Reducing Food Loss and Waste from Farm to Fork with IR Spectroscopy

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This dissertation is submitted for the degree of Doctor of Philosophy

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Lancaster Environment Centre

Dedicated to my beloved Mother and Brother
Helena Christina Burke and Thomas Alexander Burke

And to my recently departed dear friend
Rowan Bonney

Gone away, but never forgotten.

“To surrender to futility is to deprive yourself of wonder. So you might as well give it a go anyway”

– Joan Hatfield, New World Podcast

“All through my life I've had this strange unaccountable feeling that something was going on in the world, something big, even sinister, and no one would tell me what it was.”

— Douglas Adams, The Hitchhiker's Guide to the Galaxy

Declaration

This thesis has not been submitted in support of an application for another degree at this or any other university. It is the result of my own work and includes nothing that is the outcome of work done in collaboration except where specifically indicated. Many of the ideas in this thesis were the product of discussion with my supervisor Professor Martin McAinsh, Dr Mike Roberts, and Professor Francis L Martin.

Excerpts of this thesis have been published in the following conference manuscripts and academic publications.

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Abstract

Food loss and waste is an issue that is often misunderstood and to many is entirely unknown. Food loss and waste have unprecedented impacts on our economy, and society and are fundamentally an environmental disaster. Important resources go to waste along with our food and the inappropriate disposal contributes to global greenhouse gas emissions by around 10%. With a changing climate making it harder to produce food for a growing population, it is more important than ever, that food loss and waste are significantly reduced. Fruit and vegetables are the most wasted food products due to their high perishability. This research explores one avenue for addressing food loss and waste by using infrared spectroscopy as a method for detecting molecular and biochemical processes involved in fruit and vegetable degradation and subsequent spoilage. Attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy and near-infrared (NIR) spectroscopy are used to enhance our understanding of the biochemical processes occurring in post-harvest fruit stored in different temperature environments. Biochemical markers that may have important applications within the food supply chain have been described. Storage temperature conditions have shown notable effects on the biochemical signatures further supporting the applied use of post-harvest temperature control for shelf-life extension. Contributing factors to food waste include the fraudulent misrepresentation of fruit origins and farming practices, IR spectroscopy has been investigated as a method for accurate classification of these factors. Developmental processes in tomato plants have been analysed using near-infrared spectroscopy to enhance our understanding of the biochemical processes involved. Spectroscopy was paired with powerful analytical chemometric analysis to provide data exploration, biomarker identification, and classification models. These approaches provide for high accuracy results in classifications and suggest suitability for use in an applied setting for detection and reducing food loss and waste in the supply chain.

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Upon starting this project, I was in the wake of the devastating bereavement of my brother. Without the support I received, both from home, and from the many people in Lancaster, you would not be reading this acknowledgments section today. Thank you to everyone who has helped me get here, there are too many names to mention, but I will always be grateful.

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SDG – Sustainable Development Goals

FLW - Food Loss and Waste

FAO- Food and Agriculture Organisation

FSA – Food Standards Agency

DNA – Deoxyribonucleic acid

ATP - Adenine Triphosphate

GHG - Greenhouse Gas

WRAP- Waste and Resources Action Plan

MAP – Modified Atmosphere Packaging

IR – Infrared

NIR – Near Infrared

MIR – Mid Infrared

ATR-FTIR – Attenuated Total Reflectance Fourier Transform Infrared

PCA – Principal Component Analysis

PC – Principal Component

LD – Linear Discriminant

LDA- Linear Discriminant Analysis

SVM- Support Vector Machine

DPH – Days Post Harvest

VOC – Volatile Organic Compounds

PCA-LDA – Principal Component Analysis Linear Discriminant Analysis

LDL – Low-Density Lipoprotein

LVP – Leaves Vegetation Phase

LPH – Leaves Post Harvest

LFP – Leaves Fruiting Phase

BH – Before Harvest

PH – Post Harvest

1. Introduction: Infrared Spectroscopy-Linked Chemometrics: A Novel Approach to Reducing Food Loss and Waste

Achieving global food security is a central aim of the United Nations' Sustainable Development Goals (SDGs) encompassing SDG 2: Zero hunger, SDG 3: Good health and well-being, and SDG 12: Responsible consumption and production. These goals incorporate the global availability of nutritious food, alleviating hunger and promoting good health and well-being. Ensuring sustainable consumption and production patterns are key targets of SDG 12, which calls for a cut to all food loss and waste (FLW) by 50% per capita by 2030 (Fabi and English, 2018.).

1.1 What is Food Loss and Waste?

It is essential to distinguish between food loss and waste, as these concepts are related but represent distinct issues that occur throughout the food system. Typically, food loss refers to the reduction in the quantity of food, both in yield and mass, and its quality, often leading to its discarding (Hoehn et al., 2023). Losses occur before food comes into contact with the consumer, normally during production, post-harvest processing, and distribution, and encompass both the edible and inedible parts (Delgado, Schuster and Torero, 2021). In addition to physically discarded items, food loss also encompasses the concept of lost potential yield. Potential yield may refer to the reduced number of items

or the reduced biomass, representative of the gap between the yield produced and what the crop is capable of producing in optimal condition (West et al., 2014). Food waste, (see Figure 1.1) in contrast, refers to the removal of edible food from the food system, occurring post-farmgate; at retail level, in hospitality, and from the consumer household, and often is the result of consumer-associated behaviours (Jeswani, Figueroa-Torres and Azapagic, 2021).

Figure 1.1. UK contributions to food loss and waste at stages in the supply chain (Capgemini, 2023)

These definitions can become slightly muddied when observing a global system, as different organisations differ in detail. The Food and Agriculture Organisation of the United Nations (FAO, 2011) presents a tighter distinction between food loss and waste based on intentions, food losses occur unintentionally and result from systemic issues, and food waste occurs intentionally and due to behavioural issues (FAO, 2019; FAO, 2011). The EU definitions are closely aligned with the FAO, however, the incorporation of food redistribution and waste reduction is a big focus in associated EU policy. The EU acknowledges that food waste occurs at *all* stages of the supply chain (EUR- lex, 2019; Xameerah Malik et al., 2024), as opposed to only occurring post-farmgate. The Waste and Resources Action Programme (WRAP) specifically focused on the UK food system, and defines food waste as the discarding of edible food and inedible parts (Xameerah Malik et al., 2024), this includes anything from across the entire food supply chain that was intended for human consumption at some point (WRAP, 2023).

These definitions are important when recording food loss and waste data within the supply chain, as it affects the focus of food loss and waste reduction policies. The inclusion

or exclusion of important details like the product destination, the inedible parts, motivation, and associated supply chain stages can have profound effects on policy efficacy (Hanson et al., 2016). An example of this is when recording food waste volume regardless of its destination. It drives a focus for the prevention of the waste, reducing over-ordering. Including a 'waste-saving' destination, such as composting in the metric, allows supply chain actors to continue over-ordering while reducing their recorded food waste volume through composting excess stock. The focus can be altered by including inedible food parts in the volume recorded as food waste, a method for reducing volume could be through finding innovative ways to use the inedible parts (Mohamed Yusoff, Godsell and Woolley, 2024), An example of this is the generally considered inedible banana peel that is, in fact, edible and through motivation to reduce food waste, they may be incorporated into recipes.

SDG targets have been set in response to the staggering global food loss and waste statistics. It is estimated that 1/3 of all food globally is lost or wasted, of that, for example in 2022; approximately 1.05 billion tonnes of food were wasted in retail, food service, and households (FAO, 2024.). These staggering figures represent a missed opportunity to feed millions of people affected by hunger every year, coming to around 733 million people globally (FAO, 2024.), and in the UK, 7.2 million, equating to 11% of the population (Brigid Francis-Devine et al., 2024).

1.2 Achieving Food Security is Underpinned by Good Health and Nutrition

The nutritional content of the food we consume is vital to human health, reducing individual occurrences of nutrient deficiencies and diseases, and maintaining the functioning of bodily processes (Espinosa-Salas and Gonzalez-Arias, 2024). Fruit and vegetables are nutrient-rich and important sources of macro- and micronutrients (Iqbal, 2006). Good health is important for wider society and the economy, reducing the burden on health services (Woodward *et al.*, 2000). These elements further necessitate avoiding loss and waste, especially in nutritious fruit and vegetables, as they play such an important role in preserving the health of the population.

Fruit and vegetables, including tomatoes, used in this thesis as an exemplar crop, are important sources of numerous vitamins and minerals. Vitamin C (ascorbic acid) is a powerful antioxidant that reduces oxidative damage, contributes to wound healing, and plays an important role in immune function (Carr and Maggini, 2017). Bone health and blood coagulation is assisted by vitamin K which also possesses anti-inflammatory properties and contributes to lowering cancer incidence (Sadler et al., 2024). Beta carotene, a carotenoid present in tomatoes, is a precursor to vitamin A, which is important in maintaining eye health, immune function, and skin health, and preventing some associated chronic diseases (Eggersdorfer and Wyss, 2018). Lycopene, another important carotenoid, is also a potent antioxidant that is associated with reduced risk of heart disease and certain cancers (Mozos et al., 2018). Small amounts of antioxidant Vitamin E in tomatoes can help protect cell membranes from oxidative stress and damage, as well as contributing to skin health and immune function (Pruteanu et al., 2023). DNA synthesis, cell division and red blood cell formation processes use vitamin B9 (folate) which can be sourced from tomato fruit (Merrell and McMurry, 2024), as well as Biotin and Niacin (B3) which are important for energy production, metabolism and maintaining healthy hair, skin and nails (Dattola et al., 2020). Tomatoes are a source of Riboflavin, (vitamin B2) which is involved in cellular metabolism, energy production and antioxidant activity (Mahabadi et al., 2024). Vitamin B1, and thiamine plays an important role in carbohydrate metabolism, and nerve function and can aid rest, repair, and restoration through healthy sleep (Bozic and Lavrnja, 2023).

Minerals including magnesium, phosphorous, potassium and calcium are present in tomato fruit. Magnesium is an essential mineral involved in over 300 enzymatic reactions in the human body that is also important in blood sugar regulation (Pelczyńska et al., 2022). Potassium helps reduce blood pressure, magnesium and potassium influence muscle function and may reduce risk of stroke and cardiovascular disease (Godswill et al., 2020). Adenosine triphosphate (ATP), which is a crucial to essential cellular processes, contains three phosphate groups and requires phosphorous presence for its synthesis (Dunn and Grider, 2024). Phosphorous is also important for DNA synthesis and bone health (Penido and Alon, 2012). Calcium is a vital mineral for human health including bone health, muscle function and nerve transmission. Although tomatoes aren't

the most significant source, they can provide small levels of calcium (Yu and Sharma, 2024).

The nutritional content of tomatoes and other fruit and vegetables is influenced by several factors; the variety and their growing conditions will influence the plant and fruit health and dictate nutritional quality. After harvest, the nutritional content can continue to be affected through environmental influences, chemical processes, and microbial interaction (Collins et al., 2022), and these interactions must be well understood. Maintaining the optimal nutritional content and extending the quality shelf life is reliant on understanding the pre-harvest and post-harvest processes.

1.3 Climate Change: A Growing Threat to Food Security

Climate change is an increasing threat to food security making this challenge more difficult due to agricultural systems being disrupted, reducing crop yields, and the destabilisation of food production ecosystems (Kumar *et al.*, 2022, p. 4; Schmitt *et al.*, 2022). Extreme weather events are becoming more frequent, such as flooding and severe storms, precipitation is becoming more unpredictable, and temperature fluctuations are becoming more intense (Bolan *et al.*, 2024). Numerous approaches are being considered and implemented in efforts to mitigate some environmental pressures to ensure successful crops, often through the application of chemical fertilisers and pesticides (Dudley *et al.*, 2017). These practices often exacerbate the problem, weakening critical ecosystems and crucially negating sustainable agriculture (Ahmad *et al.*, 2024; Pandian *et al.*, 2024).

A successful food system relies on soil fertility (M. Tahat *et al.*, 2020), pollination, and pest regulation (van der Sluijs and Vaage, 2016) providing resilience to environmental pressures, exacerbated by climate change. Soil health is determined by a rich community of invertebrates such as nematodes and annelids and a diversity of microbes, all with fundamental roles in providing ecosystem services. Nutrient uptake, essential in crop plants is facilitated by soil organisms, as well as nutrient cycling and the enhancement of soil structure (Yadav *et al.*, 2021). Pollinator insects and birds, in addition to a diversity of non-crop plants, further contribute to the production of nutrient-rich crops and aid in resilience against pests (Laha et al., 2022; Maggi and Pardo, 2024). Biodiversity has been

lost due to mass food production through the conversion of land for agricultural use (Cabernard, Pfister and Hellweg, 2024), and monoculture farming (Suarez and Gwozdz, 2023), and encompasses the decline of a complex biological network. Biodiversity rejuvenation and ecosystem regeneration have therefore become a focus for conservationists and ecologists as a mitigation effort to restore the systems that food production relies on necessitating the development, adoption, and prioritisation of sustainable agricultural practices if food security is to be achieved. System-based approaches that incorporate the restoration of biodiversity, in addition to the mitigation of climate is critical for the wider environmental challenge of maintaining viable and stable food production (Thrupp, 2000). However, to further alleviate the rising pressures on food production, food losses, and waste must be minimised.

1.4 Food Loss and Waste (FLW) Cause Unprecedented Environmental Damage

Food production requires resources including land, water, energy, and nutrients (Ritchie, Rosado and Roser, 2022). Agricultural land use is a significant contributor to habitat loss and biodiversity decline (Benton et al., 2021.). Additionally, it contributes to fragmentation, deforestation, degrades the land, and reduces ecosystem functionality (Ortiz *et al.*, 2021). Furthermore, these land-associated impacts are further exacerbated as more land is converted to replace wasted food. The effects of food production systems on ecosystem functioning also extend to aquatic environments. For example, overfishing threatens fish stocks and the overall health of the marine environment (Emanuelsson, 2012). Water is also an important resource for agricultural practice which is a major consumer of freshwater. Water scarcity is exacerbated when food is lost and wasted due to the substantial volume of water required to produce food that is ultimately wasted along with the food that was produced using its provision (Marston *et al.*, 2021).

The release of greenhouse gas (GHG) emissions is one of the most significant impacts of FLW (Cattaneo, et al., 2021), both from the production and disposal of food waste. In production, processing and transportation, there can be significant GHG release contributing to climate change (Carlsson-Kanyama and González, 2009). This is especially more exaggerated when produce is imported, with imported food accounting

for 40% of all food in the UK ("UK Food Security Index 2024," 2024.). When food waste decomposes in landfills, due to the lack of oxygen, the anaerobic decomposition generates by-product methane, a potent GHG (Mundra and Lockley, 2024). The global warming potential of methane is around 25 times more potent than carbon dioxide, making it important concerning climate change with 8-10% of all GHG globally attributed to FLW (Smith and Wigley, 2000).

1.5 The Price of Waste: How Food Loss and Waste Impact our Economy

FLW can cause economic losses at every stage of the supply chain. These losses can relate to financial investments in growing resources, labour costs, and transport for food that ultimately is never eaten (Ishangulyyev *et al.,* 2019). Businesses and individuals are affected financially, however there are also implications to the wider economy including food price increases as companies may have to recoup their wasted costs and associated reduction in profitability (Pimentel et al., 2022). Excluding farm-associated losses, in the UK in 2021, £21.8 billion worth of food waste (edible parts) was incurred (Xameerah Malik *et al.*, 2024): manufacturing accounted for £0.85 billion, retail accounted for £0.74 billion, hospitality and food service £3.21 billion, and households accounted for £17 billion (FAO, 2024.). In the UK, at the consumer level, an average of £250 of food was wasted per person per year, or an average household of 2.4 people wasted £600, families of four wasted £1000 of food each year. (WRAP, 2023.). A more nuanced and detailed understanding of food waste variability across the UK, explained by demographic, local services and infrastructure, and other contributing factors, is key information that can be used to apply targeted approaches for reduction. The reduction throughout the entire food chain would ease the associated financial burden, help alleviate pressure on businesses and consumers, and maintain consistency of associated costs within the supply chain and food prices at the market level (Xameerah Malik *et al.*, 2024).

1.6 Food Loss and Waste: A Burden to Society

The social impacts of food loss and waste are significant, particularly in poor and vulnerable populations where the loss of resources can exacerbate the effects of food

insecurity and perpetuate social inequalities and disparities in food access (Papargyropoulou *et al.*, 2022). While currently 1.3 billion tonnes of food is wasted every year, 800 million people globally go hungry (FAO, 2023). Food loss and waste contributes to food price increases, making food less accessible and affordable to vulnerable people and populations, widening the inequality gap (World Bank, 2025). In recent years, many western countries, including the United Kingdom, have also been grappling with the effects of FLW due to economic turmoil, dubbed 'the cost of living crisis'. This has been the result of compiled factors including the consequences of the Covid-19 pandemic, increased inflation and supply chain disruptions (Gupta *et al.*, 2023). There has been a rise in the cost of essential goods and services including housing, energy, transportation and food. These rises have been the result of inflation and measures put in place for businesses to mitigate inflationary impacts. The resultant price increases have profoundly affected most of the population, more people having to squeeze household budgets and making significant sacrifices with many people struggling or unable to afford basic necessities. Consequently, the less disposable income that the population have access to, the less money that can enter the wider economy causing economic stagnation (*Cost of living crisis*, 2022).

One of the most significant factors of the cost of living crisis has been food poverty referring to individual or household's inability to not only access an adequate calorie requirement from food, but sufficient dietary nutrition due to financial constraints (Stone *et al.*, 2024). There is growing concern surrounding the growing food poverty in the UK with the increasing use of charity funded food banks. In 2023/2024, food banks in the Trusell Trust network distributed 3.12 million emergency food parcels, an increase of 94% from five years prior (Trussell Trust, 2024). There are serious impacts of food poverty on health and well-being. Lack of consumption of healthy, nutritious food can lead to malnutrition and subsequently can lead to diet-related diseases (Francis-Devine et al., 2024). Children living in food poverty in food-insecure homes become at risk of developmental problems both physically and mentally affecting educational attainment and they become at risk of long term health problems (Belsky *et al.*, 2010). Reducing food loss and waste requires a multifaceted approach and is essential to help reduce food poverty in the UK, and the wider global population. Reducing food losses will ultimately help to make more food available, alleviate price increases associated with recouping

financial losses from food losses, stretch food budgets further, reducing the financial strain on households and ensure more food reaches those in need (Xameerah Malik *et al.*, 2024). Further focus on reducing consumer-related wastage, for example through extending product shelf life can improve calorie and nutrient availability for the consumer. Policy and community initiatives are both central to such a multifaceted approach to reducing FLW. To this end, Government policy requires a greater focus on reducing FLW, tightening supply chains, improving food redistribution networks, promoting food recovery and redistribution programmes, in addition to educating consumers about food waste prevention (Patel *et al.*, 2021).

1.7 From Farm to Fork: Stages of the Food Supply Chain

Food supply chains comprise multiple stages and involve multiple processes through which food must travel before arriving on our plates (Figure 1.1). The UK food system is complex due to the requirement of delivering safe, high quality and enjoyable produce for consumers, in addition to being made up of a web of different companies and government organisations that perform different processes. Geographically this can become convoluted based on the business connections and agreed client contracts. This becomes even more complex when the actors involved are internationally based. At every stage in the supply chain there are factors that could provide reason for food losses or general supply chain disruption (Serdarasan, 2013).

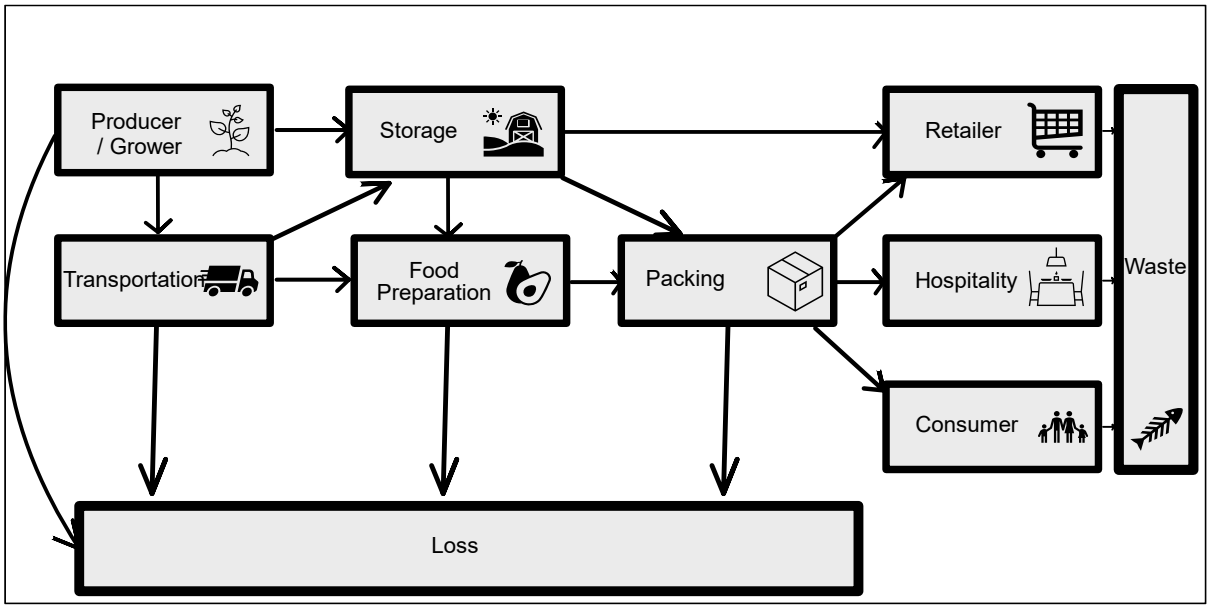

Figure 1.2. Diagram demonstrating the elements that form the supply chain and how they interact

Successful crop production relies on the availability of high-quality seeds that exhibit high gemination rates, vigorous growth, and are disease and impurity-free (Kumar *et al.*, 2023) reaching optimal crop yield and quality, avoiding losses (Prasad, Chauhan and Sripathy, 2017). The conventional production of crops, either destined for human consumption or to be used for animal feed requires a sufficient supply of agrochemicals. These might include fertilisers providing nutrients, pesticides, and herbicides to protect crop plants from diseases and pests. Agrochemicals are heavily regulated to ensure human safety and to reduce damage to the environment, levels of regulation are determined by country, adding to the challenges associated (Ahmad *et al.*, 2024). Disruptions in the supply chain, especially when dealing with international suppliers can provide vulnerability even at these early stages of the food system. Fluctuations in costs of raw materials due to these disruptions can cause the production to be unaffordable and financial losses to be either absorbed by the producer or passed down the supply chain (Katsaliaki et al., 2022). Efficient and working machinery and infrastructure are also a requirement for successful production, the upgrading and regular maintenance of equipment are crucial but also impose financial costs. Environmental stresses, including unpredictable and extreme weather events such as: droughts, floods and heatwaves,

heavily influence production and must be planned for as much as possible (Kumar et al., 2022) .

Raw agricultural products may require processing for the use of becoming primary ingredients, this stage will also involve quality control and subsequent storage. Regulatory standards will apply, associated with food safety and nutrient content dependent on the product destination. For example, for durum wheat to be used in the production of pasta, according to the European Union regulations 2019 for 'Pasta di Gragnano' (Pasta Grain) the minimum nutrient for 100g dry product should be: moisture: not exceeding 12,5 %, energy value 1 486 KJ 350 Kcal, protein 13 g, carbohydrates 73 g, fats 1g, ash max. 0,86 %. (European Union, 2019) Further characteristic regulations apply at later stages to the product made by the initial ingredient, in this case pasta (Russo *et al.*, 2021). Food loss and waste volumes may increase resulting from produce that doesn't meet regulatory standards. Maintaining quality and safety requires standards, which in turn necessitate interventions to prevent the production of substandard products (Food standards agency, 2023). Additionally, methods must be in place to redirect and use any products that haven't met requirements effectively.

Whole, non-ingredient produce may also require preparation or the application of preservation techniques, including freezing, vacuum packing, drying, or tinning. This preservation is applied to ensure food safety and to extend or prolong the product shelf life (Wiley, 1994). The application of product packaging has a number of purposes, as mentioned safety, shelf-life and protection of the product, but important information is placed on packaging related to nutrition, cooking guidelines, ingredients and can also contain information about the origin of the product (Food standards agency, 2023). Packaging is also important to business branding and as a method of selling their products (Klimchuk and Krasovec, 2013). The development of packaging requires design and production, availability of the materials and associated costs. As a result of public awareness in recent years, the considerations for sustainability of packaging are becoming more important to packaging design as sustainability is influencing consumer buying habits (Falguera et al., 2012).

Logistics management is conducted by actors in the supply chain directing and organising the transportation of products. Depending on the extent of specific business capabilities

and how many processes they are able to complete, there may be different amounts of transporting a load will undertake. Transportation may also require different sets of requirements for product preservation, like controlled temperature transportation, or fitting with government or business policies for sustainability. This might include the use of biofuel powered vehicles or choice of transportation methods that are less environmentally damaging, such as avoiding air freight. Management of logistics may have to consider challenges involving weather conditions, availability of transportation, import and export regulations, global events and associated financial costs. Product storage may be required at any stage and at multiple stages in the supply chain. This requires organisation and availability of appropriate facilities. These facilities must be equipped with strategies for inventory management and the adherence to regulatory standards. Associated energy providers and costs may influence these stages (Kamisli Ozturk, 2020).

The sale and consumption of food products happens through retail channels or within hospitality and food service. Both elements involve many processes for products to reach their endpoint. Retail involves effective stock management influenced by consumer demand, market trends, economic factors, and product availability. The food service industry also requires stock management and the assurance of a steady supply of ingredients needed for their menu. Health regulations, safety including the concentration of potential allergens in a product and maintenance of hygiene are all important factors into successful running of a business. These numerous stages are connected by interdependencies on other actors for the successful delivery of food products, this causes susceptibility to disruption and cross-system vulnerability and can cause cascading effects (Serdarasan, 2013).

1.8 Spotting the Weak Links: Key Vulnerabilities in the Food Chain

Vulnerabilities in food supply chains are becoming more prevalent. In recent years the UK has experienced several significant disruptions which may have had knock-on effects impacting FLW. These include Brexit, the global Covid-19 pandemic, and the associated rising costs of inputs. Furthermore, disruptions in transportation and logistics caused by

fuel shortages, strikes and labour shortages and infrastructure failures (Vlajic *et al.*, 2013) can lead to delays in delivery of key items, food products or critical inputs. For example, the global Covid-19 pandemic highlighted the vulnerability of the supply chain to logistical bottlenecks and elevated demand for certain products (Aday and Aday, 2020). Our 'just-in-time' supply chain provides vulnerability, a just-in-case system involving buffer stock would help to mitigate risk of disruptions, however this is more challenging for perishable goods.

Geopolitical tensions and disruption of global trade can heavily impact productivity and the successful execution of food production. Changes in trade policies, for instance Brexit (Hendry *et al.*, 2019), can affect the ability to obtain certain products, whilst tariffs may force companies to change suppliers. This may involve companies making ethical or environmental sacrifices (Kastner *et al.*, 2021), or the introduction of impact costs further down the supply chain. Policies and regulations are consistently evaluated and amended, either at a company level or at the wider governmental level often as a result of technological or scientific evidence (Figure 1.2). These might include health regulations, environmental sustainability or societal improvements. Although actors in the supply chain are considered in these policy changes, severe or sudden changes can cause uncertainty, the adoption of unfamiliar practices that may require additional learning, the acquisition of additional materials or equipment, and additional planning and investment. Economically driven factors can impose pressures on all actors in the supply chain which are often distributed unequally between actors. Inflation and currency value fluctuations impact commodity prices causing volatility and profitability of farming and food production inevitably causing food prices to be affected (Urak and Bilgic, 2023).

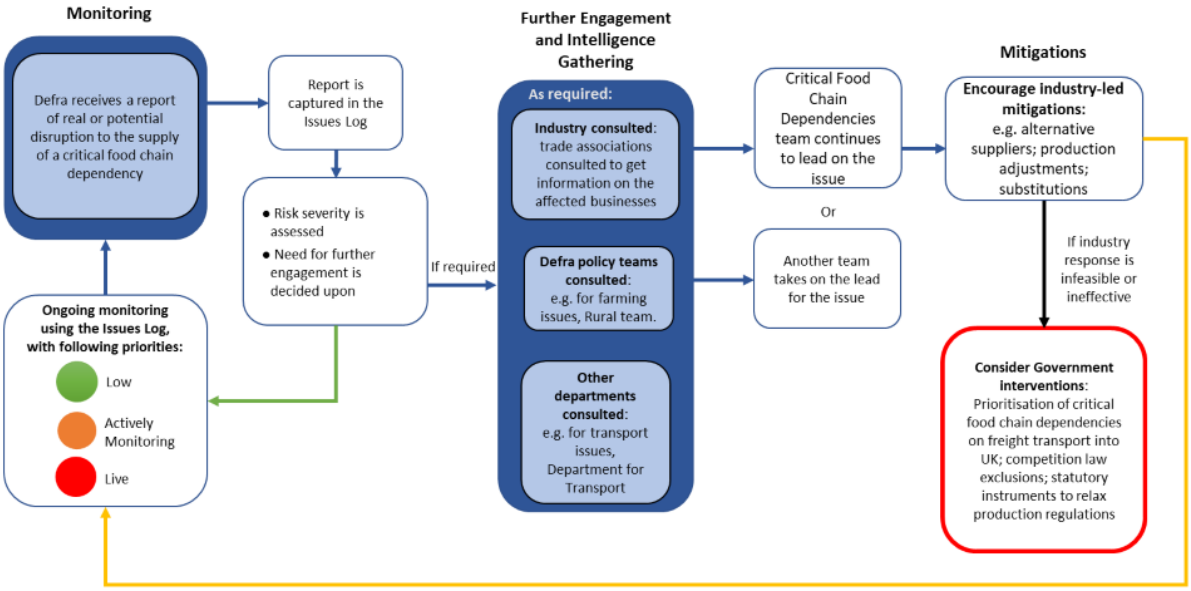

Figure 1.3: Diagram demonstrating how food system policies are devised and monitored (DEFRA, 2021)

1.9 Food Loss and Waste in the Supply Chain

Opportunities for FLW occur at every stage of the supply chain (Figure 3). Potential yield losses can occur at the growers, often in a farm or growing facility, due to reasons including weather extremes affecting crop growth and development (Iizumi and Ramankutty, 2015), diseases and pests (Ishangulyyev et al., 2019) and inappropriate harvesting techniques (Johnson *et al.*, 2019). Post-harvest, losses can arise from inappropriate handling of produce or poor storage conditions (Arah *et al.*, 2016), especially in highly perishable items such as fruits and vegetables. Some produce will be processed ready for retail, which might include trimming of inedible parts and then packaged appropriately. Aside from inefficiencies in processing, packaging defects can contribute to reduced shelf life, increase damage, and hence, enhance losses (Wohner *et al.*, 2019). Transporting produce to its destination, often for retail, requires appropriate management of temperature and handling to avoid damage and losses in transit (Figure 1.3). Upon arrival at retail, losses can occur from inventory mismanagement,

overstocking, and assigned standards associated with aesthetics (Castagna *et al.*, 2021). 70% of food waste is at the consumer level due to over-purchasing, inappropriate storage and preparation practices (WRAP, 2023), and plate waste in the hospitality sector (Dhir *et al.*, 2020).

Consumer buying habits have an important role in dictating the levels of food waste and often influence FLW earlier in the supply chain (Jones-Garcia, Bakalis and Flintham, 2022). Buying habits vary between different global nations. Italy and France are examples of cultures that tend to buy often for immediate use, prioritising quality (colour, flavour, texture, and nutritional content) over shelf-life. In the UK, an extended shelf-life is considered preferable driving the need for varieties that offer longer shelf-life but may lack in qualify characteristics including flavour, texture and aesthetic qualities. The UK's focus for products with higher a shelf-life is often attributed to less frequent food shopping in globally sourced supermarkets over locally sourced markets. These cultural differences may have been shaped through working structure and work-place locality restricting the availability of free time. Buying decisions are also heavily influenced by aesthetic standards which have been determined and perpetuated by retail organisations. Decisions based on aesthetic standards have significant impacts on food loss and waste, not just at the retailer through loss of sale, but at earlier stages in the supply chain due to sub-standard produce being rejected and destroyed.

1.10 Systemic Approaches for Reducing Food Loss and Waste

Reducing food loss and waste is an enormous challenge that requires the application of a variety of methods to succeed. This includes small-scale methods, processes, and technologies that address smaller and specific mechanisms contributing to FLW, however, there is a requirement for large-scale methods for systemic change that help to remove vulnerabilities. Global organisations have established models and frameworks that attempt to address this. The Food and Agriculture Organisation of the United Nations have developed the Food Loss and Waste Framework for global monitoring and applying interventions (Technical Platform on the Measurement and Reduction of Food Loss and Waste | Food and Agriculture Organization of the United Nations, [Accessed 6/7/2025]). Monitoring is achieved through measuring food loss and waste at various stages in the

supply chain which seeks to identify the points where the highest losses occur. Collected data is used to diagnose the causes of loss and waste, so interventions can be designed and implemented. Interventions may be relevant and applied to a range of stakeholders, including governments, industry organisations and public sector bodies.

The Food Recovery Hierarchy was developed by the United States Environmental Protection Agency (EPA) which sets prioritisation of strategies using an inverted pyramid hierarchal structure (US EPA, 2015). This hierarchy is organised as Source Reduction (prevent surplus, Feed Hungry People (redistribute food), Feed Animals, Industrial Uses (bioenergy), Composting, Landfill/Incineration (last resort). This structure aims to promote upstream solutions over downstream treatment.

A significant programme in the UK for food loss and waste reduction is the Waste and Resources Action Programme's Courtauld Commitment 2030 providing a data-driven roadmap serving as a voluntary agreement for food system actors (UK Food and Drink Pact, no date). Multi-stakeholder collaboration involves standardised measurements and transparent, accurate reporting and actions implemented to meet targets. The framework encourages collaborative working, and innovation of processes and technologies like packaging, redistribution and new ways of utilising waste products.

True Cost Accounting (TCA) framework was launched by the UN Environment Programme (UNEP) and the Global Alliance for the Future of Food. Conceptually, it incorporates external factors that are often not considered when measuring food system data, and when developing interventions. TCA is designed to quantify the costs of externalities involved in the production, processing, and consumption of food products. These costs not only incorporate the financial contributions, but additionally, they quantify the environmental and social costs that are often ignored. The aim is to assign a monetary cost used as a proxy to highlight the most expensive products to inform decision-making. Reducing these assigned costs contributes to reducing the climate impact, social impact, including human health, whilst providing a natural deflation of real product pricing, benefitting all stakeholders, including customers in the supply chain. TCA is a complex model requiring comprehensive metrics, transparency and global collaboration to compile the extensive data needed to accurately quantify TCA costs,

raising questions about realistic and feasible implementation. ('The Evaluation Framework', 2018)

Due to the complexity of the global food system, the application and functioning of systemic frameworks are equally complex. There is a requirement for maintaining continuous data collection, stringent participation, policy development is required to adapt to the changing system, and efficacy evaluation is vital for continued optimisation.

1.11 Current Strategies for Reducing Food Loss and Waste

Despite the variety of methods that can aid in reducing FLW in the supply chain, there are limitations and challenges associated with the widespread implementation. This success often depends on a variety of individual factors and contexts including geographical location, infrastructure, and economic factors (Ishangulyyev et al., 2019). Policy support, investment, and food system collaboration are required for the successful and widespread implementation of these methods. There are significant challenges when endeavouring to achieve the optimal reductions in food loss and waste needed to alleviate economic, social, and environmental impacts nationally and globally. Traditional methods and current practices have proven insufficient in effectively tackling these multifaceted issues. There is a need for innovative solutions which includes the development and utilisation of new technologies.

Mitigation strategies aimed towards reducing FLW have been developed and implemented throughout the supply chain. In early stages at the production level in farming and harvesting technological techniques can be used to optimise growing inputs including using satellite imaging (Lee *et al.*, 2010), drone-facilitated monitoring, and soil sensors enabling an advanced precision application of water and fertilisers (Javaid *et al.*, 2023). This can improve yield whilst reducing waste. Crop diversification can reduce the risk of total crop losses from pests, disease or unpredictable fluctuations in the market (Lin, 2011). The implementation of sustainable farming practices with a focus for ecosystem function and rejuvenating biodiversity can enhance crop resilience to environmental stresses and pests (Sarma *et al.*, 2024). Harvesting techniques using machinery designed to reduce damage to crops can also reduce post-harvest losses (Kaur *et al.*, 2023).

Postharvest losses can be further reduced by minimising physical handling and the opportunity for damages. Simplifying the supply chain can help with this, shortening transport distance, using local suppliers, and directly transferring goods to their end destination avoiding unnecessary drop-off points. Consistent and appropriate temperature-controlled transportation and storage can also inhibit spoilage and extend product shelf life (Jedermann *et al.*, 2014). Some products benefit from the application of specialised packaging protecting from pathogen infection and reducing exposure to oxygen, light, and moisture which all promote spoilage processes (Pascall *et al.*, 2022). This includes vacuum packaging or Modified Atmosphere Packaging (MAP) (Alegbeleye *et al.*, 2022). The drying or dehydration of produce can also be used to extend shelf life (Safwa *et al.*, 2023). This is particularly useful for lower-quality produce that is unsuitable for continuation through the supply chain (*FAO*, 2021). The redirection of sub-standard or low-grade produce for repurposing can reduce losses and waste, this could include for use as an ingredient in another product or alternative packaging like canning. Finally, the utilisation of by-products in which the inedible parts are removed in processing and repurposed for animal feed or bioenergy reduces the waste of biomass (Shurson, Chen and Dou, 2024). It is important that interventions with the aim of reducing food loss and waste are evaluated for other impacts. For example, the use of local suppliers reduces the availability of certain foods outside of their season, possibly impacting nutrient accessibility. Additionally, the use of technology to prolong shelf-life might be costly in energy or produce emissions.

Streamlined management can reduce losses through demand forecasting and inventory management (Davis, 2015). Advanced analytics and Artificial intelligence (AI) applications can aid this process by predicting consumer demand helping to reduce overstocking and waste of unsold produce (Bose, 2009). Additionally, dynamic pricing based on consumer demand predictions or products nearing their expiration can incentivise the sale of produce avoiding waste. Clearer food labelling, including shelf-life dates, can provide the consumer with more information about how to appropriately store products to maximise shelf life (Toma, Costa Font and Thompson, 2020). Some UK retailers have trialled the removal the best-before dates on perishable products, including fruit and vegetables, this includes Waitrose & Partners who aim to remove dates on 500 products to align with their pledge to remove food waste at home by 2030

(Spoiler Alert! Best Before dates removed on nearly 500 Waitrose products, [Accessed 2025). This policy aims to encourage customers to rely on their senses to assess quality and freshness, instead of potentially unreliable dates that may be contributing to waste at the consumer level. Research carried out by Love Food Hate Waste informs this policy, focusing on reducing food waste in the supply chain, suggesting that consumer freshness assessment behaviour is improved from the removal of dates, and food waste volume is positively impacted, or reduced (Charlebois, Rankin and Music, 2023). The removal of dates from food products presents the risk of a negative impact on food waste volumes, as supermarkets have less pressure to remove products from the shelves, reducing the consumer's shelf-life and spoiling earlier in the consumer's home. Additionally, consumers may be deterred from buying fresh fruit and vegetables without dates through the mistrust of product freshness. These impacts have the potential to shift food waste along the supply chain instead of reduce it, necessitating internal monitoring to accompany the policy to avoid this shift. Love Food Hate Waste has stipulated that retailers will be monitoring and controlling stock in the same way as before, using internal date codes and only the packaging date label on the packaging is removed, negating this shift (WRAP, 2022). If all else fails, surplus food may be donated to charities or food banks ensuring produce is not discarded and instead reaches vulnerable people in need (Sundin *et al.*, 2022). Although food donations have provided an important role for supplementing the diets of vulnerable people in the UK, this should be considered a last resort for addressing food poverty. Vulnerable people that rely on donations have to live on end of life and poor-quality products. Ideally, food poverty should be addressed at its route, negating the need for people to rely on food donations.

1.12 Stable Isotope Analysis Is Already Playing a Crucial Role For Food Loss and Waste Reduction

Stable isotope analyses are used in the food supply chain, playing a strategic role in reducing food loss and waste. Primarily analysis is used to tracing the origin and verify food authenticity upholding food safety and business integrity. Through research, further applications of isotope analysis are emerging.

Soil fertility analysis is a less common application of isotope analysis that provides useful information about nutrient availability, fertiliser efficiency and soil erosion (Busari, Salako and Tuniz, 2016). Understanding soil profiles can inform management of growing methods to achieve optimal conditions for high yield and quality of produce, reducing potential food loss (Stable Nitrogen Isotope Helps Scientists Optimize Water, Fertilizer Use, 2017)

There is limited exploration of the use of stable isotope analysis in relation to physiological changes in produce that occur during spoilage. Horacek and Papesch (2021) found isotopic changes in $\delta^{15}N$ and $\delta^{18}O$ isotope values when testing each day for a 21 day period. These changes, although from a limited study, demonstrate that stable isotopes may provide a useful method for spoilage detection following the compilation of characterised reference profiles (Horacek and Papesch, 2021). Extensive research and data contribution would be required to form an adequate archive and establish the robustness of spoilage isotope profiles. Spoilage characterisation using isotopes may be a potential avenue and provide a complementary method for addressing the challenge of reducing food loss and waste, for spoilage detection, and cold chain monitoring. This study seems to be a unique application of isotope analysis, highlighting an important gap in research. Further research could explore the characterisation of spoilage markers and shelf-life stages with the application of predictive models that could provide insights into isotope capabilities for predicting accurate product shelf-life.

The detection of food fraud is a common use of stable isotope analysis comparing test samples with comprehensive databases of isotopic signatures. Geographic isotope profiling can be established by looking at isotopes influenced by local climate, geology and soil characteristics seen in carbon (^{12}C, ^{13}C), nitrogen (^{14}N, ^{15}N), sulfur (^{32}S, ^{34}S), hydrogen (^{1}H, ^{2}H), and oxygen (^{16}O, ^{18}O). Additionally, growing conditions influenced by irrigation, precipitation, proximity to the sea, surface water, latitude, and longitude can be described from water-associated isotope ratios ($^{2}H/^{1}H$ and $^{18}O/^{16}O$) (Terro et al., 2025). A valuable resource of stable isotope and elemental data for a wide range of food commodities used for testing authenticity and detecting food fraud is the IsoFoodTrack database serving as a valuable resource for agencies in food control and researchers (Terro et al., 2025). The database is coupled with a user-friendly interface

providing accessibility and useful visualisation and importantly, is focused on the integration of open-access data which is crucial for system-wide standardisation. Another well-established database maintained by the European Commission is the European Wine DataBank comprised of isotopic data collected from wines across the EU, providing reference material which can be used to authenticate sugar content, water dilution levels and geographic origins (Christoph, Hermann and Wachter, 2015). The authentication of food using stable isotopes can be achieved through fingerprinting using verified samples compiling compositional profiles. High value products with established certifications of authenticity, such as Parma ham, Grana Padano cheese, and Parmigiano Reggiano, have isotopically comprised profiles which can be accessed through databases, including the Stable Isotope Ratio Analysis (SIRA) database which is widely accessible and ensures reliable authentication, instilling trust in products and their suppliers (Christoph, Hermann and Wachter, 2015).

Product authentication, although not obviously, is an important element of reducing food loss and waste. The presence of or the suspicion of fraudulent food may result in entire batches being rejected or removed from the supply chain, even if the food itself is safe and edible. This both contributes to food waste and the loss of its associated resources used during production. Without accurate and trustworthy authentication methods, mistrust and suspicion increases which in turn increases rejection incidence. Additionally, the presence of fraudulent food drives market prices down through the application of cheap prices forcing legitimate producers to overproduce or compete with deflated prices causing surpluses potentially being unsold and wasted. Authentication reduces rejection of safe and edible food, and prevents fraudulent products from flooding the markets and maintaining prices reflecting genuine demand and supply (The Cost of Food Crime Phase 2 | Food Standards Agency, 2023). Stable isotopes provide accurate and crucial methodologies in the supply chain, contributing to reducing food loss and waste.

1.13 Reducing Food Loss and Waste by Detecting Spoilage in Perishable Fruit

Understanding the spoilage-associated biochemical and molecular processes is integral to reducing food loss and waste. A combination of identification of key biomarkers using analytical techniques, along with monitoring and visible assessment can help to reduce loss and waste throughout the supply chain in addition to achieving optimal quality and food safety. The implementation of effective strategies for repurposing in place of discarding produce can significantly contribute to the reduction of waste and reduce the associated environmental impacts.

Biomarkers associated with spoilage processes are often used to detect the spoiling in fresh produce. These can include changes in pH which could indicate microbially associated spoilage, volatile organic compounds, visible analysis of colour changes, the presence of mould, off-odours and the formation of biofilm (Lorenzo *et al.*, 2017). Additionally, the physical examination of structural integrity can be applied to assess firmness. However, these indicators often present too late for the repurposing of fruits and instead lead to the discarding of the individual fruits or the entire batch. Analytical methods can be used to identify biomarkers of spoilage when visible identifiers aren't present, especially microbial spoilage. Gas chromatography (Oldham and Held, 2023) and mass spectrometry (Franco-Duarte *et al.*, 2019) or electronic noses (Bonah *et al.*, 2019) detect volatile compounds indicative of microbial spoilage. Enzyme assays can also be used to detect enzyme levels which can be attributed to the spoilage stage (Ou, Wilson and Weber, 2018). Spectrophotometry can be used to detect oxidative spoilage including lipid peroxides, protein carbonyls, and volatile oxidation (Kodali *et al.*, 2020). Furthermore, external monitoring using data loggers and sensors of the climactic storage facilities and transportation, including levels of humidity and temperature provides a preservative measure to inhibit spoilage (Taj *et al.*, 2023). These serve as preventive measures in addition to providing data to further inform future actions in augmenting preservation conditions.

1.14 Infrared Spectroscopy: Principles and Applications

The development of effective interventions and solutions to reducing food loss and waste in the supply chain is reliant on a comprehensive understanding of where and why food loss and waste occurs (Bajželj *et al.*, 2020). Infrared spectroscopy can play a role in

obtaining accurate information for strategy implementation regarding food spoilage and quality enabling better decision-making at various stages in the supply chain.

Infrared (IR) spectroscopy provides a powerful non-destructive analytical technique that is used to study the chemical and biochemical composition of samples (Othman, 2022). The identification of chemical bonds can be achieved by measuring the absorption of specific wavelengths of IR light (Johnson *et al.*, 2023). The infrared electromagnetic spectrum is divided into three main regions: near-IR (NIR), mid-IR (MIR), and far-IR. Near and mid-IR spectroscopic regions are commonly used for chemical analysis in MIR and NIR spectroscopy techniques. However, the far-infrared region (400-10 cm^{-1}; 25,000-106 nm) encompassing rotational transitions and low-frequency vibrations (*Infrared Spectroscopy*, 2013) is less commonly used due to the lack of specificity that is found in the Mid-IR region. IR spectroscopy techniques use the interaction of a sample and IR light (Figure 1.4) to understand the chemical composition (*Infrared Spectroscopy*, 2013). Molecules absorb energy when exposed to IR radiation causing the chemical bod to vibrate at specific frequencies. Vibrational modes occur in differing patterns, dictated by the molecular structure, shape, and composition. An interferogram is formed from the reflected light, which is then processed to create a spectrum. This spectrum displays molecular information based on the levels of light absorbed when interacting with the molecules in the sample, revealing its biochemical composition (*Infrared Spectroscopy*, 2013).

