapple varieties (Asikin et al., 2022; Brat et al., 2004; Elss et al., 2005; Lasekan & Hussein, 2018; Zheng et al., 2012) describe varietal differences as a key influencing factor on the quality and quantity of the aroma patterns. Quantitative differences in total ester concentrations were observed for Tainung No.6 and No.4 pineapples, with further variation in their individual concentration among these two varieties. For the ketone family of compounds, 2,5-dimethyl-4-hydroxy-3(2H)-furanone (furaneol) was found at a relatively higher concentration (76 µg/kg) in Tainung No.4 but was not found in the Tainung No.6 pineapple. Although 3-(methylthio) propanoic acid ethyl ester was present in the two varieties, the other characteristic aroma compounds of the two varieties were different (Zheng et al., 2012). Among the commonly detected compounds across many pineapple varieties like methyl-2-methylbutanoate, dimethyl malonate, methyl-2-methyl acetoacetate, methyl-2-hydroxy-2-methylbutanoate, methyl hexanoate, ethyl isohexanoate, methyl-2-methylhexanoate, methyl3-(methylthiol)-propanoate, ethyl hexanoate, y-lactone, 2,5-dimethyl-4-hydroxy-3(2H)-furanone, methyl-3-hydroxyhexanoate, 2,5-dimethyl-4-methoxy-3(2H)furanone, methyl octanoate, methyl-(4E)-octenoate and 2,4-dihydroxy-2,5-dimethyl-3(2H)-furanone, the highest FD factor was attributed to methyl-2-methylbutanoate (FD, 1024), methyl hexanoate (FD, 128) and 2,4-dihydroxy-2,5-dimethyl-3(2H)furanone (DMHF) (FD, 128), respectively. However, methyl-2-methylbutanoate was not detected in varieties like N36, Maspine (*syn*. 73-50, CO-2) and Sarawak (*syn*. Smooth Cayenne) grown in Malaysia but methyl hexanoate and DMHF contributed

significantly to the aroma profiles of most pineapple varieties (Lasekan & Hussein, 2018). Vast variation in volatile profile of different varieties and clear differences in characteristic aroma compounds like n-butyl acetate, ethyl 2-hydroxypropanoate, and (E)-beta-caryophyllene in Flhoran41 and Smooth Cayenne varieties. Large variation in the lactone class of VOCs within a given cultivar was also observed from fruit to fruit (Steingass, Langen, et al., 2015). High variation in the amount and composition of the identified VOCs among three different cultivars was also reported in Okinawan pineapple cultivars (Asikin et al., 2022)

2.5.3 Tissue type

Obtaining a uniform representative sample is an important prerequisite for aroma analysis to get consistent and reliable results. There was a significant quantitative variation in the volatile profile of 'top, middle and bottom' cross sections of the Gold cultivar (*syn*. MD2) pineapple (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010) Methyl butanoate, methyl 2-methyl butanoate, and methyl hexanoate were the 3 most abundant components representing 74% of total volatiles in Gold Cultivar pineapple samples and the most odour active contributors were methyl and ethyl 2-methyl butanoate and 2,5-dimethyl 4-methoxy 3(2H)-furanone (mesifuran). Though the aroma profile components did not vary along the fruit, the volatile compounds content significantly varied along the fruit, from 7560 to 10910 μg/kg, from the top to the bottom cross-sections of the fruit. In addition, most odour-active volatiles concentration increased from the top to the bottom 3rd of the fruit (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010). Clear qualitative variation in the aroma profile of the pulp and core of Smooth Cayenne pineapples was reported. In pulp, the characteristic aroma compounds were ethyl 2-methylbutanoate, ethyl hexanoate, 2,5-dimethyl-4-hydroxy-3(2H)-furanone (DMHF), decanal, ethyl 3-(methylthio) propionate, ethyl butanoate, and ethyl (E)-3-hexenoate; while in core the main compounds were ethyl 2-methylbutanoate, ethyl hexanoate and DMHF (Wei, Liu, Liu, Lv, et al., 2011).

2.5.4 Fruit maturity and harvest

Volatile profile of differently ripened pineapples were significantly different (Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Steingass, Langen, et al., 2015; Umano et al., 1992), confirming the effect of fruit ripeness on pineapple aroma. Contents of gamma-C6 lactones increased during post-harvest storage, reaching the highest values in MD2 pineapples harvested at full maturity, whereas the enantiomeric purity of gamma-C6 lactones significantly decreased during post-harvest maturation of green-ripe fruits (Steingass, Langen, et al., 2015). In green pineapples, the major volatile constituents were ethyl acetate (25%), ethyl 3-(methylthio) propanoate (10 %), and ethyl 3-acetoxyhexanoate (8.7 %). In ripened pineapples, ethyl

acetate (34%), threo-butane-2,3-diol diacetate (13%), and 3-hydroxy-2-butanone (8.7 %) were the major constituents. Concentrations of hydroxy and acetoxy acid esters increased during ripening was observed in pineapple varieties from the Philippines (Umano et al., 1992). Fully ripe MD2 pineapple fruits were characterised by volatiles, such as delta-octalactone, gamma-lactones, 1-(E,Z)-3,5-undecatriene and 1,3,5,8-undecatetraene, as well as various methyl esters. In contrast, post-harvest storage of green-ripe sea-freighted fruits resulted in an increased formation of ethyl esters, acetates, acetoxy esters and alcohol (Steingass et al., 2014). Volatiles derived from fermentative metabolism, such as alcohols and ethyl esters, were found in post-harvest stages of green ripe MD2 pineapple fruits (Steingass, Carle, et al., 2015). Fully ripe air-freighted MD2 pineapples were characterised by elevated concentrations of two 1,3,5,8-undecatetraene isomers, methyl 3-methylbutanoate and 4-methoxy-2,5-dimethyl-3(2H)-furanone, which have been reported as potent contributors to the pineapple flavour. Compared to fully ripened fruits, the development of volatiles of sea-freighted pineapples upon arrival in Europe was rudimentary. Postharvest storage of sea-freighted pineapples resulted in a different volatile profile due to the genesis of hydroxylated and acetoxylated methyl esters and hexanal (Steingass et al., 2016). 'Shenwan' (*syn.* Queen) pineapple fruits ripened in different seasons (spring, summer, autumn, and winter) cause significant diversity in the qualitative and quantitative volatile profile. Ten kinds of aroma components were detected in spring fruits, including four unique components. The predominant compounds were hexanoic acid methyl ester, 1,3,7-octatriene-3,7-dimethyl and octanoic acid methyl ester with relative content of 39, 26 and 10%, respectively. Nineteen kinds of aroma components were detected in summer fruits, including ten unique components. The predominant ones were butanoic acid 2-methyl-methylester, hexanoic acid methyl ester, and 2-hydroxy-N-(2-morpholinoethyl)-4-phenylbutanamide with relative content of 25, 25 and 9.6%. The eleven predominant key aroma compounds detected in autumn fruits contained hexanoic acid methyl ester, butanoic acid 2-methylmethyl ester and butyric acid methyl ester, with relative content of 58, 19 and 8.8%. Twelve kinds of aroma components were detected in winter fruits, including hexanoic acid methyl ester, octanoic acid methyl ester and cis-ocimene with relative content of 63.1, 15.8 and 7.8%. The relative contents of methyl 3-(methylthio)-propanoate in the four corresponding fruits were 0.89, 4.1, 0.45 and 1%, respectively (Liu et al., 2011).

2.5.5 Analysis

Pineapple aroma is a mixture of several classes of molecules which makes the analysis of aroma composition challenging (Lukás et al., 2013). From the literature reviewed, the four main steps of VOCs analysis were: (i) isolation and concentration; (ii) separation; (iii) identification; and (iv) sensory characterization. Homogenisation and mixing with inorganic salts (mainly sodium chloride)

were commonly employed to suppress enzyme activity but, this can affect the VOCs patterns and the analogy to sensory quality in consumption. One of the methods for VOCs isolation was liquid−liquid extraction (LLE) producing the best results with regard to quality (number of extracted VOCs) and quantity (high recovery rates). However, high workload, the lack of automation, and the extraction of non-volatile compounds are some common disadvantages of LLE. Since introduction of solid phase microextraction (SPME), this technique has been widely used in the VOCs analysis of pineapples. 28 out of the 58 evaluated studies herein used SPME for VOCs isolation. However, one of the main disadvantages of the SPME, is the strong discrimination effect of individual VOCs and classes of VOCs towards SPME matrices, which leads to insufficient extraction. A comparison of isolation techniques was published for pineapple (Akioka & Umano, 2008; Lukás et al., 2013; Pino, 2013; Teai et al., 2001; Wei et al., 2014). Application of stable isotope dilution assay (SIDA) is one way of minimising the challenges associated with SPME based analysis. Coupling GC and MS is the method of choice for VOCs analysis and the identification techniques utilised in the analysis provide different confidence levels to the results. The highest level is only possible by coelution of isotope-labelled references (SIDA) or by the standard addition method. Of the published literature considered here, only few reports (Tokitomo et al., 2005) achieved these conditions and the remaining reports may share semiquantitative data.

2.5.6 Artifacts

Artifacts are undesirable attribute of a sample or process under examination, that can mislead the results. In GC-MS analysis of pineapple VOCs, artifacts can be originated from the sample packaging, and from the analytical instrument. Some of the possible compounds that may not arise from pineapple samples are ethanol and acetone. Thermal reactions in the instrument (GC injector) are known to cause decomposition of furanones at temperatures above 160°C, and may decompose to a variety of small molecules, including acetone and other ketones, as well as alkyl furanones. MS detectors with lower stability than GC conventional detectors (e.g., FID) were known to cause divergent results. An example of the MS fragmentation reporting inconsistency is reported for ethyl 3-hydroxybutanoate (Lukás et al., 2013). Several compounds have been described as migrating compounds originating from the environment. For instance, p-xylene, cyclohexyl acetate, or 2-ethylhexanoic acid may originate from packaging material, crates, and cardboard boxes being commercially used for storage of the fruits (Lukás et al., 2013; Steingass, Carle, et al., 2015).

Table 2.3 on page 25 summarises sample details, extraction conditions, analytical methods, and VOCs identification / quantitation criteria, that could potentially influence the VOCs analysis.

Table 2.3 Sample details, extraction conditions, analytical methods, and other criteria that could influence the VOCs identification and quantitation

Reference	Material** and source	Storage	Homoge-nisation	Sample size	VOCs extraction; STD; SIDA; method	GC separation	Criteria Identification -Quantitation
(Haagen-Smit et al., 1945)	Smooth Cayenne; Hawaii	Fresh	yes	1 fruit	FD; NA; NA; NA	NA	Physico-Chemical
(Connell, 1964)	NA; Yeppoon, North Coast, Brisbane	Fresh juice	yes	475 gallons juice	FD - LLE; NA; NA; NA	Packed Column, 2m, Dl-2-eithylhexyl sebacate	RT, Physico-Chemical
(Rodin et al., 1965)	Smooth Cayenne; Hawaii	Fresh	yes, NaCl	5 batches of 50 fruit	LLE; NA; NA; NA	G.E. SF96,20% on firebrick, 6 ft x 1/4 in	MS, IR, NMR and UV
(Silverstein et al., 1965)	Smooth Cayenne; Hawaii	Fresh	yes, NaCl	Concentrat e from 250 pineapples	LLE; NA; NA; NA	G.E. SF 96 silicone, 2076 on firebrick, 6 ft X g i1/4	MS, IR, NMR and UV
(Rodin et al., 1966)	Smooth Cayenne; Hawaii	NA	NA	Concentrat e from 250 pineapples	NA	LAC 446 column, Chromosorb W 30/60-mesh, 12 ft X 5 mm ID; Carbowax 20 M, Chromosorb W, 60/80, 5 ft X 2 mm ID	MS, IR, NMR and UV
(Flath & Forrey, 1970)	Smooth Cayenne; Hawaii	Essence	yes, NaCl	9 litres juice	LLE; Yes; NA; GC-MS	Stainless steel open-tubular columns (500-foot X 0.02-inch I.D., 500-foot X 0.03-inch I.D., 1000-foot X 0.03-inch I.D)	external standards, RT
(Berger et al., 1985)	NA; from Ivory Coast	NA	NA	NA	extracted sample; yes; NA; GC-MS	SE-54 fused silica capillary, 30 m X 0.32 mm	sniffing, RT, MS, external & internal standards
(Takeoka et al., 1989)	Smooth Cayenne: green and ripened air freighted from Hawaii	Fresh, air freight	Yes, $CaCl_2$	NA	extracted sample; yes; NA; GC-MS	DB-WAX, 60 m X 0.32 mm	RI, MS, external & internal standards
(Wu et al., 1991)	NA; Fresh pineapples grown in Costa Rica	Fresh from market	yes	NA	extracted sample; yes; NA; GC-MS	fused silica capillary, 50M X 0.32 mm	RI, MS, external & internal standards
(Takeoka et al., 1991)	NA; Fresh Hawaiian pineapple extract	Fresh from market	NA	NA	extracted sample; yes; NA; GC-MS	DB-WAX, 60 m X 0.32 mm	RI, MS, external & internal standards
(Umano et al., 1992)	NA; imported from the Philippines	Stored	yes	NA	extracted sample; yes; NA; GC-MS	DB-Wax, 30 m X 0.25 mm	RI, MS, external standards, odour description
(Spanier et al., 1998)	Fresh cut chunks of Chempaka (Smooth Cayenne) variety grown in Central America	Fresh	yes	NA	extracted sample; NA; NA; GC-MS	SPB5 capillary, 60m x 0.75mm	FID, RI,MS, GC-O, no reference standards
(Teai et al., 2001)	NA: grown in French Polynesia, bought from market	Stored/marke t	yes	NA	extracted sample; NA; NA; GC-MS	HP-1, 50m x 0.32mm x 0.52µm; HP-CW20M, 50m x 0.2mm x0.2µm	FID, RI, MS, external & internal standards

Reference	Material** and source	Storage	Homoge-nisation	Sample size	VOCs extraction; STD; SIDA; method	GC separation	Criteria Identification -Quantitation
(Preston et al., 2003)	NA; from Costa Rica, Ghana, Honduras, Ivory coast, La Reunion, South Africa, and Thailand	NA	yes	13	extracted sample; yes; NA; HRGC-MS; HRGC-IRMS	DB-Wax, 30 m × 0.25 mm, 0.25 µm	RI, MS, IRMS external standards
(Brat et al., 2004)	new variety FLHORAN41 and Smooth Cayenne; grown in French West Indies	Fresh	yes	5	extracted sample; yes; NA; GC-MS	DB wax, 30 m × 0.25 mm, 0.25 µm	RI, MS, external standards
(Lamikanra & Richard, 2004)	Delmonte MD2; market	Stored/market	NA	NA	HS-SPME; single ISTD; NA; GC-MS	HP-5MS, 30m× 0.25mm, 0.25µm	RI, MS, external standards
(Elss et al., 2005)	Various cultivars; from Costa Rica, Ghana, Honduras, Ivory coast, La Reunion, South Africa and Thailand	Stored	yes	19	extracted sample; yes; NA; HRGC-MS	DB-Wax, 30m x0.25mm, 0.25 µm	RI, MS, external standards
(Tokitomo et al., 2005)	Super Sweet (F-2000) (MD2); from market in Germany	NA	yes	NA	SAFE; yes; yes; GC-MS; GC-O	CP-WAX58, 25m x 0.32mm, 0.2 µm and DB-5, 30mx 0.32mm, 0.25 µm	RI, MS, external & matching internal standards, AEDA, sniffing, GC-O, OAV
(Akioka & Umano, 2008)	NA; from Philippines, purchased from market	Stored/market	NA	NA	extracted sample; yes; NA; GC-MS, GC-O	DB-Wax, 60 m x 0.25 mm, 0.25 µm	RI, MS, GC-O, FD, external standards
(Braga et al., 2009)	Smooth Cayenne; market	NA	yes, with dry ice	NA	HS-SPME; NA; NA; GC-MS	HP-5MS, 30m x 0.25 mm, 0.25 µm	RI, MS
(Braga et al., 2010)	Smooth Cayenne; market	NA	yes, with dry ice	NA		HP-5MS, 30m x 0.25 mm, 0.25 µm	RI, MS
(M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010)	Gold cultivar: imported from Costa Rica, bought from market in Lleida	Stored/market	yes	NA	HS-SPME; yes; NA; GC-MS	Equity 5, 30 m x 0.25 mm, 0.25 µm	RI, MS, external & internal standards
(M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010)	Gold cultivar: imported from Cost Rica, bought from market in Lleida	Stored	yes	10	HS-SPME; yes; NA; GC-MS	Equity 5, 30 m x 0.25 mm, 0.25 µm	RI, MS, external & internal standards
(Liu et al., 2011)	Shenwan pineapples; China	Fresh	yes	3	HS-SPME; NA; NA; GC-MS	HP-1, 30 m x 0.25 mm, 0.1µm	MS
(Pedroso et al., 2011)	Fresh pineapple (NA); Hawaii, and Dehydrated pineapple chips; Brazil	Stored/markets	yes	NA	HS-SPME; single ISTD; NA; GCxGC-FID; GCxGC-MS	GCxGC diff columns	RI, MS
(Wei, Liu, Liu, Lv, et al., 2011)	Smooth Cayenne; China	Fresh	yes	NA	HS-SPME; NA; NA; GC-MS	HP-5MS, 30 m × 0.25 mm, 0.25 µm	MS, internal standard, no external standards

Reference	Material** and source	Storage	Homoge-nisation	Sample size	VOCs extraction; STD; SIDA; method	GC separation	Criteria Identification -Quantitation
(Wei, Liu, Liu, Zang, et al., 2011)	Tainung 17; China	Fresh, stored	yes, NaCl	NA	HS-SPME; NA; NA; GC-MS	HP-5MS, 30 m × 0.25 mm, 0.25 µm	MS
(Zheng et al., 2012)	Tainung No. 4 and No. 6; China	Fresh	yes	NA	HS-SPME; Yes; NA; GC-MS	HP-5MS, 30 m × 0.25 mm, 0.25 µm	RI, MS, external & internal standards
(Kaewtathip & Charoenrein, 2012)	Smooth Cayenne; Thailand	Stored	yes	3	HS-SPME; yes; NA; GC-MS	HP-5MS, 60 m × 0.25 mm, 0.25 µm	RI, MS, external & internal standards
(Zhang et al., 2012)	MD2 (Golden Ripe); USA	Fresh, market (stored)	NA	NA	HS-SPME; NA; NA; GC-MS	SPB-5, 60 m × 0.25 mm, 0.25 µm	MS, internal standard, no external standards
(Lukás et al., 2013)	MD 2; market	Stored	yes	NA	extracted sample; NA; NA; GC-MS	HP-5MS, 30 m × 0.25 mm, 0.25 µm; Ultra 1, 50 m × 0.32 mm, 0.52 µm; and polar DB-FFAP, 30 m × 0.25 mm, 0.25 µm	RI, MS, external & internal standards
(Pino, 2013)	Red Spanish; Cuba	Fresh	yes	NA	HS-SPME; single ISTD; NA; GC-MS	HP-5MS, 30 m × 0.25 mm, 0.25 µm	RI, MS, external & internal standards
(Liu & Liu, 2014)	NA; China	Fresh	NA	NA	HS-SPME; NA; NA; GC-MS, GC-FID	NA	MS
(Steingass et al., 2014)	MD2 (Extra Sweet); from Ghana, sourced from market in Germany	Fresh, FR and GR, stored	yes	single fruit samples	HS-SPME; single ISTD; NA; GC-MS	DB wax and HP 5MS ,30M x 0.25 mm, 0.25 µm	RI, MS, internal standards, no external standards
(Wei et al., 2014)	Shenwan; China	NA	yes	NA	HS-SPME; single ISTD; NA; GC-MS	HP-5MS ,30M x 0.325 mm, 0.25 µm	RI, MS
(Steingass, Jutzi, et al., 2015)	MD2 (Extra Sweet); from Ghana, air-freighted	Fresh,FR and GR, stored	yes	NA	HS-SPME; NA; NA; GCxGC-MS	ZB wax, 30 m × 0.25 mm, 0.5 µm; BPX5 2m × 0.15mm, 0.25 µm	RI, MS
(Steingass, Langen, et al., 2015)	MD2 (Extra Sweet); from Ghana, sourced from market in Germany	Fresh,FR and GR, stored	yes	NA	HS-SPME; yes; SIDA; GC-MS	5MS ,30M x 0.25 mm, 0.25 µm (coated with 50% 6-TBDMS-2,3-diacetyl-b-CD)	RI, MS, internal standards
(Steingass, Carle, et al., 2015)	MD2 (Extra Sweet); from Ghana, sourced from market in Germany	Fresh,FR and GR, stored	yes	NA	HS-SPME; single ISTD; NA; GC-MS	ZB wax, 30 m × 0.25 mm, 0.5 µm; BPX5 2m × 0.15mm, 0.25 µm	MS
(Steingass et al., 2016)	MD2 (Extra Sweet); from Ghana, sourced from market in Germany	Fresh,FR and GR, stored	yes	3	HS-SPME; single ISTD; NA; GC-MS	DB wax ,30M x 0.25 mm, 0.25 µm	MS

Reference	Material** and source	Storage	Homoge-nisation	Sample size	VOCs extraction; STD; SIDA; method	GC separation	Criteria Identification -Quantitation
(Sun et al., 2016)	Smooth Cayenne, Queens-land Cayenne, New Phuket, Shen-wan, Tainung17, Tainung19; China	NA	NA	NA	HS-SPME; NA; NA; GC-MS	NA	NA
(Turazzi et al., 2017)	NA; market in Brazil	Stored/marke t	yes	NA	HS-SPME; NA; NA; GC-MS	5MS ,30M x 0.25 mm, 0.25 µm	RI, MS
(Lasekan & Hussein, 2018)	Moris, Maspine, MD2, N36, Josapine and Sarawak; Malaysia	Fresh	yes	3	HS-SPME; yes; NA; GC-MS, GC-O	TG-5MS ,30M x 0.25 mm, 0.25 µm	RI, MS, GC-O, AEDA, external standards
(Orellana-Palma et al., 2020)	Golden Sweet; Chile	Stored	yes, fresh juice	NA	HS-SPME; NA; NA; GC-FID	DB-624, 60m x 0.25 mm, 1.8 µm	RI, external standards
(Steingass et al., 2021)	MD2 (Extra Sweet); from Ghana	Fresh,FR and GR, stored	yes	NA	HS-SPME; single ISTD; NA; GC-MS	DB wax, 30M x 0.25 mm, 0.25 µm	RI, MS, internal standards
(Vollmer et al., 2021)	MD2; from Ghana, air freighted, sourced from market in Germany	Stored	yes, juice	NA	HS-SPME; yes; NA; GC-MS	DB wax, 30M x 0.25 mm, 0.25 µm HP-5MS, 60 m × 0.25 mm, 0.25 µm	RI, MS, internal standards
(Zainuddin et al., 2021)	Josephine, Morris, Sarawak, MD2; local market, Malaysia	Fresh	yes	NA	HS-SPME; NA; NA; GC-MS	HP-5MS, 30M x 0.325 mm, 0.25 µm	RI, MS, external standards
(Xiao et al., 2021)	Jinzuan, Niunai and Xiangshui; China	Stored	yes, juice	NA	HS-SPME; yes; NA; GC-MS, GC-O	DB wax and DB 5 (60 m × 0.25 mm, 0.25 µm)	RI, MS, external standards, internal standards
(Asikin et al., 2022)	N67-10, Yugafu, and Yonekura; Okinawan pineapples, Japan	fresh	Yes, juice	NA	HS-SPME, yes, NA; GC-FID, GC-MS	DB wax, 60 m × 0.25 mm x 0.25 µm	RI, MS, external standards, internal standard

*** Shenwan and Morris are 'the variety 'Queen'. Gold is MD2. Sarawak is Smooth Cayenne. Tainung 4 and Tainung 6 are a Queen x Smooth Cayenne cross. Josapine is a Ruby x Queen cross. Maspine is 73-50. NA – information not available.*

2.6 Research gap and conclusions

In conclusion, pineapple VOCs have been extensively studied over several decades by many researchers. The published manuscripts available to date include works focusing on different pineapple varieties, from different geographical locations, the effect of sampling, different extraction and isolation techniques, the effect of harvest, storage and logistics, and the interaction of VOCs. Though several studies have reported the VOCs profile and key characteristic aroma compounds in pineapple, only a few studies met the guidelines specified by Molyneux, R.J. and P. Schieberle, 2007. It is important to consider the details of sampling, extraction conditions, analytical methods employed, and the VOCs identification/quantitation criteria, while referring to the data tables provided in this review (**Table 2.2** on page 13 and Appendix 1, **Table A1**). A high level of confidence in VOCs identification and quantitation exists only when the criteria (calculation of RI using GC columns of different polarities, MS fragmentation pattern, co-elution with reference materials, use of external and internal reference standard materials, and additional confirmation using GC-O) meet the guidelines. MS fragmentation pattern facilitates the tentative identification of VOCs when additionally considering the RI. However, reported MS fragmentation data are not included in this review due to the lack of sufficient published data. The authors of this review do not exclude the possibility of VOCs that are reported but not covered in this review due to the lack of access to data. Inconsistencies in reporting VOCs from several sources, including the differences in varieties, environment, logistics, storage, and analytical methods, including artifacts, demand the need for a reliable database. This review provides a detailed overview of pineapple VOCs and identifies the key aroma compounds that play a vital role in the characteristic aroma of pineapple. The subset of key pineapple aroma volatiles identified herein can be targeted in analytical method development and utilised in varietal improvements.

2.7 Publications relevant to the analysis of pineapple VOCs after publishing the literature review

To ensure the relevance and currency of this thesis, an appendix to the literature review is incorporated as Appendix 1, **Table A3**, which summarises the relevant scientific publications released after the initial review phase. This update involved a targeted search using databases focusing on literature published from February 2023 to May 2025. The newly identified studies have been integrated, highlighting recent advancements relevant to the research topic. This effort ensures that the thesis reflects the most up-to-date understanding of the field.

Chapter 3 Stable Isotope Dilution Assay and HS-SPME-GC-MS Quantification of Key Aroma Volatiles of Australian Pineapple (*Ananas comosus* var. *comosus*) Cultivars

Pineapple (*Ananas comosus* var. *comosus*), renowned for its sweet and tropical flavour, is one of the most widely consumed non-climacteric fruits globally and ranks as the third most important tropical fruit in world production (*FAO. 2023. Major Tropical Fruits Market Review – Preliminary results 2022. Rome.*, 2023; *FAO. 2024. Major Tropical Fruits Market Review – Preliminary results 2023. Rome.*, 2024). In Australia, nearly all pineapple cultivation occurs in Queensland, where favourable climatic conditions support the growth of several commercial cultivars. Among the sensory attributes that influence consumer purchasing decisions, aroma stands out as a critical quality trait. The unique aroma of pineapple arises from a complex mixture of volatile organic compounds (VOCs), including esters, terpenes, alcohols, aldehydes, and ketones, which contribute to its fruity, floral, coconut-like, and caramel-like notes.

Drawing from the key findings presented in Chapter 2, the literature review, this chapter proceeds to report the development and application of a high-throughput analytical method for the accurate quantification of key aroma VOCs in Australian-grown pineapple cultivars. The method integrates matrix-matched stable isotope dilution analysis (SIDA) with headspace solid-phase microextraction (HS-SPME) and gas chromatography-mass spectrometry (GC-MS), enabling simultaneous measurement of 26 targeted VOCs in a single analysis. Deuterium-labelled analogues of the analytes were used as internal standards, and the validated method achieved high determination coefficients (R^2 ranging from 0.9772 to 0.9999), ensuring precision and reliability. The method was applied to five popular cultivars: ‘Aus Carnival’, ‘Aus Festival’, ‘Aus Jubilee’, ‘Aus Smooth (Smooth Cayenne)’, and ‘Aussie Gold (73-50)’, revealing significant variation in VOC content and composition among them. Esters were the predominant class of volatiles, followed by terpenes, alcohols, aldehydes, and ketones. This approach addresses limitations of previous VOC isolation techniques and offers improved accuracy by mitigating matrix effects and extraction biases commonly associated with SPME.

This method development is the first application of matrix-matched SIDA combined with HS-SPME-GC-MS for quantitative analysis of key aroma volatiles in Australian pineapple cultivars. The method provides a valuable tool for breeding programs aiming to link aroma traits to fruit genetics and enhance consumer appeal through improved flavour quality. This chapter was published as ‘Stable isotope dilution assay and HS-SPME-GC-MS quantification of key aroma volatiles of Australian pineapple (*Ananas comosus*) cultivars’ in *Food Chemistry* (George et al., 2024).

Author contributions for this chapter are summarised in **Table 3.1** below.

Table 3.1 Author contributions in Chapter 3

	Jenson George	Garth Sanewski	Thoa Nguyen	Craig Hardner	Heather E. Smyth
Conceptualization	x				x
Methodology	x				x
Software	x		x		x
Validation	x				
Formal analysis	x				
Investigation	x		x		x
Resources	x	x	x		x
Data curation	x	x			x
Writing - original draft	x				
Writing - review & editing	x	x	x	x	x
Visualization	x	x	x	x	x
Supervision		x	x	x	x

3.1 Introduction

Pineapple (*Ananas comosus*), with its unique sweet flavour, is one of the most popular tropical, non-climacteric fruits consumed worldwide. It is also the third most important tropical fruit in world production (*FAO. 2023. Major Tropical Fruits Market Review – Preliminary results 2022. Rome.*, 2023). In Australia, 99% of the pineapple production is from the state of Queensland (*Australian Horticulture Statistics Handbook 2021/22*, 2022) due to the favourable climatic conditions (Liu & Liu, 2014; Garth M. Sanewski et al., 2018). Though plentiful pineapple varieties are grown worldwide, only a few of the leading types are sold commercially. The molecular basis of pineapple aroma has been studied for over 70 years, as this knowledge is a major advantage in developing superior fruit varieties with high consumer appeal (George et al., 2023). The flavourful fruit is known to contain a large number of volatile compounds at varying concentrations. Volatile-aroma compounds greatly contribute to the flavour quality of pineapple fruit by providing distinct sensory properties that are sweet, fruity, tropical, pineapple-like, caramel-like, coconut-like, etc. (George et al., 2023; Lukás et al., 2013; Siti Rashima et al., 2021; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021). They are mostly highly odorous volatile substances that are derived from the free aglycone molecules of esters, alcohols, aldehydes, terpenes, and lactones (Pino, 2013; Tokitomo et al., 2005; Zheng et al., 2012).

Although nearly 480 volatile organic compounds (VOCs) have been identified to date using different analytical techniques, only 40 compounds (key aroma compounds) are reported to contribute to the unique flavour of pineapple (Brat et al., 2004; Elss et al., 2005; George et al., 2023; Kaewtathip &

Charoenrein, 2012; Steingass, Jutzi, et al., 2015; Tokitomo et al., 2005; Umano et al., 1992; Wei, Liu, Liu, Lv, et al., 2011). The aroma of pineapple is one of the important factors attracting consumers and strengthening the marketplace (Lukás et al., 2013; Steingass et al., 2016; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021), and hence their accurate quantification is an important task.

A comparison of volatile isolation techniques was published for pineapple (Akioka & Umano, 2008; Lukás et al., 2013; Pino, 2013; Teai et al., 2001; Wei et al., 2014). Since the introduction of solid phase microextraction (SPME), this technique has been widely used in the VOCs analysis of pineapples. The majority (28 out of the 58) of the evaluated studies by George et al., 2023 (George et al., 2023) identified the use of SPME for VOCs isolation. However, one of the main disadvantages of the SPME is the strong discrimination effect of individual VOCs and classes of VOCs toward SPME fibers, which leads to insufficient extraction (Turazzi et al., 2017). Along with the matrix effects (i.e., the changes in mass spectrometric signal due to the presence of matrix compounds) and other potential sources of variation (e.g. ionic strength) can considerably impact the quantification of results, particularly their accuracy and precision (Pico et al., 2022; Yuan et al., 2013). Application of stable isotope dilution analysis (SIDA) is one way of minimising the challenges associated with SPME-based analysis, and stable isotopes of deuterium-labelled standards are commonly applied as they are readily accessible and relatively inexpensive as compared to 13C-labelled standards. SIDA provides an alternative approach to reduce variability related to sample preparation and matrix effects and to improve the recovery of the analytes (Maraval et al., 2010). Coupling gas chromatography (GC) and mass spectrometry (MS) is the method of choice for VOCs analysis, and the identification techniques utilised in the analysis provide different confidence levels to the results (George et al., 2023). The highest level is only possible by coelution of isotope-labelled references (SIDA) or by the standard addition method (Molyneux & Schieberle, 2007), and the combined analytical method of SIDA and headspace (HS) solid-phase microextraction (SPME) coupled with GC-MS [HS-SPME-GC-MS] is considered more accurate (Siebert et al., 2005) (Butkhup et al., 2011; San et al., 2017; Sanchezpalomo et al., 2005).

Therefore, the objective of this study was to develop a high-throughput method to evaluate the VOCs in different cultivars of Australian pineapples. The method incorporated matrix-matched, stable isotope diluted analysis (SIDA) - headspace (HS) - solid-phase microextraction (SPME) - gas chromatography-mass spectrometry (GC-MS). The developed method was validated and applied to measure the key aroma compounds, accurately and precisely, in selected Australian pineapple cultivars, namely 'Aus Carnival', 'Aus Festival', 'Aus Jubilee', 'Aus Smooth (Smooth Cayenne)', and 'Aussie Gold (73-50)'. The method enabled simultaneous measurement of a greater number of key

aroma compounds in one step, with a higher level of accuracy and precision in measurements compared to existing methods for pineapple, and has the potential for high throughput, thereby meeting the need for concentration data to better explore sensory contributions based on comparison to respective odour threshold information. To the best of our knowledge, the combination of matrix-matched, SIDA and HS-SPME-GC-MS has been applied for the first time for quantitative analysis of key aroma volatiles in Australian-grown pineapple cultivars. The method could contribute significantly to pursuing the accurate measurement of key aroma compounds of commercial pineapple varieties and their parent lines, thereby providing valuable insights in breeding programs seeking to link volatiles to fruit genetics.

3.2 Materials and methods

3.2.1 Chemicals, reagents, and standards

Neat reference standards of the aroma compounds listed in **Table 3.2** on page 34 (based on the 40 key aroma compounds identified in Chapter 2 (George et al., 2023)), and hyper grade for LC-MS LiChrosolv isopropanol were obtained commercially from Merck (Sigma Aldrich), New South Wales, Australia. The labelled internal standards, ethyl 2-methylbutyrate-d9 (D-7676), ethyl hexanoate-d11 (D-7060), octanal-d16 (D-6929), ethyl octanoate-d15 (D-7063) were obtained commercially from CDN isotopes, Quebec, Canada, through PM Separations Pty Ltd, Queensland, Australia.

3.2.2 Fruit material

Ripe fruit (n = 3) of five Australian commercial pineapples cultivars, 'Aus Carnival', 'Aus Festival', 'Aus Jubilee', 'Aus Smooth (Smooth Cayenne)' and 'Aussie Gold (73-50)', used for method validation were sourced from Brisbane Markets Ltd, Queensland, Australia in Jan 2023. The fruit were stored at 5°C for 24 hours and then quickly cut to remove the skin, top and bottom 1/3^{rd,} and the core. After that, the fruit pulp (edible fruit) was cut into small pieces (cubes) and milled in a ‘Retsch MM500 vario’ ball mill, to obtain homogeneous puree samples. The whole process was done in ice-cold conditions to minimise the loss of volatiles, and the resulting puree was immediately weighed into the headspace vials. The resulting vials were stored at -20°C prior to GC-MS-HS-SPME-SIDA analysis.

3.2.3 Preparation of matching matrix

It was necessary to develop a deodorised pineapple-based substrate as a ‘matched matrix’ in which to prepare the standard addition samples for optimal calibration of the SIDA method. The matched matrix was prepared by combining equal amounts of pineapple puree from several fruit samples (from another study within our laboratory, covering the genetic diversity of the pineapple fruit grown in

Queensland Australia). The moisture content of the combined puree was measured as 81.62 % (SD+/- 0.04) and the puree was freeze-dried. The resulting freeze-dried powder was further dried at 30 °C under continuous vacuum for 48 hours to get dried pineapple powder with a moisture content of 3.32 % (SD +/- 0.03). pH of the pineapple fruit samples was in the range of 3.88-4.97, with an average of 4.47 and a median of 4.53. Therefore, pH 4.5 was chosen as the target pH to prepare a suitable buffer. Sodium citrate buffer was chosen due to the high levels of citric acid in the fruit. Sodium citrate buffer (0.01 M, pH 4.5) was prepared as follows. To 800 mL Milli-Q water was added 1.3618 g sodium citrate and 0.9884 g citric acid were added and stirred to dissolve. pH of the resulting solution was recorded as 4.51 at 22 °C. The solution was then volumetrically made up to 1 L using Milli-Q water. The dried pineapple powder was reconstituted in the citrate buffer to get the pineapple matching matrix, with a pH of 4.51 and 81.6% moisture, which is used in the preparation of standard calibration solutions under section 3.2.4.

Table 3.2 Analysis parameters for the determination of twenty-six targeted aroma volatiles.

Sl. No	t_R[†]	Volatile compound	CAS No.	*Int. Std. group*	% Matrix effect	Target ion m/z	Qualifier ions m/z (%)[‡]
1	2.577	methyl isobutyrate	547-63-7	*i*	-13.5	43	71 (41), 59 (23)
2	2.923	ethyl propionate	105-37-3	*i*	-18.2	57	102 (11), 75 (10), 74 (10)
3	3.093	methyl butyrate	623-42-7	*i*	-22.3	43	74 (75), 71 (55), 59 (25)
4	3.313	3-methyl-1-butanol	123-51-3	*i*	-10.0	55	70 (70), 57 (30), 42 (80)
5	3.733	ethyl isobutyrate	97-62-1	*i*	-11.4	43	71 (43), 116 (14), 88 (9), 45 (9)
6	4.030	isobutyl acetate	110-19-0	*i*	-16.3	43	56 (45), 73 (32)
7	4.070	methyl 2-methylbutyrate	868-57-5	*i*	-13.4	57	88 (95), 85 (30), 101 (23)
8	4.107	methyl isovalerate	556-24-1	*i*	-17.6	74	85 (30), 57 (26), 41 (24)
9	4.630	ethyl butyrate	105-54-4	*i*	-35.2	43	71 (96), 88 (55)
i	*5.710*	*ethyl 2-methylbutyrate-d9*				*66*	*107 (35), 46 (50)*
10	5.863	ethyl 2-methylbutyrate	7452-79-1	*i*	-31.0	57	102 (63), 85 (35), 41 (40)
11	6.517	2-methylbutyl acetate	624-41-9	*i*	-46.1	43	70 (34), 55 (12), 73 (15)
12	7.177	methyl hexanoate	106-70-7	*ii*	-75.8	74	87 (40), 43 (35), 99 (25),
ii	*8.047*	*ethyl hexanoate-d11*				*91*	*110 (40), 50 (80)*
iii	*8.090*	*octanal-d16*				*48*	*50 (105), 62 (70), 91 (25), 110 (10)*
13	8.147	ethyl hexanoate	123-66-0	*ii*	-69.6	88	99 (50), 60 (45), 43 (85)
14	8.213	octanal	124-13-0	*iii*	_	43	56 (65), 57 (50), 84 (50), 68 (30)
15	8.233	ethyl trans-3-hexenoate	2396-83-0	*ii*	-73.0	69	142 (10), 68 (25), 88 (10)
16	8.467	methyl 3-(methylthio)propionate	13532-18-8	*i*	-14.7	74	61 (69), 134 (105), 103 (30)
17	8.577	D limonene	5989-27-5	*i*	2.7	68	67 (44), 93 (60)
18	8.747	phenylacetaldehyde	122-78-1	*iii*	_	91	120 (30), 92 (30), 65 (20)
19	8.890	2,5-dimethyl-4-methoxy-3(2H)-furanone	4077-47-8	*i*	-99.9	142	55 (15), 69 (10), 99 (8)
20	9.447	ethyl 3-(methylthio)propionate	13327-56-5	*i*	-30.2	74	61 (87), 148 (65), 103 (25)
21	9.767	methyl octanoate	111-11-5	*iv*	-59.6	74	87 (42), 55 (18), 43 (23)
iv	*10.603*	*ethyl octanoate-d15*				*91*	*105 (32), 142 (28), 121 (5)*
22	10.760	ethyl octanoate	106-32-1	*iv*	-25.3	88	57 (28), 101 (35), 73 (20)
23	10.827	α-terpineol	98-55-5	*i*	-24.6	59	93 (50), 121 (31), 43 (40)
24	10.927	decanal	112-31-2	*iii*	_	57	55 (60), 70 (47), 68 (34)
25	13.543	damascenone	23696-85-7	*i*	_	69	121 (60), 41 (20), 105 (16)
26	13.693	ethyl decanoate	110-38-3	*iv*	7.5	88	101 (41), 60 (15), 61 (15)

[†] Retention time. [‡] This % represents the associated ions relative % to the target ion shown in the previous column, not necessarily the base peak. *i, ii, iii,* and *iv* are the internal standard groups.

3.2.4 Preparation of standards and samples for analysis

A standard stock solution containing the twenty-six volatile compounds from **Table 3.2** on page 34 was prepared by accurately weighing about 5-10 mg of individual standards into a 20 mL amber volumetric flask. Contents were dissolved and made up to the mark using isopropyl alcohol (IPA) and/or in MilliQ-water (pre-cooled on ice slurry). Working Standards were prepared by diluting the stock solution using 1:1 (v/v) IPA- Milli Q water followed by Milli-Q water alone. The pineapple puree (*x* g in case of samples) or mixed reference standard solution (*x* mL), mixed internal standard solution (50 µL), 500 µL MQ-water or 500 µL matching matrix solution, and saturated NaCl solution ((4.45-*x*) mL) were placed into a 20 mL GC head space-SPME vial (Supelco, Australia) and sealed the vial with a screw cap.

Diluted solutions of the individual reference standards and labelled internal reference standards (prepared separately in IPA and/or in MilliQ-water and/or in combination) were separately injected under the same analytical conditions reported in the manuscript under section 3.2.5. and recorded their individual retention times. The NIST2014 database library was used as an additional identification tool by matching the mass spectra of the individual compounds.

3.2.5 Headspace sampling and instrumental analysis conditions

In this paper, GC-MS-HS-SPME-SIDA analysis is employed to accurately quantify the targeted key aroma compounds (**Table 3.2** on page 34). The volatile components were extracted using an SPME fiber (Supelco: 50/30µm DVB/CAR/PDMS, Stableflex, 23Ga, Gray), based on previous studies of the SPME fibers in pineapple fruit matrix (Turazzi et al., 2017), and analysed using Shimadzu GC-MS2010 gas chromatograph (Shimadzu Aus) equipped with a Shimadzu AOC 5000 multi-purpose sampler and coupled to a QP2010S mass selective detector. The conditions of the method were based on collective information from multiple references (Osman, 2020; Steingass, Carle, et al., 2015; Zainuddin et al., 2021; Zhang et al., 2012) that supported the optimum separation of the targeted volatiles as follows. The volatile compounds (from the vials prepared as per section 3.2.4) were absorbed onto the SPME fiber at 40 °C for 10 min with constant shaking in Shimadzu autosampler AOC 5000, followed by desorption (splitless injection) in the GC injection port at 250 °C for 2 min. Separation of analytes was achieved with a DB-5MS capillary column (30 m × 0.25 mm × 0.25 µm film thickness, Agilent Technologies), under an oven temperature program as follows: 40 °C hold for 2 min, then increased to 60 °C at a rate of 5 °C/min, then increased to 100 °C at a rate of 40 °C/min, and to 200 °C at a rate of 8 °C/min, and to 240 °C at a rate of 40 °C/min, and held at 240 °C for 4.5 min. Purified helium (purity 99.999%) was used as the carrier gas at 1.5 mL/min constant flow rate (split ratio 50.0). The mass spectrometer was operated in both SCAN and SIM mode from m/z 35 to

335, with 70 eV electron ionization at 230 °C, quadrupole at 250 °C (The mass spectrometer quadrupole temperature was set at 230 °C, the source was set at 250 °C, and the transfer line at 280 °C). Compounds were identified by matching their mass spectra and retention time with authenticated standards and the NIST2014 database library. The concentration represented by each major volatile peak was determined by using matching internal standard (**Table 3.2** on page 34). The method was validated according to the guidelines (NATA, 2012; *Official Methods of Analysis of AOAC INTERNATIONAL*, 2023)

3.3 Calibration and validation of the method

Matrix effect on the analysis was studied using selected standards reference materials and isotope labelled reference compounds (**Table 3.2** on page 34) prepared separately in water and in pineapple matrix (prepared as explained under sections 3.2.3 and 3.2.4). Chromatograms were compared, and the percentage differences were calculated (**Table 3.2** on page 34). Considering the existence of a matrix effect higher than 15%, all the standard solutions used hereafter for method validation were prepared in matching pineapple matrix (*Official Methods of Analysis of AOAC INTERNATIONAL*, 2023). Solutions were always made in duplicate from separately weighed reagents to ensure precision in their preparation. The stock concentrations of target analytes were in a range of 0.25g/L to 0.50g/L, and working standards were in a range of 30ppt to 700µg/L. The solutions were prepared in SPME vials for analysis (n = 8 levels of concentration x 6 different GC vials, i.e., three technical replicates each for intra-day and inter-day). The concentrations of analytes in the samples were calculated from the peak area ratios for the unlabelled and labelled compounds versus the concentration ratio.

3.3.1 Linearity and accuracy

Considering the existence of a high percentage-varying matrix effect (**Table 3.2** on page 34), matrix-matched calibration curves were prepared. The coefficients of determination (R^2) were calculated, and a t-test of the slope for verifying the linearity was also performed ($t_{experimental} > t_{critical}$). Separate recoveries were not calculated as the standards were made in matching pineapple matrix.

3.3.2 Limit of detection and limit of quantification

Limit of detection (LOD) and limit of quantification (LOQ) were calculated based on 3.3a/S and 10a/S, respectively (NATA, 2012; *Official Methods of Analysis of AOAC INTERNATIONAL*, 2023), where ‘a’ is the standard deviation of the ‘y’ intercepts and ‘S’ is the slope of the calibration curve.

3.3.3 precision: inter-day and inter-day repeatability relative standard deviation

For intra-day repeatability, standards were injected in triplicates and the % relative standard deviation (% RSD) of each of the analytes was calculated (n=3). For inter-day repeatability, the standards were injected in triplicate on two consecutive days and the % relative standard deviation (% RSD) of each of the analytes was calculated (n=6). As SPME samples cannot be re-injected from the same vial, each injection used a fresh standard vial. A maximum of 15% RSD was considered acceptable for repeatability.

3.4 Statistical analysis

To find the significance of results and to find out which specific group's means (compared with each other) are different, an ANOVA test including Tukey's HSD, and a multivariate analysis (principal component analysis - PCA) that describes similarities and differences among cultivars based on their volatile profile were performed using the XLSTAT® software premium version 2022.3.2 (Addinsoft, Paris, France).

3.5 Results and discussion

An accurate and precise analytical method involving a combination of matrix-matched HS-SPME-GC-MS and SIDA was developed using selected ion monitoring (SIM) to quantify important aroma volatiles present in selected Australian pineapple cultivars. The concentration ranges targeted for each analyte were selected by considering both the sensorially active range of each compound by referring to the odour sensory threshold concentrations (**Table 3.3** on page 39) and the indicative concentration range as previously reported for that compound in pineapples (George et al., 2023).

3.5.1 Linearity

The % matrix effect was estimated and based on the results shown in **Table 3.2** on page 34; matrix-matched calibration curves were used for quantification of the targeted pineapple volatiles. The calibration curves prepared in matching pineapple matrix showed good linearity over the reported concentration range for all compounds with good correlation (R^2) ranging from 0.9772 to 0.9999 (intra-day) and 0.9736 to 0.9999 (inter-day), and p values < 0.05 for the t-test of the slope (**Table 3.3** on page 39). Calibration curves of all the 26 compounds are provided in Appendix 2, **Figure B1**. Therefore, the method is considered linear and suitable for the application to quantify targeted aroma compounds.

3.5.2 Limit of detection and limit of quantification

In general, the LOD and LOQ values obtained for the reference compounds given in **Table 3.3** on page 39 were relatively lower than their odour threshold (**Table 3.2** on page 34). Therefore, the developed method showed very good sensitivity of detection.

3.5.3 Precision and accuracy

The % RSD values and accuracy values obtained for the reference compounds are given in **Table 3.3** on page 39, and in general, the method was accurate and precise for all the targeted compounds within the pineapple matrix. Percentage RSD values range from 1.8 to 12.7, except the observed 20.1% for 2,5-dimethyl-4-methoxy-3(2H)-furanone. Accuracy values range from 90.4 % to 113.3 % (except the observed 122.6% for methyl isobutyrate, 120.1% for 3-methyl-1-butanol, and 124.7% for Phenyl acetaldehyde). Practically, RSD values lower than 15 % are recommended for method validation (*Official Methods of Analysis of AOAC INTERNATIONAL*, 2023). However, considering the complexity of the pineapple fruit matrix, the method was considered acceptable for the purpose of measuring volatiles in pineapple.

The labelled internal standard used to quantify each target analyte, respective retention time, and the target and qualifier ions used for SIM and relative percentages are given in **Table 3.2** on page 34. The 'inverse isotope effect', where the heavier deuterated compounds elute prior to their non-labelled counterparts in nonpolar columns, was also observed in this study (Schmarr et al., 2012; Tintrop et al., 2023).

The retention indices (RI) were not calculated using n-alkane mixtures (C8-C20), in the reported analytical method developed. Rational for this deviation is provided in Appendix 2, **Supplementary Information B1**.

Table 3.3 Summary of calibration and main validation parameters for determination of twenty-six targeted aroma volatiles in pineapple pulp matrix.

Sl. No	Volatile compound	Linear range (µg/L)	LOD	LOQ	Av. %RSD	Av. % Accuracy	R^2 *calibration equation*		p-value (t-slope test)
							intra day	Inter day	
1	methyl isobutyrate	5.92 - 236.8	0.44	1.34	12.7	122.6	0.9957	0.9981	<0.0001
							y = 0.02342522x - 0.1651980	*y = 0.02282920x - 0.03504168*	
2	ethyl propionate	8.21 - 328.4	0.06	0.19	5.6	110.2	0.999	0.9999	<0.0001
							y = 0.03037692x - 0.1081646	*y = 0.03249202x - 0.07647061*	
3	methyl butyrate	16.99 - 679.6	0.29	0.88	8.3	102.3	0.9994	0.9998	<0.0001
							y = 0.03902097x - 0.1973809	*y = 0.03902097x - 0.1973809*	
4	3-methyl-1-butanol	13.97-558.8	0.51	1.55	1.8	120.1	0.9962	0.9954	<0.0001
							y = 0.002960468x - 0.04550633	*y = 0.003085409x - 0.04112401*	
5	ethyl isobutyrate	14.07 - 562.8	0.22	0.68	7.2	110.6	0.999	0.9989	0.000
							y = 0.07778468x - 0.9570591	*y = 0.07720159x - 0.9588190*	
6	isobutyl acetate	7.78 - 311.2	0.11	0.32	5.8	102.2	0.9999	0.9999	<0.0001
							y = 0.1517417x - 0.5382122	*y = 0.1517417x - 0.5382122*	
7	methyl 2-methylbutyrate	12.83 - 513.2	0.08	0.23	6.7	105.9	0.9996	0.9996	<0.0001
							y = 0.05991383x - 0.4217346	*y = 0.05991383x - 0.4217346*	
8	methyl isovalerate	12.74 - 509.6	0.06	0.19	6.4	106.6	0.9996	0.9996	<0.0001
							y = 0.06136720x - 0.4665380	*y = 0.06136720x - 0.4665380*	
9	ethyl butyrate	7.94 - 317.6	0.06	0.19	5.8	97.5	0.9998	0.9998	<0.0001
							y = 0.06924849x - 0.1284021	*y = 0.06924849x - 0.1284021*	
10	ethyl 2-methylbutyrate	8.21 - 328.4	0.10	0.29	8.5	101.3	0.9999	0.9999	<0.0001
							y = 0.1320597x - 0.4657484	*y = 0.1320597x - 0.4657484*	
11	2-methylbutyl acetate	7.12 - 284.8	0.07	0.22	6.2	93.6	0.9992	0.9992	<0.0001
							y = 0.8170604x - 0.3441047	*y = 0.8170604x - 0.3441047*	
12	methyl hexanoate	8.62 - 344.8	0.09	0.27	6.0	97.4	0.9994	0.9918	<0.0001
							$y = -0.00004942462x^2 + 0.07454985x + 0.2111702$	*$y = -0.00004942462x^2 + 0.07454985x + 0.2111702$*	
13	ethyl hexanoate	7.23 - 289.2	0.14	0.41	7.5	96.6	0.9996	0.9984	0.000
							y = 0.04815328x - 0.04148217	*y = 0.04815328x - 0.04148217*	
14	octanal	9.61 - 384.4	0.15	0.46	9.1	95.0	0.999	0.9928	0.000
							y = -0.00001121040x2 + 0.03653887x + 0.08203627	*y = - 0.00001121040x2 + 0.03653887x + 0.08203627*	
15	ethyl trans-3-hexenoate	8.64 - 345.6	0.13	0.38	5.1	101.7	0.9997	0.9913	<0.0001

Sl. No	Volatile compound	Linear range (µg/L)	LOD	LOQ	Av. %RSD	Av. % Accuracy	R^2 *calibration equation*		p-value (t-slope test)
							intra day	**Inter day**	
							$y = -0.00003933413x^2 + 0.07393936x + 0.1413647$	*$y = -0.00003933416x^2 + 0.07393936x + 0.1413647$*	
16	Methyl-3-(methylthio) propionate	24.74 - 247.4	0.37	1.11	5.6	113.3	0.9878	0.9776	0.003
							y = 0.005867739x - 0.1992945	*y = 0.005749287x - 0.1749477*	
17	D limonene	17.50 - 700.0	0.25	0.77	10.3	105.5	0.9964	0.9969	0.000
							y = 0.1721458x - 1.972685	*y = 0.1721458x -1.972685*	
18	phenylacetaldehyde	12.45 - 498.0	0.19	0.59	7.1	124.7	0.9793	0.9925	0.002
							y = 0.002155605x - 0.04415329	*y = 0.001181531x - 0.009399119*	
19	2,5-dimethyl-4-methoxy-3(2H)-furanone	15.48 - 619.2	0.49	1.48	20.1	110.9	0.9934	0.9835	0.000
							y = 0.001357199x - 0.03407528	*y = 0.001336756x - 0.04217937*	
20	ethyl 3-(methylthio)propionate	21.98 - 219.8	0.19	0.57	6.5	117.8	0.9772	0.9736	0.003
							y = 0.01266805x - 0.3287511	*y = 0.01233423x - 0.2389133*	
21	methyl octanoate	15.56 - 622.4	0.26	0.78	9.0	90.4	0.9986	0.9986	0.000
							$y = -0.001817782x^2 + 2.582725x + 11.86831$	*$y = -0.001817782x^2 + 2.582725x + 11.86831$*	
22	ethyl octanoate	8.52 - 340.8	0.31	0.92	11.0	98.7	0.9999	0.9975	0.001
							$y = -0.0005912428x^2 + 1.204494x + 3.375864$	*$y = -0.0005912428x^2 + 1.204494x + 3.375864$*	
23	α-terpineol	23.14 - 231.4	0.14	0.41	12.1	119.9	0.978	0.9854	0.002
							y = 0.01996474x - 0.5814167	*y = 0.01255025x - 0.1209035*	
24	decanal	8.22 - 328.8	0.28	0.86	13.2	100.2	0.9974	0.9897	0.002
							y = 0.01352805x - 0.06008784	*y = 0.01671388x - 0.1977710*	
25	damascenone	23.20 - 232.0	0.22	0.68	8.0	116.4	0.9778	0.9813	0.001
							y = 0.1263255x -3.185532	*y = 0.1263255x - 3.185532*	
26	ethyl decanoate	8.51 - 170.2	0.49	1.49	11.4	103.4	0.9975	0.9979	0.001
							y = 0.2549409x + 2.582623	*y = 0.2545737x + 2.626471*	

3.6 Analysis of key aroma compounds in pineapples

The ripe pineapple cultivars such as 'Aus Carnival', 'Aus Festival', 'Aus Jubilee', 'Aus Smooth (Smooth Cayenne)', and 'Aussie Gold (73-50)' used for analytical method validation were suitable for its applied usefulness. The analytes in pineapple flesh were quantified using calibration curves obtained from a matching pineapple matrix. A summary of the concentration data for the 26 key aroma volatile compounds produced by ripe 'Aus Carnival', 'Aus Festival', 'Aus Jubilee', 'Aus Smooth (Smooth Cayenne)', and 'Aussie Gold (73-50)' pineapple cultivars is reported in **Table 3.4** on page 44. The volatile compositional profile is shown in the PCA biplot given in **Figure 3.1** on page 42, which explains 76% variation in the volatile profile across the cultivars. While all fruit was considered at a commercially acceptable stage of ripeness, fruit of Aussie Gold (73-50) were considered slightly less mature than fruit of the other cultivars. Overall, ethyl and methyl esters of propanoic, butanoic, hexanoic, and octanoic acids and other ester compounds were contributing more than 50% of the total volatiles in the pineapple cultivars tested, which is in agreement with published data (George et al., 2023). The proportions of the different volatile compounds greatly varied among the cultivars. The variation was mainly due to the difference in concentration of VOCs such as methyl hexanoate, furaneol, ethyl hexanoate, ethyl butanoate, α-Terpineol, ethyl methyl butyrate, ethyl methyl propionate, methyl isobutyrate, methyl isovalerate, D-limonene, and phenylacetaldehyde. The concentration of the VOCs were also varied from the previously reported values but generally was in agreement with their relative concentration within fruit cultivars. Methyl esters of hexanoic acid and 3-(methylthio)propanoic acid were found in higher concentrations among cultivars 'Aus Festival' and 'Aus Jubilee'. The relative concentration of 2,5-dimethyl-4-methoxy-3(2H)-furanone was higher among all the fruit samples, and similar observations were reported among MD-2 and Gold cultivars (George et al., 2023). The observed concentrations of hexanoic acid ethyl ester, 3-(Methylthio)propanoic acid ethyl ester were lower than many of the reported concentrations across MD-2 and Gold cultivars, and could be due to the changes in ripeness levels of the fruit samples (George et al., 2023). Odour active compounds such as damasceneone and decanal were also found in the samples, similar to that reported in MD-2 cultivars (George et al., 2023; Vollmer et al., 2021). However, it is important to consider the details of sampling, extraction conditions, analytical methods employed, and the VOCs identification/quantitation criteria, while comparing the results with the published literature data with inconsistencies in reporting (George et al., 2023). Cultivars ‘Aus Festival’ and ‘Aus Jubilee’ produced the highest average concentration of methyl hexanoate (557.04µg/l and 595.28 µg/l) and 3-(Methylthio) propanoic acid methyl ester (596.75µg/l and 394.96µg/l).