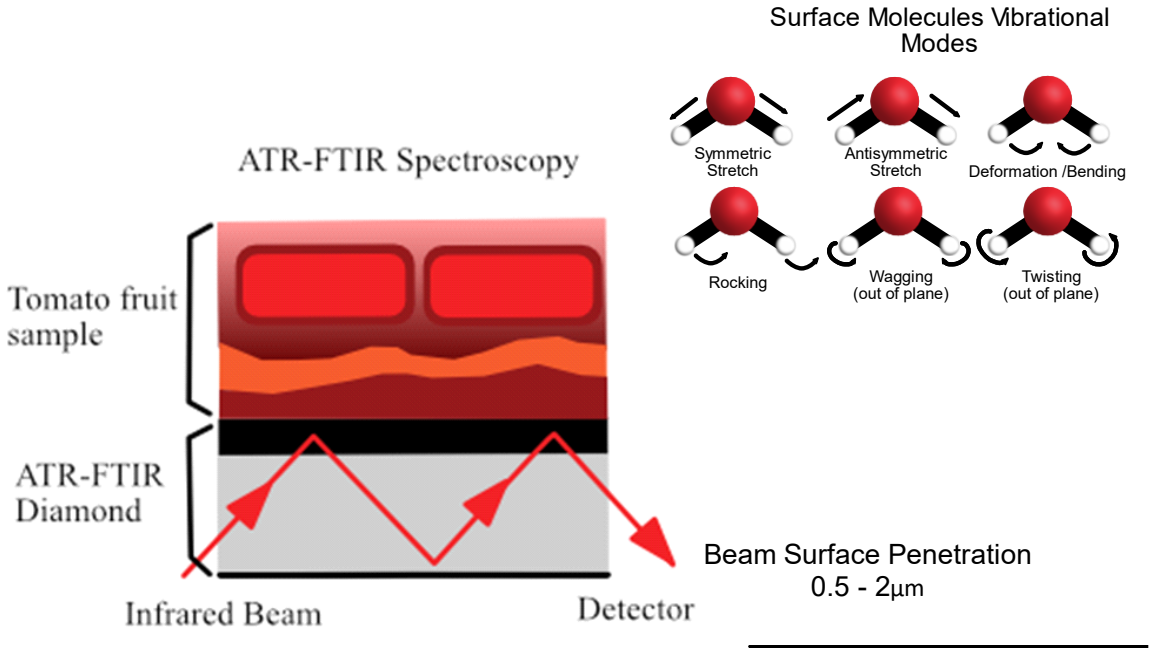

Figure 1.4. ATR-FTIR spectroscopy, reworked. ATR_FTIR laser reflecting from tomato sample with max penetration of 2μm. Types of vibrational modes of sample molecules displayed (Butler *et al.*, 2015).

This technique's versatility allows intricate analysis of solid, liquid, or gaseous states on both inorganic and organic samples. IR spectroscopy is valuable in scientific research and used in a variety of industries due to its capacity to provide detailed molecular information. Important fields of application include environmental and material sciences, healthcare, and pharmaceuticals and the applications for this technology are continuing to grow including less obvious applications in art and cultural heritage (Mokari, Guo and Bocklitz, 2023)

1.14.1 Mid-Infrared Spectroscopy (MIR)

MIR spectroscopy region is between 2500-25000 nm (4000-400 cm^{-1}) which contains the fundamental frequencies of most molecular bonds making it particularly important and invaluable in the identification of sample chemistry. The vibrational modes occur in different forms, primarily stretching and bending of the molecular bonds. Stretching occurs with the asymmetric or symmetric changing in bond length in contrast with bending which refers to the angle between bonds changing by scissoring, rocking,

wagging, or twisting (Chem LibreTexts, 2023). An absorption spectrum is produced for the sample using a MIR spectrometer, this maps the absorption intensity at wavelength or wavenumber (cm^{-1}). The fingerprint region (1800-900 cm^{-1}) of the MIR spectrum is of particular interest in biochemical analysis. Named suggestively based on a human fingerprint, it provides a unique biochemical signature associated with organic structures that can be used for highly specific identification (Chem LibreTexts, 2015). The biochemical signature describes the concentrations of chemicals present at the time of measurement, providing a tool to better understand biochemical changes. Obtaining this biochemical signatures can inform about the quality, nutritional value, development status and chemical composition which are all valuable data that can be used to optimise the food supply chain. The complexity of the information distributed in the MIR spectrum provides greater specificity than the near-infrared spectrum making it a more attractive method for obtaining precise sample detail, especially key biomarkers (Colthup, 1975a).

1.14.2 Attenuated Total Reflection Fourier Transform Infrared Spectroscopy (ATR-FTIR)

Attenuated total reflection Fourier transform infrared spectroscopy is a technique that samples within the Mid-infrared spectrum that is particularly useful when analysing solid and liquid samples. An infrared laser is directed onto a crystal that is in direct contact with the sample. This technique employs a crystal, normally diamond, germanium, or zinc selenide which have a high refractive index that receives MIR light at a specific angle producing an evanescent wave that penetrates typically between 0.5 and 5 microns (Gupta, 2017). The evanescent wave provides an absorption measurement indicative of the molecular structure of the sample. ATR-FTIR can handle a wide variety of sample types with minimal preparation, this includes powders, films, liquids, gels and solids. It also allows for real-time process monitoring including polymer curing, drug delivery and surface reactions. The versatility of this technique suggests the propensity to successfully obtain detailed biochemical information from the surface of whole fruit, providing a rapid, high-throughput and non-destructive tool valuable for use in the supply chain.

1.14.3 Near-Infrared Spectroscopy (NIR)

The near-infrared region is between 780 nm to 2500 nm (14,000 – 4000 cm^{-1}), this region can be attributed to overtones, or resonant frequencies, and combinations of molecular vibrations which are weaker than absorptions within the MIR-IR region providing a less detailed molecular fingerprint (Beć, Grabska and Huck, 2020). NIR is capable of penetrating deeper into the sample than MIR/ATR-FTIR, making it more effective in the analysis of moisture content, solid-state materials, and bulk properties like particle size and crystallinity. Moisture content is especially useful when use NIR to analyse fruit samples as it can indicate developmental stage, quality or degree of spoilage. Additionally, NIR spectrometers often being portable allowing for in-situ data acquisition whereas most mid-infrared spectrometers are often confined to laboratory spaces.

1.14.4 Chemometrics: A Powerful Analytical Tool for Large and Complex Datasets

MIR and NIR data are analysed through chemometrics, a combination of chemistry, mathematics and statistics, to extrapolate meaningful chemical information about a sample. Chemometrics is effective in manipulating and analysing complex and large datasets with extensive undescribed variables using a range of complex models to extrapolate important information. Chemometrics is a vital step in the field of spectroscopy due to the multivariate outputs forming large and complex datasets (Lavine and Workman, 2013). Modern chemical research generates vast amounts of data from analytical techniques, including spectroscopy, making it challenging to interpret. These challenges occur when using traditional, univariate methods making chemometrics essential in a multitude of industries and fields using spectroscopic technology. Chemometrics is designed to process and analyse multidimensional datasets containing multiple variables that could influence the final result simultaneously, for example in food quality analysis moisture content, chemical composition and physical properties could all be contributing to the spectral data acquired (Brereton, 1987). Chemometrics allows for precise and automated classification, assigning data points to pre-defined categories. Data reduction and visualisation is a core technique in chemometrics, simplifying complex data for the interpretation of potentially hidden patterns or trends.

Raw spectroscopic data must undergo preprocessing techniques prior to advanced statistical analysis. Preprocessing is used to standardise the data ensuring accurate analysis, in addition to noise removal or cleaning (Morais *et al.*, 2020). The skipping of this step may cause unreliable results to be drawn from the dataset. Some important preprocessing techniques used in analysing spectral data include smoothing which removes noise and distortion. Smoothing techniques including the Savitzky-Golay (SG) filter are commonly used. Normalising and scaling, which ensure that all the variables are measured on the same scale, prevent variables artificially dominating. Vector normalisation and mean centring are commonly used prior to multivariate analysis technique: principal component analysis ensuring that the variable contribute equally to the model (Jolliffe and Cadima, 2016; Zhang *et al.*, 2022). Transformation of derivatives can help to further enhance small peaks to remove background effects and understand underlying trends or patterns.

1.14.5 Multivariate Analysis

Principal component analysis (PCA) is an exploratory visualisation tool in chemometrics that reduces the dimensionality and simplifies the dataset. The model identifies directions along which the variance in the data is maximised (Jolliffe and Cadima, 2016). These directions, or principal components will represent a feature in the data. The first principal component (PC1) represents the direction in the feature space along which the data varies the most. It accounts for the largest possible variance in the data. Each subsequent principal component (PC2, PC3, and so on) represents the next orthogonal (uncorrelated) direction of maximum variance. These components capture the remaining variance in decreasing order (Analytics Vidhya, 2016). Scores and loadings are the composites of each PC, scores displaying patterns of similarity between samples and the loadings are the weights or coefficients of the original variables in the linear combination that forms each principal component (Cordella, 2012). In the context of spectral data, these can be attributed to variances at specific wavenumbers allowing for identification of significant biomarkers.

Following from PCA, Linear Discriminant Analysis (LDA) can be applied, this maximises the separation between classes that are predefined allowing for a powerful classification

tool PCA-LDA (Tominaga, 1999). It works by computing a projection that maximises the distance between the means of different classes, while maximising the variance within each class. It is useful by combining the strengths of both PCA and LDA reducing noise, handling complex datasets, revealing hidden patterns and providing robust and accurate classification.

Machine learning support vector machine is a supervised machine learning classification and regression model. It is primarily used for classification due to its robust nature of being able to find optimal boundaries between classes even when the data is not linearly separable. SVM uses a kernel function that maps and separates the data using a hyperplane, the model is then trained and tested using this separated data. SVMs are commonly used to classify spectroscopic data as well as several other data forms (Soman, et al., 2009). SVM models train on 70 % and test on 30 % of the data. SVM models are highly effective at complicated and high-dimensional data, it is less prone to overfitting than other machine learning classification models which is more reliable, it is also flexible due to the linear and non-linear classification ability. To achieve the maximum success whilst avoiding overfitting, SVM often requires a new set of preprocessing to PCA-LDA. While PCA-LDA prefers SG filter, second derivative, second polynomial, vector normalisation and mean-centering normalisation, SVM performs better using SG filter, first derivative, second polynomial, vector normalisation and 0, 1 range normalisation (Ahsan *et al.*, 2021). In the following chapters these techniques will be employed to both MIR and NIR spectroscopic data.

1.15 Infrared Spectroscopy has Diverse Applications

1.15.1 Pharmaceutical and Health

The use of IR spectroscopy for quality control and assurance is extensive in the pharmaceutical industry. It allows verification of identity of compounds and purity. This use certifies consistency of drugs for distribution. During drug development stages, polymorphism studies are conducted to help understand the drug efficacy, bioavailability and toxicity, IR spectroscopy is used in the identification of these different crystalline forms, also known as polymorphs (Mukherjee *et al.*, 2013). Further use in the field of healthcare is medical diagnostics for a variety of diseases. Analysis of samples of a

biological nature including blood, urine and tissue allows for the detection of conditions including cancer, diabetes and infections (Sakudo *et al.*, 2006; Paraskevaidi *et al.*, 2021, 2021). MIR and NIR spectroscopy have both been shown to be able to differentiate between healthy and diseased tissue specimens obtained from biopsy.

1.15.2 Forensics and Materials Analysis

The identification of substances suspected to be linked to criminal activity can be achieved through IR spectroscopy, including drugs, explosives, and fibres found in crime scenes (Fabian and Mantele, 2006). Forensic uses also include authentication of documents detecting alterations and forgeries through compositions of ink and paper (Udrițioiu *et al.*, 2012). The technologies' specificity can even analyse trace residues which can provide crucial information and evidence aiding criminal investigations (Wei *et al.*, 2024).

IR spectroscopy also has its place in cultural heritage through authentication of valuable artwork and historical artifacts (Poliszuk and Ybarra, 2014). This is through the analysis of the materials and techniques employed by the artist. Pigments in paintings and sculptures can be analysed (Carbó *et al.*, 1996) providing knowledge and information about the historical context and the age of the work by comparing the used materials to their known historical presence and use. This material identification can also aid the restoration of artwork to inform the conservationist of the appropriate materials to use (Derrick, Stulik and Landry, 2000).

In the field of material science, IR spectroscopy is crucial in polymer analysis which aids the identification of polymer types, polymerisation processes and polymer material degradation (Jenkins, 2013). This is important for property assessment like chemical, thermal, electrical and mechanical which are important to understand when allocating materials to product design. Additionally, properties including performance associated with the product designed use, such as strength, flexibility and resistance to environmental factors. Material defects and consistency in the polymer materials can be determined informing quality certification which also helps confirm compliance with legal industry standards and regulations and informs of safety, especially important in

materials used to produce food packaging, medical devices and products used by children.

1.15.3 Environmental Applications

IR spectroscopy is now an important tool used in variety of analytical applications for researching and mitigating environmental damage including the environmental impact of agricultural practices. Soil properties can be quantified including moisture content, nutrient levels, and organic matter (Ng *et al.*, 2022) which can be used to understand the condition of arable land and to monitor the implementation of new sustainable practices and land management. Pollution levels can also be monitored through IR spectroscopic analysis of water and soil (Horta *et al.*, 2015). Gases, particulates and contaminates (Ng, *et al*., 2017) can be detected and identified and the quantification of levels of carbon dioxide, methane and volatile organic compounds can also be achieved (W. Wu *et al.*, 2024). These approaches and data collection can provide important evidence and grounds for informing policy changes. The current UK policy for honey authentication procedure was informed by research conducted by Agency *et al*. (2025) using spatially offset Raman Spectroscopy (SORS) to identify sugar types and their concentrations to detect adulterated ingredients. The success and robust results from this study has contributed to the food standard agency policy, recognising it as a technique suitable for implementation at appropriate stages in the supply chain to detect fraudulent products. Additionally, a toolkit has been designed to complement the use of this technique to guide the data analysis and extrapolation of information obtained from the analytical results (Mumford et al., 2025)

The environmental damage caused by plastic pollution is becoming of increasing concern informed by studies of the degradation of plastics and how the breakdown of products impact on different environments and living organisms (US EPA, 2023). This concern has contributed to the development of alternative materials such as bioplastics providing detailed knowledge of how the polymers behave in conjunction with environmental factors (Yu & Flury, 2024). The optimisation of recycling and reusability has been enhanced with the use of IR spectroscopy (Emom *et al.*, 2024). Contaminants can be detected and removed, and the identification of plastic composition allows for accurate

sorting of plastic types so they can be effectively processed for reuse reducing the production of new plastic.

1.15.4 IR spectroscopy in the Food System

IR spectroscopy is particularly useful in the food industry and is established for use in raw material analysis, quality control (Johnson *et al.*, 2023), safety assurance (Liu, Deng and Han, 2024), fraud detection, allergen identification (Luan *et al.*, 2023) and contaminant presence (Ceniti *et al.*, 2023). Safety is of the highest priority in the food industry and critical for compliance with regulatory standards and maintaining trust from the consumer. IR spectroscopy is used in the food industry as a rapid and non-destructive analytical tool. ATR-FTIR spectroscopy provides detailed profiling information using the vibrations of molecular bonds to identify functional groups in food. Key functional groups in food analysis include: O-H (alcohols, phenols, carboxylic acids), C=O (aldehydes, ketones, esters, amides, carboxylic acids), C-H (alkanes, alkenes, alkynes), N-H (amines, amides), and C-O (alcohols, ethers, esters) (Kassem et al., 2023). It is capable of analysing a range of materials: solids, liquids, powders, and pastes. A primary use of ATR-FTIR spectroscopy is the identification of raw materials, including the detection of fats (Lucarini *et al.*, 2018), proteins (Glassford et al., 2013; Zhao *et al.*, 2021) and carbohydrates (Farooq and Ismail, 2014) which helps to verify the authenticity of ingredients, and requires little to no preparation of produce for the analysis. Bovine milkfats were successfully characterised by Windarsih, Irnawati and Rohman (2020) using FTIR spectroscopy and chemometric analysis. Adulterated ingredient: Lard oil, was successfully detected, demonstrating the accuracy of analysis characterising different fat types based on their molecular composition (Windarsih, Irnawati and Rohman, 2020). The fingerprint region is especially valuable as it can be compared with reference spectra when determining adulteration of a material or if a dilution has been applied.

ATR-FTIR is used extensively for detecting adulteration of ingredients which is a common form of food-fraud with system-wide consequences, which are sometimes even fatal (Visciano and Schirone, 2021). Low-quality oils, that have been mixed with premium oils can be detected using ATR-FTIR (Cebi, Arici and Sagdic, 2021). Additionally other

premium products including honey (Ng *et al.*, 2022; Cárdenas-Escudero, Galán-Madruga and Cáceres, 2023), spices (Dhakal *et al.*, 2019; Lafeuille *et al.*, 2020), fruit juices (Yaman and Durakli Velioglu, 2019), and wines (Dixit *et al.*, 2005) are at risk of ingredient adulteration, and ATR-FTIR can be used in the authentication process (Bayen and Elliott et al., 2024). Whey protein concentrate is an example of a product that may be adulterated with a cheaper ingredient such as wheat flour, fraudulently increasing the profitability. This adulteration poses dangerous risks due to allergens but is able to be successfully detected using ATR-FTIR spectroscopy (Martins *et al.*, 2022). Detecting fraudulent practices in the food industry is critical in maintaining customer safety. This is especially important when harmful chemicals are used as additives but accidental contact between food products and hazardous chemicals can also occur (Rather *et al.*, 2017). During processing, food may come into contact with cleaning agents, pesticides (Xiao *et al.*, 2015) or packaging residues (*EFSA*, 2024), and it is imperative for human safety that contaminants are detected so products can be removed from the supply chain. Food-borne illnesses can also occur as a result of microbial contamination at any stage in the supply chain; ATR-FTIR can provide a non-destructive method for detecting dangerous food pathogens (Tessaro *et al.*, 2023).

Customer satisfaction, brand reputation, and compliance are all important for manufacturers, all of which are associated with product quality. Composition, texture, flavour, nutritional content, and appearance, as well as food safety, are key measures of quality (Kader, 2008). ATR-FTIR can provide a valuable tool in quality control (Ríos-Reina *et al.*, 2017; Sujka *et al.*, 2017). For example, ATR-FTIR can be used for quantifying the moisture levels and fat content in raw materials including grains (Golea, Codină and Oroian, 2023), meat (Candoğan *et al,*, 2021) and dairy (Balan *et al.*, 2020) providing important insights into the quality of the ingredients. The chemical composition of grains, seeds, and processed foods can be assessed, which may need to meet certain quality standards. In dairy production, the fat content of cheese and butter (Zhao *et al.*, 2015) can be measured using ATR-FTIR, allowing immediate adjustments to be made during production, ensuring a consistent product, reducing product wastage, and ensure high-quality products every time.

ATR-FTIR is used in the monitoring of chemical reactions that affect the quality and shelf-life. An example of this is the tracking of oxidation in oils (Zhou *et al.*, 2021) and the lipid peroxidation in meat products, both of which are indicators of spoilage which can be tracked in real-time throughout the supply chain. Additionally, product processing methods including cooking, can be monitored including the Maillard reaction (Calabrò and Magazù, 2020; Yang and Hiramatsu, 2019) in baking or roasting along with other important chemical transformations including starch gelatinisation (Lu *et al.*, 2021) in baked goods which determines texture and quality. Monitoring chemical transformations allows manufacturers to optimise key variables involved in product processing, including the temperature, pressure and cooking time.

Product development is an important process in food innovation. ATR-FTIR plays an essential role in providing detailed information about the molecular structure and composition of ingredients, helping developers understand how ingredients interact with each other, how they behave during processing and how they contribute to the nutritional and sensory properties. Ingredient characterisation is one of the primary applications of ATR-FTIR in product development (Wilson and Tapp, 1999). For example, the fatty composition of oils or protein structures in dairy or plant-based ingredients or carbohydrates in starches and sugars can be analysed, and the data helps developers to select the right ingredients for the product (Köllmann *et al.*, 2023). The ingredients may influence texture, taste, structure or physical appearance. There has been a rise in meat replacement products in recent years, products that require very specific characteristics which may be determined by the use of ATR-FTIR in ingredient characterisation. Additionally, the interactions between ingredients may be monitored using ATR-FTIR, in the formulation of gluten-free baked goods, different starches, and gums may be used to mimic the properties of gluten, and ATR-FTIR can be used to analyse these interactions and fine-tune their formulations.

NIR spectroscopy can be used to analyse organic compounds including protein, fat, and carbohydrates making it a useful tool in the supply chain (Perez-Guaita *et al.*, 2021). It is often used to quantify the nutrient content of raw materials or ingredients including grains such as wheat, corn, and maize, allowing for regular and quality standards to be met (Johnson *et al.*, 2023). Chemical processes that affect the quality of cooked or

processed food products can be monitored using NIR including the production of confectionary products like caramel (Mohamed *et al.*, 2024) which involves very specific heating techniques to produce a high-quality product.

NIR can be valuable in the quality assessment of fruit and vegetables (Walsh *et al.*, 2020), measuring qualities including ripeness inferred from sugar content, moisture, and volatile compounds. NIR allows the detection of internal defects in produce such as apples, carrots, pears, and tomatoes by measuring sugar levels or detecting internal bruising (Huang, Lu and Chen, 2020) from measuring cell wall associated compounds, water content, pigment level changes and sugar composition. Tenderness quality can also be detected in meat products. These useful techniques allow for the grading of the products and for the products to be properly distributed either for high-quality product sales or for redirection to ingredients or other purposes.

NIR can be used for the detection of contaminants ensuring product safety as well as fraudulent activity including the inclusion of adulterated ingredients. Pesticide residues have been identified on strawberry fruit (Yazici, Tiryaki and Ayvaz, 2020) using NIR spectroscopy which provides a useful tool due to the availability of hand-held NIR spectrometers making it applicable for easy use *in-situ* in the supply chain. Nutrient content can be measured by NIR in a variety of food products, for example in flour, the protein content is measured to ensure it meets industry standards (Vongsvivut *et al.*, 2014). It can also assess the moisture and fat content of meat, especially ground meat, this allows for product consistency and to meet customer expectations. Sugar levels can be monitored in drinks to make sure flavour profiles are consistent as well as meet regulatory health standards.

Dry products like crisps or crackers require their environment to remain absent of moisture to maintain shelf life. Moisture levels are measured using NIR before packaging to avoid premature spoilage and for the product to maintain a crisp texture. Dough hydration levels can be measured using NIR spectroscopy (Castro-Reigía *et al.*, 2024) and this can be done in real time allowing for precision control for high-quality baked goods.

1.15.5 IR Spectroscopy could Provide a Useful Tool To Reduce Food Loss and Waste In The Supply Chain

The known capabilities and existing uses of infrared spectroscopy suggest a significant potential application as an analytical tool for addressing the complex challenge of reducing food loss and waste. Both ATR-FTIR spectroscopy and NIR spectroscopy have been identified as tools for quality assessment and shelf life, and have been used for detecting adulterated products (Bilamjian et al., 2024; Li et al., 2024). However, their use on fresh fruit and vegetable products has been less widely adopted in the supply chain. The exploration of understanding the biochemical processes involved in fresh fruit and vegetables and establishing important markers that can be used in practice is fundamental to the widespread application. The techniques provide advantages over some of the current methodologies being used, primarily the non-destructive nature of sample reading and high-throughput spectral acquisition (Workman, 2024), making it an important avenue for research to which this thesis seeks to initiate. The rapid quality controlling capabilities in both NIR and ATR-FTIR have the potential to reduce waste from misjudged products and provide options for non-destructive sorting, enabling timely processing. Moisture and composition checks may be applied to prevent spoilage in storage, and degradation detection checks can be used for monitoring during transit in the logistical and packaging supply chain stages. Food authentication is widely practiced using IR spectroscopy (Rodriguez-Saona, Giusti and Shotts, 2016), to extend its use for fruit and vegetable origin authentication may further contribute to a more resilient system, protected against the infiltration of fraudulent food products, and contribute to the reduction of food loss and waste. Both spectroscopic methods may be used at any stage in the supply chain provided the appropriate equipment is used, meaning it has the potential for use at every stage or at the most appropriate stages for supply chain and product optimisation to enhance precision farming, characterise key markers in ripening and senescence for the potential use for predictive tools for shelf-life determination. This thesis aims to explore the possibilities of using ATR-FTIR and NIR spectroscopy in a variety of ways with the aim for reducing food loss and waste.

1.15.6 Bridging The Gap Between Infrared Spectroscopy and System-Level Strategies for Reducing Food Waste

Food loss and waste are profound systemic issues that require both technological implementation and system-wide approaches (Arshad *et al.*, 2025). This thesis explores

how the use of technological tools such as infrared spectroscopy including: Attenuated Total Reflectance- Fourier Transform Infrared (ATR-FTIR) and Near-Infrared (NIR) can serve as a powerful tool for the mitigation of losses and waste that occur in a variety of ways and stages in the supply chain. The technically focused chapters seek to address a variety of places that can directly and indirectly result in food losses or waste, these include **Chapter 2** that investigates the biochemical changes that occur in fruit postharvest regardless of environment, different temperatures of postharvest storage. **Chapter 3** investigates the authentication of growing locations, knowledge that is important for authentic sale, fraudulent produce could lead to food waste so early detection can prevent future large scale discarding. **Chapter 4** sets to build an understanding of the biochemical journey from plant to postharvest spoilage aiming to optimise quality, inform decision making related to cultivation to reduce wastage. **Chapter 5** explores complementary social science approaches that look to address systemic policy, reshape the food system economy and support sustainable changes, particularly Trust Cost Accounting (TCA). The thesis looks to bridge the gap between analytical chemistry and systemic approaches and their social impact, providing a comprehensive view of combined techniques to transform food loss and waste management in the food system and strengthen national and global food security.

1.16 Aims and Objectives

The need to develop novel and innovative approaches for the maintenance of global food security and mitigate the impact of climate change on food production systems is becoming increasingly clear with a global population predicted to increase to 10.4 billion by the end of the century (United Nations, 2024). This includes the minimisation of FLW at all points throughout the supply chain. The power of IR spectroscopy for environmental monitoring and within food production systems has been demonstrated. This research seeks to explore the opportunities for using IR spectroscopy-based approaches for the high-throughput, non-destructive, and rapid analysis of produce. This research seeks to demonstrate the potential application of IR spectroscopy in the food supply chain with the over-arching goal of reducing FLW. Suggested applications include the early detection and prediction of spoilage through an increased understanding of pre

and post-harvest biology of produce, identifying fraud and classification of fruit developmental stages and processes. Specifically, the objectives of the research are:

Chapter 2: Application of Mid-Infrared Spectroscopy to Detect Storage-Induced Biochemical Changes in Fruit and Vegetables

A critical aspect of addressing the complex challenge of reducing food loss and waste is possessing a deep understanding of the biochemical changes occurring postharvest in highly perishable produce, helping to extend shelf-life, quality and improve decision-making in the supply chain. Visible degradation is not sufficient enough to fully optimise these practices due to these processes occurring at earlier stages than is visibly expressed. Assessing internal biochemical changes using existing methods is limited for use in the supply chain due to the destructive nature and lengthy analysis time which is critical for assessing produce and making decisions on the destination for best use. ATR-FTIR spectroscopy provides an alternative method that allows for non-destructive and high-throughput measurements for the monitoring of molecular changes and providing useful information informing produce quality and rapid actions to reduce loss and waste. Spoilage pathways may be linked by identifying spectral signatures forming a foundation for predictive models. Postharvest storage conditions are critical to optimising fruit quality, understanding biochemical processes under a variety of temperatures can provide informative identifiers. Post-harvest biochemical processes are already well characterised through many areas, including gene expression, metabolomics, transcriptomics, enzymatic profiling, and sugar metabolisation. Detailed documentation of spectral mapping is emerging but underdeveloped; most studies focus on endpoint comparisons related to fungal spoilage detection or shelf life estimation, however, time-course analysis has not been explored. The use of chemometric analysis of powerful datasets is limited, and spectral analysis is often interpreted from single spectra. The highly beneficial non-destructive feature has surprisingly rarely been exploited in spectral studies; instead analyses are focused on fruit parts removed and processed prior to spectral measurements. This chapter seeks to fill these gaps exploring spectral measurements of external fruit tissue, comprehensive time-series using chemometric analysis, and exploration of spectral signatures that may be linked to physiological biochemical changes for potential use as proxies for critical stages in spoilage.

Fundamentally, the study seeks to achieve the expression of signifiers of spoilage in the spectra before visible degradation occurs, providing an important basis for use in the supply chain, maximising the opportunity for waste prevention.

Research questions:

During postharvest storage of tomatoes, peppers, and lettuces, what are the notable spectral changes?

Can differentiation between produce stored at different temperatures be achieved through distinct spectral features?

Can points in time be characterised using identified spectral markers?

Can we establish informative spectral regions for tracking postharvest degradation?

Are we able to map important biochemical changes temporally?

Aims:

- Identify spectral biomarkers associated with spoilage of fruit
- Determine the effect of different post-harvest storage conditions on fruit quality

Chapter 3: Identifying Fraudulent Produce using Mid-Infrared and Near-Infrared Spectroscopy, a Comparative Study.

A growing concern in global food systems is the entry of inauthentic or fraudulent food items into the supply chain, increasing the demand for increased transparency around origin and farming practices and a necessity for methods for accurate authentication. Fraudulent misrepresentation of organic status or product origin can undermine sustainability progress. The occurrence of fraudulent food is known, the monitoring and documentation of occurrences is conducted widely in the global food system; however it is expected that a large proportion of these occurrences remains undiscovered. A variety of methods are in place for detection and verification, including DNA-based methods, stable isotopes, and ATR-FTIR is widely used for a variety of products; however, the non-

destructive use on fruit surfaces has been less explored. The use of NIR spectroscopy is less commonly used in this way due to limited specificity. The application of powerful chemometric analysis is not commonly used. Multi-modal spectroscopic techniques are explored to differentiate between the geographical origins of tomato fruits through spectral signatures, providing a unique comparison between the power and capabilities of the techniques and the specificity of the data, especially fruit surface measurements. The study further attempts to interpret the organic status and geographical origin spectral signatures by using industry-standard differentiators, stable isotopes in comparison. Isotopic ratios of growing origin may link to discriminating spectral features, providing a potential rapid and non-destructive alternative analytical method for use in the supply chain avoiding labour-intensive authentication using stable isotopes. Forming archival documented spectral profiles can build a foundation for classification models for supply chain applications, which coupled with AI models could be a powerful tool for detecting and preventing at early stages in the supply chain. Chemical profiling determined from spectral signatures can support certifications within regulatory frameworks protecting sustainability, business integrity, and consumer safety.

Research Questions:

Can NIR, ATR-FTIR and stable isotope profiles differentiate between tomatoes from different regions?

Is the organic status of tomato fruit distinguishable using NIR and stable isotope profiling?

What represent the most informative spectral and isotopic features for classification?

Does spectral analysis provide a suitable alternative for fruit origin authentication?

Aims

- To evaluate the potential of spectral analytical techniques in classifying tomatoes based on origin and growing practices.

- Compare the efficacy of IR spectroscopic techniques with industry-used stable isotopes for identifying origin chemical profiles and organic profiles of tomato fruit

Chapter 4: Tomatoes from seedling to spoilage, Near-Infrared Spectroscopy

What is known about the physiological development of tomato plants is highly detailed, as the tomato is one of the most widely studied model organisms. Our knowledge has been built from a range of experimental techniques that provide a detailed map of varying layers of processes. Gene expression studies have provided a detailed picture of genomic and genetic processes, mutants have been used to explore the roles of genes, Quantitative Trait Locus (QTL) mapping and transcriptomics, metabolomics, biochemical analyses looking at sugar profiles, acidity, pigments. Microscopy has played an important role in visualising physiological changes, phenotypic measurements. Although the knowledge is detailed and pathway-specific, the testing remains destructive. Spectral analysis has begun to be used as a non-targeted holistic view tool and is increasingly used in academic research and within the supply chain. However, the uses have been focused on product quality and have not been used to explore developmental time courses, especially linking spectral changes to known physiological landmarks. This lack of exploration may be due to certain limitations and the lack of ability to measure gene expression or signalling pathways. Linking specific physiological events to isolated features in the data is difficult due to overlap within and between spectra. The broad biochemical fingerprints obtained in spectra, may be used as indirect proxies, not direct markers, which may suggest that it is not as useful. However, building a detailed knowledge archive of spectral data for important crop plants through development may provide a foundation for developing predictive models for use in the supply chain. A significant benefit of this is the non-destructive nature of the measurements and high-throughput data recording, desirable features compared with other methods. Detailed spectral presentation of crop biochemistry has the potential to be connected to existing knowledge by specifically designed studies that run non-spectral measurements alongside spectral measurements. The implementation of stresses, environmental treatments, changes in growing conditions like nutrient concentrations during these studies could allow a highly detailed

identification of biochemical changes and how they're expressed in the spectra, in addition to characterising optimal harvest time etc. With this deeper knowledge this could inform important decisions which optimise quality, yield, and reduce losses and waste. The work in this chapter seeks to examine NIR spectral evolution in the tomato plant lifecycle, starting to fill the gap of temporal spectral data, forming the foundation for future work. The chapter offers insight into spectral signatures across plant vegetative and reproductive phases, potentially revealing important physiological transitions and enables a deeper understanding of biochemical shifts in pre- and post-harvest fruit associated with shelf-life, transportability, and nutritional content.

Research Questions

How does NIR spectral data change through tomato development and spoilage?

Can we differentiate between plant and fruit development phases using NIR spectral profiles?

What represents notable variance in spectral regions and features between developing phases?

Can we identify time point specificity through spectral signatures that reveal important biochemical and physiological transitions?

Aims

- Identify spectral biomarkers of ripening and post-harvest spoilage stages
- Identify spectral cross-overs between ripening phases and spoilage
- Identify spectral cross-overs between plant and fruit biochemical processes To lay a foundation for future predictive models based on lifecycle data

Chapter 5: A tool in the toolkit: Can true cost accounting remove siloed thinking about food loss and waste?

The complex challenge of reducing food loss and waste is a deeply rooted systemic problem therefore it cannot be achieved with technological methods alone. Governmental policies and interventions are continuously evolving focused on resolving the substantial problem. Simultaneously, other important actors and stakeholders are actively developing and implementing policies and processes that aim support the endeavour to reduce food loss and waste. These actions from individual organisations are critical to achieving this goal, however there lies a lack of functionality systemically in the absence of communication and collaboration causing inconsistencies and for actions to fail. These systemic issues occur within the national food system and are only exacerbated when observing the enormous and vastly more complex global food system. The lack of consistent definitions of food system elements between key organisations creates obstacles in formulating legislation and actions to alleviate systemic problems affecting everyone, for instance food loss and waste definitions are defined inconsistently by UK government, the EU and food waste charities like WRAP who all play significant roles in vital actions. While technical innovations including spectroscopic tools are critical to targeted approaches, these are rarely implemented within a systemic governing framework. A variety of frameworks have been developed in theoretical proposals including True Cost Accounting (TCA). Correcting externalities associated with the food system that are often ignored has been identified as a promising method for improving food security on a global scale and more specifically to support the complex challenge of reducing food loss and waste. The conceptual basis of TCA assigns an economic value to environmental, societal and health costs and benefits which form a total value of food products. These assignments represent how costly an item is intended to inform food system decision making from all actors. Currently there is a growing body of research and theory investigating TCA and proposed methods of implementation however there is a lack of consensus surrounding its feasibility and potential success. This chapter attempts to assemble insights from a diversity of perspectives representing all actors as stakeholder in the supply chain from position-influenced experiences. The perceived potential, TCA's feasibility in practice and the barriers and limitations were

explored and assessed to provide a deeper understanding of TCA framework and to form recommendations for systemic policy development.

This research was conducted collaboratively by multi-disciplinary researchers as part of the government organisation Global Food Security Network's scheme, encompassing contributions by early-career researchers to achieving global food security described by United Nations SDG goal 17. Programme participants are competitively selected and a final team is selected for their work design and awarded the role of conducting research and produce a policy think piece for publication, presentation to UK government and at the COP26 summit.

Research Questions

How is TCA applicable to the UK supply chain?

What are the limitations of TCA as a systemic approach?

How do the experiences of stakeholders representing diverse actors in the supply chain relate to TCA and can they inform to potential efficacy of TCA in practice?

Aims

- Understand the benefits and limitations of using TCA as a systemic approach for reducing food loss and waste
- Develop policy recommendations for supply-chain actors in industry and government to address system-wide food loss and waste in the context of TCA

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2 Application of Mid-Infrared Spectroscopy to Detect Storage-Induced Biochemical Changes in Fruit and Vegetables

2.1 Abstract

Culturally important tomato fruit, bell peppers, and lettuce provide nutrition to a global market, but are highly perishable and require controlled storage and transportation to maintain shelf-life. Temperature control is highly effective for extending shelf-life, maintaining produce quality, and preventing spoilage. A non-destructive, high-throughput, and cheap technology is needed that can be used throughout the supply chain to detect spoilage biomarkers for effective and timely repurposing of these crops before they perish. This study investigates the use of attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy as a rapid, quantitative method for detecting spoilage in the surface tissue of tomatoes, peppers, and lettuces stored in a variety of post-harvest storage temperatures. Chemometric multivariate analysis of the spectral fingerprint region (1800 cm^{-1} to 900 cm^{-1}) Spectral variations occurred from harvest until spoilage, the key biochemical changes were described by wavenumbers indicative of the processes involved in post-harvest fruit degradation that may serve as biomarkers. Biochemical signatures associated with time and temperature were distinct enough for machine learning models to successfully classify with high accuracy rates indicating that ATR-FTIR spectral information is suitable for classification and potential for use in the supply chain

2.2 Introduction

Food supply chains are becoming increasingly vulnerable due to a variety of pressures including rapid urbanisation (Satterthwaite *et al.*, 2010), rising input costs and decreased investment (Ching-Pong Poo et al., 2024), a lack of young farmers taking up the profession (May *et al.*, 2019), and the systemic shock from the COVID-19 pandemic (Garnett *et al.,* 2020). This vulnerability is further exacerbated by the significant impacts of climate change and the pressure to feed an increasing human population (Tchonkouang *et al.,* 2024). One of the biggest challenges currently facing agriculture is to continue providing sufficient, nutritious food for a growing population (United Nations, 2021). The current population of the UK in 2024 is 67 million, expected to increase to between 75 and 77 million by 2050 (World Population Review, 2024). The provision of sufficient safe and nutritious food is dependent on a functioning food system with successful agricultural systems and international importation of a wide variety of food products (Peng and Berry, 2019).

2.2.1 Fruit Ripening and Senescence in Climacteric Fruit

Ripening and senescence in climacteric fruit like tomatoes, differ from non-climacteric fruit like peppers primarily by ethylene dependence only exhibited in climacteric fruit. Ethylene production corresponds with the increase of respiration upregulates the process involved in ripening and senescence while non-climacteric fruit ripening and senescence processes are driven by plant hormones and transcriptional regulators (Liu et al., 2015) .

Chloroplasts present in pre-ripened climacteric fruits perform photosynthesis, tissue is green due to high levels of chlorophyll and fruit structure is firm. Sweetness is low but at this stage starches are beginning to convert into sugars (Tipu and Sherif, 2024). Transcription factors begin to increase slowly including: RIN (Ripening Inhibitor) and NOR (Non-Ripening) that work to mediate ripening, and CNR (Colourless Non-Ripening) that controls early ripening related genes. The onset of ripening, also known as the breaker stage is identifiable by visible colour change that occurs through chlorophyll degradation and accumulation of carotenoids like lycopene and β-carotene. Climacteric fruit's characteristic ethylene production is initiated and induces autocatalytic feedback

loop. Ethylene receptors trigger ripening associated gene expression resulting in structural softening from cell wall degradation from polysaccharide breakdown including pectin and hemicellulose, taste and aroma development from hydrolysis of starches into sugars, synthesis of volatile compounds including alcohols, aldehydes and esters, and pH increase reducing acidity, and the continued colour change through carotenoid accumulation (Baldwin, Goodner and Plotto, 2008). These processes continue and are accelerated throughout the ripening stage, regulated by accelerating ethylene release. During senescence these processes continue further in response to ethylene release, and important enzymes including polygalacturonase (PG) and pectinesterase (PE) remain active continuing to degrade cell wall structure. Additionally cell membranes start to degrade leading to ion leakage and further softening (Chun and Huber, 1998). Ethylene levels decrease; however, oxidative stress increases, resulting in the accumulation of reactive oxygen species (ROS) (Meitha, Pramesti and Suhandono, 2020), which in excessive levels, may carry potential human health implications. Cell death occurs, fruit structural integrity diminishes and creates opportunities for pathogen infections further accelerating senescence and spoilage.

2.2.2 Ripening and Senescence in Non-climacteric fruit

Abscisic acid (ABA) is a primary hormonal driver that undergoes transcriptional cascades in the ripening process of non-climacteric fruit. Carotenoid biosynthesis pathways facilitate the biosynthesis of ABA, which triggers functions similar to climacteric fruit by regulating the expression of ripening-associated genes (Gupta et al., 2022). Transcription factors including NAC, MYB and bHLH are upregulated which regulate processes including pigment biosynthesis: carotenoids, and specifically in pepper, capsanthin and capsorubin, while chlorophyll degrades, forming colour development. A range of enzymes, including PE, PG and PL, similar to tomato fruit, are expressed as a result of transcription factor regulation, which play a significant role in cell wall metabolism (Wang and Seymour, 2022). Conversely, enzyme expression occurs more gradually than climacteric fruit resulting in slower softening and the fruit may exhibit a longer shelf life compared with climacteric fruit. Subsequent senescence is also a slower process and more oxidative than ethylene-driven ripening

Leafy vegetables like lettuce undergo different development processes to fruit ripening and is representative of typical leaf growth. Development until commercial maturity takes between 2-5 weeks depending on the cultivar and its growing environment. The key processes exhibited during pre-harvest development include cell division and expansion in leaves, chlorophyll accumulates necessary for photosynthetic energy production, mesophyll cells accumulate sugars including sucrose and fructose contributing to flavour (Alberts et al., 2002). Through the development of the plant, a rosette head formation of leaves is formed, and mechanical protection is established through cell wall and cuticle thickening, which contributes to the structure and texture. At the physiological peak the water content is at its highest, contributing to leaf turgor, cell walls are intact, maintaining internal quality and protection from pathogen infection, and nutritional content is highest, determined by high concentrations of antioxidants, polyphenols and vitamins.

Postharvest degradation processes involved in early stages involve the upregulation of cytochrome c oxidase and mitochondrial respiration genes for ATP production to meet demands. Photosynthetic chlorophyll begins to degrade due to upregulation of enzymes, including chlorophyllase (CHC) and pheophorbide a oxygenase (PAO). Sucrose synthase (SUS) and invertase enzymes modulate sugar metabolism for energy. Lettuces produce low levels of ethylene gas induced by ACS and ACO, and can be induced in higher levels due to physical damage, pathogen exposure and exposure to external sources of ethylene. Lettuce is sensitive to ethylene, meaning senescence may be accelerated, reducing shelf life and quality, and contributing to the ripening and senescence of other fruit or vegetables within close proximity (Saltveit et al., 2003). Cell membranes undergo lipid peroxidation of the polyunsaturated fats, regulated by LOX gene, which increases in expression during senescence. This degradation also is associated with the generation of of volatile compounds from lipid hydroperoxide (HPL) and peroxygenase activity, which creates off-taste and odour. Cell wall degradation occurs throughout senescence, compromising the structural integrity, causing softening of leaves and loss of turgor. A range of senescence-associated enzymes contribute to degradation of structural components: pectin and cellulose, including PG, pectin methylesterase (PME), and PL. Wilting is caused by intercellular water loss and reduced turgor from intracellular water loss. Structural decline and cell wall breakdown, in addition to decline in phenolic

compounds, weakens leaf immunity and protection against pathogenic microbial infection further contributing to decay, reducing shelf life (Pogorelko et al., 2013).

The infrared spectrum has been explored identifying the interaction between compounds and molecular structures with infrared light and how the composition is expressed in a spectrum interferogram. Numerous studies have explored the spectral interpretation of organic tissues, and the compositional biochemistry is increasingly characterised at wavenumber-specific absorbance peaks, especially within the fingerprint region (Al-Kelani and Buthelezi, 2024).

2.2.3 The Role of Ethylene in Ripening Fruit

Ripening in climacteric fruit involves rises in respiration and ethylene production. Cell wall softening, sugar accumulation and aroma-volatile synthesis processes are coordinated by hormone Ethylene, a simple hydrocarbon gas (C2H4). Two enzymes are involved in the biosynthesis of ethylene gas; 1aminicyclopropane-1-carboxylic acid (ACC) synthase (ACS) and ACC oxidase (ACO) .

Expression of ACS genes is triggered by external stimuli including wounding or temperature changes, and maturity associated developmental cues. ACC is produced through the conversion of S-adenosylmethionine (SAM) which is catalysed by ACS (Barry, C.S., Giovannoni, J.J 2007) . The ACC is then converted to ethylene by ACO. A signalling cascade occurs once ethylene diffuses throughout the tissue to bind with ethylene receptors which upregulates ripening related genes.

System 2 ethylene is an important response and hallmark of climacteric fruit ripening, characterised by ethylene production and its autocatalytic nature. Autocatalytic ethylene production phase occurs after an initial surge in ethylene (system 1 ethylene) which activates RIN, NOR and CNR transcription factors in tomatoes. Ethylene biosynthesis is amplified through the upregulation of specific ACS and ACO genes by transcription factors (Yokotani, N. et al. 2009). This feedback loop causes system 2 ethylene level rises which dramatically accelerates ripening processes including colour changes, activation of cell wall- degrading enzymes including polygalacturonase and pectin methylesterase, sugar accumulation and the softening of fruit texture (Seymour, G.B. et al. 2013).

2.2.4 Preventing Early Spoilage in Fruit and Vegetables

Optimal climatic conditions, including appropriate temperature and relative humidity (El-Ramady *et al.*, 2015) alongside maintaining healthy agricultural systems and implementing sustainable practices are imperative for successful crop yields (Tahat *et al.*, 2020). Due to changes in climate such as: the increase in extreme weather events, rising temperatures, and less predictable precipitation, achieving sufficient crop yields is becoming more difficult, meaning it is more important than ever to minimise produce losses (Gomiero, Pimentel and Paoletti, 2011). Production must be coupled with a widely applicable and efficient system to avoid food loss and waste and extend shelf life to maintain quality, nutrition, and taste (Augustin *et al.*, 2016). Several methods can be practiced after harvest that reduce premature spoilage from occurring, the most common of which are temperature control, humidity control, and packaging design (Elik *et al.*, 2019). Other methods include ethylene inhibition and damage avoidance. Mass production of fruit and vegetables may require the application of multiple techniques to delay spoilage and maintain quality.

In some instances, fruit and vegetables may be manipulated by inhibiting the ripening stage. This is done in tomato by prematurely harvesting the fruit, and subsequently putting it into temperature-controlled storage (Augustin *et al.*, 2016). Early harvesting at the 'Breaker Stage', determined in tomatoes by incipient red colour development, delays the ripening processes and the subsequent spoilage. Fruit is stored in atmosphere-controlled containers containing gases that inhibit the natural release of ethylene. Before sale, the fruit is exposed to the synthetically produced gas; ethylene (Ebrahimi *et al.*, 2021), initiating the ethylene synthesis pathways, triggering ripening processes and continues to facilitate them with continued exposure (Liu *et al.*, 2015). Administering this process may extend shelf-life, but sacrifices flavour, aroma and colour development, potentially making the fruit less desirable to the consumer.

Measures can be taken to reduce the occurrence of mechanical damage that occurs through the supply chain to prevent incidence of pathogen infection through the damage site; a significant contributor to reduced shelf life. This might involve technical equipment, specific storage containers and additional packing materials to separate the

produce, and this extends to sufficient training for the labour workforce to implement preservative methods for handling (Li and Thomas, 2014).

Packaging can be an effective tool in maintaining produce quality, and can significantly extend the shelf life of products. 'Active Packaging' possesses additives to extend the product's shelf-life, these include natural compounds including tannins, lignans and flavonoids for their antimicrobial antioxidant properties (Singh *et al*., 2022). This has been a focus of development for several decades and encompasses a wide range of additives to achieve this purpose. A widely used example of this is 'Modified Atmosphere Packaging' (MAP) which inhibits the spoilage processes of a variety of items including meat products. An air-tight plastic packet is flushed with gas and then sealed. This is normally using carbon dioxide or a mixture of carbon dioxide and nitrogen (Muhlisin *et al.*, 2014) which significantly reduces the ability for microbial proliferation by creating an inhospitable environment. MAP is used to maintain quality, extend shelf-life, and additionally retain the product's aesthetic characteristics which is often an important driver for retailers. Plastic packaging, however, has been identified as a significant contributor to environmental pollution (Bauer *et al.*, 2022) which has motivated the development of methods that negate the need for using environmentally harmful packaging, whilst still meeting quality expectations. An important alternative is edible coatings applied directly to fruit, negating the need for extra packaging, for example: APeel Sciences ltd use cellulose-based coatings on fruit like avocados (Apeel Sciences, [Accessed: 3/7/2025]). Coatings have been widely used for several decades, however, recent technological developments have created improved and more suitable coating methods that are in line with contemporary market requirements (Vargas *et al.*, 2008; Galus *et al.*, 2020). Aside from their primary design for shelf life and quality preservation without the application of single-use materials destined for disposal, they must align with the necessity for safe human consumption and freedom of properties that negatively impact the natural environment (Jafarzadeh *et al.*, 2021). These properties that some edible coatings now provide have driven an increase in popularity (Perez-Vazquez *et al.*, 2023), however, new technological advancements are only currently used by a small number of suppliers in the main food supply chain. Sophisticated packaging may incur higher costs which are often passed on to the consumer making these products less accessible.