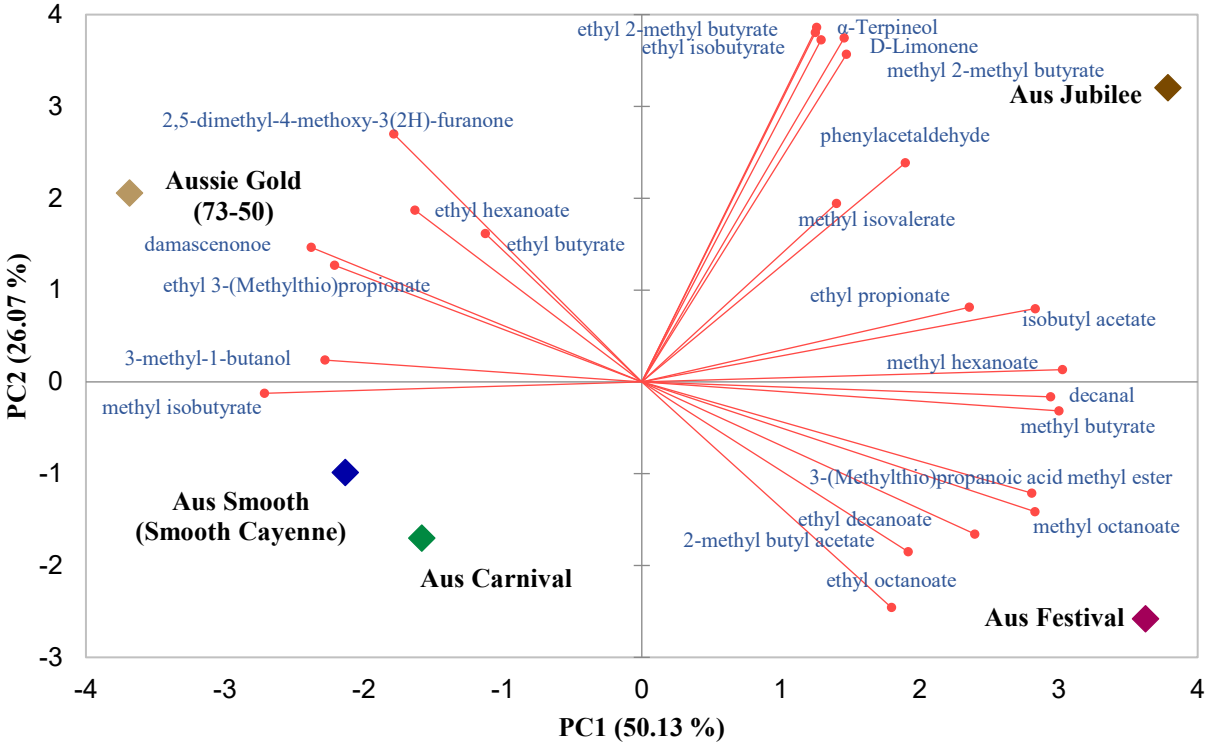


Figure 3.1 PCA biplot of volatiles data and pineapple cultivars (PC1 v PC2 76%)

To compare the odour contribution and relative importance of each compound to the aroma of the cultivars used in this study, the odour activity value (OAV) was calculated for each compound (**Table 3.4** on page 44). The OAV is the ratio between the concentration of an aroma compound and its odour threshold (Pino & Febles, 2013). Reported odour sensory thresholds and nature of the odour of each target analyte are also shown in **Table 3.4** on page 44. Among the targeted aroma compounds, fourteen compounds each in 'Aus Carnival' and 'Aus Smooth', sixteen in 'Aus Festival', fifteen in 'Aus Jubilee', and twelve compounds in 'Aussie Gold (73-50)' were having OAV>1 and considered as odour active. Though substances with high OAV (>1) are generally considered as compounds responsible for the characteristic aroma, the contribution of other VOCs and interaction (masking, additive, and synergistic effects) of the VOCs also play an important role toward the aroma of pineapples (George et al., 2023; Gonçalves, 2018; Teai et al., 2001; Xiao et al., 2021). Compounds such as, methyl isobutyrate; propanoic acid 2-methyl- ethyl ester; butanoic acid 2-methyl- methyl ester; butanoic acid ethyl ester; butanoic acid 2-methyl- ethyl ester; hexanoic acid ethyl ester; D-limonene; phenylacetaldehyde; 2,5-dimethyl-4-methoxy-3(2H)-furanone; 3-(Methylthio)propanoic acid ethyl ester; decanal; and damascenone were found odour active in all the five cultivars. The observed high OAV (OAV>1) for most of the selected VOCs, validate and confirms the usefulness of the method. The application of OAV's to compare odour volatile contribution has been reported previously (Akioka & Umano, 2008; Berger et al., 1985; Pino, 2013; Spanier et al., 1998; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Wei et al., 2014). However, the method utilised

in that study could not approach the OAV of some compounds due to the lack of a suitable internal standard to detect aroma volatiles present at low levels. Future work should consider developing method for ethyl acetate (CAS No. 141-78-6); 4-Hydroxy-2,5-dimethyl-3(2H)-furanone (CAS No. 3658-77-3); δ -octalactone (CAS No. 698-76-0); methyl 3-acetoxyhexanoate (CAS No. 21188-60-3); methyl 5-acetoxyhexanoate (CAS No. 35234-22-1); isoamyl acetate (CAS No. 123-92-2); acetaldehyde (CAS No. 75-07-0); δ -decalactone (CAS No. 705-86-2); 1-(3E,5Z)-3,5-undecatriene (CAS No. 19883-27-3); vanillin (CAS No. 121-33-5); isovaleraldehyde (CAS No. 590-86-3); 2-Methylbutyraldehyde (CAS No. 96-17-3) and 1-(E,Z,Z)-3,5,8-undecatetraene (CAS No. 29837-19-2), which were previously identified (George et al., 2023) as also key aroma compounds. In the present work, availability, separation and detection issues prevented these key aroma compounds being included. Incorporation of this additional key aroma compounds would make the method more comprehensive for the analysis of pineapple samples. The accuracy and precision achieved in the present work allow for meaningful comparisons to be made using OAVs, because the concentration data collected is sensitive and reliable.

3.7 Conclusions

An accurate and precise method was achieved for the analysis of key pineapple flavour volatiles in a model system and subsequently validated with selected Australian pineapple cultivars. The quantification of volatiles through matrix-matched calibration curves corrected the matrix effects, ensured that the differences in volatiles among cultivars were due to genetic and agronomical factors and not to analytical issues. The method of combining SIDA with HS-SPME-GC-MS was found to be highly sensitive and allowed high throughput of samples. It produced calibrations with high coefficients of determination and excellent linearity across a range of concentrations relevant to pineapple flavour. This method represents a significant improvement over current methods with the incorporation of multiple external reference standards, multiple isotope-labelled internal standards, and a matching model system of pineapple fruit matrix. The application of such a standardised, accurate and precise method allows for meaningful comparison in VOC composition and was employed as described in this thesis to measure volatiles in Australian-grown commercial pineapple cultivars and pineapples from the Australian pineapple breeding program. It could be of wider benefit in future studies involving breeding, post-harvest and target market studies, and studies aimed at exploring and optimising the flavour of commercial pineapple varieties and their parent lines to produce better-tasting fruits for consumers.

Table 3.4 Summary of the concentration (in µg/L) data for the 26 key aroma volatile compounds produced by ripe Australian commercial pineapple cultivars such as 'Aus Carnival', 'Aus Festival', 'Aus Jubilee', 'Aus Smooth (Smooth Cayenne)' and 'Aussie Gold (73-50)'

Sl. No.	Volatile compound *(Odour description)*	CAS No.	*OT# (µg/L)*	Aus Carnival (µg/L) (± SD) *OAV*	Aus Festival (µg/L) (± SD) *OAV*	Aus Jubilee (µg/L) (± SD) *OAV*	Aus Smooth (Smooth Cayenne) (µg/L) (±SD) *OAV*	Aussie Gold (73-50) (µg/L) (± SD) *OAV*	Pϕ
1	methyl isobutyrate *(fruity, sweet)*	547-63-7	*6*	24 (5) a *3.961*	15 (5) a *2.536*	16 (4) a *2.647*	19 (6) a *3.222*	23 (9) a *3.777*	0.399
2	propanoic acid, ethyl ester *(fruity, sweet)*	105-37-3	*10*	7 (2) a *0.745*	11 (1) a *1.061*	10 (1) a *0.996*	8 (2.0) a *0.814*	9.0 (2) a *0.901*	0.251
3	butanoic acid, methyl ester *(fruity, sweet)*	623-42-7	*72*	56 (13) b *0.779*	168 (54) a *2.339*	141 (38) a *1.955*	41 (13) b *0.573*	36 (15) b *0.495*	0.001
4	3-methyl-1-butanol *(pineapple, chocolate)*	123-51-3	*300*	10 (2) a *0.033*	10 (3) a *0.035*	9 (2) a *0.031*	13 (4.0) a *0.042*	13 (5) a *0.043*	0.688
5	propanoic acid, 2-methyl-, ethyl ester *(fruity, sweet)*	97-62-1	*0.1*	18 (3.0) a *183.283*	20 (3) a *196.269*	24 (7) a *241.965*	19 (2) a *188.470*	21 (3) a *211.267*	0.439
6	isobutyl acetate *(fermented, ethereal)*	110-19-0	*66*	6 (2) a *0.098*	8 (1) a *0.123*	8.0 (2) a *0.122*	6 (1) a *0.097*	7 (1) a *0.103*	0.405
7	butanoic acid, 3-methyl-, methyl ester *(fruity, apple like)*	556-24-1	*44*	14 (2) a *0.328*	14 (3) a *0.321*	18 (3.0) a *0.401*	14 (2) a *0.313*	15 (2) a *0.341*	0.337
8	butanoic acid, 2-methyl-, methyl ester *(pungent, fruity)*	868-57-5	*1*	34 (8) ab *34.168*	25 (8) b *25.350*	53 (14) a *52.631*	37 (12) ab *37.199*	22 (9) b *22.257*	0.038
9	butanoic acid, ethyl ester *(fruity)*	105-54-4	*1*	5 (1) b *5.014*	9 (4) ab *9.025*	6 (1) b *6.381*	5 (1) b *4.979*	18 (13) a *17.771*	0.120
10	butanoic acid, 2-methyl-, ethyl ester *(apple, pineapple, fruity)*	7452-79-1	*0.3*	3 (3) a *8.666*	3 (2) a *8.353*	4 (4) a *12.650*	3 (3) a *8.424*	3 (3) a *9.816*	0.982
11	1-butanol, 2-methyl-, acetate *(fermented, sweet, balsamic)*	624-41-9	*5*	1 (1) a *0.297*	5 (4) a *0.976*	2 (1) a *0.408*	2 (1) a *0.331*	2 (0) a *0.402*	0.250
12	hexanoic acid, methyl ester *(pineapple, fruity)*	106-70-7	*70*	245 (56) b *3.449*	557 (179) a *7.958*	595 (156) a *8.504*	82 (26) b *1.168*	51 (21) b *0.732*	0.000
13	hexanoic acid, ethyl ester *(pineapple, banana, fruity)*	123-66-0	*1*	7 (2) a *6.876*	8 (3) a *7.957*	8 (2) a *7.665*	8 (2) a *8.310*	11 (5) a *11.302*	0.445
14	octanal	124-13-0	_	ND	ND	ND	ND	ND	_
15	ethyl trans-3-hexenoate	2396-83-0	_	ND	ND	ND	ND	ND	_

Sl. No.	Volatile compound *(Odour description)*	CAS No.	*OT# (µg/L)*	Aus Carnival (µg/L) (± SD) *OAV*	Aus Festival (µg/L) (± SD) *OAV*	Aus Jubilee (µg/L) (± SD) *OAV*	Aus Smooth (Smooth Cayenne) (µg/L) (±SD) *OAV*	Aussie Gold (73-50) (µg/L) (± SD) *OAV*	Pϕ
16	3-(methylthio) propanoic acid methyl ester *(meaty, onion-like)*	13532-18-8	*180*	204 (36) bc *1.132*	597 (219) a *3.315*	395 (97) b *2.194*	210 (47) bc *1.167*	145 (29) c *0.805*	0.003
17	D-limonene *(citrus)*	5989-27-5	*10*	22 (4) a *2.189*	24 (7) a *2.384*	28 (4) a *2.762*	23 (6) a *2.270*	26 (6) a *2.558*	0.704
18	phenylacetaldehyde *(floral, sweet)*	122-78-1	*4*	7 (2) b *1.867*	11 (4) ab *2.817*	16 (4) a *3.992*	12 (4) ab *3.072*	10 (4) ab *2.461*	0.139
19	2,5-dimethyl-4-methoxy-3(2H)-furanone *(caramel, roasty, sweet)*	4077-47-8	*0.03*	169 (39) a *5636.261*	115 (37) a *3824.177*	160 (43) a *5318.069*	132 (42) a *4410.018*	198 (82) a *6596.288*	0.375
20	3-(methylthio) propanoic acid ethyl ester *(meaty, onion, pineapple)*	13327-56-5	*7*	39 (6) a *5.586*	39 (13) a *5.630*	38 (10) a *5.477*	41 (5) a *5.805*	46 (6) a *6.518*	0.838
21	octanoic acid, methyl ester *(fruity)*	111-11-5	*200*	50 (17) cd *0.248*	136 (44) a *0.682*	100 (27) ab *0.499*	66 (16) bc *0.332*	11 (2) d *0.055*	0.001
22	octanoic acid, ethyl ester *(fruity, winey, sweet)*	106-32-1	*192*	ND	5.1 (0.2) *0*	ND	ND	ND	_
23	α-terpineol *(floral, lilac)*	98-55-5	*330*	16 (2) a *0.049*	17 (3) a *0.052*	21 (5) a *0.064*	16 (2) a *0.050*	19 (2) a *0.057*	0.383
24	decanal *(waxy, floral, citrus)*	112-31-2	*0.1*	11 (1) bc *107.147*	13 (1) ab *131.963*	14 (1) a *139.625*	8 (1) cd *81.943*	7 (3) d *68.657*	0.000
25	damascenone *(fruity, sweet)*	23696-85-7	*0.00075*	3 (0) a *4426.408*	3 (1) a *4406.533*	3 (1) a *4424.691*	4 (1) a *5711.186*	5 (2) a *6846.974*	0.376
26	decanoic acid, ethyl ester *(sweet, fatty, nut-like)*	110-38-3	*6300*	19 (1) b *0.003*	37 (3) a *0.006*	21 (4) b *0.003*	8 (2) d *0.001*	12 (0) c *0.002*	<0.0001

ND: not detected. # previously reported odour threshold values taken from (George et al., 2023). SD is variation between individual fruits of pineapple. ϕ indicates significant difference in concentration between cultivars by ANOVA ($P<0.05$). *abcd* Different letters within a row indicate a significant difference by Tukey LSD ranking test.

Chapter 4 Relationship between key aroma compounds and sensory attributes of Australian-grown commercial pineapple cultivars

Pineapple (*Ananas comosus* var. *comosus*), celebrated for its distinctive sweet and tropical flavour, ranks as the third most important tropical fruit in global production (FAO, 2024). In Australia, pineapple cultivation is concentrated in Queensland, where favourable climatic conditions support the growth of several commercial cultivars. Despite the diversity of pineapple varieties worldwide, only a few dominate the commercial market, often selected for agronomic traits rather than flavour.

This chapter describes the application of the validated analytical method (detailed in Chapter 3) to explore and investigate the intricate relationship between chemical composition and sensory attributes across five Australian-grown commercial pineapple cultivars. The study focused on three core areas. First, consumer acceptability and sensory profiling were conducted by evaluating five commercial pineapple cultivars with input from 117 consumers and a trained sensory panel comprising 13 members. Notably, this study is the first to apply agglomerative hierarchical clustering (AHC) to map consumer preferences against sensory profiles of Australian-grown pineapple cultivars. Second, the chemical composition of the cultivars was analysed through targeted quantification of volatile organic compounds (VOCs) likely contributing to flavour. Third, the impact of flavour-associated VOCs was examined by assessing the relationships between chemical composition, sensory attributes, and consumer preferences using multivariate statistical techniques. Thus, the compositional targets of consumer quality would be established to enable the development of molecular markers of pineapple fruit quality.

This integrative approach highlights the complex interplay between chemical and sensory traits in pineapple, offering valuable insights for cultivar selection and breeding strategies aimed at enhancing fruit quality and consumer satisfaction. This chapter was published as 'Relationship between key aroma compounds and sensory attributes of Australian-grown commercial pineapple cultivars' in *Journal of Agriculture and Food Chemistry* (George et al., 2025).

Author contributions for this chapter are summarised in **Table 4.1** on page 47.

4.1 Introduction

Flavour perception in foods involves smell, taste, and chemesthesis. Chemical stimuli released during eating are transported by saliva to taste-sensitive areas, while volatile compounds travel to the nasal cavity, engaging olfactory receptors. This interaction enhances neural responses, influencing fruit

flavour perception (Colonges et al., 2022; Dubrow et al., 2022; Fan et al., 2021; Laing & Jinks, 1996; Li et al., 2024; Sari et al., 2023; Schwieterman et al., 2014; Spence, 2015; Sung et al., 2019).

Table 4.1 Author contributions in Chapter 4

	Jenson George	Ishita Pramanik	Garth Sanewski	Thoa Nguyen	Sharon Pun	David Edwards	Margaret Currie	Simone Moller	Craig Hardner	Philippa Lyons	Heather E. Smyth
Conceptualization	x		x								x
Methodology	x										x
Software	x										x
Validation	x										
Formal analysis	x	x			x	x	x	x		x	
Investigation	x				x	x	x	x			
Resources	x		x	x						x	x
Data curation	x	x	x		x					x	x
Writing - original draft	x							x			
Writing - review & editing	x	x	x	x	x			x	x	x	x
Visualization	x	x	x	x					x	x	x
Supervision			x	x					x	x	x

The specific flavour and aroma of pineapple depend on factors such as cultivar, harvest maturity, climatic conditions, agronomical practices, and postharvest handling (George et al., 2023). Important flavour-associated VOCs in pineapples are derived from sugars, organic acids, and amino acids. Recent studies suggest that an omics approach (genomics, transcriptomics, metabolomics, and flavouromics) is valuable for identifying VOCs during ripening and elucidating their content variations and sensory triggers (Charve et al., 2011; Huang et al., 2024; Z. Liu et al., 2024; Schwieterman et al., 2014; Sung et al., 2019; Tieman et al., 2012). Notably, methyl and ethyl esters, along with terpenoid compounds, emerge as characteristic aroma contributors in pineapple (Asikin et al., 2023; Asikin et al., 2024; George et al., 2024; George et al., 2023; Steingass et al., 2016).

Although some studies reported the hedonic studies of pineapple exploring the effect of VOCs on sensory properties and consumer preferences (Steingass et al., 2016; Vollmer et al., 2021), there were no previous reports on consumer preference mapping using the agglomerative hierarchical clustering (AHC) of consumer data against sensory perception of Australian-grown commercial pineapple cultivars, despite their diverse chemical compositions. Most research focuses on one or two cultivars, (George et al., 2023) but comparing several cultivars provides a broader perspective on traits impacting consumer preferences. Moreover, fruit quality is profoundly influenced by environmental conditions. For Australian-grown pineapples, understanding the relationships between pineapple chemical composition, sensory profile related to consumer liking is essential for identifying key

targets for breeding. Specifically, unravelling pineapple fruit quality at the cultivar level is essential for developing or identifying superior types in breeding programs suitable for premium markets.

To address these objectives, our study explored the following:

i) Consumer acceptability and sensory profiling: five commercial Australian-grown pineapple cultivars were evaluated. Consumer acceptability was determined using pineapple consumers (n=117) and sensory profiles developed using an experienced trained sensory panel (n=13).

ii) Chemical Composition: Through targeted analysis, we measured the concentration of VOCs that are likely to be involved in fruit flavour in the five pineapple cultivars.

iii) Impact of Flavour-Associated VOCs: We investigated how the chemical composition, specifically key aroma compounds, related to the sensory attributes and consumer preferences using multivariate statistical analysis.

4.2 Materials and methods

4.2.1 Chemicals, reagents and standards

Neat reference standards of the aroma compounds listed in Chapter 3, **Table 3.2** on page 34 (based on the 40 key aroma compounds identified in Chapter 2 (George et al., 2023), and hyper grade for LC-MS LiChrosolv isopropanol were obtained commercially from Merck (Sigma Aldrich), New South Wales, Australia. The labelled internal standards, ethyl 2-methylbutyrate-d9 (D-7676), ethyl hexanoate-d11 (D-7060), octanal-d16 (D-6929), ethyl octanoate-d15 (D-7063) were obtained commercially from CDN isotopes, Quebec, Canada, through PM Separations Pty Ltd, Queensland, Australia.

Matching aroma free sample matrix, and standard stock solution containing the reference standards of the key aroma compounds, and the sample vials for VOCs analysis were prepared by following the conditions outlined in Chapters 2 and 3 (George et al., 2024; George et al., 2023).

4.2.2 Fruit material

Approximately 30 ripe fruits of the commercially available pineapple cultivars, 'Aus Carnival', 'Aus Festival', 'Aus Jubilee', 'Aus Smooth' (Smooth Cayenne) and 'Aussie Gold' (Pineapple Research Institute 73-50), were sourced from wholesale markets and supplied in January 2023 by Favco Qld Pty Ltd, Queensland, Australia. Externally the fruit were at the first break to half-colour stage, with a °Brix of >12%. The stage of ripeness could be considered commercially acceptable according to standard practices in pineapple retail markets in Australia. The fruits were stored at 5 °C in

temperature-controlled cabinets (CARON Model 6040-3, Marietta, Ohio, USA) at the Department of Primary Industries (DPI), Coopers Plains, Queensland, Health and Food Sciences Precinct, until the samples were prepared for assessment.

4.3 Sample Preparation

Individual fruits were peeled, and the top and bottom thirds were removed. The remaining flesh was cut into four equal quarters, with cores removed. These quarters were then sliced into 1.5 mm thick segments (10-15 g each) and served to assessors in plastic pots labelled with a three-digit blinding code and a composite letter. A flow chart of sample preparation is given in Appendix 3, **Supplementary information C1.** The composite tracking codes (A, B, C, etc.) are given in Appendix 3, **Table C1,** and were used throughout consumer assessment and physicochemical analyses.

For consumer assessment, approximately ten pineapples per cultivar were needed to produce the required samples. Segments from two quarters of each fruit were used for consumer assessment, while the segments from the other two quarters were retained for chemical and physical analyses. For sensory profiling, the same cutting protocol was followed, but all fruit was used for sensory assessment.

For chemical analyses, pineapple segments from consumer testing were cut into small pieces and milled into a homogeneous puree using a ball mill (Retsch MM500 vario). This process was performed in ice-cold conditions to minimise volatile loss. The puree was immediately weighed into headspace vials and stored at -80°C for GC-MS-HS-SPME-SIDA analysis. Samples for pH, °Brix, and %TA were transferred to plastic centrifuge tubes (kept at 4-5°C using ice slurry) and immediately analysed.

4.4 Consumer and Sensory Evaluation

Consumer and sensory evaluations were conducted at the DPI sensory laboratories, which are equipped with 12 testing booths and necessary facilities. Data collection was performed using EyeQuestion® software, adhering to IFST guidelines. Informed consent was obtained from all assessors prior to the study.

4.4.1 Trained panel sensory evaluation

Descriptive sensory analysis (AS 2542.1.3:2014 adopts ISO 8586:2012) ("BS EN ISO 8586:2023: Sensory analysis. Selection and training of sensory assessors," 2023) of pineapple samples using thirteen trained sensory panellists. They participated in five training sessions to develop and refine sensory attributes. A comprehensive list of sensory attributes, definitions and reference standards is

summarised in Appendix 3, **Table C2**. Formal evaluations were performed in triplicate, using a 100-point scale to rate appearance, aroma, flavour, and texture attributes.

4.4.2 Consumer assessment

A total of 117 naïve pineapple consumers (49 males, 68 females, aged 18-65) from Brisbane, Queensland, evaluated pineapple samples. They rated appearance, aroma, flavour, texture, and overall liking on a 9-point hedonic scale. Two incomplete datasets were excluded, resulting in 115 complete datasets for analysis.

Details of the trained panel sensory evaluation and consumer assessment are provided in Appendix 3, **Supplementary information C2**.

4.5 Physicochemical analysis

4.5.1 °Brix

A 2 mL centrifuge tube containing pineapple composite puree (prepared as per section 3.2) was centrifuged at 14,000 rpm at ambient temperature in a bench-top centrifuge (Beckman Coulter Microfuge 18). Two to three drops of the supernatant were transferred to a refractometer (Atago Pocket Refractometer) and the °Brix was measured.

4.5.2 pH and titratable acidity (%TA)

The pH and the titratable acidity (*AOAC Official Method 942.15; Acidity (Titratable) of Fruit Products*, 2023; Garner et al., 2008; Sadler & Murphy, 2010; Steingass et al., 2014; Tyl & Sadler, 2017) were measured using an auto-titrator (Metrohm Eco Titrator). About 5 g of puree (section 3.2.2) was accurately weighed into a 100 mL beaker. 60 mL of MilliQ water and a stirrer bar were added to the beakers and the pH and %TA were measured by titration against standard 0.1 M Sodium hydroxide solution. The % TA was determined according to the published protocol (Garner et al., 2008) and was calculated as a percentage of citric acid, as shown below.

% TA = (V x N x mq acid x 100) / sample weight (g)

Where, V is the volume of NaOH, N is the normality of NaOH, and mq is the milliequivalent of citric acid (0.064).

4.6 Analysis of key aroma compounds by GC-MS

Sample vials (stored at -80°C, section 4.3) with pineapple puree (~0.5 g) were opened and added saturated NaCl solution (4.45 mL), and mixed internal standard solution (50 µL). The vials were

immediately sealed with the screw cap and taken for GC-MS injections. The previously developed (Chapter 3, Section 3.2.5) and the published (George et al., 2024) validated, matrix-matched-GC-MS-HS-SPME-SIDA method was employed to accurately quantify the targeted key aroma compounds.

4.7 Statistical Analysis

To determine the significance of the results and identify which specific group means differ from one another, as well as to create predictive models to find correlations between data points, several statistical methods were employed. These included agglomerative hierarchical clustering (AHC), one-way analysis of variance (ANOVA) with Tukey's honestly significant difference (HSD) test, principal component analysis (PCA), and preference mapping. These analyses were performed using the XLSTAT® software premium version 2022.3.2 (Addinsoft, Paris, France). Results were considered statistically significant if the p-value was less than 0.05. Pearson's correlations were visualised using a heatmap.

4.8 Results and discussion

4.8.1 Fruit Characteristics of Pineapple Cultivars

Table 4.2 on page 52 provides a summary of the pH, °Brix, %TA, and °Brix: %TA ratio for five pineapple cultivars and are plotted in **Figure 4.1** on page 53. There were significant differences among cultivars for all traits. The pH levels of the cultivars are ranked as follows: 'Aus Festival' > 'Aus Carnival' > 'Aus Jubilee' > 'Aussie Gold' (73-50) > 'Aus Smooth' (Smooth Cayenne). The %TA pH levels are ranked as: 'Aus Festival' < 'Aus Jubilee' < 'Aussie Gold' (73-50) < 'Aus Carnival' < 'Aus Smooth' (Smooth Cayenne). The °Brix values are ranked: 'Aus Jubilee' > 'Aus Festival' > 'Aus Carnival' > 'Aussie Gold' (73-50) = 'Aus Smooth' (Smooth Cayenne). Although °Brix are commonly used as a ripening index for fresh pineapples, the observed differences are mainly due to variations in cultivars and partly due to the differences in ripeness levels. The °Brix: %TA ratio is ranked as: 'Aus Festival' > 'Aus Jubilee' > 'Aus Carnival' > 'Aussie Gold' (73-50) > 'Aus Smooth' (Smooth Cayenne). High-quality pineapples typically exhibit a sweet taste with balanced acidity and a high °Brix to TA ratio. According to Ramsaroop and Saulo (Ramsaroop & Saulo, 2007), both sweetness perception and preference for fresh pineapple samples are linked to higher °Brix: %TA ratios. They noted that the perceived pineapple flavour aligns with sweetness perception, although their study did not assess volatile flavour compounds.

Table 4.2 ANOVA table of five pineapple cultivars and Physicochemical characteristics data such as pH, °Brix, %TA, and °Brix: %TA ratio

	pH	% TA	°Brix	°Brix: % TA
'Aus Festival'	4.22 (0.17) a	0.42 (0.05) c	15.1 (1.5) b	36.3 (6.4) a
'Aus Jubilee'	4.13 (0.15) b	0.47 (0.07) c	16.5 (1.5) a	35.7 (7.4) a
'Aussie Gold' (73-50)	3.91 (0.22) c	0.56 (0.11) b	12.7 (2.0) c	24.4 (9.4) b
'Aus Carnival'	4.17 (0.11) ab	0.57 (0.06) b	14.1 (2.1) b	25.2 (5.5) b
'Aus Smooth' (Smooth Cayenne)	3.56 (0.06) d	0.76 (0.15) a	12.7 (2.6) c	16.8 (1.9) c
Pr > F(Model)	<0.0001	<0.0001	<0.0001	<0.0001
Significant	Yes	Yes	Yes	Yes

Mean values (± SD), SD is variation between individual sample segments from consumer acceptability test of five pineapple cultivars, n ≥ 8. Different letters in the same row indicate significant statistical differences (Tukey's HSD, P ≤ 0.05).

4.8.2 Diversity of key aroma compounds within the pineapple cultivars

Table 4.4 on page 55 reports the concentration data for 22 key aroma volatile compounds in ripe 'Aus Carnival', 'Aus Festival', 'Aus Jubilee', 'Aus Smooth' (Smooth Cayenne), and 'Aussie Gold' (73-50) pineapple cultivars. Although all fruits were at a commercially acceptable ripeness, 'Aussie Gold' (73-50) was slightly less mature with lower °Brix and °Brix: %TA as evident from **Table 4.2** above. Ethyl and methyl esters of propanoic, butanoic, hexanoic, and octanoic acids, along with other esters, made up over 50% of the total volatiles, consistent with published data (George et al., 2023). The proportions of volatile compounds varied significantly among cultivars, mainly due to differences in concentrations of VOCs such as, methyl hexanoate, furaneol, ethyl hexanoate, ethyl butanoate, α-Terpineol, ethyl methyl butyrate, ethyl methyl propionate, methyl isobutyrate, methyl isovalerate, D-limonene, and phenylacetaldehyde. While concentrations of VOCs varied from previous reports, they generally aligned with relative concentrations within cultivars. 'Aus Festival' and 'Aus Jubilee' had higher concentrations of methyl esters of hexanoic acid and 3-(methylthio)propanoic acid. The relative concentration of 2,5-dimethyl-4-methoxy-3(2H)-furanone was higher across all samples, similar to MD-2 cultivar (George et al., 2023). Lower concentrations of hexanoic acid ethyl ester and 3-(methylthio)propanoic acid ethyl ester were observed compared to the MD-2 cultivar, possibly due to ripeness differences (George et al., 2023; S. Liu et al., 2024). Odour-active compounds like damascenone were also found, similar to MD-2 cultivars (George et al., 2023; Vollmer et al., 2021). 'Aus Festival' and 'Aus Jubilee' had the highest average concentrations of methyl hexanoate (732.9 µg/l and 760.0 µg/l) and 3-(methylthio)propanoic acid methyl ester (803.8 µg/l and 497.2 µg/l). However, it is important to consider sampling, extraction conditions, analytical methods, and VOCs identification/quantitation criteria when comparing results with published data (George et al., 2023).

To compare the relative importance of each compound to the aroma of the cultivars used in this study, the odour activity value (OAV) was calculated for each compound (**Table 4.4** on page 55). The OAV

is the ratio between the concentration of an aroma compound and its odour threshold (George et al., 2023). Reported odour sensory thresholds and the nature of the odour of each target analyte are also shown in **Table 4.4** on page 55. Among the targeted aroma compounds, thirteen compounds each in 'Aus Smooth', fifteen in 'Aus Festival', sixteen in 'Aus Jubilee', and twelve compounds in 'Aussie Gold (73-50)' and 'Aus Carnival' had an OAV>1 and are considered as odour active. Though substances with high OAV (>1) are generally considered as compounds responsible for the characteristic aroma, the contribution of other VOCs and interaction (masking, additive, and synergistic effects) of the VOCs also play an important role toward the aroma of pineapples (George et al., 2023; Gonçalves, 2018; Teai et al., 2001; Xiao et al., 2021). Compounds such as methyl isobutyrate; ethyl propionate; ethyl isobutyrate, methyl 2-methylbutyrate; ethyl butyrate; ethyl 2-methylbutyrate; ethyl hexanoate; D-Limonene; phenyl acetaldehyde; 2,5-dimethyl-4-methoxy-3(2H)-furanone; and damascenone were found odour active in all the five cultivars.

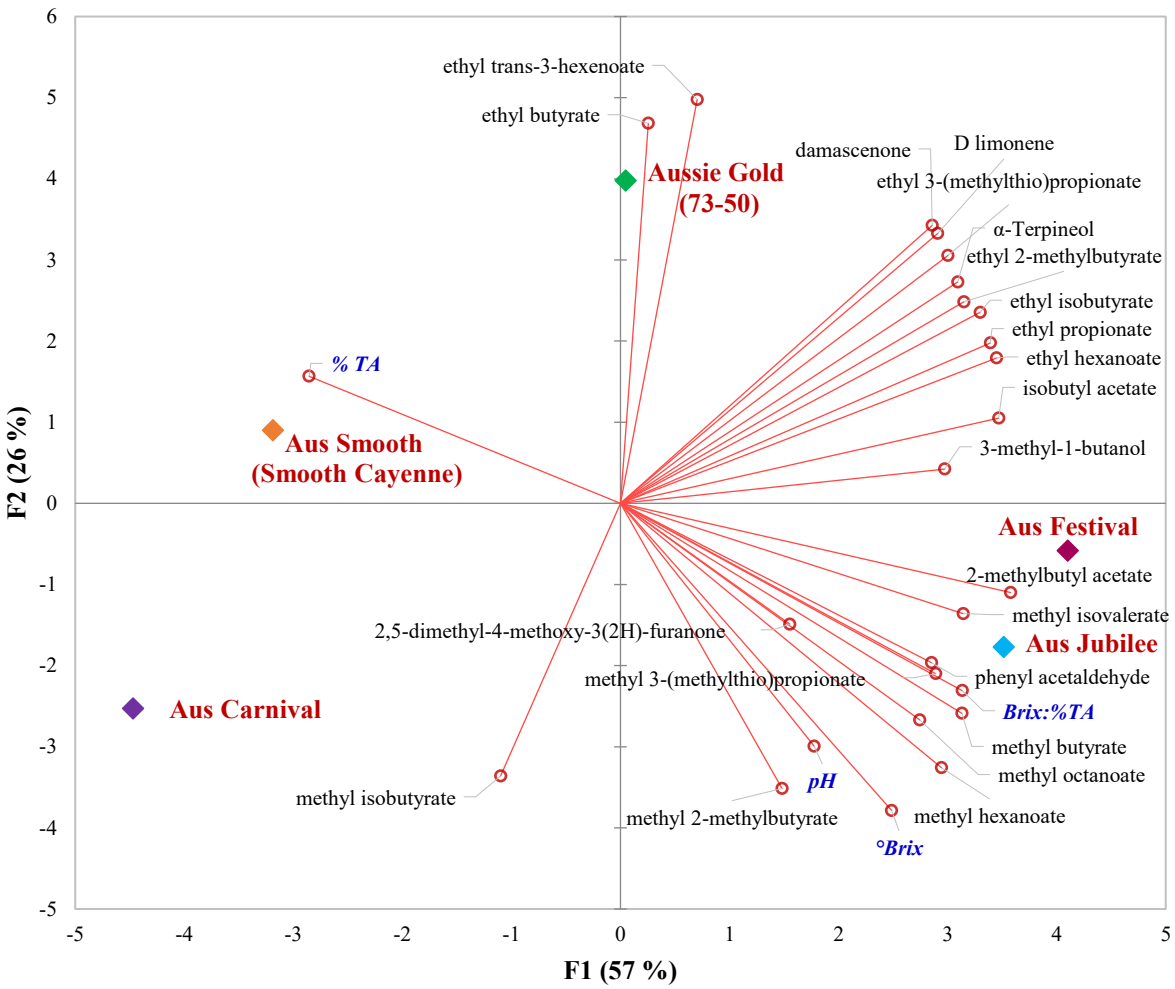


Figure 4.1 PCA biplot (PC1 v PC2 83%) of individual sample segments from consumer acceptability test of five pineapple cultivars, n ≥ 8, and non-volatile and volatile compositional data, technical replicate n =3

The non-volatile and volatile compositional profiles for the five pineapple cultivars are shown in the PCA biplot given in **Figure 4.1** on page 53, which explains 83% variation. The largest variation across the cultivar sample set (PC1 57%) was driven by the concentration of VOCs and %TA. Samples on the right were higher in VOCs generally and low in %TA. Conversely, cultivars on the left of the plot, namely 'Aus Carnival' and 'Aus Smooth' were low in VOCs and high in %TA. The second most important variation (PC2 26%) was driven by methyl and ethyl esters of propanoic, butanoic, hexanoic, and octanoic acids. Cultivars in the bottom were higher in methyl esters and low in ethyl esters. Conversely, cultivars at the top were higher in ethyl esters and low in methyl esters. In general, the proportions of the different VOCs greatly varied among cultivars. VOCs are driven by ripeness and cultivars 'Aus Festival' and 'Aus Jubilee' with higher 'Brix: %TA' ratios have higher concentrations of key targeted volatiles.

4.8.3 Consumer evaluation results

For direct comparison to physical and chemical assessments, the mean liking score for the five pineapple cultivars was calculated based on composite samples and summarised in **Table 4.4** on page 55. 'Aus Festival', 'Aus Jubilee' and 'Aus Carnival' scored highest ($p < 0.05$) for overall liking, liking of appearance, aroma, flavour and texture. Although 'Aus Gold' has comparable scores to those of 'Aus Carnival' in appearance, it still scored low in all other modalities (*aroma, flavour, texture, overall liking*) ($p<0.05$).

Table 4.3 Average composite mean liking score of five pineapple cultivars

	appearance liking	*aroma liking*	*flavour liking*	*texture liking*	*overall liking*
'Aus Festival'	7.2 a	7.1 a	7.4 a	7.0 a	7.2 a
'Aus Jubilee'	7.1 a	6.4 b	7.0 ab	6.6 ab	6.8 ab
'Aussie Gold' (73-50)	6.3 b	5.7 c	5.6 c	5.9 c	5.4 c
'Aus Carnival'	6.7 ab	6.6 ab	6.7 b	6.5 ab	6.4 b
'Aus Smooth' (Smooth Cayenne)	4.9 c	4.9 d	5.7 c	6.1 bc	5.4 c
Pr > F(Model)	<0.0001	<0.0001	<0.0001	0.003	<0.0001
Significant	Yes	Yes	Yes	Yes	Yes

Mean liking scores of individual sample segments from the consumer acceptability test of five pineapple cultivars, $n \geq 8$. Different letters in the same row indicate significant statistical differences (Tukey's HSD, $P \leq 0.05$).

Table 4.4 ANOVA table of the five pineapple cultivars and concentration of key aroma compounds and their OAVs

Volatile compound ***(Odour description)***	**OT# (µg/L)**	**'Aus Festival'**	**'Aus Jubilee'**	**'Aussie Gold 73-50'**	**'Aus Carnival'**	**Smooth Cayenne**	**Pr > F(Model)**	**Significant**
methyl isobutyrate *(fruity, sweet)*	6	20.0 (3.1) bc **3.3**	20.3 (3.4) b **3.4**	19.6 (2.9) bc **3.3**	23.8 (5.8) a **4.0**	18.1 (3.4) c **3.0**	<0.0001	Yes
ethyl propionate *(fruity, sweet)*	10	12.0 (2.1) a **1.2**	11.4 (1.7) ab **1.1**	11.4 (1.3) ab **1.1**	9.3 (3.8) c 0.9	10.3 (2.0) bc **1.0**	0.000	Yes
methyl butyrate *(fruity, sweet)*	72	221.6 (56.7) a **3.1**	179.7 (42.0) b **2.5**	30.9 (18.1) d 0.4	56.1 (24.1) c 0.8	38.5 (19.3) cd 0.5	<0.0001	Yes
3-methyl-1-butanol *(pineapple, chocolate)*	300	13.7 (2.5) a 0	12.0 (2.2) b 0	11.2 (1.5) bc 0	9.8 (3.9) c 0	11.7 (3.2) b 0	0.000	Yes
ethyl Isobutyrate *(fruity, sweet)*	0.1	23.5 (3.2) a **235.4**	23.2 (3.1) a **232.5**	23.3 (2.1) a **233.2**	19.5 (8.0) b **194.7**	21.2 (3.4) ab **212.2**	0.005	Yes
isobutyl acetate *(fermented, ethereal)*	66	8.6 (1.4) a 0.1	8.1 (1.7) ab 0.1	7.6 (1.4) b 0.1	6.3 (2.4) c 0.1	7.3 (1.4) b 0.1	<0.0001	Yes
methyl isovalerate *(fruity, apple like)*	44	33.3 (16.2) b 0.8	67.2 (34.3) a **1.5**	19.3 (8.2) c 0.4	34.2 (12.3) b 0.8	34.8 (25.6) b 0.8	<0.0001	Yes
methyl 2-methylbutyrate *(pungent, fruity)*	1	17.2 (1.8) ab **17.2**	18.5 (3.0) a **18.5**	16.6 (1.6) b **16.6**	15.9 (5.9) b **15.9**	15.8 (2.3) b **15.8**	0.021	Yes
ethyl butyrate *(fruity)*	1	7.4 (3.4) b **7.4**	7.7 (2.1) b **7.7**	28.0 (19.7) a **28.0**	6.3 (3.6) b **6.3**	6.3 (2.1) b **6.3**	<0.0001	Yes
ethyl 2-methylbutyrate *(apple, pineapple, fruity)*	0.3	1.4 (0.6) ab **4.7**	1.4 (0.4) a **4.8**	1.4 (0.5) a **4.8**	1.1 (0.4) b **3.8**	1.2 (0.3) ab **4.1**	0.068	No
2-methylbutyl acetate *(fermented, sweet, balsamic)*	5	2.9 (0.5) a 0.6	2.8 (0.6) a 0.6	2.4 (0.4) b 0.5	2.2 (0.9) b 0.4	2.2 (0.4) b 0.4	<0.0001	Yes
methyl hexanoate *(pineapple, fruity)*	70	732.9 (271.7) a **10.5**	760.0 (328.4) a **10.9**	44.4 (28.6) c 0.6	245.0 (180.4) b **3.5**	76.4 (51.6) c **1.1**	<0.0001	Yes
ethyl hexanoate *(pineapple, banana, fruity)*	1	10.5 (4.5) a **10.5**	9.8 (1.8) a **9.8**	9.8 (3.5) a **9.8**	6.9 (2.9) b **6.9**	7.8 (1.1) b **7.8**	0.000	Yes

Volatile compound ***(Odour description)***	**OT# (µg/L)**	**'Aus Festival'**	**'Aus Jubilee'**	**'Aussie Gold 73-50'**	**'Aus Carnival'**	**Smooth Cayenne**	**Pr > F(Model)**	**Significant**
ethyl trans-3-hexenoate	NA	7.0 (2.0) b	7.0 (0.9) b	10.5 (4.4) a	6.0 (3.0) b	6.9 (2.9) b	<0.0001	Yes
methyl 3-(methylthio)propionate *(meaty, onion-like)*	180	803.8 (306.1) a **4.5**	497.2 (181.0) b **2.8**	148.8 (64.4) d 0.8	213.2 (76.7) cd **1.2**	261.3 (158.1) c **1.5**	<0.0001	Yes
D limonene *(citrus)*	10	31.1 (3.6) a **3.1**	30.3 (4.8) a **3.0**	31.8 (2.9) a **3.2**	26.3 (10.9) b **2.6**	28.5 (4.4) ab **2.9**	0.010	Yes
phenylacetaldehyde *(floral, sweet)*	4	14.8 (4.6) b **3.7**	20.4 (10.7) a **5.1**	8.5 (1.3) cd **2.1**	7.5 (3.0) d **1.9**	11.5 (3.9) c **2.9**	<0.0001	Yes
2,5-dimethyl-4-methoxy-3(2H)-furanone *(caramel, roasty, sweet)*	0.03	150.9 (45.6) bc **5031.1**	203.7 (52.2) a **6789.8**	171.5 (72.4) b **5716.3**	169.1 (37.0) b **5637.4**	123.7 (37.2) c **4121.8**	<0.0001	Yes
ethyl 3-(methylthio)propionate *(meaty, onion, pineapple)*	7	51.8 (7.6) a **7.4**	49.0 (7.9) a **7.0**	51.3 (4.9) a **7.3**	42.2 (17.4) b **6.0**	46.5 (6.9) ab **6.6**	0.004	Yes
methyl octanoate *(fruity)*	200	179.4 (112.3) a 0.9	127.5 (76.3) b 0.6	13.0 (7.2) d 0.1	45.7 (30.0) cd 0.2	66.0 (65.5) c 0.3	<0.0001	Yes
α-terpineol *(floral, lilac)*	330	20.7 (2.5) ab 0.1	20.7 (3.5) ab 0.1	21.3 (2.0) a 0.1	17.5 (2.0) c 0.1	18.5 (3.3) bc 0.1	0.005	Yes
damascenone *(fruity, sweet)*	0.00075	4.3 (0.5) a **5797.2**	4.2 (0.7) a **5649.2**	4.5 (0.4) a **5933.5**	3.7 (1.5) b **4897.4**	4.0 (0.6) ab **5338.0**	0.011	Yes

Mean concentration values in µg/L. (± SD), SD is the variation between sample segments from the consumer acceptability test of 5 pineapple cultivars, n ≥ 8. Different letters in the same row indicate significant statistical differences (Tukey's HSD, P ≤ 0.05). NA: not available. OAVs > 1 are in bold.

Hierarchical clustering based on *overall liking* resulted in three distinct consumer clusters with consumers showing similar preferences in fruit profiles, as shown in **Figure 4.2** below. Details of consumer clustering analysis, AHC Dendrogram and ANOVA results are provided in Appendix 3, **Supplementary information C3, Figure C1** and Appendix 3, **Table C9**, respectively.

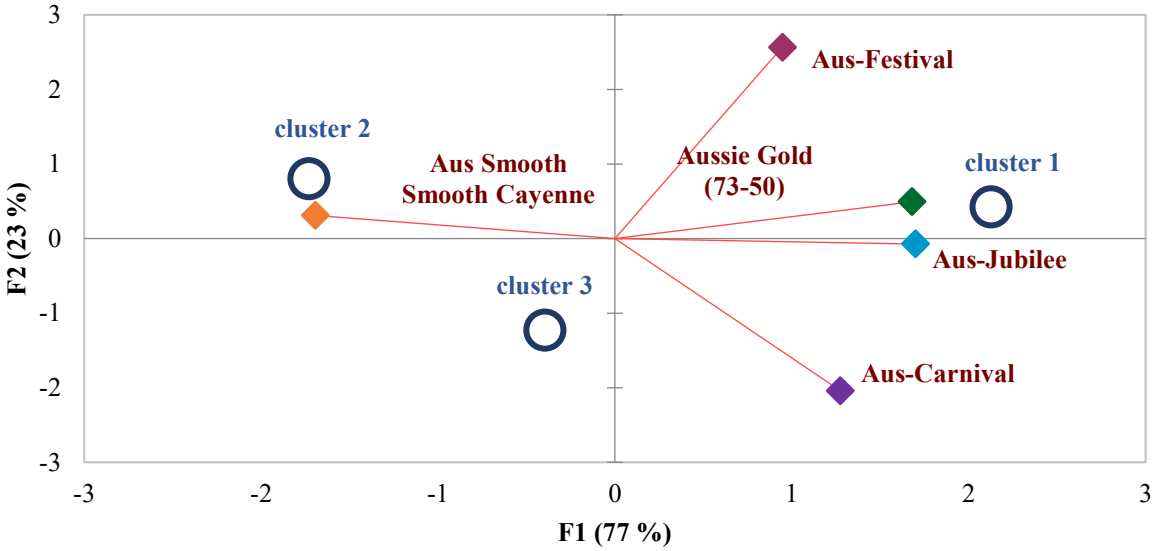


Figure 4.2 Preference map of pineapple cultivars and three consumer clusters (F1 v F2 100%).

Cluster 1 (n = 34), Cluster 2 (n = 43), and Cluster 3 (n = 38) exhibited distinct preferences for various cultivars. Based on overall liking, cluster 1 liked all pineapple cultivars; their least liked was 'Aus Gold'. Cluster 2 liked 'Aus Smooth' the most, followed by 'Aus Festival', 'Aussie Gold', and lastly. 'Aus Jubilee'. This cluster disliked 'Aus Carnival'. Cluster 3 was unique and lacked strong preferences for 'Aus Jubilee' and 'Aussie Gold', and further disliking 'Aus Festival'. This cluster liked 'Aus Carnival' and 'Aus Smooth'.

4.8.4 Sensory evaluation results

Trained panel assessment resulted in sensory profiles for each cultivar. The panel performance and quality of the sensory data was examined, and the results are given in Appendix 3, **Supplementary information C2**, **Tables C3**, **Table C4** and **Table C5**. Significant sensory attributes for appearance, aroma, flavour and texture were used to generate the PCA biplot shown in **Figure 4.3** on page 58. Sensory panel results and ANOVA table of sensory attributes are provided in Appendix 3, **Supplementary information C2**, **Tables C6**, **Table C7** and **Table C8**.

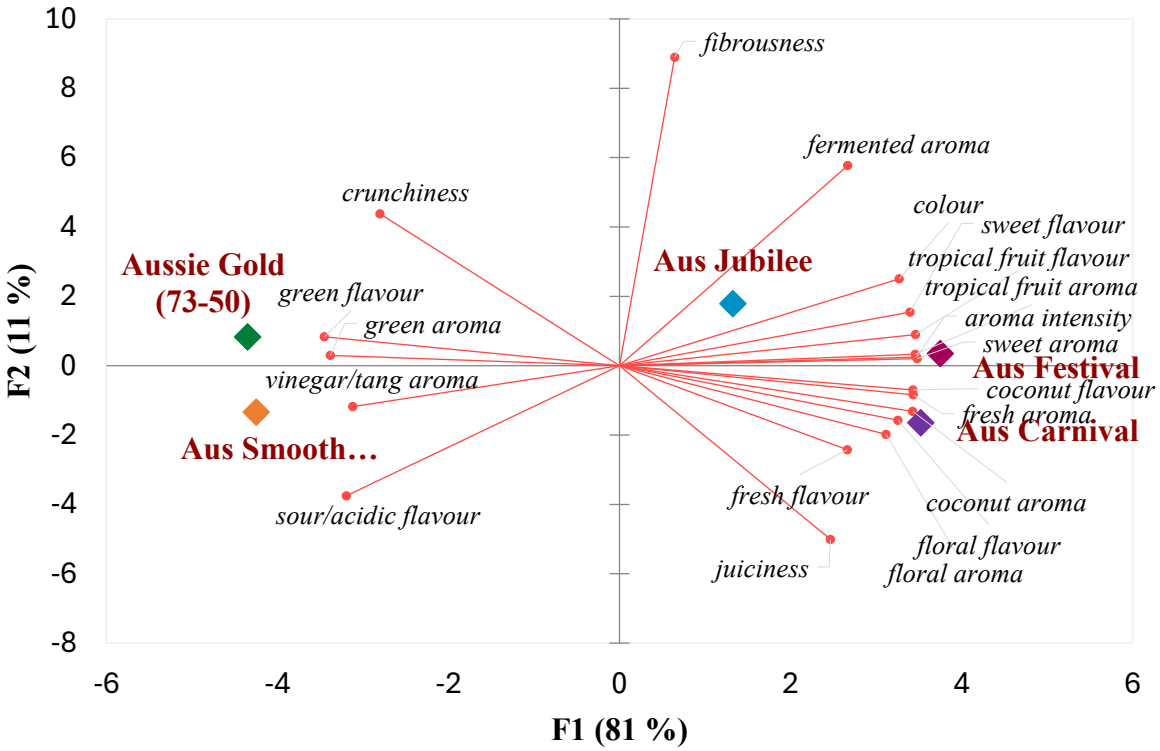


Figure 4.3 PCA biplot with sensory profiles of each pineapple cultivar (PC1 v PC2 92%)

The first two principal components (PC1 v PC2) explained 92% of the variation. The cultivars 'Aus Festival', 'Aus Jubilee' and 'Aus Carnival' were characterised by bright yellow flesh *colour*, *high aroma intensity* of *sweet, tropical fruit, coconut* and *fresh* aromas. These cultivars were also high in *sweetness, tropical fruit, coconut, fresh* and *floral* flavours, with high *juiciness*. 'Aus Carnival' had a slightly higher *vinegar/tang* aroma and *sour/acidic* flavour than 'Aus Festival' and 'Aus Jubilee. On the other end of the PC1, 'Aus Gold' and 'Aus Smooth' were characterised by light yellow flesh *colour* and low *aroma intensity* with distinct *vinegar/tang* and *green aromas*, and high *sour/acidic* and *green* flavours. These characteristic aroma and flavour attributes could be due to differences in ripeness levels as shown in **Figure 4.1** on page 53 and **Table 4.2** on page 52. Variations in fruit ripeness are reported as a key factor influencing the changes in the volatile profile of pineapple cultivars (S. Liu et al., 2024). Compared to 'Aus Smooth', 'Aus Gold' had a brighter yellow flesh *colour*, a stronger *sweet* flavour and a less *sour/acidic* flavour. Among all the cultivars, 'Aussie Gold' notably had the highest *crunchy* and lowest *juicy* texture.

4.8.5 Preference mapping: consumer clusters v sensory attributes

Preference mapping was performed to model the consumer and sensory data across the five pineapple cultivars. The resulting preference map is shown in **Figure 4.4** on page 59. The current study also

explored the 'similarity-dissimilarity' relationship between the consumer clusters and sensory attributes by the Pearson correlation matrix (Pearson (n-1)) as shown in **Table 4.5** on page 60.

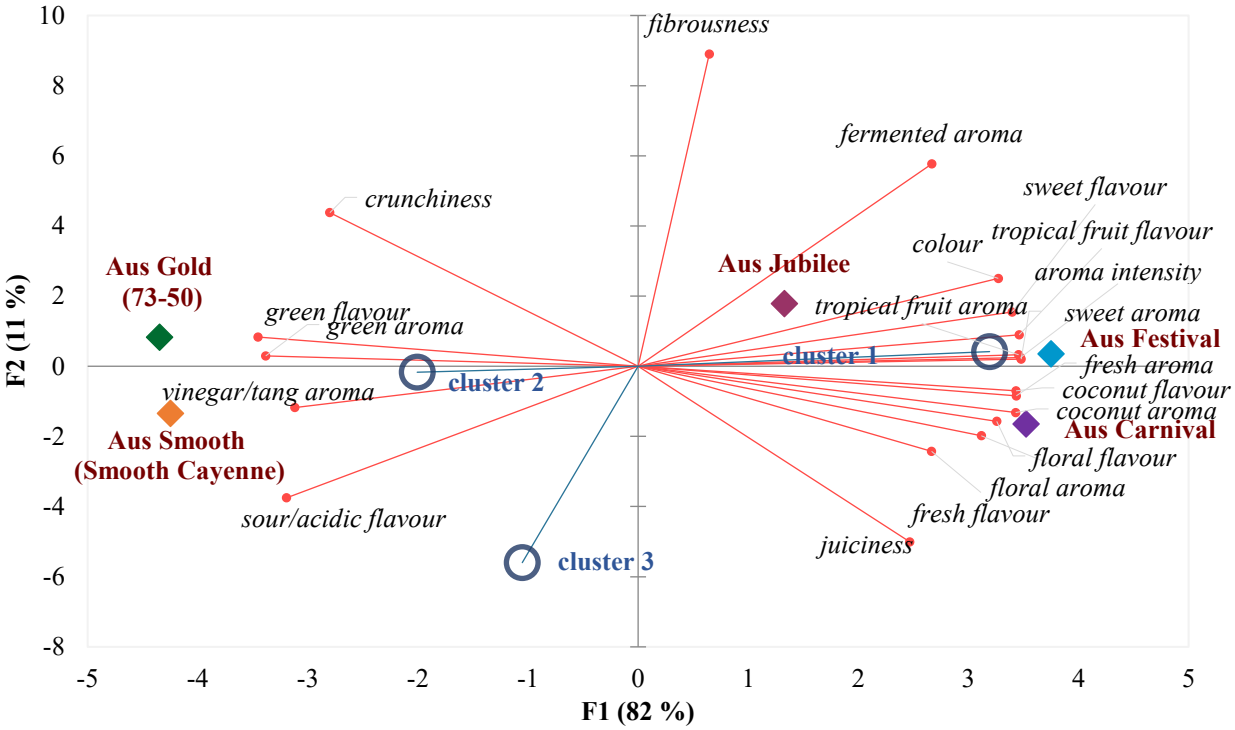


Figure 4.4 Preference map of consumer clusters and sensory attributes of five pineapple cultivars.

Consumers in cluster 1 liked all pineapple cultivars similarly but liked 'Aus Gold' slightly less for its distinct *green* and *vinegar/tang* aromas, *sour/acidic* and *green* flavours, and high *crunchy* texture. Consumers in this cluster favoured pineapples that have brighter yellow flesh *colour*, high *juiciness*, higher *aroma intensity*, *sweet, tropical fruit, coconut, fresh, floral* aromas and flavours. Consumers in this cluster favoured pineapples that have brighter yellow flesh *colour*, high *juiciness*, higher *aroma intensity*, *sweet, tropical fruit, coconut, fresh, floral* aromas and flavours and did not exhibit any liking towards distinct *green* and *vinegar/tang* aromas, *sour/acidic* and *green* flavours, and high *crunchy* texture. Consumers in cluster 2 showed a higher liking for 'Aus Smooth', particularly for its characteristic *sour/acidic*, *green* and *vinegar/tang* aroma and flavour attributes. Cluster 3 was a unique cluster where the consumers indicated their liking for 'Aus Carnival' and 'Aus Smooth', especially for their *juicy* texture. These consumers show a liking for a balance between *sour/acidic* and *fresh*, *floral* flavours.

Table 4.5 Similarity-dissimilarity matrix (Pearson (n-1)) of consumer clusters v sensory attributes

	cluster 1	cluster 2	cluster 3
cluster 1	1	-0.219	-0.459
cluster 2	-0.219	1	-0.239
cluster 3	-0.459	-0.239	1
colour	0.803	-0.641	-0.487
aroma intensity	0.871	-0.635	-0.305
sweet aroma	0.894	-0.589	-0.337
vinegar/tang aroma	-0.992	0.261	0.378
tropical fruit aroma	0.861	-0.675	-0.236
floral aroma	0.811	-0.349	-0.441
coconut aroma	0.858	-0.566	-0.281
green aroma	-0.920	0.419	0.454
fresh aroma	0.827	-0.689	-0.163
fermented aroma	0.762	-0.530	-0.423
crunchiness	-0.836	0.182	0.063
fibrousness	0.405	0.092	-0.664
juiciness	0.774	-0.099	0.052
sweet flavour	0.833	-0.686	-0.355
sour/acidic flavour	-0.847	0.566	0.540
tropical fruit flavour	0.880	-0.627	-0.349
floral flavour	0.746	-0.762	0.044
coconut flavour	0.859	-0.568	-0.341
green flavour	-0.928	0.500	0.276
fresh flavour	0.468	-0.900	0.309

The p-value threshold for a significant correlation is 0.05. The different shades of red represent a positive correlation coefficient while the different shades of blue represent a negative correlation coefficient. The intensity of the colour depends on the strength of the R2 correlation coefficient.