2.2.5 Extending Shelf-Life

The most widely practiced methods for extending shelf life and quality are the use of refrigeration and humidity regulation (Rawat, 2015) throughout the supply chain and in storage. Achieving optimal storage temperatures for produce is an effective method to extending the shelf life of fresh produce. Enzymatic activity in biochemical processes such as ripening, respiration, and consequential fruit degradation are directly affected by temperature (El-Ramady *et al.*, 2015). Respiration plays a vital role in maintaining optimal water content by mediating osmotic control and providing energy to support the maintenance of structural components. This sustains turgidity, provides the availability of water used in important molecular functions (Criddle *et al.*, 1997), and maintains structural integrity, maintaining quality and protecting from microbial infection. Enzymatic activity is increased by exposure to certain temperatures (Daniel *et al.*, 2008)and microbial colonisation (Qiu *et al.*, 2022) which accelerates fruit ripening and other metabolic processes and can result in accelerated degradation. Temperature also impacts the fruit's natural production and release of ethylene, delaying ripening. Therefore, shelf life can be extended with the slowing down of enzymatic activity using lower temperatures (Moon *et al.*, 2020).

The use of controlled temperature can be assisted with controlled humidity levels to further inhibit biochemical processes which might lead to early spoilage (Mahmood, Sultan and Miyazaki, 2019). Harvested tomato fruit stored in high humidity, reduces the need for transpiration and so reduces their overall water-loss (Montanaro, 2012). This enables the fruit to maintain turgidity, and firmness and reduce the associated structural damage that might lead to microbial infection. The use of controlled atmosphere storage facilities should be used to achieve optimal regulation of humidity levels combined with temperature control to slow down ripening, maintain physiological conditions, and extend the shelf life of tomatoes (Majidi *et al.*, 2012). Optimal post-harvest conditions are variable between different fresh fruits and vegetables, possibly varying between different varieties. Determination of these ideal conditions can only be characterised through testing. A more rigorous approach to combatting the reduction of food losses and preventing accelerated spoilage can be through understanding and defining the stages of fruit spoilage, which can be analysed by investigating the dynamics of biochemical

processes (Hoehn *et al.*, 2023). Effective analytical tools need to be established to facilitate this understanding.

2.2.6 The Role of Infrared Spectroscopy

In agriculture, the use of hyperspectral imaging is becoming more popular as it provides a non-destructive method for collecting biochemical information about plants (Morais *et al.,* 2019). Mid-infrared (MIR) spectroscopy has a range of applications, and is particularly useful due to the unique characteristics of the MIR region (2500-25,000 nm) of the electromagnetic spectrum (Ozaki, 2021). Many functional groups in organic molecules, such as carbohydrates, proteins, lipids, and cellulose, exhibit characteristic absorption bands. This allows for the detection and identification of specific chemical components in plant tissues (Movasaghi *et al.*, 2008). Additionally, the non-destructive nature of MIR spectroscopy is a substantial benefit for certain applications including shelf-life determination and fruit quality surveying (Cozzolino *et al.*, 2024). High throughput, and rapid analysis of datasets with large numbers of samples can be processed using IR spectroscopy. In the supply chain, these methods would benefit *in-situ* analysis, at different and multiple stages.

The fingerprint region of the MIR spectrum (1800-900 cm^{-1}) is of particular interest in biochemical analysis providing a unique biochemical signature associated with organic structures that can be used for highly specific identification (The Fingerprint Region, 2013). The complexity of the information distributed in the MIR spectrum provides greater specificity than the relatively simple near-infrared (NIR) spectrum (see section 1.11.3) making it a more attractive method for obtaining detailed biochemical information from samples, including key biomarkers. For example, carbohydrates are characterised by C - O stretching (1200-1000 cm^{-1}) and O - H bending (1450-1400 cm^{-1}) vibrations (Hong *et al.*, 2021) whilst proteins identified by Amide I (1700-1600 cm^{-1}) and Amide II (1600-1500 cm^{-1}) bands which arise from the C = O stretching and N - H bending vibrations of the peptide bonds (Sadat and Joye, 2020).

2.2.7 Aims and Objectives

This study investigated the potential of MIR spectroscopy as a predictive tool for reducing waste in food supply chains, focusing on fresh fruit and vegetables popular in the UK diet (YouGov, 2024). The ability of MIR to distinguish between two common commercial varieties of tomato, Arvento, a salad tomato, and Piccolo, a variety of cherry tomatoes based on the biochemical analysis, and associated spectral biomarkers, of post-harvest spoilage of fruit, was examined. Additionally, the impact of storage temperature on spoilage-related spectral biomarkers was investigated in three important and popular fresh fruit and vegetables: tomato, bell pepper, and lettuce. MIR spectroscopy was conducted on the surface of the produce, non-destructively to preserve the integrity of the product simulating the potential *in-situ* application of MIR spectroscopy in the supply chain. The resultant MIR spectra were subsequently subjected to chemometric analysis including principal component analysis (PCA), PCA coupled with linear discriminant analysis (PCA-LDA), and support vector machines (SVM) and assessed in the context of biomarkers predictive of spoilage that offer the potential for reducing waste in supply chains.

Research questions:

- During postharvest storage of tomatoes, peppers, and lettuces, what are the notable spectral changes?
- Can differentiation between produce stored at different temperatures be achieved through distinct spectral features?
- Can points in time be characterised using identified spectral markers?
- Can we establish informative spectral regions for tracking postharvest degradation?
- Are we able to map important biochemical changes temporally for the future application for predictive models?

Aims:

- Identify spectral biomarkers associated with spoilage of fruit
- Determine the effect of different post-harvest storage conditions on fruit quality

2.3 Methods

2.3.1 Plant Material and Data Acquisition

2.3.1.1 Salad and Cherry Tomato Varieties

Solanum lycopersicum var. 'Arvento' salad tomatoes provided 'loose with the vine removed' and 'Piccolo' (cherry tomatoes) were supplied by Suncrop ltd. Tomatoes were grown at Suncrop nursery in Yorkshire, they were untreated, unsprayed or 'organic'. 'Arvento' var. were stored after harvest at 12°C for 22 hours, transported on a temperature controlled lorry at 10°C for 4 hours, before storage at alternative Suncrop location in Chatteris, Cambridgeshire at 10°C for 4 days before courier transported at temperature 8-14°C for 6 hours to Lancaster Environment Centre where they were kept at 11-12°C upon arrival. 11 days from harvest, tomatoes (n = 35) were evaluated using Bruker Alpha 1 ATR-FTIR spectrometer. Seven timepoints between 11-30 days after harvest were measured to the point of spoilage and inability to continue measurements due to level of decay and integrity of the fruit.

Solanum lycopersicum var. 'Piccolo' were grown by Sterling Suffolk Ltd, Ipswich. Their production method was hydroponics in Coir grow slabs with supplementary lighting due to overwinter cropping. They remained untreated, unsprayed or 'organic'. Tomatoes were harvested and then transported at 10°C for 1.5 hours and stored at Suncrop Chatteris, Cambridgeshire site at 10°C for 3 days before being transported at 8-14°C for 6 hours to Lancaster Environment Centre where they were kept at 11-12°C upon arrival. 8 days from harvest, tomatoes (n = 35) were evaluated using Bruker Alpha 1 ATR-FTIR) spectrometer. Six timepoints between 8-28 days after harvest were measured to the point of spoilage and inability to continue measurements due to level of decay and integrity of the fruit. Variability in the timing of measurement acquisition was unavoidable due to accessibility to facilities during the COVID-19 pandemic.

2.3.1.2 Storing Fruit and Vegetables under Different Post-Harvest Temperatures

Tomato*:*

Solanum lycopersicum var. 'Roterno' tomato samples were supplied by Suncrop ltd. The tomatoes were unsprayed with synthetic pesticides and synthetic fertiliser free, defined as industry standard: 'organic'. Fruit harvested at breaker stage, and subsequently ripened using a ripening agent: Ethephon. They were stored at the producer location at 8-10°C for 7 days before being transported in a temperature-controlled vehicle at 8-14°C for a 6 hour journey from the Suncrop ltd Cambridgeshire producer location to the Lancaster Environment Centre where analysis was conducted. Upon arrival, the tomato fruit were washed with reverse osmosis (RO) water and immediately dried before storage.

The tomatoes were stored in the dark at two different temperature regimes, n = 6 : cold storage: 1-2°C, in a Prestcold cold store room in the Lancaster Environment Centre; Ambient temperature: 19-20°C in a Percival Scientific Model AR-36L3 incubator. The spectral acquisition was taken on 9, 12, 17, 19, 21, 24 and 30 days post-harvest (DPH). These tomatoes were prepared before spectral acquisition, requiring a new individual for spectral analysis at every time point. Tomatoes were cut using a sterilised scalpel into 4 quarters from the stem base, and the internal locular fluid containing the seeds was removed. Spectral readings were taken from the outer surface of the cut pieces organised by three readings on three quarters and one on the remaining quarter chosen randomly. The scalpel was sterilised using 70% (v/v) ethanol application and diffusion.

Pepper

Capsicum annuum var. 'Artega' pepper samples were provided by Suncrop Ltd. The peppers were untreated: unsprayed with synthetic pesticides and synthetic fertiliser free, defined as industry standard: 'organic'. They were stored at the producer location at 19°C for 3 days before being transported in a temperature-controlled vehicle at 8-14°C for 6 hours, then kept at 11-12°C upon arrival. Peppers were washed with reverse osmosis (RO) water and air-dried before storage.

Peppers were split into respective storage temperatures, n = 5 individuals per group and stored in the dark at three different temperature regimes: cold storage: 1-2°C in a Prestcold store room located in the Lancaster Environment Centre; medium temperature: 11-12°C in a Percival Scientific Model AR-36L3 incubator; ambient temperature: 19-20°C. Spectral acquisition was taken on 4, 7, 11, 16, 21, 25, 30 and 35 DPH. Peppers were cut using a scalpel into 3 pieces, and spectral readings were taken from cut pieces due to lack of contact with the spectrometer crystal. New individuals were cut immediately before data acquisition. Pepper spectral readings were taken from the outer surface of the cut pieces, organised by three readings on two pieces and four on the remaining third.. The scalpel was sterilised using 70% (v/v) ethanol, applied and diffused.

Lettuce*: Lactuca sativa* var. 'Da Vinci' lettuces were grown from seeds in a controlled environment room (CE room) at the Lancaster Environment Centre. Seeds were germinated on filter paper and kept in the dark for 48 hours, then the lighting sequence (400-w metal halide) was changed to a 12-hour light/dark rotation. At 7 days, the seedlings were transplanted into 40 cell plug trays for 2 weeks using John Innes no.2 compost. The plugs were then transplanted into 2-litre pots for a further 6 weeks. The CE room temperature ranged between 21°C-26°C, mean = 23.34°C and humidity mean = 63.60% from germination to harvest. After growth, the lettuces were quality controlled and chosen based on heterogeneity and minimal damage or defects. 30 lettuce heads were harvested using a sterilised (70% (v/v) ethanol) Stanley knife and distributed at random into 3 sample treatment groups (n = 10 individuals per group), these groups were put into storage conditions determined by temperature: cold storage: 1-2°C in a Prestcold cold store room located in the Lancaster Environment Centre; medium temperature: 11-12°C in a Percival Scientific Model AR-36L3 incubator; ambient temperature Percival Scientific Model AR-36L3 incubator: 19-20°C. A single leaf was removed from the base of the lettuce head using a sterilised (70% (v/v) ethanol applied and diffused) Stanley knife immediately before spectral reading. Spectral acquisition was conducted at 2, 4, 6, 8, 10, 12, and 14 DPH

2.3.1.3 Attenuated Total Reflectance - Fourier Transform Infrared (ATR-FTIR) Spectroscopy

Samples were analysed using a Bruker Alpha 1 ATR-FTIR spectrometer and Opus version 7.1 software. Readings obtained were an average of 24 scans. Between measurements, the spectrometer crystal was cleaned using Bruker isopropyl alcohol wipes. A background spectrum of air was taken between each sample measuring the signal contribution of the instrument and its surrounding environment, providing a reference which is subtracted from the sample spectra to avoid including interference from the surrounding environment.

Individual fruits were placed onto the diamond in 10 locations, a spectrum was measured at each point to provide sufficient replicates for PCA-LDA in addition to minimising the effect of natural tissue heterogeneity, potentially masking the subtle effects underpinning biomarkers of decay. The time-series measurements were continued until the physical integrity of the samples was degraded to a point that the spectrometer instrument was unable to produce usable spectra due to insufficient contact with the spectrometer crystal.

2.3.1.4 Chemometric Analysis.

Spectral data were imported into MATLAB Version: 9.10.0.1602886 (R2021a, MathWorks, Inc., Natick, MA). iRootLab version 0.17.8.22-d (Copyright 2012 Julio Trevisan, Francis L. Martin & Plamen P. Angelov) package for MATLAB was used for preprocessing and subsequent data analysis. The raw spectral data was truncated to isolate the mid-infrared biochemical fingerprint region (1800-900cm^{-1}) before applying the Savitzky-Golay (SG) smoothing filter (second-order differentiation, second-order polynomial fitting, 9 filter coefficients) to remove scattering, noise and undesired artefacts. This was followed by vector-normalisation of the data (Butler *et al.*, 2015; Skolik *et al.*, 2019; Morais *et al.*, 2020).

Exploratory analysis was conducted using principal component analysis (PCA) which reduces the dimensionality of the data, improving the interpretability of large datasets with large numbers of features. The principal component axis displaying the greatest separation and class clustering with the highest variability is selected using PCA scores

plots. In the cases where PCA alone was unable to achieve substantial separation between the classes, PCA-LDA was applied. Loadings plots were generated and key wavenumbers were identified based on the greatest variances between the spectra (Jolliffe and Cadima, 2016).

Support vector machine (SVM) machine learning models were applied to both classify time-post-harvest and the storage temperature conditions. The preprocessed spectral data are randomly split into training and test subsets (70% and 30% respectively) using 5-fold cross-validation optimisation to control the level of over or underfitting. This applied SVM used a Gaussian kernel function for capturing non-linear relationships in the data. The SVM required a different set of preprocessing methods, SG filter with first differentiation order, vector-normalisation with an additional normalisation method of min-max scaling. The SVM provided an accuracy metric described by a percentage accuracy of the prediction for each class (Brereton, 1987).

2.4 Results

2.4.1 Arvento and Piccolo Tomatoes Both Exhibit a Marked Decrease in Quality Over Time

Upon arrival, all Arvento tomato samples were visually assessed, they were ripe from recent harvesting,, firm to the touch: free from softening by ripening or spoilage They were free from visible defects, for example: bruising, shrivelling, or microbial growth. They exhibited uniform characteristic red/orange colouration, an example individual is shown in Figure 2.1. At 11 DPH (Figure 2.1A), tomatoes remained fresh, some had minor discolouration, at 14 DPH (Figure 2.1B) tomatoes remained much the same in appearance. Fruit quality began to decline by 17 DPH (Figure 2.1C) with evidence of softening and cuticle wrinkling. By 21-24 DPH (Figure 2.1D & E), there were visually noticeable soft spots exhibited through changes to shape and colour and the presence of wrinkling. At 24 DPH (Figure 2.1E) there was one individual with a minor cuticle tear emitting fluid leakage. At 27 DPH (Figure 2.1F), the fruit were becoming more difficult to take readings from due to softness. The torn individual at 27 DPH had become more obviously spoiled with heavy fluid leakage. At 30 DPH (Figure 2.1G), more than half of the

tomatoes appeared to be unfit for consumption with extensive softening, 2 occurrences of mould presence indicating an unidentified pathogen infection, 3 individuals showed signs of fluid leaks leading to complete deterioration by 33 DPH where the experiment was concluded with no spectral readings taken.

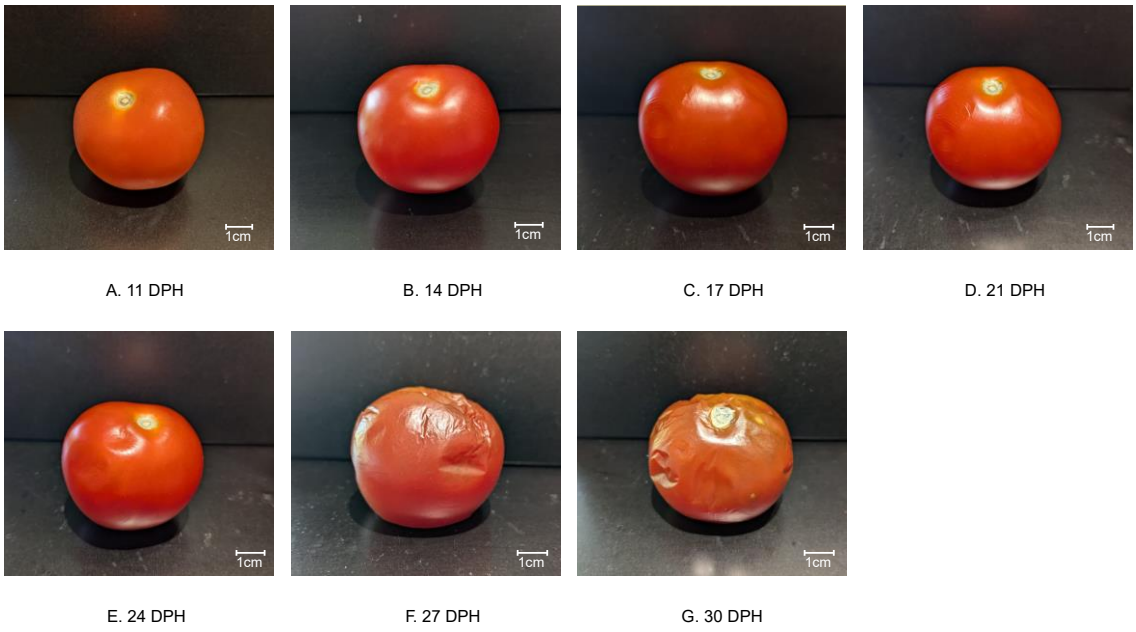

Figure 2.1. Photographic images of whole *Solanum lycopersicum* 'Arvento' tomato samples *Lactuca sativa*, at 11, 14, 17, 21, 24, 27 and 30 days post-harvest (DPH).

Piccolo tomatoes arrived on the vines, ripe, firm and vibrant red colouration. Their quality remained consistent until 22 DPH with slight softening occurrences in most individuals. At 28 DPH, softening had increased significantly with 7 individuals exhibiting split cuticles. At 31 DPH, more than half the batch were unable to be read on the spectrometer, resulting in the timepoint being abandoned and the time-series concluded. In both varieties, the remaining fruit undescribed by spoilage identifiers varied in visible quality with some individuals remaining visibly unchanged from the start of the time series.

Consistent signs of decline in the quality of Arvento tomatoes began showing from 17DPH, while acceptable quality was maintained in Piccolo until 22DPH. They both rapidly deteriorated thereafter, with more than half of Arvento being unfit for measurement by 30DPH. Cultivar-associated post-harvest marketability are highlighted

from these results, indicated by softening, cuticular wrinkling, and fluid leakage as indications, marking critical thresholds for quality loss.

2.4.2 Chemometric Analysis Revealed Differences in Spectral Signatures Between Arvento and Piccolo Tomatoes

Each tomato variety group was analysed in a time series that followed tomato fruit after harvest. Figure 2 displays the mean spectra within the fingerprint region of each category or class, the categories in this study are separated into 'days post-harvest' (DPH) time points. Figures 2.2A & C display the raw, unprocessed spectra, Figure 2.2B & D display these data after the application of preprocessing techniques.

Using the preprocessed spectra, visual separations between classes can be observed at wave numbers 1623 cm^{-1}, 1556-1530 cm^{-1} (1520-1560 cm^{-1} nitro compounds), 1217 cm^{-1} (1250-1200 cm^{-1} vinyl ether), 1166 cm^{-1} (1180-1160 cm^{-1} sulfoxide) and 1014 cm^{-1} (C - O and C - C bond stretching in polysaccharides) in Arvento tomatoes and at 1174 $cm^{-1}$and 1166 cm^{-1} (1160-1180 cm^{-1} sulfoxide) in Piccolo tomatoes (Colthup, 1975b).

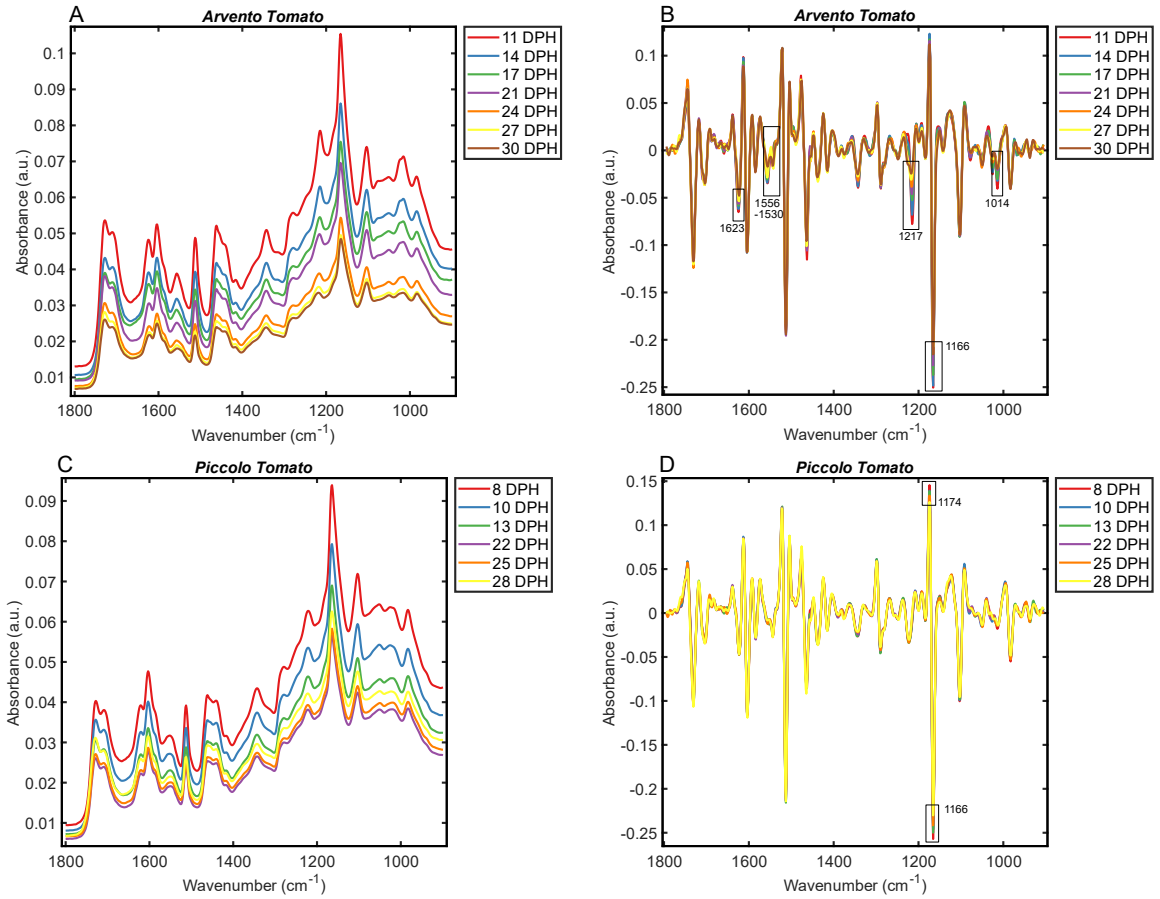

Figure 2.2. A,B) *Solanum lycopersicum* 'Arvento' tomato samples **C,D)** *Solanum lycopersicum* 'Piccolo' tomato samples **A,C)** Fingerprint region of the unprocessed data displayed using class means. Classes consist of different time points: classified by the number of days post-harvest (**DPH**). **B,D)** Class means of preprocessed data within the fingerprint region (1800-900 cm^{-1}). Preprocessing techniques include: Satvitzky-Golay filter with second differentiation order and vector normalisation.

An exploratory unsupervised PCA model was applied to the preprocessed spectral data, seen in Figure 3. PCs are orthogonal axes containing data plotted based on their variances. PC1 is the direction with the greatest variance, PC2 the second, PC3, the third etc. PCs do not correspond to single measurements. The variables that explain the variances can be explored in PCA loadings that identify the wave regions or wavenumbers that these variances occur. Visualisation of useful variances expressed in the data is explored by plotting the axes against each other in differing combinations, through this class-associated differentiation may be seen. In Arvento tomatoes (Figure 2.3A), class separation by DPH can be observed along PC2 which explains 7.46% of the variance. PC1,

2 and 3 explained 27.41% of the total variance (PC1: 13.9%, PC2: 7.46%, PC3: 6.05%). The spread of the data points within each class appears to become greater the earlier in the time series suggesting there is more variability between the individual tomatoes at earlier stages of spoilage. Overall, close clustering indicates low variability. In Piccolo tomatoes (Figure 3D), PC1, 2 and 3 accounted for 30.98% of the total variance (PC1: 12.4%, PC2: 10.9%, PC3: 7.68%). There is less visible variability between each timepoint, however, there is a clear, wide, spread within the time point classes along the PC2 axis, especially at 8 DPH, in contrast to highly concentrated data from 28 DPH. Along PC3, all timepoint classes share a similar spread and overlap with each other, suggesting that spectral similarities were not distinct enough to separate entirely.

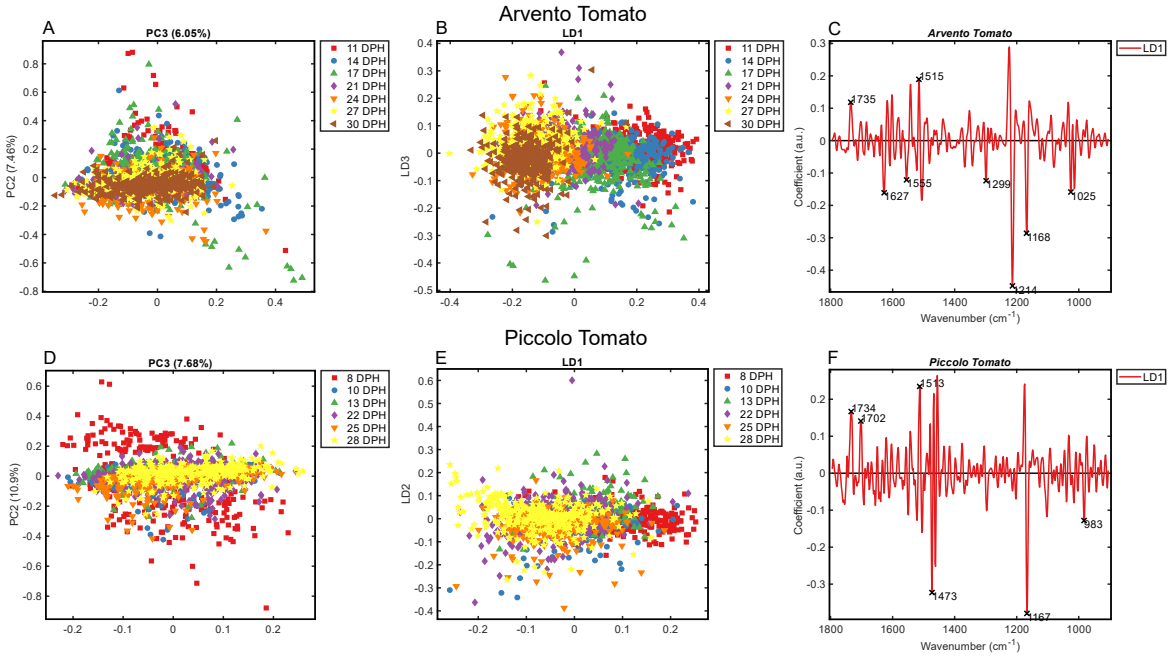

Figure 2.3. A-C) *Solanum lycopersicum* 'Arvento' tomato multivariate analyses. **D-F**). *Solanum lycopersicum* 'Piccolo' tomato multivariate analyses. **A,D**) Principal Component Analysis (PCA). **B,E**) Principal Component Analysis with Linear Discriminant Analysis (PCA-LDA), **C,F**) PCA-LDA Loadings plots with significant wavenumbers associated with greatest variances.

PCA-LDA class supervised analysis was applied and demonstrated a higher degree of separation between time point classes in both tomato varieties. In Arvento tomatoes (Figure 3B), there is a clear distribution along LD1 showing time points clustered, these time point clusters are spread along the axis in the expected temporal order. However,

the time points overlap suggesting spectral similarities. When isolating the first and last time points (11 DPH and 30 DPH), they are distinct without an overlap indicating they are highly variable from each other. This can also be described along LD1 in Piccolo tomatoes (Figure 2.3E). Loading plots associated with PCA-LDA analysis display significant wavenumbers associated with the highest variances between classes. 1735 cm^{-1}, 1627 cm^{-1}, 1555 cm^{-1}, 1515 cm^{-1}, 1299 cm^{-1}, 1214 cm^{-1}, 1168 cm^{-1} and 1025 cm^{-1} have been identified in Arvento tomatoes (Figure 3C & Table. 1) and in Piccolo tomatoes, significant wavenumbers of: 1734 cm^{-1}, 1702 cm^{-1}, 1513 cm^{-1}, 1473 cm^{-1}, 1167 cm^{-1}, and 983 cm^{-1} were identified (Figure 2.3F). Similar peak wavenumbers were identified between both tomato varieties including 1735 cm^{-1} (Arvento) and 1734 cm^{-1} (Piccolo) both associated with C = O carbonyl group stretching, typically found in esters, aldehydes and ketones. 1515 cm^{-1} (Arvento) and 1513 cm^{-1} (Piccolo) are both associated with aromatic C = C stretching or the C - C stretching vibrations within aromatic rings, additionally 1168 cm^{-1} (Arvento) and 1167 cm^{-1} (Piccolo) are associated with C - O stretching in polysaccharides or carbohydrates (Colthup, 1975b).

Table 2.1. Loadings showing the key wavelengths exhibiting the greatest variances for post-harvest *Solanum lycopersicum* 'Arvento' and 'Piccolo' tomato fruit. The temporal element of these data means these variances are associated with biochemical changes. Listed are the isolated wavenumbers from PCA loadings and their wave regions and their assigned biochemical compounds, obtained through the body of literature.

Arvento Loadings			
Wavenumber (cm-1)	**Wavenumber Range**	**Compound Assignment**	**Reference**
1735	1740-1720 1750-1715 1750-1735	C = O Aliphatic aldehydes C = O Lactones six-membered ring C = O Saturated esters	(Colthup, 1975b)
1627	1800-1600 1665-1585 1655-1560	C = O Stretching: Ketones, aldehydes, carboxylic acids d- and x-L-amino acids C = N Pyrrolines	(Colthup, 1975b)

	1660-1625	Organic nitrates	
1555	1600-1500 1605-1555	C = O Stretching vibration: Alkenes, aromatic compounds CO_2 Asymmetric stretch: Normal chain amino acids	(Colthup, 1975b)
1515	1600-1500 1530-1490	C = O Stretching vibration: Alkenes, aromatic compounds NH_3 Normal chain amino acids	(Colthup, 1975b)
1299	1330-1260	C - N Phenyl stretching: Primary aromatic amines	(Colthup, 1975b)
1214	1214-1185 1210-1310 1225-1200 1260-1180 1240-1170	C – O Ester formates Aromatic ether alkoxy C – O - C stretching: Alkyl vinyl ethers Phenols C – NH_2 Primary amines	(Colthup, 1975b)
1168	1200-1000 1210-1160	C - O Stretching: Polysaccharides C - O Streching: Saturated esters	(Colthup, 1975b)
1025	1050-1010 1025-1047 1075-1000 1125-1000 1022-1038	Aromatic ether alkoxy Aromatic ether methylene-1, 2-disoxybenzenes phenyl - CHOH- Aromatic secondary alcohols C – O Carbohydrates 1125-1000 C – NH_2 Primary amines (weak)	(Colthup, 1975b)
Piccolo Loadings			
1734	1740-1720 1835-1715 1750-1715	C = O Aliphatic aldehydes C = O Conjugated esters Lactones six-membered ring	(Colthup, 1975b)
1702	1750-1700 1710-1685	C = O Stretching: Esters C = O Aromatic aldehydes	(Colthup, 1975b)
1513	1530-1490	NH_3 Symmetric deformation: Normal chain amino acids	(Colthup, 1975b)

1473	1500-1400 1484-1390	C – H Bending NH_4 deformation: Ammonium ion	(Colthup, 1975b)
1167	1210-1160	C – O Saturated esters	(Colthup, 1975b)
983		Unassigned	

Between Arvento and Piccolo tomatoes, temporal patterns were revealed in PCA showing distinct separation. Variability and class separation emerged at early-stages along PC2, while a concentrated distribution was exhibited at later-stages in Piccolo. Supervised modelling using PCA-LDA enhanced separation in both cultivars, indicating it as a useful tool to the interpretation of post-harvest progression associated in class differences.

2.4.3 SVM Machine Learning for Classifying Time points in Piccolo and Arvento Tomatoes

A support vector machine (SVM) learning model was applied to classify tomato fruit based on their developmental time points (days post-harvest, DPH), to determine whether spectral data could reliably identify fruit age as a proxy for physiological stage, Figure 4 displays the classification accuracy rate at various time points (DPH) for Arvento and Piccolo tomato varieties. Arvento variety achieved the highest level of 68.2% model classification accuracy at 11 DPH, higher than by chance but possibly unusable for commercial classification, with lower accuracy rates as the time series progressed being lowest at 24 DPH (27.59%) (Figure 2.4A). Significant misclassification occurred between neighbouring time points, the highest misclassification was 32.07% at 30 DPH/27 DPH, a higher value than the lowest accuracy of classification. In contrast, accuracy in Piccolo, was much higher, reaching 96.12% at its highest, and lowest result of 66.16%, only slightly lower than the highest value in Arvento tomato DPH classification (Figure 2.4B). Misclassification remained at low levels throughout the model with the exception of 22 DPH against all other time-points, hitting misclassification of between 12.47% and 26.3%.

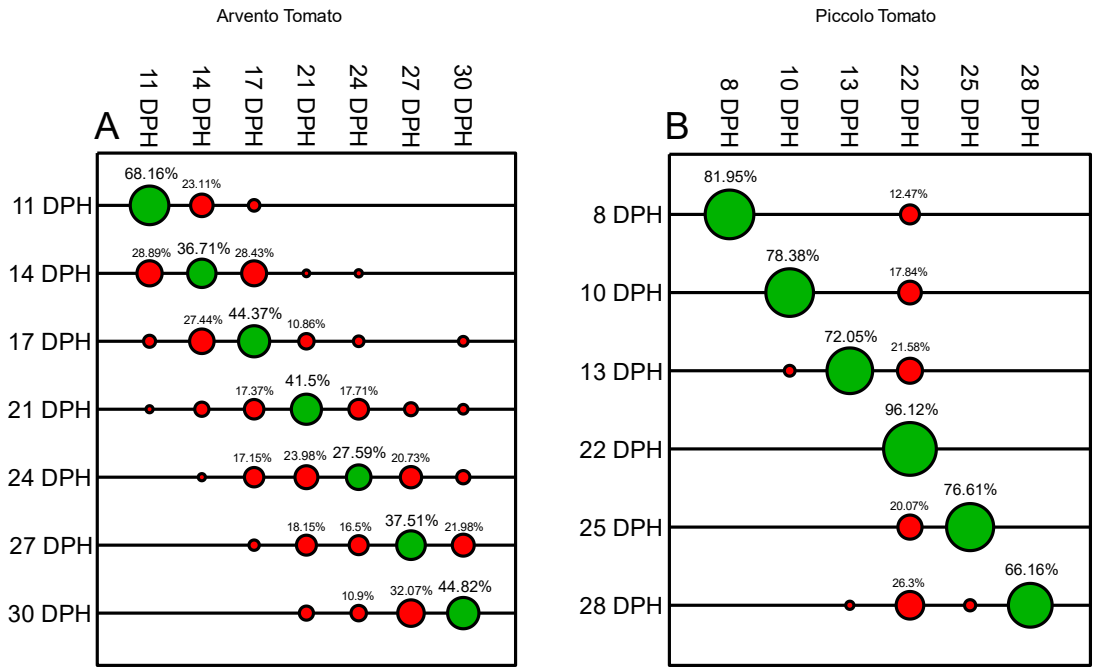

Figure 2.4. A) *Solanum lycopersicum* 'Arvento' tomato SVM confusion matrix **B)** *Solanum lycopersicum* 'Piccolo' variety SVM confusion matrix displaying accuracy percentage of the SVM model at each timepoint class, classified by days post-harvest (**DPH**).

Overall, Piccolo tomato post-harvest age was markedly more successfully classified in SVM machine-learning modelling through achieving high accuracy of up to 96.12% and misclassification was consistently low. This is compared with the frequent errors in classification between neighbouring time-points of Arvento tomatoes, and a commercially unusable score of 68.2% accuracy. These results suggest that differences in how spectral signatures track physiological post-harvest stages are cultivar-specific.

2.4.4 PCA Loadings Presented Wavenumber Associated Peak Variances Between Time Points

Neighbouring time points through the series were isolated and PCA models were performed to explore the data spread at those stages, and whether the classes naturally spread without assistance from LDA. PCA loadings were obtained to get a greater understanding of the specificity of the chemical processes of spoilage acting along the time series (Arvento: Figure 2.5, Piccolo: Figure 2.6). PCA-LDA was not performed due to

seeing largest chemical variances for both time points together without class discrimination. In every time point pairing there is significant overlap between the two time points however the data spread varies. In 17 & 21 DPH (Figure 2.5E), 17 DPH has a large spread along PC2 and PC3 axes, however, 21 DPH is largely spread along PC3 but is concentrated along PC2, suggesting that despite the large similarities in the spectra, there are spectral differences, this may be associated with a biochemical change occurring at 17 DPH that reduces at 21 DPH. This spread difference can be observed again at 27 & 30 DPH (Figure 2.5K); at 27 DPH there is a large spread on both PC2 and PC3 axes compared with 30 DPH showing a reduced variability along PC2 axis. Loadings associated with 17 & 21 DPH (Figure 2.5F) identify a distinct peak at wavenumber 1462 cm^{-1} which may be associated with the spread difference between the two time points. 1462 cm^{-1} is associated with the bending or deformation vibrations of CH_2 or CH_3 groups, particularly in lipids and fatty acids (Colthup, 1975b). At timepoint pair 27 & 30 DPH (Figure 2.5L), three prominent wavenumbers occurred: 1732 cm^{-1}, 1508 cm^{-1}, and 1473 cm^{-1}, all previously occurred earlier in the time series. The most distinct peak at 1508 cm^{-1} is associated with polyphenols, carotenoids, and proteins (Colthup, 1975), suggesting these could describe the biochemical changes displayed in this data distribution. In Piccolo tomatoes, the distribution of data variability is largely indistinct within each timepoint pair except in 8 & 10 DPH. At 8 DPH, there is a variable spread on both axes: PC1 and PC3 with 10 DPH showing a concentrated distribution along PC1, again this suggests a biochemical change happening at 8 DPH that decreases by 10 DPH.

Significant wavenumbers repeatedly occur throughout the Arvento time-series tomatoes, including 1731 cm^{-1} occurring in 11 & 14 DPH, 14 & 17 DPH, 17 & 21 DPH, and 21 & 24 DPH, and similar 1732 cm^{-1} in 27 & 30 DPH (Figure 2.5B, D, F, H, & L) both associated with fatty acids and esters. Similarly, 1511 cm^{-1} appears in 11 & 14 DPH, 14 & 17 DPH and 21 & 24 DPH (Figure 2.5B, D, & H) associated with aromatic ring vibrations related to phenolic compounds (Table 2.2). At 17 & 21 DPH a distinct peak occurs at wavenumber 1462 cm^{-1}, frequently associated with alkanes. Alkanes are major structural components in the membrane and cuticle (Rios *et al.*, 2015). At 24 & 27 DPH and 27 & 30 DPH, 1508 cm^{-1} appears as a distinct peak associated with aromatic ring vibrations.

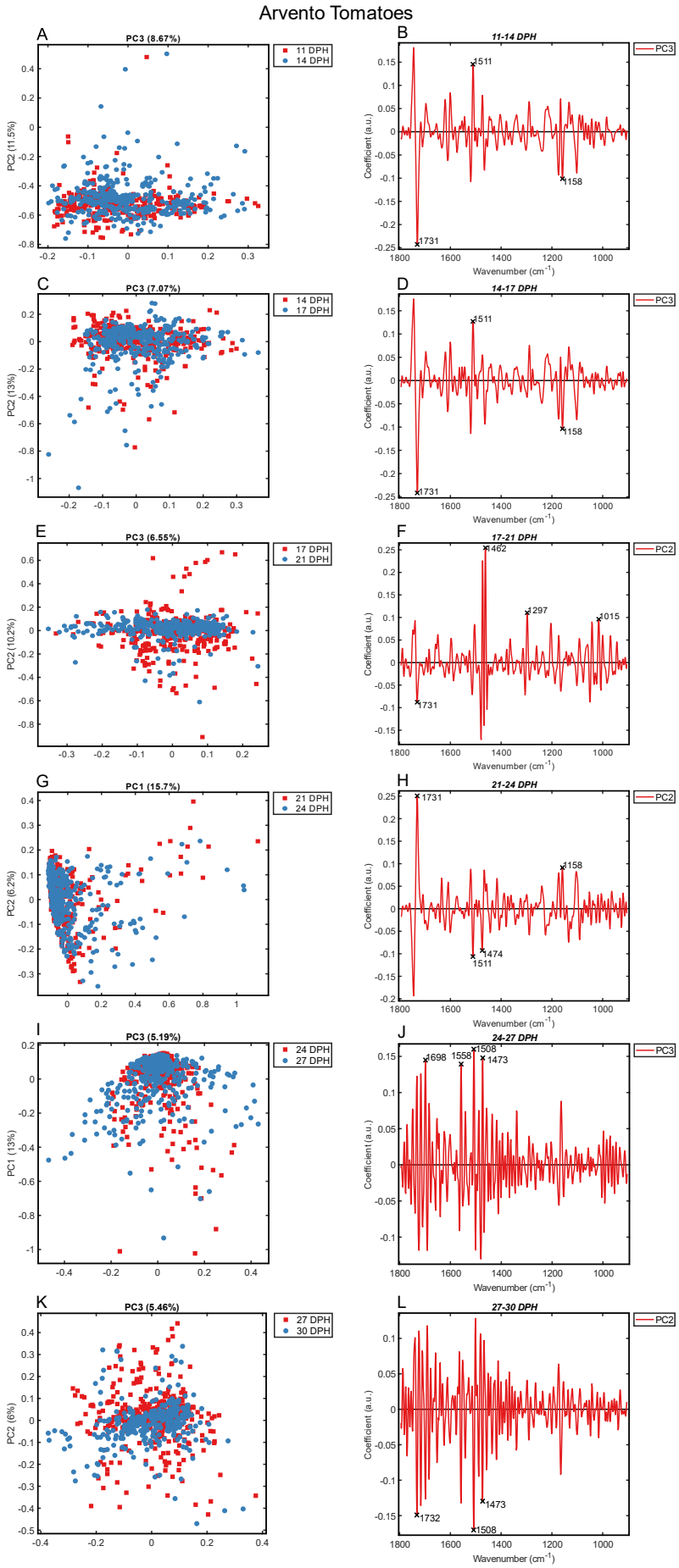
Arvento Tomatoes
A
PC3 (8.67%)
11 DPH
14 DPH
PC2 (11.5%)
B
11-14 DPH
PC3
1511
1158
1731
Coefficient (a.u.)
Wavenumber (cm-1)
C
PC3 (7.07%)
14 DPH
17 DPH
PC2 (13%)
D
14-17 DPH
PC3
1511
1158
1731
Coefficient (a.u.)
Wavenumber (cm-1)
E
PC3 (6.55%)
17 DPH
21 DPH
PC2 (10.2%)
F
17-21 DPH
PC2
1462
1297
1015
1731
Coefficient (a.u.)
Wavenumber (cm-1)
G
PC1 (15.7%)
21 DPH
24 DPH
PC2 (6.2%)
H
21-24 DPH
PC2
1731
1158
1474
1511
Coefficient (a.u.)
Wavenumber (cm-1)
I
PC3 (5.19%)
24 DPH
27 DPH
PC1 (13%)
J
24-27 DPH
PC3
1698
1558
1508
1473
Coefficient (a.u.)
Wavenumber (cm-1)
K
PC3 (5.46%)
27 DPH
30 DPH
PC2 (6%)
L
27-30 DPH
PC2
1732
1473
1508
Coefficient (a.u.)
Wavenumber (cm-1)

Figure 2.5. Principal component analysis PCA scores (**A, C, E, G, I** & **K**) and loadings plots (**B, D, F, H, J** & **L)** for *Solanum lycopersicum* 'Arvento' tomato. Consecutive time points were compared sequentially, and the highest variances for each pairwise comparison identified at specific wavenumbers.

In Piccolo variety (Figure 2.6), 1541 cm^{-1} occurs in 13 & 22 DPH, and 22 & 25 DPH, is associated with amide II band, a marker for proteins. Aromatics associated wavenumber 1507 cm^{-1} appears in 13 & 22 DPH earlier than in Arvento tomatoes where 1508 cm^{-1} appears at 24 & 27 DPH. 1464 cm^{-1}, 1457 cm^{-1}, 1457 cm^{-1} and 1467 cm^{-1} NH_4 deformation: Ammonium ion, alkanes and Boron associations appear at 10 & 13 DPH, 13 & 22 DPH, 22 & 25 DPH and 25 & 28 DPH respectively (Figure 2.6D, F, H, & J) .