4.8.6 Preference mapping: sensory attributes v key aroma compounds

The profile of key aroma compounds and the sensory profile of the five pineapple cultivars are shown in the PCA biplot given in **Figure 4.5** on page 61, which explains 89% of the variation in key aroma compounds content across the five pineapple cultivars. Volatile compounds, particularly methyl esters, located in the top-right quarter of the biplot, were the primary contributors to higher scores given by trained panellists such as *fresh* aroma, *tropical fruit* flavour and aroma, *sweet* flavour and aroma, *coconut* flavour and aroma, *floral* flavour and aroma, *aroma intensity*. Terpenoid compounds such as alpha-terpineol, limonene, damascenone, and various ethyl esters, located in the top-left quarter of the biplot, were secondary contributors to higher scores by the panellists. As a result, the cultivars 'Aus Jubilee' and 'Aus Festival' with relatively higher levels of these compounds, higher °Brix: %TA ratio (**Figure 4.1** on page 53 and **Table 4.2** on page 52), along with a balanced *juiciness* and *fibrousness, and* higher scores given by trained panellists such as *fresh* aroma, *tropical fruit*

flavour and aroma, *sweet* flavour and aroma, *coconut* flavour and aroma, *floral* flavour and aroma, *aroma intensity*, were the drivers of higher consumer acceptability.

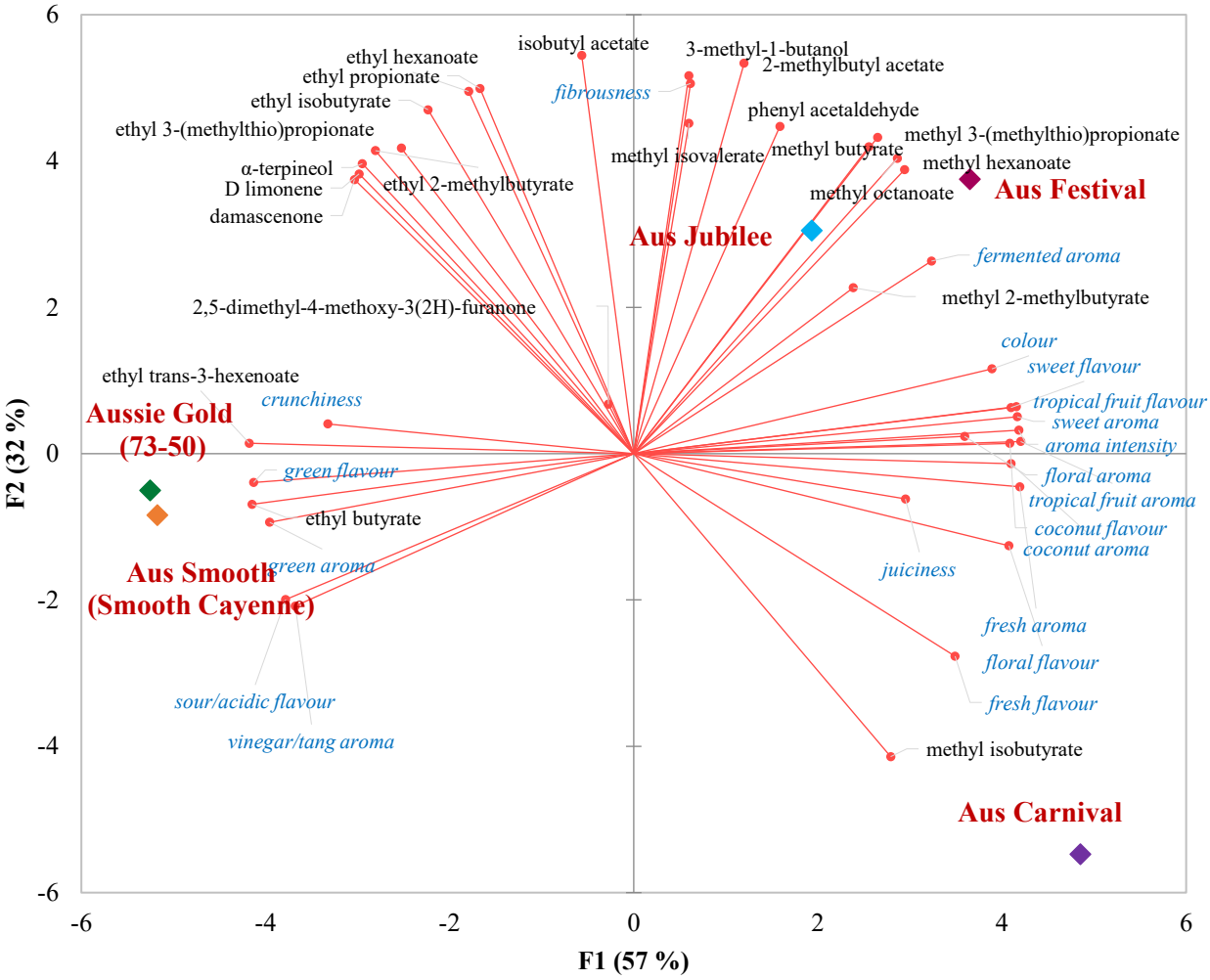


Figure 4.5 PCA biplot of the profile of key aroma compounds and the sensory profile of the five pineapple cultivars individual sample segments from consumer acceptability test, n ≥ 8 (PC1 v PC2 89%).

The cultivars 'Aussie Gold' and 'Aus Smooth' with relatively lower levels of methyl esters, lower °Brix: %TA ratio, along with higher scores given by trained panellists such as *green* flavour and aroma, *sour/acidic* flavour and *vinegar/tang* aroma, and are less in *aroma intensity*, made them least preferable for consumers. These results suggest that a balanced combination of sweetness, *tropical fruit* flavour and aroma, *sweet* flavour and aroma, *coconut* flavour and aroma, *floral* aroma and flavour could contribute to the overall flavour profile in relation to positive hedonic perception of pineapple.

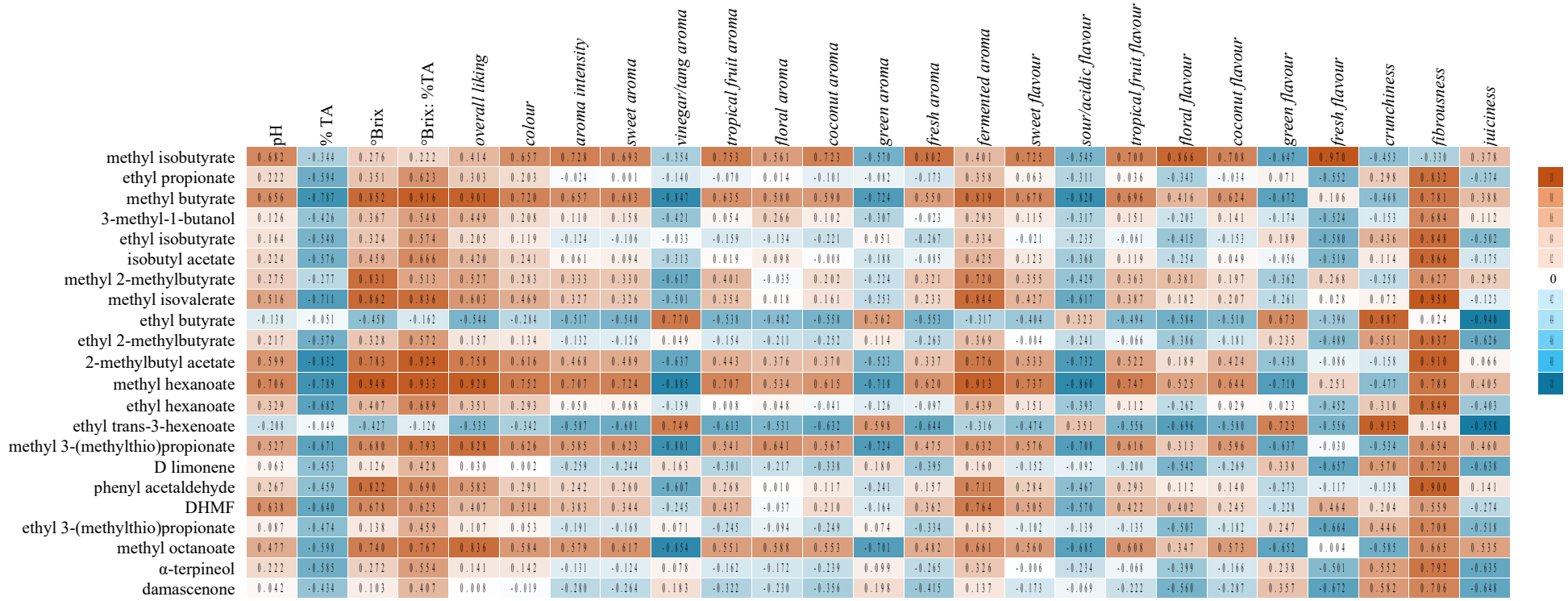
The current study also determined the relationship between the chemical composition, overall consumer liking and sensory profiles by the Pearson correlation matrix (Pearson (n-1)) as shown in **Table 4.6** on page 63. The *Overall liking* was positively correlated with °Brix, °Brix: %TA ratio,

flesh *colour*, *aroma intensity*, *sweet* flavour and aroma, *tropical* flavour and aroma, *floral* flavour and aroma, and *coconut* flavour and aroma. The *Overall liking* was negatively correlated with %TA, *vinegar/tang* aroma, *green* flavour and aroma, *sour/acidic* flavour. The *Overall liking* had a positive correlation with juiciness and fibrousness but was negatively correlated with crunchiness. These results implies that pineapple flavour could play a crucial role in the hedonic perception of pineapple. The *overall liking* was also positively correlated to majority of the targeted key aroma compounds. Compounds such as methyl isobutyrate (*fruity, sweet*), methyl butyrate (*fruity sweet*), 2-methylbutyl acetate (*fermented, sweet, balsamic*), methyl hexanoate (*pineapple, fruity*), methyl 3-(methylthio)propionate (*meaty, onion-like*), 2,5-dimethyl-4- methoxy-3(2H)-furanone (*caramel, roasty, sweet*) and methyl octanoate (*fruity*) were positively correlated to the overall liking, *sweet, tropical, floral, coconut* and *fresh*, aroma and flavour attributes.

The Pearson correlation matrix obtained in this study, could not establish a positive correlation between some of the previously reported aroma compounds. Compounds such as ethyl butyrate (*fruity*) and ethyl trans-3-hexenoate were correlated with the *vinegar/tang*, *green*, *sour/acidic* aroma and flavour attributes were negatively correlated to the overall liking.

It is important to note that, the contribution of other VOCs and interaction (masking, additive, and synergistic effects) of the key aroma compounds and other VOCs present in pineapple, also play an important role toward the aroma of pineapples (George et al., 2023; Sengar et al., 2022; Teai et al., 2001; Xiao et al., 2021).

Table 4.6 Correlation matrix (Pearson (n-1)) of individual sample segments from consumer acceptability test of pineapple, n ≥ 8 and chemical composition, overall consumer liking and sensory scales.



The p-value threshold for a significant correlation is 0.05. The different shades of blue represent a positive correlation coefficient, while the different shades of red represent a negative correlation coefficient. The intensity of the colour depends on the strength of the R2 correlation coefficient. The scale on the right indicates the interpretations of different colours.

4.9 Limitations of current study

The application of OAVs to compare odour volatile contribution has been reported previously (Akioka & Umano, 2008; Berger et al., 1985; Pino, 2013; Spanier et al., 1998; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Wei et al., 2014). However, the method utilised in that study could not approach the OAV of some compounds due to the lack of a suitable internal standard to detect aroma volatiles present at low levels. Future work should consider developing method for ethyl acetate (CAS No. 141-78-6); 4-Hydroxy-2,5-dimethyl-3(2H)-furanone (CAS No. 3658-77-3); δ-octalactone (CAS No. 698-76-0); methyl 3-acetoxyhexanoate (CAS No. 21188-60-3); methyl 5-acetoxyhexanoate (CAS No. 35234-22-1); isoamyl acetate (CAS No. 123-92-2); acetaldehyde (CAS No. 75-07-0); δ-decalactone (CAS No. 705-86-2); 1-(3E,5Z)-3,5-undecatriene (CAS No. 19883-27-3); vanillin (CAS No. 121-33-5); isovaleraldehyde (CAS No. 590-86-3); 2-Methylbutyraldehyde (CAS No. 96-17-3) and 1-(E,Z,Z)-3,5,8-undecatetraene (CAS No. 29837-19-2), which George et al., 2023 (George et al., 2023) identified as also key aroma compounds. Availability, separation and detection issues prevented these compounds from being included in the present work.

This study did not specifically test for anosmia/hyposmia to furaneol or any single compound, however, the panel was screened for sensory acuity as were trained and experienced with similar descriptive studies (Meilgaard et al., 2006). This study could not perform the aroma omission and reconstitution test in combination with GC-O, due to the unavailability of instrument, limiting the scope of identifying the impact of synergetic, masking and additive effect, and confirming the actual contributions of selected key aroma compounds towards the overall aroma of pineapple. Potential artifacts from the analytical instrument and conditions have been reported (George et al., 2023). Future work should incorporate the latest recommendations (Reinhardt & Steinhaus, 2025) to address the challenges associated with high-temperature injection of analytes. It is possible, as a future direction, to conduct aroma omission and reconstitution tests using GC-O to more accurately assess the sensory relevance of individual and interactive aroma compounds. Another major limitation of this study was the restricted diversity among the commercial cultivars selected, which consequently constrained the exploration of associations between sensory attributes and key aroma volatiles; future studies incorporating a broader range of cultivars may offer deeper insights into these relationships

4.10 Conclusions

Australian-grown commercial pineapple cultivars show significant variations in key aroma compounds, which greatly influence their sensory attributes and consumer preferences. The study found that certain key aroma compounds are associated with *sweetness*, *tropical fruit flavour*, *coconut*

notes, *floral* aroma, and overall *sweet* flavour. 'Aus Festival' and 'Aus Jubilee' were the most liked for their high levels of desirable aroma and flavour compounds, balanced *sweetness*, and *juiciness*. Conversely, 'Aussie Gold' and 'Aus Smooth' were less favoured because of their lower levels of these compounds and higher levels of *green* and *sour* flavour. Overall liking of the fruit was primarily driven by its *sweetness* and key aroma compounds. However, factors such as cultivar type, fruit maturity, environmental conditions, and their interactions can alter pineapple attributes and composition, leading to a wide range of sensory experiences. The Pearson correlation matrix showed that overall liking was positively correlated with *sweetness*, *tropical* and *floral* flavours, and *aroma intensity*, while negatively correlated with *sour* and *green* flavours. These findings highlight the importance of specific volatile compounds, like methyl and ethyl esters and terpenoid compounds, in enhancing the sensory experience and consumer acceptability of pineapples, catering to diverse consumer preferences. Additionally, ripeness was a key driver of the sensory differences observed in this study, particularly influencing green and sour flavour attributes. This aligns with findings in tropical fruits such as mango, papaya, and pineapple, where ripening stages significantly alter volatile profiles and sensory perception (e.g., sweetness, acidity, and aroma intensity). For instance, in mango, unripe stages are associated with higher levels of green and sour notes due to compounds like hexanal and cis-3-hexenol, which diminish as ripening progresses (Pino & Mesa, 2006). Similarly, pineapple and passion fruit exhibit marked changes in ester and sulphur compound concentrations during ripening, directly impacting flavour acceptability(Brat et al., 2004; Elss et al., 2005; Umano et al., 1992). These variations present a common challenge in horticultural research, where fruit availability and consistent ripeness across samples are difficult to control, often leading to variability in sensory and chemical data. Addressing this challenge requires improved postharvest handling and ripeness standardisation protocols to ensure reproducibility and comparability across studies. Despite these challenges, this study provides a better understanding of the complex relationship between compositional factors and sensory attributes linked to consumer preferences of different pineapple cultivars. The findings of this study could be used in future selection and breeding of superior pineapple cultivars.

Chapter 5 Genome-Wide Association of Volatiles Reveals Candidate Gene Markers for Pineapple Aroma

Building upon the previous research described in this thesis, which identified key aroma compounds in pineapple and elucidated their relationship to sensory perception, the study presented in this research chapter advances our understanding by exploring the genetic underpinnings of volatile organic compounds (VOCs) production. Fruit aroma and flavour volatiles are central to consumer preference and overall pineapple fruit quality, with VOCs synthesised through intricate biochemical pathways governed by genetic regulation and environmental conditions.

In this study, an integrated analysis of the chemical composition, sensory attributes, and their potential associations with the genetics of pineapple is presented. This study aims to identify genetic loci associated with traits influencing pineapple flavour and aroma, using genome-wide association studies (GWAS), including GAPIT, 3mrMLM and BGLR.

Two different pineapple populations from the Queensland Department of Primary Industries (DPI) breeding program were analysed. In 2022, 196 fruits from the Maroochy Research Facility (MRF) were assessed for compositional traits such as colour parameters, flavour rating, °Brix, pH, titratable acidity, organic acids, sugars, and key aroma volatiles. In 2024, 154 additional fruits were evaluated, with a subset undergoing similar but limited compositional analysis, and all samples subjected to sensory evaluation at the Queensland Alliance for Agriculture and Food Innovation (QAAFI) sensory laboratory.

The phenotypic data collected across both years provided a robust foundation for GWAS. Genotypic data were aligned with the F180 'Smooth Cayenne' pineapple reference genome (Fang et al, unpublished), and single-nucleotide polymorphisms (SNPs) were used to map genetic variation associated with VOC expression. Traits were categorised into *tropical fruit, cucumber, coconut, sweet/honey, fermented, floral, other, no-aroma*, and *aroma intensity* to facilitate targeted analysis. Multi-model GWAS enabled the identification of robust, significant marker-trait associations.

The findings presented here offer novel insights into the genetic control of pineapple flavour and aroma. These results not only enhance our understanding of the biochemical and sensory complexity of pineapple but also provide valuable molecular markers for breeding programs aimed at improving fruit quality and consumer appeal.

Author contributions for this chapter are summarised in **Table 5.1** on page 67.

Table 5.1 Author contributions in Chapter 5

	Jenson George	Garth Sanewski	Thoa Nguyen	Sharon Pun	Craig Hardner	Heather E. Smyth
Conceptualisation	x	x				x
Methodology	x	x				x
Software	x	x				x
Validation						
Formal analysis	x					
Investigation	x	x			x	x
Resources	x	x		x	x	x
Data Curation	x	x		x		x
Writing - Original Draft	x					
Writing - Review & Editing	x	x	x		x	x
Visualisation	x	x	x		x	x
Supervision		x	x		x	x

5.1 Introduction

Pineapple (*Ananas comosus*) is the third most important non-climacteric tropical fruit globally, valued for its sweet, aromatic flavour and nutritional benefits. Traditional breeding programmes have primarily targeted agronomic traits such as yield, disease resistance, and environmental adaptability. However, flavour, an essential determinant of consumer preference, has often been underemphasised due to its scientific complexity and the high cost of phenotyping.

Flavour in pineapple is shaped by a dynamic interplay of sugars, organic acids, and volatile organic compounds (VOCs), with VOCs being central to aroma perception. Over 480 VOCs have been identified in pineapple, though only a subset (~40) significantly contributes to its characteristic aroma profile (George et al., 2023). Esters, particularly methyl and ethyl esters, dominate the VOCs landscape, imparting fruity and tropical notes, while lactones, aldehydes, and furanones enhance sweet and floral nuances (El Hadi et al., 2013; George et al., 2025; Holt et al., 2019; Mostafa et al., 2022).

Results described in Chapters 3 and 4, involving the profiling of five Australian pineapple cultivars, revealed a suite of VOCs closely associated with favourable sensory attributes (George et al., 2024; George et al., 2025). Ester compounds emerged as the most influential contributors to sensory scoring of descriptors such as *tropical*, *sweet*, *coconut*, and *floral* aromas. Key compounds included 2-methylbutyl acetate (CAS 624-41-9), methyl isovalerate (methyl 3-methylbutanoate; CAS 556-24-1), methyl isobutyrate (methyl 2-methylpropanoate; CAS 547-63-7), methyl 3-(methylthio) propionate (methyl 3-methylsulfanylpropanoate; CAS 13532-18-8), methyl 2-methylbutyrate (CAS 868-57-5), methyl hexanoate (CAS 106-70-7), methyl octanoate (CAS 111-11-5), 3-methyl-1-butanol

(CAS 123-51-3), and phenylacetaldehyde (CAS 122-78-1), and a range of ethyl esters such as ethyl hexanoate, ethyl butyrate, and ethyl 2-methylbutyrate. Terpenoids like furaneol, α-terpineol, d-limonene, and damascenone also played a significant role in enhancing aroma complexity and consumer appeal (George et al., 2025). However, it should be noted that not all key aroma compounds were included in the previous studies (George et al., 2024; George et al., 2025).

High hedonic consumer ratings were linked to flavour profiles characterised by high °Brix to titratable acidity ratios and the presence of esters and terpenoids, while titratable acidity and green and acidic taste correlated with lower consumer preference. While this was largely due to fruit ripeness during consumer evaluation (Chapter 4), these findings underscore the importance of VOC composition in shaping pineapple flavour and provide a foundation for targeted breeding strategies.

Genome-wide association studies (GWAS) and linkage mapping have emerged as powerful tools to dissect the genetic basis of aroma traits (El Hadi et al., 2013; Holt et al., 2019; Mostafa et al., 2022). Platforms like GAPIT (Wang & Zhang, 2021) and 3VmrMLM (Zhang et al., 2020) facilitate the identification of loci associated with VOCs. Integration of GWAS with analytical platforms such as gas chromatography-mass spectrometry (GC-MS) has enabled the mapping of specific aroma compounds to genetic markers.

Despite their importance, the genetic regulation of ester biosynthesis remains incompletely understood. Several candidate genes, such as Alcohol Acyltransferase (AAT), Alcohol Dehydrogenase (ADH), Acetyl-CoA Carboxylase (ACC), Acyl-CoA synthetase (ACS), and S-Acyltransferase, are reported (Colonges et al., 2022; Fan et al., 2021; Larsen et al., 2019; Soomro et al., 2023), to be involved in the expression of VOCs in plants, fruits and vegetables, which are also regulated by developmental and environmental cues. In apples, AATs are involved in the formation of esters from alcohols and acyl-CoAs (Dudareva et al., 2013; Lai et al., 2024; Soomro et al., 2023). In fruits like strawberry and apricot, AAT expression increases during ripening, correlating with ester accumulation (Lu et al., 2024).

In this study, we integrate targeted VOCs profiling with GWAS to elucidate the genetic determinants of pineapple aroma. By evaluating genotypes cultivated under uniform conditions in Queensland, we aim to identify candidate genes and molecular markers associated with desirable flavour traits. These insights will inform the development of flavour-enhanced pineapple cultivars through precision breeding strategies.

5.2 Materials and methods

5.2.1 Chemicals, reagents and standards

Neat reference standards of the aroma compounds listed in Chapter 3, **Table 3.2** on page 34 (based on the 40 key aroma compounds identified and described in Chapter 2 (George et al., 2023), and hyper grade for LC-MS LiChrosolv isopropanol were obtained commercially from Merck (Sigma Aldrich), New South Wales, Australia. The labelled internal standards, ethyl 2-methylbutyrate-d9 (D-7676), ethyl hexanoate-d11 (D-7060), octanal-d16 (D-6929), ethyl octanoate-d15 (D-7063), were obtained commercially from CDN isotopes, Quebec, Canada, through PM Separations Pty Ltd, Queensland, Australia. Matching aroma-free sample matrix, and standard stock solution containing the reference standards of the key aroma compounds, and the sample vials for VOCs analysis were prepared by following the conditions outlined in Chapters 2 and 3 (George et al., 2024; George et al., 2023).

Authentic reference standards of citric acid (CAS No. 77-92-9, Merck Cat. No. C0759), L-malic acid, (CAS No. 97-67-6, Merck, Cat. No. M1000), fructose (CAS No. 57-48-7, Merck Cat. No. F0127), glucose (CAS No. 50-99-7, Merck Cat. No. G5767), sucrose (CAS No. 57-50-1, Merck, Cat. No. S0389) were sourced from Merck Australia. 0.1M (0.1N) sodium hydroxide solution UN1824 (SL131-2.5L-P) was sourced from Chem-Supply Pty Ltd, Australia.

5.2.2 Plant material

Pineapple (*Ananas comosus)* samples were sourced from the Queensland Department of Primary Industries (QDPI) breeding program at the Maroochy Research Facility (MRF), Nambour, during the 2022 and 2024 harvest seasons. A genetically diverse subset of about 200 accessions, representing domestic pineapple germplasm, was selected for comprehensive phenotypic and genotypic analysis, separately for the years 2022 and 2024 as shown in **Table 5.2** below. Fruits were cultivated under uniform agronomic conditions to minimise environmental variability.

Table 5.2 Samples by year and traits measured

Year	No. of Samples	Traits Assessed	GWAS Model
2022	196	pH, °Brix, %TA, Organic Acids, Sugars, Colour, Flavour Rating, Volatiles	GAPIT, BLINK, 3VmrMLM
2024	154	pH, °Brix, %TA, Sensory (Trained Panel)	BGLR

5.2.3 Sample preparation and presentation for sensory evaluation

Summer fruit samples from 2022 were halved lengthwise, and colour parameters (L, C, h, a*, b*) were measured alongside flavour ratings by the plant breeder. Approximately 300 g of the longitudinal

mid-section was vacuum-packed and stored at –20°C for physicochemical analysis. Spring fruit samples from 2024 were delivered fresh to the QAAFI sensory laboratory, University of Queensland, Long Pocket campus, and were stored in a 'climatic chamber' (aralab) at 10°C, 85% humidity, for 2 days. On the day of sensory studies, the individual fruits were peeled, and the top and bottom thirds were removed. The remaining flesh was cut into four equal quarters, with cores removed. These quarters were then sliced into 1.5 mm thick segments (10-15 g each) and served to assessors in plastic pots labelled with a three-digit blinding code and a composite letter. The fruit samples were then evaluated fresh by a trained sensory panel. A subset of these samples was also analysed for colour parameters, while another subset was stored at –20°C for subsequent physicochemical testing. For both the 2022 and 2024 samples, chemical analysis involved partial thawing, dicing, and homogenisation using a Retsch MM500 vario ball mill under ice-cold conditions to preserve volatile compounds. Homogenates were aliquoted into headspace vials and stored at –80°C for volatile analysis. Additional aliquots were used to measure °Brix, pH, titratable acidity (TA), and to profile sugars and organic acids. The primary objective of this study was to generate phenotypic data to link VOCs with sensory traits, and to facilitate a GWAS aimed at identifying correlations between these traits and underlying genetic markers.

5.3 Flavour rating

For 2022 samples, a simple and in situ system was developed by the plant breeder to provide background information for sorting, with flavour ratings conducted while the samples were still fresh, prior to vacuum packing. The initial 1-7 scale (n=1) served as a guide for selecting samples for further analysis. Given the high volume of samples (approximately 50 or more per day), it was challenging to rate them with more detailed definitions. However, the 1-7 scale proved effective. The flavour ratings were as follows: *acid* =1, *bland/unpleasant*=2, *slight flavour*=3, *sweet*=4, *aromatic/coconut*=5, *fruity*=6, *floral*=7. The term "aromatic" was used to encompass all aromatic profiles that could not be easily separated into distinct notes.

5.4 Sensory Evaluation

A descriptive sensory evaluation, 'Check-All-That-Apply' (CATA), was conducted on the 2024 sample set using a semi-trained panel at the QAAFI sensory laboratory, University of Queensland, Long Pocket campus. A List of CATA attributes is summarised in Appendix 4, Table D3. This study was approved by the Human Ethics Committee of the University of Queensland and the Australian National Statement of Ethical Conduct in Human Research (approval number: 2019002607). The study employed RedJade® sensory software for data collection and panel management. Among the

14 trained panellists (comprising 4 males and 10 females) aged between 28 and 61 years, 12 individuals, as available, participated in sensory evaluation sessions conducted over an 18-day period. Each panellist had prior experience in descriptive analysis and underwent refresher training prior to the study. The panellists attended a 60-minute training session on the first day of assessment, which focused on CATA attributes, sample trial assessment, and familiarisation with the smelling and eating protocol under the guidance of the panel leader. During formal evaluation, the panel assessed aroma attributes across 15 or more distinct samples using a consensus vocabulary developed in alignment with previous tropical fruit aroma studies (Chapter 4). Sessions were conducted under controlled lighting and temperature conditions, with randomised sample presentation to minimise bias. Over 18 non-consecutive days spanning three months, a total of 327 individual fruit samples were evaluated. The number of samples assessed per day ranged from 15 to 31. Some samples were repeated across sessions, although not in a systematic pattern.

5.5 Physicochemical Analysis:

°Brix: A 2 mL centrifuge tube containing pineapple composite puree (prepared as per section 3.2.2) was centrifuged at 14,000 rpm at ambient temperature in a bench-top centrifuge (Beckman Coulter Microfuge 18). Two to three drops of the supernatant were transferred to a refractometer (Atago Pocket Refractometer), and the °Brix was measured.

5.5.1 pH, °Brix and Titratable Acidity

The °Brix, pH and titratable acidity of the samples were measured using the previously explained conditions outlined under Chapter 4, sections 4.5.1 and 4.5.2, respectively.

5.5.2 Organic acids and sugars by HPLC

5.5.2.1 Sample extraction

Approximately 5 g of the puree was accurately weighed into two 50 mL centrifuge tubes, and 15 mL MilliQ water was added. The contents were mixed and sonicated for 10 minutes with occasional shaking. Extracts were centrifuged for 10 min at 4000 rpm at 20°C, and the resulting supernatant was decanted into another 50 mL centrifuge tube. The residue left behind was re-extracted 2 more times in the same way using the same volume of MilliQ water. The combined supernatants were made up to 50 mL with the extracting solution and mixed well. The resulting diluted solution was filtered through a 13 mm 0.45 µm nylon syringe filter into two glass HPLC vials for organic acid and sugar analysis.

5.5.2.2 HPLC Method for Organic Acids

The filtered (0.45 µm Nylon syringe filter) extracts were analysed using a Shimadzu HPLC system consisting of a system controller (SCL-10Avp), degasser (DGU-14A), low pressure gradient forming switching valve (FCV-10ALvp), pump (LC-10ATvp), auto-sampler (SIL-20ATHT), column oven (CTO-10Avp), photodiode array detector (SPD-M10Avp), and equipped with LabSolutions software. Chromatographic separation was performed with an ion-exclusion column (BIO-RAD Aminex HPX-87H, 300 x 7.8 mm, Cat. No. 125-0140) and a matching guard column at 50°C. The mobile phase consisted of 0.01N (5mM) H_2SO_4 in MilliQ water (prepared by adding 280 µL of conc H_2SO_4 to approximately 250 mL of MilliQ water, then diluting to 1 L volumetrically). Separation was achieved by isocratic elution at a flow rate of 0.6 mL/min over 20 mins. The injection volume was 20 µL, and detection was monitored at 210 nm. Calibration equations were determined from the correlation between peak area and standard citric and malic acid concentrations. The citric and malic acid contents of the pineapple flesh were calculated using the calibration equations and expressed as mg/g FW after applying the appropriate dilution factors.

5.5.2.3 HPLC Method for Sugars

The samples were filtered (0.45 µm Nylon syringe filter) and analysed using a Shimadzu HPLC system consisting of a system controller (SCL-10Avp), degasser (DGU-14A), low pressure gradient forming switching valve (FCV-10ALvp), pump (LC-10ATvp), auto-sampler (SIL-20ATHT), column oven (CTO-10Avp), RI detector (RID-10A), and equipped with LabSolutions software. RP-HPLC was conducted using an NH2 column (Supelco LC-NH2, 5 µm, 4.6 x 250 mm) and matching guard column at 40°C. The mobile phase consisted of 85% v/v acetonitrile in water. Separation was achieved by isocratic elution at a flow rate of 1 mL/min over 20 mins. The injection volume was 10 µL. Calibration equations were determined from the correlations between peak area and standard fructose, glucose, and sucrose concentrations. The fructose, glucose, and sucrose content of the pineapple flesh was calculated using the calibration equations and expressed as mg/g FW after applying the appropriate dilution factors.

5.5.3 Volatile Analysis by GC-MS

For 2022 samples, sample vials (stored at -80°C, section 5.2.3) with pineapple puree (~0.5 g) were opened and added saturated sodium chloride solution (4.45 mL), and mixed internal standard solution (50 µL). The vials were immediately sealed with the screw cap and taken for GC-MS injections. The previously developed (Chapter 3, Section 3.2.5) and the published (George et al., 2024) validated, matrix-matched-GC-MS-HS-SPME-SIDA method was employed to accurately quantify the targeted

key aroma compounds. The 2024 samples were not tested for their VOC profile or the profiling of sugars and organic acids due to the unavailability of a GC-MS instrument and other associated resources.

5.6 Statistical analysis

Using multivariate statistical analysis, this chapter investigated the intricate relationship between the chemical composition, sensory profile, and varietal differences of samples harvested in the years 2022 and 2024. These analyses were performed using the XLSTAT® software premium versions 2022.3.2-2025.1.0 (Addinsoft, Paris, France).

5.7 Genotyping and SNP Analysis

Molecular marker development: Freeze-dried leaf base samples (white tissue) were supplied to Diversity Arrays Pty Ltd for DArTseq marker development. Based on a previous study, the combination of restriction enzymes PstI and MseI was considered as suitable (Kilian et al., 2016). Seedling DNA samples were processed in digestion/ligation reactions, and the data processed by DArT PL's proprietary SNP and silico-DArT calling algorithms contained in the software program DArTsoft14 as per Kilian et al., 2012 (Kilian et al., 2012) and Sanewski et al. (2017). (Sanewski, 2020)

Marker sequences were aligned against the unpublished version 4 of the phased, long-read genome assembly of the pineapple cultivar 'Smooth Cayenne' clone F180 (F180v4HA and F180v4HB) (Personal communication, J. Fang, QAAFI, 2024).

5.7.1 Marker analyses

A total of 40,686 SNP markers for 1,024 taxa were produced and aligned to the F180v4 haplotype assemblies by Diversity Arrays Pty Ltd and provided in a HapMap format file. The markers were filtered by call rate (>95%) and minor allele frequency (>0.025). Markers on duplicated positions were removed. Taxa with very high null allele counts were removed. Missing marker calls were imputed using the LD KNNi algorithm in TASSEL 5.2.93 (Bradbury et al., 2007; Money et al., 2015). The accuracy of imputation was tested by masking 10% and comparing the imputed file with the original. The accuracy was 95%. Markers not positioned on any of the 25 chromosomes were removed. A total of 11,987 markers remained for analysis. The marker file was further filtered to include only the taxa of interest in the current study.

5.8 Genome-Wide Association Study (GWAS)

A genome-wide association study (GWAS) was conducted to identify single-nucleotide polymorphisms (SNPs) associated with biochemical and sensory traits in pineapple. The analysis was performed in R (v4.3.2) using the GAPIT and 3VmrMLM packages. Multi-loci mixed linear models were applied with principal components (PC3) and kinship (Van Raden) to account for population structure and relatedness. Phenotypic data included key aroma compounds and sensory attributes, which were analysed alongside genotypic data comprising SNP markers (196 samples × 11,987 markers in 2022, and 154 samples ×11,987 markers in 2024). Model fit was assessed using quantile-quantile (QQ) and Scree plots. Manhattan and QQ plots were generated to visualise significant associations and model performance.

5.9 Bayesian Generalised Linear Regression (BGLR)

The Bayesian Generalised Linear Regression (BGLR) package was used with the logistic regression model to analyse binary-type and categorical Check-All-That-Apply (CATA) sensory data collected from 2024 samples (Pérez & de los Campos, 2014).

5.10 Results and discussion

5.10.1 Metabolomic Diversity Among Pineapple Genotypes

To assess genotypic variation, the minimum, maximum, and range of all measured metabolites and fruit quality traits were evaluated. Analysis of variance (ANOVA) was conducted using genotype codes, incorporating compositional data, sensory flavour scores, flavour rating and colour ratings. Principal component analysis (PCA), performed using XLSTAT, served as an unsupervised method to identify traits contributing to phenotypic variability and to evaluate the influence of genetic background on fruit quality and metabolite profiles.

PCA revealed clear genetic differentiation among pineapple genotypes. Separate PCA plots for the 2022 and 2024 datasets (**Figure 5.1** on page 76 and **Figure 5.2** on page 77), which included non-volatile traits (pH, °Brix, titratable acidity, sugars, organic acids), sensory ratings, and VOCs, demonstrated substantial chemical diversity. The PCA explained 27% of total variance in 2022 and 58% in 2024, underscoring the potential of integrating metabolomic and genomic data in pineapple breeding programs. An additional PCA conducted exclusively on the 2022 samples for VOCs was included to confirm the specific influence of VOCs on the genetic variation among samples, and the PCA biplot is presented in Appendix 4, **Figure D1**.

For the 2022 pineapple samples (n=1), 26 key aroma compounds were profiled, including esters, lactones, aldehydes, and furanones - classes known to define the fruity aroma of pineapple. Esters such as methyl hexanoate, methyl butanoate, ethyl hexanoate, and methyl 2-methylbutanoate were the most abundant and consistently detected across genotypes. These findings align with prior studies identifying esters as dominant contributors to pineapple aroma (George et al., 2024; George et al., 2023; George et al., 2025) (Steingass, Jutzi, et al., 2015). As previously reported (George et al., 2025), a high °Brix to titratable acidity ratio, combined with desirable aroma compounds, was significantly associated with preferred sensory attributes such as *tropical fruit, floral, fruity, sweet/honey, and aromatic/coconut* notes - key drivers of consumer liking.

Limitations such as the lack of sample reproducibility and the absence of VOCs data for the 2024 pineapple samples hindered direct correlation between VOCs profiles and sensory attributes. Working with seasonal horticultural crops such as pineapple, mango and strawberry presents significant challenges due to the narrow harvest windows, variability in fruit ripeness, and the high cost of field trials, all of which are further compounded by climatic unpredictability; for instance, mango cultivars exhibit marked differences in flowering and fruit set under varying microclimatic conditions, affecting both yield and quality (Hafiz Mohkum Hammad, 2025). Despite these constraints, this study provides a foundational framework for future research into the genetic and biochemical determinants of pineapple flavour.

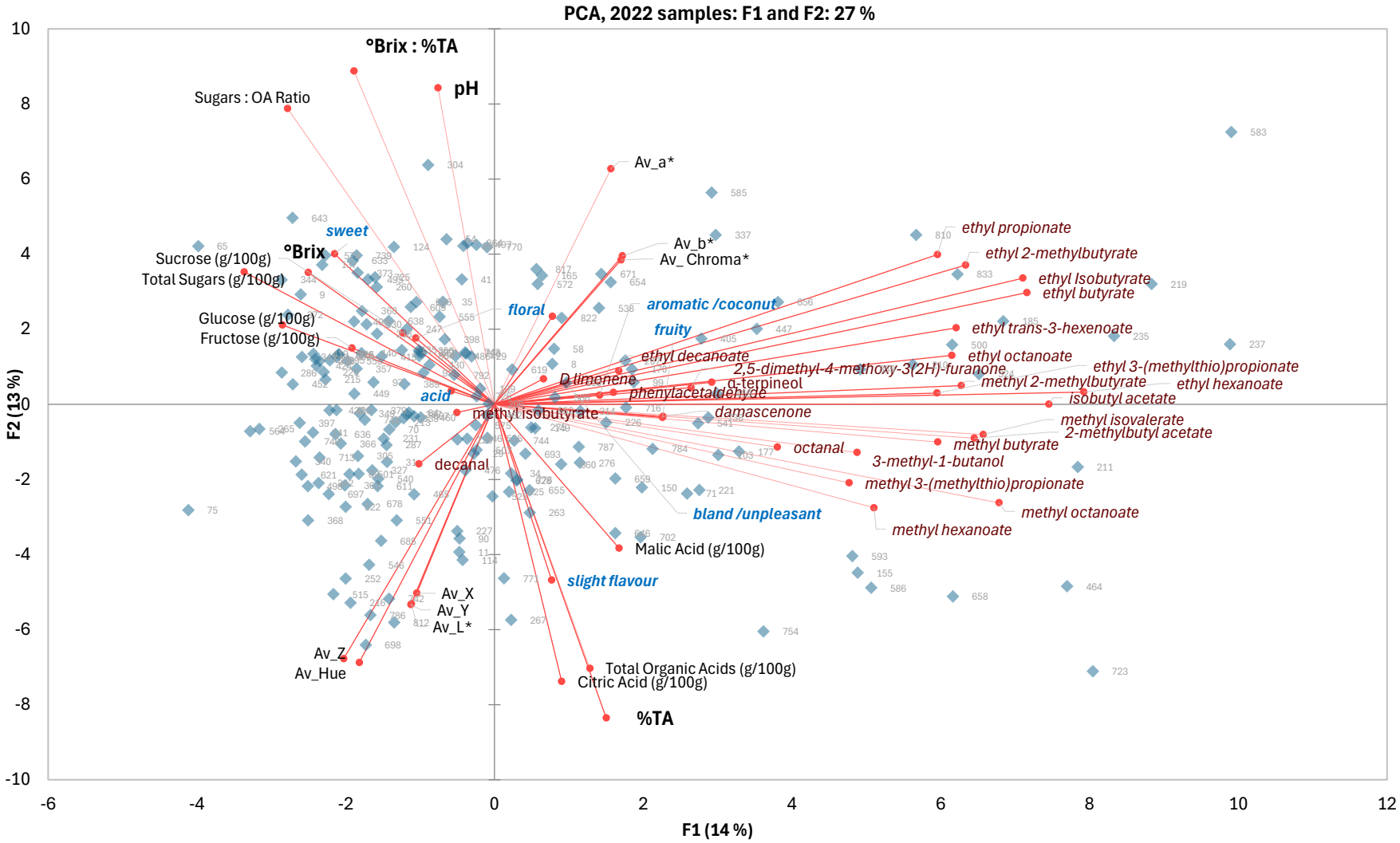


Figure 5.1 PCA 2022 non-volatile, flavour rating, and volatile data showing the diversity of genetic population samples (n=1)

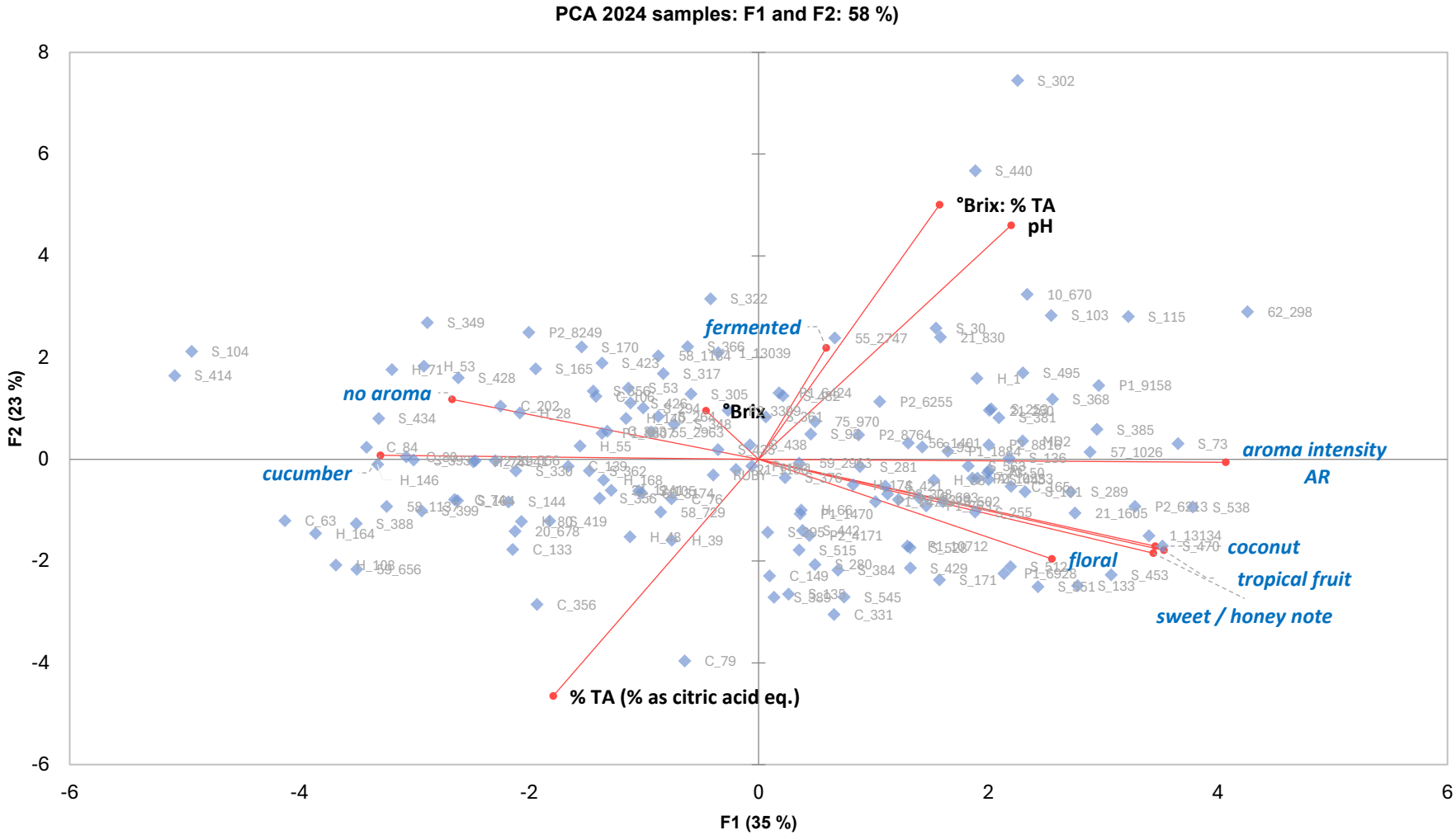


Figure 5.2 PCA 2024 non-volatile and sensory attributes (CATA) showing the diversity of genetic population samples (n=1)

5.10.2 Genome-Wide Association Studies (GWAS)

From the genome-wide association study (GWAS) conducted on the 2022 summer harvest samples of pineapple using the HA and HB haplotype reference assembly, loci were identified that are associated with VOCs biosynthesis. GWAS was performed using three multi-loci mixed linear models - 3 Variance-Component Multi-locus Random_SNP-effect Mixed Linear Models (3VMrMLM) (X. Li et al., 2023), Fixed and Random Model Circulating Probability Unification (FarmCPU) (Liu et al., 2016), and Bayesian-information and Linkage-disequilibrium Iteratively Nested Keyway (BLINK) (Huang et al., 2019). FarmCPU and BLINK were implemented in the GAPIT framework. GWAS (from multi-loci mixed linear models (MLM) with principal components (PC3) and kinship (Van Raden) to account for population structure and relatedness) results for HA and HB type files are provided in Appendix 4, **Table D1 and Table D2.**

5.10.2.1 Comparative Insights

Upon comparison of the GWAS results for HA and HB type files from Appendix 4, **Table D1** and **Table D2,** the genetic markers and candidate genes associated with VOCs between the two datasets. The analysis focuses on shared and unique markers, chromosomes, and gene associations, with visualisations to highlight key findings. Both datasets share significant markers on chromosomes 1–7, 9–13, and 16–25.

5.10.2.2 Significant Markers per Chromosome

The overlay chart **Figure 5.3** below compares and illustrates the number of significant markers across chromosomes in both datasets. This helps identify chromosomes with high marker density for potential volatile organic compound-related traits.

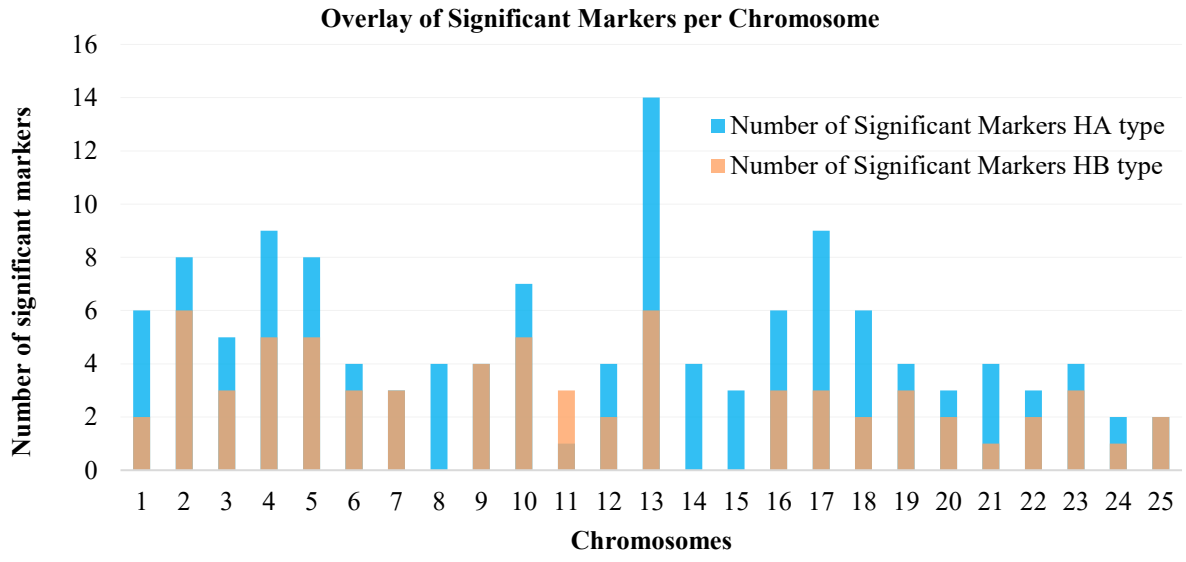


Figure 5.3 Overlay Chart - Significant Markers per Chromosome in HA and HB Datasets

5.10.2.3 Significant SNP Associations and QTL Hotspots

The GWAS identified several single-nucleotide polymorphisms (SNPs) significantly associated with VOCs traits in pineapple. These associations span diverse VOC classes, including esters, aldehydes, alcohols, and terpenoids. The results provided in Appendix 4, **Table D1** present these SNPs, detailing their chromosomal positions, p-values, and proximal candidate genes. Broadly, results from HA- and HB-haplotype reference assemblies complemented each other and identified similar chromosomes and markers, and HB type featured some additional markers. Chromosomes 2, 4, 5, 10, 13, and 17 exhibited high densities of significant SNPs, indicating the presence of potential QTL hotspots responsible for VOCs regulation.

5.10.2.4 Top SNP Markers

The most frequently associated SNP markers are visualised below in **Figure 5.4** below . These loci were consistently identified across multiple GWAS models, suggesting robust genetic control of VOCs traits in the diversity panel used in this study. Several SNPs were found to be associated with multiple VOC traits, implying shared genetic regulation or pleiotropic effects. Noteworthy examples are given in **Table 5.3** on page 80**.** These loci were consistently identified across multiple GWAS models, reinforcing their potential as robust genetic determinants of aroma traits.

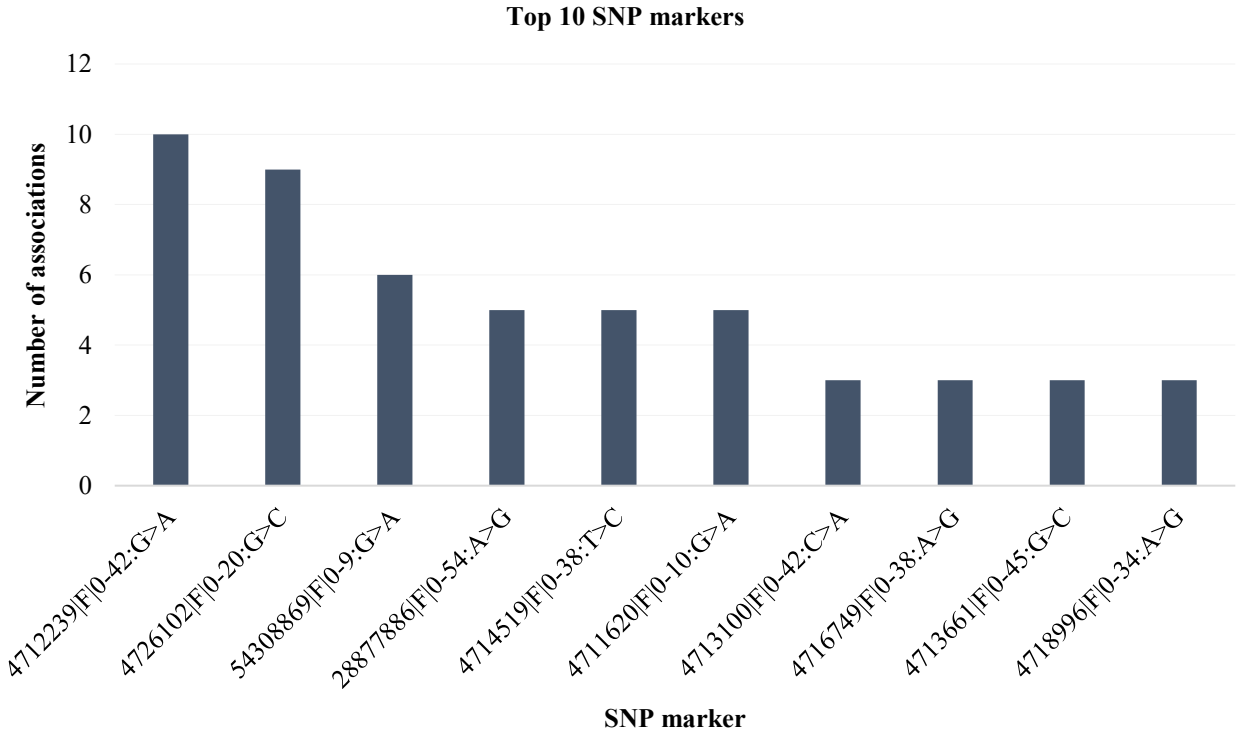


Figure 5.4 Top 10 SNP Markers Associated with VOCs Traits

Table 5.3 Frequency of SNPs associated with multiple VOCs traits

Chr	SNP Marker	VOC	Frequency
23	4712239|F|0-42:G>A	2-methyl butyl acetate	5
		3-methyl-1-butanol	5
12	4726102|F|0-20:G>C	methyl isovalerate	1
		isobutyl acetate	1
		ethyl octanoate	1
		ethyl isobutyrate	2
		ethyl hexanoate	1
		ethyl decanoate	1
		ethyl butyrate	1
		ethyl-2-methyl butyrate	1
21	54308869|F|0-9:G>A	ethyl butyrate	2
		ethyl-2-methyl butyrate	2
		ethyl propionate	2
23	4714519|F|0-38:T>C	methyl isovalerate	5
	4711620|F|0-10:G>A	phenyl acetaldehyde	5
14	28877886|F|0-54:A>G	DHMF	5
	4713100|F|0-42:C>A	DHMF	3
4	4716749|F|0-38:A>G	methyl isobutyrate	1
		methyl butyrate	1
		methyl 2-methyl butyrate	1
13	4713661|F|0-45:G>C	phenyl acetaldehyde	1
		methyl isovalerate	1
		ethyl decanoate	1
8	4718996|F|0-34:A>G	2-methyl butyl acetate	3

5.10.2.5 Candidate Genes and Functional Roles

A linkage disequilibrium decay analysis was also conducted (results shown in Appendix 4, **Figure D2**), and candidate genes located within ±270 kb of significant SNPs were curated and annotated based on their putative roles in VOCs biosynthesis are given in **Table 5.4** on page 81. These genes participate in key metabolic pathways, including fatty acid metabolism, esterification, terpenoid biosynthesis, and amino acid-derived transformations.

Table 5.4 Proposed candidate genes and their role in VOCs biosynthesis

Candidate Gene	Chr: Position	Marker	Associated VOCs	Gene ID	Dist (Kb)	Proposed Biosynthetic Role *(Reference)*
Aldo-keto reductases	23: 11,710,077	4711620|F|0-10:G>A	Phenylacetaldehyde	HA018773.1	265	Catalyse NAD(P)H-dependent reduction of aldehydes/ketones to alcohols, contributing to VOCs formation (Xiao et al., 2024)
	23: 11,413,316	4712239|F|0-42:G>A	2-methyl butyl acetate, methyl isovalerate, 3-methyl-1-butanol)	HA018768.1 HA018769.1 HA018770.1 HA018771.1 HA018773.1	46 43 40 37 32	AKRs contribute by reducing the aldehyde precursors to their corresponding alcohols, which are then esterified Formed from leucine via the Ehrlich pathway, where AKRs reduce the intermediate 3-methylbutanal to the alcohol form. (Hyndman et al., 2003)
	23: 11,484,768	4714519|F|0-38:T>C	methyl isovalerate	HA018768.1 HA018769.1 HA018770.1 HA018771.1 HA018773.1	117 102 92 76 40	
Benzyl Alcohol O-Benzoyltransferase	14: 77,515	28877886|F|0-54:A>G	DHMF	HA011938.1 HA011939.1 HA011940.1 HA011941.1 HA011942.1	90 93 99 103 116	Transfers benzoyl groups to alcohols, forming aromatic esters involved in floral scent. the enzyme is part of the BAHD acyltransferase family, which is known to catalyse the formation of esters and other volatiles in plants. (Kargar et al., 2021) (Basu et al., 2003)
	12: 16,268,110	4726102|F|0-20:G>C	methyl isovalerate, isobutyl acetate, ethyl octanoate, ethyl isobutyrate, ethyl decanoate, ethyl-3-methylthio propinoate, ethyl-2-methyl butyrate	HA011197.1	13	
GDSL esterase/lipase	3: 15,453,675	4713100|F|0-42:C>A	DHMF, ethyl decanoate	HA012566.1	134	Hydrolyse or synthesize ester bonds, modifying fatty acid-derived VOCs (reported in apples, pear, peach). (Cao et al., 2018)
	6: 15,713,325	54316670|F|0-52:G>A	methyl 2-methyl butyrate	HA005453.1	146	
	6: 14,175, 875	4712476|F|0-17:A>G	ethyl octanoate	HA005346.1	167	
	4: 19,352, 236	4712947|F|0-18:C>T	methyl hexanoate, ethyl propionate,	HA004203.1	111	
	1: 1,776,844	4717468|F|0-64:C>T	ethyl propionate	HA000177.1	55	
	16: 12,952,360	28880797|F|0-11:G>A	ethyl propionate	HA013967.1	32	
S-Acyltransferase	1: 1,776,844	4717468|F|0-64:C>T	ethyl propionate,	HA000166.1	32	Catalyse acyl group transfer, forming esters from alcohols and acyl-CoA (Schomburg & Schomburg, 2006).
	5: 15,189,973	28877549|F|0-16:C>T	ethyl trans-3-hexenoate	HA004615.1 HA004618.1	189 131	
	6: 2,218,622	28877005|F|0-31:C>A	ethyl trans-3-hexenoate	HA005189.1	142	
Alcohol Dehydrogenase (ADH)	14: 15,453,675	4713100|F|0-42:C>A	DHMF	HA012577.1	42	Convert aldehydes to alcohols, key step in VOCs biosynthesis (Jörnvall et al., 1994). DHMF is Formed via sugar degradation and Maillard-like reactions; ADH may play a role in reducing intermediate aldehydes.
	23: 1,292,707	4718140|F|0-11:A>G	methyl isobutyrate,	HA018505.1	10	These fruity esters are formed by esterification of alcohols (e.g., ethanol, butanol) with acyl-CoA derivatives. ADH is essential for producing the alcohol substrates.
	23: 13,123,023	54308869|F|0-9:G>A	ethyl butyrate, ethyl-2-methyl butyrate, ethyl propionate	HA017597.1	167	

serine/threonine-protein kinase	8: 16,078,526	4718996|F|0-34:A>G	2-methyl butyl acetate	HA007079.1 HA007080.1	50 64	May regulate enzymes in VOCs biosynthesis via phosphorylation (Heierhorst et al., 2000). Serine/threonine-protein kinases (STPKs) influence the expression of genes encoding enzymes such as alcohol dehydrogenases (ADHs), which produce 2-methylbutanol, and alcohol acyltransferases (AATs), which catalyse the formation of esters
Acetyl-CoA Carboxylase (ACC)	24: 13,009,295	4727640|F|0-46:A>T	ethyl hexanoate	HA019557.1	203	Produces malonyl-CoA, precursor for fatty acid-derived VOCs. (Yang et al., 2020). These esters are formed by alcohol acyltransferases (AATs) that combine ethanol with acyl-CoA derivatives (e.g., hexanoyl-CoA, butyryl-CoA).
	21: 13,123,023	54308869|F|0-9:G>A	ethyl butyrate	HA017622.1	70	
	21: 13,123,023	54308869|F|0-9:G>A	ethyl-2-methyl butyrate,	HA017597.1	167	
	14: 14,785,656	4712775|F|0-35:C>T	ethyl hexanoate	HA012465.1	220	
Acetyltransferase	10: 6,318,164	4712984|F|0-62:A>G	ethyl butyrate	HA008622.1	142	Transfers acetyl groups to alcohols, forming acetate esters. (Millat et al., 2014)
	8: 16,078,526	4718996|F|0-34:A>G	2-methyl butyl acetate, ethyl propionate	HA007062.1	139	
acyl-coenzyme A thioesterase	12: 1,284,054	4715358|F|0-29:T>A	ethyl-3-methylthio propinoate	HA004933.1	67	The proposed biosynthetic pathway involving acyl-CoA thioesterase (ACOT) begins with the catabolism of methionine, which is converted into 3-methylthiopropionic acid through transamination and decarboxylation. This intermediate is then activated to 3-methylthiopropionyl-CoA, which can be hydrolysed by ACOT to regulate precursor levels and prevent toxicity. Finally, alcohol acyltransferase (AAT) catalyses the esterification of 3-methylthiopropionyl-CoA with ethanol to produce the volatile compound ethyl-3-methylthiopropionate.
Acyl Carrier Protein	25: 9,400,834	4712394|F|0-6:C>G	ethyl decanoate	HA019768.1	41	ACP is well-established as a central scaffold protein in fatty acid biosynthesis, which provides the precursors for many volatile esters found in fruits and vegetables. (Swigoňová et al., 2009)
	10: 10,517,834	54311942|F|0-13:G>A	ethyl trans-3-hexenoate	HA008661.1	8	
acyl-Co A synthetase	19: 1,800,357	28877433|F|0-16:A>G	methyl octanoate	HA016031.1	145	These enzymes activate fatty acids by converting them into acyl-CoA esters, a necessary step before esterification into volatiles like methyl octanoate. (Chornyi et al., 2024)
carboxylesterase	17: 11,988,154	4722450|F|0-18:G>A	2-methyl butyl acetate	HA014674.1	15	These esters are typically formed by alcohol acyltransferases (AATs) and may be hydrolysed or regulated by carboxylesterases. (Lian et al., 2018)
	10: 13,491,757	4718506|F|0-41:C>A	methyl 2-methyl butyrate	HA008809.1 HA008810.1	48 41	
acyl-Co A	23: 1,292,707	4718140|F|0-11:A>G	methyl isobutyrate	HA018485.1	201	These esters are formed by combining alcohols (e.g., methanol, ethanol) with acyl-CoA derivatives of fatty acids or amino acid-derived acids. (Yang et al., 2017)
	14: 14,795,781	4709745|F|0-43:C>T	ethyl octanoate, ethyl hexanoate	HA012500.1	51	
Methionine S-methyltransferase	19: 1,270,467	28878735|F|0-29:A>T	methyl-3-methyl thio propionate	HA015983.1	58	This enzyme catalyses the methylation of L-methionine using S-adenosyl-L-methionine (SAM) as the methyl donor, forming S-methylmethionine (SMM). SMM is a key intermediate in sulphur-containing volatile biosynthesis, including compounds like methyl-3-methylthio propionate. (Schomburg et al., 2006)

QQ plots and Manhattan plots further supported the validity of these associations by showing deviation from expected distributions, indicating potential true positives. Representative examples include:

Gene ID: HA011197.1, with the proposed candidate 'Benzyl alcohol O-benzoyltransferase' on 'Chr-12: 4726102|F|0-20:G>C' was associated with 7 VOCs and implicated in the biosynthesis of esters including ethyl-2-methyl butyrate (**Figure 5.5** below), ethyl hexanoate (**Figure 5.6** below), isobutyl acetate (**Figure 5.7** on page 84), and other ester compounds. Gene ID: HA018773.1 and HA018768.1-HA018771.1 and HA018773.1, with the proposed candidate 'Aldo-keto reductases on 'Chr-23: 4711620|F|0-10:G>A, 4712239|F|0-42:G>A and 4714519|F|0-38:T>C were associated with 5 VOCs and implicated in the biosynthesis of phenyl acetaldehyde (**Figure 5.9** on page 84) 3-methyl-1-butanol, and different esters such as 2-methyl butyl acetate (**Figure 5.8** on page 84) and methyl isovalerate. The proposed candidate 'GDSL esterase/lipase' on 'Chr-1:4717468|F|0-64:C>T, Chr-3: 4713100|F|0-42:C>A, Chr-4: 4712947|F|0-18:C>T, Chr-6: 54316670|F|0-52:G>A, Chr-6: 4712476|F|0-17:A>G, and Chr-16: 28880797|F|0-11:G> were associated with several VOCs such as ethyl decanoate (HA012566.1), methyl 2-methyl butyrate (HA005453.1), Ethyl octanoate (HA000177.1), methyl hexanoate and ethyl propionate (HA004203.1, HA013967.1).

These genes are central to VOCs production in pineapple and represent promising targets for functional validation and breeding applications.

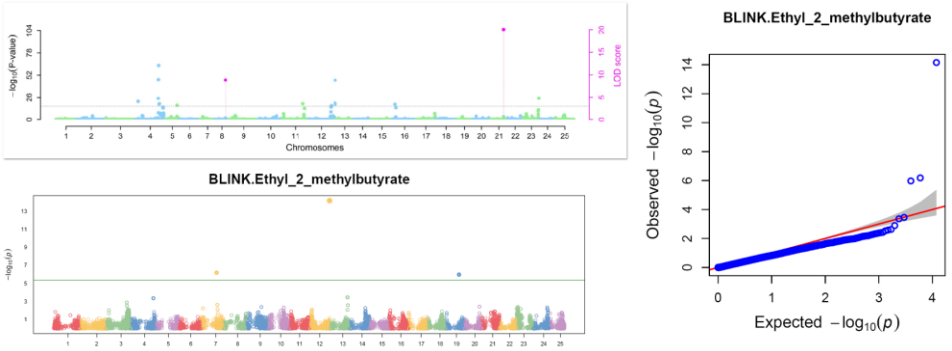


Figure 5.5 QQ and Manhattan plots of ethyl-2-methyl butyrate

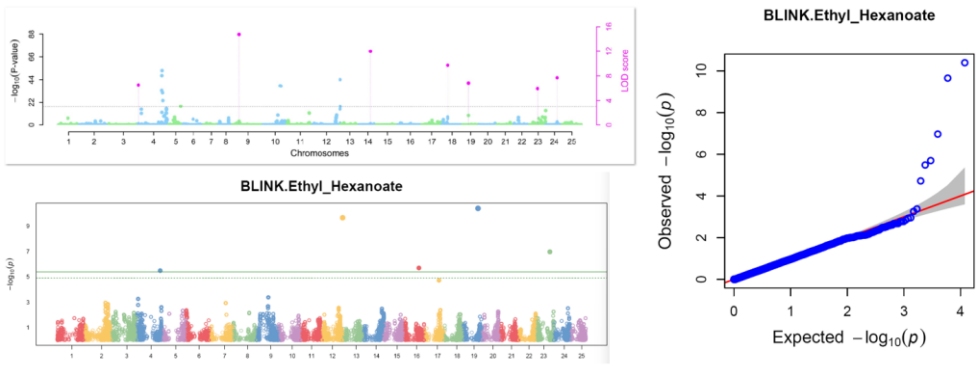


Figure 5.6 QQ and Manhattan plots of ethyl hexanoate

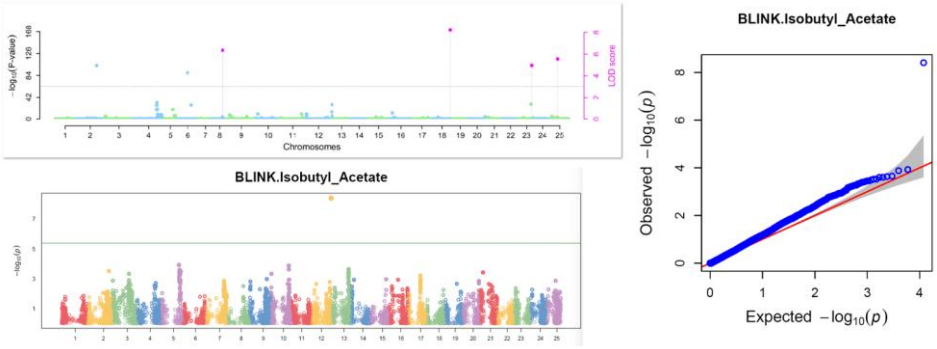


Figure 5.7 QQ and Manhattan plots of isobutyl acetate

Figure 5.8 QQ and Manhattan plots of 2-methylbutyl acetate

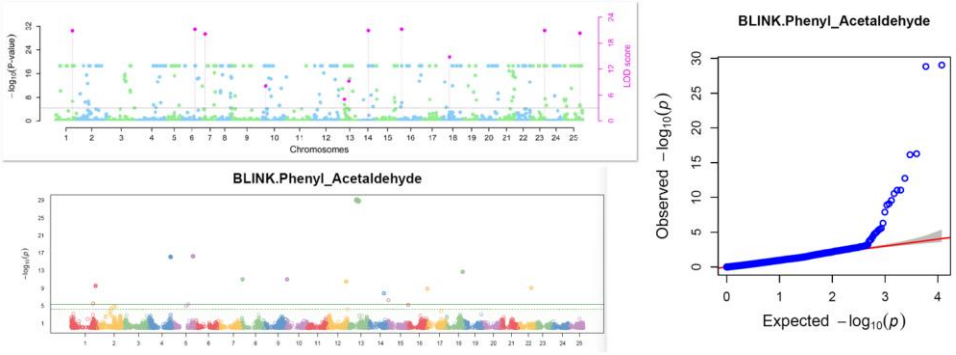


Figure 5.9 QQ and Manhattan plots of phenylacetaldehyde

5.10.3 Link to volatile organic compounds and aroma profiles

A range of VOCs were significantly associated with the identified loci, contributing to diverse aroma profiles such as esters (methyl butyrate, ethyl hexanoate, 2-methyl butyl acetate, methyl butyl acetate, methyl isobutyrate, ethyl octanoate), furanones (2,5-dimethyl-4-methoxy-3(2H)-furanone-DHMF), and terpenes. These compounds contribute to fruity, sweet, floral, and fermented aroma notes. Findings from the study in Chapter 4 (George et al., 2025) confirmed the sensory relevance of key volatiles, reinforcing their role in shaping consumer perception. The biosynthesis of these aroma compounds is regulated by gene expression, transcription factors, and epigenetic mechanisms.

5.10.3.1 Biosynthetic Pathways and Regulatory Insights

The biosynthesis of VOCs in pineapple involves multiple interconnected metabolic pathways. Compounds such as methyl isovalerate, ethyl propionate, and 2-methyl butyl acetate share several genes, indicating the genetic overlap in their formation. Many VOCs are synthesised through common routes, including the Ehrlich pathway, which produces branched-chain esters, fatty acid metabolism, which contributes to the formation of ethyl esters, and sulphur-containing pathways, which involve methionine-derived compounds. Esters are primarily synthesised via esterification of fatty acids, a process catalysed by enzymes such as alcohol acyltransferases (AATs) and acyl-CoA synthetases (ACS) (Colonges et al., 2022; Soomro et al., 2023). These enzymes facilitate the combination of alcohols and acyl-CoA molecules to form a wide variety of ester compounds that contribute to the characteristic aroma of pineapple. Furanones and terpenoids are produced through either the mevalonate or methylerythritol phosphate (MEP) pathways, both of which involve terpene synthases (TPS) (Chen et al., 2017). In particular, furaneol, a key aroma compound, is formed in fruits such as strawberry, tomato, and pineapple from d-fructose-1,6-diphosphate via an unknown enzyme that produces 4-hydroxy-5-methyl-2-methylene-3(2H)-furanone. This intermediate is subsequently reduced by an enone oxidoreductase (Schwab et al., 2008). Alcohols and aldehydes, which also contribute significantly to pineapple aroma, are derived from amino acid and fatty acid metabolism. Their formation is mediated by enzymes such as alcohol dehydrogenase (ADH), lipoxygenase (LOX), and hydroperoxide lyase (HPL).

Table 5.5 below presents a comprehensive overview of the VOCs contributing to pineapple's distinctive aroma, detailing their chemical classifications, representative compounds, biosynthetic routes, and the key enzymes involved in their formation.

Table 5.5 Class of VOCs and their associated pathways

Class of Compound	Examples	Pathway	Key Enzymes
Esters	Methyl hexanoate, Ethyl butyrate	Fatty Acid Biosynthesis, Esterification	Alcohol acyltransferase (AAT), Acyl-CoA synthetase (ACS)
Terpenoids	Limonene, Linalool	Terpenoid Biosynthesis	Terpene synthases TPS
Alcohols	3-Methyl-1-butanol	Amino Acid-Derived Pathways	Alcohol dehydrogenase (ADH)
Aldehydes	phenylacetaldehyde	Fatty Acid Biosynthesis	Lipoxygenase (LOX), Hydroperoxide lyase (HPL), Aromatic amino acid aminotransferase (AAAT), Aldo-keto reductase (AKR)

Figure 5.10 on page 86 illustrates the ester biosynthesis process, highlighting the connection between fatty acid metabolism and ester formation through enzymes like alcohol acyltransferase (AAT) and acyl-CoA synthetase (ACS). These diagrams synthesise findings from both literature and experimental data. The regulation of these pathways is tightly linked to fruit development and is

sensitive to environmental factors, a pattern also observed in other fruits such as mango, guava, apple, and kiwifruit (L.-X. Li et al., 2023; Souleyre et al., 2022). Recent studies (Lu et al., 2024; Yang et al., 2025; Asikin et al., 2022; Bai et al., 2022; George et al., 2023) (Lu et al., 2024; Yang et al., 2025) (Asikin et al., 2022; Bai et al., 2022; George et al., 2023) further supports the influence of external conditions on VOCs biosynthesis.

Notably, variation in quantitative trait loci (QTL) associated with esters like ethyl hexanoate offers promising targets for marker-assisted selection (MAS). A deeper understanding of the genetic and environmental controls governing these pathways is crucial for enhancing aroma profiles through breeding strategies and postharvest practices.

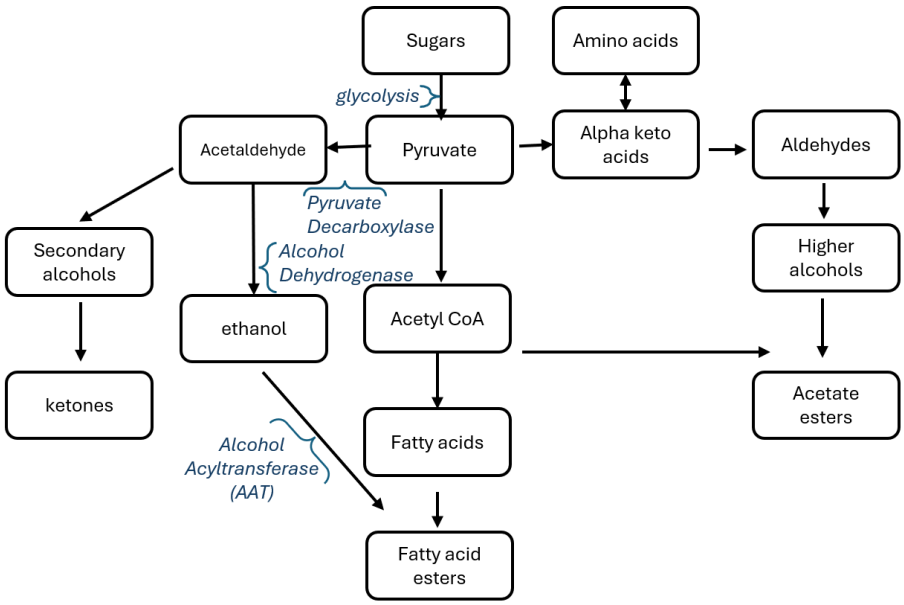


Figure 5.10 Simplified diagram of the ester biosynthesis pathway (recreated for esters from the results and based on S. Lai et al. 2024 and Kelly Colonges et al., 2022).

For the 2024 pineapple samples, GWAS analysis was challenging due to the binary nature of the data and absence of strong, easily detectable association signals. This suggests a lack of loci with large phenotypic effects on sensory attributes, as well as limitations inherent to the sensory data itself. Additionally, many VOCs in pineapple may not be sufficiently abundant or consistently expressed across genotypes to support well-powered GWAS using small populations, leading to poor model fit. However, the BGLR results of the measured sensory trait as '*other*' with a span of around more than 95 attributes, with a major subcategory of *other-alcohol, other-banana, other-chemical, other-citrus, other-green,* and *other-savoury,* showed significant associations as shown in **Table 5.7** on page 87. Since these subcategories of the 'other' category could potentially relate to many VOCs, it is more likely that a shared pathway leads to the formation of these chemicals. Moreover, there could be a

polymorphism in a gene further along the pathways involved in sugar or amino acid production, which in turn are substrates for VOCs synthesis. This indicates the need for a more focused sensory study that incorporates VOCs data to better understand this process associations. From the 2022 sample, one of the breeder-flavour ratings marked as '*aromatic flavour'* was significantly associated in the GWAS study results, as shown in **Table 5.6** below, indicating the possibilities of associations of several volatiles involved in the formation of flavour compounds in pineapple.

Table 5.6 GWAS study results for the '*aromatic flavour'* category of the flavour rating for 2022 samples

Phenotype	Chr: Position	SNP (Marker)	Gene ID	Proposed candidate	Dist (Kb)
aromatic flavour	6: 13,824,859	28877035|F|0-12:C>T	HA005326.1	Alpha-humulene 10-hydroxylase	169
			HA005346.1	GDSL esterase/lipase	184
			HA005344.1	Ethylene-responsive transcription factor	161
			HA005321.1	premnaspirodiene oxygenase	186
	10: 12,487,587	28882356|F|0-13:A>G	HA008726.1	anthranilate O-methyltransferase	191
			HA008728.1	formate--tetrahydrofolate ligase	155
			HA008731.1	glutamate decarboxylase-like	117
			HA008741.1	glucan endo-1,3-beta-glucosidase	15
			HA008742.1	tyrosine-protein phosphatase	181
			HA008743.1	protein disulfide isomerase	192

Table 5.7 BGLR results for the 'other' category of the sensory traits for 2024 samples

Chr: Position	SNP	P.value	MAF	Program
4: 2,250,892	100058025|F|0-16:C>T	1.88E-13	0.03	BLINK
8: 1,700,730	4718629|F|0-32:T>A	2.37E-10	0.24	BLINK
8: 12,347,857	28877373|F|0-5:T>C	4.04E-06	0.16	BLINK
11: 2,827,203	28877677|F|0-21:G>A	1.16E-19	0.06	FarmCPU
11: 2,064,392	4717235|F|0-6:G>C	1.60E-17	0.05	BLINK
11: 1,922,120	4713522|F|0-8:G>A	8.47E-17	0.06	FarmCPU
11: 3,054,712	4716007|F|0-45:C>T	5.51E-08	0.1	FarmCPU
12: 1,5916,142	28880027|F|0-34:A>G	2.39E-10	0.06	FarmCPU
12: 15,876,507	28879759|F|0-15:A>G	6.48E-10	0.06	FarmCPU
12: 13,328,342	28883297|F|0-13:A>T	1.57E-09	0.15	FarmCPU
13: 15,157,841	4718848|F|0-62:C>T	5.79E-08	0.03	FarmCPU
14: 491,082	28875556|F|0-24:G>C	1.56E-06	0.13	BLINK
16: 12,887,398	54313139|F|0-18:G>A	2.01E-38	0.04	BLINK
16: 1,263,921	54313047|F|0-11:C>T	2.33E-37	0.06	BLINK
16: 500,702	4716414|F|0-33:G>A	5.12E-24	0.05	BLINK
16: 12,887,398	54313139|F|0-18:G>A	6.66E-23	0.04	FarmCPU
16: 1,263,921	54313047|F|0-11:C>T	5.98E-08	0.06	FarmCPU
17: 665,222	100222993|F|0-16:A>T	4.44E-49	0.02	BLINK
17: 665,222	100222993|F|0-16:A>T	3.07E-18	0.02	FarmCPU
18: 13,036,577	4710212|F|0-38:T>A	3.10E-18	0.04	BLINK
19: 2,135,792	4720640|F|0-15:A>G	1.58E-07	0.1	BLINK
22: 1,941,147	4713422|F|0-18:A>G	1.47E-21	0.03	FarmCPU
22: 1,941,147	4713422|F|0-18:A>G	1.62E-07	0.03	BLINK

Given these constraints, our analysis focused on the most robust genotype-phenotype associations identified in the 2022 samples. These included associations that formed distinct peaks in Manhattan

plots, indicative of single loci with large effects on VOC concentrations across more varieties. A notable limitation of the present study is the restriction of candidate gene identification to an LD decay distance of 270Kb surrounding the targeted VOCs, which represent the terminal products of complex biosynthetic pathways. This approach may have excluded linked genetic regulators further distant that may be involved in precursor formation, such as genes associated with sugar biosynthesis, ethylene signalling, and other metabolic processes that contribute to the overall aroma and flavour profile of pineapple (El Hadi et al., 2013). Emerging evidence suggests that VOC profiles in fruits are shaped not only by final enzymatic steps but also by earlier metabolic events, including carbohydrate flux, hormonal regulation, and transcriptional control (Abbas et al., 2023; El Hadi et al., 2013). For instance, ethylene-responsive genes and sugar biosynthesis pathways have been implicated in modulating aroma compound production in various fruit species (Abbas et al., 2023). These upstream components may exert direct or indirect influence on VOC biosynthesis and should be considered in future investigations. To enhance the resolution and interpretability of genetic associations in pineapple aroma research, future studies should expand the genomic search space beyond the current threshold. Additionally, methodological improvements, such as the application of advanced statistical models, increased population sizes, and integration of multi-omics approaches (e.g., transcriptomics, metabolomics, and epigenomics), will be essential for capturing the full spectrum of genetic contributors to aroma traits (Yow et al., 2023). While more advanced GWAS models with larger populations with greater diversity and a more comprehensive sensory panel methodology may enhance detection in future studies, our current approach, multiple multi-loci, mixed linear models with a relatively small population and sensory panel, highlights the most promising associations. This provides a foundation for identifying candidate genes involved in pineapple aroma biosynthesis and supports the development of marker-assisted selection strategies for flavour improvement.

5.10.4 Implications for Breeding

This study represents the first integration of genomics, metabolomics, and sensory data to unravel the genetic basis of pineapple aroma in Australian-grown cultivars. The identification of strong genotype–phenotype associations and candidate genes lay a solid foundation for the implementation of marker-assisted selection (MAS) in pineapple breeding. Future research directions include fine-mapping of key loci using whole-genome sequencing, functional validation of candidate genes, and the application of clustered regularly interspaced short palindromic repeats (CRISPR) and other gene-editing technologies to enhance desirable traits. These findings will inform consumer-focused breeding programs aimed at improving fruit flavour. Moreover, extending this integrative approach

to other tropical fruits, such as mango, peach, and strawberry, will contribute to a broader understanding of the genetic architecture underlying aroma volatile production across parental lines (varieties/ population samples).

5.11 Conclusions

Pineapple produces a complex and diverse array of VOCs that define its characteristic aroma and flavour, key attributes influencing consumer preference. Despite their importance, these traits have been under-utilised in breeding programs due to the intricate biochemistry of VOC biosynthesis and the limitations of high-throughput phenotyping. This study incorporated a comprehensive multi-omics approach integrating gas chromatography-mass–mass spectrometry (GC-MS), sensory evaluation, and genome-wide association studies (GWAS) to unravel the genetic architecture underlying pineapple aroma. GC-MS analysis revealed a diverse spectrum of aroma-active VOCs, including esters, lactones, ketones, and terpenes, with significant variation observed across breeding lines. Among these, esters emerged as the most abundant and widely distributed class, playing a dominant role in defining the fruit's aromatic profile.

Sensory panel evaluations confirmed that key VOCs, particularly esters and furanones, are positively correlated with overall consumer liking. This sensory validation underscores the relevance of these compounds as breeding targets for flavour enhancement. The integration of sensory data with metabolomic profiles provided a robust framework for linking chemical composition to perceived aroma quality. Metabolite-GWAS revealed that a relatively small number of genomic regions exert major control over VOCs abundance. The identified QTL were enriched for candidate genes involved in VOCs biosynthesis, including aldo-keto reductase, benzoyl alcohol-benzoyl transferase, GDSL esterase/lipase, alcohol acyltransferases (AATs), acyl-CoA synthetases, and oxidoreductases, enzymes known to catalyse key steps in ester, aldehyde, alcohol and furanone formation.

A robust association was detected between ester production and a candidate AAT gene and acyl-CoA, which catalyses the final step in ester biosynthesis. Use of a stringent multi-model GWAS approach enabled the identification of loci associated with VOCs and candidate genes predictive of VOC profiles. These genomic markers enable the development of predictive models for aroma traits, supporting the feasibility of marker-assisted selection (MAS) in pineapple breeding.

In conclusion, this study establishes a genomic and biochemical framework for the improvement of pineapple flavour. By linking VOC composition to sensory perception and genetic determinants, this study provides actionable insights for genomics-assisted breeding strategies aimed at enhancing aroma and consumer appeal in future pineapple cultivars.

Chapter 6 Conclusions and Future Research Directions

The breeding of tropical fruit varieties has shifted from a production-focused approach to a consumer-driven strategy, emphasising flavour, aroma, and sensory appeal. Advances in volatilomics, flavouromics, sensory-consumer evaluations, and genomics have revolutionised marker-assisted selective breeding, enabling the development of superior cultivars tailored to consumer preferences. Despite these advances, there are limited examples of applications for sensory quality in aiding breeding efforts. This research aimed to identify key aroma compounds in Australian-grown pineapple cultivars, develop robust analytical methodologies for their quantification, and apply these tools to profile varieties from the Queensland Department of Primary Industries (DPI) breeding program and commercial sources. The findings support molecular marker discovery and marker-assisted selection (MAS) strategies for flavour enhancement. This research has also provided valuable insights into the aroma chemistry, sensory attributes, and genetic basis of pineapple flavour, highlighting key volatile organic compounds (VOCs) that contribute to its distinctive profile. One of the main strengths of the current research was the successful establishment of a multidisciplinary approach involving analytical chemistry, sensory science, and fruit genetics. This integrated framework enabled a more holistic understanding of fruit quality traits and provided a solid foundation for linking biochemical data with genetic and sensory insights.

6.1 Summary of Achievements

The comprehensive review (George et al., 2023) of existing literature identified over 480 VOCs in pineapples, with about 40 recognised as aroma active. These compounds include esters, aldehydes, ketones, lactones, sulphur-containing compounds, and terpenoids, which vary substantially across cultivars, ripeness stages, and post-harvest conditions. Analytical techniques such as gas chromatography-mass spectrometry (GC-MS), gas chromatography-olfactometry (GC-O), and stable isotope dilution analysis (SIDA) have played a critical role in refining VOC identification methods, although challenges remain in standardising protocols and establishing a comprehensive database. By applying matrix-matched SIDA-HS-SPME-GC-MS, this study quantified 26 key aroma-active VOCs across five commercial pineapple cultivars grown in Australia (George et al., 2024). Significant differences in VOC composition were observed, with esters being the most prevalent class, followed by terpenes, alcohols, aldehydes, and ketones. Odour activity values (OAVs) indicated that compounds like damascenone, decanal, and 2,5-dimethyl-4-methoxy-3(2H)-furanone play crucial roles in pineapple aroma. The novelty of this work lies in the development of a matrix-matched approach specifically tailored for pineapple, effectively addressing genotype-specific matrix effects and enhancing quantification accuracy. This method marks a substantial advancement over previous

techniques by enabling precise measurement of volatiles within complex fruit matrices. Notably, it represents the first application of a matrix-matched SIDA for pineapple volatiles, facilitating the comprehensive, single-step quantification of 26 aroma-active compounds. This detailed profiling establishes a valuable benchmark for future volatilomics research in tropical fruits.

This pioneering study of key aroma compounds, sensory evaluation and consumer preference studies of Australian-grown commercial pineapple cultivars (George et al., 2025) established a strong link between pineapple flavour perception and specific VOCs, particularly methyl and ethyl esters, terpenoids, and the °Brix to titratable acidity (TA) ratio. Cultivars 'Aus Festival' and 'Aus Jubilee' were preferred for their sweetness and tropical fruit notes, whereas 'Aus Smooth' and 'Aussie Gold' were perceived as more acidic, with vinegary and green flavour attributes reducing consumer acceptance. Importantly, this work is among the first to integrate sensory data with volatile profiles and genomic information across a broad breeding population. The application of advanced statistical methods such as principal component analysis (PCA) and preference mapping further validated the importance of key aroma compounds in shaping consumer perception.

This study is the first ever approach to identify potential candidate gene markers associated with the formation of VOCs that are associated with Australian-grown pineapples' sensory properties. Genomic analyses revealed strong links between genotypes and VOC biosynthesis traits. GWAS identified key loci associated with ester production, particularly those connected to the AAT1 gene, which encodes alcohol acyltransferase. Association mapping tools showed that flavour traits can be reliably inferred from genetic data, supporting the potential for marker-assisted selection (MAS). Although expanding population sizes, improving VOC detection methods, and diversifying sensory evaluation approaches could further enhance GWAS resolution, the current multi-locus mixed linear model has successfully proposed promising candidate genes.

6.2 Limitations of the Study

Despite the robustness of the matrix-matched SIDA-HS-SPME-GC-MS method, several methodological and logistical challenges persist. The gold-standard analytical approach, headspace solid-phase microextraction (HS-SPME) coupled with gas chromatography–mass spectrometry (GC-MS) and stable isotope dilution analysis (SIDA), is labour-intensive, expensive, time-consuming, and highly sensitive to sample preparation conditions. Limitations related to suitable internal standards prevented the detection of some aroma volatiles present at low levels. A key limitation of the current analytical approach is the absence of Gas Chromatography-Olfactometry (GC-O), which could have

helped the identification of VOCs specifically contributing towards subtle notes such as coconut-like aromas through aroma omission and reconstitution analysis.

Sensory and instrumental data are inherently different in nature; while instrumental methods provide precise quantification of individual VOCs, sensory perception arises from the complex interaction of VOCs within a matrix. Differences in panel training, perception thresholds, and cultural preferences further contributed to variability in sensory data, limiting the resolution of consumer preference mapping. A notable limitation in the sensory evaluation of fresh pineapple is the restricted number of samples that can be assessed per session, as the fruit's high bromelain content, the cysteine protease enzyme (Siti Rashima et al., 2021), can cause oral irritation, including bleeding of the lips and gums, among panellists. The sensory data were constrained by the limited diversity of evaluated cultivars and variability in ripeness, which hindered the ability to definitively associate specific VOCs with distinct sensory notes such as coconut, floral, or tropical aromas. This critical limitation should be addressed in future studies to enhance the reliability of sensory-chemical correlations. This limitation underscores the need for broader sensory profiling in future studies. Fruit ripeness emerged as a key determinant of sensory attributes, consistent with findings in tropical fruits like mango, papaya, and earlier research on pineapple, where ripening stages significantly alter volatile profiles and sensory perceptions such as sweetness, acidity, and aroma intensity due to compounds like hexanal and cis-3-hexenol, diminishing with ripening (Pino & Mesa, 2006). Similarly, previous studies on tropical fruit such as pineapple and passion fruit have shown marked changes in ester and sulphur compound concentrations during ripening, directly affecting flavour acceptability (Brat et al., 2004; Elss et al., 2005; Umano et al., 1992). These variations pose common challenges in horticultural research, where controlling fruit availability and ripeness across samples can be difficult, leading to variability in sensory and chemical data. These limitations hinder the scalability of the method for large breeding populations and reduce reproducibility across studies. The limitations in aligning chemical data with sensory profiles underscore the need for improved experimental design.

Although the use of a 270 Kb LD decay distance for candidate gene identification aligns with standard GWAS methodology and is not inherently limiting, the genetic linkage analysis in this study may have overlooked more distant regulatory elements. The absence of LD heatmaps for each chromosome prevents verification of potential long-range linkages beyond 270 Kb, which could include upstream regulators involved in precursor biosynthesis pathways such as sugar metabolism and ethylene signalling. Future research should broaden the genomic search space and incorporate multi-omics approaches, such as genetic, transcriptomic, metabolomic, and epigenomic factors influence fruit flavour traits (Zheng et al., 2024), to capture the full complexity of metabolic

regulation underlying pineapple aroma traits. In particular, ribonucleic acid (RNA) co-expression studies could help identify additional genes expressed alongside specific candidate genes, offering insights into regulatory networks. Given that RNA expression data for ripening pineapple is already available, this analysis is feasible and could significantly enhance candidate gene discovery. The genetic dissection of sensory traits in tropical fruits such as pineapple remains a significant challenge due to the complex and emergent nature of aroma perception. As described in Chapter 2, the literature review (George et al., 2023), pineapple aroma is shaped by a diverse array of VOCs, including esters, terpenes, lactones, and aldehydes, that interact in synergistic, additive, or masking ways to produce distinct sensory impressions. The subsequent study in Chapter 4 (George et al., 2025) further emphasised that no single VOC is solely responsible for a sensory note; rather, it is the relative abundance and interaction of multiple compounds that define the overall aroma profile. This concept aligns with the foundational work of Richard Axel and Linda Buck, winners of the 2004 Nobel prize, who showed that the human olfactory system interprets aroma as a mosaic, where each VOC functions like a pixel in a broader sensory image (Watts, 2004). While advances in quantitative trait loci (QTL) mapping and genome-wide association studies (GWAS) have facilitated the identification of genetic loci associated with individual VOCs, translating these findings into predictable sensory outcomes remains elusive. This is largely due to the non-linear and context-dependent nature of aroma perception, which is influenced by compound thresholds, matrix effects, and human variability. The complexity of aroma perception, shaped by synergistic and masking interactions among VOCs, poses challenges in translating genetic loci into predictable sensory outcomes. Limited biological replication, the relatively small number of samples that can be evaluated by a sensory panel, inaccuracy of assessment and asynchronous fruit ripening further reduced the statistical power of phenotypic evaluations, hindering effective implementation of MAS and GS. Improved genetic linkage analysis will help refine the identification of molecular markers involved in VOC biosynthesis. Simulation-based studies have recently proposed optimised breeding schemes that balance genetic gain with diversity conservation, particularly for low-heritability traits such as aroma (Gill et al., 2022). To overcome current limitations, future studies should incorporate larger and more genetically diverse populations and apply sensory-informed GWAS models to better link VOCs with perceptual traits. However, the feasibility of expanding sensory panel evaluations must be revisited, particularly for fresh pineapple, due to the oral irritation caused by its high bromelain content. This challenge underscores the need for innovative sensory methodologies or alternative model systems that can safely and effectively assess flavour perception at scale, ultimately enhancing the precision of marker-assisted selection for flavour traits. This would enhance the precision of marker-assisted selection for flavour traits.

6.3 Future Research Directions

Together, this study successfully established a multidisciplinary framework integrating analytical chemistry, sensory science, and fruit genetics/biotechnology. This approach enabled a comprehensive understanding of fruit quality traits and facilitated the linkage of biochemical data with genetic and sensory insights. Despite its strengths, several areas could be further enhanced. Building on the findings of this research, several future directions are proposed to address current limitations and advance the field of tropical fruit aroma profiling and breeding.

°Brix measurements using a refractometer should be adjusted for acidity and supported by HPLC profiling of sugars and acids (Paull & Chen, 2003; Paull & Duarte, 2025) and gravimetric analysis, to report accurate total soluble solids (TSS). Incorporating near-infrared spectroscopy (Seki et al., 2023; Tantinantrakun et al., 2023) will further enhance the estimation of dry matter and sugar content. Continuous access to analytical instrumentation would have enabled consistent analysis of VOCs, using the matrix-matched GC-MS SIDA headspace method, particularly across all harvests in genetic population samples. Incorporating Gas Chromatography-Olfactometry (GC-O) could have revealed additional key aroma compounds, including subtle notes such as coconut-like aromas that may be overlooked in targeted analyses. High-throughput VOC phenotyping using platforms such as Proton Transfer Reaction Time-of-Flight Mass Spectrometry (PTR-ToF-MS) offers a rapid and efficient alternative to traditional GC-MS for screening large breeding populations. These platforms support the processing of high sample volumes and enable parallel research streams, significantly accelerating data acquisition. Although the analytical method developed in this study effectively addresses matrix effect challenges by incorporating diverse genetic samples from breeding programs, ongoing breeding efforts that introduce new varieties necessitate periodic method updates, including reassessment of matrix effects, to ensure continued accuracy in VOC quantification and data reliability. To enhance analytical precision, future studies should expand the VOCs profiling framework to include certain key aroma compounds (George et al., 2024; George et al., 2023) that were previously undetectable due to internal standard limitations. Incorporating aroma omission and reconstitution tests alongside Gas Chromatography-Olfactometry (GC-O) will enable deeper insights into the synergistic, masking, and additive effects of VOCs. Additionally, updated protocols to mitigate high-temperature injection artifacts (Reinhardt & Steinhaus, 2025) will improve analytical reliability. Integrating machine learning and predictive modelling will be essential for deciphering complex VOC interactions and predicting sensory outcomes from chemical profiles. To address limitations in replication and instrumentation, future studies should adopt high-throughput platforms like PTR-ToF-MS and GC-O, and develop sensory tools tailored for genetic linkage analysis.

Biological replication in this study was limited, particularly within commercial and breeding populations, due to constraints in fruit availability. To enhance statistical robustness, future studies should aim for improved replication, ideally 20 or more differentiated fruit samples per harvest for commercial populations and at least three for genetic populations. Incorporating samples from multiple consecutive years would allow for a more comprehensive assessment of seasonal variability and trait stability. An ideal future study would involve comprehensive sensory profiling of 20–30 cultivars at peak ripeness, followed by consumer preference testing and VOC analysis. Preference mapping could then identify volatile markers linked to distinct flavour types, guiding streamlined analytical and genomic workflows. Broader cultivar diversity and multi-year sampling will be essential for improving trait stability assessments and reproducibility. Tailored sensory tools designed for integration with genetic linkage analysis are needed to better connect sensory data with genetic datasets. To ensure the reliability of sensory and chemical analyses, it is essential to standardise ripeness assessment protocols and conduct sampling during the peak season. Specifically, samples should be collected at a time of year and at a ripeness stage that maximises the expression of VOCs. Future sensory studies should evaluate 20–30 fruits at optimal ripeness using trained panels to capture the full spectrum of flavour variation. Future sensory studies should incorporate pre-panel °Brix/TSS or NIR measurements to stratify fruit samples by sweetness, thereby enhancing the interpretability of consumer liking scores (Harker et al., 2009; Harker et al., 2008; Hunter et al., 2020). This approach will support more robust sensory–chemical correlations and improve predictive modelling of consumer preferences. To mitigate variability in sensory responses and reduce the risk of adverse effects, it is advisable to pre-screen panellists for individual sensitivity to high levels of acidity and bromelain, a proteolytic enzyme abundant in fresh pineapple (Siti Rashima et al., 2021) Seasonality and ripeness variability significantly influenced sensory and volatile profiles, as observed in other tropical fruits (Brat et al., 2004; Yahia & Yahia, 2019), underscoring the need for consistent sampling across seasons and ripeness stages. A major gap remains in reliably associating specific VOCs with sensory attributes. Therefore, improving instrumental accuracy alone may not enhance relevance to consumer perception. Bridging this gap requires methodologies that translate the volatile matrix into perceptual relevance, such as using synthetic VOC mixtures at varying concentrations to establish categorical ratings by trained sensory panels, and incorporation of aroma omission and reconstitution experiments via GC-O. Robust sensory evaluation frameworks, including expanded panels, broader cultivar coverage, and assessment of anosmia/hyposmia among participants, are essential to refine aroma variability interpretation (Watts, 2004). To support market segmentation and targeted breeding, future research should incorporate descriptive profiling and consumer testing across a wider range of

cultivars. Standardising ripeness protocols and postharvest handling will be key to improving reproducibility and data quality.

Tropical fruit breeding programs face persistent challenges, including high costs, lengthy field trials, asynchronous ripening, and limited biological replicates. These constraints are well-documented (Gill et al., 2022; Vieira et al., 2025; Yahia & Yahia, 2019). Recent multi-omics studies in mango, guava, and pineapple have begun to elucidate biosynthetic and regulatory networks underlying aroma traits through integrated genomics, transcriptomics, and metabolomics (Lomax et al., 2024). This complexity underscores the need for multivariate techniques such as PLS regression and preference mapping to identify VOC combinations linked to specific flavour profiles. To strengthen the genetic basis of aroma traits, sensory-informed GWAS models should be employed by combining trained panel data with genotypic and metabolomic datasets. This approach will facilitate the identification of markers linked to perceptually significant traits. For resource-limited breeding programs, cost-effective genotyping strategies such as low-density SNP arrays with imputation are recommended to support marker-assisted selection (MAS). Consumer-focused breeding strategies, including preference mapping and emotional response analysis, will ensure alignment between breeding targets and market expectations. Further progress will require detailed mapping of key loci via whole-genome sequencing, functional validation of candidate genes, and the application of gene-editing technologies like CRISPR to enhance desirable traits.

6.4 Final Remarks

Collectively, this study underscores the strategic value of integrating analytical chemistry, sensory science, and genomics to enhance flavour traits in pineapple. Despite inherent methodological complexities, the findings establish a robust foundation for future breeding initiatives aimed at optimising consumer-preferred aroma profiles. The advancement of molecular breeding techniques, coupled with expanded multi-omics approaches, is poised to accelerate the development of superior cultivars that align with market demands and bolster competitiveness within tropical horticulture. These integrative strategies effectively bridge molecular insights with sensory perception, enabling more precise and efficient enhancement of fruit quality traits. Extending this framework to other tropical fruits, such as mango, peach, and strawberry, will deepen our understanding of the genetic regulation of aroma volatile biosynthesis across diverse species and populations. Implementation of these approaches will empower breeders to develop pineapple varieties with distinct flavour profiles, including coconut, floral, or melon notes, complemented by unique visual attributes such as colour, thereby enhancing consumer appeal and market differentiation.

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Appendices

Appendix 1 Supplementary information for Chapter 2

Table A1: Combined list of all the VOCs reported to the date of publication

Sl.No.	IUPAC Name	Reported name	CAS No.	M.W.
Esters				
1	(2-methyl-5-prop-1-en-2-ylcyclohex-2-en-1-yl) acetate	Carvyl acetate (Steingass, Carle, et al., 2015)	97-42-7	194.27
2	(E)-2-methylbut-2-enoic acid	Methyl 2-methyl-(E)-2-butenoate (Steingass et al., 2014)	80-59-1	100.12
3	[(2E)-3,7-dimethylocta-2,6-dienyl] acetate	geranyl acetate (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	105-87-3	196.29
4	[(E)-hex-2-enyl] acetate	(E)-2-Hexen-1-ol acetate (Steingass, Carle, et al., 2015)	2491-18-9	142.20
5	[(Z)-hex-3-enyl] acetate	(Z)-3-Hexen-1-ol acetate (Steingass, Carle, et al., 2015; Steingass et al., 2021)	3681-71-8	142.2
6	1-methoxypropan-2-yl acetate	1-Methoxy-2-propyl acetate (Steingass, Carle, et al., 2015)	108-65-6	132.16
7	1-phenylethyl acetate	1-Phenylethyl acetate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	93-92-5	164.20
8	2-butoxyethyl acetate	2-Butoxyethyl acetate (Steingass, Carle, et al., 2015)	112-07-2	160.21
9	2-ethylhexyl acetate	2-Ethylhexyl acetate (Connell, 1964; Steingass, Carle, et al., 2015)	103-09-3	172.26
10	2-methylbutyl acetate	2-Methylbutyl acetate (Akioka & Umano, 2008; Asikin et al., 2022; Liu et al., 2011; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Zainuddin et al., 2021; Zhang et al., 2012; Zheng et al., 2012)	624-41-9	130.18
11	2-methylbutyl hexanoate	2-Methylbutyl hexanoate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Zainuddin et al., 2021)	2601-13-0	186.29
12	2-methylheptan-2-yl acetate	2-Heptanol acetate (Steingass, Carle, et al., 2015)	5921-82-4	172.26
13	2-methylpentyl formate	2-Methylpentyl formate (Steingass, Carle, et al., 2015)	381670-34-4	130.18
14	2-methylpropyl acetate	2-Methyl-1-propyl acetate (Asikin et al., 2022; Mohd Ali et al., 2020; Orellana-Palma et al., 2020; Pino, 2013; Steingass, Carle, et al., 2015; Takeoka et al., 1989; Turazzi et al., 2017; Umano et al., 1992)	110-19-0	116.16
15	2-methylpropyl formate	2-Methyl-1-propyl formate (Lukás et al., 2013)	542-55-2	120.13
16	2-oxopropyl acetate	Acetoxyacetone (Flath & Forrey, 1970; Marta Montero-Calderón et al., 2010; Po & Po, 2012; R.A., 1980)	592-20-1	116.11
17	2-phenylethyl acetate	2-Phenylethyl acetate (Elss et al., 2005; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Vollmer et al., 2021)	103-45-7	164.2
18	3-acetyloxybutan-2-yl acetate	threo-Butane-2,3-diol diacetate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021)	1114-92-7	174.19
19	3-acetyloxybutyl acetate	1,3-Butanediol diacetate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	1117-31-3	174.19
20	3-methylbut-2-enyl hexanoate	3-Methyl-2-butenyl hexanoate (Steingass, Carle, et al., 2015)	76649-22-4	184.27
21	3-methylbut-2-enyl acetate	3-Methyl-2-butenyl acetate (Asikin et al., 2022; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021)	1191-16-8	128.17

Sl.No.	IUPAC Name	Reported name	CAS No.	M.W.
22	3-methylbut-3-enyl acetate	3 - methylbut - 3 - enyl acetate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	5205-07-2	128.17
24	3-methylbutyl butanoate	butanoic acid, 3-methyl butyl ester (Spanier et al., 1998)	106-27-4	158.24
25	3-methylbutyl decanoate	3-Methylbutyl decanoate (Steingass, Carle, et al., 2015)	2306-91-4	242.40
26	3-methylbutyl acetate	3-Methylbutyl acetate (Akioka & Umano, 2008; Asikin et al., 2022; Elss et al., 2005; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Umano et al., 1992; Vollmer et al., 2021; Zhang et al., 2012)	123-92-2	130.18
27	3-methylbutyl hexanoate	3-Methylbutyl hexanoate (Steingass et al., 2021)	2198-61-0	186.29
28	3-O-ethyl 1-O-methyl propanedioate	ethyl methyl malonate (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Umano et al., 1992; Vollmer et al., 2021)	6186-89-6	146.14
29	3-oxobutan-2-yl acetate	3-acetoxy-2-butanone (Steingass, Carle, et al., 2015; Umano et al., 1992)	4906-24-5	130.14
30	4-acetyloxybutyl acetate	1,4-Butanediol diacetate (Steingass, Carle, et al., 2015)	628-67-1	174.19
31	4-O-ethyl 1-O-methyl butanedioate	ethyl methyl butanedioate (Steingass et al., 2021)	627-73-6	160.17
32	benzyl acetate	Benzyl acetate (Asikin et al., 2022; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Teai et al., 2001)	140-11-4	150.17
33	bis(2-methylpropyl) benzene-1,2-dicarboxylate	diisobutyl phthalate (Marta Montero-Calderón et al., 2010; Umano et al., 1992)	84-69-5	278.34
34	butan-2-yl acetate	acetic acid 1-methylpropyl ester (Spanier et al., 1998)	105-46-4	116.16
35	butyl formate	1-Butyl formate (Flath & Forrey, 1970; Marta Montero-Calderón et al., 2010; R.A., 1980)	592-84-7	102.13
36	butyl acetate	n-Butyl acetate (Brat et al., 2004; Elss et al., 2005; Lasekan & Hussein, 2018; Liu & Liu, 2014; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Turazzi et al., 2017)	123-86-4	116.16
37	cyclohexyl acetate	Cyclohexyl acetate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	622-45-7	142.20
38	dibutyl benzene-1,2-dicarboxylate	dibutyl phthalate (Marta Montero-Calderón et al., 2010; Umano et al., 1992)	84-74-2	278.34
39	diethyl butanedioate	Diethyl butanedioate (Steingass, Carle, et al., 2015; Steingass et al., 2021)	123-25-1	174.19
40	diethyl carbonate	Diethyl carbonate (Akioka & Umano, 2008; Elss et al., 2005; Flath & Forrey, 1970; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Turazzi et al., 2017; Vollmer et al., 2021)	105-58-8	118.13
41	diethyl pentanedioate	Diethyl pentanedioate (Braga et al., 2009; Steingass, Carle, et al., 2015)	818-38-2	188.22
42	diethyl propanedioate	diethyl propanedioate (Berger et al., 1985; Steingass et al., 2021)	105-53-3	160.17
43	dimethyl butanedioate	dimethyl succinate (Elss et al., 2005; Lukás et al., 2013; Marta Montero-Calderón et al., 2010)	106-65-0	146.14
44	dimethyl pentanedioate	Dimethyl pentanedioatec (Steingass, Carle, et al., 2015)	1119-40-0	160.17
45	dimethyl propanedioate	dimethyl malonate (Akioka & Umano, 2008; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Flath & Forrey, 1970; Lasekan & Hussein, 2018; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Po & Po, 2012; R.A., 1980; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Wu et al., 1991; Xiao et al., 2021)	108-59-8	132.11
46	ethyl (E)-hex-3-enoate	Ethyl (E)-3-hexenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Xiao et al., 2021; Zheng et al., 2012)	26553-46-8	142.2

Sl.No.	IUPAC Name	Reported name	CAS No.	M.W.
47	ethyl (Z)-hex-3-enoate	Ethyl (Z)-3-hexenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Umano et al., 1992)	64187-83-3	142.2
48	ethyl (Z)-oct-3-enoate	ethyl (Z) - 3 - octenoate (Marta Montero-Calderón et al., 2010)	69668-87-7	170.25
49	ethyl 5-oxohexanoate	ethyl 5 - oxohexanoate (Marta Montero-Calderón et al., 2010)	13984-57-1	158.19
50	ethyl hexanoate	Ethyl hexanoate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Braga et al., 2010; Brat et al., 2004; Elss et al., 2005; Flath & Forrey, 1970; Kaewtathip & Charoenrein, 2012; Lamikanra & Richard, 2004; Lasekan & Hussein, 2018; Lukás et al., 2013; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Pedroso et al., 2011; Pickenhagen, 1989; Pino, 2013; Po & Po, 2012; Preston et al., 2003; R.A., 1980; Ravichandran et al., 2020; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Wu et al., 1991; Xiao et al., 2021; Zainuddin et al., 2021; Zhang et al., 2012; Zheng et al., 2012)	123-66-0	144.21
51	ethyl octadecanoate	ethyl octadecanoate (Berger et al., 1985; Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010; Teai et al., 2001)	111-61-5	312.5
52	ethyl tetradecanoate	ethyl tetradecanoate (Brat et al., 2004; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Takeoka et al., 1989)	124-06-1	256.42
53	ethyl (2E,4E)-deca-2,4-dienoate	Ethyl 2,4-decadienoate (Steingass, Carle, et al., 2015)	37549-74-9	196.29
54	ethyl (2E,4Z)-deca-2,4-dienoate	Ethyl decadienoate (Pino, 2013; Steingass, Carle, et al., 2015; Vollmer et al., 2021)	3025-30-7	196.29
55	ethyl (E)-3-phenylprop-2-enoate	Ethyl cinnamate (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass et al., 2021; Teai et al., 2001; Zheng et al., 2012)	103-36-6	176.21
56	ethyl (E)-hept-4-enoate	Ethyl (E)-4-heptenoate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Vollmer et al., 2021)	54340-70-4	156.22
57	ethyl (E)-hex-2-enoate	(Berger et al., 1985; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021; Xiao et al., 2021)	27829-72-7	142.2
58	ethyl (E)-oct-2-enoate	ethyl (E)-2-octenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021)	7367-82-0	170.25
60	ethyl (E)-oct-3-enoate	ethyl (E)-3-octenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021)	26553-47-9	170.25
61	ethyl (E)-octadec-9-enoate	ethyl (E)-octadec-9-enoate (Lukás et al., 2013)	6114-18-7	310.5
62	ethyl (Z)-dec-4-enoate	Ethyl (Z)-4-decenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021)	7367-84-2	198.3
63	ethyl (Z)-hept-4-enoate	Ethyl (Z)-4-heptenoate (Steingass et al., 2021; Steingass et al., 2014)	39924-27-1	156.22
64	ethyl (Z)-oct-4-enoate	ethyl (Z)-4-octenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014)	34495-71-1	170.25
65	ethyl (Z)-oct-5-enoate	Ethyl (Z)-5-octenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021)	72820-74-7	170.25
66	ethyl 2-hydroxy-2-methylbutanoate	ethyl 2-hydroxy-2-methylbutanoate (Elss et al., 2005; Steingass, Carle, et al., 2015; Umano et al., 1992)	77-70-3	146.18
67	ethyl 2-hydroxy-3-methylbutanoate	Ethyl 2-hydroxy-3-methylbutanoate (Elss et al., 2005; Steingass, Carle, et al., 2015; Steingass et al., 2021; Umano et al., 1992)	7/06/2441	146.18
68	ethyl 2-hydroxyhexanoate	ethyl 2-hydroxyhexanoate (Elss et al., 2005; Umano et al., 1992)	52089-55-1	160.21
69	ethyl 2-hydroxypropanoate	ethyl lactate (Brat et al., 2004; Connell, 1964; Elss et al., 2005; R.A., 1980; Teai et al., 2001; Umano et al., 1992)	97-64-3	118.13
70	ethyl 2-methylbutanoate	Ethyl 2-methylbutanoate (Akioka & Umano, 2008; Asikin et al., 2022; Brat et al., 2004; Elss et al., 2005; Lamikanra & Richard, 2004; Lukás et al., 2013; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pino, 2013; Po & Po, 2012; Preston et al., 2003; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Steingass, Langen, et al., 2015; Sun et al., 2016; Takeoka et al., 1989; Tokitomo et al.,	7452-79-1	130.18

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		2005; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Wei, Liu, Liu, Zang, et al., 2011; Xiao et al., 2021; Zainuddin et al., 2021; Zheng et al., 2012)		
71	ethyl 2-methylpropanoate	Ethyl 2-methylpropionate (Akioka & Umano, 2008; Asikin et al., 2022; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pickenhagen, 1989; Pino, 2013; Po & Po, 2012; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Takeoka et al., 1989; Tokitomo et al., 2005; Vollmer et al., 2021; Wei, Liu, Liu, Zang, et al., 2011; Zainuddin et al., 2021)	97-62-1	116.16
72	ethyl 2-phenylacetate	Ethyl 2-phenylacetate (Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021)	101-97-3	164.2
73	ethyl 3-acetyloxy-2-methylbutanoate	ethyl 3-acetoxy-2-methylbutanoate (Steingass et al., 2021; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021)	139564-43-5	188.22
74	ethyl 3-acetyloxybutanoate	Ethyl 3-acetoxybutanoate (Steingass, Carle, et al., 2015; Umano et al., 1992)	27846-49-7	174.19
75	ethyl 3-acetyloxyhexanoate	Ethyl 3-acetoxy hexanoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Wu et al., 1991)	21188-61-4	202.25
76	ethyl 3-acetyloxyoctanoate	ethyl 3-acetoxyoctanoate (Umano et al., 1992; Wu et al., 1991)	85554-66-1	230.3
77	ethyl 3-acetyloxypentanoate	ethyl 3-acetoxypentanoate (Umano et al., 1992)	27846-50-0	188.22
78	ethyl 3-hydroxy-2-methylbutanoate	ethyl 3-hydroxy-2-methylbutanoate (Steingass, Carle, et al., 2015; Umano et al., 1992)	27372-03-8	146.18
79	ethyl 3-hydroxybutanoate	Ethyl 3-hydroxybutanoate (Lukás et al., 2013; Steingass et al., 2021; Turazzi et al., 2017; Umano et al., 1992)	5405-41-4	132.16
80	ethyl 3-hydroxyhexanoate	Ethyl 3-hydroxyhexanoate (Braga et al., 2009; Elss et al., 2005; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Zheng et al., 2012)	2305-25-1	160.21
81	ethyl 3-hydroxyoctanoate	ethyl 3-hydroxyoctanoate (Elss et al., 2005; Steingass, Carle, et al., 2015; Umano et al., 1992)	7367-90-0	188.26
82	ethyl 3-hydroxypentanoate	ethyl 3-hydroxypentanoate (Umano et al., 1992)	54074-85-0	146.18
83	ethyl 3-methylbutanoate	Ethyl 3-methylbutanoate (Akioka & Umano, 2008; Elss et al., 2005; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Takeoka et al., 1989; Turazzi et al., 2017; Vollmer et al., 2021; Xiao et al., 2021; Zainuddin et al., 2021)	108-64-5	130.18
84	ethyl 4-acetyloxybutanoate	ethyl 4-acetoxybutanoate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Umano et al., 1992)	25560-91-2	174.19
85	ethyl 4-acetyloxyhexanoate	Ethyl 4-acetoxyhexanoate (Steingass et al., 2021; Umano et al., 1992)	121308-81-4	202.25
86	ethyl 4-acetyloxyoctanoate	ethyl 4-acetoxyoctanoate (Pickenhagen, 1989; Takeoka et al., 1989; Umano et al., 1992; Wu et al., 1991)	121312-01-4	230.3
87	ethyl 4-acetyloxypentanoate	ethyl 4-acetoxypentanoate (Umano et al., 1992)	27846-52-2	188.22
88	ethyl 4-hydroxyhexanoate	ethyl 4-hydroxyhexanoate (Pickenhagen, 1989; Umano et al., 1992)	101853-50-3	160.21
89	ethyl 4-hydroxyoctanoate	ethyl 4-hydroxyoctanoate (Umano et al., 1992)	57753-66-9	188.26
90	ethyl 5-acetyloxyhexanoate	Ethyl 5-acetoxyhexanoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Umano et al., 1992; Wu et al., 1991)	35234-24-3	202.25
91	ethyl 5-acetyloxyoctanoate	Ethyl 5-acetoxyoctanoate (Steingass, Carle, et al., 2015; Umano et al., 1992)	35234-25-4	230.3
92	ethyl 5-hydroxyhexanoate	ethyl 5-hydroxyhexanoate (Pickenhagen, 1989; Umano et al., 1992)	20266-62-0	160.21
93	ethyl 5-hydroxyoctanoate	ethyl 5-hydroxyoctanoate (Berger et al., 1985; Pickenhagen, 1989; Umano et al., 1992)	75587-05-2	188.26
94	ethyl acetate	Ethyl acetate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Connell, 1964; Flath & Forrey, 1970; Haagen-Smit et al., 1945; Lamikanra & Richard, 2004; Lukás et al., 2013; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pino, 2013; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021;	141-78-6	88.11