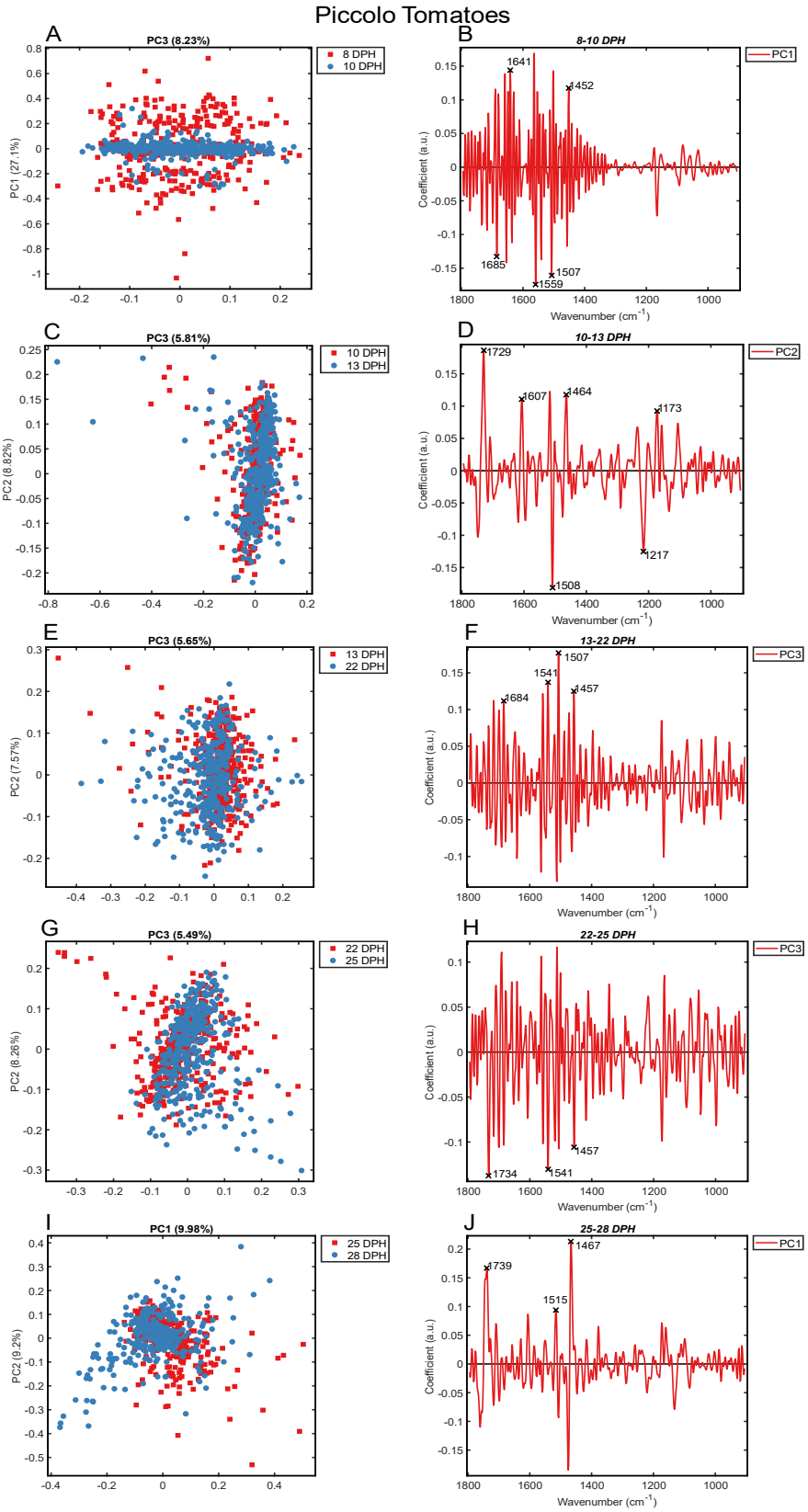
Piccolo Tomatoes
A
PC3 (8.23%)
8 DPH
10 DPH
PC1 (27.1%)
B
8-10 DPH
PC1
1641
1452
1685
1507
1559
Coefficient (a.u.)
Wavenumber (cm-1)
C
PC3 (5.81%)
10 DPH
13 DPH
PC2 (8.82%)
D
10-13 DPH
PC2
1729
1607
1464
1173
1217
1508
Coefficient (a.u.)
Wavenumber (cm-1)
E
PC3 (5.65%)
13 DPH
22 DPH
PC2 (7.57%)
F
13-22 DPH
PC3
1507
1541
1457
1684
Coefficient (a.u.)
Wavenumber (cm-1)
G
PC3 (5.49%)
22 DPH
25 DPH
PC2 (8.26%)
H
22-25 DPH
PC3
1457
1734
1541
Coefficient (a.u.)
Wavenumber (cm-1)
I
PC1 (9.98%)
25 DPH
28 DPH
PC2 (9.2%)
J
25-28 DPH
PC1
1467
1739
1515
Coefficient (a.u.)
Wavenumber (cm-1)

Figure 2.6. Principal component analysis PCA scores (**A, C, E, G** & **I**) and loadings plots (**B, D, F, H** & **J)** for *Solanum lycopersicum* 'Piccolo' tomato. 2 closest time points have been isolated and highest variances identified at specific wavenumbers

Table 2.2. Loadings showing the key wavelengths exhibiting the greatest variances for post-harvest *Solanum lycopersicum* 'Arvento' and 'Piccolo' tomato fruit. The temporal element of these data means these variances are associated with biochemical changes at adjacent time-points. Listed are the isolated wavenumbers from PCA loadings and their wave regions and their assigned biochemical compounds, obtained through the body of literature.

Arvento (Figure 5)				
DPH	**Wavenumber (cm-1)**	**Wavenumber Range**	**Compound Assignment**	**Reference**
11-14	1731	1750-1700 1740-1720 1735-1715 1750-1714	C = O Stretching vibrations in carbonyl groups: Esters, aldehydes, and ketones C = O Aliphatic aldehydes C = O Conjugated esters Lactones, six-membered ring	(Colthup, 1975b)
	1511	1530-1490	C=C stretching: Aromatic compounds NH_3 Normal chain amino acids	(Colthup, 1975b)
	1158	1300-1000	C-O stretching or C-C stretching in some cases. Alcohols, Ethers, and Esters	(Colthup, 1975b)
14-17	1731	1750-1700 1740-1720 1735-1715 1750-1714	C = O stretching vibrations in carbonyl groups: Esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)

			C = O Conjugated esters Lactones, six-membered ring	
	1511	1600-1500 1530-1490	C=C stretching: Aromatic compounds NH_3 Normal chain amino acids	(Colthup, 1975b)
	1158	1300-1000	C-O stretching or C-C stretching in some cases. Alcohols, Ethers, and Esters	(Colthup, 1975b)
17-21	1731	1750-1700 1740-1720 1735-1715 1750-1714	C = O stretching vibrations in carbonyl groups: Esters, aldehydes, and ketones C = O Aliphatic aldehydes C = O Conjugated esters Lactones six-membered ring	(Colthup, 1975b)
	1462	1470-1440 1484-1390 1465-1330	CH_2 bending vibrations (scissoring) in alkanes NH_4 deformation: Ammonium B – N Boron	(Colthup, 1975b)
	1297	1330-1260	C - N Phenyl stretching: Primary aromatic amines	(Colthup, 1975b)
	1015	1050-1010 1075-1000 1125-1000	C - O stretching vibrations: Primary alcohols or ethers Aromatic ether alkoxy phenyl – CHOH - Aromatic secondary alcohols C - O stretching carbohydrates	(Colthup, 1975)

21-24	1731	1750-1700 1740-1720 1735-1715 1750-1714	C = O stretching vibrations in carbonyl groups: Esters, aldehydes, and ketones C = O Aliphatic aldehydes C = O Conjugated esters Lactones six-membered ring	(Colthup, 1975b)
	1511	1600-1500 1530-1490	C=C stretching: Aromatic compounds NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
	1474	1470-1440 1484-1389	C-H bending: Aliphatic chains or aromatic rings NH_4 deformation: Ammonium ion	(Colthup, 1975b)
	1158	1300-1000	C – O stretching: Ethers, alcohols and esters	(Colthup, 1975b)
24-27	1698	1700-1670 1710-1640	C = O singly conjugated ketones Thiol esters	(Colthup, 1975b)
	1558	1600-1500 1600-1550 1605-1555	C = C stretching vibrations: Aromatic compounds, C = C β-carotene CO_2 stretch: Normal chain amino acids	(Quijano-Ortega *et al.*, 2020) (Colthup, 1975b)
	1508	1600-1500 1530-1490	C = C stretching vibrations: Aromatic compounds NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
	1473	1484-1389	NH_4 deformation: Ammonium ion	(Colthup, 1975b)

27-30	1732	1740-1720 1735-1715 1750-1714	C = O stretching vibrations in carbonyl groups: Esters, aldehydes, and ketones C = O Aliphatic aldehydes C = O Conjugated esters Lactones six-membered ring	(Colthup, 1975b)
	1508	1600-1500 1530-1490	C = C stretching vibrations: Aromatic compounds NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
	1473	1484-1389	NH_4 deformation: Ammonium ion	(Colthup, 1975b)
Piccolo (Figure 2.6)				
8-10	1685	1710-1685 1710-1639	C = O Aromatic aldehydes Thiol esters	(Colthup, 1975b)
	1641	1680-1620 1680-1640 1670-1630 1653-1635 1655-1560 1660-1625	C = C stretching: Protein amide I bands C = O doubly conjugated ketones Hydroxy aryl ketones Phenyl vinyl ether C = N Pyrrolines Organic nitrates	(Colthup, 1975b)
	1559	1600-1500 1600-1550 1605-1555	C = C stretching: Aromatic compounds C = C β-carotene CO_2 Normal chain amino acids	(Quijano-Ortega *et al.*, 2020) (Colthup, 1975b)
	1507	1530-1490	NH_4 deformation: Normal chain amino acids	(Colthup, 1975b)

	1452	1470-1440 1484-1389 1465-1330	CH_2 bending vibrations or C-H bending in aliphatic structures. CH_2 bending vibrations (scissoring) in alkanes, C = C stretching in aromatic rings NH_4 deformation: Ammonium ion B – N Boron	(Colthup, 1975b)
10-13	1729	1740-1720 1750-1714	C = O Aliphatic aldehydes Lactones six-membered ring	(Colthup, 1975b)
	1607	1680-1600 1640-1580 1665-1585 1655-1559	C = C stretching in aromatic systems C= O 1, 3-Diketones, enol form 1640-1580 NH_3 deformation α-L-amino acids C = N Pyrrolines	(Colthup, 1975b)
	1508	1530-1490	NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
	1464	1470-1440 1484-1390 1465-1330	CH_2 bending vibrations or C-H bending in aliphatic structures. CH_2 bending vibrations (scissoring) in alkanes, C = C stretching in aromatic rings NH_4 deformation: Ammonium ion B – N Boron	(Colthup, 1975b)

	1217	1210-1310 1225-1200 1260-1180 1170-1240	Aromatic ether alkoxy C – O - C stretching: Alkyl vinyl ethers Phenols C – NH_2 primary amines (strong)	(Colthup, 1975b)
	1173	1210-1160 1191-1171 1170-1240	C - O Saturated esters CH – NH – C Secondary amines C – NH_2 primary amines (strong)	(Colthup, 1975b)
13-22	1684	1700-1670 1710-1639	C = O singly conjugated ketones Thiol esters	(Colthup, 1975b)
	1541	1600-1500 1620-1539	C = C stretching in aromatic rings. Pyrrolines	(Colthup, 1975b)
	1507	1600-1500 1530-1490	C = C stretching vibrations: Aromatic compounds NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
	1457	1470-1440 1484-1389	CH_2 bending vibrations or C-H bending in aliphatic structures. CH_2 bending vibrations (scissoring) in alkanes, C = C stretching in aromatic rings NH_4 deformation: Ammonium ion	(Colthup, 1975b)

22-25	1734	1750-1700 1740-1719	C = O stretching vibration in carbonyl groups: Esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
	1541	1620-1539	Pyrrolines	(Colthup, 1975b)
	1457	1470-1440 1484-1389 1465-1330	CH_2 bending vibrations or C-H bending in aliphatic structures. CH_2 bending vibrations (scissoring) in alkanes, C = C stretching in aromatic rings NH_4 deformation: Ammonium ion B – N Boron	(Colthup, 1975b)
25-28	1739	1750-1700 1740-1720 1740-1735	C = O stretching vibration in carbonyl groups: Esters, aldehydes, and ketones C = O Aliphatic aldehydes C = O Propionates	(Colthup, 1975b)
	1515	1600-1500 1530-1490	C = C stretching in aromatic rings NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
	1467	1470-1440 1484-1389 1465-1330	CH_2 bending vibrations or C-H bending in aliphatic structures. CH_2 bending vibrations (scissoring) in alkanes, C = C stretching in aromatic rings NH_4 deformation: Ammonium ion	(Colthup, 1975b)

			B – N Boron	

These results have highlighted patterns suggesting cultivar specific timing of changes in lipid, phenolic compounds and proteins postharvest are detectable without supervised methods. This was indicated through the use of pairwise PCA of neighbouring timepoints that revealed recurring biochemical signals. For example, fatty acids and esters at 1731-1732 cm^{-1} repeatedly were isolated as the greatest variances in Arvento, in addition to 1151 cm^{-1} associated with phenolic compounds repeatedly appearing along the time-course.

2.4.5 Storage Temperature had a Marked Effect on Spoilage Rates in Tomato, Pepper and Lettuce

Tomato: Upon arrival, Roterno tomatoes were firm, exhibited characteristic red/orange colouration, minimal softening no decay and no infection incidence. There were no visible changes in tomatoes stored at ambient temperature (19-20°C) until 19 DPH when three individuals displayed a slight loss of colour and structure and displayed mild softening. At 21 DPH, ambient tomatoes exhibited slight wrinkling whilst remaining 'saleable' based on visual observation; four individuals exhibited softened spots. In contrast, refrigerated tomatoes (1-2°C) remained firm and edible with no blemishes or infection incidence, although one individual showed signs of softening compared to the rest. The general structural integrity of the ambient-stored batch had declined by 24 DPH, but less prominently in the refrigerated tomatoes. This integrity loss made it more difficult to obtain spectral readings due to loss of contact with the spectrometer crystal. At 30 DPH, 1 individual from the refrigerated tomatoes was lost as physical contact was unable to be made to obtain spectral scans. In ambient tomatoes, cuticle breakages had occurred in two ambient individuals causing water loss however spectral readings were able to be taken. An unidentified pathogen incidence had also occurred in another ambient tomato, this was determined by the presence of a green fuzzy mould at the stem base. Remaining refrigerated tomatoes at 30 DPH exhibited further softening but were considered edible but categorised as difficult to sell. At 33 DPH, more than three of the tomatoes in ambient and one in refrigerated lost their structural integrity resulting in the time point being abandoned, concluding the time series.

Pepper: Upon arrival, red Artega peppers were fresh, firm and ripe with minimal softening no decay and no infection incidence. Quality remained consistent both visibly and texturally until 16 DPH where noticeable softening spots were present in ambient temperature (19-20°C) stored fruit. In peppers stored in the storeroom (11-12°C) and refrigerated (1-2°C) fruit remained unchanged. By 25 DPH, softening had occurred in storeroom and ambient temperature fruit, however, refrigerated remained relatively unchanged. At 21 DPH, ambient stored peppers displayed more softening but would still be considered as edible. Storeroom peppers were also exhibiting softening in two individuals. 25 DPH remained consistent of spoilage effects from 21 DPH across all groups. The initial occurrence of mild softening occurred in refrigerated peppers at 30 DPH. Discolouration; fading of red colour, wrinkling and dehydration was visibly apparent in all fruit stored at ambient with three individuals displaying strong internal black colouration which could be attributed to pathogen infection, and one individual with minor black internal spotting. Storeroom peppers displayed softening, and dehydration at 30 DPH in four individuals. At 35 DPH, ambient and storeroom fruit were soft, floppy, dehydrated, further developed blackening and considered unfit for sale. Refrigerated fruit remained edible with minor softening, but would be considered low quality for sale. At 38 DPH, refrigerated peppers remained structurally intact for readings to be acquired however, the time-series was concluded when degradation compromised the ability for spectral acquisition in four ambient individuals and two storeroom peppers. This was determined due to severe surface wrinkling and tissue breakdown causing insufficient contact with the spectrometer crystal.

Lettuce: Visual observations were taken accompanied with photographs (Figure 2.7) of Da vinci lettuce samples at 0, 7 and 14 DPH from each storage condition: Refrigerated (1-2°C), Storeroom (11-12°C) and Ambient (19-20°C). At 0 DPH, lettuce samples were homogenous in appearance with fresh, compact heads. The leaves appeared healthy with characteristic green colouring with red leaf tips. There was no visible damage, wilting, colour abnormalities or visible pathogen incidence. At 7 DPH, refrigerated lettuces remained largely unchanged. Storeroom lettuces displayed minor signs of wilting, shrivelling and colour fading. Ambient structural integrity had declined and had become flat in shape, signs of browning were apparent. By 14 DPH, refrigerated lettuces displayed wilting and browning. Leaves were no longer crisp in texture or appearance. Storeroom

lettuces became shrivelled from dehydration, requiring physical unravelling before spectral readings. Overall, their structure was significantly deteriorated. Ambient lettuces had noticeably browned, normally caused by a reduction in ascorbic acid and an increase in enzymes including lipoxygenase (Zhang et al., 2023). The lettuce had also acquired a prominent limp structure from loss of turgor. All the lettuces across all storage conditions were visibly past the point of sale, with storeroom and ambient being considered unfit for consumption.

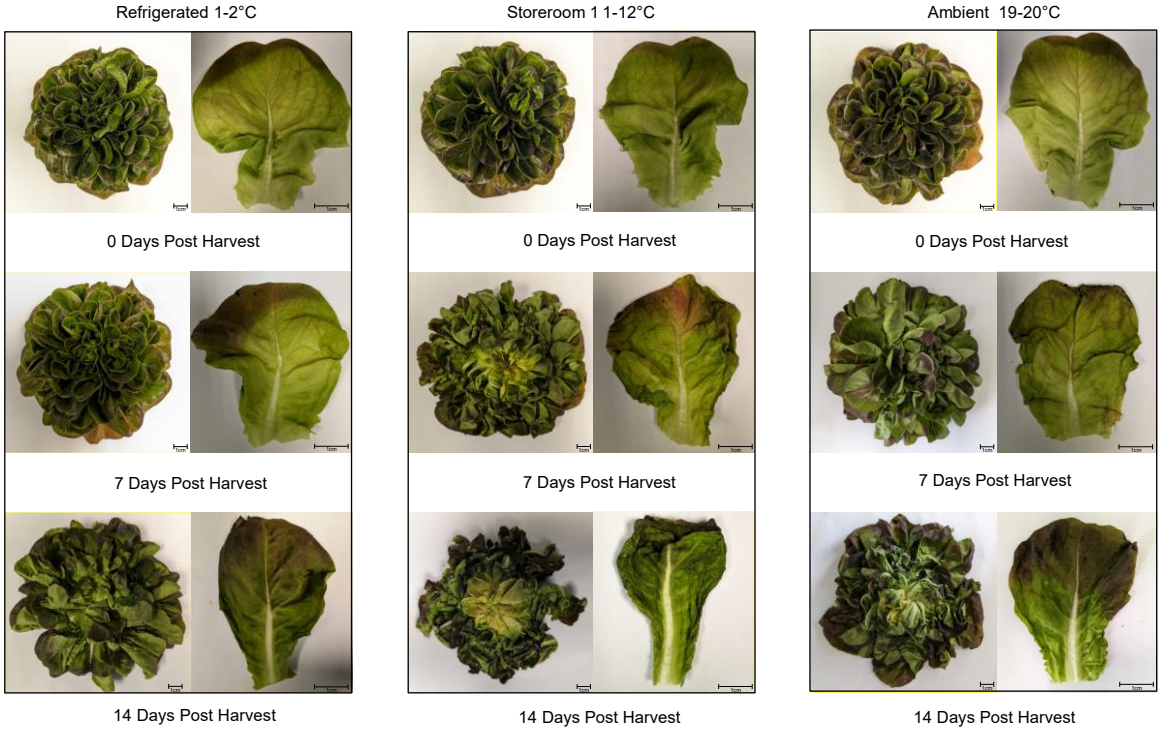

Figure 2.7. Photographic images of whole *Lactuca sativa*, 'Da vinci' lettuces and a single removed leaf at three stages: 0, 7 and 14 DPH from three storage temperature conditions: Refrigerated (1-2°C), Storeroom (11-12°C) and Ambient (19-20°C)

2.4.6 Multivariate Analysis of Different Storage temperatures in Tomatoes, Peppers and Lettuces

The effects of storage temperature and DPH on the spectral properties of produce were analysed separately. Figure 8 shows the fingerprint region of the unprocessed and pre-processed spectra for tomato, pepper and lettuce. Preprocessed spectra show separations in tomato spectra at 1020-1030 cm^{-1}: sulfoxide cm^{-1}, 1060-1110 cm^{-1} primary alcohols, 1200-1250 cm^{-1} vinyl ether, 1330-1370 cm^{-1} sulfone, 1460 cm^{-1} alkanes, 1520-1560 cm^{-1} nitro compounds, 1620 cm^{-1} unsaturated ketone, 1720 cm^{-1} carboxylic acid; in peppers at 1160-1180 cm^{-1} sulfoxide, 1470 cm^{-1} alkane, 1490 cm^{-1} and 1510 cm^{-1} nitro compound, 1600 cm^{-1} conjugated alkenes, 1720 cm^{-1} carboxylic acid; in lettuces: 960 cm^{-1} alkenes, 1720 cm^{-1} aliphatic ketones (Colthup, 1975b)

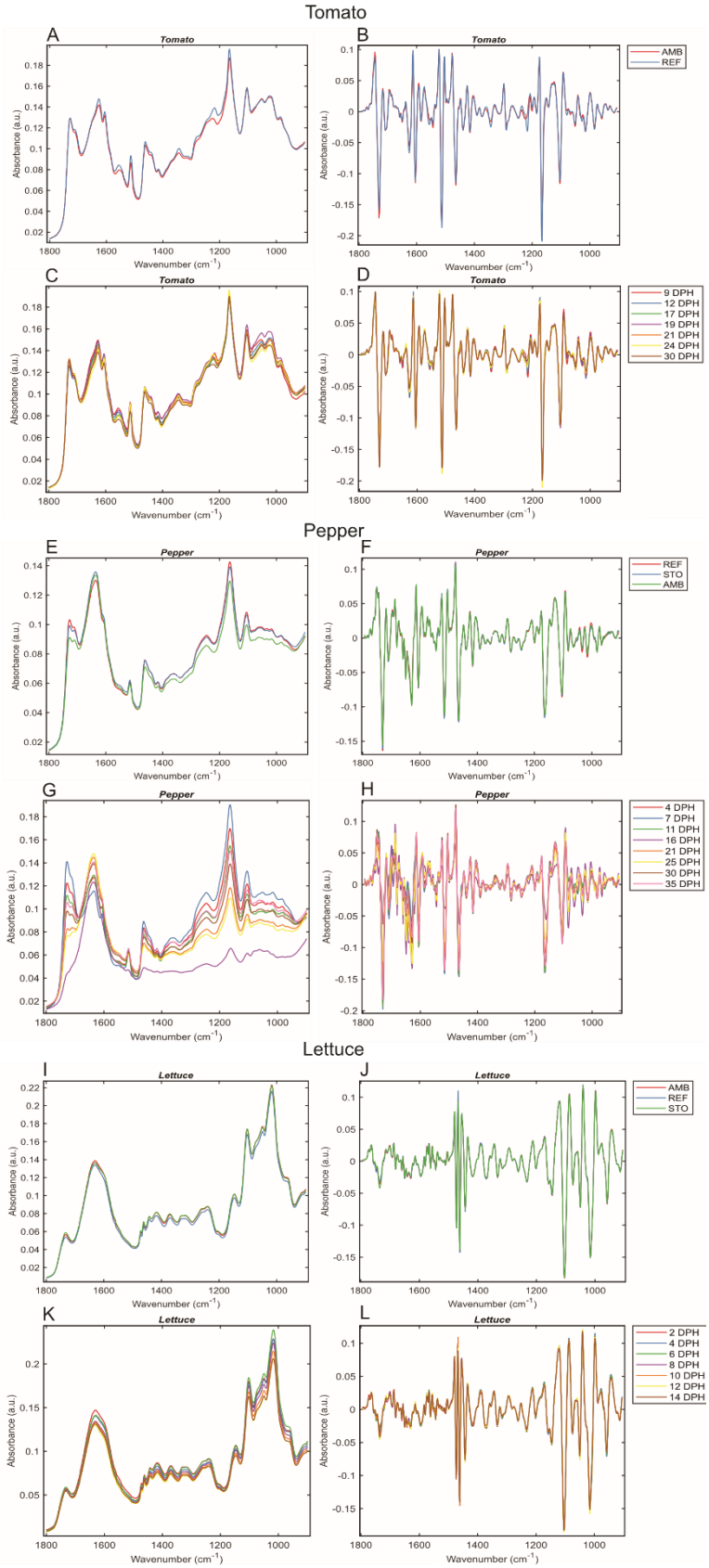

Figure 2.8. A-D) *Solanum lycopersicum* 'Roterno' tomato samples **E-H)** *Capsicum annuum* 'Artega' pepper and **I-L)** *Lactuca sativa*, 'Da vinci' lettuces. **A, C, E, G, I, K)** Fingerprint

region and **B, D, F, H, J, L)** Pre-processed fingerprint regions are displayed and organised by both storage conditions: **AMB** Ambient (19-20°C), **STO** Store Room (11-12°C) and **REF** Refrigerated (1-2°C) and time classes classified by **DPH**

PCA analysis of refrigerated tomato fruit stored at 1-2°C displayed widespread clustering along PC1 and PC2 axes. Along PC2 ambient tomatoes: 19-12°C exhibited a more concentrated clustering, which was largely separate from the refrigerated tomatoes with minor overlap. Along PC1 axis, both storage conditions overlapped almost entirely, suggesting that this feature was experienced in both storage groups however PC2 describes a biochemical feature that distinguishes the two groups by 13.2% of the variance in the data (Figure 2.9A). Further analysis using PCA-LDA, revealed only one describing feature in the data specifically related to differences between temperature condition classes (Figure 2.9B). There was notable clustering of tomatoes within each temperature, spectral differences between each condition, the mean values of each group did not align but the data distributions exhibited a large overlap suggesting spectral similarities overall. PCA provided a more complex visualisation of tomatoes (Figure 2.9C) at different time points (DPH). Clustering could be seen within 30 DPH, however, a portion of these data points were separate and scattered across the PC1 and PC2 space. Smaller and multiple clusters could be seen in all time points. No single DPH clustered entirely. This suggests that the smaller cluster groups within time points share similarities, but differ from other time points within their class. There is no obvious temporally organised distribution. Clustering was seen in contrast, PCA-LDA provided some clearer separation between time points across LD1 and LD2 axes (Figure 2.9D) however there is heavy overlapping suggesting large spectral similarities between time points throughout the time series. Clustering can be observed most prominently in 24 DPH and 30 DPH towards the end of the time series. 9 DPH and 12 DPH, early stages are completely distinct from late stage time points 24 PH and 30 DPH.

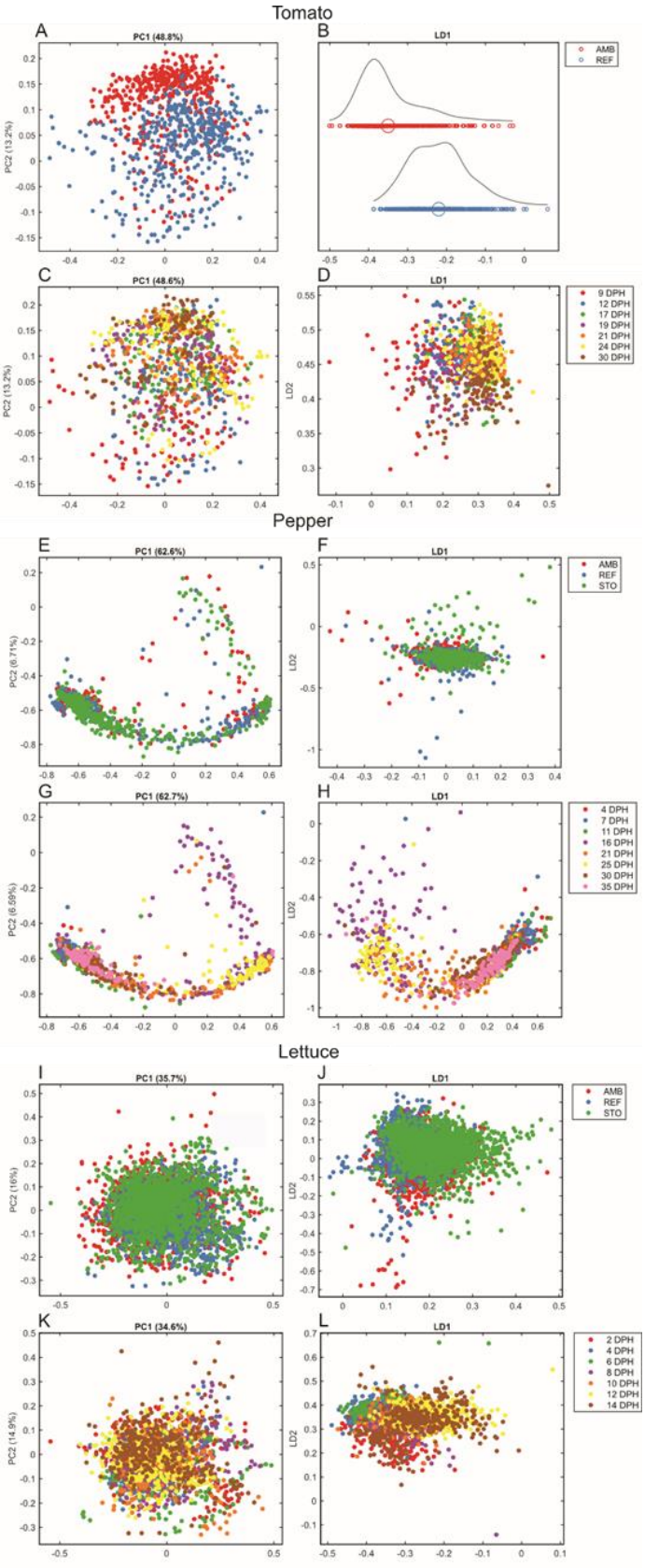

Figure 2.9. A-D) *Solanum lycopersicum* 'Roterno' tomato samples **E-H)** *Capsicum annuum* 'Artega' pepper and **I-L)** *Lactuca sativa*, 'Da vinci' lettuces. **A, C, E, G, I, K)** Principal

Component Analysis PCA. **B, D, F, H, J, L)** Principal Component Analysis with Linear Discriminant Analysis PCA-LDA. With the exception of **F**, PCA-LDA are plotted LD1 against LD2. With only one feature in the data, **B** was restricted to LD1 only. Analysis was conducted using both storage condition classes including **AMB** Ambient (19-20°C), **STO** Store Room (11-12°C) and **REF** Refrigerated (1-2°C) and using time classes classified by **DPH:** Days post-harvest.

PCA-LDA loadings (Figure 10A) provided significant wavenumbers of 1735 cm^{-1}, 1603 cm^{-1}, 1561 cm^{-1}, 1508 cm^{-1}, 1473 cm^{-1}, 1215 cm^{-1}, and 1161 cm^{-1} explained the greatest variances between ambient and refrigerated tomatoes. The largest peak at 1215 cm^{-1} is associated with ethers, esters and phenols. Tomatoes, over time (Figure 10B), showed peak variances at wavenumbers: 1700 cm^{-1}, 1650 cm^{-1}, 1454 cm^{-1}, 1161 cm^{-1}, 1082 cm^{-1}, 1051 cm^{-1}, 1015 cm^{-1}. The highest peaks, representing the greatest variance were at 1082 cm^{-1} and 1015 cm^{-1}. These represent similar spectral regions that are associated with amines, carbohydrates and ethers. PCA-LDA scores (Figure 9L) displayed distinct separation between 9 DPH and 30 DPH. Peak variances occurred at 1714 cm^{-1}, 1606 cm^{-1}, 1504 cm^{-1}, 1408 cm^{-1}, 1341 cm^{-1}, 1217 cm^{-1}, 1161 cm^{-1}, 1082 cm^{-1}, 1017 cm^{-1} (Figure 10C). The most distinct peak occurred at 1017 $cm^{-1,}$ associated with C – O alcohols and ethers, and carbohydrates (Table 2.2).

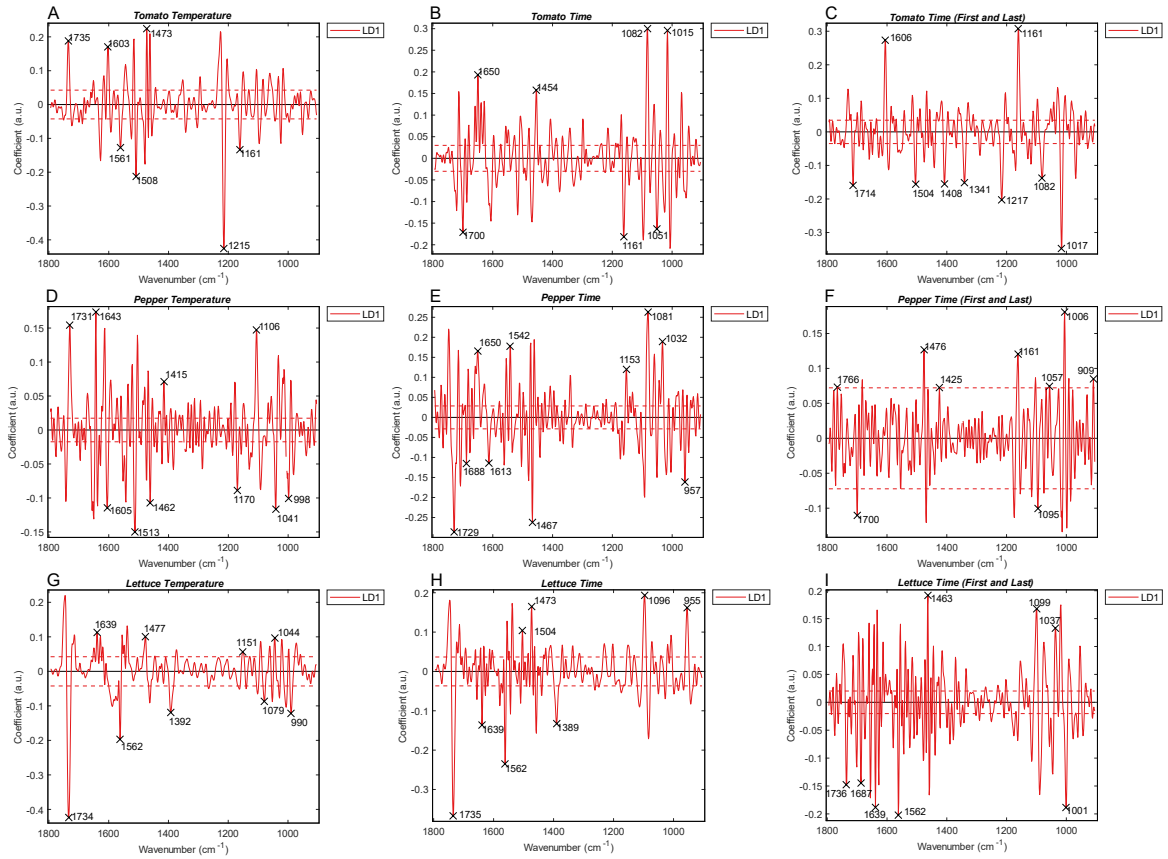

Figure 2.10: PCA-LDA loadings for *Solanum lycopersicum* 'Roterno' tomato samples **(T),** *Capsicum annuum* 'Artega' pepper **(P)** and *Lactuca sativa*, 'Da vinci' lettuces **(L)** by storage condition **(1)**, time **(2)** first and last time points **(3)**

SVM machine learning classifier models were trained and run for storage temperature classification and subsequently DPH classification providing varied rates of accuracy. 94.89% of accurate classification was achieved in refrigerated 1-2°C samples against storeroom 11-12°C (Figure 2.11A). When classifying ambient against refrigerated, the model accuracy rate was 95.61%. DPH classification rates were less successful, ranging from 61.48% to 73.27%, 21 DPH, and 12 DPH respectively (Figure 2.11B).

Table 2.3. Loadings showing the key wavenumbers that exhibit the greatest variances between storage temperature conditions for post-harvest *Solanum lycopersicum* 'Roterno' tomato fruit, *Capsicum annuum* var. 'Artega' pepper and *Lactuca sativa* var. 'Da Vinci' lettuces

Storage temperature		

Wavenumber (cm^{-1})	**Wavenumber Range**	**Compound Assignment**	**References**
Tomato Temperature (Figure 2.10A)			
1735	1740-1720 1750-1735 1750-1715 1735 1740-1735	C = O stretching vibration in carbonyl groups, typically seen in esters, aldehydes, and ketones C = O Aliphatic aldehydes Saturated esters Lactones six-membered ring C = O n-butyrates/ isobutyrates C = O Propionates	(Colthup, 1975b)
1603	1650-1600 1640-1580 1665-1585 1600-1621 1655-1558	C = C stretching vibrations in aromatic compounds C = O 1,3 diketones, enol form NH_3 deformation: α-L-amino acids C = O amido acids C = N Pyrrolines	(Colthup, 1975b)
1561	1605-1555 1655-1558	CO_2 stretching: Normal chain amino acids C = N Pyrrolines	(Colthup, 1975b)
1508	1600-1500 1530-1490	C = C stretching in aromatic ring stretching NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
1473	 1484-1388	CH_2 bending vibrations in alkanes NH_4 deformation: Ammonium ion	(Colthup, 1975b)
1215	1210-1310	C – O stretching vibrations: Esters, ethers, or phenols Aromatic ether alkoxy	(Colthup, 1975b)

	1225-1200 1260-1180 1170-1240	C – O – C stretching alkyl vinyl ethers Phenols C – NH_2 primary amines (strong)	
1161	1260-1180 1210-1158	C – O – C stretching vibrations in ethers or esters C – O Saturated esters	(Colthup, 1975b)
Tomato Time (Figure 2.10B)			
1700	1700-1670 1710-1640	C = O carbonyl stretching vibration, ketones, aldehydes, and carboxylic acids C = O singly conjugated ketones Thiol esters C = O α-amido acids	(Colthup, 1975b)
1650	1670-1630 1650 1665-1585 1653-1635 1655-1560 1660-1625	C = C stretching vibration in alkenes C = O stretch in amide I band protein O – hydroxyl aryl ketones C = C fumarates NH3 deformation α-L-amino acids asymmetric Phenyl vinyl ether C = N Pyrrolines R – O – NO_2 organic nitrates	(Colthup, 1975b)
1454	1484-1388	CH_2 or CH_3 alkanes NH_4 deformation: Ammonium ion	(Colthup, 1975b)
1161	1210-1158	C – O Saturated esters	(Colthup, 1975b)
1082	1090-1066	C – O stretching vibrations: Alcohols, ethers, or carbohydrates CH_2 – NH_2 Aliphatic primary amines	(Colthup, 1975b)

1051	1035-1060 1075-998	Acetate made from primary alcohols phenyl -CHOH- Aromatic secondary alcohols	(Colthup, 1975b)
1015	1050-1010 1075-1000 1125-1000	C – O stretching vibrations: Primary alcohols or ethers Aromatic ether alkoxy phenyl – CHOH – Aromatic secondary alcohols C – O stretching carbohydrates	(Colthup, 1975b)
Tomato Time: First and Last (Figure 2.10C)			
1714	1725-1705 1724-1695	C = O stretching vibration in carbonyl groups, esters, aldehydes, or ketones C = O dialkyl ketones C = O α-amido acids	(Colthup, 1975b)
1606	1640-1580 1665-1585 1600-1621 1655-1558	C = C stretching in aromatic compounds or alkenes C = O 1,3 diketones, enol form NH_3 deformation α-L-amino acids C = O amido acids C = N Pyrrolines	(Colthup, 1975b)
1504	1530-1490	C = C stretching vibrations in aromatic compounds NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
1408	1393-1425 1484-1388	CH_2 bending vibrations: alkanes or aromatic systems CO_2 stretching: Normal chain amino acids NH_4 deformation: Ammonium ion	(Colthup, 1975b)

1341	1390-1330 1342-1320 1380-1332 1380-1310	C – H bending or deformation in alkanes Phenols solid state Secondary aromatic amines C – N Phenyl Aromatic amine dimethyl anilines B – O boron	(Colthup, 1975b)
1217	1210-1310 1225-1200 1260-1180 1170-1240	C – O stretching in esters, ethers, or phenolic compounds Aromatic ether alkoxy C–O–C stretch alkyl vinyl ethers Phenols C – NH_2 primary amines (strong)	(Colthup, 1975b)
1161	1210-1158	C – O Saturated esters	(Colthup, 1975b)
1082	1125-1000 1090-1066	C – O stretching vibrations, alcohols, ethers, or carbohydrates C – O Carbohydrates CH_2 – NH_2 Aliphatic primary amines	(Colthup, 1975b)
1017	1050-1010 1075-1000 1125-1000	C – O stretching in alcohols or ethers Aromatic ether alkoxy Phenyl – CHOH – Aromatic secondary alcohols C – O Carbohydrates	(Colthup, 1975b)
Peppers Temperature (Figure 2.10D)			
1731	1740-1718	C = O stretching vibrations: Esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)

1643	1670-1630 1710-1640 1665-1585 1653-1635 1655-1560 1660-1625, 1285-1268	C = C stretching: Alkenes or C = O stretching of the amide I band proteins C = O o-hydroxyl aryl ketones Thiol esters NH_3 deformation: α-L-amino acids Phenyl vinyl ether C = N Pyrrolines R – O – NO_2 Organic nitrates	(Colthup, 1975b)
1605	1640-1580 1665-1585 1605-1555 1600-1621 1655-1558	C = C stretching vibrations in aromatic compounds C = O 1,3 diketones, enol form Benzoates (ring) NH_3 deformation: α-L-amino acids CO_2 normal chain amino acids C = O Amido acids C = N Pyrrolines	(Colthup, 1975b)
1513	1530-1490	N – O asymmetric stretching in nitro compounds or aromatic ring stretching vibrations NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)
1462	1484-1390 1330-1465	CH_2 bending vibrations (scissoring) in alkanes C-H bending in aromatic systems NH_4 deformation: Ammonium ion B – N boron	(Colthup, 1975b)
1415	1393-1425 1484-1388	CH_2 or CH_3 bending vibrations, alkanes, or the symmetric stretching of carboxylate ions	(Colthup, 1975b)

		CO_2 stretching: Normal chain amino acids NH_4 deformation: Ammonium ion	
1170	1210-1160 1170-1240	C – O Saturated esters C – NH_2 Primary amines (strong)	(Colthup, 1975b)
1106	1125-1000	C – O – C stretching vibrations in ethers or esters, polysaccharides C – O Carbohydrates	(Colthup, 1975b)
1041	1035-1060 1025-1047 1075-1000 1125-1000	C – O stretching vibrations, alcohols or ethers C – N stretching in amines Acetate made from primary alcohols Aromatic ether methylene-1, 2-disoxybenzenes phenyl – CHOH – Aromatic secondary alcohols C – O Carbohydrates	(Colthup, 1975b)
998	1000-675	C = C bending in alkenes or out-of-plane bending vibrations in aromatic compounds.	(Colthup, 1975b)
Pepper Time (Figure 10E)			
1729	1740-1725 1740-1718	C = O stretching vibration in carbonyl groups, esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
1688	1700-1668 1690-1620 1690-1685	C = O stretching in conjugated carbonyl compounds C = N stretching in imines C = O singly conjugated ketones	(Colthup, 1975b)
1650	1670-1630 1710-1640	C = C stretching vibrations, alkenes	(Colthup, 1975b)

	1665-1585 1653-1635 1655-1560 1660-1625, 1285-1268	C = O stretch amide I band proteins C = O O-hydroxyl aryl ketones Thiol esters NH_3 deformation α-L-amino acids Phenyl vinyl ether C = N Pyrrolines R – O – NO_2 Organic nitrates	
1613	1620-1600 1640-1580 1665-1585 1620-1610 1655-1558	C = C stretching vibrations in aromatic rings or conjugated alkenes C = O 1,3 diketones, enol form Isophthalates (ring) NH_3 deformation: α-L-amino acids C = C alkyl vinyl ether C = N Pyrrolines	(Colthup, 1975b)
1542	1550-1520 1550-1540 1620-1538	N – O asymmetric stretching in nitro compounds or N – H bending and C – N stretching amide II band in proteins Pyrrolines	(Colthup, 1975b)
1467	1370-1450 1600-1450 1484-1388	CH_2 or CH_3 bending vibrations in alkanes C – H bending in aromatic rings NH_4 deformation: Ammonium ion	(Colthup, 1975b)
1153	1250 -1150	C – O stretching vibrations, esters, ethers, or alcohols.	(Colthup, 1975b)
1081	1125-1000 1090-1066	C – O – C stretching ethers or esters, polysaccharides C – O Carbohydrates	(Colthup, 1975b)

		CH_2 – NH_2 Aliphatic primary amines	
1032	1050-1010 1075-1000 1125-1000 1022-1038	Aromatic ether alkoxy Phenyl – CHOH – aromatic secondary alcohols C – O Carbohydrates C – CH_2 primary amines (weak)	(Colthup, 1975b)
957	990-900	Out-of-plane bending vibrations in alkenes or aromatic rings.	(Colthup, 1975b)
Pepper Time: First and Last (Figure 2.10F)			
1766	1765-1740 1775-1738	C = O stretching vibration in carbonyl groups, esters, lactones, or anhydrides Lactones type I and type II	(Colthup, 1975b)
1700	1700-1670 1724-1695	C = O carbonyl stretching vibration, ketones, aldehydes, and carboxylic acids C = O singly conjugated ketones C = O α-amido acids	(Colthup, 1975b)
1476	1484-1388	CH_2 or CH_3 bending vibrations in alkanes, C – H bending in aromatic systems NH_4 deformation: Ammonium ion	(Colthup, 1975b)
1425	1450-1360 1393-1425 1484-1388	CH_2 bending vibrations in alkanes or aromatic ring stretching vibrations COO- stretching carboxylate groups Carboxylic acid salt	(Colthup, 1975b)

		CO_2 stretching: Normal chain amino acids NH_4 deformation: Ammonium ion	
1161	1210-1158	C – O Saturated esters	(Colthup, 1975b)
1095	1125-1000	C – O – C stretching vibrations in ethers or esters, polysaccharides C – O Carbohydrates	(Colthup, 1975b)
1057	1035-1060 1075-1000 1125-1000	C – O stretching vibrations, alcohols, ethers, or glycosidic linkages in sugars Acetate made from primary alcohols Phenyl – CHOH – Aromatic secondary alcohols C – O Carbohydrates	(Colthup, 1975b)
1006	1125-1000	C – O stretching in alcohols or ethers, ring vibrations in aromatic systems C – O Carbohydrates	(Colthup, 1975b)
909	990-900	Out-of-plane C-H bending in alkenes or aromatic compounds.	(Colthup, 1975b)
Lettuce Temperature (Figure 2.10G)			
1734	1740-1718	C = O stretching vibration in carbonyl groups, esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
1639	1640-1580 1665-1585	C = C stretching vibrations in alkenes or conjugated systems, C = O stretching amide I band proteins C = O 1,3 diketones, enol form	(Colthup, 1975b)

	1653-1635 1660-1620	NH_3 deformation: α-L-amino acids Phenyl vinyl ether C = N Pyrrolines R – O – NO_2 Organic nitrates	
1562	1605-1555 1655-1558	C = C stretching in aromatic rings CO_2 stretching: normal chain amino acids C = N Pyrrolines	(Colthup, 1975b)
1477	1484-1388	CH_2 bending vibrations in alkanes or aromatic ring stretching vibrations C – H bending in alkyl groups NH_4 deformation: Ammonium ion	(Colthup, 1975b)
1392	1450-1360 1484-1388	COO- stretching of carboxylate ions Carboxylic acid salt NH_4 deformation: Ammonium ion	(Colthup, 1975b)
1151	1300-1000	C – O stretching vibrations, esters, ethers, or phenols.	(Colthup, 1975b)
1079	1125-1000 1090-1066	C – O – C stretching in ethers or esters C – O stretching in alcohols or carbohydrates C = O Carbohydrates CH_2 – NH_2 aliphatic primary amines	(Colthup, 1975b)
1044	1035-1060 1050-1010 1025-1047 1075-1000 1125-1000	C – O stretching in alcohols, ethers, C – N stretching in amines Acetate made from primary alcohols Aromatic ether alkoxy Aromatic ether methylene-1, 2-disoxybenzenes	(Colthup, 1975b)

		Phenyl – CHOH -Aromatic secondary alcohols C – O Carbohydrates	
990		C – H Out-of-plane bending vibrations in alkenes or aromatic systems	(Colthup, 1975b)
Lettuce Time (Figure 2.10H)			
1735	1740-1720 1750-1735 1750-1715 1735 1740-1735	C = O stretching vibration esters, aldehydes, and ketones C = O Aliphatic aldehydes Saturated esters Lactones six-membered ring C = O n-butyrates/ isobutyrates C = O Propionates	(Colthup, 1975b)
1639	1640-1580 1665-1585 1653-1635 1655-1560 1660-1625 1285-1268	C = C stretching vibrations in alkenes or conjugated systems C = O stretching amide I band proteins C = O 1,3 diketones, enol form NH_3 deformation: α-L-amino acids Phenyl vinyl ether C = N Pyrrolines R – O – NO_2 Organic nitrates	(Colthup, 1975b)
1562	1605-1555 1655-1558	C = C stretching in aromatic rings CO_2 stretching: Normal chain amino acids C = N Pyrrolines	(Colthup, 1975b)
1504	1530-1490	C = C stretching vibrations: Aromatic compounds or vibrations in conjugated systems	(Colthup, 1975b)

		NH_3 deformation: Normal chain amino acids	
1473	1484-1388	CH2 bending vibrations in alkanes NH4 deformation: Ammonium ion	(Colthup, 1975b)
1389	1450-1360 1390-1330 1260-1178	CH_2 bending vibrations C – H bending in alkanes. C – N stretching in some organic compounds Carboxylic acid salt Phenols solid state	(Colthup, 1975b)
1096	1125-1000	C – O stretching, alcohols and ethers C – N stretching in amines C = O Carbohydrates	(Colthup, 1975b)
955	990-900	C – H Out-of-plane bending vibrations in aromatic compounds. Organic heterocycles.	(Colthup, 1975b)
Lettuce Time: First and Last (Figure 2.10I)			
1736	1740-1720 1740-1735	C = O stretching vibrations esters, aldehydes, ketones and carboxylic acids C = O Aliphatic aldehydes C = O Propionates	(Colthup, 1975b)
1687	1700-1670 1710-1638	C = O singly conjugated ketones Thiol esters	(Colthup, 1975b)
1639	1640-1580	C = C stretching vibrations in alkenes or conjugated systems, C = O stretching amide I band proteins	(Colthup, 1975b)

	1665-1585 1653-1635 1655-1560 1660-1625	C = O 1,3 diketones, enol form NH_3 deformation: α-L-amino acids Phenyl vinyl ether C = N Pyrrolines R – O – NO_2 Organic nitrates	
1562	1600-1500 1605-1555 1655-1558	C = C stretching in aromatic rings CO_2 stretching: Normal chain amino acids C = N Pyrrolines	(Colthup, 1975b)
1463	1484-1390 1330-1465	CH_2 bending vibrations (scissoring) in alkanes C-H bending in aromatic systems NH_4 deformation: Ammonium ion B – N boron	(Colthup, 1975b)
1099	1125-1000	C – O Carbohydrates	(Colthup, 1975b)
1037	1035-1060 1050-1010 1075-1000 1125-1000 1125-1000 1022-1038	C – O stretching in secondary alcohols, ethers. Acetate made from primary alcohols Aromatic ether alkoxy Phenyl – CHOH – Aromatic secondary alcohols C – O Carbohydrates C – NH_2 Primary amines (weak)	(Colthup, 1975b)
1001	1075-1000 1125-1000	Out-of-plane bending vibrations in aromatic rings, bending modes in heterocyclic compounds Phenyl – CHOH – Aromatic secondary alcohols C – O Carbohydrates	(Colthup, 1975b)

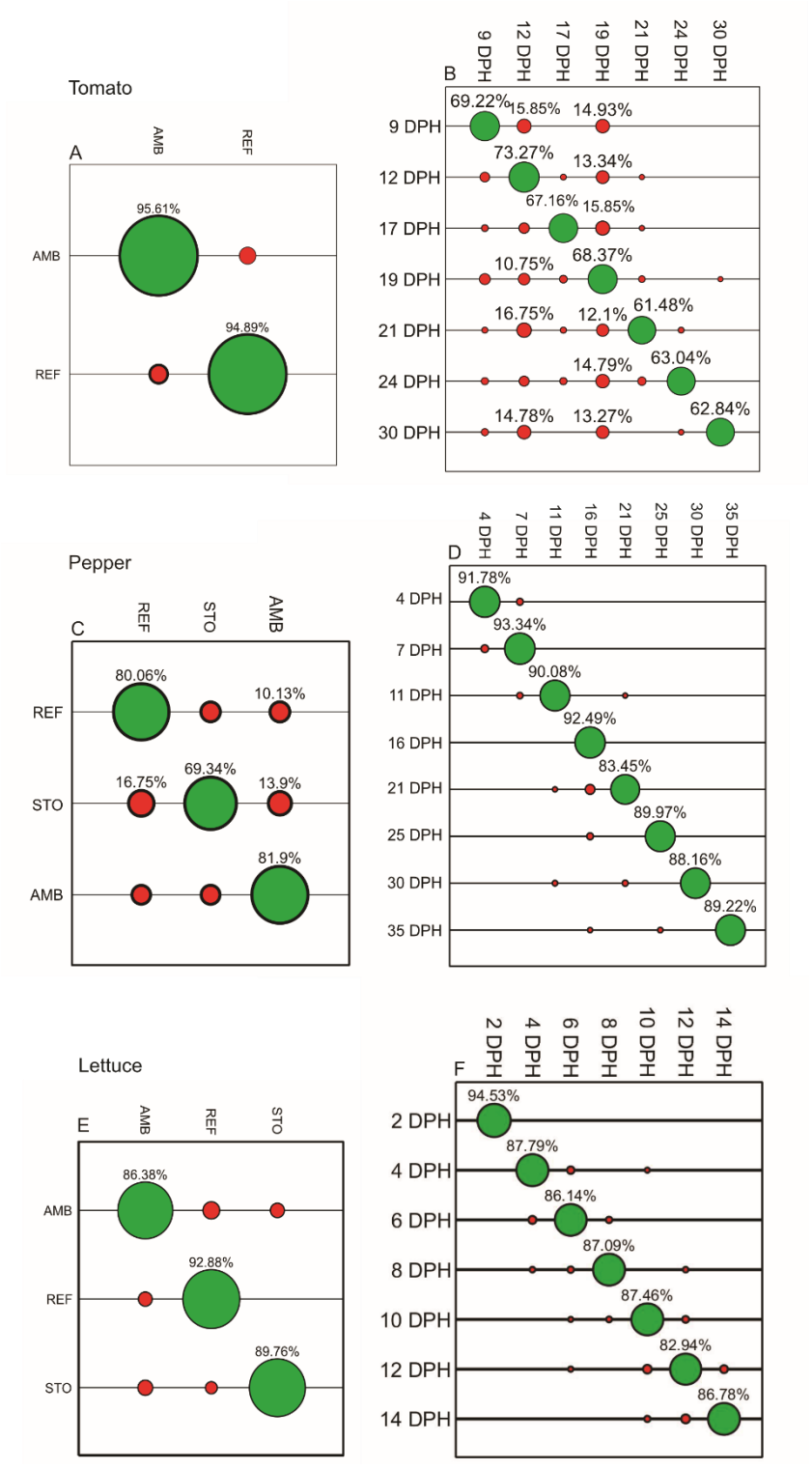

Figure 2.11. Machine learning models: Support Vector Machine (SVM) confusion matrices for feature classification. **A,B)** *Solanum lycopersicum* 'Roterno' tomato samples **C,D)** *Capsicum annuum* 'Artega' peppers and **E,F)** *Lactuca sativa*, 'Da vinci' lettuces. Support Vector Machine learning models performed on both **A,C,E)** storage condition:

Storage conditions include **AMB** Ambient (19-20°C), **STO** Store Room (11-12°C) and **REF** Refrigerated (1-2°C). **B,D,F)** Spectra are displayed in **DPH** Days post-harvest.

2.4.7 PCA-LDA Loadings of Different Storage temperatures in Tomatoes, Peppers and Lettuces

Storage temperatures in peppers showed clustering in all storage conditions along PC2 explained by 6.71% of the data variance (Figure 2.9E). Along this axis minimal separation between the storage conditions were observed. PC1 axis which explains 62.6% of the data displays wide distribution of the data however there is an observed split, which is not defined by temperature classes. PCA-LDA (Figure 2.9F) showed heavy clustering in all storage temperatures with no separation along LD1 or LD2. This is in contrast to PCA analysis of DPH (Figure 2.9G) where clear clustering is observed in all time points with the exception of 16 DPH which is widely distributed along PC2 axis suggesting an important biochemical variation between the tomatoes in this time point. There was a significant overlap between 11 DPH, 21 DPH, 30 DPH and 35 DPH and separately 16 DPH, and 25 DPH. This suggests these two groups share spectral similarities. When PCA-LDA (Figure 2.9H) was applied, there was minimal separation, however, the groupings observed in the PCA model remained consistent suggesting the PCA-LDA made marginal difference to further separate the classes.

PCA-LDA loadings identified important wavenumbers between storage conditions including: 1731 cm^{-1}, 1643 cm^{-1}, 1605 cm^{-1}, 1513 cm^{-1}, 1462 cm^{-1}, 1415 cm^{-1}, 1170 cm^{-1}, 1106 cm^{-1}, 1041 cm^{-1}, 998 cm^{-1}, largely associated with aromatic compounds. When time classes were analysed, 1729 cm^{-1}, 1688 cm^{-1}, 1650 cm^{-1}, 1613 cm^{-1}, 1542 cm^{-1}, 1467 cm^{-1}, 1153 cm^{-1}, 1081 cm^{-1}, 1032 cm^{-1}, 957 cm^{-1} with the largest peaks at 1729 cm^{-1} and 1081 cm^{-1} both associated with esters, aldehydes and ketones. Wavenumbers from the first and last time point were 1766 cm^{-1}, 1700 cm^{-1}, 1476 cm^{-1}, 1425 cm^{-1}, 1161 cm^{-1}, 1095 cm^{-1}, 1057 cm^{-1}, 1006 cm^{-1}, 909 cm^{-1}, the highest peak at 1006 cm^{-1} Despite the minor separation between these time points, the highest variance at 1006 cm^{-1} is associated with carbohydrates, ethers and alcohols. There are indicated shifts in aromatic compounds, esters, aldehydes, and ketones between early and late time points during storage, reflecting the progression of fruit ripening and degradation processes.

This is further supported by a machine learning model trained on the data (Figure 2.11C & D), initially using storage temperature as the class. This model performed with accuracy rates of: storeroom: 69.35%, refrigerated: 80. 06% and ambient: 81.90%. When SVM models were run on classes determined by DPH, the model achieved higher accuracy rates ranging from 83.45% at 21 DPH to 93.34% at 7 DPH.

Lettuce PCA analysis showed no clear separation between storage condition classes (Figure 2.9I &J). When PCA-LDA was applied, there was a clearer view of clustering, however across both LD1 and LD2 axes, minimal separation was exhibited between each condition, suggesting that there was very little difference in spectral signatures. When PCA analysis was conducted on lettuces measured at different time points, there is no clear separation along PC1 or PC2 axes, however, when PCA-LDA was applied there were more distinct clustering within the time points, especially visible in 2 DPH, 6 DPH, 12 DPH and 14 DPH. Separations were observed between 2 DPH 6 DPH and 12 DPH. Lettuce between storage temperatures: 1734 cm^{-1}, 1639 cm^{-1}, 1562 cm^{-1}, 1477 cm^{-1}, 1392 cm^{-1}, 1151 cm^{-1}, 1079 cm^{-1}, 1044 cm^{-1}, 990 cm^{-1}, the highest peak at 1734 cm^{-1} associated with esters, aldehydes and ketones lettuce over time: 1735 cm^{-1}, 1639 cm^{-1}, 1562 cm^{-1}, 1504 cm^{-1}, 1473 cm^{-1}, 1389 cm^{-1}, 1096 cm^{-1}, 955 cm^{-1}, the heist peak at 1735 cm^{-1}. First and last: 1736 cm^{-1}, 1687 cm^{-1}, 1639 cm^{-1}, 1562 cm^{-1}, 1463 cm^{-1}, 1099 cm^{-1}, 1037 cm^{-1}, 1001 cm^{-1}, the highest peak at 1463 cm^{-1} associated with alkanes, aromatics, ammonium ion and boron (Table 2.2).

2.4.8 Multivariate Analyses of Neighbouring Time Points

Spoilage-related processes in fruit may occur corresponding to a temporal sequence, but this may be influenced by storage conditions. PCA and subsequent PCA-LDA were performed on adjacent time points throughout the time course experiments to further understand the specificity of temporally associated processes and how they were influenced by storage temperature. In tomato, (Figure 2.12) there was a distinct separation between the two storage temperatures in PCA analysis and subsequent PCA-LDA analysis; this was particularly prominent at 19 & 21 DPH and 21 & 24 DPH. This separation became more prominent as the time series progressed chronologically. The highest variances have been identified at peak wavenumbers at each timeslot. In tomato

(Figure 2.12) peak wavenumbers have been identified at 9 & 12 DPH: 1605 cm^{-1} and 1515 cm^{-1}, 12 & 17 DPH, 1616 cm^{-1} and 1215 cm^{-1}, 17 & 19 DPH: 1616 cm^{-1} and 1473 cm^{-1}, 19 & 21 DPH: 1627 cm^{-1}, 1215 cm^{-1} and 1167 cm^{-1}, 21 & 24 DPH: 1736 cm^{-1} and 1215 cm^{-1}, 24 & 30 DPH: 1736 cm^{-1} and 1215 cm^{-1}. (Table 2.3) 1215 cm^{-1} occurs at multiple time groups, associated with C - O stretching vibrations, particularly in esters, ethers, or phenols.

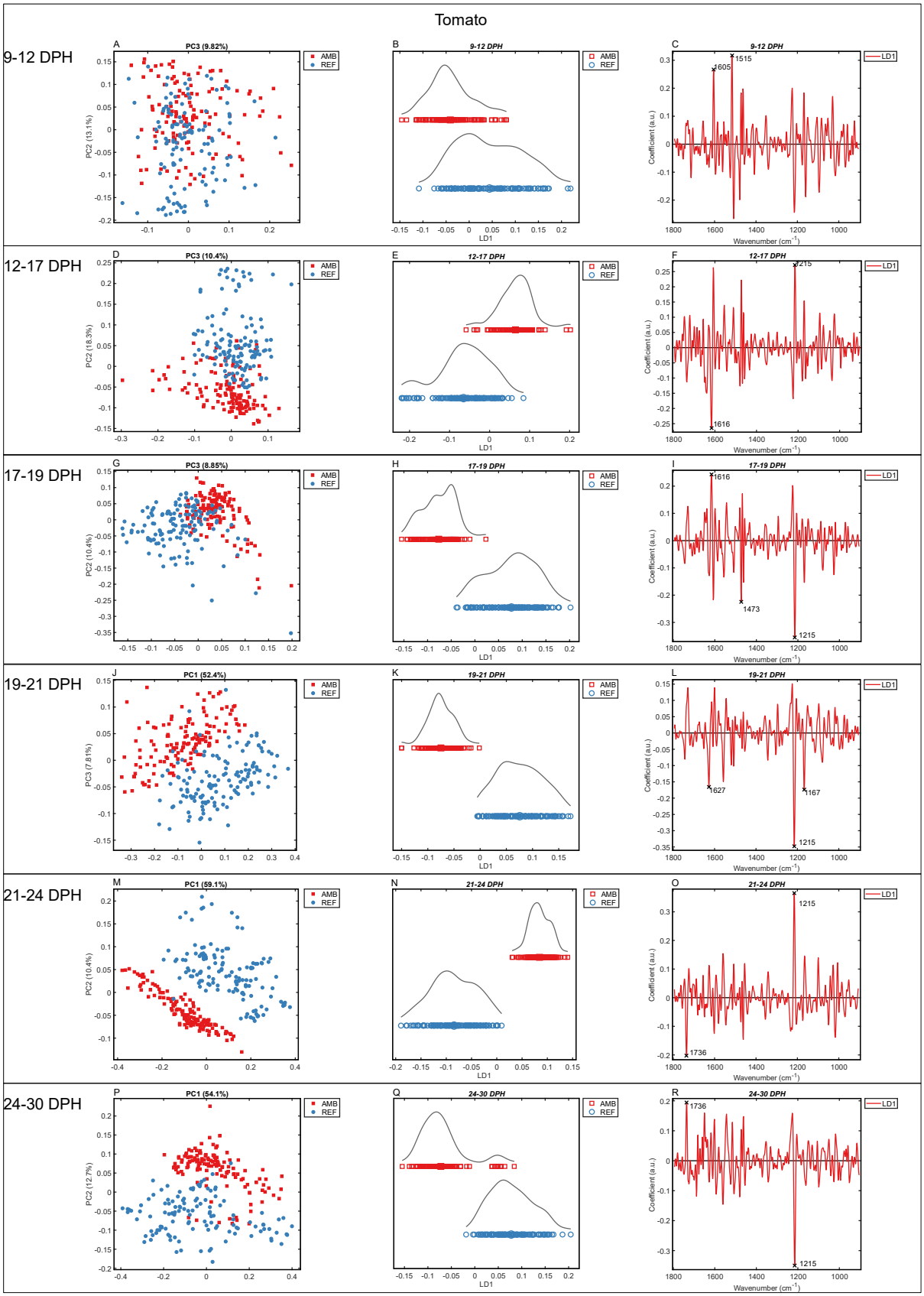
Tomato
9-12 DPH
12-17 DPH
17-19 DPH
19-21 DPH
21-24 DPH
24-30 DPH
A
PC3 (9.82%)
PC2 (13.1%)
B
9-12 DPH
C
9-12 DPH
1515
1605
D
PC3 (10.4%)
PC2 (18.3%)
E
12-17 DPH
F
12-17 DPH
1215
1616
G
PC3 (8.85%)
PC2 (10.4%)
H
17-19 DPH
I
17-19 DPH
1616
1473
1215
J
PC1 (52.4%)
PC3 (7.81%)
K
19-21 DPH
L
19-21 DPH
627
1167
1215
M
PC1 (59.1%)
PC2 (10.4%)
N
21-24 DPH
O
21-24 DPH
1215
1736
P
PC1 (54.1%)
PC2 (12.7%)
Q
24-30 DPH
R
24-30 DPH
1736
1215
AMB
REF
LD1
Coefficient (a.u.)
Wavenumber (cm-1)

Figure 2.12. Principal component analysis PCA scores (**A, D, G, J, M** & **P**), Principal component analysis with linear discriminant analysis PCA-LDA scores (**B, E, H, K, N** & **Q**), and loadings plots (**C, F, I, L, O** & **R)** for *Solanum lycopersicum* 'Arvento' tomato. 2 closest timepoints have been isolated and highest variances identified at specific wavenumbers. PCA score plots (**A-P**) are plotted using two principal components, orthogonal axes displaying data points plotted using variances. PCA-LDA scores plots (**B-Q**) are plotted using on principal component axis.

Table 2.4. Loadings showing the key wavelength variance between storage temperature conditions for post-harvest *Solanum lycopersicum* 'Roterno' tomato fruit, *Capsicum annuum* var. 'Artega' pepper and *Lactuca sativa* var. 'Da Vinci' lettuces associated with biochemical changes at adjacent time points.

Storage Temperature by Timepoint				
Tomato (Figure 2.12)				
DPH	**Wavenumber (cm^{-1})**	**Wavenumber Range**	**Compound Assignment**	**References**
9-12	1605	1680-1600 1640-1580 1665-1585 1605-1555 1655-1559	C = C stretching vibrations in aromatic compounds C = O 1,3-diketones, enol form Benzoates (ring) NH_3 deformation: α-L-amino acids CO_2 stretching: Normal chain amino acids C = N Pyrrolines	(Colthup, 1975b)
	1515	1600-1500 1530-1490	C = C stretching aromatic rings, phenolic compounds or flavonoids p - Cymene monocyclic, terpene NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)

12-17	1616	1680-1600 1640-1580 1665-1585 1620-1610 1655-1559	C = C stretching in aromatic systems C = O 1,3-diketones, enol form NH_3 deformation: α-L-amino acids C = C alkyl vinyl ether C = N Pyrrolines	(Colthup, 1975b)
	1215	1210-1310 1225-1200 1260-1180 1170-1240	Aromatic ether alkoxy C - O - C stretching alkyl vinyl ethers Phenols C - NH_2 primary amines (strong)	(Colthup, 1975b)
17-19	1616	1680-1600 1640-1580 1665-1585 1620-1610 1655-1559	C = C stretching in aromatic systems C = O 1,3-diketones, enol form NH_3 deformation: α-L-amino acids C = C alkyl vinyl ether C = N Pyrrolines	(Colthup, 1975b)
	1473	1470-1440 1484-1389	CH_2 bending vibrations in alkanes, alkyl chains NH4 deformation: Ammonium ion	(Colthup, 1975b)
19-21	1627	1680-1600 1640-1580 1665-1585 1655-1560 1660-1625 1285-1269	C = C stretching vibrations in polyenes, carotenoids C = O 1,3-diketones, enol form NH_3 deformation: α-L-amino acids C = N Pyrrolines	(Colthup, 1975b)

			R - O - NO_2 Organic nitrates	
	1215	1210-1310 1225-1200, 1260-1180 1170-1240	Aromatic ether alkoxy C- O - C stretching alkyl vinyl ethers Phenols C – NH_2 primary amines (strong)	(Colthup, 1975b)
	1167	1300-1000 1210-1159	C - O stretching vibrations in alcohols or phenols C - O Saturated esters	(Colthup, 1975b)
21-24	1736	1740-1719	C = O Carbonyl stretching vibrations in aldehydes, ester, carboxylic acids and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
	1215	1210-1310 1225-1200 1260-1180 1170-1240	Aromatic ether alkoxy C - O - C stretching alkyl vinyl ethers Phenols C - NH_2 primary amines (strong)	(Colthup, 1975b)
24-30	1736	1740-1720 1740-1735	C = O Carbonyl stretching vibrations in aldehydes, ketones, esters and carboxylic acids C = O Aliphatic aldehydes C = O Propionates	(Colthup, 1975b)
	1215	1210-1310 1225-1200 1260-1180	Aromatic ether alkoxy C - O - C stretching alkyl vinyl ethers Phenols	(Colthup, 1975b)

		1170-1240	C - NH_2 primary amines (strong)	
Pepper (Figure 2.13)				
4-7	1728	1740-1719	Ester or carbonyl stretching C = O Aliphatic aldehydes	(Colthup, 1975b)
	1606	1680-1600 1640-1580 1665-1585 1600-1621 1655-1559	C = C stretching in aromatic compounds or alkenes C = O 1,3-diketones, enol form NH_3 deformation: α-L-amino acids C = O amido acids C = N Pyrrolines	(Colthup, 1975b)
7-11	1728	1740-1719	Ester or carbonyl stretching C = O Aliphatic aldehydes	(Colthup, 1975b)
	1606	1680-1600 1640-1580 1665-1585 1600-1621 1655-1559	C = C stretching in aromatic compounds or alkenes C = O 1,3-diketones, enol form NH_3 deformation: α-L-amino acids C = O amido acids C = N Pyrrolines	(Colthup, 1975b)
11-16	1093	1200-1000	C - O - C stretching vibrations in ethers or esters.	(Colthup, 1975b)
	1032	1050-1010 1025-1047 1075-1000 1125-1000 1022-1038	Aromatic ether alkoxy Aromatic ether methylene-1, 2-disoxybenzenes Phenyl - CHOH - Aromatic secondary alcohols C - O Carbohydrates C - NH2 primary amines (weak)	(Colthup, 1975b)

16-21	1103	1125-1000	C - O Carbohydrates	(Colthup, 1975b)
	1041	1035-1060 1050-1010 1025-1047 1075-1000 1125-1000	Acetate made from primary alcohols Aromatic ether alkoxy Aromatic ether methylene-1, 2-disoxybenzenes Phenyl - CHOH - Aromatic secondary alcohols C - O Carbohydrates	(Colthup, 1975b)
21-25	1721	1750-1700 1725-1705 1724-1695	C = C stretching in conjugated systems or aromatic rings C = O Amide I band in proteins Dialkyl ketones C = O α-amido acids	(Colthup, 1975b)
	1629	1680-1600 1640-1580 1665-1585 1655-1560 1660-1625, 1285-1269	C = C stretching in conjugated systems or aromatic rings C = O Amide I band in proteins C = O 1,3-diketones, enol form NH_3 deformation: α-L-amino acids C = N Pyrrolines R - O - NO_2 Organic nitrates	(Colthup, 1975b)
25-30	1517	1600-1500 1530-1490	C = C stretching of aromatic compounds NH_3 deformation: Normal chain amino acids	(Colthup, 1975b)

	1463	1470-1440 1484-1390 1330-1465	CH_2 bending vibrations (scissoring) in alkanes C-H bending aromatic systems NH_4 deformation: Ammonium ion B - N Boron compounds	(Colthup, 1975b)
30-35	1688	1700-1669	C = O singly conjugated ketones	(Colthup, 1975b)
	1651	1670-1630 1665-1585 1653-1635 1655-1560 1660-1625	C = O O-hydroxyl aryl ketones NH_3 deformation: α-L-amino acids Phenyl vinyl ether C = N Pyrrolines R - O - NO_2 Organic nitrates	(Colthup, 1975b)
Lettuce (Figure 2.14)				
2-4	1732	1740-1719	C = O Aliphatic aldehydes	(Colthup, 1975b)
	1639	1665-1585 1653-1635 1655-1560 1660-1625 1285-1269	C = O O-hydroxyl aryl ketones NH_3 deformation α-L-amino acids Phenyl vinyl ether C = N Pyrrolines R - O - NO_2 Organic nitrates	(Colthup, 1975b)
4-6	1732	1740-1719	C = O stretching esters, aldehydes, or ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
	1099	1200-1000	C – O Stretching vibrations ethers	(Colthup, 1975b)

6-8	1068	1200-1000 1075-1000 1090-1067	C - O stretching vibrations, esters, ethers, alcohols, polysaccharides and complex carbohydrates Phenyl - CHOH - Aromatic secondary alcohols CH_2 - NH_2 Aliphatic primary amines	(Colthup, 1975b)
	1734	1750-1700 1740-1719	C = O stretching vibration in carbonyl groups, esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
	1006	1200-1000 1075-1000 1125-1000	C - O stretching in alcohols or ethers Phenyl - CHOH - Aromatic secondary alcohols C - O Carbohydrates	(Colthup, 1975b)
8-10	1734	1750-1700 1740-1719	C = O stretching vibration in carbonyl groups, esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
	1639	1680-1600 1670-1630 1665-1585 1653-1635 1655-1560 1660-1625	C = C stretching vibrations in alkenes or conjugated systems C = O stretching amide I band proteins C = O O-hydroxyl aryl ketones NH_3 deformation: α-L-amino acids Phenyl vinyl ether C = N Pyrrolines	(Colthup, 1975b)

			R - O - NO_2 Organic nitrates	
	1734	1750-1700 1740-1719	C = O stretching vibration in carbonyl groups, esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
	1640	1670-1630 1710-1640 1640 1665-1585 1653-1635 1655-1560 1660-1625	C = O O-hydroxyl aryl ketones Thiol esters C = O acrylates C = C methacrylates NH_3 deformation: α-L-amino acids Vinyl ether Phenyl vinyl ether C = N Pyrrolines R - O - NO_2 Organic nitrates	(Colthup, 1975b)
	1558	1600-1500 1605-1555	C = C stretching vibrations aromatic compounds CO_2 stretching: Normal chain amino acids	(Colthup, 1975b)
12-14	1456	1470-1440 1484-1389	CH_2 bending vibrations C - H bending in aliphatic chains or cyclic compounds NH_4 deformation: Ammonium ion	(Colthup, 1975b)
	1734	1750-1700 1740-1719	C = O stretching vibration in carbonyl groups, esters, aldehydes, and ketones C = O Aliphatic aldehydes	(Colthup, 1975b)
	1538	1600-1500	C = C stretching in aromatic compounds	(Colthup, 1975b)
	1099	1125-1000	C - O Carbohydrates	(Colthup, 1975b)

In pepper (Figure 2.13), the separation between the three storage temperatures was less distinct in the PCA analysis however PCA-LDA allowed greater separation at 11 & 16 DPH, 16 & 21 DPH, and 30 & 35 DPH. PCA-LDA allowed for clear clustering of storage conditions, early stage time points showing larger variability within and between classes with significant overlap, however, chronological analysis shows increasing clustering in conjunction with increased separation. Time point pair 25 & 30 DPH and 30 & 35 DPH display prominent separation and clustering, the greatest variance was shown at wavenumbers 1517 cm^{-1} at 25 & 30 DPH and 1651 cm^{-1} at 30 & 35 DPH. Peak wavenumbers identified along the time-series were 4 & 7 DPH: 1728 cm^{-1} and 1606 cm^{-1}, 7 & 11 DPH: 1728 cm^{-1} and 1606 cm^{-1}, 11 & 16 DPH: 1093 cm^{-1} and 1032 cm^{-1}, 16 & 21 DPH: 1103 cm^{-1} and 1041 cm^{-1}, 21 & 25 DPH: 1721 cm^{-1} and 1629 cm^{-1}, 25 & 30 DPH: 1517 cm^{-1} and 1463 cm^{-1} and 30 & 35 DPH: 1688 cm^{-1} and 1651 cm^{-1} (Table. 2.3).

In lettuce (Figure 2.14), PCA analyses showed minimal separation between storage temperatures in all time point groups, with the exception of some outlier groups in 2 & 4 DPH which might be explained by unrelated chemical differences. Separation between storage temperatures was observed in the PCA-LDA analysis in every timepoint pairing, the storage groups were not strongly clustered suggesting continuous biochemical change occurrences along the time series and a mismatch in the rate of spoilage in these different conditions. Minor overlapping occurred suggesting the presence of spectral similarities. Lettuce wavenumbers have been identified at 2 & 4 DPH: 1732 cm^{-1}, 1639 cm^{-1} and 1096 cm^{-1}, 4 & 6 DPH: 1732 cm^{-1}, 1099 cm^{-1} and 1068 cm^{-1}, 6 & 8 DPH: 1734 cm^{-1} and 1006 cm^{-1}, 8 & 10 DPH: 1734 cm^{-1} and 1639 cm^{-1}, 10 & 12 DPH: 1734 cm^{-1}, 1640 cm^{-1}, 1558 cm^{-1} and 1456 cm^{-1}, 12 & 14 DPH: 1734 cm^{-1},1538 cm^{-1} and 1099 cm^{-1}. Similar wavenumbers 1732 and 1734 occur throughout the time series, associated with C = O stretching vibration in carbonyl groups, typically seen in esters, aldehydes, and ketones (Table 2.3).

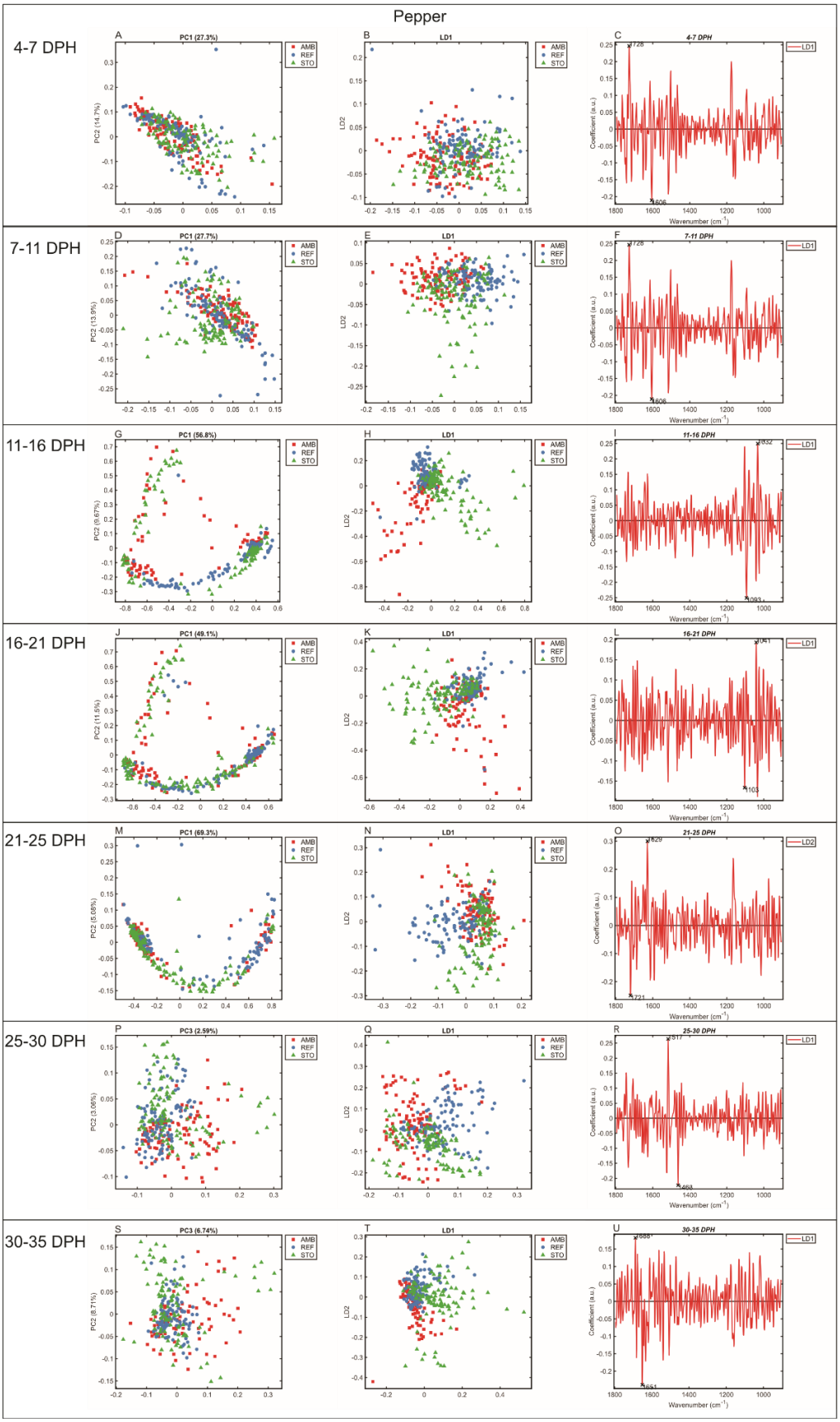
Pepper
4-7 DPH
7-11 DPH
11-16 DPH
16-21 DPH
21-25 DPH
25-30 DPH
30-35 DPH
AMB
REF
STO
Wavenumber (cm-1)
Coefficient (a.u.)

Figure 2.13. Principal component analysis PCA scores (**A, D, G, J, M, P** & **S**), Principal component analysis with linear discriminant analysis PCA-LDA scores (**B, E, H, K, N, Q,** & **T**), and loadings plots (**C, F, I, L, O, R** & **U)** for *Capsicum annuum var.* 'Artega' pepper. 2 closest timepoints have been isolated and highest variances identified at specific wavenumbers

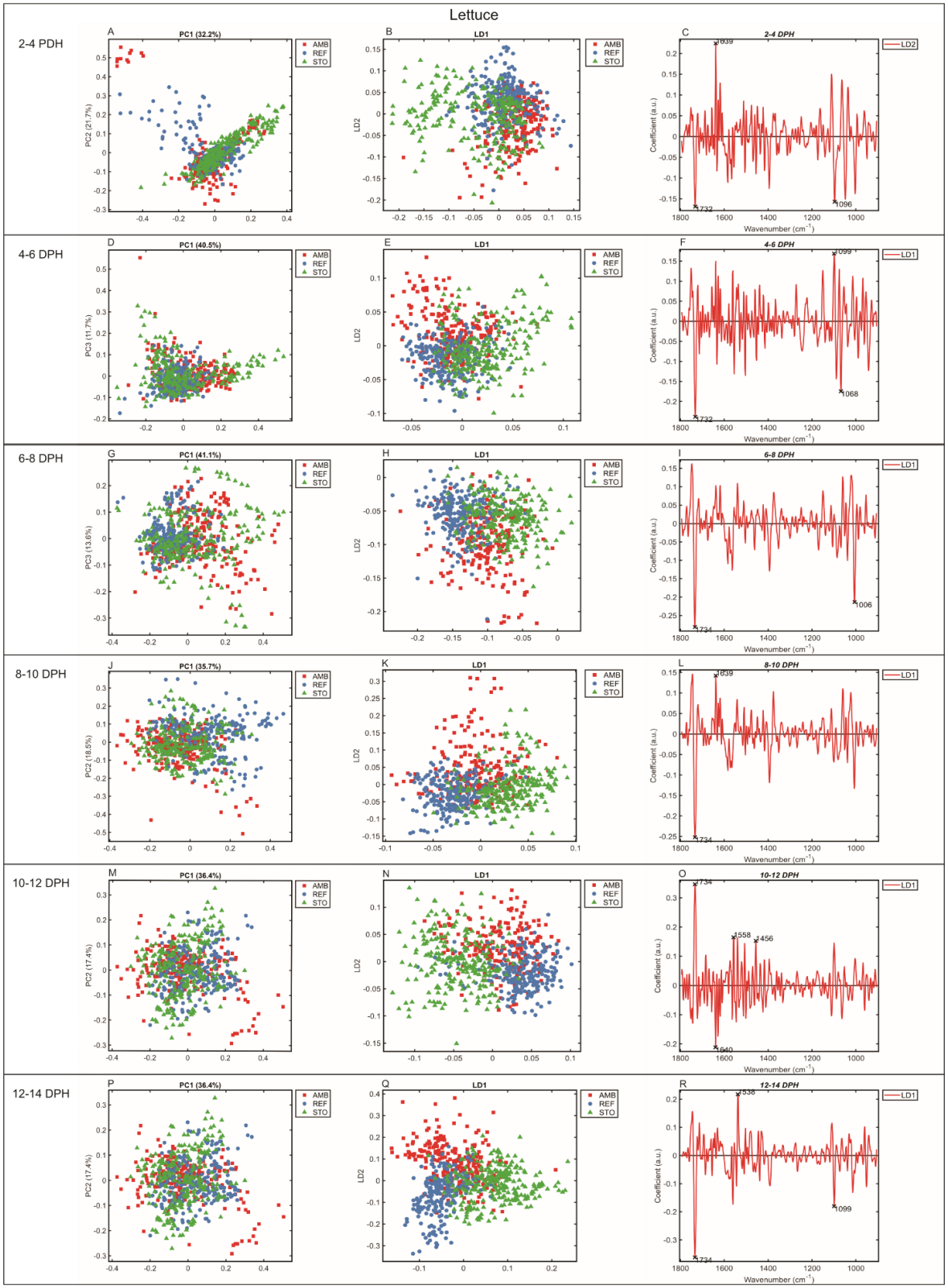

Figure 2.14. Principal component analysis PCA scores (**A, D, G, J, M** & **P**), Principal component analysis with linear discriminant analysis PCA-LDA scores (**B, E, H, K, N** & **Q**),

and loadings plots (**C, F, I, L, O** & **R)** for *Lactuca sativa* var. 'Da Vinci' lettuces. 2 closest timepoints have been isolated and highest variances identified at specific wavenumbers

2.5 Discussion

Before reaching the consumer, an alarming 20-50% of all produced fruit and vegetables are lost or wasted along the supply chain (Gustavsson *et al.*, 2011). In addition, FLW contributes to 8-10% of global greenhouse gasses and to mitigate the impacts of climate change as a whole, actions must be taken to reduce FLW. This study aimed to explore the post-harvest spoilage processes of important fruit and vegetables in relation to a variety of storage conditions and to identify key spectral biomarkers that may be used as a proxy for senescence stages, even when influenced by storage temperature variations. Biochemical markers could play an important role for the targeted categorisation of senescence stage of postharvest fruit and vegetable produce in the supply chain. This would be particularly useful prior to the emergence of visual identifiers of spoilage that present too late for effective product management to reduce FLW. Accurate classification may further indicate produce shelf life and inform decision making to reduce FLW. To this end, the potential for MIR to classify the biochemical compositional status of produce based on its post-harvest spectral signature and associated spectral biomarkers was examined in this study using three tomato varieties, pepper, and lettuce.

2.5.1 Exploratory PCA and PCA-LDA Analysis Provided a Useful Method for Understanding the Biochemical Processes Occurring in Postharvest Fruit and Vegetables

Storage is a vital element in the supply chain and is required at multiple stages including during transportation. Understanding the biochemical processes that occur during storage and how the storage conditions such as temperature affects products can help inform actors in the food system on how best to store fruit and vegetables to achieve optimal shelf-life and quality (Gidado *et al.*, 2024). These temporal indicators contribute to the understanding of how key nutrients change over time and in relation to storage temperature. For example these findings highlight changes in lycopenes, important

antioxidants for human health, shown in tomatoes at key stages through senescence. This understanding may inform the maintenance of key nutrients in produce, important for human health. Additionally, detailed understanding guides reducing waste, improving economic profitability. Food loss and waste reduction are pivotal to mitigation of climate change and other related environmental impacts. PCA-LDA loading wavenumbers were able to provide some understanding of chemical processes that were affected by temperature (Figure 2.10A, D, & G). Despite the associated PCA-LDA scores plots (Figure 2.9B, F & J) varying in visual separation between the temperatures, and clustering in temperatures, SVM machine learning models (Figure 2.11A, C & E) supported the reliability of the spectral information obtained. To understand how the biochemical processes changed over time, spectral readings were taken from regular time points, after harvest until full degradation which provided some important insights. Postharvest spoilage processes are less understood than preharvest ripening and senescence (Liu *et al.*, 2022). Postharvest spoilage processes are attributed to a continuation of preharvest ripening processes (Palumbo *et al.*, 2022), whilst being true, less is known about the specificity of these processes and how they differ from how they behave before harvest. Analyses between neighbouring time points in tomatoes (Figure 2.5, 2.6 & 2.12), peppers (Figure 2.13) and lettuces (Figure 2.14) enabled a detailed understanding of when chemical processes occurred, detail that might be missed when analysing the time series as a whole. Observing the greatest variances between isolated timepoints provided specificity to changes occurring at targeted time points. By removing non-targeted time point data, it removed skew caused by averaging across the full time series, which can obscure nuanced or transient chemical changes specific to particular stages of spoilage or storage response. The detection compounds shown to occur at specific time points may be used as proxy biomarkers potentially indicative of spoilage stages with high specificity.

2.5.2 Sugars Play an Important Role in Postharvest Spoilage in Fruit

Sugars provide a substrate for respiration and the synthesis of ATP, important for fuelling molecular processes, but sugars can also modulate biosynthesis of hormones,

including ethylene, a key hormone involved in ripening, synthesised in climacteric fruits like tomatoes and bananas (Li *et al.*, 2016), and which continues to be released post-harvest, continuing ripening, but not in non-climacteric fruit. Cellulose is an important polysaccharide and cell wall component present in fruit and vegetables that provides structural integrity, contributing to the shape and firmness (Alberts *et al.*, 2002). During ripening, senescence, and subsequent spoilage, cellulose in cell walls along with a matrix of hemicellulose and pectin, breaks down, weakening the structural integrity of the fruit (Bhagia *et al.*, 2022). The loss of this integrity is important to spoilage processes as visual and textural characteristics deteriorate and can result in water loss (Gidado *et al.*, 2024). In the late stages of spoilage, the cuticle can become torn and ruptured from spoilage degradation processes like water loss and additionally resulting from mechanical movement causing damage. This provides opportunities for pathogen infection further accelerating degradation (Wan *et al.*, 2021). Key wavenumbers 1161 cm^{-1}, 1167 cm^{-1}, and 1168 cm^{-1} displayed peaks representing high variances, these wavenumbers have been shown to be associated with cellulose (Movasaghi, *et al.*, 2008) suggesting there were changes in cellulose occurring, likely in volume or structural composition. These were observed in all tomato varieties as a distinction between the early and late stages of spoilage (Figure 2.10C, Figure 2.3C & F). Cellulose was also observed as important changes in Arvento tomatoes between 11 and 24 DPH and again at 27 and 30 DPH, significant wrinkling and softening presented by 24 DPH, and fluid leakage was observed by 27 DPH supporting these key changes in cellulose. Similarly, cellulose was observed as a key compound in peppers, especially between 11 and 21 DPH by wavenumbers 1093 cm^{-1} and 1106 cm^{-1}. This provides some important insight as visual and textural softening only appeared at 16 DPH, however, the appearance of these wavenumbers suggests that cellulose degradation is occurring earlier than is visibly detectable. As such, these wavenumbers may be used as spoilage biomarkers that if identified in produce in the supply chain, could be used to indicate early spoilage informing decision-making focussed on produce optimisation and reducing FLW. An important caveat is that the changes that occur in cellulose in ripening stages could be misinterpreted as early spoilage. This limitation drives the need for obtaining a detailed understanding of developmental processes exhibited in infrared spectra to qualify validity of biomarkers. 1106 cm^{-1} was a key difference between peppers stored in different temperature

environments. This indicates that cellulose is impacted by temperature and further supports its use as a biomarker of spoilage. Lettuce is particularly vulnerable to spoilage causing a short shelf-life in comparison to other fruit and vegetables. Lettuce have delicate cell walls, vulnerable to damage due to being thinner, less lignified and containing fewer structural components. They rely on their high water content to maintain its turgidity and crisp texture and structure (Giannakourou and Tsironi, 2021). The cellulose degradation in lettuce is often driven by bacterial pathogens including *Pseudomonas sp*. that thrive in high moisture environments, typical of leafy green vegetables (Allende, *et al*., 2004). Cellulose degradation causes loss of turgor, and loss of water resulting in limpness and wilting. Cellulose breakdown also results in increased vulnerability to bruising providing entry points for pathogens accelerating spoilage further. Lettuce kept in refrigerated conditions, remained texturally intact for considerably longer than lettuces stored in higher temperatures, 11-12°C and ambient 19-20°C. Overall, cellulose was observed to be an important biochemical change throughout the spoilage process at wavenumber 1096 cm^{-1} and identified as a key difference between storage temperatures at 1151 cm^{-1}.

Further validation could be conducted to confirm that cellulose degradation is the corresponding process to these spectral differences. This could be achieved by conducting enzymatic assays, chemical quantification of enzyme content and microscopic observations.

2.5.3 The Presence of Alcohols May Provide a Key Biomarker for Spoilage

Other important wavenumbers associated with sugars and starches, both of which have important roles in degradation were in tomatoes: 1082 cm^{-1} (Figure 2.10), 1025 cm^{-1} (Figure 2.3); peppers: 1032 cm^{-1} (Figure 2.13), 1041 cm^{-1} (Figure 2.10), 1081 cm^{-1} (Figure 2.10), and 1057 cm^{-1} (Figure 2.10); and lettuce: 1044 cm^{-1} (Figure 2.10) and 1057 cm^{-1} (Figure 2.10). Sucrose, fructose, and glucose are readily available in plant tissues and serve as energy sources for microorganisms that drive spoilage such as fungi and bacteria (Chen *et al.*, 2023). Access to energy sources accelerates microbial proliferation,

increasing microbe-produced enzyme accumulation, including amylases which further accelerate the breakdown of key structural components in fruit including polysaccharides like starches. (Gopinath *et al.*, 2017). The degradation of starch can alter osmotic balance and turgor pressure, contributing to the softening and collapse of internal tissue structures during spoilage.

Fermentation is another process conducted by microbes that contributes to off-flavours and odours. Fermentation by-products include organic acids, alcohols, and volatile organic compounds (VOCs) which produce sourness and sometimes sulphurous odours (Rajendran, *et al.,* 2023) VOCs were observed as key biochemical changes in tomatoes, peppers, and lettuce. Wavenumbers associated with VOCs were highlighted in tomatoes in all three varieties in almost all time points, making their use as biomarkers of spoilage processes difficult. However, key differences between tomatoes from different temperature storage were observed at 1603 cm^{-1} and 1508 cm^{-1}, both associated with C = C stretching in aromatic compounds suggesting that these are impacted by temperature. The presence of alcohols may indicate fermentation processes from microbes. These were identified in tomatoes at 11 and 14 DPH in Arvento 1158 cm^{-1}, and 19 and 21 DPH in Roterno at 1167 cm^{-1}. Alcohols are described assignments to key wavenumbers identified as one of the largest changes in tomato biochemistry: 1082 cm^{-1},1017 cm^{-1} and 1015 cm^{-1}. In peppers 1153 cm^{-1} and 1057 cm^{-1} were key chemical changes and 1006 cm^{-1} in lettuce over time. A more useful indicator of spoilage might be associated with the presence of phenyl - CHOH – aromatic secondary alcohols, which might include 2-Phenylethanol, an aromatic alcohol that is known to be produced through non-pathogenic microbial fermentation including *Bacillus licheniformis* (Xu *et al.*, 2019) and it acts as an anti-microbial compound (F. Wu *et al.*, 2024). The synthesis of this compound may be a reactionary defence mechanism to the increasing presence of pathogenic microbes. 2-Phenylethanol has been identified to inhibit *Botrytis cinerea* mycelium growth (Zou *et al.*, 2023), a fungal disease that severely affects tomatoes, peppers, and lettuce. Phenyl - CHOH – aromatic secondary alcohols were identified as a key difference between storage temperatures in peppers and lettuces at 1041 cm^{-1} and 1044 cm^{-1}, respectively. In peppers and lettuce it also represented one of the largest chemical changes in the whole time series at 1032 $cm^{-1,}$ specifically in pepper at 11-

16DPH, and 1037 cm^{-1}, along the whole timeseries. This compound was also observed as a biochemical change at 16 and 21 DPH in peppers at 1041 cm^{-1} and 6 and 8 DPH in lettuce. The presence of internal blackening in ambient peppers was observed at 30 DPH which might be attributed to several pathogenic infections including *Botrytis cinerea* (Gray Mold) which causes internal black rot, *Colletotrichum spp*. or *Alternaria alternata* (Raynaldo *et al.*, 2024). Further research would be required to confirm a relationship between the occurrence of 2-Phenylethanol and the infection visibly observed between 14 and 9 days after.