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		Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Xiao et al., 2021; Zhang et al., 2012)		
95	ethyl benzoate	Ethyl benzoate (Braga et al., 2009; Flath & Forrey, 1970; Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Xiao et al., 2021)	93-89-0	150.17
96	ethyl butanoate	Ethyl butanoate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pedroso et al., 2011; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Xiao et al., 2021; Zainuddin et al., 2021)	105-54-4	116.16
97	ethyl decanoate	Ethyl decanoate (Braga et al., 2009; Elss et al., 2005; Kaewtathip & Charoenrein, 2012; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pedroso et al., 2011; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Wei, Liu, Liu, Lv, et al., 2011)	110-38-3	200.32
98	ethyl dodecanoate	Ethyl Laurate (Braga et al., 2009; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Takeoka et al., 1989; Teai et al., 2001)	106-33-2	228.37
99	ethyl formate	Ethyl formate (Braga et al., 2009; Marta Montero-Calderón et al., 2010; R.A., 1980)	109-94-4	74.08
100	ethyl furan-2-carboxylate	Ethyl 2-furoate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	614-99-3	140.14
101	ethyl heptanoate	Ethyl heptanoate (Elss et al., 2005; Flath & Forrey, 1970; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2017; Steingass et al., 2014; Vollmer et al., 2021; Xiao et al., 2021; Zhang et al., 2012)	106-30-9	158.24
102	ethyl hex-5-enoate	Ethyl 5-hexenoate (Lamikanra & Richard, 2004; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021)	54653-25-7	142.2
103	ethyl hexa-2,4-dienoate	Ethyl hexadienoate (Steingass et al., 2021; Vollmer et al., 2021)	2396-84-1	140.18
104	ethyl hexadecanoate	ethyl hexadecanoate (Berger et al., 1985; Umano et al., 1992)	628-97-7	284.5
105	ethyl methyl carbonate	Ethyl methyl carbonate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	623-53-0	104.10
106	ethyl nonanoate	Ethyl nonanoate (Braga et al., 2009; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; R.A., 1980; Sengar et al., 2022; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Wei, Liu, Liu, Lv, et al., 2011)	123-29-5	186.29
107	ethyl octanoate	Ethyl octanoate (Kaewtathip & Charoenrein, 2012; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Pedroso et al., 2011; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass, Jutzi, et al., 2015; Turazzi et al., 2017; Vollmer et al., 2021; Zheng et al., 2012) (Asikin et al., 2022; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Flath & Forrey, 1970; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pickenhagen, 1989; R.A., 1980; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992)	106-32-1	172.26
108	ethyl pentanoate	Ethyl pentanoate (Asikin et al., 2022; Elss et al., 2005; Flath & Forrey, 1970; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pedroso et al., 2011; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021; Xiao et al., 2021; Zainuddin et al., 2021; Zhang et al., 2012)	539-82-2	130.18
109	ethyl prop-2-enoate	Ethyl 2-propenoate (Elss et al., 2005; Steingass et al., 2021; Vollmer et al., 2021; Zainuddin et al., 2021)	140-88-5	100.12
110	ethyl propanoate	Ethyl propanoate (Akioka & Umano, 2008; Asikin et al., 2022; Elss et al., 2005; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Umano et al., 1992; Vollmer et al., 2021; Zainuddin et al., 2021)	105-37-3	102.13

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111	hexyl acetate	n-Hexyl acetate (Elss et al., 2005; Lukás et al., 2013; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Vollmer et al., 2021)	142-92-7	144.21
112	hexyl hexanoate	n-Hexyl hexanoate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Xiao et al., 2021)	6378-65-0	200.32
113	methyl (2S,3S)-3-acetyloxy-2-methylbutanoate	Methyl 3-acetoxy-2-methylbutanoate (Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Umano et al., 1992; Vollmer et al., 2021)	151004-71-6	174.19
114	methyl (4E)-octa-4,7-dienoate	methyl octadienoate (Marta Montero-Calderón et al., 2010)	189440-77-5	154.21
115	methyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate	methyl linolenate (Berger et al., 1985)	7361-80-0	292.5
116	methyl (9Z,12Z)-octadeca-9,12-dienoate	methyl (Z, Z) - 9,12 - octadecadienoate (Berger et al., 1985)	112-63-0	294.5
118	Methyl (E)-4-hexenoate	Methyl (E)-4-hexenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Vollmer et al., 2021)	14017-81-3	127.16
119	methyl (E)-but-2-enoate	methyl (E) - 2 – butenoate (Mohd Ali et al., 2020; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014)	623-43-8	100.12
120	methyl (E)-hex-2-enoate	2-hexanoic acid methyl ester (Spanier et al., 1998)	2396-77-2	128.17
121	methyl (E)-hex-3-enoate	methyl 3 - hexenoate (Spanier et al., 1998; Steingass et al., 2021; Wu et al., 1991)	2396-78-3	128.17
122	methyl (E)-oct-2-enoate	methyl 2 - octenoate (M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2017)	7367-81-9	156.22
123	methyl (Z)-hept-4-enoate	Methyl (Z)-4-heptenoate (Steingass et al., 2021; Steingass et al., 2017; Steingass et al., 2014; Vollmer et al., 2021)	39924-30-6	142.2
124	methyl (Z)-oct-3-enoate	methyl (Z) - 3 - octenoate (Marta Montero-Calderón et al., 2010)	69668-85-5	156.22
125	methyl (Z)-octadec-9-enoate	methyl (Z) - 9 - octadecenoate (Marta Montero-Calderón et al., 2010)	112-62-9	296.5
126	methyl (Z)-octadec-9-enoate	Methyl oleate (Berger et al., 1985)	112-62-9	296.50
127	methyl 2-methyl-3-oxobutanoate	methyl 2 - methyl - 3 - oxobutanoate (Marta Montero-Calderón et al., 2010)	17094-21-2	130.14
128	methyl 3-hydroxyhexanoate	3-hexanoic acid methyl ester (Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Flath & Forrey, 1970; Kaewtathip & Charoenrein, 2012; Lukás et al., 2013; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Turazzi et al., 2017; Umano et al., 1992; Wu et al., 1991)	21188-58-9	146.18
129	methyl 4-hydroxybutanoate	methyl 4 - hydroxy butanoate (Marta Montero-Calderón et al., 2010)	925-57-5	118.13
130	methyl 6-methyl-3-oxoheptanoate	4-heptanoic acid methyl ester (Spanier et al., 1998)	104214-14-4	172.22
131	methyl decanoate	Methyl decanoate (Braga et al., 2009; Kaewtathip & Charoenrein, 2012; Lasekan & Hussein, 2018; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Pedroso et al., 2011; R.A., 1980; Sengar et al., 2022; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2017; Steingass et al., 2014; Takeoka et al., 1989; Teai et al., 2001; Turazzi et al., 2017; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Xiao et al., 2021; Zheng et al., 2012)	110-42-9	186.29
132	methyl hex-4-enoate	methyl (Z) - 4 - hexenoate (Steingass, Carle, et al., 2015)	13894-60-5	128.17
133	methyl hexadecanoate	methyl hexadecanoate (Berger et al., 1985; Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010; Teai et al., 2001)	112-39-0	270.5
135	methyl octadecanoate	methyl octadecanoate (Berger et al., 1985; Marta Montero-Calderón et al., 2010; Teai et al., 2001)	112-61-8	298.5
136	methyl pyridine-3-carboxylate	methyl nicotinate (Elss et al., 2005; Marta Montero-Calderón et al., 2010)	93-60-7	137.14
137	methyl (2E,4E)-deca-2,4-dienoate	Methyl 2,4-decadienoate (Steingass, Carle, et al., 2015)	7328-33-8	182.26

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138	methyl (2E,4E)-hexa-2,4-dienoate	methyl (E,E)-2,4-hexadienoate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	689-89-4	126.15
139	methyl (E)-3-phenylprop-2-enoate	Methyl cinnamate (Marta Montero-Calderón et al., 2010; Steingass et al., 2021; Zheng et al., 2012)	103-26-4	162.18
140	methyl (E)-hex-2-enoate	Methyl (E)-2-hexenoate (Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Zainuddin et al., 2021)	13894-63-8	128.17
141	methyl (E)-hex-3-enoate	Methyl (E)-3-hexenoate (Akioka & Umano, 2008; Asikin et al., 2022; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Vollmer et al., 2021; Xiao et al., 2021; Zainuddin et al., 2021)	13894-61-6	128.17
142	methyl (E)-oct-3-enoate	Methyl (E)-3-octenoate (Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Vollmer et al., 2021)	35234-16-3	156.22
143	methyl (E)-pent-3-enoate	Methyl 3-pentenoate (Steingass, Carle, et al., 2015)	818-58-6	114.14
144	methyl (Z)-dec-4-enoate	Methyl (Z)-4-decenoate (Akioka & Umano, 2008; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2017; Steingass et al., 2014; Takeoka et al., 1989; Vollmer et al., 2021)	7367-83-1	184.27
145	methyl (Z)-hex-3-enoate	Methyl (Z)-3-hexenoate (Akioka & Umano, 2008; Asikin et al., 2022; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Umano et al., 1992; Vollmer et al., 2021; Zainuddin et al., 2021)	13894-62-7	128.17
146	methyl (Z)-oct-2-enoate	Methyl (E)-2-octenoate (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2017; Steingass et al., 2014; Takeoka et al., 1989)	68854-59-1	156.22
147	methyl (Z)-oct-4-enoate	Methyl (Z)-4-octenoate (Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989)	21063-71-8	156.22
148	methyl (Z)-oct-5-enoate	Methyl (Z)-5-octenoate (Akioka & Umano, 2008; Steingass et al., 2021; Steingass et al., 2017; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Vollmer et al., 2021)	41654-15-3	156.22
149	methyl 2-ethyl-3-methyl-2-(2-oxoethyl)butanoate	butanoic 3-methyl ethyl ester (Spanier et al., 1998)	175698-14-3	186.25
150	methyl 2-hydroxy-2-methylbutanoate	methyl 2-hydroxy-2-methylbutanoate (Akioka & Umano, 2008; Asikin et al., 2022; Elss et al., 2005; Lukás et al., 2013; Steingass, Jutzi, et al., 2015; Turazzi et al., 2017; Umano et al., 1992)	32793-34-3	132.16
151	methyl 2-hydroxy-3-methylbutanoate	Methyl 2-hydroxy-3-methylbutanoate (Elss et al., 2005; Steingass, Carle, et al., 2015; Steingass et al., 2021)	17417-00-4	132.16
152	methyl 2-hydroxyhexanoate	Methyl 2-hydroxyhexanoate (Mohd Ali et al., 2020; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Umano et al., 1992)	68756-64-9	146.18
153	methyl 2-hydroxypropanoate	methyl lactate (Elss et al., 2005; Teai et al., 2001; Umano et al., 1992)	547-64-8	104.1
154	methyl 2-methylbutanoate	Methyl 2-methylbutanoate (Akioka & Umano, 2008; Braga et al., 2010; Brat et al., 2004; Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Lamikanra & Richard, 2004; Lukás et al., 2013; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pickenhagen, 1989; Pino, 2013; Po & Po, 2012; Preston et al., 2003; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Wei, Liu, Liu, Zang, et al., 2011; Wu et al., 1991; Xiao et al., 2021; Zainuddin et al., 2021)	868-57-5	116.16
155	methyl 2-methylheptanoate	heptanoic acid-2-methyl methyl ester (Spanier et al., 1998)	51209-78-0	158.24
156	methyl 2-methylpropanoate	Methyl 2-methylpropanoate (Akioka & Umano, 2008; Asikin et al., 2022; Lukás et al., 2013; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pickenhagen, 1989; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Tokitomo et al., 2005; Turazzi et al., 2017; Vollmer et al., 2021; Xiao et al., 2021; Zainuddin et al., 2021)	547-63-7	102.13
157	methyl 2-phenylacetate	Methyl 2-phenylacetate (Kaewtathip & Charoenrein, 2012; Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021)	101-41-7	150.17
158	methyl 3-acetyloxy-2-methylbutanoate	methyl 3-acetoxy-2-methylbutanoate (Steingass et al., 2016; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021)	139564-42-4	174.19

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159	methyl 3-acetyloxybutanoate	Methyl 3-acetoxybutanoate (Elss et al., 2005; Lukás et al., 2013; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991)	89422-42-4	160.17
160	methyl 3-acetyloxyhexanoate	Methyl 3-acetoxy hexanoate (Flath & Forrey, 1970; Kaewtathip & Charoenrein, 2012; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991)	21188-60-3	188.22
161	methyl 3-acetyloxyoctanoate	methyl 3-acetoxyoctanoate (R.A., 1980; Steingass, Carle, et al., 2015; Umano et al., 1992; Wu et al., 1991)	35234-21-0	216.27
162	methyl 3-hydroxy-2-methylbutanoate	methyl 3-hydroxy-2-methylbutanoate (Lukás et al., 2013; Steingass, Carle, et al., 2015; Umano et al., 1992)	34293-67-9	132.16
163	methyl 3-hydroxy-3-methylbutanoate	methyl 3-hydroxy-3-methylbutanoate (Elss et al., 2005; Steingass, Carle, et al., 2015; Umano et al., 1992)	6149-45-7	132.16
164	methyl 3-hydroxybutanoate	Methyl 3-hydroxybutanoate (Brat et al., 2004; Elss et al., 2005; Lukás et al., 2013; Mohd Ali et al., 2020; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2014; Takeoka et al., 1989; Umano et al., 1992)	1487-49-6	118.13
165	methyl 3-hydroxyoctanoate	methyl 3-hydroxyoctanoate (Elss et al., 2005; R.A., 1980; Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Teai et al., 2001; Umano et al., 1992; Wu et al., 1991)	7367-87-5	174.24
166	methyl 3-hydroxypentanoate	methyl 3-hydroxypentanoate (Steingass, Carle, et al., 2015; Umano et al., 1992)	56009-31-5	132.16
167	methyl 3-methylbutanoate	Methyl 3-methylbutanoate (Akioka & Umano, 2008; Asikin et al., 2022; Elss et al., 2005; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Tokitomo et al., 2005; Vollmer et al., 2021; Xiao et al., 2021)	556-24-1	116.16
168	methyl 4-acetyloxyhexanoate	Methyl 4-acetoxyhexanoate (Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Steingass, Langen, et al., 2015; Takeoka et al., 1989; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991)	112059-09-3	188.22
169	methyl 4-acetyloxyoctanoate	methyl 4-acetoxyoctanoate (Pickenhagen, 1989; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Wu et al., 1991)	60121-04-2	216.27
170	methyl 4-hydroxyhexanoate	Methyl 4-hydroxyhexanoate (Umano et al., 1992; Vollmer et al., 2021)	101853-52-5	146.18
171	methyl 4-hydroxyoctanoate	methyl 4-hydroxyoctanoate (Umano et al., 1992)	101853-51-4	174.24
172	methyl 4-methylpentanoate	Methyl 4-methylpentanoate (R.A., 1980; Steingass, Carle, et al., 2015; Wu et al., 1991)	2412-80-8	130.18
173	methyl 5-acetyloxyheptanoate	methyl 5-acetoxyheptanoate (Umano et al., 1992)	139564-44-6	202.25
174	methyl 5-acetyloxyhexanoate	Methyl 5-acetoxyhexanoate (Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Lamikanra & Richard, 2004; Lukás et al., 2013; Mohd Ali et al., 2020; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991)	35234-22-1	188.22
175	methyl 5-acetyloxyoctanoate	Methyl 5-acetoxyoctanoate (Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2014; Steingass, Langen, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Wu et al., 1991)	35234-23-2	216.27
176	methyl 5-hydroxyhexanoate	methyl 5-hydroxyhexanoate (Elss et al., 2005; Pickenhagen, 1989; Steingass et al., 2016; Umano et al., 1992)	62593-13-9	146.18
177	methyl 5-hydroxyoctanoate	methyl 5-hydroxyoctanoate (Pickenhagen, 1989; Umano et al., 1992)	101853-49-0	174.24
178	methyl 5-oxopentanoate	Methyl 5-oxo-pentanoate (Steingass, Carle, et al., 2015)	6026-86-4	130.14
179	methyl acetate	Methyl acetate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Connell, 1964; Flath & Forrey, 1970; Liu & Liu, 2014; Lukás et al., 2013; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Xiao et al., 2021; Zainuddin et al., 2021; Zhang et al., 2012)	79-20-9	74.08
180	methyl benzoate	methyl benzoate (Elss et al., 2005; Gonçalves, 2018; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Xiao et al., 2021)	93-58-3	136.15

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181	methyl butanoate	Methyl butanoate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Lasekan & Hussein, 2018; Lukás et al., 2013; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Pedroso et al., 2011; Pickenhagen, 1989; Pino, 2013; Po & Po, 2012; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Takeoka et al., 1989; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Wei, Liu, Liu, Zang, et al., 2011; Wu et al., 1991; Xiao et al., 2021; Zainuddin et al., 2021)	623-42-7	102.13
182	methyl dec-4-enoate	Methyl dec-4-enoate (Kaewtathip & Charoenrein, 2012)	1191-02-2	184.27
183	methyl dodecanoate	Methyl laurate (Berger et al., 1985; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	111-82-0	214.34
184	methyl heptanoate	Methyl heptanoate (Akioka & Umano, 2008; Asikin et al., 2022; Elss et al., 2005; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Pedroso et al., 2011; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Vollmer et al., 2021; Xiao et al., 2021; Zhang et al., 2012)	106-73-0	144.21
185	methyl hex-5-enoate	Methyl 5-hexenoate (Akioka & Umano, 2008; Braga et al., 2009; Lamikanra & Richard, 2004; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pedroso et al., 2011; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Umano et al., 1992; Vollmer et al., 2021; Zainuddin et al., 2021)	2396-80-7	128.17
186	methyl hexanoate	methyl hexanoate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2010; Brat et al., 2004; Elss et al., 2005; Flath & Forrey, 1970; Kaewtathip & Charoenrein, 2012; Lamikanra & Richard, 2004; Lasekan & Hussein, 2018; Lukás et al., 2013; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Pedroso et al., 2011; Pickenhagen, 1989; Pino, 2013; Po & Po, 2012; Preston et al., 2003; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Takeoka et al., 1989; Teai et al., 2001; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Wei, Liu, Liu, Zang, et al., 2011; Xiao et al., 2021; Zainuddin et al., 2021; Zhang et al., 2012; Zheng et al., 2012)	106-70-7	130.18
187	methyl nonanoate	Methyl nonanoate (Braga et al., 2009; Kaewtathip & Charoenrein, 2012; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Xiao et al., 2021)	1731-84-6	172.26
188	methyl oct-4-enoate	Methyl 4-octenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Wei, Liu, Liu, Lv, et al., 2011)	21063-71-8	156.22
189	methyl octanoate	methyl octanoate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Flath & Forrey, 1970; Kaewtathip & Charoenrein, 2012; Lamikanra & Richard, 2004; Lasekan & Hussein, 2018; Lukás et al., 2013; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pedroso et al., 2011; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Wu et al., 1991; Xiao et al., 2021; Zainuddin et al., 2021; Zheng et al., 2012)	111-11-5	158.24
190	methyl pentanoate	Methyl pentanoate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Flath & Forrey, 1970; Lasekan & Hussein, 2018; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Xiao et al., 2021; Zainuddin et al., 2021; Zhang et al., 2012)	624-24-8	116.16
191	methyl prop-2-enoate	Methyl 2-propenoate (Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2014; Vollmer et al., 2021)	96-33-3	86.09
192	methyl propanoate	Methyl propanoate (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Vollmer et al., 2021; Xiao et al., 2021; Zainuddin et al., 2021)	554-12-1	88.11
193	NA	Ethyl 3-acetoxy-2-methylbutanoate (diasteroemers) (Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021)	NA	188.22

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194	NA	Methyl 3-acetoxy-2-methylbutanoate (diasteroemers) (Steingass et al., 2016; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021)	NA	174.19
195	NA	Methyl (E)-4-hexenoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Vollmer et al., 2021)	NA	128.17
196	pentyl acetate	n-Pentyl acetate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015)	628-63-7	130.18
197	pentyl hexanoate	Pentyl hexanoate (Flath & Forrey, 1970; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; R.A., 1980; Sengar et al., 2022)	540-07-8	186.29
198	prop-2-enyl hexanoate	2 - propenyl hexanoate (Marta Montero-Calderón et al., 2010)	123-68-2	156.22
199	propan-2-yl acetate	1-Methylethyl acetate (Steingass et al., 2014)	108-21-4	102.13
200	propan-2-yl dodecanoate	Isopropyl dodecanoate (Steingass, Carle, et al., 2015)	10233-13-3	242.40
201	propyl 2-methylpropanoate	2-Propyl 2-methylpropionate (R.A., 1980)	644-49-5	130.18
202	propyl formate	1-Propyl formate (R.A., 1980)	110-74-7	88.11
203	propyl hexanoate	n-Propyl hexanoate (Steingass, Carle, et al., 2015)	626-77-7	158.24
204	propyl 2-methylbutanoate	Propyl 2-methylbutanoate (Pickenhagen, 1989; Steingass, Carle, et al., 2015)	37064-20-3	144.21
205	propyl acetate	n-Propyl acetate (Akioka & Umano, 2008; Elss et al., 2005; Flath & Forrey, 1970; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pickenhagen, 1989; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Xiao et al., 2021)	109-60-4	102.13
206	NA	erythro-butane-2,3-diol diacetate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Umano et al., 1992)	17998-02-6	174.19
207	NA	methyl 2- acetoxy butanoate (Marta Montero-Calderón et al., 2010)	NA	160.17
208	NA	threo-Butane-2,3-diol diacetate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021)	79297-93-1	174.19
Alcohols				
209	(3E,6Z)-nona-3,6-dien-1-ol	(E,Z)-3,6-Nonadien-1-ol (Vollmer et al., 2021)	56805-23-3	140.22
210	(E)-hex-2-en-1-ol	(E) - 2 - hexen - 1 - ol (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	928-95-0	100.16
211	(E)-oct-2-en-1-ol	(E)-2-Octen-1-ol (Steingass, Carle, et al., 2015)	18409-17-1	128.21
212	(Z)-hex-3-en-1-ol	(Z)-3-hexenol (Pickenhagen, 1989; Takeoka et al., 1989; Umano et al., 1992)	928-96-1	100.16
213	[(2R,3S)-3-hydroxybutan-2-yl] acetate	erythro-3-acetoxy-2-butanol (Umano et al., 1992)	NA	132.16
214	[(2R,3S)-3-hydroxybutan-2-yl] acetate	threo-3-acetoxy-2-butanol (Umano et al., 1992)	NA	132.16
215	2-(4-methylphenyl)propan-2-ol	p-cymen-8-ol (Elss et al., 2005; Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Umano et al., 1992)	1197-01-9	150.22
216	2,3-dimethylbutan-2-ol	2,3 - dimethyl - 2 - butanol (R.A., 1980)	594-60-5	102.17
217	2,3-dimethylundec-1-en-3-ol	2,3-Dimethyl-undec-1-en-3-ol (Zheng et al., 2012)	NA	198.34

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218	2,6-dimethoxy-4-prop-2-enylphenol	4 - allyl - 2,6 - dimethoxy phenol (Marta Montero-Calderón et al., 2010)	6627-88-9	194.23
219	2-butoxyethanol	2 - butoxy - ethanol (Marta Montero-Calderón et al., 2010)	111-76-2	118.17
220	2-ethylhexan-1-ol	2-ethyl-1-hexanol (Marta Montero-Calderón et al., 2010)	104-76-7	130.23
221	2-methylbut-3-en-2-ol	2-methyl-3-buten-2-ol (Akioka & Umano, 2008; Brat et al., 2004; Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Umano et al., 1992; Xiao et al., 2021)	115-18-4	86.13
222	2-methylbutan-1-ol	2-Methyl-1-butanol (Steingass et al., 2014)	137-32-6	218.41
223	2-methylbutan-2-ol	2-methyl-2-butanol (Marta Montero-Calderón et al., 2010)	75-85-4	88.15
224	2-methylpentan-2-ol	2 - methyl pentan - 2 - ol (R.A., 1980)	590-36-3	102.17
225	2-methylpropan-1-ol	2-Methyl-1-propanol (Elss et al., 2005; Flath & Forrey, 1970)	78-83-1	74.12
226	2-methylpropan-2-ol	tert - butanol (Marta Montero-Calderón et al., 2010)	75-65-0	74.12
227	2-phenylethanol	2-Phenylethanol (Elss et al., 2005; Pickenhagen, 1989; Steingass et al., 2016; Steingass et al., 2021; Takeoka et al., 1989; Teai et al., 2001; Wu et al., 1991)	60-12-8	122.16
228	2-prop-2-enylphenol	2 - allylphenol (Marta Montero-Calderón et al., 2010)	1745-81-9	134.17
229	3-(2-hydroxyethyl)phenol	(3 - hydroxyphenyl) ethyl alcohol (Marta Montero-Calderón et al., 2010)	13398-94-2	138.16
230	3-methylbut-2-en-1-ol	3-methyl-2-butenol (Asikin et al., 2022; Marta Montero-Calderón et al., 2010; Umano et al., 1992)	556-82-1	86.13
231	3-methylbut-3-en-1-ol	3 - methyl - 3 - butan - 1 - ol (Marta Montero-Calderón et al., 2010)	763-32-6	86.13
232	3-methylbut-3-en-2-ol	3-methyl-3-buten-2-ol (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	10473-14-0	86.13
233	3-methylbutan-1-ol	3-Methylbutanol (Orellana-Palma et al., 2020; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Takeoka et al., 1989; Umano et al., 1992; Wu et al., 1991)	123-51-3	88.15
234	3-methylpentan-2-ol	3 - methyl pentan - 2 – ol (Marta Montero-Calderón et al., 2010; Wu et al., 1991)	565-60-6	102.17
235	3-methylpentan-3-ol	3 - methyl pentan - 3 - ol (Marta Montero-Calderón et al., 2010; R.A., 1980)	77-74-7	102.17
236	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	coniferilic alcohol (Marta Montero-Calderón et al., 2010)	32811-40-8	180.2
237	4-ethenyl-2-methoxyphenol	4 - vinyl guaiacol (Marta Montero-Calderón et al., 2010)	7786-61-0	150.17
238	4-ethenylphenol	4 - vinyl phenol (Marta Montero-Calderón et al., 2010)	2628-17-3	120.15
239	5-(1-hydroxyethyl)oxolan-2-one	Solerol (Elss et al., 2005; Marta Montero-Calderón et al., 2010)	27610-27-1	130.14
240	5-methyl-2-propan-2-ylcyclohexan-1-ol	Menthol (Asikin et al., 2022; Marta Montero-Calderón et al., 2010; Umano et al., 1992)	1490-04-6	156.26
241	butan-1-ol	Butanol (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Turazzi et al., 2017; Xiao et al., 2021; Zhang et al., 2012)	71-36-3	74.12
242	decan-1-ol	1 - decanol (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Sengar et al., 2022; Steingass, Carle, et al., 2015)	112-30-1	158.28
243	dodecan-1-ol	1 - dodecanol (Berger et al., 1985; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	112-53-8	186.33
244	ethanol	Ethanol (Akioka & Umano, 2008; Asikin et al., 2022; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pino, 2013; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Turazzi et al., 2017; Vollmer et al., 2021; Wu et al., 1991; Zhang et al., 2012)	64-17-5	46.07

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245	furan-2-ylmethanol	furfuryl alcohol (Marta Montero-Calderón et al., 2010)	98-00-0	98.1
246	heptan-1-ol	Heptanol (Asikin et al., 2022; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Turazzi et al., 2017; Xiao et al., 2021)	111-70-6	116.2
247	hexan-1-ol	1-Hexanol (Asikin et al., 2022; Braga et al., 2009; Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Takeoka et al., 1989; Turazzi et al., 2017; Umano et al., 1992; Wu et al., 1991; Xiao et al., 2021)	111-27-3	102.17
248	hexan-2-ol	2 - hexanol (Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010)	626-93-7	102.17
249	hexan-3-ol	3 - hexanol (Marta Montero-Calderón et al., 2010; Takeoka et al., 1989)	623-37-0	102.17
250	methanol	Methanol (Akioka & Umano, 2008; Marta Montero-Calderón et al., 2010; R.A., 1980)	67-56-1	32.04
251	NA	erytro - 3 - acetoxy - 2 - butanol (Marta Montero-Calderón et al., 2010)	NA	132.16
252	NA	erytro - 3 - hydroxy - 2 - butanol (Marta Montero-Calderón et al., 2010)	NA	
253	nonan-1-ol	1-Nonanol (Braga et al., 2009; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wei et al., 2014; Wei, Liu, Liu, Zang, et al., 2011)	143-08-8	144.25
254	oct-1-en-3-ol	1-Octen-3-ol (Steingass, Carle, et al., 2015; Vollmer et al., 2021)	3391-86-4	128.21
255	octan-1-ol	1-octanol (Asikin et al., 2022; Braga et al., 2009; Steingass, Carle, et al., 2015; Sun et al., 2016; Turazzi et al., 2017; Wei, Liu, Liu, Zang, et al., 2011)	111-87-5	130.23
256	pent-1-en-3-ol	1 - penten - 3 - ol (Marta Montero-Calderón et al., 2010)	616-25-1	86.13
257	pentan-1-ol	1-Pentanol (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	71-41-0	88.15
258	pentan-2-ol	2 - pentanol (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Wu et al., 1991)	6032-29-7	88.15
259	pentan-3-ol	3 - pentanol (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	584-02-1	88.15
260	phenylmethanol	Benzyl alcohol (Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2014; Umano et al., 1992)	100-51-6	108.14
261	propan-1-ol	1-Propanol (Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; R.A., 1980; Zhang et al., 2012)	71-23-8	60.1
262	propan-2-ol	Isopropyl alcohol (Steingass, Carle, et al., 2015)	67-63-0	60.10
263	undecan-1-ol	1-Undecanol (Steingass, Carle, et al., 2015)	112-42-5	172.31
Aldehydes				
264	(2E)-3,7-dimethylocta-2,6-dienal	Geranial (Pickenhagen, 1989; Steingass, Carle, et al., 2015)	141-27-5	152.23
265	(2E,4E)-deca-2,4-dienal	(E,E)-2,4-Decadienal (Steingass, Carle, et al., 2015)	25152-84-5	152.23
266	(2E,4E)-hepta-2,4-dienal	(E,E)-2,4-Heptadienal (Steingass, Carle, et al., 2015; Vollmer et al., 2021)	4313-03-5	110.15
267	(2E,4E)-hexa-2,4-dienal	(E,E)-2,4-Hexadienal (Steingass, Carle, et al., 2015)	142-83-6	96.13
268	(2E,4E)-nona-2,4-dienal	(E,E)-2,4-Nonadienal (Steingass, Carle, et al., 2015)	5910-87-2	138.21
269	(2E,4Z)-hepta-2,4-dienal	(E,Z)-2,4-Heptadienal (Vollmer et al., 2021)	4313-02-4	110.15

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270	(2E,6Z)-nona-2,6-dienal	(E,Z)-2,6-Nonadienal (Steingass, Carle, et al., 2015)	557-48-2	138.21
271	(2Z)-3,7-dimethylocta-2,6-dienal	Neral (Steingass, Carle, et al., 2015)	106-26-3	152.23
272	(E)-dec-2-enal	(E)-2-Decenal (Steingass, Carle, et al., 2015; Vollmer et al., 2021)	3913-81-3	154.25
273	(E)-dodec-2-enal	(E)-2-Dodecenal (Vollmer et al., 2021)	20407-84-5	182.3
274	(E)-hept-2-enal	(E)-2-Heptenal (Pickenhagen, 1989; Steingass, Carle, et al., 2015; Vollmer et al., 2021)	18829-55-5	112.17
275	(E)-hex-2-enal	(E) - 2 - hexenal (Pickenhagen, 1989; Steingass, Carle, et al., 2015; Takeoka et al., 1989)	6728-26-3	98.14
276	(E)-non-2-enal	(E)-2-Nonenal (Steingass, Carle, et al., 2015; Steingass et al., 2016; Vollmer et al., 2021)	18829-56-6	140.22
277	(E)-oct-2-enal	(E)-2-Octenal (Steingass, Carle, et al., 2015; Vollmer et al., 2021)	2548-87-0	126.2
278	(E)-pent-2-enal	(E)-2-Pentenal (Pickenhagen, 1989; Steingass, Carle, et al., 2015)	1576-87-0	84.12
279	(E)-undec-2-enal	(E)-2-Undecenal (Steingass, Carle, et al., 2015; Vollmer et al., 2021)	53448-07-0	168.28
280	(Z)-2-butyloct-2-enal	2-butyl-2-octenal (Umano et al., 1992)	13019-16-4	182.3
281	1,1-diethoxyethane	1,1 - diethoxyethane (Flath & Forrey, 1970)	105-57-7	118.17
282	2-methylbutanal	2-methylbutanal (Pickenhagen, 1989; Pino, 2013)	96-17-3	86.13
283	2-methylpentanal	2-Methylpentanal (Steingass, Carle, et al., 2015; Turazzi et al., 2017)	123-15-9	100.16
284	2-phenylacetaldehyde	Phenylacetaldehyde (Braga et al., 2009; Elss et al., 2005; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Pino, 2013)	122-78-1	120.15
285	3-methylbutanal	3-methylbutanal (Pickenhagen, 1989; Pino, 2013)	590-86-3	86.13
286	4-hydroxy-3,5-dimethoxybenzaldehyde	Syringaldehyde (Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Teai et al., 2001; Wu et al., 1991)	134-96-3	182.17
287	4-hydroxy-3-methoxybenzaldehyde	Vanillin (Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Teai et al., 2001; Tokitomo et al., 2005; Umano et al., 1992; Wu et al., 1991)	121-33-5	152.15
288	4-hydroxybenzaldehyde	p - hydroxybenzaldehyde (Marta Montero-Calderón et al., 2010; Pickenhagen, 1989; Wu et al., 1991)	123-08-0	122.12
289	5-methylfuran-2-carbaldehyde	5 - methylfurfural (Marta Montero-Calderón et al., 2010)	620-02-0	110.11
290	acetaldehyde	Acetaldehyde (Akioka & Umano, 2008; Braga et al., 2009; Marta Montero-Calderón et al., 2010; Pino, 2013; R.A., 1980; Steingass et al., 2021; Steingass et al., 2014; Xiao et al., 2021)	75-07-0	44.05
291	benzaldehyde	Benzaldehyde (Akioka & Umano, 2008; Elss et al., 2005; Marta Montero-Calderón et al., 2010; Orellana-Palma et al., 2020; Pickenhagen, 1989; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Xiao et al., 2021)	100-52-7	106.12
292	decanal	Decanal (Akioka & Umano, 2008; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Sun et al., 2016; Turazzi et al., 2017; Vollmer et al., 2021; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Xiao et al., 2021; Zheng et al., 2012)	112-31-2	156.26
293	dodecanal	Dodecanal (Sengar et al., 2022; Steingass, Carle, et al., 2015)	112-54-9	184.32
294	formaldehyde	Formaldehyde (Connell, 1964; Marta Montero-Calderón et al., 2010; R.A., 1980)	50-00-0	30.03
295	furan-2-carbaldehyde	Furfural (Braga et al., 2009; Elss et al., 2005; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Steingass et al., 2017; Teai et al., 2001; Umano et al., 1992; Zhang et al., 2012)	98-01-1	96.08

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296	heptanal	heptanal (Braga et al., 2009; Pedroso et al., 2011; Spanier et al., 1998; Steingass, Carle, et al., 2015)	111-71-7	114.19
297	hexanal	Hexanal (Asikin et al., 2022; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; Lasekan & Hussein, 2018; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Pedroso et al., 2011; Spanier et al., 1998; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2017; Steingass et al., 2014; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Xiao et al., 2021)	66-25-1	100.16
298	nonanal	Nonanal (Akioka & Umano, 2008; Asikin et al., 2022; Berger et al., 1985; Braga et al., 2009; Brat et al., 2004; Elss et al., 2005; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Sun et al., 2016; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Wei, Liu, Liu, Zang, et al., 2011)	124-19-6	142.24
299	octanal	Octanal (caprilic aldehyde) (Braga et al., 2009; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass, Jutzi, et al., 2015; Tokitomo et al., 2005; Vollmer et al., 2021; Zheng et al., 2012)	124-13-0	128.21
300	pentanal	Pentanal (Steingass, Carle, et al., 2015; Takeoka et al., 1989)	110-62-3	86.13
301	propanal	propanal (Marta Montero-Calderón et al., 2010; R.A., 1980)	123-38-6	58.08
302	tetradecanal	Tetradecanal (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	124-25-4	212.37
303	tridecanal	Tridecanal (Sengar et al., 2022; Steingass, Carle, et al., 2015)	10486-19-8	198.34
304	undecanal	Undecanal (Braga et al., 2009; Pedroso et al., 2011; Steingass, Carle, et al., 2015)	112-44-7	170.29
Acids				
305	(E)-3-phenylprop-2-enoic acid	cinamic acid (Marta Montero-Calderón et al., 2010)	140-10-3	148.16
306	2-methylbutanoic acid	2-methylbutyric acid (Marta Montero-Calderón et al., 2010; Teai et al., 2001)	116-53-0	102.13
307	2-phenylacetic acid	Phenylacetic acid (Marta Montero-Calderón et al., 2010; Tokitomo et al., 2005; Wu et al., 1991)	103-82-2	136.15
308	3-methylbutanoic acid	3-methylbutyric acid (Umano et al., 1992)	503-74-2	102.13
309	acetic acid	acetic acid (Braga et al., 2009; Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Turazzi et al., 2017; Umano et al., 1992; Xiao et al., 2021; Zhang et al., 2012)	64-19-7	60.05
310	benzoic acid	Benzoic acid (R.A., 1980; Vollmer et al., 2021)	65-85-0	122.12
311	butanoic acid	Butanoic acid (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Tokitomo et al., 2005; Vollmer et al., 2021)	107-92-6	88.11
312	decanoic acid	Decanoic acid (Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Xiao et al., 2021)	334-48-5	172.26
313	heptanoic acid	Heptanoic acid (Steingass, Carle, et al., 2015; Vollmer et al., 2021; Xiao et al., 2021)	111-14-8	130.18
313	tetradecanoic acid	tetradecanoic acid (Braga et al., 2009)	544-63-8	228.37
313	pentadecanoic acid	pentadecanoic acid (Braga et al., 2009)	1002-84-2	242.40
314	hexadecanoic acid	hexadecanoic acid (Braga et al., 2009)	57-10-3	256.42

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315	hexanoic acid	Hexanoic acid (Asikin et al., 2022; Brat et al., 2004; Lasekan & Hussein, 2018; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Sun et al., 2016; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Xiao et al., 2021; Zainuddin et al., 2021)	142-62-1	116.16
316	nonanoic acid	Nonanoic acid (Orellana-Palma et al., 2020; Steingass, Carle, et al., 2015; Vollmer et al., 2021; Xiao et al., 2021)	112-05-0	158.24
317	octadec-9-enoic acid	Octadec-9-enoic acid (Lukás et al., 2013)	2027-47-6	282.5
318	octadecanoic acid	Octadecanoic acid (Berger et al., 1985; Lasekan & Hussein, 2018; Lukás et al., 2013)	57-11-4	284.5
319	octanoic acid	Octanoic acid (Asikin et al., 2022; Brat et al., 2004; Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Xiao et al., 2021; Zheng et al., 2012)	142-07-2	144.21
320	pentanoic acid	Pentanoic acid (Steingass, Carle, et al., 2015; Xiao et al., 2021)	109-52-4	102.13
321	propanoic acid	propanoic acid (Marta Montero-Calderón et al., 2010; Umano et al., 1992)	79-09-4	74.08
Ketones				
322	(5Z)-octa-1,5-dien-3-one	(Z) - 1,5 - octadien - 3 – one (Marta Montero-Calderón et al., 2010)	65767-22-8	124.18
323	(E)-1-(2,6,6-trimethylcyclohexa-1,3-dien-1-yl)but-2-en-1-one	β-Damascenone (Pino, 2013; Steingass, Carle, et al., 2015; Tokitomo et al., 2005; Vollmer et al., 2021)	23726-93-4	190.28
324	(E)-4-(2,6,6-trimethylcyclohexen-1-yl)but-3-en-2-one	(E)-β-Ionone (Vollmer et al., 2021)	14901-07-6	192.3
325	(E)-oct-3-en-2-one	(E)-3-Octen-2-one (Steingass, Carle, et al., 2015)	18402-82-9	126.20
326	1-hydroxypropan-2-one	Hydroxyacetone (Marta Montero-Calderón et al., 2010; Umano et al., 1992)	116-09-6	74.08
327	1-phenylethanone	Acetophenone (Steingass, Carle, et al., 2015; Xiao et al., 2021)	98-86-2	120.15
328	2,10,10-trimethyltricyclo[7.1.1.02,7]undec-6-en-8-one	2,10,10-Trimethyltricyclo[7.1.1.0(2,7)]undec-6-en-8-one (Wei, Liu, Liu, Lv, et al., 2011)	NA	204.31
329	2,2,6-trimethylcyclohexan-1-one	2,2,6-Trimethylcyclohexanone (Vollmer et al., 2021)	2408-37-9	140.22
330	2,5-dimethylfuran-3-one	2,5 - dimethyl - 3(2H) -furanone (Marta Montero-Calderón et al., 2010)	14400-67-0	112.13
331	2,6,6-trimethylcyclohex-2-en-1-one	2,6,6-Trimethyl-2-cyclohexen-1-one (Vollmer et al., 2021)	20013-73-4	138.21
332	3-hydroxypyran-2-one	3 - hydroxy - (2H) - pyran - 2 -one (Elss et al., 2005)	496-64-0	112.08
333	3-methylbutan-2-one	3 - methyl - 2 - butanone (Elss et al., 2005)	563-80-4	86.13
334	4-hydroxy-4-methylpentan-2-one	4-Hydroxy-4-methylpentan-2-one (Steingass et al., 2021)	123-42-2	116.16
335	6-methylhept-5-en-2-one	6-Methyl-5-hepten-2-one (Braga et al., 2009; Elss et al., 2005; Steingass, Carle, et al., 2015; Steingass et al., 2014; Vollmer et al., 2021)	110-93-0	126.2
336	heptan-2-one	2-Heptanone (Elss et al., 2005; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Steingass, Carle, et al., 2015; Takeoka et al., 1989)	110-43-0	114.19
337	hexan-2-one	2 – hexanone (Marta Montero-Calderón et al., 2010)	591-78-6	100.16

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338	hexan-3-one	3 - hexanone (Marta Montero-Calderón et al., 2010)	589-38-8	100.16
339	nonan-2-one	2-Nonanone (Steingass, Carle, et al., 2015)	821-55-6	142.24
340	octan-3-one	3-Octanone (Steingass, Carle, et al., 2015)	106-68-3	128.21
341	pent-1-en-3-one	1-Penten-3-one (Pickenhagen, 1989; Steingass, Carle, et al., 2015)	1629-58-9	84.12
342	pentan-2-one	2-Pentanone (Elss et al., 2005; R.A., 1980; Teai et al., 2001; Wu et al., 1991)	107-87-9	86.13
343	pentan-3-one	3 – pentanone (R.A., 1980)	96-22-0	86.13
344	propan-2-one	Acetone (Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass et al., 2017; Umano et al., 1992)	67-64-1	58.08
Lactones				
345	5-dodecyloxolan-2-one	γ - palmitolactone (Marta Montero-Calderón et al., 2010)	730-46-1	254.41
346	(3R)-3-hydroxy-4,4-dimethyloxolan-2-one	pantolactone (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Teai et al., 2001)	599-04-2	130.14
347	(6R)-6-ethyloxan-2-one	delta-Heptalactone (Elss et al., 2005; Marta Montero-Calderón et al., 2010)	108943-43-7	128.17
348	(6S)-6-heptyloxan-2-one	delta-Dodecalactone (isomer) (Elss et al., 2005; Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010)	108943-47-1	198.3
349	4-hydroxy-2,3-dimethyl-2H-furan-5-one	3 - hydroxy - 4,5 - dimethyyl -2(5H) – furanone (Marta Montero-Calderón et al., 2010)	28664-35-9	128.13
350	5-acetyloxolan-2-one	solerone (Elss et al., 2005; Marta Montero-Calderón et al., 2010)	29393-32-6	128.13
351	5-butyloxolan-2-one	gamma-Octalactone (Asikin et al., 2022) (Lasekan & Hussein, 2018; Mohd Ali et al., 2020; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Turazzi et al., 2017; Vollmer et al., 2021) (Brat et al., 2004; Elss et al., 2005; Kaewtathip & Charoenrein, 2012; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; Po & Po, 2012; R.A., 1980; Steingass et al., 2014; Teai et al., 2001; Tokitomo et al., 2005; Umano et al., 1992; Wu et al., 1991; Zheng et al., 2012)	104-50-7	142.2
352	5-ethyloxolan-2-one	gamma-Hexalactone (Asikin et al., 2022; Brat et al., 2004; Elss et al., 2005; Lukás et al., 2013; Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991)	695-06-7	114.14
353	5-hexyloxolan-2-one	gamma decalactone (Elss et al., 2005; Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Langen, et al., 2015; Teai et al., 2001; Tokitomo et al., 2005; Vollmer et al., 2021; Wu et al., 1991)	706-14-9	170.25
354	5-methyloxolan-2-one	γ - valerolactone (Marta Montero-Calderón et al., 2010)	108-29-2	100.12
355	5-octyloxolan-2-one	gamma dodecalactone (Elss et al., 2005; Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010; Steingass et al., 2016; Steingass et al., 2014; Takeoka et al., 1989; Teai et al., 2001; Tokitomo et al., 2005; Umano et al., 1992)	7/05/2305	198.3
356	5-pentyloxolan-2-one	gamma nonalactone(Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991)	104-61-0	156.22
357	5-propyloxolan-2-one	gamma heptalactone (Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2014)	105-21-5	128.17
358	6-butyloxan-2-one	delta-Nonalactone (Marta Montero-Calderón et al., 2010; Sengar et al., 2022; Turazzi et al., 2017)	3301-94-8	156.22

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359	6-heptyloxan-2-one	δ - dodecalactone	713-95-1	198.3
360	6-methyloxan-2-one	delta-hexalactone (Brat et al., 2004; Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991)	823-22-3	114.14
361	6-pentyloxan-2-one	delta-decalactone(Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Tokitomo et al., 2005; Umano et al., 1992; Vollmer et al., 2021)	705-86-2	170.25
362	6-propyloxan-2-one	delta-Octalactone (Asikin et al., 2022; Vollmer et al., 2021; Xiao et al., 2021; Zainuddin et al., 2021) (Mohd Ali et al., 2020; Steingass et al., 2021) (Lasekan & Hussein, 2018; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass, Langen, et al., 2015) (Brat et al., 2004; Elss et al., 2005; Marta Montero-Calderón et al., 2010; Po & Po, 2012; R.A., 1980; Steingass et al., 2014; Teai et al., 2001; Tokitomo et al., 2005; Umano et al., 1992; Wei et al., 2014; Wu et al., 1991; Zheng et al., 2012)	698-76-0	142.2
363	oxolan-2-one	gamma-butyrolactone (Brat et al., 2004; Elss et al., 2005; Lasekan & Hussein, 2018; Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Teai et al., 2001; Umano et al., 1992; Xiao et al., 2021)	96-48-0	86.09
Furan – terpene - class of compounds				
364	2-pentylfuran	2-Pentylfuran (Steingass, Carle, et al., 2015)	3777-69-3	138.21
365	2-[(2R,5S)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	(Z)-Linalool oxide (furanoid) (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	5989-33-3	170.25
366	1-(furan-2-yl)ethanone	2-acetylfuran (Umano et al., 1992)	1192-62-7	110.11
367	2-(5-ethenyl-5-methyloxolan-2-yl)propan-2-ol	linalool oxide (R.A., 1980; Umano et al., 1992)	60047-17-8	170.25
368	2-[(2R,5R)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	linalool oxide (trans-furanoid) (R.A., 1980)	34995-77-2	170.25
369	2-methyloxolan-3-one	2-methyltetrahydrofuran-3-one (Marta Montero-Calderón et al., 2010)	3188-00-9	100.12
370	4-hydroxy-2,5-dimethylfuran-3-one	2,5-Dimethyl-4-hydroxy-2,3-dihydro-3-furanone (Asikin et al., 2022; Brat et al., 2004; Flath & Forrey, 1970; Lasekan & Hussein, 2018; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wu et al., 1991; Zhang et al., 2012)	3658-77-3	128.13
371	4-methoxy-2,5-dimethylfuran-3-one	2,5-dimethyl-4-methoxy-3(2H)-furanone (Asikin et al., 2022; Brat et al., 2004; Elss et al., 2005; Lasekan & Hussein, 2018; Mohd Ali et al., 2020; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2017; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Zainuddin et al., 2021; Zhang et al., 2012)	4077-47-8	142.15
372	5-(hydroxymethyl)furan-2-carbaldehyde	5-(Hydroxymethyl)furfural (Elss et al., 2005; Teai et al., 2001; Umano et al., 1992; Wei, Liu, Liu, Lv, et al., 2011)	67-47-0	126.11
373	(5E)-6,10-dimethylundeca-5,9-dien-2-one	(E)-Geranylacetone (Vollmer et al., 2021)	3796-70-1	194.31
374	1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	Camphor (Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Umano et al., 1992)	76-22-2	152.23
375	(2E)-3,7-dimethylocta-2,6-dien-1-ol	geraniol (Asikin et al., 2022; Elss et al., 2005; Lasekan & Hussein, 2018; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010)	106-24-1	154.25
376	(1aR,4aS,7R,7aR,7bS)-1,1,7-trimethyl-4-methylidene-2,3,4a,5,6,7,7a,7b-octahydro-1aH-cyclopropa[e]azulene	(−)-Alloaromadendrene (Zheng et al., 2012)	25246-27-9	204.35
377	(1aR,4R,7bS)-1,1,4,7-tetramethyl-1a,2,3,4,4a,5,6,7b-octahydrocyclopropa[e]azulene	α-Gurjunene (Steingass, Carle, et al., 2015; Steingass et al., 2021)	489-40-7	204.35

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378	(1E,6E,8S)-1-methyl-5-methylidene-8-propan-2-ylcyclodeca-1,6-diene	germacrene D (Marta Montero-Calderón et al., 2010)	23986-74-5	204.35
379	(1R)-1,3-dimethyl-8-propan-2-yltricyclo[4.4.0.02,7]dec-3-ene	α-Copaene (Asikin et al., 2022; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Takeoka et al., 1989; Vollmer et al., 2021)	3856-25-5	204.35
380	(1R)-7-methyl-4-methylidene-1-propan-2-yl-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	delta Muurolene (Asikin et al., 2022)	120021-96-7	204.35
381	(1R,2S,3S,6S,8S)-6-methyl-7-methylidene-3-propan-2-yltricyclo[4.4.0.02,8]decane	(+)-Sativene (Wei, Liu, Liu, Lv, et al., 2011)	3650-28-0	204.35
382	(1R,4aR,8aS)-7-methyl-4-methylidene-1-propan-2-yl-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	γ-Muurolene (Asikin et al., 2022; Takeoka et al., 1989)	30021-74-0	204.35
383	(1R,4aS,8aS)-7-methyl-4-methylidene-1-propan-2-yl-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	Gamma -Cadinene	1460-97-5	204.35
384	(1R,4E,9S)-4,11,11-trimethyl-8-methylidenebicyclo[7.2.0]undec-4-ene	β-Caryophyllene (Sengar et al., 2022; Sun et al., 2016; Wei, Liu, Liu, Lv, et al., 2011)	87-44-5	204.35
385	(1R,5S,6R,7S,10R)-10-methyl-4-methylidene-7-propan-2-yltricyclo[4.4.0.01,5]decane	β-Cubebene (Wei, Liu, Liu, Lv, et al., 2011)	13744-15-5	204.35
386	(1S)-4,7-dimethyl-1-propan-2-yl-1,2-dihydronaphthalene	α-Calacorene (Sun et al., 2016; Wei, Liu, Liu, Lv, et al., 2011)	21391-99-1	200.32
387	(1S)-4-methyl-1-propan-2-ylcyclohex-3-en-1-ol	4 - terpinenol (Marta Montero-Calderón et al., 2010)	2438-10-0	154.25
388	(1S,2S,3R,4S,6R,7R,8S)-1,2-Dimethyl-8-propan-2-yltetracyclo[4.4.0.02,4.03,7]decane	(+)-Cycloisosativene (Liu & Liu, 2014; Sun et al., 2016)	22469-52-9	204.35
389	(1S,4aS,8aR)-4,7-dimethyl-1-propan-2-yl-1,2,4a,5,6,8a-hexahydronaphthalene	α-Muurolene (Akioka & Umano, 2008; Braga et al., 2009; Liu et al., 2011; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Teai et al., 2001; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Zheng et al., 2012)	10208-80-7	204.35
390	(1S,4S)-1,4-dimethyl-7-propan-2-ylidene-2,3,4,5,6,8-hexahydro-1H-azulene	β-Guaiene (Sun et al., 2016; Wei, Liu, Liu, Lv, et al., 2011)	88-84-6	204.35
391	(1S,6R,7R)-1-methyl-3-methylidene-8-propan-2-yltricyclo[4.4.0.02,7]decane	β – ylangene (Marta Montero-Calderón et al., 2010)	20479-06-5	204.35
392	(1S,8aR)-4,7-dimethyl-1-propan-2-yl-1,2,3,5,6,8a-hexahydronaphthalene	δ - cadinene (Asikin et al., 2022; Brat et al., 2004; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Takeoka et al., 1989; Wei, Liu, Liu, Lv, et al., 2011)	483-76-1	204.35
393	(1Z,6Z)-cyclodeca-1,6-diene	1,6-Cyclodecadiene (Zheng et al., 2012)	1124-79-4	136.23
394	(3E)-3,7-dimethylocta-1,3,6-triene	(E)-β-Ocimene (Asikin et al., 2022; Lasekan & Hussein, 2018; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2017; Steingass, Jutzi, et al., 2015)	3779-61-1	136.23
395	(3E,5E)-undeca-1,3,5-triene	1-(3E,5E)-3,5-Undecatriene (Berger et al., 1985; Braga et al., 2009; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2014; Sun et al., 2016; Takeoka et al., 1989)	19883-29-5	150.26
396	(3E,5E,8Z)-undeca-1,3,5,8-tetraene	(E,E,Z)-Undeca-1,3,5,8-tetraene (Akioka & Umano, 2008; Asikin et al., 2022; Braga et al., 2009; Liu et al., 2011; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Takeoka et al., 1989; Tokitomo et al., 2005; Vollmer et al., 2021; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011; Wei, Liu, Liu, Zang, et al., 2011)	50277-31-1	148.24
397	(3E,5Z)-undeca-1,3,5-triene	1-(3E,5Z)-3,5-undecatriene (Akioka & Umano, 2008; Berger et al., 1985; Braga et al., 2009; Kaewtathip & Charoenrein, 2012; Lasekan & Hussein, 2018; Mohd Ali et al., 2020; Marta Montero-Calderón et al., 2010; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Sun et al., 2016; Takeoka et al., 1989; Tokitomo et al., 2005; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011; Wei, Liu, Liu, Zang, et al., 2011; Xiao et al., 2021)	19883-27-3	150.26

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398	(3R,4aR,8aR)-5,8a-dimethyl-3-prop-1-en-2-yl-2,3,4,4a,7,8-hexahydro-1H-naphthalene	α-Selinene (Steingass, Carle, et al., 2015; Steingass et al., 2021)	473-13-2	204.35
399	(3R,4aS,5R)-4a,5-dimethyl-3-prop-1-en-2-yl-2,3,4,5,6,7-hexahydro-1H-naphthalene	Valencene	4630-07-3	204.35
400	(3Z)-3,7-dimethylocta-1,3,6-triene	(Z)-β-Ocimene (Steingass, Carle, et al., 2015; Vollmer et al., 2021; Wei et al., 2014; Wei, Liu, Liu, Lv, et al., 2011)	3338-55-4	136.23
401	(3Z,5E,8Z)-undeca-1,3,5,8-tetraene	(Z,E,Z)-undeca-1,3,5,8-tetraene [1, 2,7, 9, 12]	29837-19-2	148.24
402	(4Z,6Z)-3a,4,6,9a-tetramethyl-2,3,8,9-tetrahydro-1H-cyclopenta[8]annulene	1,2,4,8-Tetramethylbicyclo[6.3.0]undeca-2,4-diene		204.35
403	(5R)-2-methyl-5-[(2S)-6-methylhept-5-en-2-yl]cyclohexa-1,3-diene	α – zingiberene (Marta Montero-Calderón et al., 2010)	495-60-3	204.35
404	(5S)-4,10,11,11-tetramethyltricyclo[5.3.1.01,5]undec-9-ene	α – patchoulene (Marta Montero-Calderón et al., 2010)	560-32-7	204.35
405	(7aS)-1,1,7,7a-tetramethyl-2,3,5,6,7,7b-hexahydro-1aH-cyclopropa[a]naphthalene	(+)-Calarene (Wei, Liu, Liu, Lv, et al., 2011)	17334-55-3	204.35
406	1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane	1,8 - cineol (Elss et al., 2005)	470-82-6	154.25
407	1,4-dimethyl-7-prop-1-en-2-yl-1,2,3,3a,4,5,6,7-octahydroazulene	γ – gurjunene (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Takeoka et al., 1989)	22567-17-5	204.35
408	1-ethenyl-1-methyl-2,4-bis(prop-1-en-2-yl)cyclohexane	β-Elemene (Asikin et al., 2022; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass, Jutzi, et al., 2015; Wei, Liu, Liu, Lv, et al., 2011)	33880-83-0	204.35
409	1-ethenyl-2-[(E)-hex-1-enyl]cyclopropane	(±)-Dictyopterene A (Zheng et al., 2012)	22822-99-7	150.26
410	1-methyl-4-isopropyl-; 4-Isopropyl-1-methyl-1,4-cyclohexadiene	γ-Terpinene (Steingass, Carle, et al., 2015; Sun et al., 2016)	99-85-4	136.23
411	1-methyl-4-prop-1-en-2-ylbenzene	Dehydro-p-cymene (Steingass, Carle, et al., 2015; Vollmer et al., 2021)	1195-32-0	132.2
412	1-methyl-4-prop-1-en-2-ylcyclohexene	Limonene (Brat et al., 2004; Elss et al., 2005; Lukás et al., 2013; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Sun et al., 2016; Takeoka et al., 1989; Umano et al., 1992; Xiao et al., 2021)	138-86-3	136.23
413	1-methyl-4-propan-2-yl-7-oxabicyclo[2.2.1]heptane	1,4 - cineol (Elss et al., 2005; Marta Montero-Calderón et al., 2010)	470-67-7	154.25
414	1-methyl-4-propan-2-ylbenzene	p-Cymene (Brat et al., 2004; Elss et al., 2005; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Teai et al., 2001; Umano et al., 1992; Vollmer et al., 2021)	99-87-6	134.22
415	1-methyl-4-propan-2-ylidenecyclohexene	α-Terpinolene (Akioka & Umano, 2008; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014)	586-62-9	136.23
416	2-(4-methylcyclohex-3-en-1-yl)propan-2-ol	α-Terpineol (Akioka & Umano, 2008; Steingass, Carle, et al., 2015; Steingass et al., 2014)	98-55-5	154.25
417	2,2,4-trimethylheptane	heptane 2, 2, 4-trimethyl (Spanier et al., 1998)	14720-74-2	142.28
418	2,2,5-trimethylhexane	hexane 2,2,5-trimethyl (Spanier et al., 1998)	3522-94-9	128.25
419	2,6,6-trimethylbicyclo[3.1.1]hept-2-ene	α - pinene (Brat et al., 2004; Lamikanra & Richard, 2004; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Takeoka et al., 1989; Zainuddin et al., 2021)	80-56-8	136.23
420	2,6,6-trimethylcyclohexene-1-carbaldehyde	β-Cyclocitral (Steingass, Carle, et al., 2015; Vollmer et al., 2021)	432-25-7	152.23
421	2-[(2R,4aR)-4a,8-dimethyl-2,3,4,5,6,7-hexahydro-1H-naphthalen-2-yl]propan-2-ol	γ – eudesmol (Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015)	1209-71-8	222.37