2.5.4 Pigmentation Degradation was Observed in Key Wavenumbers Before it was Visually Expressed

During spoilage, there were observed changes in the colour of the fruit. In Arvento tomatoes, discolouration started to appear between 14 and 17 DPH and by 30 DPH in peppers. Wavenumber 1731 cm^{-1} observed as a peak biochemical variance in tomatoes, in peppers: 1688 cm^{-1} and 1651 cm^{-1}. These wavenumbers are associated with aldehydes and ketones, which can be attributed to pigment degradation pathways. Pigment changes include carotenoids, such as lycopene, in tomatoes (González-Peña *et al.*, 2023), and capsanthin in peppers (Gómez-García and Ochoa-Alejo, 2013). Aldehydes and ketones were identified as key differences between storage temperatures in tomatoes, peppers, and lettuce, suggesting that pigmentation degradation is affected by the temperature at which they are stored. Wavenumber associated with changes in aldehydes and ketones are also observed in earlier time points compared with visually observed discolouration, for example in Piccolo tomatoes (Figure 2.6) as early as 8 and 10 DPH 1641 cm^{-1}, 1685 cm^{-1}, and 1559 cm^{-1}, and 1728 cm^{-1} at 4 and 7 DPH in peppers, and 1732 cm^{-1} as early as 2 and 4 DPH in lettuce all indicative of aldehydes and ketones were identified before visual colour changes. These could serve as important biomarkers for early spoilage. These findings are described physiologically; however, the identification of these biochemical changes using surface spectral measurements is novel, especially when observed temporally. Further work to more closely map these changes using an improved

robust design would be beneficial, especially if conducted alongside chemical analysis including pigment extraction and quantification.

2.5.5 Key Ripening and Spoilage Hormone Ethylene was Affected by Postharvest Storage Temperature

The presence of ethylene could be attributed to the presence of C = C stretching combined with characteristic C – H out of plane bending (Coates, 2006) band. This was observed in Piccolo tomato fruit, especially early-stage post-harvest. To further validate this spectral signature and prescribed association to ethylene, ethylene quantification analyses would be beneficial. Gas chromatography is a useful tool for this, while less suitable for paired use in the supply chain, conducting gas chromatography simultaneously with spectral analysis in a research context would provide validation of the wavenumber assignments. One of the largest differences between peppers kept in different storage conditions was the presence of ethylene, characterised by wavenumbers 1643 cm^{-1} and 998 cm^{-1}. This may be indicative of the rates of ethylene becoming inhibited by lower temperatures (Qi *et al.*, 2021). Ethylene-associated wavenumbers were also identified in peppers across the time-series indicating that ethylene levels vary during spoilage. Interestingly, although elevated ethylene would have been expected in tomatoes during spoilage (Tucker *et al.*, 2017) were not observed in any of the three tomato varieties. However, ethylene release has been shown to be inconsistent between different tomato varieties and can be affected by environmental pressures (Zhao, *et al.*, 2021) which may contribute to this anomaly.

2.5.6 Spectral Biomarkers as Reliable Indicators of Spoilage were Supported by High Performance of Machine Learning Models

Machine learning models were highly effective at classifying tomatoes, peppers, and lettuce that were stored in different temperatures (Figure 2.11A, C & E). This suggests that the spectral signatures associated with the differences between storage conditions

are reflective of the temperature-dependent process underlying spoilage under each condition. Whilst the analysis was conducted with the inclusion of fruit or vegetables from all time points in the series, the model nevertheless was still able to classify with high accuracy rates. In pepper and lettuce (Figure 2.11D & F), SVM models were successfully able to identify the time points with high accuracy, again this was despite the fact that they were stored in different temperatures. In tomatoes, the SVM model (Figure 2.11B) achieved lower classification rates than peppers and lettuces, a higher number of misclassifications also occurred but was still able to classify well. These high success rates show that these classification models are robust, and the spectral signatures are distinct both throughout different spoilage stages in time and when different storage conditions are applied. Temperature conditions have also been shown they are key influences to maintaining the shelf life of produce, with post-harvest refrigeration being highly successful at inhibiting spoilage and microbial infection (Wang *et al.*, 2023). These analytical techniques have exhibited a promising ability to detect key chemical changes that may be used as proxies for senescence and spoilage before visual identifiers occur, making this a valuable tool for food system optimisation. This potential emphasises the importance of further exploration of using ATR-FTIR spectroscopy and chemometric analytical modelling to address the challenge of reducing food loss and waste.

2.6 Limitations

The biological composition of the fruit and leaf tissues may be influenced by factors that occur during the growing period, including differing weather conditions, nutrient availability, or plant physiological states. Compositional concentrations that might be affected by these conditions include sugars, water, organic acids, and structural polysaccharides, all of which contribute to the mid-infrared spectra. In this study, replicates were obtained to account for heterogeneity in the batches, in addition to technical replication to account for surface heterogeneity however, the variability between pre-harvest conditions was not extensively accounted for, only limited by the provision of fruit from an industry producer that executes standardised growing procedures. This represents a limitation of the work as the ability to separate the biochemical variation between ripening and senescence, and the external environmental

influences is not fully resolved. Further studies would benefit from multiple experimental runs, the systematic variation controlled within the study, or the use of reference tagged samples. An example of a useful physiological reference dataset that spectral data would ideally be anchored to is those used in isotope mapping or isoscaping. Currently, such datasets for ATR-FTIR spectra in ripening or post-harvest senescence spoilage are not currently available to provide sufficient resolution.

2.6.1 Omitted Marker Gene Validation of Post-Harvest Tomato Spectra

Molecular validation was initially planned to complement the spectroscopic analysis using qPCR to assess the expression of marker genes known to be associated with ripening and senescence in tomato fruit. Due to logistical reasons and time-constraints associated with the COVID-19 pandemic, it was not possible to complete this element of the study however in future work, this paired component between RNA expression and spectroscopic analysis would provide a novel and robust method of observing the biochemical composition of fruits and leaf tissue during ripening and senescence. The intended genes for this experiment included: PG, CEL2, PL, PE, EXP1, ACO. Pectinesterase (PE), pectate lyase (PL) and polygalacturonase (PG) are enzymes that play a crucial role in breaking down and degrading pectin in the ripening and senescence processes involved in cell wall degradation and fruit softening (Wang et al., 2018). Their distinct roles occur sequentially with partial overlapping, making their timing useful indicators of ripening stages and are commonly used as marker genes for fruit ripening and senescence. PE hydrolyses the ester bonds between methanol and galacturonic acid in pectin, also known as de-esterification, and occurs in the early to mid-stages of ripening, initiating the loosening of cell walls. PL uses a process called β-elimination which cleaves α-1,4-glycosidic bonds of methylated pectin, occurring in the mid to late stages of ripening and senescence. PG also acts on α-1,4-glycosidic bonds by hydrolysing working best on non-methylated pectin occurring in late stages of ripening (Wang et al., 2018).

1-aminocyclopropane-1-carboxylic acid oxidase (ACO) is a key enzyme catalyses ethylene production and plays a crucial role in converting ACC into ethylene in the biosynthesis pathway leading to the cascading loop of system 2 ethylene. Not only is ethylene crucial for ripening but the increasing volumes of ethylene gas accelerate these

processes in senescence and fruit spoilage (Houben and Van de Poel, 2019). ACO is a key marker gene to indicate ripening and senescence and importantly can be used to detect external stresses that might induce ethylene production causing early spoilage.

α-expansin 1 (EXP1) is not expressed in unripe fruit and is specifically upregulated during the ripening process, making it a useful marker. Its role in fruit softening is through the encoding of an expansin protein that disrupts the connectivity of cell wall components, including cellulose and hemicellulose, weakening its structure and softening the fruit (Perrot, Pauly and Ramírez, 2022).

Cell wall modification can be attributed to the expression of CEL2 encoding an endo-1,4-β-glucanase enzyme that primarily assists the breakdown of cellulose. The expression of CEL2 is upregulated by ripening alongside other enzymes including PG and EXP1 in a coordinated effort in cell wall degradation (Perrot, Pauly and Ramírez, 2022). Its expression is also influenced by other factors that determine the plant's overall health including management practices and environmental conditions which provides another useful marker to indicate a reduced shelf life, low quality or identify supply chain issues.

Lipoxygenase (LOX) should be considered as a potential key marker gene due to the rise of expression upon the initiation of senescence. Membrane degradation, oxidative stress and lipid peroxidation are hallmarks of senescence and are associated with LOX (Figueroa et al., 2021). The oxygenation of polyunsaturated fatty acids is catalysed by LOX enzymes, which form precursors for jasmonic acid and volatile aldehydes. Expression of LOX primarily occurs in the onset of senescence, making it a key indicator of post-harvest degradation, however its expression can also be instigated in response to stresses that induce early senescence (Iakimova et al., 2024), reducing shelf life and quality further emphasising its relevance and importance for connecting it to spectral signatures for use in the supply chain.

A recommendation for further work is to map key marker gene expression such as these listed, paired with fruit biochemical spectral signature analysis, with the inclusion of isolated peak wavenumbers that occur during ripening and senescence. This would

provide a more robust and novel method for understanding the biochemical story by using established reference data to validate the spectral results. Limitations with the study in this chapter would be addressed to eliminate uncertainties related to influences from external factors.

2.7 Conclusions

These data and the associated analyses provide valuable insights into the intricate relationship between storage conditions and spoilage in tomatoes, peppers and lettuce and highlight how this is reflected in changes in their MIR spectra. Significant differences in spectral absorbances were identified through the use of PCA-LDA and SVM models allowing for accurate classification of both storage temperature and spoilage stages in all three produce types and varieties. In particular, key wavenumbers contributing to variations between storage conditions in the spectral signature of produce include processes related to structural integrity and enzymatic activities. It is possible therefore that these present potential spectral biomarkers for changes in produce quality during storage that can be quickly detected using non-destructive spectroscopic analysis accompanied with chemometric analysis and machine learning approaches.

It will be important that further research validates these findings across a wider range of produce in order to compile a comprehensive archive of spectroscopic data describing biomarkers detectable at different stages of spoilage which can be used throughout the supply chain as reference data for models that can be rapidly deployed *in-situ*. However, additional studies investigating the correlation between spectroscopic data and physiological parameters, such as ethylene release, senescence genetic markers, and ripening stages, would provide a further understanding of how spectral biomarkers relate to the spoilage processes.

Overall the advances in understanding of potential spectral biomarkers for spoilage made in this study contribute to essential knowledge that can be used to improve supply chain efficiency, post-harvest practices for maintaining quality, shelf life, and thus the reduction in FLW. This work has provided the groundwork for further study using MIR

spectroscopy on fruit surface and demonstrated the ability of data models to manipulate complex and large datasets that are comprised of extensive variables, and perform well when classifying features. This offers the possibility of the development of advanced high-throughput and automated analytical techniques based on this approach, improving the efficiency of these processes and ultimately benefitting consumers and the supply chain as a whole.

2.8 References

MATLAB License Number: 906220

Operating System: Microsoft Windows 10 Pro Version 10.0 (Build 19045)

Java Version: Java 1.8.0_202-b08 with Oracle Corporation Java HotSpot(TM) 64-Bit Server VM mixed mode

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3. Identifying Fraudulent Produce using Mid Infrared and Near Infrared Spectroscopy, a Comparative Study.

3.1 Abstract

Food fraud causes irreparable damage to an already vulnerable global food system and negatively affects every stakeholder. Tomatoes are a culturally important fruit that provides nutrition to a global market and represents the livelihoods of many communities. The authenticity of fruit origin is vital to ensure the associated actors in the supply chain don't lose out. Fruit labelling provides important information about the produce, including its origin, however this information may be fraudulent in some cases. Fraudulent mislabelling misrepresents legitimate, for fraudulent production, at the detriment of reliant grower communities.

Existing commercial methods for detecting fraudulent food are often slow, destructive, and expensive. A non-destructive, high-throughput, and cheap technology must become readily available to detect origin fraud for the infiltration and prevention of food criminals. This study investigates the use of attenuated total reflection-Fourier transform infrared (ATR-FTIR)and near infrared (NIR) spectroscopy as a rapid, quantitative method for detecting biochemical differences between origins from the surface tissue of

tomatoes. Stable isotope signatures were obtained to provide an industry standard reference for spectral interpretation. Fruit spectra from three UK, and one Netherlands' locations were analysed using chemometric multivariate analysis of the fingerprint region (1800 cm^{-1} to 900 cm^{-1}). Distinct chemical peaks were detected which represent biomarkers associated with growing locality and conditions. NIR spectroscopy did not perform well when identifying conventional and organic tomato spectral signatures. Machine learning modelling shows high accuracy in categorising different origins in both MID and NIR spectra. ATR-FTIR provides a low-cost method for in vivo detection of biochemical differences and biomarkers of origin.

3.2 Introduction

The current (2024) population of the UK is approx. 67, 891m and is projected to rise to nearly 77 million by 2050 (UK Population, 2024). Feeding this growing population will rely on the national food system to meet the increased demands for food. The UK has become heavily reliant on the wider global system to import food products, creating an important shift to a requirement for sustained availability of products that would otherwise be inaccessible from the UK, or outside the UK during growing seasons (Food Standards Agency, 2022). This shift in the availability of food products has profoundly benefitted the consumer for convenience, improved nutrition, and enhanced and diversified consumers' food experience. Inevitably, the food system has become complex. Whilst these complexities do not pose problems when food supply chains are efficiently run, outside influences and uncontrollable problems can arise, potentially with significant negative consequences. These can be difficult to isolate and subsequently can create systemic vulnerability in food supply chains (Newell, et al., 2022) Many external factors can escalate these vulnerabilities, including the changing climate (Forzieri *et al.*, 2018) The introduction of fraudulent food products into the supply chain, known as food fraud or 'economically motivated adulteration (EMA)', is also becoming an increasing problem (van Ruth, et al.,2017). This represents a human-augmented problem that is exploitative and importantly exacerbates the vulnerability in the supply chain and the wider food system (Gussow and Mariët, 2022).

Food fraud or EMA is a global problem that can be seriously harmful to consumers, food businesses, and wider society (Manning, 2018). There are also significant economic

consequences resulting from food fraud. Although the true figure is likely underestimated food fraud is thought to cost the UK an alarming £12 billion a year. True accountability is infeasible due to the nature of the undetected criminality. Critically, the Food Standards Agency estimates that approximately 10-30% of all food sold commercially is fraudulent (Food Standards Agency, 2020). As such, it has the propensity to impact every part of the supply chain in direct and nuanced ways: economically, environmentally, societally, and in some instances fatally. Despite 'Food Fraud' being a synonymous problem within any global food system, there is still no single, standardised definition. Food fraud can be described as the intentional adulteration of a food product for financial advantage. However, the most popular definition of food fraud used in the scientific literature is: *"the deliberate and intentional substitution, addition, tampering or misrepresentation of food, food ingredients or food packaging: of false or misleading statements made about a product, for economic gain"* (Spink, 2011; Wilkes, 2021)

The UK Government has characterised different forms of food fraud using the following categories: Adulteration, substitution, misrepresentation/mislabelling, counterfeiting, theft, diversion, over-run, and unlawful processing and documentation fraud (see Table 3.1). These characterisations are important for the effective identification and implementation of preventative measures.

Table 3.1: Food fraud categories defined by UK government department: National Food Crime Unit (NFCU) (Food Standards Agency, 2024)

Adulteration	An undeclared ingredient is included in a product to lower production costs or fake its quality. In China in 2008, melamine was added to baby formula to increase its apparent protein content.
Substitution	An ingredient of high value is replaced with one of lower value. This includes dilution of liquids, for example, replacing honey with sugar syrup or extra virgin olive oil with a lower-value oil (such as nut oil).
Misrepresentation/mislabelling	A product is marketed or labelled to incorrectly portray its quality, safety, species, geographic origin or freshness. For example, by claiming a product is organic when it is not.
Counterfeiting	A known brand's name, packaging, recipe or food processing method is copied, and counterfeit food is presented as a legitimate product.
Theft	Legitimate products are stolen and enter the market through criminal or less regulated routes.
Diversion	Legitimate food meant for one market is unlawfully diverted to another, or food waste is diverted back into the supply chain. For example, waste meat offcuts may be diverted for use in processed meals
Over-run and unlawful processing	Excess unreported product is sold, or techniques or premises used for processing are unauthorised. For example, slaughtering meat in unlicensed facilities.
Documentation fraud	False documents are made and used for the purpose of selling or marketing a fraudulent product.

3.2.1 The Hidden Damages to the Food System

Fraud causes damages to legitimate businesses as when fraudulent products enter the food system, they often compete by low price setting, out-competing their legitimate rivals (Lord *et al.*, 2017) They're also able to undercut prices due to illegal and cheaper practices in the production process. This is displayed in a variety of ways: using cheap ingredients or materials, cheaper packaging materials, misrepresenting product origin and authenticity status, inappropriate production processes, illegitimate transportation, and exploiting their workforce (Robson *et al.*, 2021). These elements allow fraudsters to drive down the sale price making their products more desirable over the legitimate products in the market while maximising profits. In turn, legitimate producers may be forced to decrease their pricing to become competitive to their financial detriment. Knowledge of legitimate brand practices, whether that resides in environmental, economic, or social responsibility, creates a business reputation that promotes consumer loyalty (Aramburu and Pescador, 2019). Fraudulent misrepresentation can harm this relationship causing damage, that may be marginal for large businesses, but potentially irreparable to more vulnerable smaller businesses who rely on their established reputation (Pickett and Pickett, 2002). Loss of confidence and loyalty resulting from fraud can extend to unimplicated businesses by association, causing further supply chain damage (Petrucelli, 2013).

3.2.2 The Societal Fallout from Fraudulent Food

Every element that contributes to the production and sale of food products is at risk of being frauded. There are several consequences of food fraud that are felt by society, including: loss of consumer trust, economic impact, market distortion, loss of nutrition, and other potentially more serious health risks (Hellberg, Everstine and Sklare, 2020). The use of illegal practices can also impact those working within the global food supply chain. This might involve financial gain through the exploitation of workers and other forms of cutting costs that can potentially create dangerous working environments (Onyeaka *et al.*, 2022). These practices may be less obvious or completely unknown to the end-product user, or to other supply chain actors higher in the supply chain. The development and adoption of company practices that protect and prevent corruption can be difficult, especially in places that do not have sufficient infrastructure in place that

protect the labour workforce (Spink, 2019). The consideration for external impacts from the food system is heavily nuanced and requires access to knowledge of systemic processes that aren't publicly accessible. There is a need for transparency in the supply chain, using globally recognised metrics and the application of clear labelling to inform the consumer (Budler *et al.,* 2023). The implementation of these measures makes fraudulent behaviour and exploitative practices more difficult.

3.2.3 Food Fraud is a Danger to Public Health

An important social impact of food fraud is the compromising of public health (Hellberg *et al*., 2020). Food safety is put at risk through the event of food fraud and provides opportunities for unintentional food risk incidents posing serious threats to public health. Detection and prevention of fraudulent food entering the food system are vital in assuring public safety. Several incidents of this nature have led to significant health disasters including excess fatalities (Spink and Moyer, 2011). Toxic oil syndrome affected 20,000 people resulting from illicitly sold rapeseed oil processed through the denaturation using 2% aniline, commonly used to create inedible industrial oil (Posada *et al.*, 2001). A multisystem disease epidemic resulted in several hundred deaths and many thousands were left with permanent disabilities (de la Paz *et al*., 2001; Gelpí *et al*., 2002) and chronic symptoms. This action of adulteration was deemed deliberate with the intent of financial profiteering. The intentional adulteration of food products was similarly practiced in what has been referred to as the 'Chinese Milk Scandal of 2008' through the addition of the organic but highly toxic compound melamine to baby formula (Ross, 2012). The incorporation of Melamine, normally used in plastic and fertiliser production, masked a protein-diluted product making it cheaper to produce and allowing for a larger profit. Six fatalities, 52,000 hospitalisations, and mild kidney and urinary conditions affecting 25,000 children were the catastrophic consequences of this illegal activity (Wang *et al.,* 2021). The gravity of this incident was exacerbated by the failure to detect the compound which could be attributed to inadequate testing methods or the associated inadequate administration. Legislation at the time also allowed the exemption of the two largest dairy producers (Pei *et al*., 2011) from thorough testing and scrutiny, which further compounded the negligence in preventing the tragedy (Brooks et al., 2017).

Reactionary policy change to significant public health incidents has included the implementation of informative food package labelling in the UK (Boden *et al.,* 2005). This has been partially driven by serious, sometimes fatal allergen reaction incidents. In the last 2 decades, there has been a global surge in the prevalence of food-related allergies, prompting a significant research focus. Food allergies have been diagnosed in 2 million people, autoimmune coeliac disease accounts for 600,000 diagnoses (Food Standards Agency, 2024), and between 1990 and 2007, food allergen anaphylactic incidents (Gupta *et al.*, 2007) have increased by 500%. The public health implication of the insurgence of food allergies, and the danger of intentional adulteration necessitates preventative, accurate, and robust testing (Luan *et al.*, 2023).

3.2.4 Fraud in the Food System: Another Environmental Threat

Food production can be exhaustive of resources and puts pressure on the environment. Therefore using production methods that cause the least damage is imperative to mitigate against climate change. This responsibility falls on both the organisations involved and the consumers making the best buying choices within their means (Thangam *et al.,* 2024). Consumer perception has a substantial influence on these decisions and the resulting environmental impact of food production systems (Szabo and Webster, 2021). A growing number of consumers are now considering environmental, ethical, and societal factors when making purchasing decisions (Popovic *et al.,* 2019), especially in regions where consumers have the financial means to act on their values. Food fraud poses a threat to efforts to mitigate environmental damage. Fraudulent adulteration using non-sustainable resources and ingredients in place of environmentally sound ones, can go undetected in environmental data and further exacerbate the climate impact (Lindley, 2021). Upon the detection of fraud, the resulting action may involve removing and destroying the affected products, causing food waste, resources and the associated damages to the environment (Cavazos *et al.*, 2023). The misrepresentation of business practices conveying a message of sustainability can mislead customers. Businesses may exploit this deception to generate financial profits, whilst causing concealed damage to the environment (de Freitas Netto *et al.*, 2020). Unsustainable ingredient adulteration, inappropriate packaging, undisclosed misuse of chemicals,

destructive land-use practices, misrepresentation of energy sources, falsification of emissions data, untested water contamination, illegal waste disposal, and undeclared pollution are some examples of damaging practices (Cavazos *et al.*, 2023). Provision of inaccurate environmental data due to concealment or falsification misleads general understanding detrimentally influencing future policy and practice implementation and potentially perpetuating environmental problems (Cochrane *et al.*, 2024).

3.2.5 Food Provenance, Origin Matters

The origin of food products is important for a number of reasons. When considering environmental implications, the distance the product has travelled has important significance, understanding the origin of the product will allow the consumer to make informed decisions (Walaszczyk and Galińska, 2020) It is also important to know the location of products to better understand the production methods. Availability of the provenance information will allow for consumers, food system stakeholders, and authorities to make educated decisions based on these aspects (Reid and Rout, 2016). Producing regions may use varying practices that should be understood in the buying and consumption of these products (Cozzolino, 2015). Within the consumer market, there may be premiums associated with provenance of various products including various fruit and vegetables. These premiums may be influenced by a specific standard of taste, quality, or unique characteristics (Li *et al.*, 2017). Provenance misrepresentation results in customers feeling defrauded or misled and the devaluing of associated provenance value. The availability of provenance information creates a trust-oriented relationship influenced by the authenticity of ethical production, environmental impact, and quality.

Certifications might be required to authenticate the validity of certain high-value products. The most common form of food fraud in the context of provenance is the improper labelling of a product's origin which is more problematic when products require authenticity status (Kotsanopoulos, 2022). Protected Designation of Origin (PDO) and Protected Geographical Indication (PGI) are two forms of authenticity certifications, devised and used within the EU, that are required for certain product validity (European Commission, 2023). Products that require this authenticity include olive oils, wines including Champagne (PDO), and some cheeses including Orkney Scottish Island Cheddar (PGI). PDO products require “every part of the production, processing, and preparation

process must take place in the specific region", however for PGI products require "at least one of the stages of production, processing or preparation takes place in the region."(European Commission, 2023)

The UK has adopted a certification scheme for healthy planting stock of fruit and vegetables: The fruit propagation certification scheme (FPCS) (*Fruit Propagation Certification Scheme*, 2023) that after accreditation is achieved, requires regular inspections and assessments involving laboratory analysis for grading categorisation. The conservation of this certification involves continuous documentation, financial contribution, and adherence to specific growing conditions. A set of complicated and time-intensive procedures that add value to the associated status and pose a significant obstacle for businesses that act illegitimately. The rainforest alliance has an active certification for traceability of fresh fruit and vegetables (Alliance, 2023) implemented in 2023 which provides accessibility to the product journey, informing consumers, other actors in the supply chain and contributing to relevant data. Rainforest alliance have included a royalty incentive for participation to support producers and other supply chain actors, helping to reduce vulnerability and mitigate impact from fraudulent organisations. Schemes like these have a preventative nature and the implementation of these schemes, public awareness of their legitimacy and applied labelling can provide transparency throughout the supply chain and to the end user (Ulberth, 2020; Manning *et al.*, 2024).

3.2.6 Detecting Food Fraud

The testing of food products to confirm their provenance is often not required by law, but instead is carried out by individual suppliers within supply chains who wish to protect themselves against marketing adulterated produce (Hong *et al.*, 2017). There are many forms of testing that can be used on various food products to establish their provenance depending on the requirements of the testing regimes; rapid, cheap, powerful, simple, and environmentally friendly. The food industry currently uses a range of scientific, technological, and analytical methods to detect food fraud. Many of these are paired with advanced statistical and machine-learning models including chemometrics (Vinothkanna *et al.*, 2024) (Table 3.2). Together, these methods aim to identify fraudulent practices such as ingredient adulteration, mislabelling, substitution, and contamination. For

example, Stable Isotope Ratio Analysis (SIRA) is already well recognised as a technique for confirming the origin of produce within supply chains (Zhao *et al.*, 2023).

Table 3.2: Methods used for food fraud detection

Method of food fraud detection	**Reference**
Nuclear Magnetic Resonance Spectroscopy (NMR)	(Sobolev *et al.*, 2019)
Infrared Spectroscopy (IR)	(Aslam *et al.*, 2023)
Mass Spectrometry (MS)	(Zambonin, 2021)
Polymerase Chain Reaction (PCR)	(Mafra *et al.*, 2008)
DNA Barcoding	(Barcaccia *et al.,* 2016)
Stable Isotope Ratio Analysis (SIRA):	(O'Sullivan *et al.*, 2022)
Isotope Ratio Mass Spectrometry (IRMS)	(Li *et al.*, 2023)
Chromatography: High-Performance Liquid Chromatography (HPLC), Gas Chromatography (GC), Thin Layer Chromatography (TLC)	(Sherma and Rabel, 2018)
Electronic Nose and Tongue	(Mahanti *et al.*, 2024)
Enzyme-Linked Immunosorbent Assay (ELISA)	(González-Martínez *et al*., 2018)
Microscopy: Light and Electron Microscopy	(Oliveira *et al.*, 2024)
Metabolomics	(Tan and Zhou, 2024)
Proteomics	(Varunjikar *et al.*, 2024)
Traceability and Blockchain Technology, RFID and QR Codes	(Loke and Ann, 2020)

3.2.7 Stable Isotope Authentication of Food

The stable isotope signature of food products is often unique to their place of origin and the type of produce (Camin *et al.*, 2017). Consequently, the analysis of stable isotopes is used in the supply chain for the testing of a wide range of products for the detection of food fraud. Food and beverage products can be analysed for oxygen, sulphur, hydrogen, nitrogen and carbon stable isotopes using isotope ratio mass spectrometry techniques (Rossmann, 2001). Testing frequently focuses on high-value products to establish their authenticity. Organic fruit and vegetables are considered a high-value product in

conjunction with conventionally grown produce. This is due to the higher financial costs and increased difficulty involved in organic production. Organics also hold a higher ethical value due to the improved safety, health, and environmental impact (Wang *et al.*, 2020). This value differential presents an opportunity and a financial motivation for fraudsters to misrepresent conventional produce for organics (Manning and Kowalska, 2021). Nitrogen isotope values are used to test for organically grown produce. Organic fertilisers support nitrogen isotopic values which typically range between 10‰ and 20‰ and are often made from peat, manure and sewage sludge. Synthetic fertilisers have much lower nitrogen isotope values of approx. between 3‰ and 5‰, comprised of substances such as ammonia and potash (Bateman *et al*., 2007). These value discrepancies, in addition to processes such as ammonia volatilisation and nitrification, allow for stable isotope measurements to discriminate between organic and synthetically grown produce (Chesson *et al*., 2018).

Stable isotopes are also well suited to distinguishing and verifying the origin of product, the most commonly frauded aspect, based on: growing conditions, topography, geology, and climate (Brombin *et al*., 2022). Geographical origin stable isotope testing makes a direct comparison between the isotopic fingerprint of a sample and material used as a reference verified from a geographic location. (Brodie *et al.*, 2011).

3.2.8 IR Spectroscopy for Food Authentication

The use of mid-infrared (MIR), near-infrared (NIR), and RAMAN spectroscopy are considered rapid and powerful techniques for detecting the chemical composition and molecular structure of food. This has been demonstrated in the analysis of olive oils (Galtier *et al*., 2007). Using NIR spectral analysis, percentages of fatty acids and free fatty acid contents have been predicted through chemometric models. In addition, the classification of five geographical locations of olive oil origins was achieved, despite the variety of cultivars. The use of spectroscopic methods is often used in the analysis of identifying the presence of adulterated compounds, additives, and product manipulation (Cozzolino, 2015; Feng *et al.*, 2021; Ruggiero *et al.*, 2022). The biochemical status of organic samples can be influenced by an extensive range of contributors, from growing conditions, cultivars and postharvest management. The use of chemometrics allows to isolate key variables explained by origin-associated characteristics, for example, growing

conditions. Soil composition, nutrients, irrigation, geology, weather conditions and even microbial interactions may all contribute to the sample biochemistry and the spectral signature of the sample (Guindo et al., 2023). Reference spectra of a verified product is compared to validate authenticity.

The presence of fraudulent food in the supply chain poses dangerous risks with highly detrimental consequences that can affect all actors in the supply chain (Manning, 2024). Avoiding these consequences is reliant on the availability of effective and reliable detection methods that can be applied throughout the supply chain.

IR spectra can be influenced by differences in soil mineral composition, climate and local agronomic practices, as these elements affect biochemical profiles including secondary metabolites, sugars and organic acids. These variations in the spectra may provide an indicator of provenance. It is expected that the differences between farming practices used in organic and conventionally grown fruit, which alter nutrient availability, stress responses, and phytochemical composition, may lead to measurable shifts in IR absorption levels.

This study aims to further understand how growing locations and organic growing practices influence the biochemistry of tomato fruit and how this is represented in the spectral signatures obtained from MIR and NIR spectroscopic techniques.

Research Questions:

Can NIR, ATR-FTIR and stable isotope profiles differentiate between tomatoes from different regions?

Is the organic status of tomato fruit distinguishable using NIR and stable isotope profiling?

What represent the most informative spectral and isotopic features for classification?

Does spectral analysis provide a suitable alternative for fruit origin authentication?

Aims

- To evaluate the potential of spectral analytical techniques in classifying tomatoes based on origin and growing practices.

- Compare the efficacy of IR spectroscopic techniques with industry-used stable isotopes for identifying origin chemical profiles and organic profiles of tomato fruit.

3.3 Methods

3.3.1 Fruit Origin, Transportation and Storage

Tomato fruit were sourced from four verified locations, three UK-based growers located in Cambridgeshire, Norfolk and West Sussex, and one in the Netherlands (Table 3.3). All tomatoes were conventionally grown (non-organic), and supplied by Suncrop Ltd through its established grower network. Cultivars included: Capricia, Roterno and Xandor, although consistent cultivar access was not possible logistically. Cultivar-dependent spectral variations was controlled for through the sourcing of Roterno cultivar from both Ca, Cambridgeshire and West Sussex. All fruit was obtained from larger batches destined for sale at a high-value UK retailer and redirected immediately after harvest, ensuring 'retail-ready' ripeness and quality. The fruit was selected for uniformity based on size, colour, ripeness, undamaged, and exhibiting consistent colouration across the fruit surface. This conforms to the selection criteria used by Suncrop Ltd's industry standards as a prime supplier for premium UK supermarket Waitrose.

Fruit were transported under industry standard conditions in temperature-controlled vehicles at 10-12°C to the Suncrop Ltd depot in Chatteris, Cambridgeshire where they were stored at 10°C for between 1-2 days, before an onward courier transported to the Lancaster Environment Centre (8-14°C; 6 hour transit). On arrival, the fruit were washed using deionized water and dried and subjected to spectral analysis.

Table 3.3. Growth methods and locations for tomatoes supplied by Suncrop ltd.

Country	County	Location	Type	Variety	Growing type	Irrigation	Growth media
UK	Cambridgeshire	Fen Drayton	Classic	Roterno	Conventional	Unknown	Unknown
NL	Zuid Holland	Westland/De Lier	Classic	Capricia	Conventional	Borehole and roof/reservoir recirculation	Rockwool
UK	Norfolk	Norwich	Classic	Xandor	Conventional	Reservoir and recirculation	Rock Wool

UK	West Sussex	Barnham	Classic	Roterno	Conventional	Reservoir and recirculation	Rockwool

For each biological replicate, spectral measurements were taken at 20 locations to account for tissue heterogeneity and blemishes using both MIR and NIR spectroscopic techniques. Additional tomatoes from each location batch were collected and sent to a verified authentication testing organisation: Food Forensics Ltd for stable isotope analysis. This organisation is used as standard by Suncrop ltd, thus mirroring industry testing practice.

To explore the use of portable NIR readers, in-situ measurements were taken from on the vine cocktail tomato fruit *Solanum lycopersicum* cv. Brioso cultivar from both conventionally grown fruit and organically grown fruit. Stable isotope analysis was conducted by Food Forensics to provide a reference to NIR spectra obtained and to compare spectral profiles with isotopic profiles associated with farming practices.

3.3.2 ATR-FTIR Spectroscopy Analytical Techniques

Ten tomatoes from each geographic location were analysed by Mid Infrared (MIR) and Near Infrared (NIR) spectroscopy. In addition, a representative sample from each sample batch were redirected to Food Forensics Ltd, Norfolk, for stable isotope analysis. MIR spectral readings were taken using a Bruker Alpha 1 Attenuated Total Reflectance – Fourier Transform Infrared (ATR-FTIR), Opus software, and analysed using iRootlab for Matlab software programme. Between each sample measurement the spectrometer crystal was cleaned using isopropyl alcohol wipes (Bruker Optics, Coventry, U.K.), and each time, background spectra were taken to account for ambient atmospheric conditions.

3.3.3 NIR Spectroscopy Analytical Techniques

NIR spectral readings were taken using a handheld NIR spectrometer device: NIRvascan ASP-NIR-M-Reflect (Allied Scientific Pro, Gatineau, Quebec, Canada) and ISC NIRScan software mobile app. The data was analysed using iRootlab for Matlab (R2021a) software programme. The spectrometer crystal was cleaned between measurements using

isopropyl alcohol wipes (Bruker Optics, Coventry, U.K.), and each time, background spectra were taken to account for ambient atmospheric conditions.

3.3.4 Stable Isotope Analytical Techniques

Stable isotope analysis was commissioned to an industry standard, Food Forensics Ltd is used as standard by Suncrop Ltd. Testing for provenance and conventional versus organic fruit was performed. Tomatoes from the same batch were subsequently used in the described spectroscopic studies. Provenance was assessed on the basis of Carbon, Nitrogen, Hydrogen, and Oxygen isotopes. Photosynthetic pathways in plants can vary as result of environmental including the availability of water and light intensity, which are reflecting in $\delta^{13}C$ values (Kochetova et al., 2022). Regional climate and geography influence the isotopic signatures related to $\delta^{18}O$ and $\delta^{2}H$ (Ariel, 2025). Soil sulphur sources, fertiliser type and proximity to marine environments may be indicated by $\delta^{34}S$ (Blanz et al., 2024). Their match to UK-based isotopic signatures was initially tested, and further PCA analysis was used to test against a reference sample. Analysis of organics and conventional tomatoes used the isotopes of Nitrogen to establish their growing method.

3.3.5 Data Analysis and Validation

The spectral data was imported from OPUS software for analysis using MATLAB R2021a (MathWorks, Inc., Natick, MA). Matlab analysis was performed using interface package iRootLab version 0.17.8.22-d (Copyright 2012 Julio Trevisan, Francis L. Martin & Plamen P. Angelov). MID Infrared spectra were cut to the fingerprint region (1800-900cm^{-1}), Near infrared spectral techniques automatically produce spectra between (1700-900cm^{-1}) negating the requirement for cutting down. Savitzky–Golay smoothing (second-order derivative, 9 filter coefficient, second-order polynomial fitting) was applied to improve the signal-to-noise ratio. Normalisation techniques: Vector normalisation and mean centring were applied.

Exploratory analysis: principal component analysis (PCA), was performed on the preprocessed data. This technique places each spectrum as a data point onto planes of space. Data is distributed within the model along axes or principal components (PCS) using the variances. PCs are responsible for explaining the spread of the data. PCs are mapped orthogonally to each other, these form the scores and associated loadings that

attribute to wavenumbers where the largest variances lie which can be used as possible spectral markers.

To further maximise class separability supervised analysis: principal component analysis with linear discriminant analysis was applied. Classification support vector machine (SVM) model was applied, a linear classifier with a nonlinear kernel transformation which is used to capture non-linear data relationships. The SVM model used k-fold cross-validation whereby the dataset was randomly divided into 5 (k) subsets, the model was trained 5 (k) times, each time using 4 (k-1) folds for training, and the remaining fold for validation. This process helps to improve the performance of the model, avoid overfitting, and provide a more reliable estimate of the effectiveness of the model. Preprocessing methods differed from those used in multivariate analysis to achieve the highest accuracy in classification. 1st order derivative, 9 filter coefficient, second order polynomial fitting was applied followed by vector normalisation and 0,1 range normalisation.

3.4 Results

3.4.1 Multivariate Analysis of MIR and NIR

Processed spectra before multivariate analysis from tomatoes grown in four the geographical locations studied showed some separation along wave regions 1744 cm^{-1} , 1730 cm^{-1} , 1643 cm^{-1} , 1215 cm^{-1} , 1101 cm^{-1} in mid-infrared, and 1682 nm, 1664 nm, 1404 nm, 1154 nm (Figure 1).

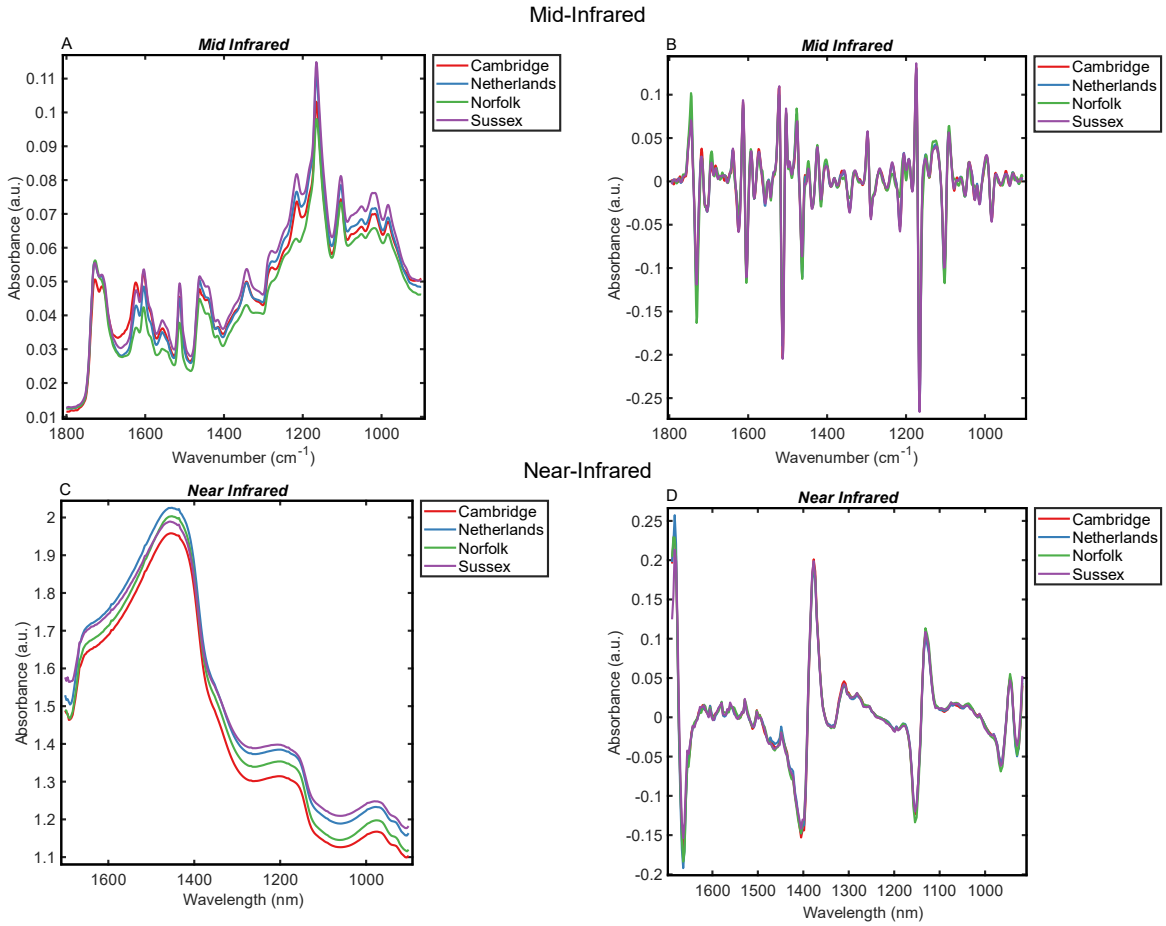

Figure 3.1. Infrared spectra of *Solanum lycopersicum* tomatoes grown in four geographical locations. **A**) Mean raw mid-infrared spectra of the fingerprint region 1800-900 cm-1 **B**) Mean pre-processed mid-infrared spectra. **C**) Mean raw near-infrared spectra 1700-900 nm **D**) Mean pre-processed near-infrared spectra.

Separation was observed in PCA analysis between all geographical tomato origins along PC1 which accounts for 32.3% of the variance of the data. Further analysis using a PCA-LDA supervised approach, identified only one feature in the data to which the class variance is explained in Figure 3.2. PCA-LDA displays an observable separation of classes with clear clustering. Overlap of class clustering occurs in Sussex tomatoes, which partially overlaps with Netherlands and Cambridge. Norfolk remains separate from all other locations. Cambridge and West Sussex were both Roterno variety which provided expectation that they could be indistinct in these analyses if these tests were using genetic similarity as the data feature. In these models, the shared cultivars were clustered and distinct, with some overlap, suggesting that the features in the data were not exhibiting cultivar classification. To improve robustness, testing multiple growing batches from

multiple years would be beneficial and smooth time related anomalies that may be skewing spectral profiles within the batches.

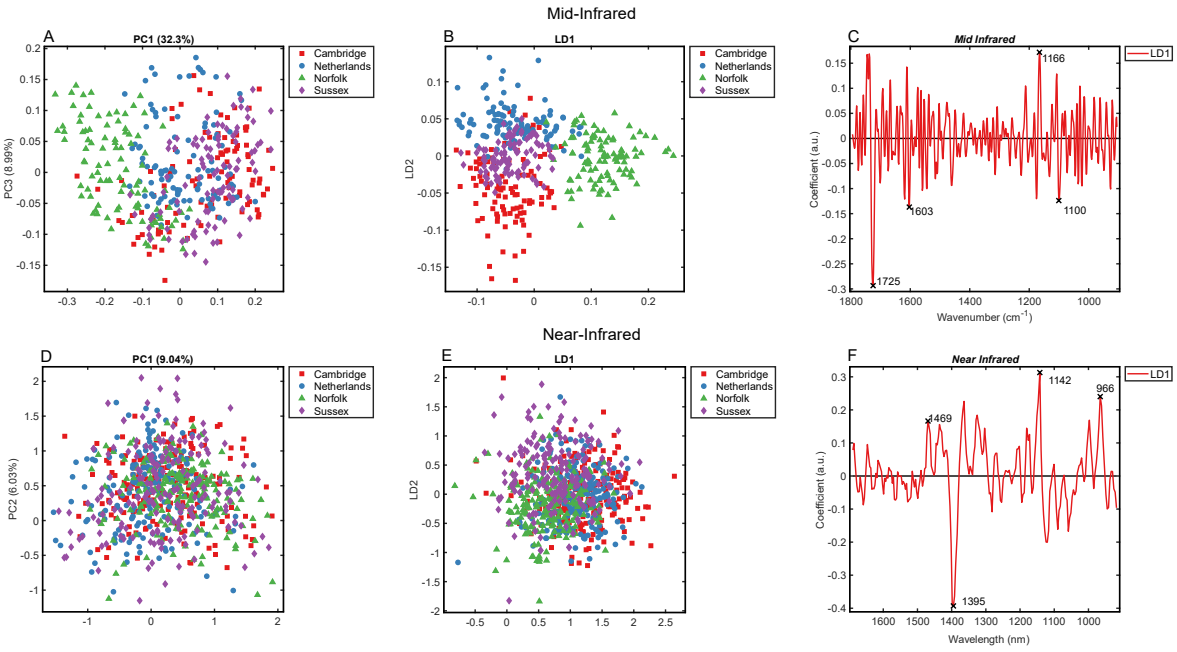

Figure. 3.2 *Solanum lycopersicum* tomatoes grown in four geographical locations. **A, D)** PCA multivariate analysis **B, E)** PCA-LDA supervised multivariate analysis **C, F)** PCA-LDA loadings. **A-C)** Mid-infrared **B- F)** Near-infrared

NIR analysis showed much less prominent class separation. PCA has no distinguishable class-associated clustering, and no outliers were identified in the dataset. When PCA-LDA was performed, some separation and clustering is achieved but there was heavy overlapping between all locations, and several individuals remained unaligned with their class cluster. Clustering is more visible in the Netherlands, Norfolk, and Sussex however Cambridge samples are less obviously clustered and have higher variance distribution along both LD1 and LD2.

Mid-infrared loadings for provenance drew out wavenumbers: 1725 cm^{-1}, 1603 cm^{-1}, 1166 cm^{-1}, and 1100 cm^{-1}. These are associated with 1725 cm^{-1}: C = O stretching in esters and lipids, 1603 cm^{-1}: C = C stretching in aromatic compounds (phenolics, carotenoids), 1166 cm^{-1}: C - O stretching in polysaccharides and esters, 1100 cm^{-1}: C – O - C stretching in cell wall polysaccharides. In NIR, wavelengths 1469 nm: C - H bending overtones in lipids and fatty acids, 1395 nm: CH_3 and CH_2 bending overtones in carbohydrates and lipids, 1142 nm: combination bands of C - H and C - O in

polysaccharides and esters, 966 nm: C - H out-of-plane bending in carotenoids and polysaccharides (Table 3.5).

Table 3.4. PCA-LDA loadings from MIR and NIR spectra obtained from *Solanum lycopersicum* tomatoes grown in four geographical locations. MIR loadings represent wavenumbers where the greatest peak variances occur, associated with fundamental vibrational modes, useful for identifying specific functional groups and molecules. NIR loadings represent the greatest peak variances related to overtones and combinations of these vibrations, offering insights into overall composition and properties.

Wavenumber	**Wave range**	**Chemical Association**	**Reference**
MIR cm^{-1}			
1725	1725 1750-1700 1725-1705 1724-1695	C = O Esters, methacrylates, maleates, fumarates, nezoates, phthalates, terephthalates, isothalates C = C stretching in conjugated systems or aromatic rings C = O Amide I band in proteins Dialkyl ketones C = O α-amido acids	(Colthup, 1975a)
1603	1665-1585 1605-1555 1600-1621 1655-1558	NH_3 deformation: α-L-amino acids CO_2 stretching: Normal chain amino acids C = O amido acids C = N Pyrrolines	(Colthup, 1975a)
1166	1300-1100	C - O stretching vibrations: esters and carboxylic acids	(Colthup, 1975a)

	near 1150-1050 1210-1158 1200-1000	C - O stretching: alcohols C-O-C stretching vibrations in ethers or esters C - O Saturated esters C – O stretching starches	
1100	1125-1000 1200-1000	Tertiary alcohols phenols, C - O Carbohydrates C – O stretching starches	(Colthup, 1975a)
Wavelength			
NIR nm			
1469	1600-1400 1550-1450 1470-1440 1600–1460	O – H stretch and O – H band combination and the H – O – H deformation combination: starch First overtone of the hydroxyl group., The first overtone of the NH stretch primary amines In heterocyclic amines such as pyrroles, indoles and carbazoles: first overtone NH stretching, Hydrogen-bonded alcohols	(Konstantinos *et al.,* 2017)
1395	1437–1389	Polysaccharides OH stretch 1st overtone	(Konstantinos *et al.,* 2017)
1142	1143-1142	C - H Aromatic hydrocarbons	(Williams *et al.*, 2019)
966	966	Water	(Konstantinos *et al.,* 2017)

3.4.2 SVM Machine Learning Classification Models

SVM machine learning models were applied to both MIR and NIR data (Figure 3.3). SVM classification of tomatoes from four geographically different growth locations or provenance, differentiated by their associated growing conditions (Cambridge, Netherlands, Norfolk, and Sussex), provide varying classification success accuracy scores based on MIR and NIR spectral data. Mid-infrared SVM classification achieved highly accurate results across the four geographical locations. Cambridge achieved 90.77% correctly classified samples, the lowest accuracy achievement, this compares with the Netherlands achieving the highest classification percentage of 95.99%. There were low misclassifications across the whole model. Overall, the classification accuracy was high in this SVM model. Across the models there is a small but notable percentage of misclassifications indicating a struggle for classification between class boundaries but negates the occurrence of the model memorising data causing overfitting.

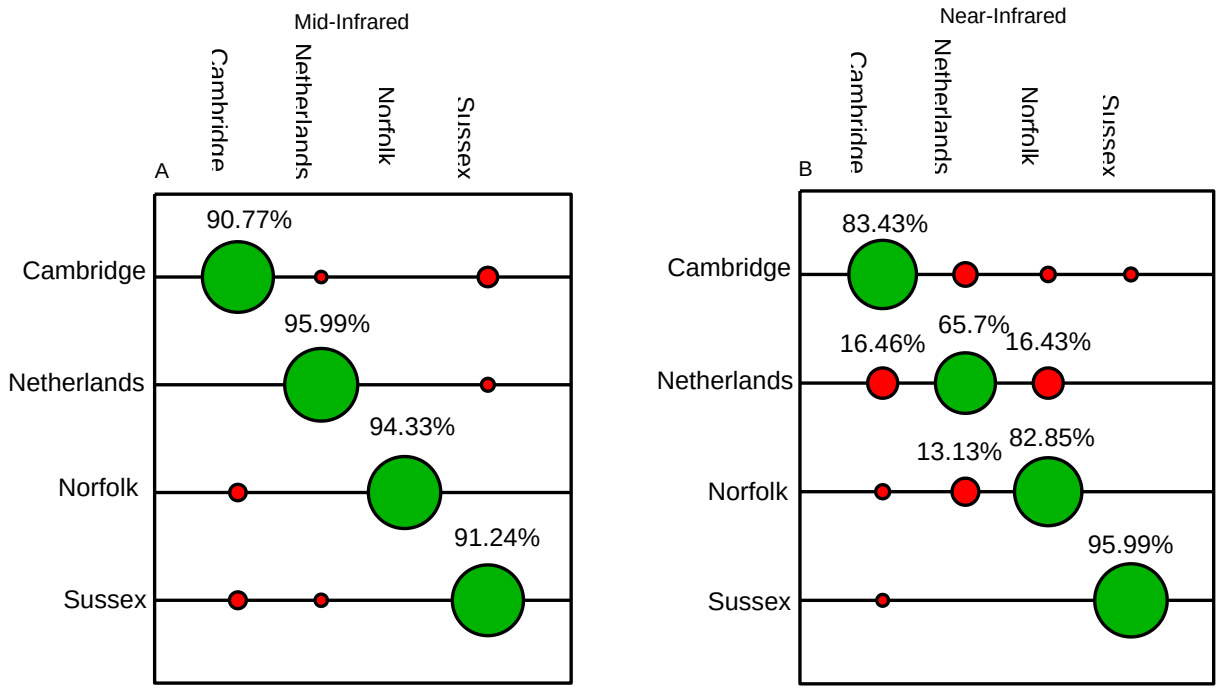

Figure. 3.3 *Solanum lycopersicum* tomato SVM confusion matrix grown in four geographical locations. **A)** Mid-infrared **B)** Near-infrared

In NIR SVM classification, more variation was observed between the growing locations. Netherlands, the highest classification in the mid-infrared SVM model, decreased to

65.7% with a misclassification rate of 16.46%. Sussex achieved the highest accuracy rating of 95.99%, Cambridge and Norfolk following with 83.43% and 82.85% respectively. Overall, classification accuracy across the NIR model was high, despite the decrease in accuracy from the MIR region with the most significant decrease appearing in the Netherlands suggesting more spectral overlap. In both models, Sussex achieved accuracy higher than 90% suggesting these were the most distinct spectra from both infrared regions.

Overall, these data show that MIR spectral achieves a higher specificity which has allowed the models to achieve better classification over NIR. MIR by nature allows for higher specificity generally (Sales *et al.*, 2015), however, the high performance in models demonstrates they are both useful, and both have the potential to be used in industry to identify tomato fruit that are suspected to come from inauthentic localities by testing against authenticated samples. Classification can be attributed to origin, not cultivar differences, demonstrated by high accuracy classification between Cambridgeshire and Sussex tomatoes that are both Roterno variety. These share the same genetics but with different growing conditions, growing conditions providing a proxy for their growth origin.

3.4.3 Stable Isotope Analysis for Provenance

ANOVA analyses of stable isotope ratios were conducted in tomatoes from four growing regions: Cambridgeshire, Netherlands, Norfolk, and Sussex from the same batches provided for spectral analysis (Table. 2, full reports in appendix). Raw data is unavailable due to policy of industry protocol (Food Forensics ltd)

Table. 3.5 Stable isotope test results of *Solanum lycopersicum* tomatoes grown in four geographical locations tested for origin authenticity against reference samples previously provided by the authentication team. P values represent confidence of similarities of carbon, nitrogen, hydrogen and oxygen isotopic values between the independent reference tomatoes and the samples resulting in a pass/fail overall result.

Origin	**ANOVA against reference sample**				**Pass/Fail**
	P(δ13C)	**P(δ15N)**	**P(δ2H)**	**P(δ18O)**	
Cambridgeshire	0.41	0.3	0.07	0.07	Pass
Norfolk	0.71	0.09	0.73	0.38	Pass
Netherlands	0.35	0.78	0.69	0.78	Pass
West Sussex	0.1	0.15	0.68	0.38	Pass

Carbon ($\delta^{13}C$), nitrogen ($\delta^{15}N$), hydrogen ($\delta^{2}H$), and oxygen ($\delta^{18}O$) isotope levels were tested against reference samples from the same growing locations. This assessment aimed to assess the deviation of the sample tomatoes from the reference samples in relation to the isotopic composition. ANOVA p values were obtained, and a significant difference was determined against the reference. Across all isotopes in all regions, all tests received a pass value denoting that there was no significant differences between the samples and the references. Carbon isotope ANOVA resulted in p-values ranging from 0.1 in Sussex to 0.71 in Norfolk, all greater than the significance threshold of $p < 0.05$. Approaching significance but not reaching the significance threshold of 0.05 in nitrogen isotopes was p= 0.09 in Norfolk, highest p-value was found when the Netherlands was tested at $p = 0.71$. $p = 0.07$ was achieved in hydrogen and oxygen isotopes in Cambridgeshire, both closely approaching the significance threshold. Other regions in these isotopes achieved much higher p-values further supporting analysis for no significant differences between all regions, and their references in all stable isotopes tested.

3.4.4 Comparing the use of IR and Stable Isotopes for the organic certification of produce.

Preprocessed spectra before multivariate analysis of organically and conventionally grown Brioso tomatoes showed observable spread at wavenumbers 1680 nm, 1639-1579 nm, 1448 nm, 1401 nm in near-infrared (Figure 3.4). These may hint at differences in proteins, aromatic groups, carbohydrates and water (Konstantinos et al., 2017) however, multivariate analysis is required for a more reliable classification due to residual noise and data complexity (Zhang *et al.*, 2022).

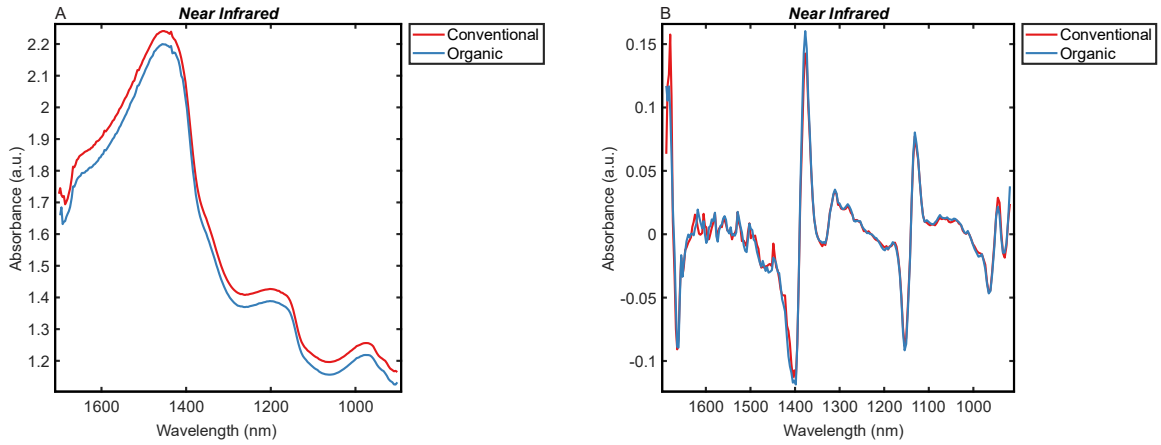

Figure. 3.4 Near Infrared spectra of *Solanum lycopersicum* tomato grown conventionally and organically. **A)** Mean raw near-infrared spectra **B)** Mean pre-processed near-infrared spectra.

In multivariate analysis, PC1 accounted for 19.5% of the variance, and PC2 for 12.03% (Figure 3.5A). Conventionally-grown and organically-grown tomato groups show considerable overlap, but some minor clustering is visible along PC1 axis.

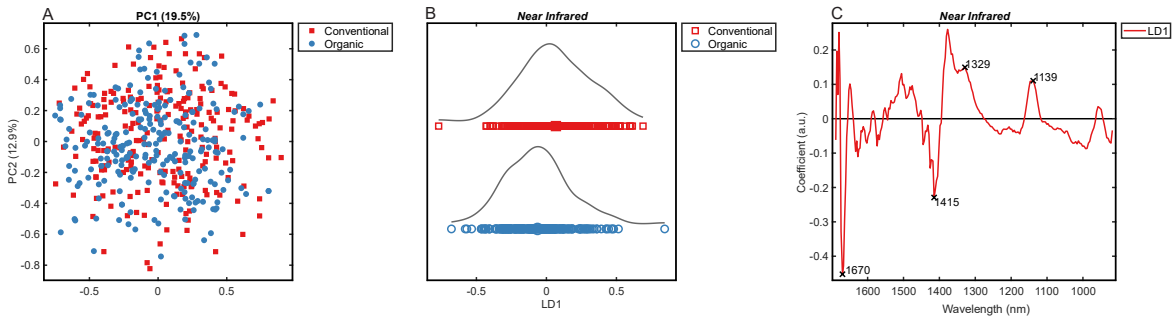

Figure. 3.5 *Solanum lycopersicum* tomatoes grown conventionally and organically. **A)** Near-infrared PCA multivariate analysis **B)** PCA-LDA supervised multivariate analysis **C)** PCA-LDA loadings.

PCA-LDA analysis enhanced the classification between organic and conventional (Figure 5B). The first linear discriminant (LD1) displayed some separation through the data distribution however there was nevertheless a marked overlap. Although there was some improvement from PCA alone, PCA-LDA approach did not perform to high accuracy in conventional tomatoes over organics. Along LD1, loadings wavenumbers were noted at 1670 nm, 1415 nm, 1329 nm, and 1139 nm. 1670 nm is associated with condensed tannins, 1415 nm is linked to alcohols and polysaccharides, 1329 nm is unassigned, and 1139 nm is assigned to aromatics (Table 3.6). Despite these wavelengths being drawn as the highest variations, the separation between the scores in PCA-LDA (Figure 3.5B) is low, and the poor performance in SVM machine learning model (Figure 3.6), these cannot be relied on.

Table 3.5. PCA-LDA loadings from NIR spectra obtained from *Solanum lycopersicum* tomatoes grown conventionally and organically

Wavelength	**Wavenumber range**	**Chemical Association**	**References**
NIR nm			
1670	1670 Near 1670 Near 1672 Near 1690 Near 1660	Condensed tannins CH Protein Sucrose CH_3 methyl Cis-unsaturation	(Dryden, 2003) (Ingle *et al.*, 2016) (Weyer and Lo, 2006a) (Sundaram *et al.*, 2011)

			(Nicolaï *et al.*, 2014)
1415	Near 1416 1400-1440 1437-1389 1400-1600	O - H O Alcohols, Phenols C -H combination C - H methylene (CH_2) Hydrocarbons, aliphatic alcohols, with first overtones Polysaccharides OH stretch 1st overtone, fatty acids determination,. O – H stretch and O – H band combination and the H – O –H deformation combination: starch First overtone of the hydroxyl group.	(Weyer and Lo, 2006a; Konstantinos G. Kyprianidis and Jan Skvaril, 2017)
1329			
1139	Near 1140	Aromatics for benzene in CCl4	(Weyer and Lo, 2006a)

SVM classification model (Figure 3.6) performed with varying accuracy of classification. Correct classification of organically grown tomatoes was highly accurate at 83.43% however a large misclassification value was obtained of 16.57%. The SVM model struggled with classification of conventionally grown tomatoes with a higher percentage of misclassifications than correct classifications, 43.18 and 56.82%, respectively. This poor classification and high misclassification suggests that the SVM is unsuitable for use in industry for classification of organically grown tomatoes.

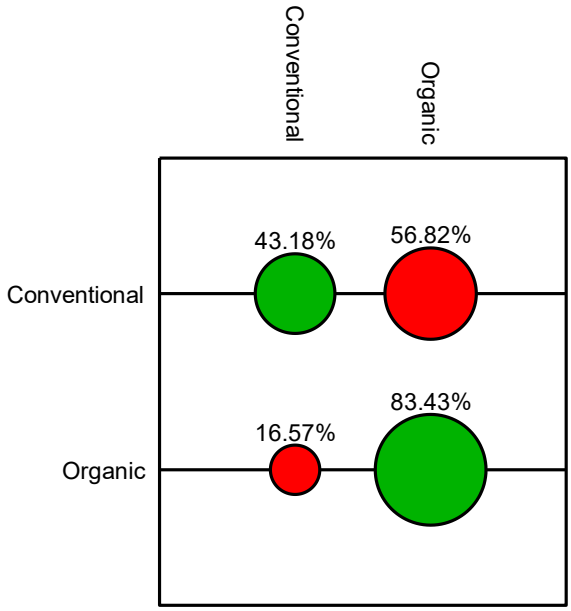

Figure. 3.6 *Solanum lycopersicum* tomato SVM confusion matrix grown conventionally and organically displaying the classification performance accuracy values.

3.4.4 Stable Isotope Analysis

Stable isotope analysis (Table 3.6) verified the authenticity of organic fruit and the inauthenticity of the conventionally grown tomatoes based on the values of $\delta^{15}N$. Organically grown Brioso tomatoes displayed values of 6.53 ± 0.15‰ fitting within the threshold of +2.5 to +45.2‰ (Inácio, Chalk and Magalhães, 2015) in contrast with conventionally grown Brioso tomatoes displaying value of 0.56 ± 0.05‰, corresponding with the conventional threshold of $\delta^{15}N$ −3.9 to +5.7‰.

Table. 3.6 Stable isotope test results of *Solanum lycopersicum* tomatoes tested for authenticity of organic growing methods testing for nitrogen values. Test was conducted against expected organic isotopic profiles, results express whether they fit the profile (pass) or whether they do not fit the expected profile (warning)

Farming practice	**T-Test**	**Test Result**
	δ 15NAIR ± σ* (‰)	
Conventional	0.56 ± 0.05	Warning
Organics	6.53 ± 0.15	Pass

3.5 Discussion

This study investigated the application of two approaches for assessing differences between tomato fruit from different growing conditions, and geographical localities, and comparing conventional and organic farming practices. This was explored using the spectral and isotopic characteristics of fruit and the application of multivariate analysis and machine learning techniques.

3.5.1 Geographical Origin was Successfully Classified with High Performance in MIR

Key wavenumbers were identified using PCA-LDA multivariate analysis describing the biggest spectral differences between the localities. Polysaccharides are key components of tomato fruit cell walls. The main polysaccharides in tomatoes are pectin, hemicellulose and cellulose. Another important polysaccharide is starch which plays an important role in fruit ripening. Wavenumber 1166 cm^{-1} and 1100 cm^{-1} may be associated with starch, a component that may be influenced by climatic conditions and growing environments (Brummell *et al.*, 1999) Climatic factors present at the different growing locations can influence the biochemical signature in tomato fruit. For example the presence of water and its molecular interactions. The irrigation regime and soil moisture may be associated with spectral indicators. O – H stretch and combination bands 1400 to 1600 nm is associated with variations in starch content (Konstantinos *et al.,* 2017), possibly reflecting plant stresses occurring from climatic stresses. Important wavelength was identified in the NIR spectrum at 1469 nm which occurs in this band, indicating that starch content may be indicative of the growing conditions. In the MIR spectrum, 1100 cm^{-1} and 1166 cm^{-1} were also highlighted as a key wavenumbers, this is associated with C – O stretching vibrations in the glycosidic linkages of starch polymers (Colthup, 1975). Starch content has been shown to be affected by a variety of external influences including temperature (Zepeda et al., 2022). 1100 cm^{-1} (C–O stretching in polysaccharides) could vary with environmental factors that impact cell wall composition, such as water and nutrient access. These could play important roles when discriminating between tomato origins. This is further supported by wavenumbers that were identified in the NIR region: 1469 nm, 1395 nm, 1142 nm and 966 nm. Also indicative of polysaccharides O – H

stretching (Tsuchikawa and Siesler, 2003; Krongtaew et al., 2010). This signature may also be influenced based on genetic variation and carbohydrate profiles. Irrigation methods varied between the growing locations (Table 3.3), growers in the Netherlands used borehole and roof and reservoir recirculation, both Norfolk and West Sussex used reservoir and recirculation and it was unknown what irrigation method was used in tomatoes grown in Cambridgeshire. Despite similarities in these methods, recirculation frequency, and compounds present in the water reservoirs used to irrigate is unknown and are likely to differ between locations, all potentially influencing starch content .

Variations between tomatoes grown in different geographical locations were observed in the tomato spectroscopic analysis of the MIR and NIR regions. In the MIR region, notable wavenumbers were identified as associated with lipids, aromatic compounds and polysaccharides: 1725, 1603, 1166 and 1100 cm^{-1} respectively, 1725 cm^{-1} (C=O stretching) may vary with organic acid and ester content (Colthup, 1975). , potentially influenced by temperature and soil fertility .

With the exception of Cambridgeshire tomatoes, all were grown using rockwool as the growing substrate. Rockwool is used in hydroponic systems and provides a substrate to attach. As it is inert, it does not contribute nutrients, so the plants rely on precise nutrient additions. Nitrogen is a key nutrient required for cultivation which is required to be added through fertiliser. (Verdoliva *et al.*, 2021). The fertiliser composition applied to these tomatoes was not available, but even subtle differences in the form and quantity of nitrogen may influence the biochemistry of the fruit. NIR spectral analysis highlighted key wavenumber 1469 nm, which along with starch association, may also be attributed to NH stretching in the 1450 to 1550 nm region (Konstantinos., et al). Nitrogen may represent a key indicator for the growing regime, which, with a reference, can be connected to growing locations.

1469 nm in the NIR spectrum may be attributed to differences in hydrogen-bonded alcohols found in region 1460 nm to 1600 nm (Weyer and Lo, 2006a) that may be associated with phenolic compounds. Environmental factors play key roles in the presence of phenolic compounds in tomato fruit (Araya *et al.*, 2021) including temperature, and availability of mineral nutrients such as nitrogen, phosphorous, potassium and calcium (Dumas *et al.*, 2003). Differences in phenolic compounds between

growing origin may be related to the provision of nutrients in applied fertilisers. This association may further be supported by the identification of 1166 cm-1 and 1100 cm-1 in the MIR spectrum, both associated with C – O stretching in hydrogen-bonded hydroxyl groups of alcohols and phenolic compounds (Colthup, 1975a). Aromatic hydrocarbons appearing at 1142 nm correspond to C – H stretch overtones found in the NIR spectrum. Also indicative of contributions to flavour and aroma a vulnerable to environmental influences including light intensities and humidity (Williams, Manley and Antoniszyn, 2019). Even subtle differences can influence concentrations in the fruit and influence the spectral signatures suggesting these have a potential for use as an indicative biomarker of growing conditions.

3.5.2 Limitations have been Identified that may Compromise the Reliability of Origin Spectral Signatures

This study included three varieties, Roterno grown in Cambridgeshire and West Sussex, Xandor grown in Norfolk and Capricia in the Netherlands. Whilst some separation between tomatoes from different regions was observed in PCA, there was nevertheless a noteable overlap between samples from Sussex, the Netherlands, and Cambridgeshire. PCA-LDA approach was applied, which improved the separation between locations, particularly Norfolk which exhibited a distinct cluster separate from the other regions. This overlapping suggests similarities in obtained spectra which complicated the distinction between geographical locations. Separations were more prominent in MIR than in NIR which was to be expected as the MIR region is generally more specific than in NIR. Factors such as climate and soil conditions may influence the chemical compositions of associated fruit grown in their geographical locations (Donhouedé *et al.*, 2023) but these may overlap due to shared agricultural practices and similarities in climate conditions.

Using SVM models to classify geographical locations showed promising results, both in MIR and NIR, with MIR performing with higher accuracy for locales. MIR SVM achieved highly accurate results ranging between 90.77% and 95.99% while NIR achieved accuracy ranging between 65.77% and 95.99%, the most variable location being the Netherlands which achieved the lowest accuracy result in NIR compared with the highest accuracy in MIR. Misclassification occurrence increased in NIR SVM suggesting the model

had more difficulty differentiating between spectral features between the geographical regions.

Isotopic analysis proved successful in authenticating each geographical location based on ANOVA significance values of carbon, hydrogen, nitrogen and oxygen with each p-value not meeting significance threshold of $p = 0.05$. Cambridgeshire approached significance at $p = 0.07$ in hydrogen and oxygen stable isotopes suggesting variations from their reference but outside of significance.

When making comparisons to spectroscopic analysis there can be some conclusions drawn. There is an overlap between information obtained from stable isotopes and MIR/NIR spectra. For example, high $\delta^{13}C$ could correlate with molecular spectral features including sugars and carbohydrates and $\delta^{18}O$ might correlate with molecular vibrations that are water-related in NIR spectra (O-H stretching vibrations). Additionally, $\delta^{15}N$ might correlate with nitrogen-containing compounds, including proteins or amino acids, detectable in both MID and NIR spectra. Environmental factors including water availability, soil type, and climate can impact the molecular composition in addition to the stable isotope ratio forming indicators for food origin which provides opportunity for these methods to be compared however there are factors that could complicate the use in practice due to data magnitude and the use of appropriate statistical and multivariate processes.

3.5.3 NIR Spectral Signatures of Conventional and Organic Tomatoes Showed Minimal Separation in Multivariate Analytical Models

Organic and conventional farming practices have the propensity to impact the molecular and chemical composition of fruit produce based on the nutrient supply and pest management practices that affect the biosynthesis of certain compounds. Assessing the distinction between organic and conventionally grown tomatoes through NIR analysis showed some separation along the identified wavenumbers as 1670 nm, associated with C = O carbonyl compounds that may include organic acids, esters and some metabolites linked to flavour and aroma, 1415 nm related to the O–H stretch first overtone is often linked to water content and polysaccharides, including pectin and cellulose. 1329 nm C –

H combination band founds in carbohydrates and lipids. Soluble solids as sugars (Ilic, 2011; Oliveira *et al.*, 2013), phenolics (Ilic, 2011; Vinha *et al.*, 2014), and carotenoids (Ilic, 2011) have been shown to be present in higher quantities in fruit from organic farming than in conventionally grown (Çakmakçı and Çakmakçı, 2023) supporting these wavenumbers as possible indicators of farming practice. 1139 nm C – H stretch of aromatic hydrocarbons, phenolic and flavour compounds influences by soil biodiversity inducing production of more phenolic compounds for natural defence. Few studies have successfully found notable differences in the nutritional content between organic and conventionally produced food. An extensive review by Dangour et al (2009) explored the results of 55 crop studies concluding that nitrogen is significantly higher in conventional crops and organic crops exhibit significantly higher levels of phosphorous, however the remaining 8 of 11 nutritional categories, there were no difference (Dangour et al., 2009) This further supports the unreliability of nutritional constituents to determine organics and conventionally grown produce.

The PCA analysis revealed a significant overlap between the two growing methods that suggests the tomatoes share many similarities in their chemical compositions despite their different growing techniques. The lack of separation prevents clear discrimination between organic and conventional cultivation based on the overall spectral profiles, indicating that the growing method may not produce sufficiently distinct biochemical changes detectable by this technique alone. When PCA-LDA was applied, there was an enhancement in separation, particularly along LD1 axis corresponding to the key features associated with differences between organic and conventionally grown tomatoes. SVM classification provided varying results in accuracy with organic samples being successfully classified at 83.43%. The model struggled to classify conventional tomatoes with a higher misclassification rate of 56.82%. This disparity could be related to a higher variability in influences from conventional farming practices causing variability in chemical profiling. This could be in conjunction with to a large cross-over to organically grown tomatoes making them difficult to classify. Organic farming practices are seemingly more distinct allowing for better classification. Stable isotope testing for organically grown tomatoes focussed on the presence of nitrogen, this is due to the plant uptake of nitrogen which differs between the nitrogen form from synthetic and organic fertiliser. The presence of $\delta^{15}N$ will range between −3.9 to +5.7‰ in conventionally

grown and +2.5 to +45.2‰ (Inácio, Chalk and Magalhães, 2015) in organically grown produce. NIR spectroscopy proved insufficient as a tool to distinguish tomatoes grown using these alternative practices; stable isotope ratio analysis remains the most reliable method in this case. Further study would benefit from a greater sample size to improve power. ATR-FTIR spectroscopy to test for spectroscopic differences between these growing methods would be advantageous due to the increased specificity that the mid infrared region provides in comparison to the NIR used in this study. Physiological measurements acting to validate spectroscopic signatures would be useful to analysing and validating the capabilities of the spectroscopic technique.

3.6 Block Chain

Infrared spectroscopy can detect biochemical differences in tomato fruit that can be attributed to growing conditions. To be used effectively, reference data of produce to compare against an authenticated growing origin is necessary. To further enhance a method for tamper-proof records providing supply chain traceability, block chain technology can be applied in conjunction with spectroscopic data. Block chains provide signatures that cannot be altered without detection, these signatures are recorded into a blockchain ledger, with a new signature added to the chain at each point in the supply chain (Jeanneret medina, Baudet and Lebraty, 2024). This can be used to log important data, including temperature changes, GPS locations, and additional test results, for example, new spectroscopic or isotope analyses. The use of impenetrable data technology like blockchain allows for a transparent method for real-time monitoring, traceability, and enhanced accuracy for food fraud detection.

3.7 Conclusions

This study demonstrated the potential of MIR and NIR spectroscopy coupled with multivariate analysis and machine learning techniques, distinguishing fruit origin but was unsuccessful at recognising farming practices. Of the two techniques, MIR spectroscopy proved the most reliable for distinguishing and classifying tomatoes on the basis of the geographical origin of tomato fruit; however NIR spectroscopy still proved effective, although the misclassification rate was higher. Since MIR and NIR spectroscopy both proved effective for the classification of fruit on this basis, the choice of technique

can be decided based on more practical needs. NIR spectroscopy may be chosen for high portability, whereas MIR may be chosen for higher accuracy when portability isn't a necessity. SVM provided a reliable approach for classification overall with the exception of singularly identifying conventionally grown tomatoes. In these cases, the use of an organic control might be needed for successful use in practice, and stable isotopes remained the preferable method, currently used in industry. Findings could provide a foundation for implementing further study with a necessity for augmented power and improved robustness. Extensive studies could form the groundwork for application of the methodology in the supply chain for authenticating fruit growing conditions representing origin.

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4. Characterising Near Infrared Spectroscopic Signals of Leaf Tissue and Fruit as Tomato Plants Evolve from Seedling to Spoilage.

Author's note: The spectral data acquisition for the experiments described in this chapter was conducted by Lancaster University student Ed Hill-King. The author performed all subsequent data processing, chemometric analysis, interpretation, and the preparation of the results presented herein.

4.1 Abstract

The changing climate is making food production ever more challenging, meaning it is vital to food security that production is made more efficient and less wasteful. One of the ways we can address these issues is by first gaining a deep understanding of the biochemical processes involved in post-harvest spoilage and how these are related to ripening and

senescence. Additionally, methods for gathering this vital information *in-situ* may provide dynamic insights into these processes, especially with the dramatically changing environmental landscape.

This study investigates the use of near-infrared spectroscopy (1700 – 900 nm) to investigate tomato plants during their developmental phases, from seedling to fruit spoilage. A handheld, portable spectrometer is used for the acquisition of biochemistry in tomato plant leaves and fruit for *in-situ* application. Distinct chemical peaks were detected may represent biomarkers associated with plant development phases are described. Machine learning modelling shows high accuracy in categorising developmental phases in leaves and tomatoes. It was demonstrated that near-infrared spectroscopy has potential for *in-situ* analysis of fruit.

4.2 Introduction

Solanum lycopersicum tomato fruit, one of the most widely cultivated and consumed fruits, contributes to a healthy and nutritious diet for millions of people globally. Tomatoes are rich in essential micronutrients that significantly support human health and immune function combating the prevention of chronic diseases. Vitamins A, C and antioxidants including lycopene are key nutrients that tomatoes provide aid in the fight of infections and play a role to maintaining healthy skin and vision. Lycopene protects cells from oxidative stress (Mohd Hassan *et al.*, 2019) and lowers levels of 'bad cholesterol' Low-Density Lipoprotein (LDL) (Mozos *et al.*, 2018). These benefits have a profound impact, especially in communities where sufficient healthcare is less available. Aside from the health benefits, tomatoes are culturally important and integral components in traditional cuisines across the globe helping to shape cultural identity in a diversity of cultures (Lang, 2004). Understanding the biochemical processes of tomato plant development and its relationship with fruit ripening and spoilage are therefore crucial for maximising nutritional benefit and reducing food waste. By understanding these complex interactions, there lies opportunities to use predictive models that can determine the optimal harvest time, ensuring fruit is picked at peak quality. Additionally, monitoring plant or leaf biochemical markers can provide early indicators of fruit health and potential spoilage, enabling targeted interventions to extend shelf life.

The biochemical and molecular processes involved in fruit ripening and fruit senescence are well understood and serve as a useful template for understanding the processes involved in spoilage. The ripening processes in fruit, continue after harvest and this leads to certain spoilage processes (Bapat *et al.*, 2010). Tomatoes are composed of a complex assortment of organic compounds that undergo significant changes throughout ripening and spoilage. Sugars, volatile compounds, organic acids and antioxidants are some important categories of chemicals that have varying contributions to the quality, nutritional content and aesthetic descriptors that affect consumer perception (Paolo *et al.*, 2018). Observable physical changes include the colour, texture, acidity, aromas and flavour. Importantly during ripening, there are developments in nutritional content including an increase in sugar content (Kanayama, 2017), vitamins, minerals and antioxidants (Jesús Periago *et al.*, 2009). In the later stages of the ripening process, this is followed by the enzymatic breakdown of these nutrients (Quinet *et al.*, 2019), making it important that the fruit is consumed at the optimal point.

Enzymatic reactions play significant roles through both ripening and spoilage in tomatoes. Tomato ripening is regulated by polygalacturonase, pectin methylesterase, cellulase and β-galactosidase enzymes (Payasi *et al.*, 2009). Enzymatic activity continues after harvest, produced by the fruit or microorganisms. Enzymatic reactions can generate reactive oxygen species (Corpas *et al.*, 2023) that can damage cellular components accelerating the deterioration of the fruit quality (Meitha *et al.*, 2020). Polygalacturonase is one of the key enzymes involved in tomato spoilage catalysing hydrolysis of pectin (Chun and Huber, 1998), a major component of the tomato cell wall and complex polysaccharide. This degradation of polygalacturonase in turn leads to cell wall breakdown (Gross and Wallner, 1979). Pectin bond molecule glycosidic bonds are cleaved by polygalacturonase resulting in the release of oligogalacturonides and breakdown products (Abbott and Boraston, 2008). Additionally, the pectin-associated enzyme, pectin methylesterase, breaks down pectin molecules leading to the formation of free carboxyl groups (Wu *et al.,* 2018). Subsequently, this reaction causes pectin to become susceptible to polygalacturonase breakdown further causing fruit softening. Hydrolysation of cellulose and hemicellulose, further important components of plant cell walls, are broken down by cellulase and hemicellulase enzymes (Zeng *et al.,* 2017) contributing to over-ripening. Enzymatic reactions are heavily influenced by

environmental pressures and conditions (Biais *et al.*, 2014). Controlling these factors using proper storage can minimise enzymatic spoilage and help preserve quality and optimise shelf life.

During both the ripening and spoilage stages in tomato, there are significant changes in the texture of the fruit. This is related to changes in the water content which contributes to the texture, and breakdown of cell wall components catalysed by enzymes like pectinases leading to softening and loss of structural integrity (Prasanna *et al.,* 2007). Shelf life can also be influenced by water content, changes happen through water uptake from the surrounding environment and losses occur through processes including transpiration, respiration and evaporation (Gidado *et al.*, 2024). Shrinking and loss of turgor occur through water losses and high moisture promotes the proliferation of microbes (Aung *et al.,* 2018). Fruit quality is heavily attributed to texture and firmness, softness is an indicator of lower quality or late shelf life by consumers, influencing their buying decisions, and water content monitoring may help avoid these problems. Taste and texture can be affected by acidity levels (S. Wang *et al.*, 2022). Acidic sourness can result in unpalatable flavours potentially causing the discarding of fruit at the consumer level. pH can be influenced by several factors including the growing conditions, storage conditions, enzymatic activity, and presence of microbial colonies (S. Wang *et al.*, 2022). However, accumulation of fructose, glucose and sucrose sugars (Sun *et al.*, 2022) contribute to flavour profiles of sweetness helping to regulate acidity levels.

Aesthetics play a large role in influencing consumer decisions (Latino *et al.,* 2023). Tomato fruit typically start growing green, chlorophyll degradation leads to the loss of the green colouration during ripening, and accumulation of pigments like anthocyanins and carotenoids including lycopene and β-carotene develop the ripe fruit colour (Kapoor *et al.*, 2022). Commercial tomato varieties are often chosen for their red colour pigmentation (Chang *et al.*, 2024) although a wide variety of colours exist in less commonly sold varieties (Flores *et al.*, 2017). During spoilage, pigmentation further develops in intensity and at the end of shelf life can develop into browning due to enzymatic reactions and oxidation of pigments (Moon *et al.*, 2020). Consumer buying decisions can be influenced by colour intensity, hue and uniformity which are associated with the ripeness and quality (Chang *et al.*, 2024). The characterisation of these processes

in NIR spectral signatures paired with predictive models using leaf tissue, pre-harvest fruit and post-harvest data could provide powerful tools to dictate appropriate practices for optimisation.

Colonisation of microbes can occur potentially influencing ripening due to their production of enzymes and metabolites which could either inhibit or accelerate the fruit ripening processes (Li *et al.*, 2024). Some strains of *Pseudomonas syringae* produce volatile organic compounds that inhibit the synthesis of ethylene causing the delay in tomato ripening or spoilage (Cellini *et al.*, 2021), however, other strains can cause diseases like bacterial speck which is detrimental to plant health (El-Fatah *et al.*, 2023). After harvest, microbial growth is a key driver of spoilage processes; fungus and bacterial populations can proliferate on fruit surfaces and infect the internal tissue through perforations further accelerating decay. Microbial contamination can occur at any stage in the supply chain and each additional processing point increases the likelihood of damage and contamination (Karanth *et al.*, 2023).

Ethylene gas, a ripening hormone is important in the initiation of tomato fruit ripening processes along with climacteric rise in respiration rate. Ethylene is released as a gas and acts as a self-stimuli for release further progressing ripening and subsequently spoilage (Cellini *et al.*, 2021). This hormone triggers many of the biochemical and physiological changes that occur in the fruit throughout both stages. Furthermore, ethylene production can be induced as a stress response to mechanical damage, pathogen infection or unfavourable environmental conditions further contributing to fruit deterioration (Bapat *et al.*, 2010). Ripening is controlled by ethylene encouraging the accumulation of lycopene and beta carotene displayed visually by the transition from green to red skin colour in tomatoes, additionally, ethylene plays a role in instigating pectin degradation, starch to sugar conversion, water uptake and protease activity degrading structural proteins making the outer cuticle of the fruit softer and more palatable for consumption. Ethylene also initiates synthesis and production of volatile compounds and flavonoids improving the taste and smell of the fruit. Exogenous ethylene is used to synthetically ripen fruit such as bananas (Liu *et al.*, 2015). In industry, tomatoes are often harvested before high endogenous ethylene release and optimal ripening to enable a longer shelf life. The produce is kept at pre-harvest quality throughout transit until close to the sale point

where they are exposed to synthetically produced ethylene to induce ripening. These produce often lack the full flavour, texture and taste that a naturally ripened fruit and this is reflected in the price by retailers. Fruit that are picked still attached to the vine are naturally ripened but often incur additional price value of around 200% in general supermarkets (Hewajulige and Premaseela, 2020).

The similarity between the processes that determine optimal suitability of tomato for consumption suggests that there is an optimal chemical composition for the harvest, storage and retail of fruit. In recent years, the agricultural industry has witnessed a growing demand for efficient and non-destructive techniques to monitor the quality and shelf life of fresh produce (Saad *et al.*, 2015). Among these, near-infrared (NIR) spectroscopy has emerged as a powerful analytical tool capable of providing rapid and comprehensive insights into the biochemical composition of agricultural products (Beć, Grabska and Huck, 2020). In particular, the application of NIR spectroscopy in the study of tomato quality has garnered significant attention due to the widespread consumption and economic importance of this fruit (Xu *et al.*, 2024)

Some significant implications in the productivity of agriculture rely on critical processes including the development of tomato plants starting from the early stages of planting and continuing throughout the plant lifespan. The external factors that provide the optimal growing environment are integral to plant health and will determine the health and development of fruit produced by the plants (VanDerZanden, 2019). The monitoring of plants might be considered an important procedure when looking to produce the highest quality produce that would be considered fit for sale, allowing for a deeper understanding of the conditions that might be favourable or that might inhibit plant health. This study uses Near-Infrared (NIR) spectroscopy to non-invasively monitor and map the development of tomato plants, starting from their initial leaf growth, fruit maturation on the plant and post-harvest spoilage. It aims to characterise developmental stages in both plant and fruit, to isolate informative biochemical changes at targeted time points and form a foundation to understand the complex interactions between vegetative plant tissue, leaves and fruit, and how that is represented in spectra. Predictive models that use leaf biochemical spectral signatures to discern the optimum harvest time of fruit and detect quality deficiencies that may affect nutritional content, vulnerability to pathogen

infection and shelf life of the fruit would be invaluable, especially for use in the supply chain. This study attempts to provide a basis for future study that explores such analytical techniques.

4.2.1 Plant developmental processes that may be observed in the NIR Spectra

Spectra produced using NIR differ significantly from ATR-FTIR in the depth of penetration, chemical sensitivity, spectral region and resolution resulting in a different biochemical signature.

In leaves, NIR has the potential for identifying water content through the interpretation of O-H stretch overtones, proteins at N-H and C-H combinations, chlorophyll, lipids and waves at C-H stretch combinations and lignification/cell walls (Beć et al., 2020). Fruit development NIR spectra may show soluble sugars at C-H stretch and O-H combination, starch breakdown with C-O and C-H overtones in polysaccharides, organic acids through COOH and OH stretch, pectin and cell wall degradation and carotenoids (Golic, Walsh and Lawson, 2003). After abscission or harvest of fruit and during senescence, water loss may be observed, lipid peroxidation through C-H overtone changes, protein degradation through decrease in N-H or C-H bands and volatile organic compounds (Tranbarger and Tadeo, 2025).

The application of NIR spectroscopy *in situ* offers a transformative tool for actors across the supply chain, from farmers to distributors. By providing real-time data on the physiological state of the plants and fruits, combined with potential application of predictive models, stakeholders can make informed decisions on harvest timing, storage conditions, and distribution logistics. This proactive approach has the potential to significantly reduce post-harvest losses, optimise resource use, and enhance overall product quality. Ultimately, the integration of NIR spectroscopy into agricultural practices promotes sustainable management and improves economic outcomes by ensuring that tomatoes reach consumers at their peak quality and freshness. The versatility of the methods allows spectral measurements to be applied at any stage in the supply chain allowing for comprehensive and powerful monitoring. Importantly at producer stage, measurements can be taken throughout the entire plant cultivation

period informing real-time amendments of growing practices to ensure high-quality produce, reducing opportunities for crop losses. The use of plant tissue to provide plant quality data allows for initiation of monitoring from early seedling stages, accounting for approximately 6 weeks before fruit develops on the plant. Nutrient and other growing conditions can be tailored to improve plant health, which may improve the fruit quality, including nutritional content, shelf-life, resilience and even improve aesthetic characteristics that contribute to saleability. The technique requires complex analysis to effectively extract valuable information from the data, meaning that there are significant limitations to the successful application in the supply chain. Further work should focus on developing AI tools to complete the analysis allowing the user to quickly obtain reliable results

What is known about the physiological development of tomato plants is highly detailed, as the tomato is one of the most widely studied model organisms. Our knowledge has been built from a range of experimental techniques that provide a detailed map of varying layers of processes. Gene expression studies have provided a detailed picture of genomic and genetic processes. Mutants have been used to explore the roles of genes through quantitative locus mapping, in addition to the use of transcriptomics, metabolomics, and biochemical analyses looking at sugar profiles, acidity, and pigments. Microscopy has played an important role in visualising physiological changes and describing phenotypic measurements. Although the knowledge is detailed and pathway-specific, the testing remains destructive. Spectral analysis has begun to be used as a non-targeted holistic tool and is increasingly used in academic research and within the supply chain. However, the uses have been focused on product quality and have not been used to explore developmental time courses, especially linking spectral changes to known physiological landmarks. Linking specific physiological events to isolated features in the data is difficult due to overlap within and between spectra. The broad biochemical fingerprints obtained in spectra, may be used as indirect proxies, not direct markers, which may suggest that it is not as useful. However, building a detailed knowledge archive of spectral data for important crop plants through development may provide a foundation for developing predictive models for use in the supply chain. A significant benefit of this is the non-destructive nature of the measurements, and high through-put data recording. Detailed spectral presentation of crop biochemistry has the potential to be connected to existing

knowledge by specifically designed studies that run non-spectral measurements, such as genetic assays, alongside spectral measurements. The implementation of stresses, environmental treatments, changes in growing conditions like nutrient concentrations during these studies could allow a highly detailed identification of biochemical changes and how they're expressed in the spectra, and have the potential for accurate and precise characterisation of optimal harvest time. With this deeper knowledge this could inform important decisions which optimise quality, yield and reduce losses and waste. The work in this chapter seeks to examine NIR spectral evolution in the tomato plant lifecycle, starting to fill the gap of temporal spectral data, forming the foundation for future work. The chapter offers insight into spectral signatures across plant vegetative and reproductive phases potentially revealing important physiological transitions and enables a deeper understanding of biochemical shifts in pre- and post-harvest fruit associated with shelf-life, transportability and nutritional content.

Due to limitations in the experimental conditions, there are gaps and inconsistencies in the time-series, resulting in an incomplete picture. Future work would benefit from improved specificity to individual leaves, individual plants and individual fruit. Additionally reference data using paired techniques including genetic expression would provide a more robust characterisation of spectral markers and allow for the use of predictive tools.

This chapter aims to: (1) determine the changes occurring in the spectral signature of Piccolo tomatoes during ripening, senescence, and spoilage, and (2) to explore the application of NIR spectroscopy as a diagnostic tool for assessing the quality and shelf life of Piccolo tomatoes throughout their post-harvest journey. Through a combination of spectroscopic analysis, chemometric modelling, and data interpretation, this research aims to provide valuable insights into the factors influencing tomato quality and the potential of NIR spectroscopy for optimising post-harvest management practices in the tomato industry.

Research Questions

- How does NIR spectral data change through tomato development and spoilage?
  Can we differentiate between plant and fruit development phases using NIR spectral profiles?
  What represents notable variance in spectral regions and features between developing phases?
  Can we identify time point specificity through spectral signatures that reveal important biochemical and physiological transitions?

Aims

- Identify spectral biomarkers of ripening and post-harvest spoilage stages
- Identify spectral cross-overs between ripening phases and spoilage
- Identify spectral cross-overs between plant and fruit biochemical processes
  To lay a foundation for future predictive models based on lifecycle data

4.3 Methods

4.3.1 Plant material

Solanum lycopersicum Piccolo (cherry) tomato plants were grown from seed (Garden Seeds Market Ltd., UK). An initial 60 seeds were germinated and sown in Levington John Innes Seed compost in seed containers (3 x3 x 4”) cells. 30 uniform seedlings were re-potted into 18-litre plant pots in Levingtons M3 potting compost. Plants were grown at a 16-hour light regime, 24°C day temperature, 18°C night (Supplementary) in glasshouses at the Lancaster Environment Centre, Lancaster University. Plants were watered once per day to soil capacity. Spectral readings were taken from the first true leaves at regular time points. Spectral readings were also taken from fruits from senescence to their natural abscission from the plant and subsequently followed until spoilage.

4.3.2 NIR Spectroscopy

Spectral readings were measured on initial true leaves at time points (days 4, 7, 16, 19, 23, 27, 31, 35, 38, 49, 53, 57, 62, 65, 70, 75, 80, 82, 91, 93, 100, and 105). The continuation of spectral measurements were taken from randomly selected leaves on the same plants. Limitations of this study arise as repeats of the same leaves occur in early measurements due to the lack of leaves available. as the plant matures and more leaves become available, the variation of leaf measurements increases. In future studies, specific leaves would be followed throughout the time series for continuity. Spectral readings were also taken from fruits from emergence, through ripening and senescence to abscission, and subsequently followed until spoilage. Spectral absorbances were measured using a handheld NIR spectrometer device: NIRscan ASP-NIR-M-Reflect (Allied Scientific Pro, Gatineau, Quebec, Canada) and associated DLP NIRscan Nano GUI v2.1.0 software. The spectrometer crystal was cleaned between measurements using isopropyl alcohol wipes (Bruker Optics, Coventry, U.K.), and each time, background spectra were taken to account for ambient atmospheric conditions.

Readings were an average of six individual scans taken automatically and were taken at two locations on each biological replicate. For leaves, one reading was taken on the top of the leaf and one on the underside of the leaf. This variation in surface readings were conducted to reduce surface bias, and account for heterogeneity between the adaxial and abaxial sides of the leaves for a more robust dataset. For tomato fruit readings were taken from two locations at random on the fruit avoiding visible tissue abnormalities. Multi-location readings were taken to provide sufficient replicates for multivariate analysis and to obtain a representative reading of the natural tissue heterogeneity accounting for tissue blemishes.