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422	3,7,7-trimethylbicyclo[4.1.0]hept-3-ene	3-Carene (Steingass, Carle, et al., 2015; Sun et al., 2016)	13466-78-9	136.23
423	3,7-dimethylocta-1,6-dien-3-ol	Linalool (Elss et al., 2005; M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010; Marta Montero-Calderón et al., 2010; R.A., 1980; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Umano et al., 1992; Wu et al., 1991)	78-70-6	154.25
424	3-methyl-6-propan-2-ylcyclohex-2-en-1-one	Piperitone (Steingass, Carle, et al., 2015)	89-81-6	152.23
425	3-methylidene-6-propan-2-ylcyclohexene	β – phellandrene (Brat et al., 2004; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	555-10-2	136.23
426	3R,4aS,8aR)-8a-methyl-5-methylidene-3-prop-1-en-2-yl-1,2,3,4,4a,6,7,8-octahydronaphthalene	beta selinene (Braga et al., 2009; Steingass et al., 2021; Steingass et al., 2014; Takeoka et al., 1989; Wei, Liu, Liu, Lv, et al., 2011)	17066-67-0	204.35
427	4,10-dimethyl-7-propan-2-yltricyclo[4.4.0.01,5]dec-3-ene	α-Cubebene (Sun et al., 2016; Wei, Liu, Liu, Lv, et al., 2011)	17699-14-8	204.35
428	4,4,7a-trimethyl-6,7-dihydro-5H-1-benzofuran-2-one	Dihydroactinidiolide (Vollmer et al., 2021)	15356-74-8	180.24
429	4,7-dimethyl-1-propan-2-yl-1,2,4a,5,6,8a-hexahydronaphthalene	α-Amorphene (Akioka & Umano, 2008; Steingass et al., 2021)	483-75-0	204.35
430	(1S,4aR,8aS)-7-methyl-4-methylidene-1-propan-2-yl-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	γ -Amorphene (Wei, Liu, Liu, Lv, et al., 2011)	6980-46-7	204.35
431	4-methyl-1-propan-2-ylcyclohex-3-en-1-ol	1-Terpinen-4-ol (Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021)	562-74-3	154.25
432	4-methylidene-1-propan-2-ylbicyclo[3.1.0]hexane	sabinene (Brat et al., 2004; Liu & Liu, 2014; Marta Montero-Calderón et al., 2010)	3387-41-5	136.23
433	6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptane	β – pinene (Takeoka et al., 1989; Xiao et al., 2021)	127-91-3	136.23
434	7-methyl-3-methylideneocta-1,6-diene	β-Myrcene (Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021)	123-35-3	136.23
435	8a-methyl-5-methylidene-3-prop-1-en-2-yl-1,2,3,4,4a,6,7,8-octahydronaphthalene	β-Selinene (Steingass et al., 2021; Takeoka et al., 1989; Wei, Liu, Liu, Lv, et al., 2011)	19069-44-4	204.35
436	cyclooctatetraene	1,3,5,7-cyclooctatetraene (Zainuddin et al., 2021)	629-20-9	104.15
437	NA	4,9-Muuroladiene (Zheng et al., 2012)	NA	204.35
438	NA	(E,E)-α-Farnesene (Steingass, Carle, et al., 2015)	502-62-4	204.35
Phenols				
439	3-methylphenol	3-methylphenol (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015)	108-39-4	108.14
440	4-ethylphenol	4-ethylphenol (M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Umano et al., 1992)	123-07-9	122.16
441	2-methoxy-4-prop-2-enylphenol	Eugenol (clove oil) (Asikin et al., 2022; Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Steingass et al., 2014; Teai et al., 2001; Vollmer et al., 2021; Wu et al., 1991)	97-53-0	164.2
442	4-prop-2-enylphenol	p-Allylphenol (Asikin et al., 2022; Marta Montero-Calderón et al., 2010; R.A., 1980; Silverstein et al., 1965; Teai et al., 2001)	501-92-8	134.17

Sl.No.	IUPAC Name	Reported name	CAS No.	M.W.
443	phenol	Phenol (Marta Montero-Calderón et al., 2010; Steingass, Carle, et al., 2015; Umano et al., 1992; Wu et al., 1991; Xiao et al., 2021)	108-95-2	94.11
Sulphur containing compounds				
444	3-methylsulfanylpropan-1-ol	3-(methylthio)propanol (Steingass et al., 2021; Umano et al., 1992)	505-10-2	106.19
445	3-isothiocyanatoprop-1-ene	Allyl isothiocyanate (Marta Montero-Calderón et al., 2010)	57-06-7	99.16
446	3-methylsulfanylpropanal	3 - (methylthio) - propanal (Marta Montero-Calderón et al., 2010)	3268-49-3	104.17
447	(methyldisulfanyl)methane	dimethyl disulfide (Marta Montero-Calderón et al., 2010; R.A., 1980; Teai et al., 2001; Xiao et al., 2021; Zhang et al., 2012)	624-92-0	94.2
448	(methyltrisulfanyl)methane	dimethyl trisulfide (Marta Montero-Calderón et al., 2010; Takeoka et al., 1991)	3658-80-8	126.3
448	2-methylsulfanylethyl acetate	2-(Methylthio) ethyl acetate (Steingass, Carle, et al., 2015)	5862-47-5	134.20
449	3-methylsulfanylpropyl acetate	3-(methylthio)propyl acetate (Elss et al., 2005; Steingass et al., 2021; Steingass, Jutzi, et al., 2015; Umano et al., 1992)	16630-55-0	148.23
450	ethyl (Z)-3-methylsulfanylprop-2-enoate	ethyl 3 - (methylthio) - (Z) - 2 -propenoate (Steingass, Carle, et al., 2015; Takeoka et al., 1991)	136115-66-7	146.21
451	ethyl 4-methylsulfanylbutanoate	ethyl 4 - (methylthio) butanoate (Marta Montero-Calderón et al., 2010)	22014-48-8	162.25
452	ethyl (E)-3-methylsulfanylprop-2-enoate	Ethyl 3-(methylthio)-(E)-2-propenoate (Steingass, Carle, et al., 2015; Takeoka et al., 1991; Vollmer et al., 2021)	136115-65-6	146.21
453	ethyl 2-methylsulfanylacetate	Ethyl 2-(methylthio)acetate (Braga et al., 2009; Steingass et al., 2021; Steingass et al., 2014; Vollmer et al., 2021)	4455-13-4	134.2
454	ethyl 3-methylsulfanylpropanoate	ethyl 3-(methylthio)propanoate (Brat et al., 2004; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011)	13327-56-5	148.23
455	methanethiol	methyl mercaptan (methanethiol) (Marta Montero-Calderón et al., 2010; R.A., 1980)	74-93-1	48.11
456	methyl (E)-3-methylsulfanylprop-2-enoate	methyl 3 - (methylthio) - (E) - 2 - propenoate (Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015; Takeoka et al., 1991)	15904-85-5	132.18
457	methyl (Z)-3-methylsulfanylprop-2-enoate	methyl 3 - (methylthio) - (Z) - 2 - propenoate (Steingass, Carle, et al., 2015; Takeoka et al., 1991)	15904-84-4	132.18
458	methyl 2-methylsulfanylacetate	methyl (methylthio)acetate (Elss et al., 2005; Umano et al., 1992)	16630-66-3	120.17
459	methyl 3-methylsulfanylpropanoate	Methyl 3-(methylthio)propanoate (Akioka & Umano, 2008; Asikin et al., 2022; Brat et al., 2004; M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010; Marta Montero-Calderón et al., 2010; Pino, 2013; Steingass, Carle, et al., 2015; Steingass et al., 2016; Steingass et al., 2021; Steingass et al., 2014; Steingass, Jutzi, et al., 2015; Turazzi et al., 2017; Umano et al., 1992; Vollmer et al., 2021; Wei, Liu, Liu, Lv, et al., 2011)	13532-18-8	134.2
460	methyl 4-methylsulfanylbutanoate	Methyl 4-(methylthio)butanoate (Steingass, Carle, et al., 2015; Steingass et al., 2021; Steingass et al., 2014; Turazzi et al., 2017)	53053-51-3	148.23
461	O-methyl 2-methylpropanethioate	methyl thioisobutyrate	NA	118.2
462	S-methyl ethanethioate	ethanethioic acid -S-methyl ester (Steingass, Carle, et al., 2015)	1534-08-3	90.15
Miscellaneous compounds				

Sl.No.	IUPAC Name	Reported name	CAS No.	M.W.
463	benzene	benzene (Marta Montero-Calderón et al., 2010; R.A., 1980)	71-43-2	78.11
464	(3Z,6E)-3,7,11-trimethyldodeca-1,3,6,10-tetraene	(Z,E)-α-Farnesene (Steingass, Carle, et al., 2015)	26560-14-5	204.35
465	(E)-4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]heptan-1-yl)but-3-en-2-one	(E)-β-Ionone-5,6-epoxide (Vollmer et al., 2021)	23267-57-4	208.3
466	1,4-xylene	p-Xylene (Lukás et al., 2013; Steingass, Carle, et al., 2015; Steingass, Jutzi, et al., 2015)	106-42-3	106.16
467	2,3,3-trimethylpentane	pentane 2,3,3-trimethyl (Spanier et al., 1998)	560-21-4	114.23
468	2-Methyl-2-phenylbutane	tert-Pentylbenzene (Asikin et al., 2022)	2049-95-8	148.24
469	3-hydroxybutan-2-one	3-hydroxy-2-butanone (acetoin) (Braga et al., 2009; Elss et al., 2005; Steingass, Carle, et al., 2015; Umano et al., 1992)	513-86-0	88.11
470	4,4,7-trimethyl-2,3-dihydro-1H-naphthalene	α-Ionene (Steingass, Carle, et al., 2015)	475-03-6	174.28
471	4-ethenyl-1,2-dimethoxybenzene	3,4-Dimethoxystyrene (Zheng et al., 2012)	6380-23-0	164.2
472	anisole	Methoxybenzene (Anisole) (Steingass, Carle, et al., 2015)	100-66-3	108.14
473	butane-2,3-diol	2,3-Butanediol (Elss et al., 2005; Steingass, Carle, et al., 2015; Steingass et al., 2021; Takeoka et al., 1989)	513-85-9	90.12
474	butane-2,3-dione	2,3-Butanedione (Elss et al., 2005; R.A., 1980; Tokitomo et al., 2005)	431-03-8	86.09
475	N,N-dimethylformamide	N ,N-dimethylformamide (Marta Montero-Calderón et al., 2010; Umano et al., 1992)	68-12-2	73.09
476	NA	β-Farnesene (Steingass, Carle, et al., 2015)	18794-84-8	204.35
477	naphthalene	Naphthalene (Vollmer et al., 2021)	91-20-3	128.17
478	nonylcyclopropane	Nonylcyclopropane (Wei, Liu, Liu, Lv, et al., 2011)	74663-85-7	168.32
479	tetradecane	Tetradecane (Asikin et al., 2022)	629-59-4	198.39
480	(4E,6E)-2,6-dimethylocta-2,4,6-triene	Alloocimene (Liu et al., 2011)	673-84-7	136.23
481	heptadecane	Heptadecane (Liu et al., 2011)	629-78-7	240.5
482	(1R,2R)-1-(Fluoromethyl)-2-vinylcyclopropane	trans-1(fluoromethyl)-2-vinylcyclopropane (Liu et al., 2011)	NA	100.13
483	2-hydroxy-3,5,5-trimethylcyclohex-2-en-1-one	2-hydroxy-3,5,5-trimethylcyclohex-2-en-1-one (Liu et al., 2011)	4883-60-7	154.21
484	icosane	Eicosane (Lasekan & Hussein, 2018; Liu et al., 2011)	112-95-8	282.5
485	toluene	Toluene (Steingass, Carle, et al., 2015)	108-88-3	92.14

Table A2: Compilation of scientific aims for pineapple VOCs measurements

Year	Reference	Aim
1945	(Haagen-Smit et al., 1945)	Investigation of chemical composition of volatile oil from the winter and summer crops of pineapple
1964	(Connell, 1964)	Investigation of VOCs of pineapple
1965	(Rodin et al., 1965)	Isolation and identification of major character impact component for pineapple flavour
1965	(Silverstein et al., 1965)	Isolation and identification of novel flavour aroma compounds in pineapple
1966	(Rodin et al., 1966)	Identification of volatile compound with a focus on sulphur containing compounds
1970	(Flath & Forrey, 1970)	A first-time review of the reported pineapple VOCs and isolation and identification of novel flavour aroma compounds in pineapple
1971	(F.P Mehrlich & Felton, 1971)	Review of the reported pineapple VOCs till 1970
1980	(R.A., 1980)	A book chapter reviewing VOCs till 1971
1985	(Berger et al., 1985)	Identification of novel VOCs in pineapple using GC-MS and their sensory properties
1989	(Takeoka et al., 1989)	Identification of VOCs by GC-MS; identification of key aroma compounds using OAVs; and sensory description of key aroma compounds
1990	(Engel et al., 1990)	A book chapter reviewing VOCs in pineapple till 1987 and other fruits volatiles
1991	(Wu et al., 1991)	Identification of free and glycosidically bound VOCs in pineapple
1991	(Takeoka et al., 1991)	Identification of additional pineapple volatiles
1991	(Berger, 1991)	A book chapter briefly reviewing VOCs in pineapple and other fruits volatiles
1992	(Umano et al., 1992)	Identification of volatile compounds by GC-MS, identification of new compounds and odour description of key aroma compounds
1993	(Hodgson & Hodgson, 1993)	A book chapter summarising VOCs in pineapple from 1945-1989
1998	(Spanier et al., 1998)	Identification of volatiles in fresh-cut and stored pineapple chunks using GC, GC-O and GC-MS
2001	(Teai et al., 2001)	Identification of volatile compounds in fresh pineapples by GC-MS
2003	(Preston et al., 2003)	Evaluation of the authenticity of flavour by studying the isotopic ratio of pineapple volatiles using GC-MS
2004	(Brat et al., 2004)	Characterisation of volatiles of new pineapple variety in comparison with Smooth Cayenne by using GC-MS
2004	(Lamikanra & Richard, 2004)	Identification of VOCs in pineapple using low-temperature SPME GC-MS methods to study the effect of UV-induced stress on VOCs of cut fruit

Year	Reference	Aim
2005	(Elss et al., 2005)	Study of the aroma profile of pineapple fruit and pineapple products using high-resolution GC-MS
2005	(Tokitomo et al., 2005)	Characterisation of key aroma compounds in fresh pineapple by application of AEDA, followed by quantifications using SIDA, calculation of OAV, along with sensory studies
2008	(Akioka & Umano, 2008)	Assessment of potent odorants of pineapple aroma using GC-MS and GC-O
2009	(Braga et al., 2009)	Investigation of VOCs composition of fresh pineapple and samples dried under normal and modified conditions using the SPME GC-MS
2010	(Braga et al., 2010)	Study of changes in volatile composition of pineapple during the drying process in normal and modified atmosphere using the SPME GC-MS
2010	(M. Montero-Calderón, M. A. Rojas-Graü, I. Aguiló-Aguayo, et al., 2010)	Study of the effect of modified packaging on the volatile profile of fresh-cut pineapple using GC-MS
2010	(M. Montero-Calderón, M. A. Rojas-Graü, & O. Martín-Belloso, 2010)	Determination of aroma profile and OAV of pineapple and how they are affected by position inside the fruit
2010	(Marta Montero-Calderón et al., 2010)	Book chapter with a major review of the pineapple VOCs, and sensory characteristics till 2005
2011	(Liu et al., 2011)	Comparison of the aroma components of pineapple fruits ripened in different seasons using GC-MS
2011	(Pedroso et al., 2011)	Demonstration of improvement in pineapple volatiles identification using the two-dimensional GC technique
2011	(Wei, Liu, Liu, Lv, et al., 2011)	Investigation of volatiles and OAV of pineapple pulp and core using HS-SPME-GC-MS
2011	(Wei, Liu, Liu, Zang, et al., 2011)	To demonstrate the benefits of SPME and use that methodology to determine the changes and distribution of aroma volatile compounds in pineapple fruit during postharvest storage
2012	(Zheng et al., 2012)	Identification and determination of the compounds responsible for the characteristic aromas of the two pineapple varieties, and illustrating differences in aroma compounds between the two varieties
2012	(Po & Po, 2012)	A book chapter briefly reviewing VOCs in pineapple till 2010 and other fruits volatiles
2012	(Kaewtathip & Charoenrein, 2012)	Use the HSPME–GC–MS technique to study the effect of freezing and thawing cycles on volatile aroma compounds of pineapple
2012	(Zhang et al., 2012)	Investigation of changes in volatile compounds of pineapple products baked at different temperatures
2013	(Lukás et al., 2013)	Study of volatile and non-volatile constituents of MD2 pineapple and the effect of different processing conditions on VOCs profile
2013	(Pino, 2013)	Determination of aroma profile and odour active compounds of pineapple by application of the AEDA and odour activity values.
2014	(Liu & Liu, 2014)	Investigation of the influence of elevated temperature postharvest treatments on the physicochemical quality and aroma components of pineapple fruits harvested during the winter
2014	(Steingass et al., 2014)	Study of the influence of harvest maturity and fruit logistics on pineapple aroma profile
2014	(Wei et al., 2014)	Development of a method of extraction and detection of aroma volatile compounds in pineapple using HS-SPME-GC-MS and determination of the key aroma compounds
2015	(Steingass, Jutzi, et al., 2015)	Monitoring the development of volatiles along the whole supply chain

Year	Reference	Aim
215	(Steingass, Langen, et al., 2015)	Application of chirospecific analysis to authenticate pineapple fruit maturity by quantitative analysis of lactones using HS-SPME-GC-MS
2015	(Steingass, Carle, et al., 2015)	Characterisation of pineapple aroma compounds by comprehensive 2D GC-MS and monitoring the ripening-dependent metabolic changes in the VOCs of pineapple.
2016	(Steingass et al., 2016)	Study of the assignment of distinctive volatiles of differently ripened and post-harvest handled pineapple
2016	(Sun et al., 2016)	A book chapter with a brief overview of the pineapple VOCs and analytical results of six pineapple cultivars
2017	(Turazzi et al., 2017)	Optimisation of the conditions for VOCs extraction of minimally processed pineapple fruit samples, and then to identify the VOCs by GC-MS.
2018	(Lasekan & Hussein, 2018)	Classification of different pineapple varieties based on volatile fingerprinting
2020	(Mohd Ali et al., 2020)	A comprehensive review of the nutritional values, volatile compounds and food products of pineapple
2020	(Orellana-Palma et al., 2020)	Evaluation of the viability of a non-thermal technology to protect valuable quality properties (including volatiles) in pineapple juice compared by the traditional evaporation technique
2021	(Steingass et al., 2021)	Study of the influence of fruit logistics on the volatile profile of fresh-cut pineapple
2021	(Vollmer et al., 2021)	Identification of the effect of continuous pressure change technology on the volatile profile, sensory profile and consumer acceptance of pineapple juice.
2021	(Zainuddin et al., 2021)	Systematic classification of pineapple by combining chemometrics, sensory analysis and chromatographic fingerprint of volatile, and phenolic compositions
2021	(Xiao et al., 2021)	Study of the interaction of esters and sulphur compounds in pineapple
2022	(Asikin et al., 2022)	Study of the VOCs in three Okinawan pineapple cultivars

Table A3: Publications relevant to the analysis of pineapple VOCs after publishing the literature review

Authors and Journal	Title and DOI	Focus	Method and VOCs	Main Findings
Porto et al. (2023); Processes	Effect of Atmospheric Cold Plasma on the Aroma of Pineapple Juice: Improving Fresh and Fruity Notes and Reducing Undesired Pungent and Sulphurous Aromas; 10.3390/pr11082303	Investigated how atmospheric cold plasma (ACP) treatment alters the aroma profile of pineapple juice.	HS-SPME-GC-MS; 17	ACP improved fresh and fruity notes by converting methyl esters to ethyl esters. Reduced pungent and sweet off notes. Thioesters were more stable but contributed to sulphurous aromas. Optimal aroma improvement occurred at 50 Hz.
Spence (2023); International Journal of Gastronomy and Food Science	Are pineapples really delicious? The history of the pineapple's taste/flavour and the role of varietal and terroir; 10.1016/j.ijgfs.2023.100682	A historical and sensory exploration of pineapple flavour, emphasising the influence of varietals and terroir.	Literature review and sensory science discussion.	Cultural, historical, and varietal factors shape pineapple flavour perception. Terroir and cultivar significantly influence flavour profiles. Consumer expectations of deliciousness are context-dependent.
Nordin et al. (2023); Foods	Comparison of Phenolic and Volatile Compounds in MD2 Pineapple Peel and Core; 10.3390/foods12112233	Characterised phenolic and volatile compounds in MD2 pineapple peel and core.	GC-MS; 38 in peel, 23 in core	Peel had higher phenolic content and antioxidant activity. Core had a higher sweetness index. Key volatiles included furfural derivatives and DDMP.
Ravichandran et al. (2023); International Journal of Food Science & Technology	Effect of high shear homogenisation on physicochemical, microstructure, particle size and volatile composition of residual pineapple pulp; 10.1111/ijfs.15984	Studied how high shear homogenization (HSH) affects the physicochemical and volatile profile of pineapple pulp.	GC-MS 10 selected VOCs	HSH reduced particle size and altered microstructure: improved homogeneity and potentially enhanced aroma release.
Liu et al. (2024); BioWeb of Conferences	Volatile compounds of fresh pineapple (*Ananas comosus cv. Josapine*) in different harvest periods; 10.1051/bioconf/202412401021	Investigated how harvest timing affects volatile profiles in Josapine pineapples.	GC-MS 112 VOCs; 9 main VOCs	Seasonal variation significantly influenced aroma compound composition. Esters and terpenes varied with harvest time, affecting flavour quality.
Lai et al. (2024); Food Chemistry	Discrimination of internal browning in pineapple during storage based on changes in volatile compounds; 10.1016/j.foodchem.2023.137358	Used volatile profiles to detect internal browning during storage.	HS-SPME-GC-MS; 30	Certain volatiles (e.g., esters, aldehydes) were markers of browning. Volatile profiling is a promising non-destructive method for quality control.
George et al. (2024); Food Chemistry	Stable isotope dilution assay and HS-SPME-GC-MS quantification of key aroma volatiles of Australian pineapple (Ananas comosus) cultivars 10.1016/j.foodchem.2024.139956	Quantified key aroma volatiles in Australian pineapple cultivars using stable isotope dilution.	HS-SPME-GC-MS with stable isotope dilution assay; focused on 26 key aroma compounds.	Identified and quantified key volatiles contributing to cultivar-specific aroma. Provided a robust method for aroma profiling in breeding and quality control.
Asikin et al. (2024); International Journal of Food Science & Technology	Gas chromatography–mass spectrometry-based electronic nose, glycosidically bound volatile, and alcohol-acyltransferase activity profiles of Okinawan pineapple; 10.1111/ijfs.17155	Explored volatile profiles, glycosidically bound volatiles, and enzyme activity in Okinawan pineapple.	HS-e nose-GC-MS; Compared the VOCs profile of 3 cultivars	Alcohol-acyltransferase activity correlated with ester formation. Glycosidically bound volatiles contributed to aroma complexity. E-nose effectively differentiated samples.
George et al. (2025); Journal of Agricultural and Food Chemistry	Relationship between Key Aroma Compounds and Sensory Attributes of Australian Grown Commercial Pineapple Cultivars; DOI: 10.1021/acs.jafc.4c12482	Investigated the relationship between key aroma compounds and sensory attributes of Australian pineapple cultivars.	HS-SPME-GC-MS with stable isotope dilution assay; focused on 26 key aroma compounds	Identified key aroma compounds contributing to sensory attributes. Provided insights into cultivar-specific aroma profiles of Australian pineapples.
Nordin et al. (2024); Journal of Agriculture and Food Research	Microencapsulation of bioactive volatile compounds from MD2 pineapple peel Extract using spray-drying and foam-mat drying; 10.1016/j.jafr.2024.101539	Studied microencapsulation of bioactive volatile compounds from MD2 pineapple peel.	GC-MS; Qualitative screening of VOCs	Microencapsulation preserved bioactive volatile compounds. Improved stability and release of volatiles.
George J (2024); Food Australia	Sensory and consumer science: Unveiling the aromatic secrets of Australian pineapple; NA	Explored the aromatic secrets of the Australian pineapple.	Sensory and consumer science.	Provided insights into consumer perceptions of pineapple aroma. Highlighted varietal differences.

Appendix 2 Supplementary information for Chapter 3

Supplementary information B1: The retention indices (RI) were not calculated using n-alkane mixtures (C8-C20), in the reported analytical method developed.

Rational for this deviation: A set of key aroma compounds were targeted for the method development, based on our recently published literature review titled as "Review of the Aroma Chemistry of Pineapple (*Ananas comosus*)" (George et al., 2023). Neat authentic reference standards of the aroma compounds listed in Table 1 of the manuscript FOODCHEM-D-24-00503 (based on the 40 key aroma compounds identified by George et al., 2023 (George et al., 2023)) were purchased commercially (in March 2022) from Merck (Sigma Aldrich), New South Wales, Australia. The labelled internal standards were procured commercially (in Dec 2022) from CDN isotopes, Quebec, Canada, through PM Separations Pty Ltd, Queensland, Australia. As an integral part of the method developed, diluted solutions of the individual reference standards and labelled internal reference standards, were separately injected under the reported analytical conditions in the manuscript and recorded their individual retention times. NIST2014 database library was used as an additional identification tool by matching the mass spectra of the individual compounds. The developed method did not identify any unknown molecules other than the targeted compounds listed in the reported method, to eliminate any potential error.

Once the mixed standard solution was prepared (using the individual reference compounds) with known concentrations of individual compounds, their retention times were recorded. The ratio of the retention time of the individual compounds with the labelled internal standard was calculated. These ratios named as retention factor* in **Table B1**. These retention factors were found to be constant across the analysis (multiple repeated injections of the mixed reference standard solutions of varying concentrations on different days; n >30) under each internal standard group. This observation was used to confirm that the individual reference compounds are not eluting at a different retention time other than the reported values and maintaining their relative elution order across multiple injections.

Calculation details:

e.g. 1: Sl.No.1: methyl isobutyrate

Average Retention time of methyl isobutyrate = 2.570 (min)

Internal standard group = 1 (ethyl 2-methyl butyrate-d9)

Average Retention time of ethyl 2-methyl butyrate-d9 = 5.704 (min)

Retention factor* = 2.570 / 5.704

= 0.451

e.g. 2: Sl.No.1: methyl hexanoate

Average Retention time of methyl hexanoate = 7.172 (min)

Internal standard group = 2 (ethyl hexanoate -d11)

Average Retention time of ethyl hexanoate -d11= 8.047 (min)

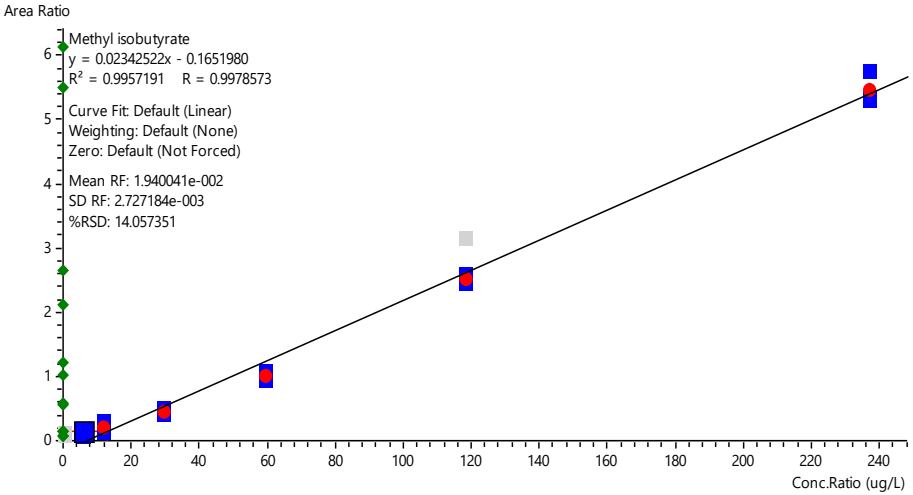
Retention factor* = 7.172 / 8.047

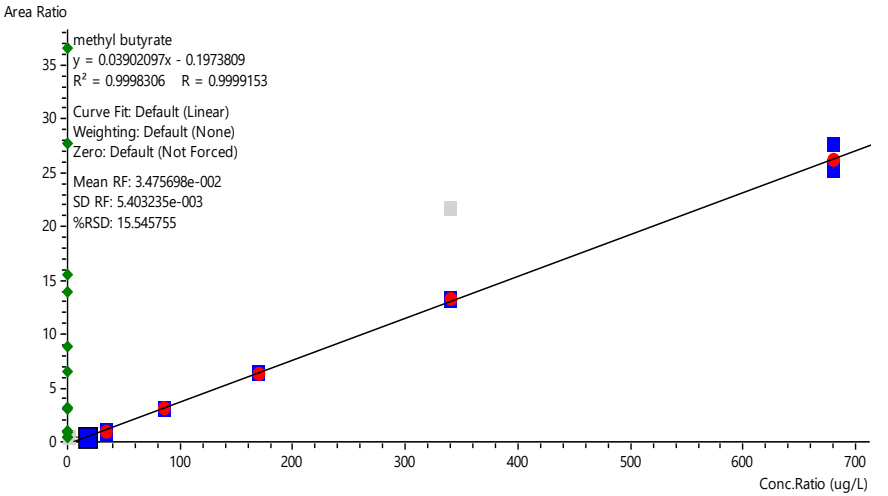
= 0.891

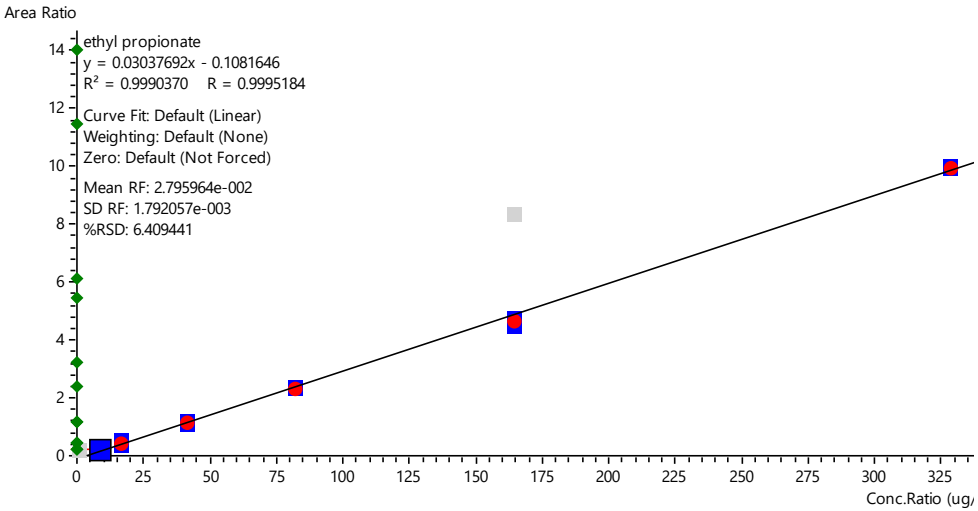
Table B1: The ratio of retention time of the individual compounds with that of the labelled internal standard under same internal standard group (groups i, ii, iii and iv)

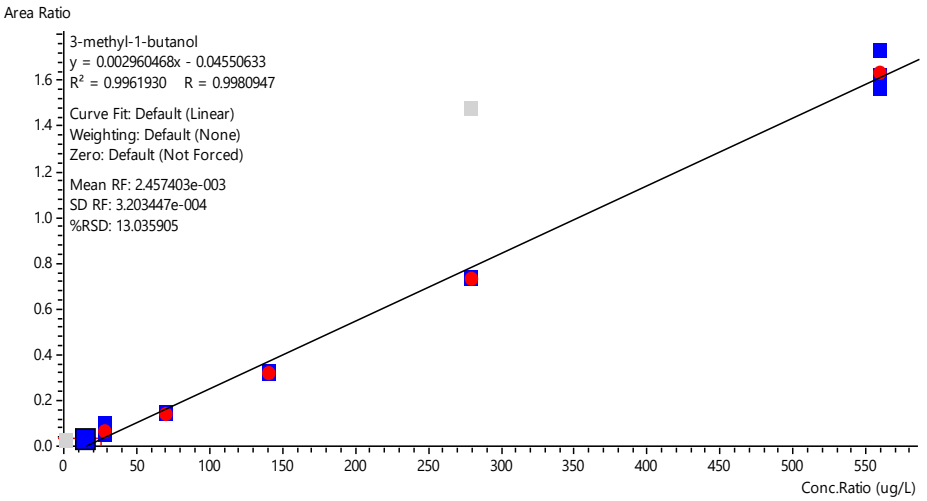
Sl. No.	Name	Individual RT	Analyte Type	Internal standard group	Observed RI	Average RT (n > 30)	Average Retention factor* (n > 30)
1	methyl isobutyrate	2.575	Target	*i*	839	2.570	0.451
2	ethyl propionate	2.921	Target	*i*	874	2.919	0.512
3	methyl butyrate	3.093	Target	*i*	892	3.090	0.542
4	3-methyl-1-butanol	3.313	Target	*i*	913	3.313	0.581
5	ethyl isobutyrate	3.736	Target	*i*	950	3.733	0.655
6	isobutyl acetate	4.039	Target	*i*	977	4.031	0.707
7	methyl 2-methyl butyrate	4.095	Target	*i*	980	4.086	0.716
8	methyl isovalerate	4.103	Target	*i*	983	4.094	0.718
9	ethyl butyrate	4.632	Target	*i*	1030	4.625	0.811
10	*ethyl 2-methyl butyrate-d9*	*5.709*	*ISTD*	*i*	*1122*	*5.704*	*1.000*
11	ethyl 2-methyl butyrate	5.864	Target	*i*	1134	5.853	1.026
12	2-methyl butyl acetate	6.494	Target	*i*	1186	6.482	1.136
13	methyl hexanoate	7.185	Target	*ii*	1232	7.172	0.891
14	*ethyl hexanoate -d11*	*8.052*	*ISTD*	*ii*	*1290*	*8.047*	*1.000*
15	*octanal-d16*	*8.099*	*ISTD*	*iii*	*1293*	*8.092*	*1.000*
16	ethyl hexanoate	8.162	Target	*ii*	1297	8.145	1.012
17	octanal	8.202	Target	*iii*	1301	8.216	1.015
18	ethyl trans 3-Hexenoate	8.253	Target	*ii*	1302	8.231	1.023
19	3-(Methylthio)propanoic acid methyl ester	8.483	Target	*i*	1313	8.467	1.484
20	D-Limonene	8.597	Target	*i*	1319	8.577	1.504
21	phenylacetaldehyde	8.746	Target	*iii*	1327	8.746	1.081
22	2,5-dimethyl-4-methoxy-3(2H)-furanone	8.892	Target	*i*	1334	8.878	1.557
23	ethyl 3-(Methylthio)propionate	9.447	Target	*i*	1362	9.450	1.657
24	methyl octanoate	9.795	Target	*iv*	1377	9.764	0.921
25	*ethyl octanoate -d15*	*10.603*	*ISTD*	*iv*	*1414*	*10.600*	*1.000*
26	ethyl octanoate	10.782	Target	*iv*	1420	10.757	1.015
27	alpha-Terpineol	10.853	Target	*i*	1422	10.829	1.899
28	decanal	10.868	Target	*iii*	1426	10.924	1.350
29	damascenonoe	13.564	Target	*i*	1518	13.544	2.375
30	ethyl decanoate	13.698	Target	*iv*	1523	13.686	1.291

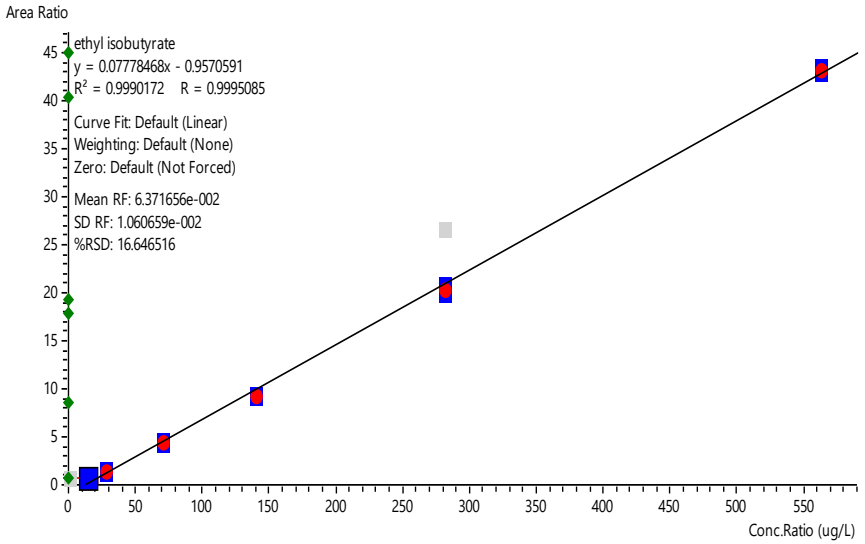
Figure B1: Calibration curves- Intra-day

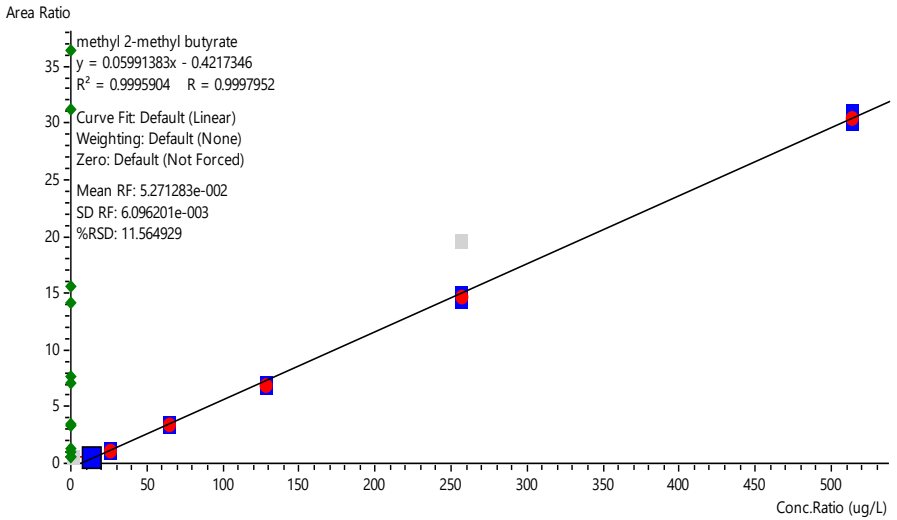


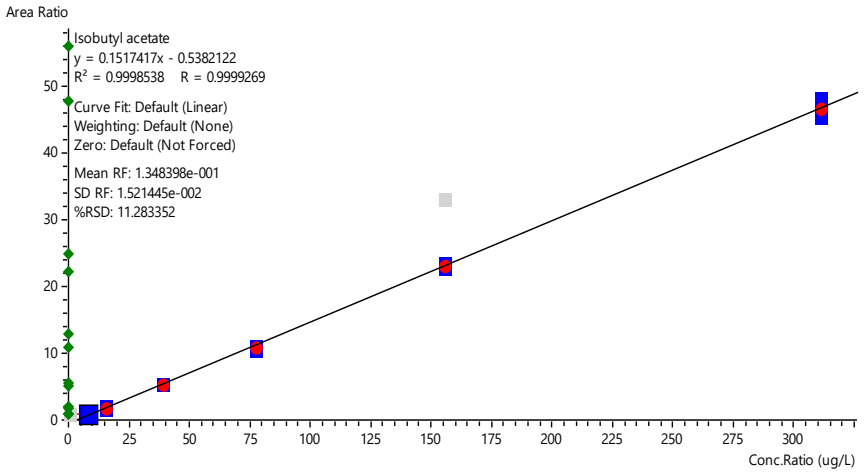


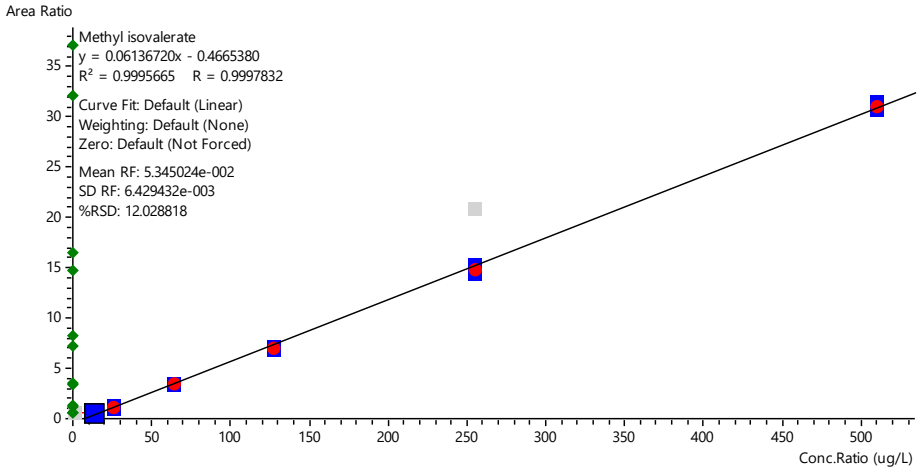


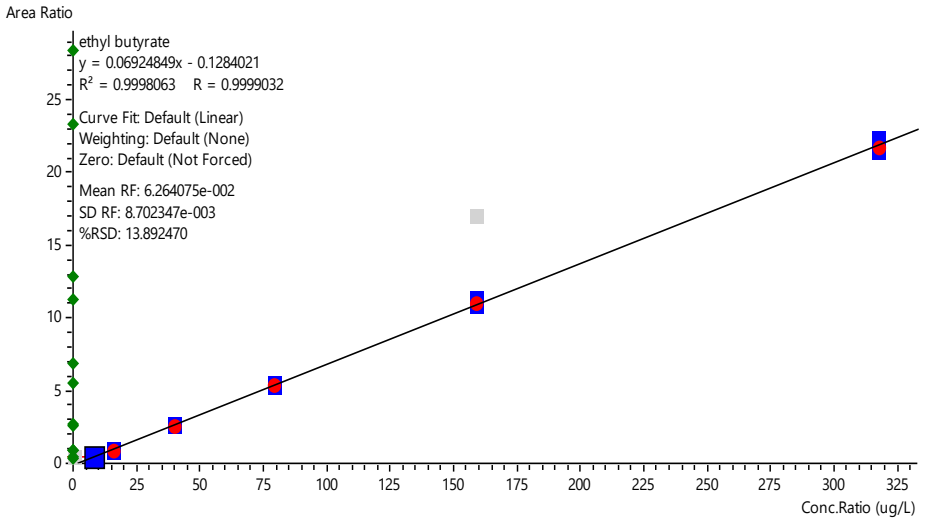


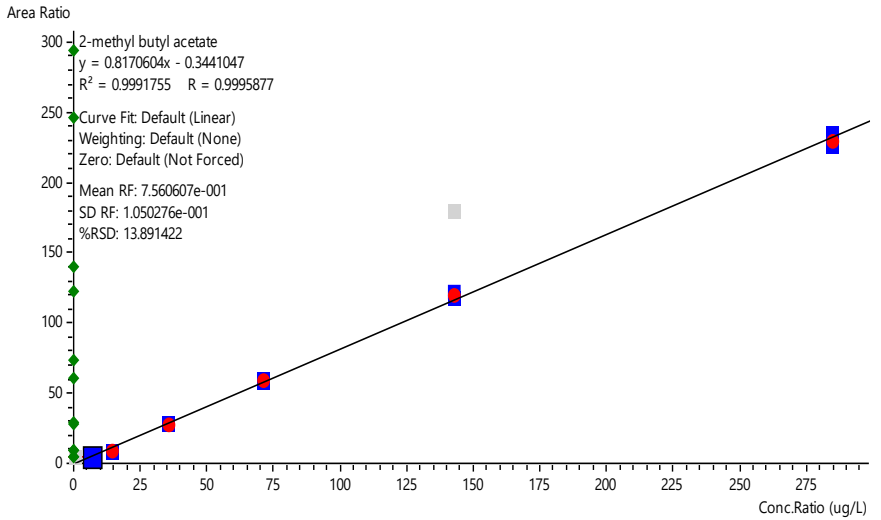

Area Ratio
ethyl isobutyrate
y = 0.07778468x - 0.9570591
R² = 0.9990172 R = 0.9995085
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 6.371656e-002
SD RF: 1.060659e-002
%RSD: 16.646516
Conc.Ratio (ug/L)

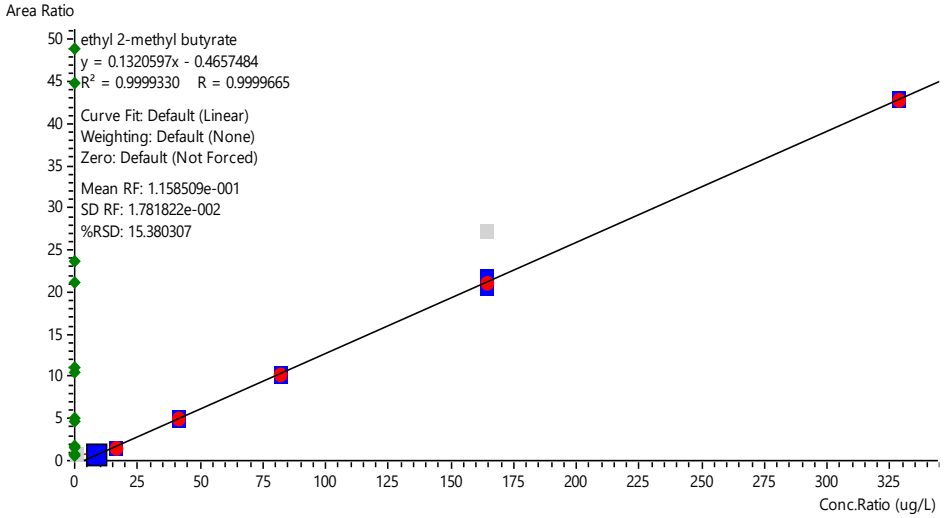

Area Ratio
methyl 2-methyl butyrate
y = 0.05991383x - 0.4217346
R² = 0.9995904 R = 0.9997952
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 5.271283e-002
SD RF: 6.096201e-003
%RSD: 11.564929
Conc.Ratio (ug/L)

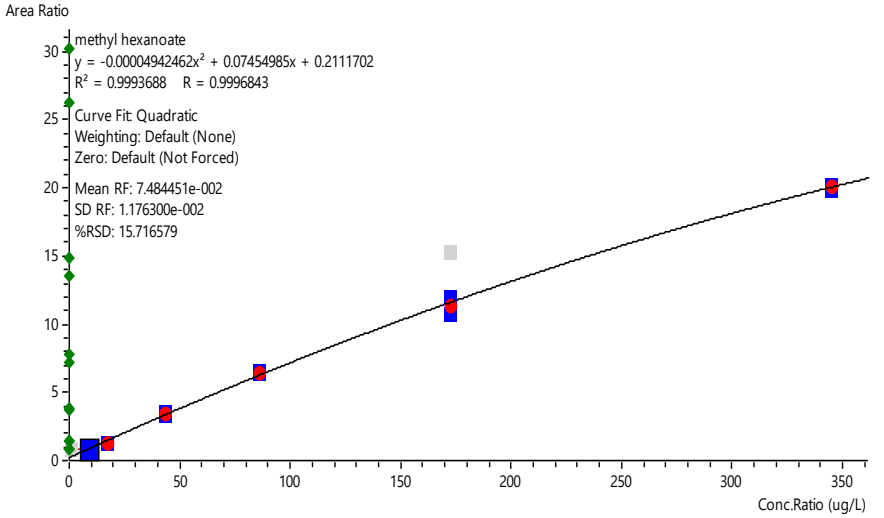

Area Ratio
Isobutyl acetate
y = 0.1517417x - 0.5382122
R² = 0.9998538 R = 0.9999269
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.348398e-001
SD RF: 1.521445e-002
%RSD: 11.283352
Conc.Ratio (ug/L)

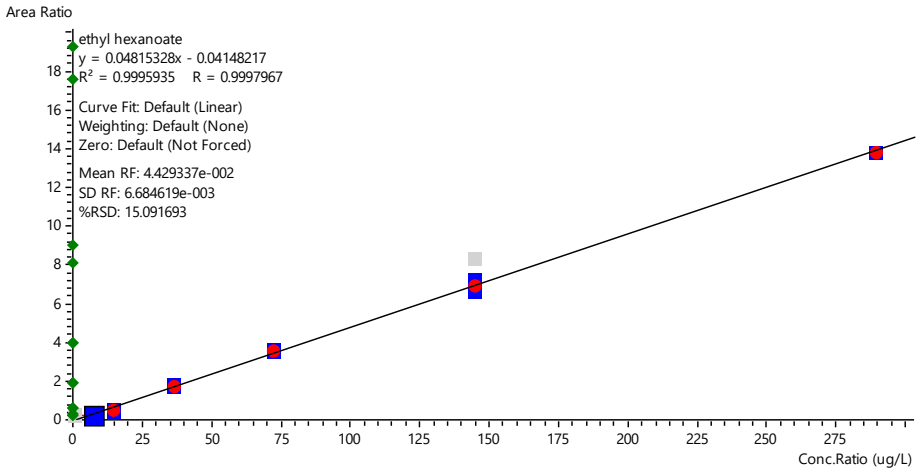

Area Ratio
Methyl isovalerate
y = 0.06136720x - 0.4665380
R² = 0.9995665 R = 0.9997832
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 5.345024e-002
SD RF: 6.429432e-003
%RSD: 12.028818
Conc.Ratio (ug/L)

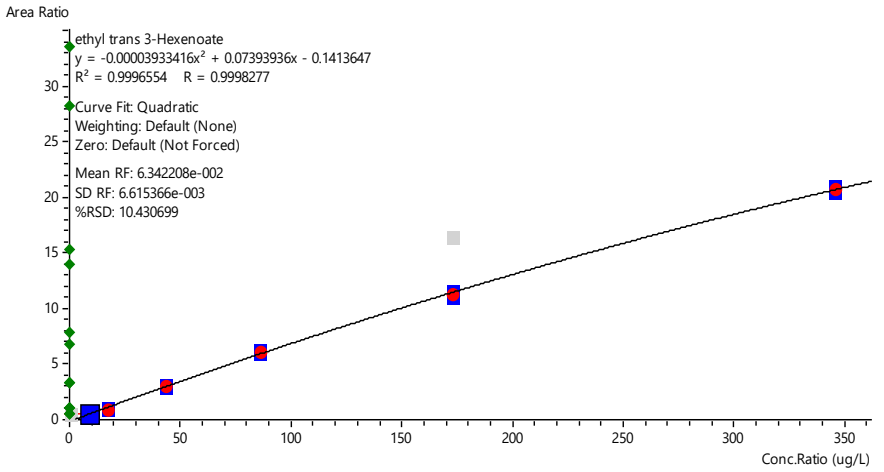

Area Ratio
ethyl butyrate
y = 0.06924849x - 0.1284021
R² = 0.9998063 R = 0.9999032
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 6.264075e-002
SD RF: 8.702347e-003
%RSD: 13.892470
Conc.Ratio (ug/L)

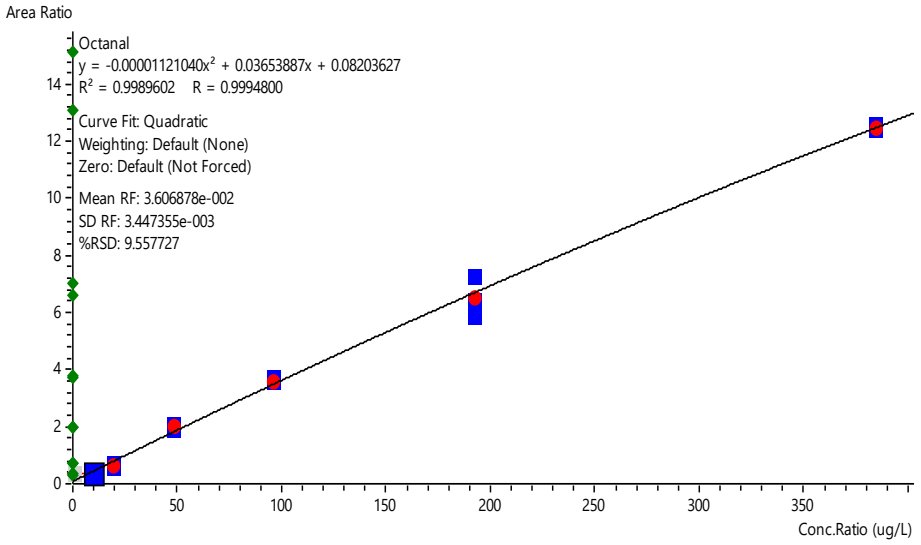

Area Ratio
2-methyl butyl acetate
y = 0.8170604x - 0.3441047
R² = 0.9991755 R = 0.9995877
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 7.560607e-001
SD RF: 1.050276e-001
%RSD: 13.891422
Conc.Ratio (ug/L)

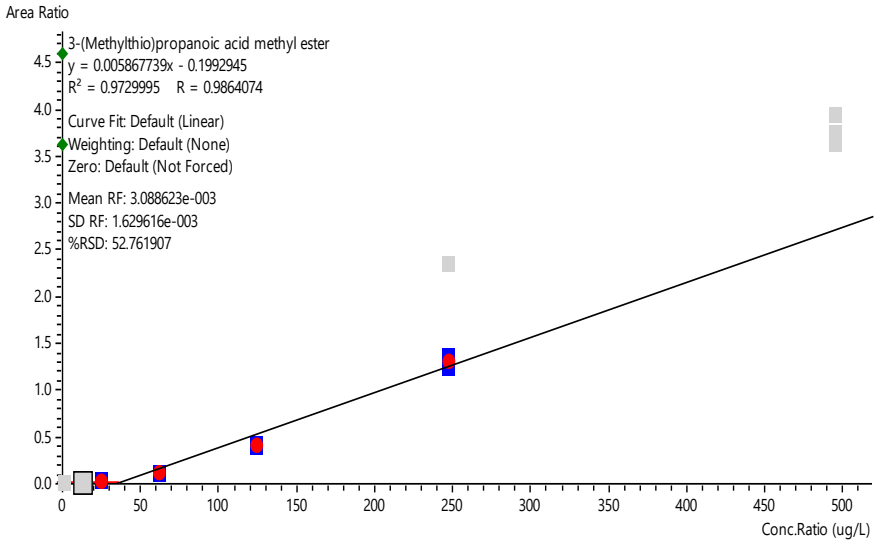

Area Ratio
ethyl 2-methyl butyrate
y = 0.1320597x - 0.4657484
R² = 0.9999330 R = 0.9999665
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.158509e-001
SD RF: 1.781822e-002
%RSD: 15.380307
Conc.Ratio (ug/L)

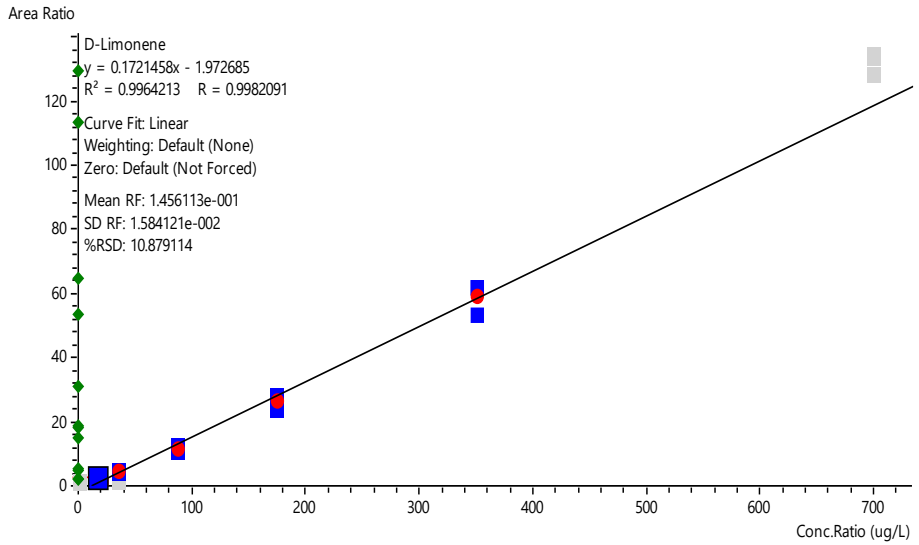

Area Ratio
methyl hexanoate
y = -0.00004942462x² + 0.07454985x + 0.2111702
R² = 0.9993688 R = 0.9996843
Curve Fit: Quadratic
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 7.484451e-002
SD RF: 1.176300e-002
%RSD: 15.716579
Conc.Ratio (ug/L)

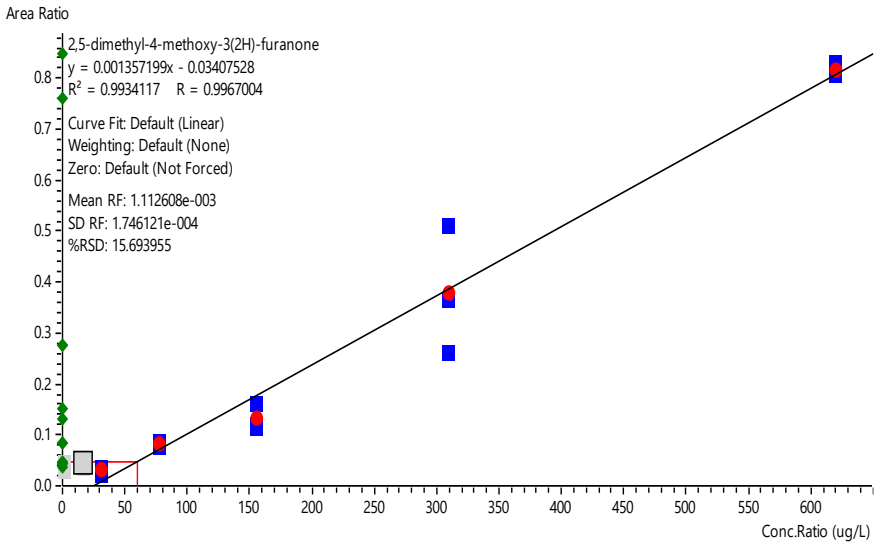

Area Ratio
ethyl hexanoate
y = 0.04815328x - 0.04148217
R² = 0.9995935 R = 0.9997967
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 4.429337e-002
SD RF: 6.684619e-003
%RSD: 15.091693
Conc.Ratio (ug/L)

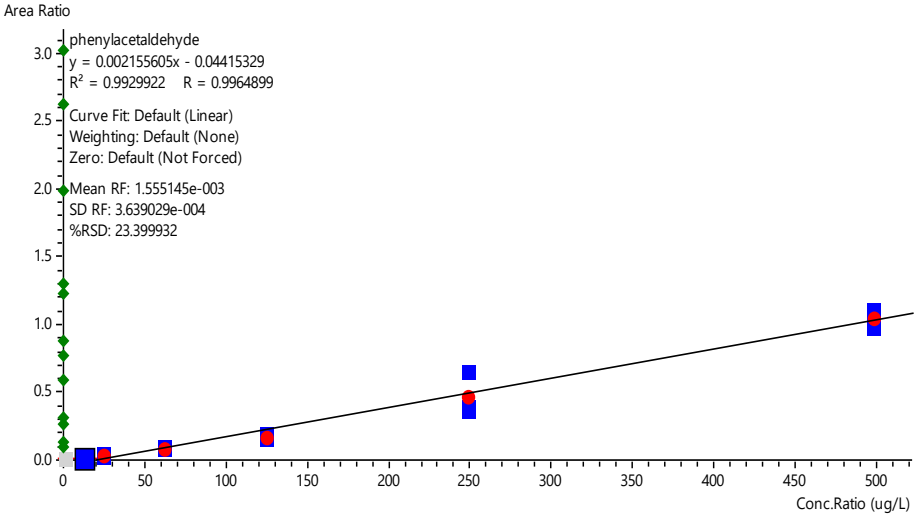

Area Ratio
ethyl trans 3-Hexenoate
y = -0.00003933416x² + 0.07393936x - 0.1413647
R² = 0.9996554 R = 0.9998277
Curve Fit: Quadratic
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 6.342208e-002
SD RF: 6.615366e-003
%RSD: 10.430699
Conc.Ratio (ug/L)

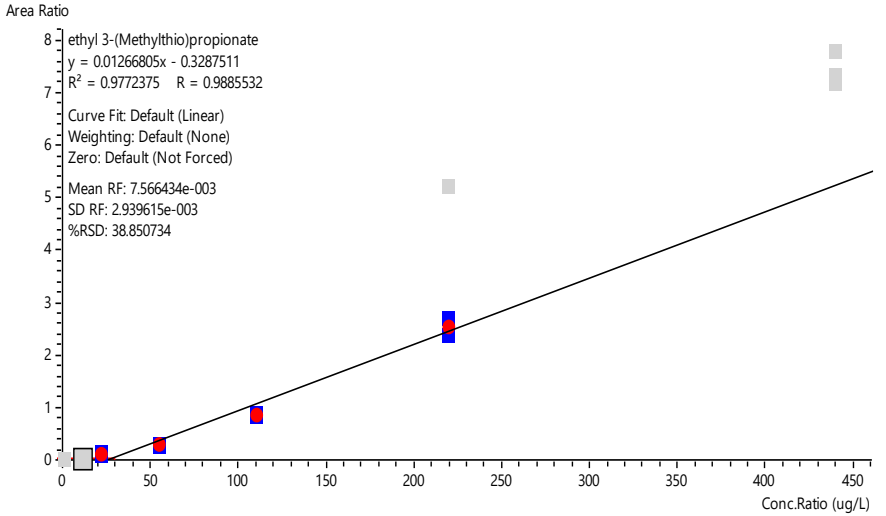

Area Ratio
Octanal
y = -0.00001121040x² + 0.03653887x + 0.08203627
R² = 0.9989602 R = 0.9994800
Curve Fit: Quadratic
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 3.606878e-002
SD RF: 3.447355e-003
%RSD: 9.557727
Conc.Ratio (ug/L)

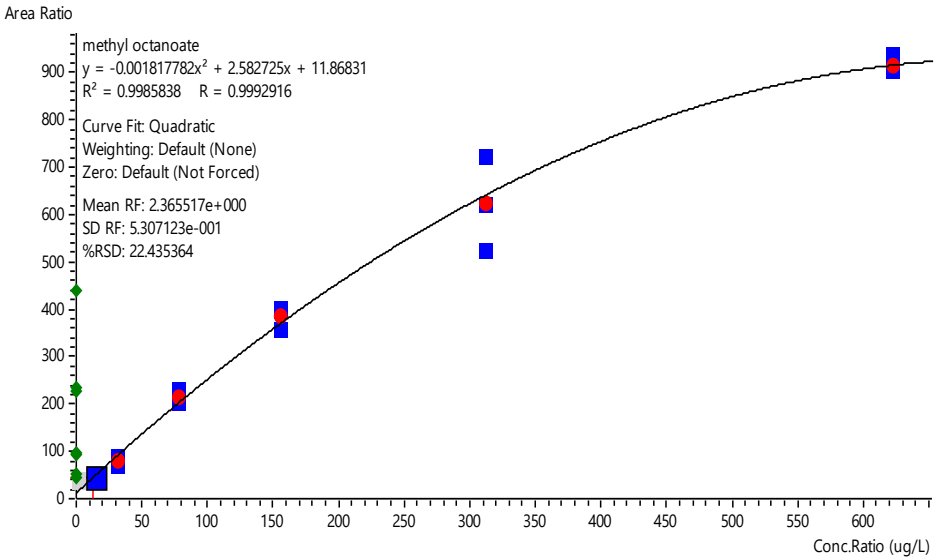

Area Ratio
3-(Methylthio)propanoic acid methyl ester
y = 0.005867739x - 0.1992945
R² = 0.9729995 R = 0.9864074
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 3.088623e-003
SD RF: 1.629616e-003
%RSD: 52.761907
Conc.Ratio (ug/L)

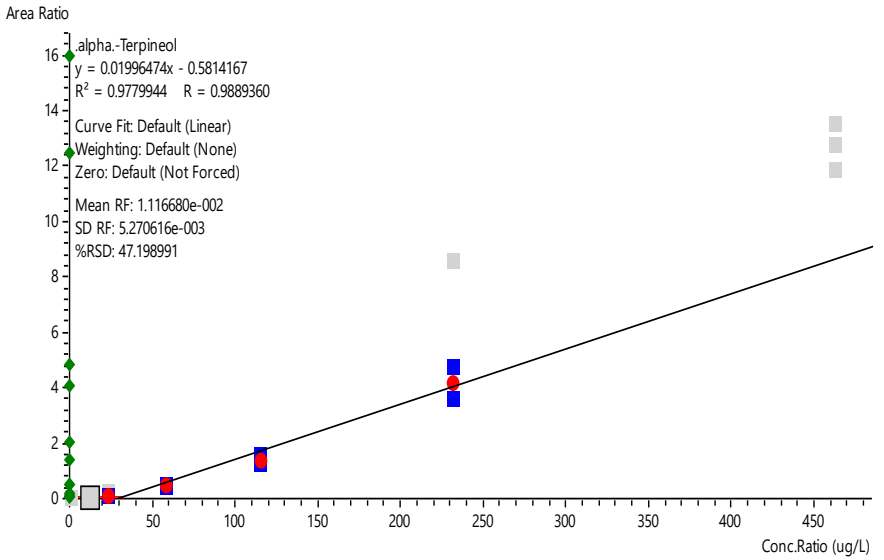

Area Ratio
D-Limonene
y = 0.1721458x - 1.972685
R² = 0.9964213 R = 0.9982091
Curve Fit: Linear
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.456113e-001
SD RF: 1.584121e-002
%RSD: 10.879114
Conc.Ratio (ug/L)

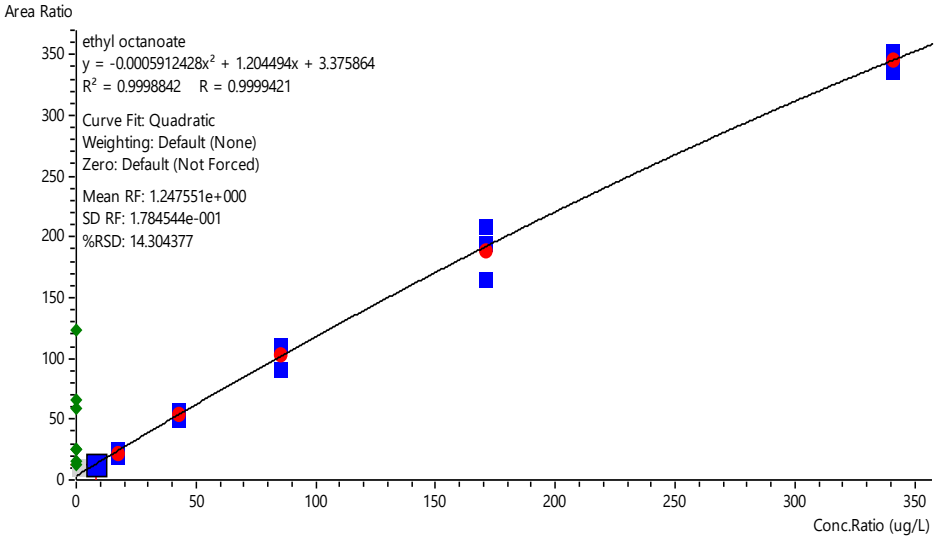

Area Ratio
2,5-dimethyl-4-methoxy-3(2H)-furanone
y = 0.001357199x - 0.03407528
R² = 0.9934117 R = 0.9967004
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.112608e-003
SD RF: 1.746121e-004
%RSD: 15.693955
Conc.Ratio (ug/L)

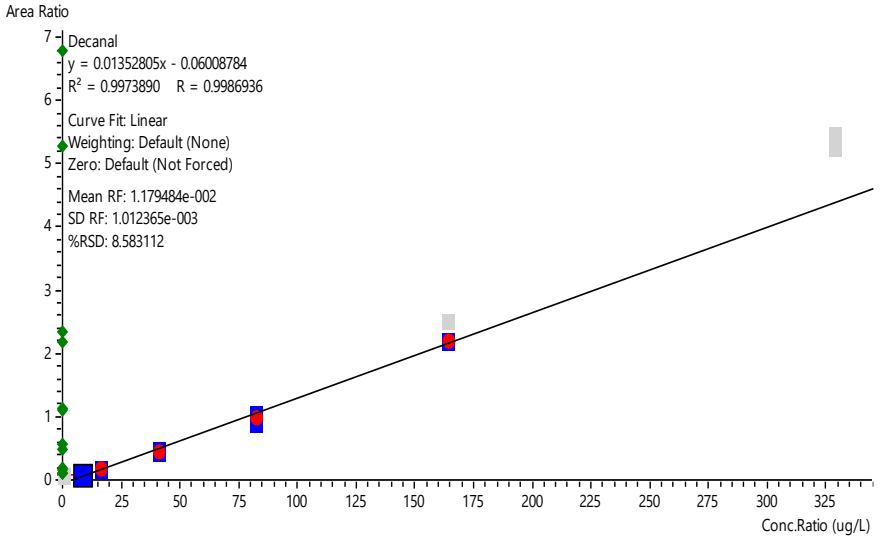

Area Ratio
phenylacetaldehyde
y = 0.002155605x - 0.04415329
R² = 0.9929922 R = 0.9964899
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.555145e-003
SD RF: 3.639029e-004
%RSD: 23.399932
Conc.Ratio (ug/L)

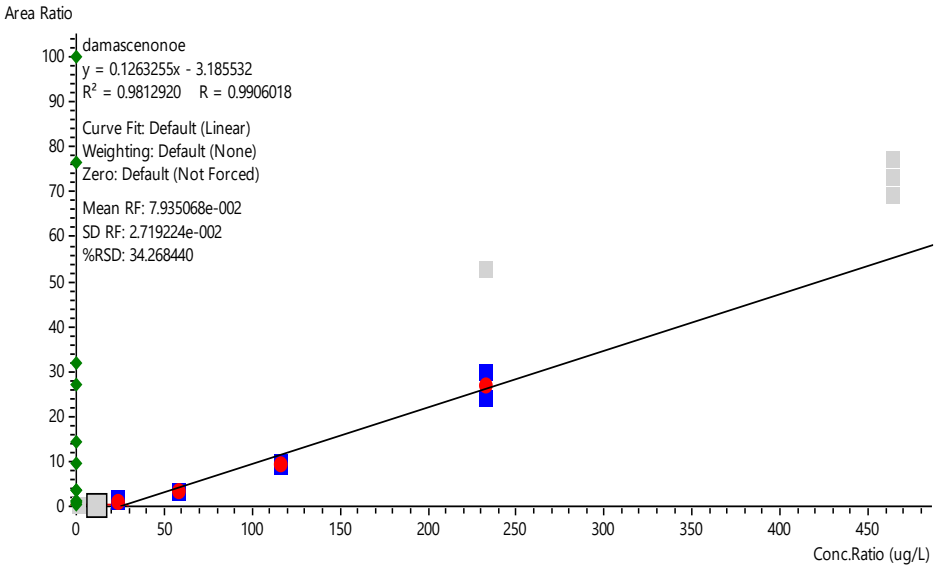

Area Ratio
ethyl 3-(Methylthio)propionate
y = 0.01266805x - 0.3287511
R² = 0.9772375 R = 0.9885532
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 7.566434e-003
SD RF: 2.939615e-003
%RSD: 38.850734
Conc.Ratio (ug/L)

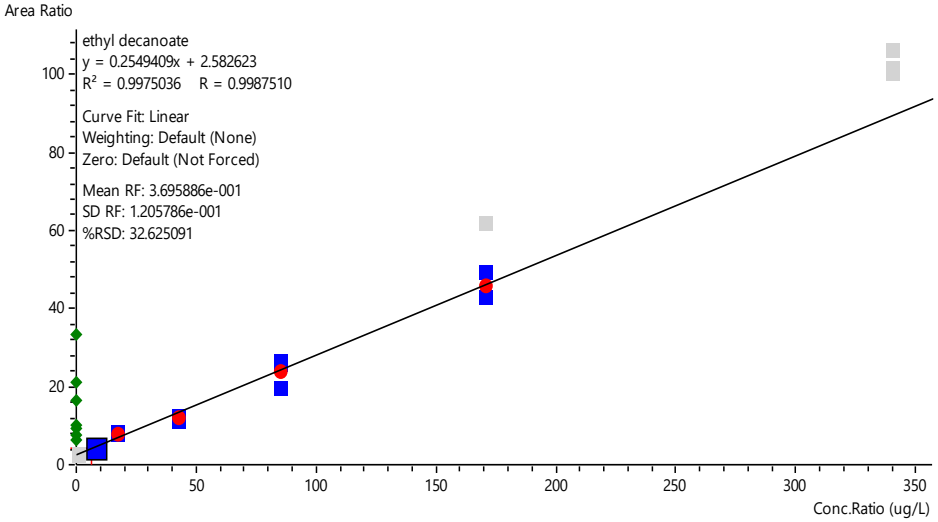

Area Ratio
methyl octanoate
y = -0.001817782x² + 2.582725x + 11.86831
R² = 0.9985838 R = 0.9992916
Curve Fit: Quadratic
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 2.365517e+000
SD RF: 5.307123e-001
%RSD: 22.435364
Conc.Ratio (ug/L)


Area Ratio
alpha.-Terpineol
y = 0.01996474x - 0.5814167
R² = 0.9779944 R = 0.9889360
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.116680e-002
SD RF: 5.270616e-003
%RSD: 47.198991
Conc.Ratio (ug/L)


Area Ratio
ethyl octanoate
y = -0.0005912428x² + 1.204494x + 3.375864
R² = 0.9998842 R = 0.9999421
Curve Fit: Quadratic
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.247551e+000
SD RF: 1.784544e-001
%RSD: 14.304377
Conc.Ratio (ug/L)


Area Ratio
Decanal
y = 0.01352805x - 0.06008784
R² = 0.9973890 R = 0.9986936
Curve Fit: Linear
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 1.179484e-002
SD RF: 1.012365e-003
%RSD: 8.583112
Conc.Ratio (ug/L)


Area Ratio
damascenonoe
y = 0.1263255x - 3.185532
R² = 0.9812920 R = 0.9906018
Curve Fit: Default (Linear)
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 7.935068e-002
SD RF: 2.719224e-002
%RSD: 34.268440
Conc.Ratio (ug/L)


Area Ratio
ethyl decanoate
y = 0.2549409x + 2.582623
R² = 0.9975036 R = 0.9987510
Curve Fit: Linear
Weighting: Default (None)
Zero: Default (Not Forced)
Mean RF: 3.695886e-001
SD RF: 1.205786e-001
%RSD: 32.625091
Conc.Ratio (ug/L)

Appendix 3 Supplementary information for Chapter 4

Supplementary information C1: Flow chart- Sample preparation

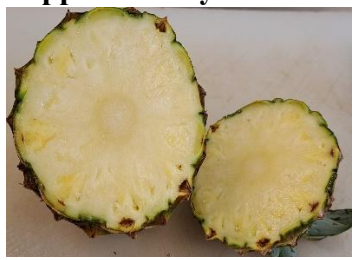


Image 1

Image 2

Image 3

Image 4

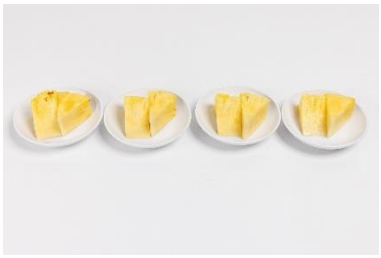


Image 5

Image 4: pineapple quarters, after removing cones as shown in image 3

Image 5: Segments for consumer / sensory studies

Image 6: Segments for compositional analysis (further chopped before milling)

Image 7: Pineapple composite puree (after milling) for compositional analysis

Image 6

Image 7

Table C1: Blinding codes and tracking letters for pineapple segment composites

Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor
Aus-Carnival	103	A	participant010	Aus-Festival	760	A	participant002	Aus-Jubilee	356	A	participant006
Aus-Carnival	103	A	participant055	Aus-Festival	760	A	participant012	Aus-Jubilee	356	A	participant060
Aus-Carnival	103	A	participant058	Aus-Festival	760	A	participant070	Aus-Jubilee	356	A	participant097
Aus-Carnival	103	A	participant110	Aus-Festival	760	A	participant074	Aus-Jubilee	356	A	participant073
Aus-Carnival	103	A	participant111	Aus-Festival	760	A	participant103	Aus-Jubilee	356	A	participant114
Aus-Carnival	103	A	participant117	Aus-Festival	760	A	participant119	Aus-Jubilee	356	A	participant005
Aus-Carnival	103	A	participant011	Aus-Festival	760	A	participant003	Aus-Jubilee	356	A	participant007
Aus-Carnival	103	A	participant042	Aus-Festival	760	A	participant076	Aus-Jubilee	356	A	participant074
Aus-Carnival	103	A	participant052	Aus-Festival	760	A	participant058	Aus-Jubilee	356	A	participant098
Aus-Carnival	103	A	participant059	Aus-Festival	760	A	participant105	Aus-Jubilee	356	A	participant059
Aus-Carnival	103	A	participant099	Aus-Festival	760	A	participant110	Aus-Jubilee	356	A	participant064
Aus-Carnival	103	A	participant114	Aus-Festival	760	A	participant072	Aus-Jubilee	356	A	participant110
Aus-Carnival	103	A	participant053	Aus-Festival	760	A	participant092	Aus-Jubilee	356	A	participant004
Aus-Carnival	103	A	participant056	Aus-Festival	760	A	participant106	Aus-Jubilee	356	A	participant112
Aus-Carnival	103	B	participant004	Aus-Festival	760	B	participant052	Aus-Jubilee	356	B	participant062
Aus-Carnival	103	B	participant064	Aus-Festival	760	B	participant065	Aus-Jubilee	356	B	participant094
Aus-Carnival	103	B	participant101	Aus-Festival	760	B	participant055	Aus-Jubilee	356	B	participant012
Aus-Carnival	103	B	participant005	Aus-Festival	760	B	participant060	Aus-Jubilee	356	B	participant106
Aus-Carnival	103	B	participant065	Aus-Festival	760	B	participant094	Aus-Jubilee	356	B	participant063
Aus-Carnival	103	B	participant113	Aus-Festival	760	B	participant011	Aus-Jubilee	356	B	participant107
Aus-Carnival	103	B	participant070	Aus-Festival	760	B	participant013	Aus-Jubilee	356	B	participant003
Aus-Carnival	103	B	participant103	Aus-Festival	760	B	participant064	Aus-Jubilee	356	B	participant072
Aus-Carnival	103	B	participant106	Aus-Festival	760	B	participant097	Aus-Jubilee	356	B	participant118
Aus-Carnival	103	B	participant007	Aus-Festival	760	B	participant114	Aus-Jubilee	356	B	participant071
Aus-Carnival	103	B	participant063	Aus-Festival	760	B	participant104	Aus-Jubilee	356	B	participant093
Aus-Carnival	103	B	participant066	Aus-Festival	760	B	participant010	Aus-Jubilee	356	C	participant013
Aus-Carnival	103	B	participant100	Aus-Festival	760	B	participant054	Aus-Jubilee	356	C	participant116
Aus-Carnival	103	B	participant002	Aus-Festival	760	B	participant098	Aus-Jubilee	356	C	participant002
Aus-Carnival	103	B	participant068	Aus-Festival	760	C	participant057	Aus-Jubilee	356	C	participant052
Aus-Carnival	103	B	participant074	Aus-Festival	760	C	participant109	Aus-Jubilee	356	C	participant061
Aus-Carnival	103	C	participant067	Aus-Festival	760	C	participant115	Aus-Jubilee	356	C	participant100
Aus-Carnival	103	C	participant069	Aus-Festival	760	C	participant063	Aus-Jubilee	356	C	participant105
Aus-Carnival	103	C	participant092	Aus-Festival	760	C	participant053	Aus-Jubilee	356	C	participant057
Aus-Carnival	103	C	participant104	Aus-Festival	760	C	participant093	Aus-Jubilee	356	C	participant055
Aus-Carnival	103	C	participant003	Aus-Festival	760	C	participant118	Aus-Jubilee	356	C	participant092
Aus-Carnival	103	C	participant061	Aus-Festival	760	C	participant004	Aus-Jubilee	356	C	participant011
Aus-Carnival	103	C	participant075	Aus-Festival	760	C	participant056	Aus-Jubilee	356	C	participant065
Aus-Carnival	103	C	participant006	Aus-Festival	760	C	participant073	Aus-Jubilee	356	D	participant053
Aus-Carnival	103	C	participant013	Aus-Festival	760	C	participant005	Aus-Jubilee	356	D	participant056
Aus-Carnival	103	C	participant060	Aus-Festival	760	C	participant059	Aus-Jubilee	356	D	participant054

Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor
Aus-Carnival	103	C	participant093	Aus-Festival	760	C	participant113	Aus-Jubilee	356	D	participant104
Aus-Carnival	103	C	participant012	Aus-Festival	760	D	participant007	Aus-Jubilee	356	D	participant010
Aus-Carnival	103	C	participant062	Aus-Festival	760	D	participant078	Aus-Jubilee	356	D	participant070
Aus-Carnival	103	C	participant105	Aus-Festival	760	D	participant100	Aus-Jubilee	356	D	participant103
Aus-Carnival	103	D	participant016	Aus-Festival	760	D	participant067	Aus-Jubilee	356	D	participant058
Aus-Carnival	103	D	participant023	Aus-Festival	760	D	participant101	Aus-Jubilee	356	D	participant099
Aus-Carnival	103	D	participant098	Aus-Festival	760	D	participant006	Aus-Jubilee	356	D	participant101
Aus-Carnival	103	D	participant057	Aus-Festival	760	D	participant071	Aus-Jubilee	356	E	participant020
Aus-Carnival	103	D	participant072	Aus-Festival	760	D	participant062	Aus-Jubilee	356	E	participant047
Aus-Carnival	103	D	participant097	Aus-Festival	760	D	participant077	Aus-Jubilee	356	E	participant001
Aus-Carnival	103	D	participant014	Aus-Festival	760	D	participant081	Aus-Jubilee	356	E	participant009
Aus-Carnival	103	D	participant077	Aus-Festival	760	D	participant099	Aus-Jubilee	356	E	participant045
Aus-Carnival	103	D	participant094	Aus-Festival	760	D	participant111	Aus-Jubilee	356	E	participant049
Aus-Carnival	103	D	participant116	Aus-Festival	760	D	participant116	Aus-Jubilee	356	E	participant018
Aus-Carnival	103	D	participant018	Aus-Festival	760	D	participant061	Aus-Jubilee	356	E	participant023
Aus-Carnival	103	D	participant054	Aus-Festival	760	D	participant117	Aus-Jubilee	356	E	participant044
Aus-Carnival	103	D	participant008	Aus-Festival	760	E	participant022	Aus-Jubilee	356	E	participant046
Aus-Carnival	103	D	participant085	Aus-Festival	760	E	participant043	Aus-Jubilee	356	E	participant111
Aus-Carnival	103	E	participant017	Aus-Festival	760	E	participant091	Aus-Jubilee	356	E	participant083
Aus-Carnival	103	E	participant073	Aus-Festival	760	E	participant008	Aus-Jubilee	356	E	participant109
Aus-Carnival	103	E	participant079	Aus-Festival	760	E	participant014	Aus-Jubilee	356	E	participant119
Aus-Carnival	103	E	participant084	Aus-Festival	760	E	participant075	Aus-Jubilee	356	F	participant108
Aus-Carnival	103	E	participant015	Aus-Festival	760	E	participant086	Aus-Jubilee	356	F	participant015
Aus-Carnival	103	E	participant043	Aus-Festival	760	E	participant040	Aus-Jubilee	356	F	participant091
Aus-Carnival	103	E	participant080	Aus-Festival	760	E	participant048	Aus-Jubilee	356	F	participant017
Aus-Carnival	103	E	participant081	Aus-Festival	760	E	participant068	Aus-Jubilee	356	F	participant048
Aus-Carnival	103	E	participant109	Aus-Festival	760	E	participant085	Aus-Jubilee	356	F	participant087
Aus-Carnival	103	E	participant001	Aus-Festival	760	E	participant088	Aus-Jubilee	356	F	participant016
Aus-Carnival	103	E	participant009	Aus-Festival	760	E	participant023	Aus-Jubilee	356	F	participant019
Aus-Carnival	103	E	participant050	Aus-Festival	760	E	participant069	Aus-Jubilee	356	F	participant021
Aus-Carnival	103	E	participant112	Aus-Festival	760	E	participant066	Aus-Jubilee	356	F	participant038
Aus-Carnival	103	E	participant071	Aus-Festival	760	E	participant079	Aus-Jubilee	356	F	participant041
Aus-Carnival	103	E	participant078	Aus-Festival	760	E	participant089	Aus-Jubilee	356	F	participant050
Aus-Carnival	103	E	participant020	Aus-Festival	760	F	participant018	Aus-Jubilee	356	G	participant008
Aus-Carnival	103	E	participant076	Aus-Festival	760	F	participant083	Aus-Jubilee	356	G	participant040
Aus-Carnival	103	F	participant039	Aus-Festival	760	F	participant021	Aus-Jubilee	356	G	participant113
Aus-Carnival	103	F	participant045	Aus-Festival	760	F	participant039	Aus-Jubilee	356	G	participant078
Aus-Carnival	103	F	participant046	Aus-Festival	760	F	participant041	Aus-Jubilee	356	G	participant088
Aus-Carnival	103	F	participant019	Aus-Festival	760	F	participant107	Aus-Jubilee	356	G	participant117
Aus-Carnival	103	F	participant047	Aus-Festival	760	F	participant019	Aus-Jubilee	356	G	participant079
Aus-Carnival	103	F	participant021	Aus-Festival	760	F	participant080	Aus-Jubilee	356	G	participant014
Aus-Carnival	103	F	participant107	Aus-Festival	760	F	participant016	Aus-Jubilee	356	G	participant022

Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor
Aus-Carnival	103	F	participant119	Aus-Festival	760	F	participant038	Aus-Jubilee	356	G	participant039
Aus-Carnival	103	F	participant022	Aus-Festival	760	F	participant051	Aus-Jubilee	356	G	participant043
Aus-Carnival	103	F	participant044	Aus-Festival	760	F	participant108	Aus-Jubilee	356	G	participant085
Aus-Carnival	103	F	participant048	Aus-Festival	760	F	participant015	Aus-Jubilee	356	G	participant051
Aus-Carnival	103	F	participant090	Aus-Festival	760	F	participant042	Aus-Jubilee	356	H	participant042
Aus-Carnival	103	F	participant091	Aus-Festival	760	G	participant050	Aus-Jubilee	356	H	participant080
Aus-Carnival	103	F	participant108	Aus-Festival	760	G	participant087	Aus-Jubilee	356	H	participant081
Aus-Carnival	103	F	participant115	Aus-Festival	760	G	participant020	Aus-Jubilee	356	H	participant089
Aus-Carnival	103	G	participant032	Aus-Festival	760	G	participant046	Aus-Jubilee	356	H	participant030
Aus-Carnival	103	G	participant088	Aus-Festival	760	G	participant084	Aus-Jubilee	356	H	participant033
Aus-Carnival	103	G	participant033	Aus-Festival	760	G	participant112	Aus-Jubilee	356	H	participant069
Aus-Carnival	103	G	participant038	Aus-Festival	760	G	participant045	Aus-Jubilee	356	H	participant084
Aus-Carnival	103	G	participant051	Aus-Festival	760	G	participant001	Aus-Jubilee	356	H	participant090
Aus-Carnival	103	G	participant087	Aus-Festival	760	G	participant009	Aus-Jubilee	356	H	participant026
Aus-Carnival	103	G	participant118	Aus-Festival	760	G	participant044	Aus-Jubilee	356	H	participant115
Aus-Carnival	103	G	participant027	Aus-Festival	760	G	participant047	Aus-Jubilee	356	H	participant029
Aus-Carnival	103	G	participant083	Aus-Festival	760	G	participant090	Aus-Jubilee	356	H	participant067
Aus-Carnival	103	G	participant089	Aus-Festival	760	G	participant017	Aus-Jubilee	356	H	participant077
Aus-Carnival	103	G	participant041	Aus-Festival	760	G	participant049	Aus-Jubilee	356	H	participant086
Aus-Carnival	103	G	participant049	Aus-Festival	760	H	participant028	Aus-Jubilee	356	I	participant031
Aus-Carnival	103	G	participant086	Aus-Festival	760	H	participant026	Aus-Jubilee	356	I	participant066
Aus-Carnival	103	G	participant028	Aus-Festival	760	H	participant035	Aus-Jubilee	356	I	participant075
Aus-Carnival	103	G	participant040	Aus-Festival	760	H	participant024	Aus-Jubilee	356	I	participant025
Aus-Carnival	103	H	participant030	Aus-Festival	760	H	participant034	Aus-Jubilee	356	I	participant068
Aus-Carnival	103	H	participant024	Aus-Festival	760	H	participant037	Aus-Jubilee	356	I	participant028
Aus-Carnival	103	H	participant026	Aus-Festival	760	I	participant029	Aus-Jubilee	356	I	participant037
Aus-Carnival	103	H	participant029	Aus-Festival	760	I	participant033	Aus-Jubilee	356	I	participant034
Aus-Carnival	103	H	participant031	Aus-Festival	760	I	participant036	Aus-Jubilee	356	I	participant076
Aus-Carnival	103	I	participant034	Aus-Festival	760	I	participant027	Aus-Jubilee	356	J	participant024
Aus-Carnival	103	I	participant036	Aus-Festival	760	I	participant030	Aus-Jubilee	356	J	participant027
Aus-Carnival	103	I	participant025	Aus-Festival	760	J	participant031	Aus-Jubilee	356	J	participant035
Aus-Carnival	103	I	participant037	Aus-Festival	760	J	participant025	Aus-Jubilee	356	J	participant036
Aus-Carnival	103	I	participant035	Aus-Festival	760	J	participant032	Aus-Jubilee	356	J	participant032

Table C1(continued)

Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor
Aussie Gold (73-50)	874	A	participant068	Smooth Cayenne	498	A	participant061
Aussie Gold (73-50)	874	A	participant077	Smooth Cayenne	498	A	participant004
Aussie Gold (73-50)	874	A	participant093	Smooth Cayenne	498	A	participant083
Aussie Gold (73-50)	874	A	participant104	Smooth Cayenne	498	A	participant029
Aussie Gold (73-50)	874	A	participant010	Smooth Cayenne	498	A	participant056
Aussie Gold (73-50)	874	A	participant070	Smooth Cayenne	498	A	participant087
Aussie Gold (73-50)	874	A	participant099	Smooth Cayenne	498	A	participant005
Aussie Gold (73-50)	874	A	participant094	Smooth Cayenne	498	A	participant053
Aussie Gold (73-50)	874	A	participant105	Smooth Cayenne	498	A	participant057
Aussie Gold (73-50)	874	A	participant003	Smooth Cayenne	498	A	participant065
Aussie Gold (73-50)	874	A	participant069	Smooth Cayenne	498	A	participant084
Aussie Gold (73-50)	874	A	participant078	Smooth Cayenne	498	A	participant052
Aussie Gold (73-50)	874	B	participant038	Smooth Cayenne	498	A	participant080
Aussie Gold (73-50)	874	B	participant041	Smooth Cayenne	498	A	participant081
Aussie Gold (73-50)	874	B	participant048	Smooth Cayenne	498	B	participant069
Aussie Gold (73-50)	874	B	participant006	Smooth Cayenne	498	B	participant071
Aussie Gold (73-50)	874	B	participant050	Smooth Cayenne	498	B	participant085
Aussie Gold (73-50)	874	B	participant012	Smooth Cayenne	498	B	participant086
Aussie Gold (73-50)	874	B	participant092	Smooth Cayenne	498	B	participant010
Aussie Gold (73-50)	874	B	participant100	Smooth Cayenne	498	B	participant031
Aussie Gold (73-50)	874	B	participant101	Smooth Cayenne	498	B	participant030
Aussie Gold (73-50)	874	B	participant002	Smooth Cayenne	498	B	participant068
Aussie Gold (73-50)	874	B	participant011	Smooth Cayenne	498	B	participant089
Aussie Gold (73-50)	874	B	participant042	Smooth Cayenne	498	B	participant063
Aussie Gold (73-50)	874	B	participant117	Smooth Cayenne	498	B	participant070
Aussie Gold (73-50)	874	B	participant103	Smooth Cayenne	498	B	participant110
Aussie Gold (73-50)	874	C	participant005	Smooth Cayenne	498	C	participant059
Aussie Gold (73-50)	874	C	participant106	Smooth Cayenne	498	C	participant107
Aussie Gold (73-50)	874	C	participant044	Smooth Cayenne	498	C	participant112
Aussie Gold (73-50)	874	C	participant071	Smooth Cayenne	498	C	participant013
Aussie Gold (73-50)	874	C	participant116	Smooth Cayenne	498	C	participant054
Aussie Gold (73-50)	874	C	participant035	Smooth Cayenne	498	C	participant058
Aussie Gold (73-50)	874	C	participant043	Smooth Cayenne	498	C	participant064
Aussie Gold (73-50)	874	C	participant051	Smooth Cayenne	498	C	participant002
Aussie Gold (73-50)	874	C	participant076	Smooth Cayenne	498	C	participant117
Aussie Gold (73-50)	874	C	participant098	Smooth Cayenne	498	C	participant012
Aussie Gold (73-50)	874	C	participant007	Smooth Cayenne	498	C	participant091
Aussie Gold (73-50)	874	C	participant013	Smooth Cayenne	498	C	participant006
Aussie Gold (73-50)	874	C	participant097	Smooth Cayenne	498	C	participant033
Aussie Gold (73-50)	874	C	participant118	Smooth Cayenne	498	C	participant060
Aussie Gold (73-50)	874	D	participant115	Smooth Cayenne	498	C	participant073
Aussie Gold (73-50)	874	D	participant004	Smooth Cayenne	498	C	participant114
Aussie Gold (73-50)	874	D	participant039	Smooth Cayenne	498	D	participant003
Aussie Gold (73-50)	874	D	participant049	Smooth Cayenne	498	D	participant011
Aussie Gold (73-50)	874	D	participant108	Smooth Cayenne	498	D	participant044
Aussie Gold (73-50)	874	D	participant119	Smooth Cayenne	498	D	participant105
Aussie Gold (73-50)	874	D	participant040	Smooth Cayenne	498	D	participant007
Aussie Gold (73-50)	874	D	participant046	Smooth Cayenne	498	D	participant077
Aussie Gold (73-50)	874	D	participant080	Smooth Cayenne	498	D	participant090
Aussie Gold (73-50)	874	D	participant109	Smooth Cayenne	498	D	participant119
Aussie Gold (73-50)	874	D	participant045	Smooth Cayenne	498	D	participant047
Aussie Gold (73-50)	874	D	participant047	Smooth Cayenne	498	D	participant055
Aussie Gold (73-50)	874	E	participant021	Smooth Cayenne	498	D	participant062
Aussie Gold (73-50)	874	E	participant056	Smooth Cayenne	498	D	participant078
Aussie Gold (73-50)	874	E	participant023	Smooth Cayenne	498	D	participant079
Aussie Gold (73-50)	874	E	participant091	Smooth Cayenne	498	D	participant113
Aussie Gold (73-50)	874	E	participant110	Smooth Cayenne	498	D	participant088
Aussie Gold (73-50)	874	E	participant073	Smooth Cayenne	498	D	participant116
Aussie Gold (73-50)	874	E	participant020	Smooth Cayenne	498	E	participant076

Cultivar	Blinding code	Tracking letter	assessor	Cultivar	Blinding code	Tracking letter	assessor
Aussie Gold (73-50)	874	E	participant067	Smooth Cayenne	498	E	participant092
Aussie Gold (73-50)	874	E	participant083	Smooth Cayenne	498	E	participant099
Aussie Gold (73-50)	874	E	participant112	Smooth Cayenne	498	E	participant042
Aussie Gold (73-50)	874	E	participant057	Smooth Cayenne	498	E	participant074
Aussie Gold (73-50)	874	E	participant084	Smooth Cayenne	498	E	participant093
Aussie Gold (73-50)	874	F	participant009	Smooth Cayenne	498	E	participant098
Aussie Gold (73-50)	874	F	participant019	Smooth Cayenne	498	E	participant108
Aussie Gold (73-50)	874	F	participant054	Smooth Cayenne	498	E	participant016
Aussie Gold (73-50)	874	F	participant072	Smooth Cayenne	498	E	participant041
Aussie Gold (73-50)	874	F	participant114	Smooth Cayenne	498	E	participant072
Aussie Gold (73-50)	874	F	participant016	Smooth Cayenne	498	E	participant109
Aussie Gold (73-50)	874	F	participant085	Smooth Cayenne	498	E	participant008
Aussie Gold (73-50)	874	F	participant089	Smooth Cayenne	498	E	participant019
Aussie Gold (73-50)	874	F	participant022	Smooth Cayenne	498	E	participant097
Aussie Gold (73-50)	874	F	participant066	Smooth Cayenne	498	E	participant106
Aussie Gold (73-50)	874	F	participant081	Smooth Cayenne	498	E	participant009
Aussie Gold (73-50)	874	F	participant088	Smooth Cayenne	498	E	participant014
Aussie Gold (73-50)	874	F	participant001	Smooth Cayenne	498	F	participant001
Aussie Gold (73-50)	874	F	participant055	Smooth Cayenne	498	F	participant015
Aussie Gold (73-50)	874	F	participant075	Smooth Cayenne	498	F	participant118
Aussie Gold (73-50)	874	F	participant087	Smooth Cayenne	498	F	participant017
Aussie Gold (73-50)	874	G	participant014	Smooth Cayenne	498	F	participant066
Aussie Gold (73-50)	874	G	participant090	Smooth Cayenne	498	F	participant103
Aussie Gold (73-50)	874	G	participant018	Smooth Cayenne	498	F	participant020
Aussie Gold (73-50)	874	G	participant053	Smooth Cayenne	498	F	participant115
Aussie Gold (73-50)	874	G	participant008	Smooth Cayenne	498	F	participant045
Aussie Gold (73-50)	874	G	participant017	Smooth Cayenne	498	F	participant075
Aussie Gold (73-50)	874	G	participant113	Smooth Cayenne	498	F	participant101
Aussie Gold (73-50)	874	G	participant015	Smooth Cayenne	498	F	participant018
Aussie Gold (73-50)	874	G	participant052	Smooth Cayenne	498	F	participant039
Aussie Gold (73-50)	874	G	participant061	Smooth Cayenne	498	F	participant046
Aussie Gold (73-50)	874	G	participant074	Smooth Cayenne	498	F	participant094
Aussie Gold (73-50)	874	G	participant064	Smooth Cayenne	498	F	participant100
Aussie Gold (73-50)	874	G	participant107	Smooth Cayenne	498	F	participant104
Aussie Gold (73-50)	874	G	participant111	Smooth Cayenne	498	G	participant049
Aussie Gold (73-50)	874	H	participant063	Smooth Cayenne	498	G	participant051
Aussie Gold (73-50)	874	H	participant029	Smooth Cayenne	498	G	participant022
Aussie Gold (73-50)	874	H	participant059	Smooth Cayenne	498	G	participant111
Aussie Gold (73-50)	874	H	participant062	Smooth Cayenne	498	G	participant038
Aussie Gold (73-50)	874	H	participant079	Smooth Cayenne	498	G	participant021
Aussie Gold (73-50)	874	H	participant030	Smooth Cayenne	498	G	participant050
Aussie Gold (73-50)	874	H	participant086	Smooth Cayenne	498	G	participant023
Aussie Gold (73-50)	874	H	participant028	Smooth Cayenne	498	G	participant043
Aussie Gold (73-50)	874	H	participant058	Smooth Cayenne	498	H	participant035
Aussie Gold (73-50)	874	H	participant031	Smooth Cayenne	498	H	participant034
Aussie Gold (73-50)	874	I	participant032	Smooth Cayenne	498	H	participant040
Aussie Gold (73-50)	874	I	participant060	Smooth Cayenne	498	H	participant048
Aussie Gold (73-50)	874	I	participant065	Smooth Cayenne	498	H	participant024
Aussie Gold (73-50)	874	I	participant024	Smooth Cayenne	498	H	participant067
Aussie Gold (73-50)	874	I	participant033	Smooth Cayenne	498	H	participant036
Aussie Gold (73-50)	874	I	participant027	Smooth Cayenne	498	I	participant025
Aussie Gold (73-50)	874	J	participant026	Smooth Cayenne	498	I	participant027
Aussie Gold (73-50)	874	J	participant034	Smooth Cayenne	498	I	participant032
Aussie Gold (73-50)	874	J	participant037	Smooth Cayenne	498	I	participant026
Aussie Gold (73-50)	874	J	participant025	Smooth Cayenne	498	J	participant028
Aussie Gold (73-50)	874	J	participant036	Smooth Cayenne	498	J	participant037

Supplementary information C2.

Consumer and Sensory evaluation:

Both consumer and sensory assessments took place in sensory booths at the DPI sensory laboratories. This facility is equipped with 12 individual testing booths, with neutral backgrounds, daylight-equivalent lights, ambient temperatures (22°C), tablets and tables for group discussion. Data collection was completed using EyeQuestion® cloud software (version 5.12.15 (Build 73)) for both evaluations. Both consumer and sensory assessments conducted in line with the Professional Food Sensory Group of the Institute for Food Science and Technology (IFST) guidelines for ethical and professional practices for the sensory analysis of food. Informed consent was collected from all assessors (trained panel and naïve consumers) before the study commenced.

Trained panel sensory evaluation:

Descriptive sensory analysis (AS 2542.1.3:2014 adopts ISO 8586:2012) ("BS EN ISO 8586:2023: Sensory analysis. Selection and training of sensory assessors," 2023) was conducted on the pineapple samples, using 13 trained sensory panellists (1 male, 12 females; average age of panel 46 years), representing diverse nationalities and ethnic backgrounds, selected for their sensory acuity.

The panellists attended four training sessions (120 mins each). The first day of training involved the generation of sensory attributes for the lexicon through consensus. The remaining training sessions were focused on attribute and lexicon refinement, sample assessment, and establishment and familiarisation of the eating protocol under the guidance of the panel leader. The final lexicon included one appearance, 13 aroma, 11 flavour, three in-mouth texture, two afterfeel and four aftertaste attributes. A comprehensive list of sensory attributes, definitions and reference standards is summarised in **Table C2**. Trained panellists attended a mock evaluation session (120 min) prior to the formal evaluations.

Formal evaluations were conducted in triplicate (approximately 20 mins each). Samples were presented one at a time in a balanced sequential monadic design. A 100-point unstructured line scale ranging from low/none to high was used to rate each attribute. Trained panel started by rating the appearance attribute and cutting the sample in half to evaluate the aroma attributes. One half of the cut sample was used to evaluate the flavour attributes, while the other was used for texture attributes. Only the significant sensory attributes were recorded during the formal session. Water and plain water crackers (Captain's Table crackers, Australia) were provided as palate cleanser between samples, and a 10-min break was provided between sessions.

Table C2: Sensory attributes list definitions and reference standards

Attribute	Definition	Reference / Scale
Appearance		
colour	The graduation of flesh colour intensity	Low (white yellow) to high (yellow)
Aroma		
intensity	Overall aroma intensity	Low to high
sweet	Caramel/honey/fruit syrup aroma	Honey and canned pineapple juice solution / none to high
vinegar/tang	Pungent aroma associated with vinegar	Diluted apple cider vinegar / none to high
tropical fruits	Sweet tropical aroma of passionfruit/pineapple	Fresh passionfruit and pineapple / none to high
floral	Fresh floral jasmine aroma	Fresh jasmine flower / none to high
coconut	Aroma of fresh and dried coconut/coconut cream	Fresh coconut flesh, coconut cream and dried coconut / none to high
green	Vine /cucumber aroma	Cucumber, tomato vine / none to high
metallic	Aroma of metallic can with fruit removed	Can with canned pineapple removed / none to high
vegetal	Savoury aroma of tinned sweetcorn	Tinned sweetcorn juice / none to high
fresh	Aroma of fresh mint	Fresh mint leaves / none to high
peppery	Warm spiced aroma of black pepper	Crushed black peppercorns / none to high
fermented	Off aroma of overripe fruit	Overripe rockmelon / none to high
eggy/sulphurous	Off aroma of boiled egg	Boiled egg / none to high
Texture		
crunchiness	Crunchiness of the sample when chewing in the mouth	Low (mushy when chewing) High (breaks up into pieces, firmer) / low to high
fibrousness	The presence of fibres in the mouth cavity	Raw celery (high) / low to high
juiciness	The amount of juice released from the sample during the first 3 bites	Canned mandarin segment (high) / low to high
Flavour		
sweet	Flavour of caramel/honey/syrup	Honey and tinned pineapple juice solution / low to high
sour/acidity	Tart flavour of green apple/lemon/green grapes	Fresh green apples slices, lemon slices and green grape / low to high
tropical fruit	Flavour of mango/passionfruit	Fresh passionfruit and mango / low to high
floral	Flavour associated with fresh jasmine	Fresh jasmine flower / none to high
coconut	Flavour of fresh and dried coconut	Coconut cream and dried coconut / none to high
green	Flavour of vine fruit/cucumber	Fresh cucumber and tomato vine / none to high
metallic	Metallic flavour, like that tasted in tinned fruit	Can of tinned pineapple (pineapple removed) / none to high
vegetal	Flavour of savoury tinned sweetcorn	Sweetcorn from a can / none to high
fresh	Flavour of fresh mint	Fresh mint leaves (torn) / none to high
peppery	Warm spiced aromatic flavour of black pepper	Crushed black peppercorns / none to high
fermented	Off flavour associated with overripe fruit	Overripe rockmelon / none to high
Aftertaste/feel		
astringent	Drying/numbing/puckering sensation of mouth or tongue	None to high
fibrous/fibrosity	Number of fibres left in the mouth following mastication	None to high
bitter	Bitter aftertaste	None to high
sour	Sour/acidic aftertaste	None to high
sweet	Sweet aftertaste of honey/syrup	None to high
Metallic	Metallic aftertaste, like that tasted in tinned fruit	None to high

Table C3: Quality of sensory data**:** Statistical analysis (min, max, mean, SD and CV) of five pineapple samples, 13 panellists, 3 replicates and interactions for each sensory attribute obtained by a mixed model analysis of variance.

Sensory attributes	min	max	Mean	SD	CV (%)
Aroma attributes					
colour	2	86	51	33	65
aroma intensity	7	82	48	36	75
sweet aroma	3	85	42	38	91
vinegar/tang aroma	7	33	15	22	143
tropical fruit aroma	4	70	37	36	97
floral aroma	3	27	14	24	173
coconut aroma	3	81	38	40	106
green aroma	3	36	18	26	149
fresh aroma	0	21	11	22	205
fermented aroma	0	21	10	23	240
Flavour attributes					
sweet flavour	7	89	52	31	59
sour/acidic flavour	16	94	60	27	70
tropical fruit flavour	6	77	68	26	71
floral flavour	1	32	52	31	177
coconut flavour	0	75	60	27	101
green flavour	4	60	68	26	124
fresh flavour	6	21	52	31	194
Texture attributes					
crunchiness	31	85	52	31	61
fibrousness	47	73	60	27	45
juiciness	42	88	68	26	39

Table C4: Statistical analysis (F ratios and significance for effects of 5 pineapple samples, 13 panellists, 3 replicates and interactions for each sensory attribute obtained by a mixed model analysis of variance).

Sensory attributes	Sample	Panellist	Replicate	Sample × panellist	Sample × replicate	Panellist × replicate
Aroma attributes						
colour	44	5	0	1	4	0
Pr > F	<0.0001	0.173	0.901	0.497	0.001	1.000
aroma intensity	49	2	0	2	2	1
Pr > F	<0.0001	0.087	0.652	0.003	0.131	0.825
sweet aroma	32	2	0	2	3	1
Pr > F	<0.0001	0.062	0.965	0.001	0.015	0.966
vinegar/tang aroma	2	4	2	2	1	2
Pr > F	0.092	0.002	0.247	0.011	0.413	0.056
tropical fruit aroma	33	2	1	1	1	1
Pr > F	<0.0001	0.040	0.455	0.101	0.363	0.702
floral aroma	5	4	0	4	1	1
Pr > F	0.005	0.000	0.735	<0.0001	0.684	0.229
coconut aroma	16	0	0	3	2	1

Sensory attributes	Sample	Panellist	Replicate	Sample × panellist	Sample × replicate	Panellist × replicate
Pr > F	<0.0001	0.910	0.801	<0.0001	0.026	0.247
green aroma	7	3	2	1	1	1
Pr > F	0.013	0.010	0.258	0.269	0.695	0.207
fresh aroma	4	6	2	3	1	2
Pr > F	0.013	<0.0001	0.177	<0.0001	0.453	0.006
fermented aroma	6	3	1	2	0	3
Pr > F	0.002	0.003	0.266	0.000	0.910	0.000
Flavour attributes						
sweet flavour	39	1	0	1	3	1
Pr > F	<0.0001	0.860	0.859	0.149	0.006	0.153
sour/acidic flavour	38	1	5	1	1	1
Pr > F	<0.0001	0.395	0.067	0.152	0.341	0.535
tropical fruit flavour	24	4	1	1	2	1
Pr > F	<0.0001	0.003	0.316	0.079	0.017	0.238
floral flavour	6	11	0	3	1	1
Pr > F	0.002	<0.0001	0.958	<0.0001	0.208	0.457
coconut flavour	28	1	0	2	2	1
Pr > F	<0.0001	0.363	0.641	<0.0001	0.164	0.816
green flavour	7	4	0	1	4	1
Pr > F	0.009	0.005	0.864	0.094	0.000	0.857
fresh flavour	2	10	-4	3	0	1
Pr > F	0.087	<0.0001	<0.0001	<0.0001	0.929	0.924
Texture attributes						
crunchiness	5	1	3	2	4	1
Pr > F	0.016	0.530	0.092	0.010	0.000	0.216
fibrousness	0	1	0	3	2	2
Pr > F	0.738	0.560	0.848	<0.0001	0.027	0.021
juiciness	3	2	0	2	6	1
Pr > F	0.078	0.100	0.655	0.013	<0.0001	0.122

Statistically significant F ratios indicated by *** (p<0.0001), ** (p < 0.01), * (p < 0.05), ns not significant.

Table C5: Panel performance

Judge\Descriptors	J01	J02	J03	J04	J05	J06	J07	J08	J09	J10	J11	J12	J13
Discrimination	9	8	5	14	14	10	11	14	10	8	9	6	6
Repeatability	13	16	13	18	17	13	16	17	15	19	16	19	16
No interaction	10	14	16	14	13	16	17	18	17	19	9	16	12
Total	32	38	34	46	44	39	44	49	42	46	34	41	34

Ideal value is 57.

Table C6 ANOVA table of pineapple cultivars and sensory panel results (aroma attributes), including Tukey ranked means text.

	colour	*aroma intensity*	*sweet aroma*	*vinegar/tang aroma*	*tropical fruit aroma*	*floral aroma*	*coconut aroma*	*green aroma*	*fresh aroma*	*fermented aroma*
Aus Festival	82.5 a	77.0 a	74.5 a	9.8 b	57.2 ab	25.7 a	67.8 a	6.9 b	15.3 a	13.9 ab
Aus Jubilee	63.3 c	58.3 b	51.7 b	11.5 b	48.8 b	9.9 b	38.0 b	17.1 ab	12.4 ab	19.3 a
Aus Carnival	70.5 b	77.2 a	70.4 a	13.7 ab	62.5 a	20.6 a	68.0 a	11.8 b	17.8 a	10.2 ab
Aus Gold	32.3 d	16.5 c	7.7 c	23.1 a	9.8 c	5.8 b	6.5 c	26.4 a	4.1 b	4.6 bc
Aus Smooth	4.1 e	10.4 c	4.5 c	18.4 ab	6.0 c	6.5 b	7.8 c	25.5 a	3.8 b	0.0 c
Pr > F(Model)	<0.0001	<0.0001	<0.0001	0.046	<0.0001	0.000	<0.0001	0.002	0.008	0.002
Significant	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

Mean values of individual samples from sensory study samples of pineapple, n ≥ 8. Different letters in the same row indicate significant statistical differences (Tukey's HSD, P ≤ 0.05).

Table C7 ANOVA table of pineapple cultivars and sensory panel results (flavour attributes), including Tukey ranked means text.

	sweet flavour	*sour/acidic flavour*	*tropical fruit flavour*	*floral flavour*	*coconut flavour*	*green flavour*	*fresh flavour*
Aus Festival	87.4 a	21.5 d	71.7 a	16.7 a	71.3 a	5.8 c	10.6 ab
Aus Jubilee	74.5 b	30.4 cd	58.1 b	16.8 a	39.4 b	18.8 b	12.7 ab
Aus Carnival	86.0 a	38.4 c	68.9 ab	24.9 a	67.4 a	7.8 c	18.7 a
Aus Gold	34.5 c	66.1 b	23.2 c	4.4 b	8.3 c	46.0 a	8.1 b
Aus Smooth	16.2 d	86.0 a	16.1 c	5.3 b	4.3 c	38.9 a	6.9 b
Pr > F(Model)	<0.0001	<0.0001	<0.0001	0.000	<0.0001	<0.0001	0.139
Significant	Yes	Yes	Yes	Yes	Yes	Yes	No

Mean values of individual samples from sensory study samples of pineapple, n ≥ 8. Different letters in the same row indicate significant statistical differences (Tukey's HSD, P ≤ 0.05).

Table C8 ANOVA table of pineapple cultivars and sensory panel results (texture attributes), including Tukey ranked means text.

	crunchiness	*fibrousness*	*juiciness*
Aus Festival	36.3 c	62.6 a	76.8 ab
Aus Jubilee	54.0 b	66.0 a	66.3 b
Aus Carnival	36.4 c	54.4 a	78.6 a
Aus Gold	79.3 a	59.5 a	45.6 c
Aus Smooth	51.6 b	56.8 a	71.2 ab
Pr > F(Model)	<0.0001	0.330	<0.0001
Significant	Yes	No	Yes

Mean values of individual samples from sensory study samples of pineapple, n ≥ 8. Different letters in the same row indicate significant statistical differences (Tukey's HSD, P ≤ 0.05).

Supplementary information C3: results from consumer clustering analysis

Naïve consumers (n= 117) were recruited by a specialised recruitment agency, comprising regular fresh pineapple consumers based in Brisbane, Queensland, Australia. The consumers included 49 males and 68 females aged 18 to 65 years. Pineapple samples were cut in half and served one at a time in a balanced, sequential monadic design. Compositive tracking code for each sample was entered in the questionnaire by consumers when they received a sample. Consumers followed the same eating protocol as the trained panel and were asked to rate the liking of appearance and aroma before they tasted the sample, after which they evaluated the liking of flavour, texture and overall liking on a 9-point hedonic scale (1=dislike extremely to 9 =like extremely). Two consumers were removed from the final dataset due to incomplete data, resulting in 115 complete datasets for analysis

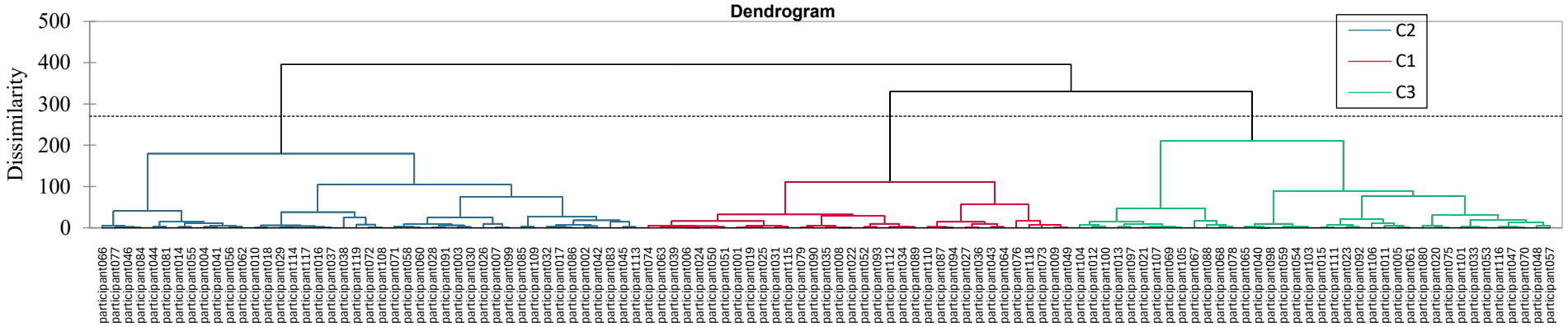


Figure C1: Agglomerative hierarchical clustering (AHC) for consumers (number of classes = 3). Incomplete data sets are excluded from AHC analysis

Table C9: Analysis of variance from cluster analysis

Variable	Pr > F	Significant
Smooth Cayenne	0.885	No
Aus-Jubilee	**<0.0001**	**Yes**
Aus-Carnival	**<0.0001**	**Yes**
Aus-Festival	**<0.0001**	**Yes**
Aussie Gold (73-50)	0.085	No

Appendix 4 Supplementary information for Chapter 5

Table D1: GWAS results of FarmCPU (*i*), BLINK (*ii*), and 3VmrMLM(*iii*) using HA type

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
2-methyl butyl acetate (624-41-9) *Fermented, sweet, balsamic*	*ii*	4: 18,293,787	4716239|F|0-63:T>C	HA003981.1	AP2-like ethylene-responsive transcription factor	7.03E-11	14.4	0.06	483
	iii	4: 17,991,616	4716239|F|0-63:T>C	HA003981.1	AP2-like ethylene-responsive transcription factor		16.8		182
	iii	8: 16,078,526	4718996|F|0-34:A>G	HA007062.1	acetyltransferase		9.90		139
	iii	8: 16,078,526	4718996|F|0-34:A>G	HA007079.1	serine/threonine-protein kinase		9.90		50
	iii	8: 16,078,526	4718996|F|0-34:A>G	HA007080.1	serine/threonine-protein kinase		9.90		64
	ii	15: 11,594,865	54316260|F|0-6:T>C	HA012907.1	acyl-coenzyme A oxidase		11.9	0.05	460
	iii	15: 11,013,487	54316260|F|0-6:T>C	HA012887.1	serine/threonine-protein kinase		15.6		339
	iii	17: 11,988,154	4722450|F|0-18:G>A	HA014677.1	Acyltransferase		15.5		38
	iii	17: 11,988,154	4722450|F|0-18:G>A	HA014674.1	Carboxylesterase		15.5		15
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018768.1	Aldo-keto reductases		8.5		46
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018769.1	Aldo-keto reductases		8.5		43
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018770.1	Aldo-keto reductases		8.5		40
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018771.1	Aldo-keto reductases		8.5		37
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018773.1	Aldo-keto reductases		8.5		32
	i, ii	3: 4,132,770	4716516|F|0-31:A>T	HA002437.1, HA002425.1, HA002426.1	GDSL esterase/ lipase, UDP-Glycosyltransferase, Histone-lysine N-methyletransferase SUVH2-like	3.05E-16		0.10	
	iii	3: 11,652,254	28876791|F|0-45:A>G	HA002485.1	GDSL esterase/lipase		21.2		1236
	iii	3: 11,652,254	28876791|F|0-45:A>G	HA002486.1	GDSL esterase/lipase		21.2		1326
2,5-dimethyl-4-methoxy-3(2H)-furanone [DHMF] (4077-47-8) *caramel, roasty, sweet*	*iii*	4: 17,760,638	54312756|F|0-55:T>C	HA003959.1	GDP-Man:Man(3)GlcNAc(2)-PP-Dol alpha-1,2-mannosyltransferase		7.5		101
	iii	6: 666,856	4718537|F|0-63:T>C	HA005035.1	Peptide chain release factor		13.2		58
	iii	14: 77,515	28877886|F|0-54:A>G	HA011938.1	Benzyl Alcohol O-Benzoyltransferase		10.1		90
	iii	14: 77,515	28877886|F|0-54:A>G	HA011939.1	Benzyl Alcohol O-Benzoyltransferase		10.1		93
	iii	14: 77,515	28877886|F|0-54:A>G	HA011940.1	Benzyl Alcohol O-Benzoyltransferase		10.1		99
	iii	14: 77,515	28877886|F|0-54:A>G	HA011941.1	Benzyl Alcohol O-Benzoyltransferase		10.1		103

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
	iii	14: 77,515	28877886|F|0-54:A>G	HA011942.1	Benzyl Alcohol O-Benzoyltransferase		10.1		116
	iii	14: 15,453,675	4713100|F|0-42:C>A	HA012566.1	GDSL Esterase/Lipase		4.6		134
	iii	14: 15,453,675	4713100|F|0-42:C>A	HA012577.1	Alcohol Dehydrogenase (ADH)		4.6		42
	iii	14: 15,453,675	4713100|F|0-42:C>A	HA012599.1	Methyltransferase		4.6		76
	iii	16: 11,696,912	4709243|F|0-49:A>T	HA013835.1	Fatty Acid Hydroxylase		15.0		135
	iii	18: 2,264,533	4718089|F|0-61:T>C	HA015189.1	UDP-Glycosyltransferase (UGT)		37.9		1169
	iii	19: 14,793,028	54312048|F|0-30:T>C	HA016469.1	Amino acid transporter		8.8		101
	iii	22: 2,076,544	4717211|F|0-15:C>G	HA017909.1	UDP-Glycosyltransferase (UGT)		6.7		1275
	ii	3: 10,482,530	4711967|F|0-50:T>C	HA002451.1	peroxygenase-like	2.03E-06	27.8	0.11	97
	i	24: 8,821,885	28883629|F|0-22:A>G	HA019113.1	aldehyde oxidase	2.34E-10		0.04	66
	i	22: 13,446,541	54316124|F|0-62:C>T	HA018264.1	peroxidase	2.54E-09		0.14	90
	i	3: 20,165,055	54311817|F|0-17:T>C	HA003175.1	pectin acetylesterase	6.67E-09		0.06	9
	i	21: 10,156,471	28880522|F|0-22:C>T	HA017329.1	acetyltransferase	5.77E-08		0.05	8
	i	7: 14,436,785	4711538|F|0-22:T>A	HA006105.1	Dual-specificity RNA methyltransferase	7.90E-07		0.11	45
	i, ii	19: 12,091,995	4713680|F|0-26:C>A	HA016178.1, HA016179.1, HA016180.1	Alpha-Humulene synthase-like x3	1.10E-12	15.9	0.36	21
α- terpineol (98-55-5) *floral, lilac*	*iii*	19: 12,529,138	4713680|F|0-26:C>A	HA016204.1	peroxidase		15.3		23
	i	25: 10,186,158	4712117|F|0-51:C>G	HA019868.1	GDSL esterase/lipase	3.34E-08		0.14	1
	i	11: 1,286,656	4718619|F|0-32:A>G	HA009425.1	Ethylene-responsive transcription facto	3.67361E-07		0.43	155
	i	17: 13,996,462	4710392|F|0-20:C>A	HA014931.1	Serine hydroxymethyltransferase	6.97423E-07		0.34	69
	ii	1: 1,738,230	4712576|F|0-6:A>G	HA000163.1	terpene synthase		42.7		20
	ii	1: 19,608,916	4717175|F|0-67:C>T	HA000832.1	Phytoene synthase	2.68463E-10		0.05	46
phenylacetaldehyde (122-78-1) *floral, sweet*	*ii, i*	4: 18,152,283	28879439|F|0-31:C>G	HA004015.1	Peroxidase	7.22E-17		0.04	30
	i, ii	5: 16,021,765	28881466|F|0-40:C>T	HA004674.1	L-ascorbate oxidase homolog	5.17E-17		0.06	69
	i	5: 10,534,309	4709277|F|0-5:G>T	HA004539.1	Arogenate dehydrogenase	1.20777E-12		0.05	495
	i	5: 12,218,713	4719032|F|0-64:C>T	HA004552.1	L-galactono-1,4-lactone dehydrogenase	1.84E-16		0.05	60

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
	iii	1: 18,955,160	4716871|F|0-54:A>G				102.3		
	iii	6: 14,218,878	4716366|F|0-13:T>A	HA005344	Ethylene Responsive TF ERF020		134.8		233
	iii	7: 2,167,403	4728040|F|0-12:A>T	HA005945.1	leucoanthocyanidin reductase		29.3		154
	iii	10: 950,430	28881270|F|0-45:A>T	HA008492.1	Glycerol kinase		8.0		9
	iii	13: 4,555,807	4713661|F|0-45:G>C	HA011331.1	lipoxygenase		5.0		312
	iii	13: 12,718,708	28874642|F|0-11:A>G	HA011499.1	Glucan endo-1,3-beta-glucosidase		9.2		72
	iii	14: 14,064,628	28875576|F|0-25:A>G	HA012397.1	Ubiquinone biosynthesis protein		106.8		3
	iii	16: 1,116,874	4709905|F|0-52:G>A	HA013539.1	ubiquitin-protein ligase		136.5		38
	iii	18: 10,600,202	4723688|F|0-35:A>G	HA015319.1	Acyl carrier protein		14.8		37
	iii	23: 11,710,077	4711620|F|0-10:G>A	HA018768.1	Aldo-keto reductases		107.4		343
	iii	23: 11,710,077	4711620|F|0-10:G>A	HA018769.1	Aldo-keto reductases		107.4		328
	iii	23: 11,710,077	4711620|F|0-10:G>A	HA018770.1	Aldo-keto reductases		107.4		317
	iii	23: 11,710,077	4711620|F|0-10:G>A	HA018771.1	Aldo-keto reductases		107.4		302
	iii	23: 11,710,077	4711620|F|0-10:G>A	HA018773.1	Aldo-keto reductases		107.4		265
	iii	25: 11,164,867	4724194|F|0-8:C>G	HA019957.1	Aldose reductase (AR)		45.9		225
	ii	8: 999,480	54312250|F|0-11:G>A	HA006662.1	glycosyltransferase	9.11266E-12		0.04	5
	i, ii	10: 963,198	28881270|F|0-45:A>T	HA008498.1	N-alpha-acetyltransferase	2.03597E-11		0.04	61
	ii	12: 14,984,154	4709137|F|0-56:G>T	HA011029.1	serine/threonine-protein kinase	2.79036E-11		0.03	2
	ii	13: 7,176,315	4709574|F|0-26:C>G	HA011346.1	2-hydroxyacyl-CoA lyase	9.09E-30		0.04	1
	i, ii	13: 8,451,372	4710543|F|0-53:A>T	HA011346.1	2-hydroxyacyl-CoA lyase	1.46E-29		0.03	1274
	i	13: 7,176,315	4709574|F|0-26:C>G	HA011346.1	2-hydroxyacyl-CoA lyase	2.16E-16		0.04	1
	i	13: 9,162,023	54313654|F|0-20:G>A	HA011372.1	UDP-glucose 4-epimerase	7.24E-13		0.03	143
	i	13: 9,299,314	4711667|F|0-52:C>T	HA011372.1	UDP-glucose 4-epimerase	7.24E-13		0.03	6
	i	13: 10,401,534	28871917|F|0-20:G>T	HA011392.1	Glycosyltransferase	1.77734E-11		0.03	95
	i	13: 10,493,546	54309273|F|0-57:G>C	HA011392.1	Glycosyltransferase	1.77734E-11		0.03	3
	ii	14: 12,836,896	28875576|F|0-25:A>G	HA012278.1	GDSL esterase/lipase		124.3		18

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
	i	17: 11,331,824	4711218|F|0-17:C>G	HA014598.1	long chain base biosynthesis protein	1.49421E-12		0.08	1529
	i	17: 12,358,537	4713761|F|0-47:C>T	HA014717.1	Serine/threonine-protein kinase	6.5366E-11		0.08	8
	i	17: 11,411,438	4710933|F|0-68:A>G	HA014598.1	long chain base biosynthesis protein	1.71E-20		0.07	103
	ii	18: 13,545,501	100160119|F|0-24:C>G	HA015634.1	laccase	1.76E-13		0.02	12
	i	4: 18,497,849	54308383|F|0-39:T>A	HA004049.1	folylpolyglutamate synthase isoform	2.01E-09		0.05	120
	i	6: 1,784,120	4713871|F|0-44:C>T	HA005166.1	serine/threonine-protein kinase	1.98E-07		0.15	25
	ii	12: 16,268,110	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase	2.68E-08		0.02	13
	iii	4: 16,741,865	54310142|F|0-33:G>A	HA003859.1	Casein kinase		3.5		1
	iii	6: 15,834,204	4715100|F|0-15:A>G	HA005499.1	esterase		6.7		122
	iii	13: 4,555,807	4713661|F|0-45:G>C	HA011346.1	2-hydroxyacyl-CoA lyase		6.0		2621
methyl isovalerate (556-24-1) *fruity, apple-like*	*iii*	18: 634,650	4709741|F|0-12:T>C	HA015153.1	acetylesterase		3.4		140
	iii	23: 11,484,768	4714519|F|0-38:T>C	HA018768.1	Aldo-keto reductases (AKRs)		118.2		117
	iii	23: 11,484,768	4714519|F|0-38:T>C	HA018769.1	Aldo-keto reductases		118.2		102
	iii	23: 11,484,768	4714519|F|0-38:T>C	HA018770.1	Aldo-keto reductases		118.2		92
	iii	23: 11,484,768	4714519|F|0-38:T>C	HA018771.1	Aldo-keto reductases		118.2		76
	iii	23: 11,484,768	4714519|F|0-38:T>C	HA018773.1	Aldo-keto reductases		118.2		40
	i	13: 14,309,093	4708841|F|0-46:G>T	HA011626.1	acyl-CoA synthetase	0.000262236		0.49	305
	i	16: 14,966,413	4712209|F|0-29:T>C	HA014239.1	Methylenetetrahydrofolate reductase	9.84E-07		0.04	22
	i, ii	4: 18,376,903	4716749|F|0-38:A>G	HA004049.1	folylpolyglutamate synthase isoform	5.67E-11		0.04	374
methyl isobutyrate (547-63-7) *fruity, sweet*	*iii*	23: 1,292,707	4718140|F|0-11:A>G	HA018485.1	acyl-coenzyme A		10.7		201
	iii	23: 1,292,707	4718140|F|0-11:A>G	HA018505.1	alcohol dehydrogenase				10
	i	13: 10,658,846	54314352|F|0-32:G>A	HA011396.1	ubiquitin-conjugating enzyme E2 26 isoform	3.26657E-07		0.06	7
	i, ii	4: 18,376,903	4716749|F|0-38:A>G	HA004049.1	folylpolyglutamate synthase isoform	2.81E-10		0.04	374
methyl butyrate (623-42-7) *fruity, sweet*	*iii*	2: 15,554,785	28879688|F|0-47:A>G	HA001539.1	ethylene-responsive transcription factor		7.2		47
	iii	25: 7,983,393	28873954|F|0-11:G>A	HA019657.1	glyoxysomal fatty acid beta-oxidation multifunctional protein		12.9		536
	i, ii	6: 15,713,325	54316670|F|0-52:G>A	HA005457.1	ketoacyl-CoA synthase	1.19E-14		0.08	119

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
	i, ii	6: 15,724,621	28877336|F|0-41:G>C	HA005433.1	fatty-acid desaturase	4.79E-13		0.07	381
	ii	1: 20,238,019	28880933|F|0-13:G>A	HA000928.1	serine/threonine-protein kinase	3.61958E-08	12.5	0.06	2
	iii	2: 14,364,441	54307575|F|0-15:A>G	HA001441.1	serine/threonine-protein kinase		12.2		18
	iii	4: 18,531,348	28876316|F|0-11:G>A	HA004060.1	S-formylglutathione hydrolase		11.5		49
	iii	10: 922,390	54308776|F|0-64:C>G	HA008493.1	hydroxyproline O-galactosyltransferase		10.7		25
	iii	13: 8,747,891	4710595|F|0-53:G>A	HA011364.1	Serine/threonine-protein kinase		8.3		84
	iii	15: 13,782,258	4719120|F|0-40:G>A	HA013159.1	Lysosomal Pro-X carboxypeptidase		6.3		1
methyl-3-methyl thio propionate (13532-18-8) *meaty, onion-like*	*iii*	16: 110,403	54307869|F|0-38:A>G	HA013437.1	Sugar carrier protein C		8.3		12
	iii	16: 12,623,194	54307431|F|0-30:G>T	HA013934.1	S-acyltransferase		19.0		17
	iii	18: 9,417,872	28877850|F|0-29:C>T	HA015267.1	thioredoxin reductase		15.7		135
	iii	19: 1,270,467	28878735|F|0-29:A>T	HA015983.1	Methionine S-methyltransferase		5.8		58
	iii	20: 11,627,957	4709262|F|0-57:T>C	HA016782.1	Beta-galactosidase		6.3		6
	iii	24: 14,132,560	4711736|F|0-17:C>T	HA019561.1	UDP-D-apiose/UDP-D-xylose synthas		11.7		1263
	ii	10: 161,745	4712632|F|0-48:A>G	HA008409.1	diacylglycerol kinase	7.8476E-07	5.8	0.23	50
	ii	15: 9,518,829	4711125|F|0-8:T>C	HA012841.1	glucose-induced degradation protein 4 homolo	1.73825E-07	66.7	0.16	588
	i	2: 17,678,633	4709381|F|0-21:G>A	HA001768.1	enoyl-CoA hydratase	9.66E-07		0.09	35
	i, ii	4: 18,376,903	4716749|F|0-38:A>G	HA004049.1	folylpolyglutamate synthase isoform	2.88E-23		0.04	1
	iii	4: 16,741,865	54310142|F|0-33:G>A	HA003859.1	Casein kinase		4.9913		1
	iii	10: 13,491,757	4718506|F|0-41:C>A	HA008809.1	carboxylesterase		26.8999		48
methyl 2-methyl butyrate (868-57-5) *pungenet, fruity*	*iii*	10: 13,491,757	4718506|F|0-41:C>A	HA008810.1	carboxylesterase		26.8999		41
	iii	16: 1,162,385	28883715|F|0-43:T>A	HA013539.1	ubiquitin-protein ligase		110.4795		8
	i	6: 15,713,325	54316670|F|0-52:G>A	HA005453.1	GDSL esterase/lipase At1g28570	2.14E-09		0.08	146
	i	6: 15,724,621	28877336|F|0-41:G>C	HA005476.1	dihydroflavonol 4-reductase	4.18E-09		0.07	13
	i	7: 12,847,529	4716322|F|0-35:G>A	HA006023.1	phenylalanine--tRNA ligase beta subunit	1.56156E-07		0.08	2
	ii	8: 16,314,472	54311855|F|0-64:G>T	HA007102.1	trifunctional UDP-glucose 4,6-dehydratase/UDP-4-keto-6-deoxy-D-	7.70E-09		0.07	9

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
					glucose 3,5-epimerase/UDP-4-keto-L-rhamnose-reductase				
	i	17: 12,327,893	28882449|F|0-21:C>T	HA014700.1	CoA ligase	2.75E-10		0.06	129
	iii	8: 16,291,825	54307798|F|0-7:A>T	HA007102.1	trifunctional UDP-glucose 4,6-dehydratase/UDP-4-keto-6-deoxy-D-glucose 3,5-epimerase/UDP-4-keto-L-rhamnose-reductase		6.4		13
	iii	18: 14,562,957	28874076|F|0-18:G>A	HA015781.1	ubiquitin-protein ligase		8.2		31
isobutyl acetate (110-19-0) *fermented, ethereal*	*iii*	23: 11,725,671	4709276|F|0-26:A>G	HA018777.1	lipid-transfer protein		4.9		193
	iii	25: 8,957,917	4715870|F|0-39:C>T	HA019724.1	S-Adenosylmethionine Synthase		5.6		30
	i, ii	12: 16,268,110	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase	3.89333E-09		0.02	13
	i	21: 7,363,264	4719832|F|0-26:A>G	HA017262.1	Lipoyl synthase	3.28E-08		0.40	584
	i, ii	9: 10,241,124	4713076|F|0-33:T>C	HA007618.1	hydroxyacyl-(acyl-carrier-protein) dehydratase	2.78E-13	16.3	0.15	588
	i, ii	12: 16,268,110	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase-like	1.02E-21	51.6	0.02	13
	iii	4: 17,850,096	28879439|F|0-31:C>G	HA003985.1	Serine/threonine-protein kinase		17.2		5
	iii	5: 14,294,012	4715533|F|0-59:C>T	HA004594.1	hydroxymethylglutaryl-CoA lyase		24.7		9
	iii	5: 16,317,057	54315506|F|0-68:A>G	HA004698.1	Ubiquitin-conjugating enzyme E2-17 kDa		38.5		86
	iii	6: 14,175,875	4712476|F|0-17:A>G	HA005346.1	GDSL esterase/lipase		46.9		167
	iii	14: 16,473,558	4714422|F|0-20:T>A	HA012648.1	Caffeoylshikimate esterase		12.1		620
ethyl octanoate (106-32-1) *banana, pineapple, brandy*	*iii*	23: 143,699	4718138|F|0-18:C>T	HA018350.1	serine/threonine-protein kinase		6.6		14
	i	14: 14,795,781	4709745|F|0-43:C>T	HA012500.1	acyl-CoA-binding domain-containing protein		10.6		51
	i	14: 14,795,781	4709745|F|0-43:C>T	HA012465.1	Acetyl-coenzyme A carboxylase		10.6		230
	i, ii	17: 11,367,038	54313905|F|0-35:A>G	HA014601.1	sinapine esterase	1.59E-20		0.06	9
	i, ii	20: 12,491,326	4710127|F|0-38:T>C	HA016871.1	sucrose synthase	5.64557E-11		0.09	14
	i	14: 14,734,326	28883171|F|0-28:A>G	HA012488.1	ascorbate transporter	3.33852E-08		0.09	1
	i, ii	22: 12,155,768	4712248|F|0-42:A>T	HA018117.1	calcium-transporting ATPase 8, plasma membrane-	4.0853E-07		0.03	11
	i	20: 12,727,799	54315558|F|0-27:G>T	HA016908.1	endoglucanase	8.91098E-07		0.06	2
	i, ii	10: 16,470,683	28877382|F|0-18:G>A	HA009207.1	ubiquitin-protein ligase	9.18901E-07		0.07	14

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
ethyl isobutyrate (97-62-1) *fruity, sweet*	*i, ii*	4: 19,097,779	4708466|F|0-11:A>G	HA004156.1	Ethylene-responsive transcription factor	2.22961E-12		0.06	11
	i, ii	7: 12,701,743	28882510|F|0-51:A>G	HA006020.1	Dicarboxylate transporter	1.40896E-22		0.03	36
	i	9: 12,324,883	4718622|F|0-64:T>C	HA007733.1	crocetin glucosyltransferase	9.01E-07	3.5	0.27	27
	i, ii	12: 16,268,110	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase	3.06536E-38		0.02	13
	iii	12: 17,723,093	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase		106.6		1442
	iii	23: 3,290,292	4709764|F|0-31:C>T	HA018655.1	elongator complex protein		13.6		18
	iii	25: 744,804	4714342|F|0-46:C>T	HA019563.1	Acyltransferase		3.2		344
ethyl hexanoate (123-66-0) *pineapple, banana, fruity*	*i*	13: 14,384,396	4722213|F|0-14:A>G	HA011677.1	UDP-glycosyltransferase	6.25527E-08		0.08	81
	i	17: 931,495	4711978|F|0-38:C>T	HA014405.1	N-alpha-acetyltransferase	3.83782E-08		0.11	1
	ii	17: 2,697,205	100134607|F|0-15:C>A	HA014468.1	Very-long-chain 3-oxoacyl-CoA reductase	4.26304E-11		0.01	6044
	ii	23: 983,441	54313351|F|0-26:A>G	HA018470.1	threonylcarbamoyladenosine tRNA methylthiotransferase		33.8		2
	iii	4: 44,581	4711470|F|0-25:C>T	HA003192.1	glycosyltransferase family 64 protein		6.5		5
	iii	9: 10,890,248	4718687|F|0-53:A>T	HA007618.1	3-hydroxyacyl-(acyl-carrier-protein) dehydratase		14.7		61
	iii	14: 14,785,656	4712775|F|0-35:C>T	HA012500.1	Acyl Co-A		12.0		61
	iii	14: 14,785,656	4712775|F|0-35:C>T	HA012465.1	Acetyl-Coenzyme A Carboxylase Carboxyl Transferase		12.0		220
	iii	18: 10,123,887	4709720|F|0-11:C>T	HA015298.1	ubiquitin-protein ligase		9.8		57
	iii	19: 9,769,372	28883636|F|0-21:T>C	HA016108.1	serine/threonine-protein kinase		6.8		1047
	iii	23: 2,458,943	4724123|F|0-28:T>C	HA018627.1	CoA Ligase		5.9		217
	iii	24: 13,009,295	4727640|F|0-46:A>T	HA019557.1	biotin carboxyl carrier protein of acetyl-CoA carboxylase		7.7		203
ethyl decanoate (110-38-3) *fruity, sweet, and slightly oily aroma*	*i,ii*	12: 16,268,110	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase	2.22E-10		0.02	13
	i, ii	19: 11,647,875	4724689|F|0-16:C>A	HA016172.1	serine/threonine-protein kinase	4.05E-11		0.42	95
	ii	23: 10,579,533	28873541|F|0-32:G>A	HA018751.1	adenylyltransferase and sulfurtransferase	1.08E-07		0.10	1
	ii	2: 6,573,414	4715727|F|0-36:G>A	HA001335.1	GDSL esterase/lipase At2g04570	4.57993E-37	47.0	0.07	2810
	ii	2: 10,924,533	28880674|F|0-11:C>T	HA001345.1	Lipase	1.05678E-22		0.09	1
	ii	2: 15,077,568	28875297|F|0-13:T>G	HA001486.1	(R,S)-reticuline 7-O-methyltransferase	1.40202E-20		0.11	10

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
	ii	9: 2,004,657	4715776|F|0-8:C>G	HA007482.1	ubiquitin-protein ligase	7.61698E-18		0.06	2
	ii	13: 12,258,284	4710228|F|0-39:A>G	HA011460.1	Serine/threonine-protein kinase	3.87823E-17		0.04	156
	ii	13: 10,658,846	54314352|F|0-32:G>A	HA011392.1	Glycosyltransferase	3.3341E-16		0.06	163
	ii	4: 19,572,786	54315313|F|0-61:G>A	HA004220.1	Calvin cycle protein CP12-2, chloroplastic	3.80894E-15		0.03	2
	ii	2: 18,053,220	54310273|F|0-9:C>T	HA001822.1	Alpha,alpha-trehalose-phosphate synthase (UDP-forming)	6.95251E-15		0.07	6
	ii	2: 14,797,703	54315499|F|0-55:A>T	HA001457.1	Serine/threonine-protein kinase	3.54493E-14		0.08	121
	iii	3: 14,857,828	4712077|F|0-33:C>T	HA002581.1	(+)-neomenthol dehydrogenase		25.1		5
	iii	9: 2,523,694	100157638|F|0-9:C>G	HA007519.1	Benzyl Alcohol O-Benzoyltransferase (BEBT)		95.1		469
	iii	13: 8,962,092	4713143|F|0-7:G>C	HA011364.1	Serine/threonine-protein kinase		36.2		129
	iii	22: 12,147,370	4712248|F|0-42:A>T	HA018123.1	beta-glucuronosyltransferase		104.5		67
	iii	25: 9,400,834	4712394|F|0-6:C>G	HA019768.1	Acyl Carrier Protein (ACP)		111.5		41
	i, ii	9: 2,509,038	100157638|F|0-9:C>G	HA007488.1	Ethylene-responsive transcription factor	9.51602E-41		0.03	407
	i	13: 11,358,488	4715691|F|0-41:T>A	HA011430.1	serine/threonine-protein kinase	9.51588E-40	41.8	0.03	111
	i, ii	13: 4,785,367	4713661|F|0-45:G>C	HA011346.1	2-hydroxyacyl-CoA lyase	5.09937E-39		0.04	2391
	ii	17: 11,367,038	54313905|F|0-35:A>G	HA014601.1	esterase-like	1.08409E-27		0.06	9
	i	18: 391,408	4718613|F|0-7:C>T	HA015140.1	ATP synthase delta chain, chloroplastic	4.78579E-26		0.04	35
	i, ii	5: 16,311,791	54307338|F|0-48:T>G	HA004703.1	methylesterase	6.92938E-24		0.05	34
	i	5: 18,102,657	28881635|F|0-8:C>T	HA004933.1	acyl-coenzyme A thioesterase	2.3449E-23		0.05	67
	i	18: 9,992,191	4709720|F|0-11:C>T	HA015289.1	Haloacid dehalogenase	1.66267E-20		0.03	64
	i	16: 10,480,032	28874077|F|0-32:T>C	HA013703.1	monodehydroascorbate reductase	5.32998E-18		0.02	559
	i	4: 18,917,875	4711335|F|0-30:G>A	HA004129.1	Heparan-alpha-glucosaminide N-acetyltransferase	7.414E-12		0.04	26
	i, ii	12: 15,182,992	4715754|F|0-28:T>A	HA011055.1	serine/threonine-protein kinase	5.40214E-08		0.14	20
	ii	12: 16,268,110	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase	1.92779E-22		0.02	13
ethyl butyrate	*i, ii*	10: 3,264,074	28879330|F|0-65:T>C	HA008599.1	peroxidase	5.38E-08		0.26	223

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
(105-54-4) *fruity*	*i, ii*	10: 10,423,764	54311942|F|0-13:G>A	HA008661.1	3-oxoacyl-(acyl-carrier-protein) synthas	7.20E-08		0.34	102
	iii	3: 3,723,882	4724974|F|0-19:A>G	HA002415.1	sterol 3-beta-glucosyltransferase		6.1		598
	iii	10: 6,318,164	4712984|F|0-62:A>G	HA008622.1	Acetyltransferase		6.7		142
	iii	19: 12,593,580	4717183|F|0-6:G>A	HA016221.1	Pectinesterase		5.9		144
	iii	21: 10,961,390	28881299|F|0-19:C>T	HA017386.1	Geranylgeranyl Pyrophosphate Synthase (GGPPS)		4.9		196
	iii	21: 13,123,023	54308869|F|0-9:G>A	HA017622.1	Acetyl-CoA Carboxylase (ACC)		13.3		70
	iii	21: 13,123,023	54308869|F|0-9:G>A	HA017597.1	Alcohol Dehydrogenase (ADH)		13.3		167
ethyl-3-methylthio propinoate (13327-56-5) *meaty, onion, pineapple*	*i, ii*	12: 16,268,110	4726102|F|0-20:G>C	HA011152.1	CoA ligase	2.85857E-12		0.02	334
	iii	12: 1,284,054	4715358|F|0-29:T>A	HA004933.1	acyl-coenzyme A thioesterase		12.9		67
	iii	12: 16,391,039	4709188|F|0-53:T>G	HA011197.1	Benzyl Alcohol O-Benzoyltransferase		4.8		110
	iii	13: 13,351,976	4718056|F|0-31:A>C	HA011569.1	UDP-glycosyltransferase		4.4		42
	iii	8: 16,803,497	28881179|F|0-16:G>A	HA007160.1	diacylglycerol O-acyltransferase		8.9		17
ethyl-2-methyl butyrate (7452-79-1) *apple, pineapple, fruity*	*iii*	21: 13,123,023	54308869|F|0-9:G>A	HA017622.1	Acetyl-CoA Carboxylase (ACC)		23.1		70
	iii	21: 13,123,023	54308869|F|0-9:G>A	HA017597.1	Alcohol Dehydrogenase (ADH)		23.1		167
	ii	7: 12,701,743	28882510|F|0-51:A>G	HA006020.1	Dicarboxylate transporte	6.52071E-07		0.03	35
	i, ii	12: 16,268,110	4726102|F|0-20:G>C	HA011197.1	benzyl alcohol O-benzoyltransferase	7.01385E-15		0.02	13
decanal (112-31-2) *sweet, aldehydic, fresh, orange, waxy, and floral*	*ii*	21: 2,731,731	4721013|F|0-31:C>T	HA017277.1	aldehyde oxidase	1.97E-16	5.6	0.18	5622
	iii	1: 4,706,113	4716403|F|0-11:G>A	HA000397.1	ubiquitin protein ligase		28.1		296
	iii	2: 11,918,588	4721013|F|0-31:C>T	HA001342.1	Protein FATTY ACID EXPORT		6.8		1578
	ii	10: 16,470,683	28877382|F|0-18:G>A	HA009201.1	serine--glyoxylate aminotransferase	3.21631E-09		0.07	18
	ii	8: 16,406,790	54315103|F|0-34:T>A	HA007123.1	clavaminate synthase	1.45889E-07		0.09	69
	i	3: 15,180,935	28880511|F|0-30:A>T	HA002605.1	pectinesterase	0.000364246		0.49	51
damascenone (23696-85-7) *fruity, sweet*	*iii*	2: 2,179,947	54309111|F|0-51:G>A	HA001237.1	Omega-6 Fatty Acid Desaturase		19.6		44
	iii	13: 14,519,918	54312061|F|0-5:G>T	HA011677.1	UDP-glycosyltransferase		5.4		54
	iii	13: 14,519,918	54312061|F|0-5:G>T	HA011678.1	O-glucosyltransferase		5.4		47
	iii	16: 14,654,603	4712209|F|0-29:T>C	HA014200.1	trans-2-enoyl-CoA reductase		8.5		20

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
	i	13: 11,358,488	4715691|F|0-41:T>A	HA011430.1	serine/threonine-protein kinase	0.000687554		0.03	111
	iii	2: 15,050,364	4709026|F|0-57:T>C	HA001486.1	(R,S)-reticuline 7-O-methyltransferase		7.0		17
	iii	3: 3,327,295	54315846|F|0-37:A>G	HA002389.1	bifunctional L-3-cyanoalanine synthase/cysteine synthase		5.9		171
	iii	3: 16,855,923	54314322|F|0-13:T>C	HA002757.1	peroxidase		10.8		45
	iii	4: 3,069,736	4709375|F|0-7:G>T	HA003546.1	Glutathione transferase		8.5		3
	iii	12: 17,327,123	28883917|F|0-15:T>C	HA011197.1	benzyl alcohol O-benzoyltransferase		5.1		1046
3-methyl-1-butanol (123-51-3) *strong, alcoholic smell with a banana oil or hot alcohol-like flavour*	*iii*	23: 717,632	4718475|F|0-18:A>G	HA018436.1	histone-lysine N-methyltransferase		10.2		4
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018768.1	Aldo-keto reductases		6.9		46
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018769.1	Aldo-keto reductases	1.84E-08	6.9		43
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018770.1	Aldo-keto reductases	1.84E-08	6.9		40
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018771.1	Aldo-keto reductases	1.84E-08	6.9		37
	iii	23: 11,413,316	4712239|F|0-42:G>A	HA018773.1	Aldo-keto reductases	1.84E-08	6.9		32
	iii	23: 11,724,983	4713357|F|0-60:T>C	HA018773.1	aldo-keto reductase		5.1		280
	iii	1: 272,681	4717915|F|0-47:T>G	HA000018.1	Oxidoreductase		5.0		101
Octanal (124-13-0) *strong, fruity, and orange-like aroma*	*iii*	5: 15,658,178	28879428|F|0-39:A>G	HA004653.1	arabinosyltransferase		6.5		9
	iii	23: 694,898	4716760|F|0-31:G>C	HA018436.1	histone-lysine N-methyltransferase		4.3		26
	iii	2: 15,981,582	4718655|F|0-15:C>G	HA001588.1	ubiquitin carboxyl-terminal hydrolase		4.8		42
methyl octanoate (111-11-5) *pleasant, fruity aroma with hints of citrus and wine*	*iii*	19: 1,800,357	28877433|F|0-16:A>G	HA016031.1	Acyl-CoA Synthetase		4.5		145
	iii	25: 8,959,706	28876644|F|0-5:A>G	HA019724.1	S-Adenosylmethionine Synthase (SAM Synthase)		4.6		32
	iii	2: 15,461,320	4714620|F|0-30:A>G	HA001526.1	serine/threonine-protein kinase		12.8		26
methyl hexanoate (106-70-7) *pleasant, fruity aroma, often described as reminiscent of pineapple and/or cheese*	*iii*	4: 19,352,236	4712947|F|0-18:C>T	HA004203.1	GDSL Esterase/Lipase		4.3		111
	iii	4: 19,352,236	4712947|F|0-18:C>T	HA004209.1	Acetate/Butyrate--CoA Ligase		4.3		161
	iii	15: 12,585,826	4709286|F|0-65:A>C	HA004548.1	NADPH:quinone oxidoreductase		4.9		446
ethyl propionate (105-37-3) *fruity, with notes of pineapple, grapes, and tropical fruit, along with a hint of rum and butterscotch*	*iii*	1: 1,776,844	4717468|F|0-64:C>T	HA000166.1	S-Acyltransferase		5.9		32
	iii	1: 1,776,844	4717468|F|0-64:C>T	HA000177.1	GDSL Esterase/Lipase		5.9		55
	iii	4: 19,273,848	54315271|F|0-15:A>G	HA004203.1	GDSL Esterase/Lipase		19.3		190

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
	iii	5: 5,696,645	54307556|F|0-12:T>C	HA004524.1	Mevalonate Kinase		7.0		432
	iii	5: 15,762,268	4717806|F|0-21:A>G	HA004653.1	arabinosyltransferase		5.3		113
	iii	8: 16,187,249	54311855|F|0-64:G>T	HA007062.1	Acetyltransferase (Alcohol Acyltransferase - AAT)		9.9		248
	iii	16: 12,952,360	28880797|F|0-11:G>A	HA013967.1	GDSL Esterase/Lipase (GELP)		7.5		32
	iii	16: 12,952,360	28880797|F|0-11:G>A	HA013969.1	Acyl-Coenzyme A Oxidase (ACOX)		7.5		44
	iii	21: 13,123,023	54308869|F|0-9:G>A	HA017622.1	Acetyl-CoA Carboxylase (ACC)		15.1		70
	iii	21: 13,123,023	54308869|F|0-9:G>A	HA017597.1	Alcohol Dehydrogenase (ADH)		15.1		167
	iii	5: 15,189,973	28877549|F|0-16:C>T	HA004615.1	S-Acyltransferase		8.1		189
	iii	5: 15,189,973	28877549|F|0-16:C>T	HA004618.1	S-Acyltransferase		8.1		131
ethyl trans-3-hexenoate (2396-83-0) *sour, green, and slightly fruity*	*iii*	6: 2,218,622	28877005|F|0-31:C>A	HA005189.1	S-Acyltransferase		4.1		142
	iii	6: 14,994,470	100136059|F|0-18:T>C	HA005398.1	histone-lysine N-methyltransferase		18.3		47
	iii	10: 10,517,834	54311942|F|0-13:G>A	HA008661.1	3-oxoacyl-(acyl-carrier-protein) synthase		5.2		8.3
	iii	10: 13,481,227	28878804|F|0-26:A>G	HA008810.1	carboxylesterase		10.7		30

Table D2: GWAS results of FarmCPU (*i*), BLINK (*ii*), and 3VMrMLM (*iii*) using HB type

Phenotype (VOC) (Cas No.) *aroma quality*	Program	Chr: Position	Marker	Gene ID	Proposed candidate	P value	LOD score	MAF	Distance (Kb)
2-methyl butyl acetate (624-41-9) *Fermented, sweet, balsamic*	*iii*	4: 4,037,597	4713780|F|0-11:T>C	HB003593.1	CDPK-related kinase		8.4		25
	ii	4: 18,299,631	54307313|F|0-44:G>A	HB004054.1	Acyl carrier protein 1, chloroplastic	9.15E-07		0.26	15
2,5-dimethyl-4-methoxy-3(2H)-furanone [DHMF] (4077-47-8) *caramel, roasty, sweet*	*i, ii*	3: 4,041,148	4716516|F|0-31:A>T	HB002416.1	UDP-glycosyltransferase 92A1	5.56E-15		0.09	1059
	i	19: 2,932,946	4715047|F|0-55:A>G	HB016082.1	beta-fructofuranosidase	2.12E-09		0.42	On
	i	22: 13,342,667	4710633|F|0-14:G>A	HB018291.1	RNA 2'-O-methyltransferase	2.64E-11		0.18	102
α- terpineol (98-55-5) *floral, lilac*	*i*	11: 1,214,885	4718619|F|0-32:A>G	HB009424.1	Acyl-coenzyme A	1.95E-07		0.43	28
	i	25: 9,923,284	4712117|F|0-51:C>G	HB019874.1	GDSL esterase/lipase	2.14E-07		0.14	1
phenylacetaldehyde (122-78-1) *floral, sweet*	*i, ii*	1: 19,045,190	4717175|F|0-67:C>T	HB000836.1	Phytoene synthase	3.79E-12		0.05	46
	i, ii	4: 17,850,096	28879439|F|0-31:C>G	HB003988.1	Peroxidase	8.21E-19		0.04	30

	i, ii	5: 11,104,966	4719032|F|0-64:C>T	HB004529.1	NADPH:quinone oxidoreductase	4.05E-24		0.05	111
	i, ii	5: 8,592,876	4709277|F|0-5:G>T	HB004507.1	26S protease regulatory subunit	2.00E-19		0.05	392
	i, ii	5: 2,765,847	54307303|F|0-53:T>G	HB004477.1	aminotransferase TAT2 isoform	9.37E-14		0.05	35
	i, ii	10: 15,419,548	28883534|F|0-36:A>G	HB009045.1	ketoacyl-CoA synthase	3.38E-12		0.05	42
	i, ii	13: 9,610,260	54313654|F|0-20:G>A	HB011344.1	serine/threonine protein phosphatase	3.67E-12		0.03	87
	i, ii	13: 9,747,611	4711667|F|0-52:C>T	HB011344.1	serine/threonine protein phosphatase	3.67E-12		0.03	224
	i, ii	13: 9,014,840	4710543|F|0-53:A>T	HB011344.1	serine/threonine protein phosphatase	6.50E-23		0.03	508
	i, ii	13: 7,324,299	4709574|F|0-26:C>G	HB011323.1	2-hydroxyacyl-CoA lyase	2.80E-16		0.04	1
	i	17: 10,997,267	4710933|F|0-68:A>G	HB014614.1	sinapine esterase	3.35E-26		0.07	54
	i	17: 11,983,407	4713761|F|0-47:C>T	HB014733.1	serine/threonine-protein kinase	6.14E-13		0.08	9
methyl isovalerate (556-24-1) *fruity, apple-like*	*i*	4: 18,184,568	54308383|F|0-39:T>A	HB004031.1	glucan endo-1,3-beta-glucosidase	1.99E-09		0.05	42
	i	19: 12,704,557	28883216|F|0-16:A>G	HB016205.1	leucine aminopeptidase	8.10E-08		0.45	87
methyl isobutyrate (547-63-7) *fruity, sweet*	*i, ii*	4: 18,074,935	4716749|F|0-38:A>G	HB004019.1	Acyl carrier protein 2, mitochondrial	2.80E-11		0.04	24
	i	21: 11,421,883	28881823|F|0-9:C>G	HB017413.1	amino-acid acetyltransferase NAGS1	6.58E-07		0.35	137
	i	2: 16,889,923	4709220|F|0-68:A>C	HB001795.1	GDSL esterase/lipase	6.47E-08		0.46	28
	iii	9: 1,783,600	28874553|F|0-62:T>C	HB007473.1	ubiquitin-protein ligase		58.8		151
methyl butyrate (623-42-7) *fruity, sweet*	*i, ii*	6: 14,257,404	54316670|F|0-52:G>A	HB005458.1	ketoacyl-CoA synthase	2.74E-17		0.08	117
	i, ii	6: 14,268,607	28877336|F|0-41:G>C	HB005458.1	ketoacyl-CoA synthase	5.38E-16		0.07	129
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	5.59E-08		0.02	13
methyl-3-methyl thio propionate (13532-18-8) *meaty, onion-like*	*ii*	10: 162,816	4712632|F|0-48:A>G	HB008389.1	diacylglycerol kinase	1.93E-07		0.23	50
	iii	1: 19,658,351	28878122|F|0-18:A>G	HB000933.1	serine/threonine-protein kinase		12.4		3
methyl 2-methyl butyrate (868-57-5) *pungenet, fruity*	*i*	6: 14,257,404	54316670|F|0-52:G>A	HB005458.1	ketoacyl-CoA synthase	1.86E-07		0.08	117
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	2.86E-08		0.02	13
	i	18: 634,653	4717310|F|0-15:C>T	HB015175.1	serine/threonine-protein kinase	2.85E-07		0.06	26
isobutyl acetate (110-19-0) *fermented, ethereal*	*i*	2: 16,970,097	28876740|F|0-44:A>G	HB001804.1	Pectinesterase	1.72E-07		0.07	1
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	3.89E-09		0.02	13
	i, ii	9: 11,979,751	4713076|F|0-33:T>C	HB007593.1	12-oxophytodienoate reductase	1.41E-13		0.15	26
ethyl octanoate (106-32-1) *banana, pineapple, brandy*	*i*	10: 15,289,777	54308671|F|0-19:C>T	HB009045.1	ketoacyl-CoA synthase	7.86E-08		0.05	42
	iii	2: 3,355,201	4717439|F|0-48:G>A	HB001299.1	Arogenate dehydrogenase 2, chloroplasti		20.3		685
	iii	5: 11,104,966	4719032|F|0-64:C>T	HB004526.1	Acyl-CoA synthetases (ACSs)		9.5		394

	i, ii	10: 16,431,095	28877382|F|0-18:G>A	HB004529.1	NADPH:quinone oxidoreductase	3.49E-09		0.07	108
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	1.92E-20		0.02	13
	i, ii	17: 10,952,834	54313905|F|0-35:A>G	HB011163.1	benzyl alcohol O-benzoyltransferase	2.24E-17		0.06	13
	i, ii	20: 12,112,729	4710127|F|0-38:T>C	HB016925.1	phytoene synthase	3.36E-10		0.09	3
	ii	7: 11,953,447	28882510|F|0-51:A>G	HB006006.1	Dicarboxylate transporter	9.96E-12		0.03	29
ethyl isobutyrate (97-62-1) *fruity, sweet*	*i, ii*	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	9.90E-31		0.02	13
	i, ii	23: 983,724	54313351|F|0-26:A>G	HB018514.1	acyl-coenzyme A	5.88E-10		0.10	108
	i	9: 3,311,157	4718318|F|0-42:A>G	HB007514.1	benzyl alcohol O-benzoyltransferase	5.71E-07		0.46	220
	ii	10: 15,289,777	54308671|F|0-19:C>T	HB009003.1	Pyruvate dehydrogenase	1.82E-08		0.05	200
	ii	10: 15,289,777	54308671|F|0-19:C>T	HB009045.1	ketoacyl-CoA synthase	1.82E-08		0.05	172
	ii	10: 15,289,777	54308671|F|0-19:C>T	HB009048.1	ketoacyl-CoA synthase	1.82E-08		0.05	204
	iii	12: 2,651,004	28877644|F|0-17:G>A	HB010504.1	alkane hydroxylase		10.4		62
ethyl hexanoate (123-66-0) *pineapple, banana, fruity*	*ii*	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	6.05E-11		0.02	13
		16: 11,307,082	28879069|F|0-10:G>A	HB013828.1	glycoprotein 3-alpha-L-fucosyltransferase	1.88E-07		0.48	39
	i, ii	19: 12,307,894	4724689|F|0-16:C>A	HB016191.1	alpha-humulene synthase	3.77E-10		0.42	114
	ii	23: 10,353,653	28873541|F|0-32:G>A	HB018782.1	adenylyltransferase and sulfurtransferase	8.61E-08		0.10	80
	i	24: 13,009,295	4727640|F|0-46:A>T	HB019392.1	O-acyltransferase WSD1-like	3.11E-07		0.23	149
	i	25: 8,555,516	4710550|F|0-37:A>G	HB019725.1	Dihydrolipoyl dehydrogenase	4.09E-08		0.09	2
	i	25: 8,555,516	4710550|F|0-37:A>G	HB019705.1	acetyltransferase	4.09E-08		0.09	318
	ii	2: 13,002,960	28877263|F|0-11:T>G	HB001383.1	acyl-coenzyme A oxidase 3, peroxisomal	3.84E-19		0.04	1085
	ii	2: 13,002,960	28877263|F|0-11:T>G	HB001432.1	Fatty-acid-binding protein	3.84E-19		0.04	153
	ii	2: 14,094,476	28882888|F|0-20:C>T	HB001487.1	O-methyltransferase	9.11E-13		0.10	18
	ii	2: 14,094,476	28882888|F|0-20:C>T	HB001498.1	N-alpha-acetyltransferase	9.11E-13		0.10	116
	ii	5: 15,503,480	54307338|F|0-48:T>G	HB004686.1	serine/threonine-protein kinase	3.87E-42		0.05	35
ethyl decanoate (110-38-3) *fruity, sweet, and slightly oily aroma*	*ii*	11: 15,196,158	4714020|F|0-11:C>T	HB010103.1	Allene oxide synthase	5.33E-16		0.05	40
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	6.51E-21		0.02	13
	ii	12: 13,649,084	28879915|F|0-61:C>T	HB010715.1	dihydrodipicolinate reductase	4.02E-12		0.11	6
	iii	6: 14,175,878	54315386|F|0-20:G>T	HB005458.1	ketoacyl-CoA synthase		26.3		36
	iii	7: 897,827	54316213|F|0-68:C>T	HB005885.1	3,4-dihydroxy-2-butanone kinase		48.0		4
	iii	10: 15,289,777	54308671|F|0-19:C>T	HB009041.1	GDSL esterase/lipase		26.6		108

	i, ii	13: 4,555,807	4713661|F|0-45:G>C	HB011314.1	serine/threonine-protein kinase	1.61E-42		0.04	190
	i, ii	13: 11,936,264	4715691|F|0-41:T>A	HB011409.1	serine/threonine-protein kinase	2.64E-41		0.03	100
	i, ii	16: 10,200,012	28874077|F|0-32:T>C	HB013732.1	glutamate-1-semialdehyde 2,1-aminomutase	8.60E-12		0.02	68
	ii	17: 10,952,834	54313905|F|0-35:A>G	HB014614.1	sinapine esterase	1.73E-16		0.06	9
	i, ii	18: 10,123,887	4709720|F|0-11:C>T	HB015301.1	Haloacid dehalogenas	2.97E-18		0.03	64
	i, ii	18: 313,107	4718613|F|0-7:C>T	HB015146.1	ATP synthase	4.01E-13		0.04	34
	ii	22: 10,385,680	28880312|F|0-35:C>G	HB018020.1	glucuronosyltransferase	1.16E-12		0.04	9
	ii	3: 842,018	4711324|F|0-40:T>G	HB002184.1	long-chain-alcohol O-fatty-acyltransferase	7.85E-07		0.30	289
	ii	3: 842,018	4711324|F|0-40:T>G	HB002237.1	aldo-keto reductase	7.85E-07		0.30	162
ethyl butyrate (105-54-4) *fruity*	*i, ii*	10: 3,275,185	28879330|F|0-65:T>C	HB008577.1	peroxidase	5.94E-12		0.26	226
	i, ii	10: 10,517,834	54311942|F|0-13:G>A	HB008649.1	3-oxoacyl-(acyl-carrier-protein) synthase	7.47E-12		0.34	102
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	2.42E-14		0.02	13
	i	4: 18,020,516	28873732|F|0-64:T>C	HB004034.1	S-formylglutathione hydrolase	1.98E-07		0.03	149
ethyl-3-methylthio propinoate (13327-56-5) *meaty, onion, pineapple*	*i*	4: 18,020,516	28873732|F|0-64:T>C	HB004019.1	Acyl carrier protein 2, mitochondrial	1.98E-07		0.03	30
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	2.93E-10		0.02	13
	i	16: 12,789,419	28873582|F|0-19:T>C	HB013961.1	long chain acyl-CoA synthetase	2.19E-08		0.20	200
	i, ii	12: 17,723,093	4726102|F|0-20:G>C	HB011163.1	benzyl alcohol O-benzoyltransferase	7.24E-15		0.02	13
	iii	4: 19,273,848	54315271|F|0-15:A>G	HB004191.1	Nicotianamine synthase		12.9		3
	iii	7: 2,167,403	4728040|F|0-12:A>T	HB005937.1	leucoanthocyanidin reductase		21.1		10
ethyl-2-methyl butyrate (7452-79-1) *apple, pineapple, fruity*	*iii*	20: 11,106,274	54307747|F|0-39:A>G	HB016777.1	Acyl-CoA		13.1		183
	iii	23: 1,274,379	4714737|F|0-61:T>C	HB018532.1	alcohol dehydrogenase		14.8		3
	iii	24: 12,767,814	54307967|F|0-5:T>C	HB019331.1	Ethylene-responsive transcription factor		8.5		112
	iii	25: 744,804	4714342|F|0-46:C>T	HB019593.1	serine/threonine-protein phosphatase		19.3		164
decanal (112-31-2) *sweet, aldehydic, fresh, orange, waxy, and floral*	*i, ii*	10: 16,431,095	28877382|F|0-18:G>A	HB009179.1	carboxyl-terminal-processing peptidase	3.28E-10		0.07	11
damascenone (23696-85-7) *fruity, sweet*	*iii*	2: 16,442,612	54314329|F|0-55:T>C	HB001731.1	amino acid transporter		17.1		1
	iii	3: 14,566,765	28883478|F|0-14:T>C	HB002569.1	(+)-neomenthol dehydrogenase		5.7		25
octanal (124-13-0) *strong, fruity, and orange-like aroma*	*iii*	5: 16,531,874	28877274|F|0-44:T>C	HB004799.1	kinesin-like protein		4.4		2
	iii	7: 16,531,874	28877274|F|0-44:T>C	HB006425.1	ATP-dependent 6-phosphofructokinase		7.1		8
	iii	10: 15,419,548	28883534|F|0-36:A>G	HB009041.1	GDSL esterase/lipase		7.7		22

ethyl propionate (105-37-3) *fruity, with notes of pineapple, grapes, and tropical fruit, along with a hint of rum and butterscotch*	*iii*	9: 14,428,873	4726550|F|0-48:A>T	HB007752.1	Histidine protein methyltransferase	4.4	13
ethyl trans-3-hexenoate (2396-83-0) *sour, green, and slightly fruity*	*iii*	13: 15,024,837	4722213|F|0-14:A>G	HB011657.1	Polynucleotide 3'-phosphatas	7.1	27
	iii	11: 14,640,813	4718382|F|0-26:G>A	HB010018.1	dihydroceramide fatty acyl 2-hydroxylase	4.0	69

Table D3: Check-All-That-Apply (CATA) questionnaire table for aroma attributes

aroma attributes								
tropical fruit	cucumber	coconut	sweet / honey note	fermented	floral	other	no aroma	other
0=☐ 1=☐	0=☐ 1=☐	0=☐ 1=☐	0=☐ 1=☐	0=☐ 1=☐	0=☐ 1=☐	0=☐ 1=☐	0=☐ 1=☐	Explanation

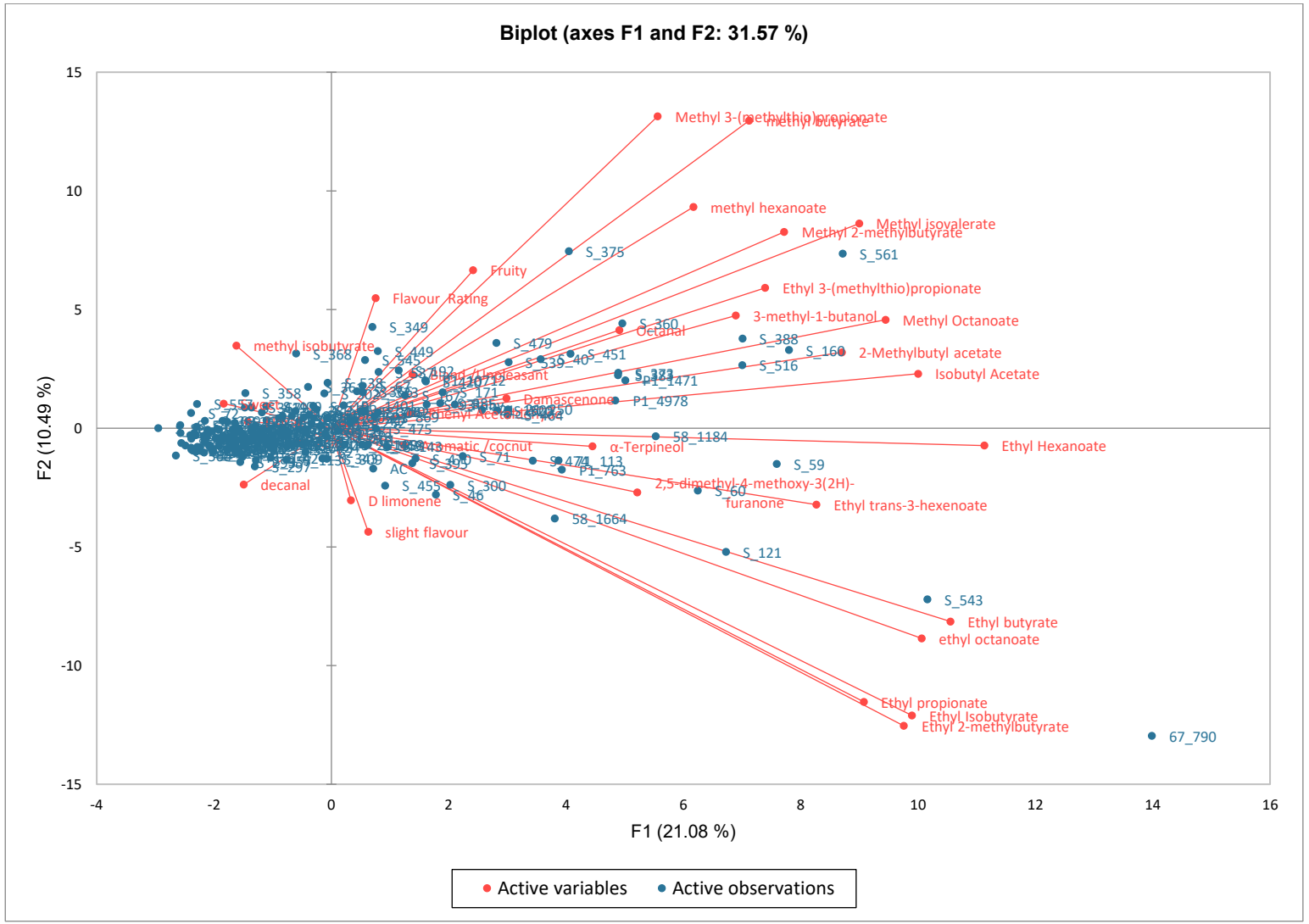


Figure D1: Genetic variation of 2022 samples PCA without non-volatiles and colour values

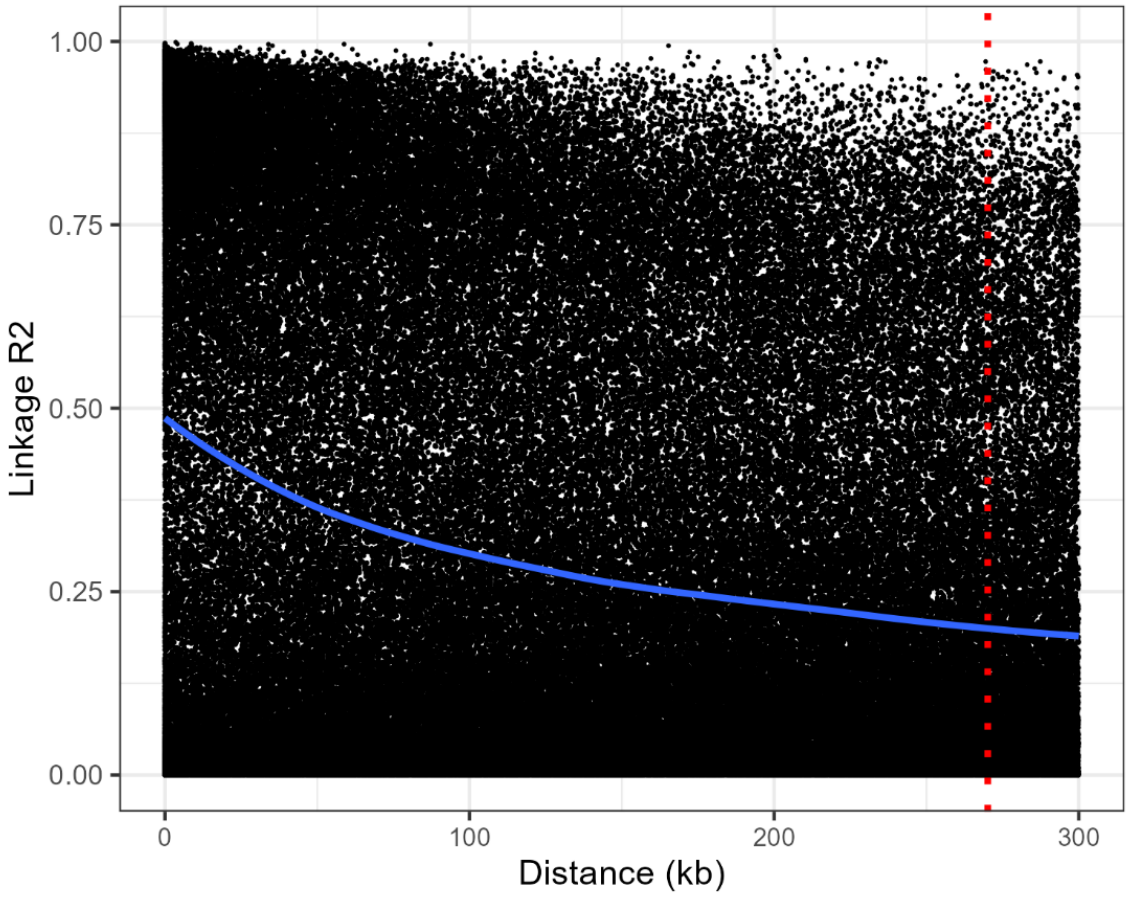


Figure D2: Linkage disequilibrium (LoessCurve_plot_F180v4HA_25chromos) plot