Measurements were taken from leaves, from the first appearance of true leaves, on day 4 and were continued until day 82. For tomato fruit, readings were taken from the first emergence on day 35, initiating the pre-harvest fruit stage. The first tomatoes abscised from the plants on day 57. After abscission, ‘harvest’ readings (post-harvest fruit stage) were continued until spoilage at which point it was no longer possible to take readings

due to insufficient contact between the sample and the spectrometer crystal. The final readings were taken on day 105.

4.3.3 Data Analysis and Validation

The data was imported and organised in Microsoft® Excel® for Microsoft 365 MSO (Version 2206 Build 16.0.15330.20260) 64-bit. Analysis was completed using iRootlab-0.17.8.22-d (Copyright 2012 Julio Trevisan, Francis L. Martin & Plamen P. Angelov) for Matlab (v.R2021a) software programme. Savitzky–Golay smoothing (second-order derivative, 9 filter coefficient, second-order polynomial fitting) was applied to improve the signal-to-noise ratio. Normalisation techniques: Vector normalisation and mean centring were applied to spectral data.

Exploratory analysis was performed on the preprocessed data using principal component analysis (PCA). This technique places each spectrum as a data-point onto planes of space distributed using the variance of the data after reducing the data into a small number of principal components (PCs), these are responsible for explaining the spread of the data. PCs are mapped orthogonal to each other, these form the scores and associated loadings. Loadings display the largest variances at specific wavenumbers, which can be used as potential spectral markers.

To further maximise class separability supervised analysis: principal component analysis with linear discriminant analysis was applied. Classification support vector machine (SVM) model was applied, a linear classifier with a nonlinear kernel transformation which is used to capture non-linear data relationships. The SVM model used k-fold cross-validation whereby the dataset was randomly divided into 5 (k) subsets, the model was trained 5 (k) times, each time using 4 (k-1) folds for training, and the remaining fold for validation. This process helps to improve the performance of the model, avoid overfitting, and provide a more reliable estimate of the effectiveness of the model. Preprocessing methods differed from those used in multivariate analysis to achieve the highest accuracy in classification. 1st order derivative, 9 filter coefficient, second order polynomial fitting was applied followed by vector normalisation and 0,1 range normalisation.

4.4 Results

4.4.1 Multivariate Analysis

Chemometric analysis of tomato plants was conducted from NIR spectra taken from *Solanum lycopersicum* 'Piccolo' tomato plant constituents including leaves from first true leaf initiation through to plant maturity, in addition to fruit ripening and senescence until the natural abscission of fruit, followed by post-harvest fruit recordings until spoilage. Figure 4.1 displays the unprocessed and preprocessed leaf and fruit spectra. Spectral readings were taken from specific plants. Different leaves from those plants were read, the plant forming the biological replicates rather than the individual leaves. Plants were followed through the time series, continuing during the fruiting period and postharvest. Figure 4.1B-E fruit spectra showed distinct wave shapes which differed between tomatoes before they were harvested and after harvest, suggesting their spectral signatures were very distinctly different. Fruit naturally harvested (abscised) at varying points and at different times. Measurements were grouped between BH and PH based on before abscission or after abscission, regardless of the date or time point, allowing to visualise the biochemistry based on abscission status. Before harvest fruit are classified by their individual harvest points meaning the number of individuals (n) at each time point varies.

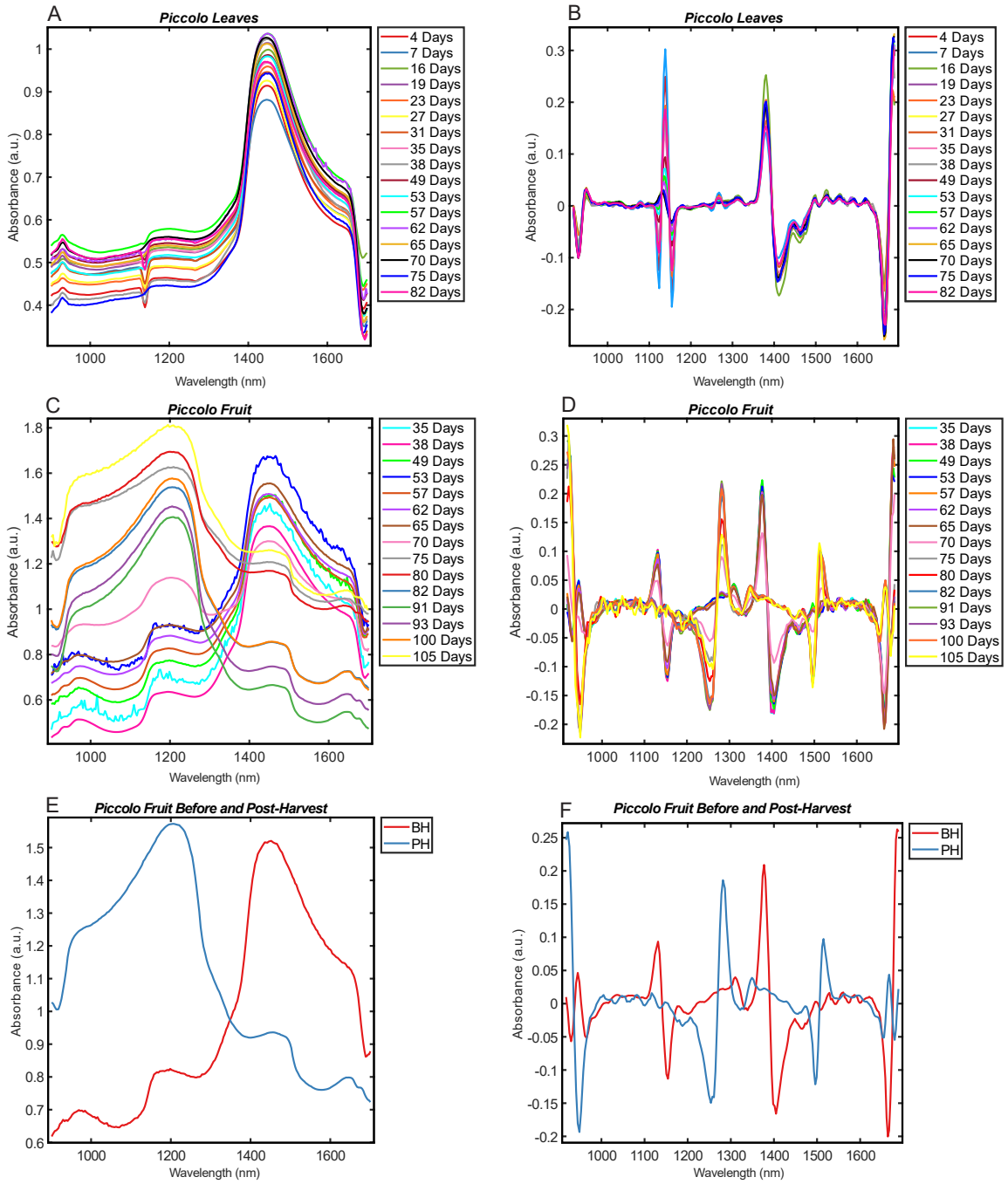

Figure 4.1. NIR spectra from *Solanum lycopersicum* 'Piccolo' tomato plant constituents including leaves and fruit throughout plant development, ripening and post-harvest spoilage of fruit. **A)** Unprocessed mean values of NIR of tomato plant leaves **B)** Means of preprocessed NIR leaf spectra. Preprocessing techniques include: Satvitzky-Golay filter with second differentiation order and vector normalisation. **C)** Unprocessed mean NIR of fruit **D)** Pre-processed mean fruit NIR spectra **E)** Mean before (BH) and post-harvest (PH) fruit spectra **F)** Preprocessed fruit spectra BH and PH

PCA models were subsequently applied to the preprocessed spectral data (Figure 2). PC axes and LD axes were decided based on observational interpretation of the best distribution and clustering of the data. PCA-LDA loadings were chosen based on the LD axis that best described class-associated clustering and separation allowing for biochemical insights related to class variances. Time-series organised PCA analysis displayed notable clustering and separation between days in tomato leaves (Figure 4.2A). Identifiable cluster groups can be observed in late-stage time points including 53, 57, 62, 65 and 75 days. Late-stage clustering appears grouped together, and spread temporally. PCA-LDA furthered focused the clustering within the time points (Figure 4.2B). The spread was more evenly distributed between the time points, with even levels of overlap along the time-series. Associated loadings plot revealed important wavenumbers associated with the greatest variances, including peaks at 1139 nm, 1392 nm, 1422 nm, and 1674 nm associated with lipids, proteins, starches and aliphatic alcohols.

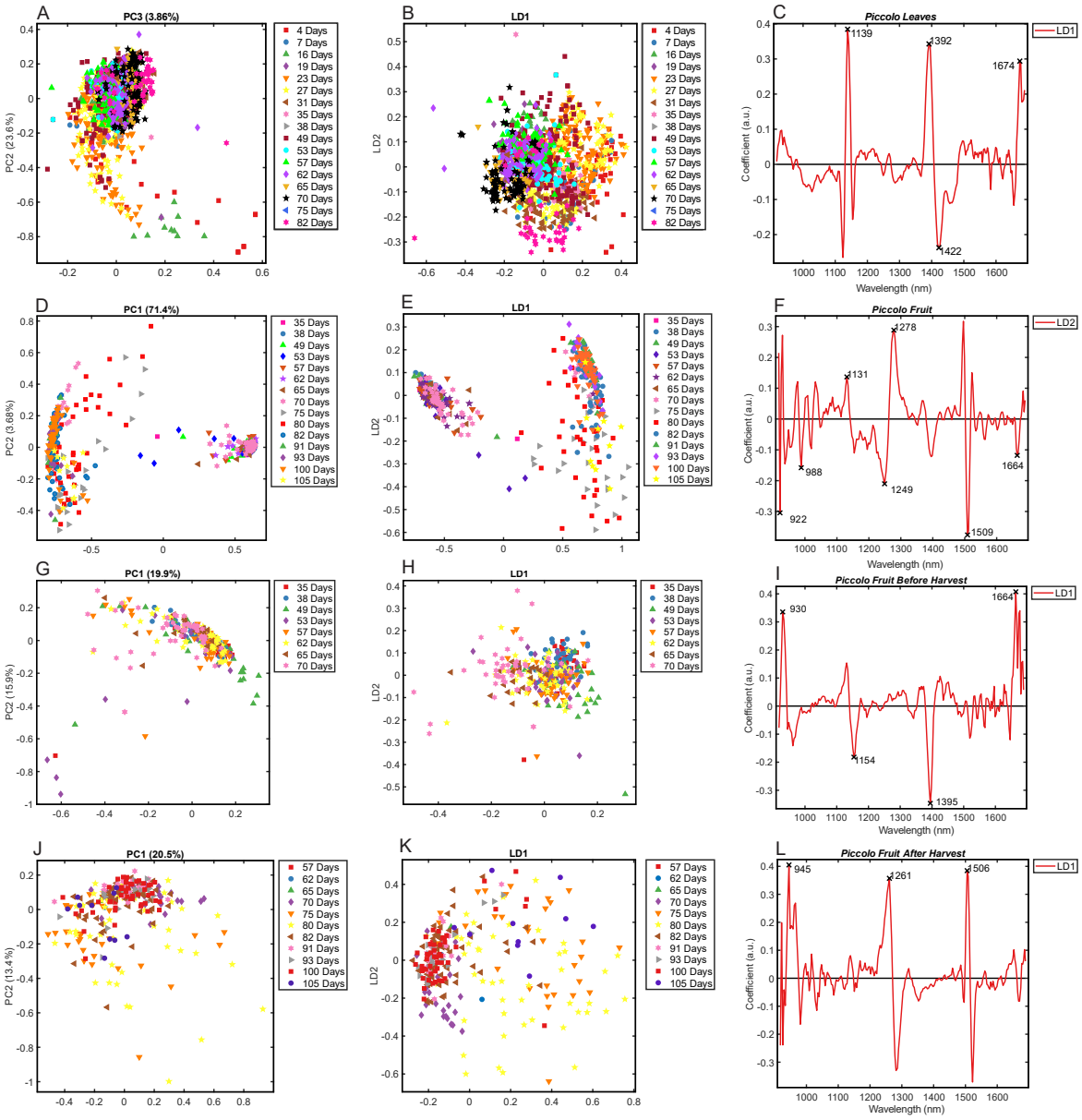

Figure 4.2. A-C) Multivariate analyses of *Solanum lycopersicum* 'Piccolo' tomato leaf NIR spectra. **D-F)** Multivariate analyses of fruit throughout development on the plant and after harvest. **G-I**) Multivariate analyses of fruit before harvest. **J-K)** Multivariate analyses of fruit after harvest. **A,J**) Principal Component Analysis (PCA). **B,K**) Principal Component Analysis with Linear Discriminant Analysis (PCA-LDA). **C,L**) PCA-LDA Loadings plots with significant wavenumbers associated with greatest variances.

From day 35, the fruiting period presented on the plants and spectra were recorded and followed through ripening and subsequent post-harvest spoilage. PCA exploratory

analysis displayed some clustering of time points, most prominently in days 70 and 100. A significant split in the data occurred separating into two grouped data clusters, comprised of multiple time points in each group with no visible overlaps. This suggests that there was a spectral signature that distinctly separated the two groups. When PCA-LDA was applied, this split remained, with even further defined clustering of the individual time points, prominent examples included: 49, 62, 70, and 93 days in one group, and 80, 82, 100, and 105 days in the other. Key wavenumbers that were drawn from tomato fruit ripening and spoilage included: 922 nm, 988 nm, 1131 nm, 1249 nm, 1278 nm, 1509 nm, and 1664 nm associated with carbohydrates, lipids, proteins n-alkenes, and starches respectively.

Some clustering was also observed along the before-harvest series (Figure 4.2G & H) and post-harvest series (Figure 4.2J & K). Wavenumbers of significant changes within pre-harvest tomatoes during ripening included: 930 nm, 1154 nm, 1394 nm, and 1667 nm. Post-harvest wavenumbers included 945 nm, 1261 nm and 1506 nm commonly associated carbohydrates including sugars like sorbitol and starches.

Plant development was categorised in three stages: vegetation stage prior to fruit initiation, the fruiting period, and the post-harvest phase. Leaf spectra were collected throughout all stages which displayed significant clustering and separation in the PCA-LDA analysis (Figure 4.3A) and the distribution was organised in temporal order.

Table 4.1. PCA-LDA loadings from NIR spectra obtained from *Solanum lycopersicum* tomato leaves and fruit, wavenumbers observed in PCA-LDA loadings representing peak variances are listed with their chemical assignments.

Tomato Leaves and Fruit			
Wavelength (nm)	**Waveregion (nm)**	**Chemical Association**	**Reference**
Leaves			

1139	992-1139	O - H, N - H, and C - H bonds combinations and overtones protein, lipid, and moisture content	(Konstantinos *et al.,* 2017)
1392	1389-1437	Polysaccharides OH stretch first overtone, fatty acids	(Pérez-Vich *et al.*, 1998)
1422	1390-1437 1400-1600 1400-1440	OH stretch first overtone: Polysaccharides O – H stretch, O – H band combination, H – O– H deformation combination: Starch First overtone of the hydroxyl group First overtones: Aliphatic alcohols and phenols water	(Sundaram *et al.*, 2011)
1674	1674	C - H protein	(Ingle *et al.*, 2016)
Fruit			
922	918-922	O - H bonds, water content	(Konstantinos *et al.,* 2017)
988	975-989 near 990	Second overtone of primary amides carbohydrates overtones or combinations O - H and C - H	(Schulz *et al.*, 1998)
1131	992–1139	Sugar (°Brix) Malic acid	(Weyer and Lo, 2006b)
1249	1150-1250	C - H vibrations fatty acids	(Sundaram *et al.*, 2011)

1278	1260–1270	The second overtone CH_3 and CH_2 asymmetrical stretching of n-alkane C – H and O – H bonds fat and water content	(Konstantinos *et al.,* 2017)
1509	1400-1600	O – H stretch and O – H band combination and the H – O – H deformation combination: starch First overtone of the hydroxyl group.	(Konstantinos *et al.,* 2017)
1664	Near 1660	Cis-unsaturation	(Sundaram *et al.*, 2011)
Fruit BH			
930	930-945	C - H stretch vibrations in carbohydrates	(Konstantinos *et al.,* 2017)
1154	1150-1250	Water (weak), fatty acids	(Sundaram *et al.*, 2011)
1395	1389-1437	Polysaccharides O - H stretch 1st overtone Fatty acids stretching of carboxylate groups ($–COO^-$)	(Konstantinos *et al.,* 2017)
1667	Near 1660	Cis-unsaturation	(Sundaram *et al.*, 2011)
Fruit PH			
945	930-945	C - H stretch vibrations in carbohydrates	(Konstantinos *et al.,* 2017)

1261	1260–1270	C - H and C - N stretching modes combination	(Konstantinos *et al.,* 2017)
1506	near 1504 1400-1600	Sorbitol O – H stretch and O – H band combination and the H – O – H deformation combination starch. First overtone of the hydroxyl group.	(Cho, Sohn and Kwon, 1998) (Konstantinos *et al.,* 2017)

4.4.2 Interpretation of Tomato Plant Developmental Stages

To evaluate the potential of near-infrared (NIR) spectroscopy as a tool for real-time crop monitoring and harvest timing, spectral data from tomato leaves were analysed across key developmental stages—from early vegetative growth through fruiting to post-harvest senescence. Additionally, fruit was analysed across stages, including pre-harvest ripening and post-harvest senescence. By applying principal component analysis followed by linear discriminant analysis (PCA-LDA), this section examines whether distinct spectral profiles reflect underlying biochemical shifts over time. Understanding these shifts could provide a non-destructive means to track physiological changes in the plant, enabling better decision-making around fertilisation, harvest scheduling, and quality assessment. Key spectral features at 1139 nm, 1392 nm, 1422 nm, and 1674 nm—linked to lipids, proteins, polysaccharides (e.g., starch), and alcohols, respectively—offer insight into the biochemical processes underpinning these developmental transitions.

Minor overlapping occurred between leaves from all phases of leaf development which suggests spectral similarities through the temporal progression between these stages. The first phase: vegetative (LVP) and the last phase: leaves post-harvest (LPH) were separate with no overlap, showing they have become distinct from each other (Figure 4.3A). Categorisation of leaf stages based on fruit phases was conducted to observe whether fruit stages have a notable impact on plant biochemistry. Further work should seek to explore the correlative dependence between plant biochemistry and fruit. This

may inform a detailed view of the dependant biochemical pathways and allow for methods to be developed using plant tissue to predict biochemical processes, the timeline and developmental phase. Peaks in PCA-LDA loadings were located at 1139 nm, 1392 nm, 1422 nm, and 1674 nm representing lipids, proteins, polysaccharides including starches, and alcohol respectively (Table 4.2)

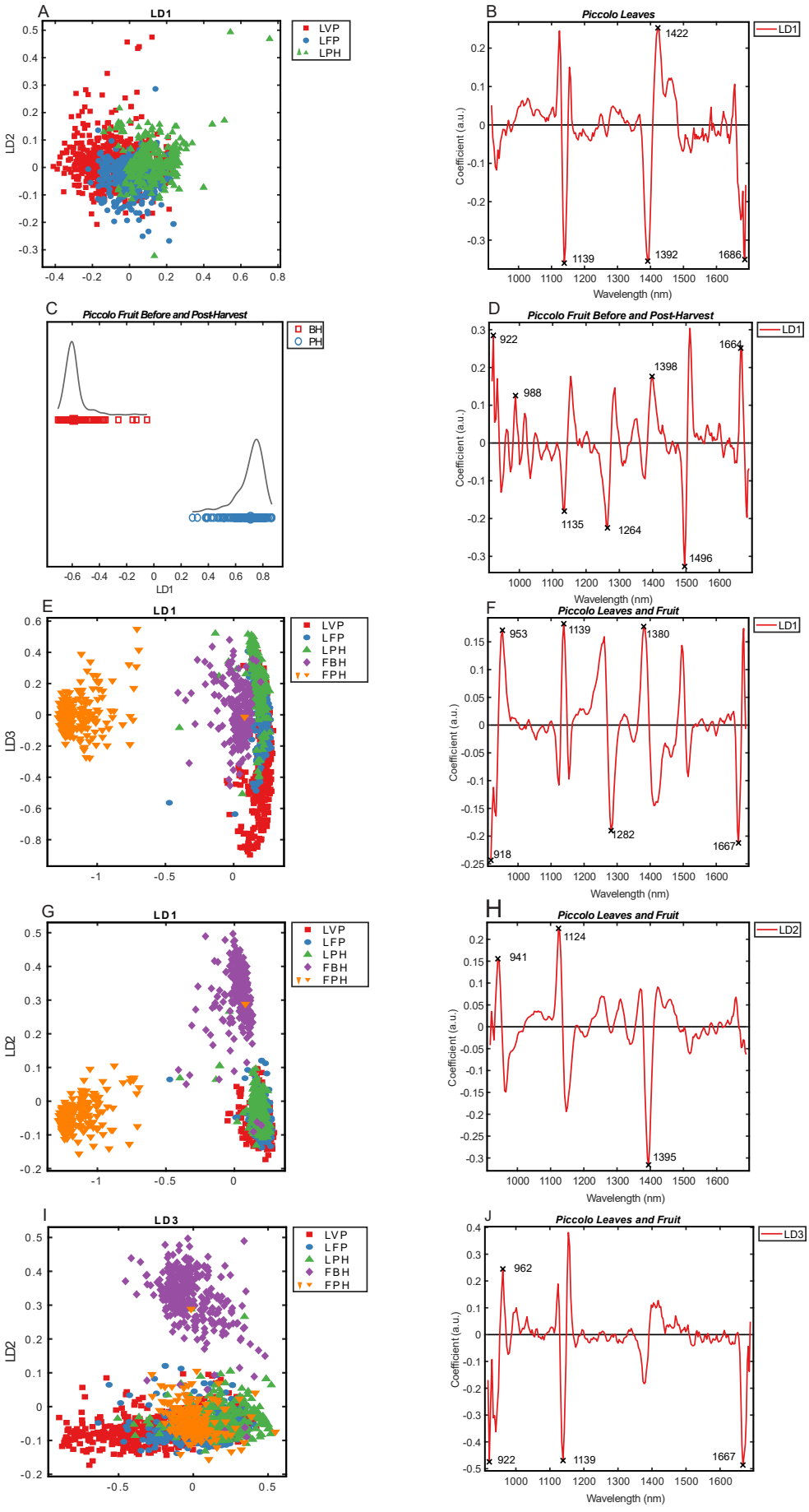
A
LD1
LD2
LVP
LFP
LPH
B
Piccolo Leaves
LD1
Coefficient (a.u.)
Wavelength (nm)
1422
1139
1392
1686
C
Piccolo Fruit Before and Post-Harvest
BH
PH
LD1
D
Piccolo Fruit Before and Post-Harvest
LD1
922
988
1135
1264
1398
1496
1664
E
LD1
LD3
LVP
LFP
LPH
FBH
FPH
F
Piccolo Leaves and Fruit
LD1
953
1139
1380
1282
918
1667
G
LD1
LD2
H
Piccolo Leaves and Fruit
LD2
941
1124
1395
I
LD3
J
Piccolo Leaves and Fruit
LD3
962
922
1139
1667

Figure 4.3. PCA-LDA scores **(A-I)** and associated loadings plots **(B-J)** of *Solanum lycopersicum* 'Piccolo' tomato plant organs **A,B)** Leaf spectra collected during Plant vegetative phase (LVP), Leaves during 'Fruiting Phase' (LFP) until fruit shedding, and 'Post-harvest' (LPH) .**C,D)** Piccolo fruit spectra were recorded before harvest (BH) defined by fruit on the plant before abscission, and post-harvest (PH) defined by fruit after abscission, regardless of the date and time point the abscission occurred at. **E-J)** Leaf and Fruit development and post-harvest phases Leaf vegetative phase (LVP) defined by leaf tissue before any fruit emerge on the plant, leaf fruiting phase (LFP) defined by the initial emergence of fruit on the plant until the first fruit abscises, and leaf post-harvest (LPH) defined by leaf tissues measured after the first fruit abscises from the individual plant , fruit before harvest (FBH), defined by first emergence of fruit until abscission, and fruit post-harvest (FPH) defined by abscission and continued measurements off the plant until spoilage.

Table 4.2. Loadings showing the key wavenumbers representing biochemical changes for *Solanum lycopersicum* tomato plant organs: Leaves and Fruit from plant development stages: Vegetative, fruiting and post-harvest.

Tomato Plant Development Phases			
Wavelength (nm)	**Wavelength region (nm)**	**Chemical Association**	**Reference**
Leaves			
1139	992–1139 Near 1140	O - H, N - H, and C - H bonds combinations and overtones protein, lipid, and moisture content Aromatics for benzene	(Weyer and Lo, 2006b)
1392	1350-1400	Polysaccharides OH stretch first overtone	(Pérez-Vich *et al.*, 1998)

	1389-1437	Fatty acids	
1422	1389-1437 1400-1440	O - H stretch first overtone Polysaccharides. Phenols aliphatic alcohols first overtones water O – H band combination and the H – O – H deformation combination, starch content. first overtone of the hydroxyl group.	(Nicolaï *et al.*, 2014)
1686	Near 1585-1665	NH_3 deformation: α-L-amino acids CO_2 stretching: Normal chain amino acids	Peirs et al. (2002a)
Fruit BH PH			
922	918–922	O - H bonds, water: internal water volume or concentration	(Pérez-Vich *et al.,* 1998)
988	near 990	Carbohydrate overtones or combinations O - O and C -H - O and C - H	(Schulz *et al.*, 1998)
1135	922-1139	O - H, N - H, and C - H bonds combinations and overtones protein, lipid, and moisture content	(Weyer and Lo, 2006b)
1264		Unassigned	

1398	1350-1400 1437–1389 1000–2000	Polysaccharides OH stretch 1st overtone fatty acids Firmness, acidity	(Sundaram *et al.*, 2011)
1496	1496 1400-1600 1460–1600	Amide bonds in hydrogen-bonded alcohols, O – H stretch and O – H band combination and the H – O – H deformation combination: starch first overtone of the hydroxyl group The first overtone of the N - H stretch of primary amines	(Nicolaï *et al.*, 2014)
1664	near 1660 1660-1670	Cis-unsaturation Condensed tannins	(Nicolaï *et al.*, 2014) (Dryden, 2003)
Leaves and Fruit			
LD1			
918	918–922	O - H bonds, water content	(Pérez-Vich *et al.,* 1998)
953	953	Vibrational overtones O - H and C - H bonds, water and carbohydrates	(Konstantinos *et al.,* 2017)

1139	Near 1140	Aromatics for benzene	(Weyer and Lo, 2006a)
1282	Near 1260–1270	C – H and O – H bonds vibration, fat and water Second overtone CH_3 and CH_2 asymmetrical stretching of n-alkane	(Prieto *et al.*, 2011) (Weyer and Lo, 2006a)
1380	1350-1400 1437–1389	Polysaccharides O - H stretch first overtone, fatty acids	(Pérez-Vich *et al.,* 1998)
1667	near 1660 1660-1670	Cis-unsaturation Condensed tannins	(Nicolaï *et al.*, 2014) (Dryden, 2003)
LD2			
941	930–945	C-H stretch vibrations in carbohydrates, this range may provide insight into carbohydrate levels in the plant tissue.	(Jerry Workman Jr and Lois Weyer, 2007)
1124	992–1139	O - H, N - H, and C - H bonds combinations and overtones protein, lipid, and moisture content	(Konstantinos *et al.*, 2017)

1395	1350-1400 1340-1483	Polysaccharides OH stretch 1st overtone stretching of carboxylate groups ($-COO^-$) Fatty acids	(Konstantinos *et al.*, 2017)
LD3			
922	918–922	O -H bonds, water content	(Pérez-Vich *et al.,* 1998)
962	962	O - H bonding Alkyl alcohols, water content	(Konstantinos *et al.*, 2017)
1139	Near 1140	Aromatics for benzene	(Weyer and Lo, 2006a)
1667	near 1660 1660-1670	Cis-unsaturation Condensed tannins	(Nicolaï *et al.*, 2014) (Dryden, 2003)

Before-harvest (BH) fruit clustered with complete separation from post-harvest (PH) tomatoes (Figure 4.3C), suggesting their spectral signatures reflect distinct biochemical profiles of tomatoes that dramatically changed when the fruit abscised from the plant. Tomato fruit PCA-LDA loadings provided peak changes at 922 nm, 988 nm, 1135 nm, 1264 nm, 1398 nm, 1496 nm, and 1664 nm associated with water content, carbohydrates, primary amines, lipids, proteins, and starches (Table 4.2).

Leaf and fruit phases showed clustering in all development phases. Different features in the data were visualised using combinations of LD1, LD2, and LD3 axes, these displayed significant separation in differing phase groups based on these features. LD1 axis displayed significant separation of post-harvest fruit from all other phases, whereas all

leaf phases were heavily overlapped suggesting similarities between these phases. Before-harvest fruit was closely connected to leaf phases with minor overlap. Conversely, the distribution of data is distinctly different in LD2 with heavy overlap between all leaf phases and post-harvest fruit. However, LD2 displays significant and distinct separation in before-harvest fruit from all other leaf phases and with post-harvest fruit. LD3 feature axis shows a temporally distribution of leaf phases in the order: vegetative phase, fruiting, and post-harvest leaves; these are clustered with minimal overlap. This temporal organisation of leaf data suggests that the spectral feature changes through time, enough that the phases become distinct between young plant to maturity. Both fruit phases overlap with each other, but they overlap with before-harvest leaves, suggesting this feature is associated with a biochemical change that is synonymous during pre-harvest leaf and fruit phase and continues in post-harvest fruit but not in leaves. These features may be explained by the wavenumbers drawn from PCA-LDA loadings plots (Table 4.2). LD1 had peak changes at 918 nm, 953 nm, 1139 nm, 1282 nm 1380 nm, and 1667 nm, associated with water, carbohydrates, proteins, fats and polysaccharides. These peak wavenumbers are likely to relate to the distinct separation in post-harvest fruit. LD2 showed peaks at 941 nm, 1124 nm, and 1395 nm, related to cell wall polysaccharides, fats and proteins metabolism and organic acids likely explaining significant changes in ripening processes in before-harvest fruit distinguishing these from all leaf phases and post-harvest fruit. 922 nm, 962 nm, 1139 nm, 1667 nm wavenumbers showed peak changes along LD3 axis, related to water, alkyl alcohols protein and fats.

4.4.3 Neighbouring Time Point Analysis Provided Greater Specificity

Wavenumbers were identified from PCA-LDA loadings at each neighbouring time points attributing to the chemical changes occurring between them (Table 4.3) characterising the temporal progression of fruit through pre-harvest to post-harvest spoilage.

Table 4.3. Loadings showing the key wavenumbers representing biochemical changes for *Solanum lycopersicum* tomato fruit at neighbouring time points

Fruit at Neighbouring Time points				
Time	**Wavelength (nm)**	**Wavelength region (nm)**	**Chemical Association**	**References**
35-38	1395	1350-1400 1389-1437	Polysaccharides OH stretch first overtone Fatty acids stretching of carboxylate groups ($-COO^-$)	(Pérez-Vich *et al.,* 1998; Konstantinos *et al.,* 2017)
	1655	near 1660	Cis-unsaturation	(Nicolaï *et al.*, 2014)
39-49	1398	1350-1400 1437–1389	Polysaccharides OH stretch first overtone Fatty acids	(Pérez-Vich *et al.,* 1998; Konstantinos *et al.,* 2017)
	1677	Near 1674	C - H Protein	(Ingle *et al.*, 2016)
49-53	918	918–922	O - H bonds, water	Konstantinos *et al.,* 2017)
	1671	1672	Sucrose	(Jerry Workman Jr and Lois Weyer, 2007)
53-57	918	918–922	O - H bonds, water	Konstantinos *et al.,* 2017)

	1621	1640-1612 1615-1636 1621	C -H stretch first overtone of terminal methylene groups of vinyl and vinylidene CH_2 stretching structures: ethylene	(Jerry Workman Jr and Lois Weyer, 2007)
	1674	1674	C - H Protein	(Ingle *et al.*, 2016)
57-62	1151	1153 1150-1250	CH_3 and CH_2 second overtone asymmetrical stretching of n-alkane Fatty acids	(Pérez-Vich, Velasco and Fernández-Martínez, 1998) (Peirs et al. (2002a)
	1395	1350-1400 1437–1389	Polysaccharides O - H stretch first overtone Fatty acids stretching of carboxylate groups ($–COO^–$)	(Pérez-Vich, Velasco and Fernández-Martínez, 1998)
	1636	1640-1612	Cellulose (dry) weak C - H stretch first overtone of terminal methylene groups of	(Jerry Workman Jr and Lois Weyer, 2007)

			vinyl and vinylidene structures	
	1670	1260–1270	The second overtone CH_3 and CH_2 asymmetrical stretching of n-alkane C – H and O – H bonds fat and water content	(Konstantinos *et al.,* 2017)
62-65	937	930–945	C - H stretch vibrations in carbohydrates	(Jerry Workman Jr and Lois Weyer, 2007)
	1395	1350-1400 1389-1437	Polysaccharides O - H stretch First overtone stretching of carboxylate groups ($–COO^-$)	(Pérez-Vich, Velasco and Fernández-Martínez, 1998) Peirs et al. (2002a)
	1686	near 1690	methyl (CH_3) C - H absorption bands	(Jerry Workman Jr and Lois Weyer, 2007
65-70	1686	near 1690	methyl (CH_3) C - H absorption bands	(Jerry Workman Jr and Lois Weyer, 2007)

70-75	945	930–945	C - H stretch vibrations in carbohydrates,	(Sundaram *et al.*, 2011)
	1664	Near 1660	Cis-unsaturation	(Nicolaï *et al.*, 2014)
75-80	937	930–945	C - H stretch vibrations in carbohydrates	(Pérez-Vich, Velasco and Fernández-Martínez, 1998)
	969	Near 970	O – H water overtones	(Jerry Workman Jr and Lois Weyer, 2007
	1249	1150-1250	C - H vibrations fatty acids	(Pérez-Vich, Velasco and Fernández-Martínez, 1998)
	1282	1260–1270	The second overtone CH_3 and CH_2 asymmetrical stretching of n-alkane C – H and O – H bonds fat and water content	(Konstantinos *et al.,* 2017)
	1689	near 1690	methyl (CH_3) C - H absorption bands	(Jerry Workman Jr and Lois Weyer, 2007

80-82	966	966	water absorption	(Konstantinos G. Kyprianidis and Jan Skvaril, 2017)
	1522	1400-1600 1000–2000	O – H stretch and O – H band combination and the H – O – H deformation combination: starch First overtone of the hydroxyl group, hydrogen-bonded alcohols	(Konstantinos G. Kyprianidis and Jan Skvaril, 2017)
82-91	937	930–945	C - H stretch vibrations in carbohydrates	(Pérez-Vich, Velasco and Fernández-Martínez, 1998)
91-93	918	918–922	O - H bonds, water content,	Konstantinos G. Kyprianidis and Jan Skvaril, 2017;
	953	953	Vibrational overtones O - H and C - H bonds, water and carbohydrate	(Konstantinos G. Kyprianidis and Jan Skvaril, 2017)

93-100	1217	1150-1250 1216	C - H vibrations fatty acids Sorbitol	(Pérez-Vich, Velasco and Fernández-Martínez, 1998)
	918	918–922	O - H bonds water content,	Konstantinos G. Kyprianidis and Jan Skvaril, 2017;
100-105	1275	Near 1260-1270	C – H and O – H bonds fat and water content	(Konstantinos G. Kyprianidis and Jan Skvaril, 2017)
	1509	1400-1600 1460–1600	O – H stretch and O – H band combination and the H – O – H deformation combination: starch First overtone of the hydroxyl group, hydrogen-bonded alcohols,	(Konstantinos G. Kyprianidis and Jan Skvaril, 2017)

Support vector machine (SVM) machine learning models were applied to leaf and tomato spectra using multiple classification organisations. Leaf SVM (Figure 4.4A) performance was unreliable. Accuracy rates reached a maximum performance of correct classification of 38 days of 60.04%, a rate above random, this is followed by 58.18% at 19 days, and

54.93% at 23 days. Other successful classification rates were much lower. Additionally, misclassification rates were high, some reaching very high rates of 75%, 72.16 and 50%. This is in contrast to developmental stage (Figure 4.4B) classification accuracy which was much more successful, achieving high accuracy in vegetation and fruiting phases of 77.02% and 73.27% although lower accuracy 48.46% was achieved for post-harvest leaves.

Fruit SVM model (Figure 4.4C) achieved some high accuracy rates including at: 38, 53, 70, 82 days of 75.26, 66.63, 64.03, and 62.53% respectively. However low accuracy rates were also achieved, sometimes unable to achieve any correct classification. Misclassifications were also achieved in varying levels ranging from 10% to 75%. Overall this SVM was inconsistent and unreliable. This reflected a similar result from the before-harvest fruit series (Figure 4.4E) and post-harvest fruit series (Figure 4.4F). Some high accuracy results were achieved including 76.01% and 79.29% at 38 and 70 days and 64.81% at 82 days however very high misclassifications were also obtained, including 100% misclassification. Fruit was more successfully classified when organised by before-harvest and post-harvest (Figure 4.4D) achieving very high rates of 97.2% in before-harvest and 100% in post-harvest. Leaf and fruit data organised by developmental stage also achieved highly accurate results, especially in fruit categories. Some misclassification results occurred in leaf phases, the highest in post-harvest of 35.11%, correct classification on post-harvest leaves achieved 43.2% the lowest in the model however the model overall was reliable in correctly classifying developmental phases.

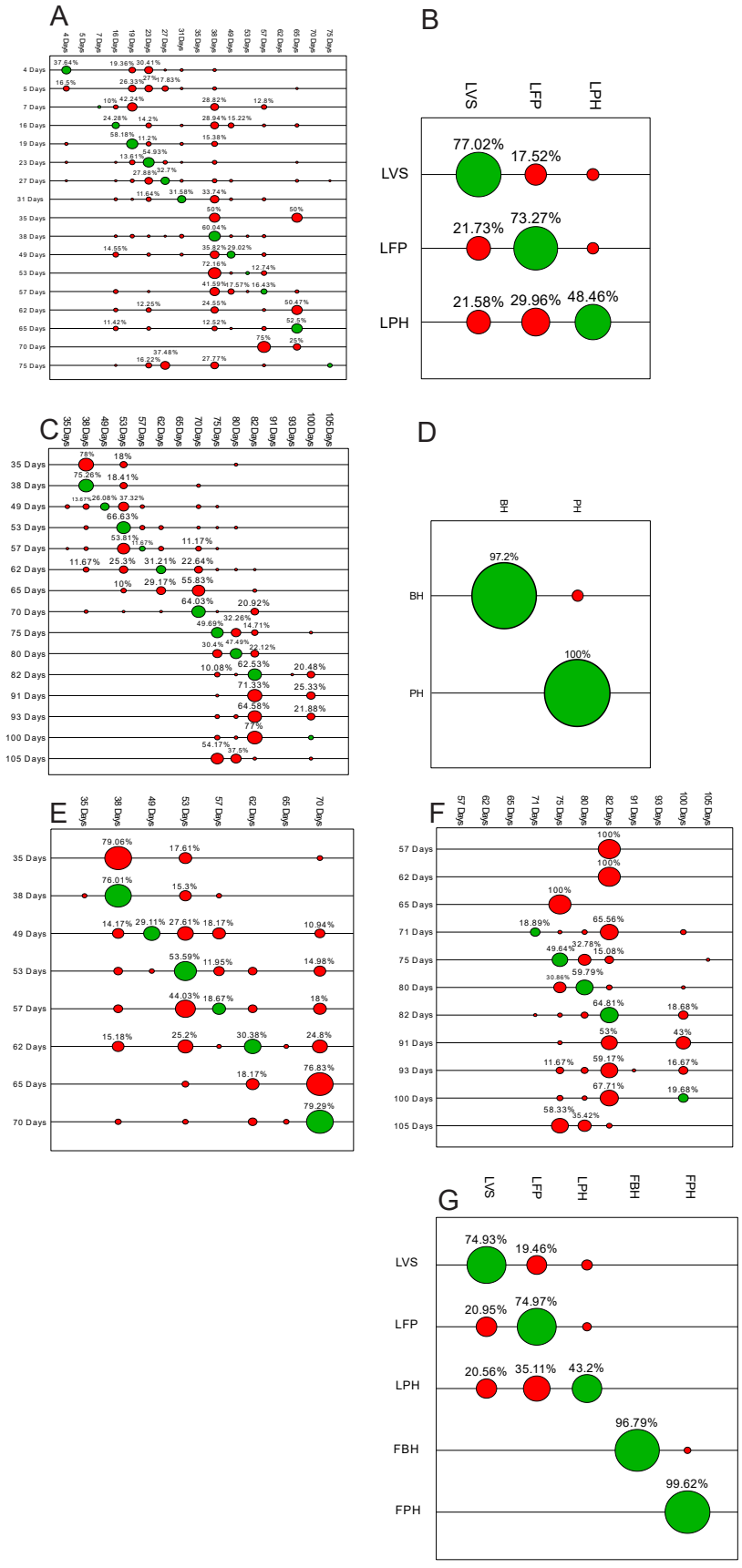
A
B
LVS
LFP
LPH
77.02%
17.52%
21.73%
73.27%
21.58%
29.96%
48.46%
C
D
BH
PH
97.2%
100%
E
F
G
FBH
FPH
74.93%
19.46%
20.95%
74.97%
20.56%
35.11%
43.2%
96.79%
99.62%

Figure 4.4 Support Vector Machines (SVM) classification accuracy confusion matrices of NIR spectral analysis of *Solanum lycopersicum* 'Piccolo' tomatoes. **A)** Piccolo leaf spectra, days from cotyledon emergence. **B)** Plant development phases: Leaf vegetative phase (LVP), leaf fruiting phase (LFP) and leaf post-harvest (LPH) **C)** Fruit development, days from cotyledon emergence **D)** Fruit before (BH) and post-harvest (PH) **E)** Fruit before harvest, days after cotyledon emergence **F)** Fruit post-harvest, days after cotyledon emergence **G)** Leaf and Fruit development and post-harvest phases Leaf vegetative phase (LVP), leaf fruiting phase (LFP) and leaf post-harvest (LPH), fruit before harvest (FBH) and fruit post-harvest (FPH)

4.5 Discussion

An extensive body of research has characterised molecular compound absorbance and their interactions with specific wavelengths and regions in the NIR portion of the electromagnetic spectrum. These characterisations helped to inform the composition of the spectral signatures obtained from plant tissues. The peak variances and biochemical changes during pre-harvest fruit (Figure 4.2I) appeared at: 930 nm and 1154 nm could be associated with cell wall components such as pectins or polysaccharides and fatty acids (Konstantinos G. Kyprianidis and Jan Skvaril, 2017) which may contribute to fruit softening during ripening (Shi *et al.*, 2023). 1395 nm is associated with the stretching of carboxylate groups ($–COO^-$) found in organic acids that typically decrease through ripening, reducing fruit acidity (Batista-Silva *et al.*, 2018). 1664 nm represents C = O protein stretching that may relate to the enzymatic breakdown of proteins during ripening, potentially through microbial enzyme breakdown from early spoilage processes. After-harvest a different set of biochemical changes (Figure 4.2L) were identified. 1261 nm may represent the lipid peroxidation contributing to off-flavours and odours, this is determined by the C-O stretching in esters and lactones (Kodali *et al.*, 2020). Aromatic compounds or phenolics are pigments that contribute to colour and flavour that break down during spoilage which could be associated with C = C stretching at 1506 nm (Simkova *et al.*, 2024).

4.5.1 NIR and chemometric analysis reveals distinct changes in spectral signature of Piccolo tomatoes associated with ripening, senescence, and spoilage

The PCA analysis revealed distinct clustering and separation patterns in tomato plant spectral data that illustrated changes related to the temporal progression of tomato leaf and fruit development, ripening, and post-harvest processes.

In leaves (Figure 4.2C) C - O stretching at 1139 nm is likely associated with proteins and lipids that may reflect structural components in the cell wall changing through leaf maturation (Alberts *et al.*, 2002). Carboxylate groups could be linked to organic acids that may play a role in photosynthesis and could be attributed to 1392 nm. 1422 nm C - H bending of lipids and fatty acids and 1686 nm C - O stretching of amides or proteins, potentially through synthesis in leaf development.

Peaks in PCA-LDA loadings were located at 1139 nm, 1392 nm, 1422 nm, 1686 nm representing biochemical changes that leaves undergo during plant development that correspond to metabolic needs. Leaf maturation and expansion involve changes in structural components of the cell wall which could be attributed to the C-O stretching in carbohydrates at 1139 nm. Metabolic adjustments in the leaf during growth especially associated with photosynthesis and respiration processes occur, these processes are linked with organic acids like malic or citric acid that could relate to the stretching vibrations of carboxylate groups at 1392 nm (Lehmann *et al.*, 2016). Protection and support of leaf integrity is reliant on membrane and cuticle formation, this important process is associated with an increase in fatty acids and lipids corresponding with C-H bending at 1422 nm. Protein synthesis occurs during leaf development represented by C=O stretching of amides and proteins at 1686 nm.

Analysis of tomato leaves provided distinct clustering in PCA, especially observed in the late developmental phases indicating that as the plant matures, biochemical changes become prominent (Figure 3. PCA-LDA further refined these clusters, showing clearer separations between the time-points. During early vegetation development, cell wall development requires the availability and/or synthesis of carbohydrates in addition to

surplus energy storage. Wavenumber 1139 nm was identified as important peak change for leaf development, often associated with carbohydrate presence including cellulose, hemicellulose and pectins in the cell walls (Abbott and Boraston, 2008). Carbohydrate changes may also be represented but the deformation of C-H bonds in carbohydrates at 1422 nm, relating to the accumulation of simple sugars and starches in developing leaves. C-N stretching in proteins, crucial during early growth and enzymatic functions metabolism and building structural components may also be attributed to 1139 nm wavenumber. 1672 nm corresponds with sucrose, often utilised during fruit ripening as a signalling compound instigating other developmental processes(Durán-Soria *et al.*, 2020) Some key developmental processes may be attributed to these protein indicators, including alterations in protein folding and degradation (Heinz Fabian and Werner Mantele, 2006). 1392 nm reflects lipid biosynthesis (Lewis and McElhaney, 2013) required for cell membrane expansion and protein activity needed for growth. When looking at the individual time points groups, 1139 nm was an important peak change between 7-16 days and 62-65 days. This wavelength is assigned to benzene ring structures, key to a variety of key secondary metabolites including phenolics, flavonoids, tannins, lignin precursors and salicylic acid which all are involved in processes occurring throughout developmental phases (Simkova et al., 2024).

Tomato fruit spectral signatures in PCA analysis revealed two overall data clusters (Figure 4.2D), comprising of early fruiting time points, and post-harvest time points suggesting that the ripening and spoilage processes exhibit clear biochemical profiles. Notable biochemical shifts in the transition between developmental phases of tomato plants were captured through the PCA-LDA analysis. Distinct biochemical profiles were indicated in the fruit from the clear spectral separation of before and post-harvest fruit. Pectins, carbohydrates and lipids have been identified by associated wavenumbers (Table 4.2), highlighting the complex changes including softening and other textural alterations due to enzymatic processes. These spectral signatures reveal that the biochemical mechanisms that are involved in fruit ripening are not only significant for the sensory qualities but also critical for understanding their shelf life and post-harvest quality. PCA-LDA further enhanced the separation and clustering (Figure 4.3C&D). PCA and PCA-LDA analysis further supports this with significant separation of class groups when organised specifically by before and after harvest in tomato fruit. Key

wavenumbers that determined the greatest biochemical changes for tomato fruit along the entire time-series included 992 nm, 1131 nm, 1249 nm, 1278 nm, 1509, 1664 nm. Fruit structure undergoes ongoing change throughout ripening and spoilage. Softening occurs through ripening adding to the edible texture and softening continues post-harvest, accelerated by enzymatic interaction. These structural changes occur through cell wall constituent breakdown including pectins and through cellulose and hemicellulose carbohydrate changes. These may be explained by C-H out-of-plane bending at 922 nm and C-O stretching in carbohydrates at 1135 nm. Cellulose, hemicellulose, and pectin, all major carbohydrate components of plant cell walls. developmental transitions such as ripening, senescence, or pathogen defence undergo processes including cleavage, rearrangement, or synthesis of these polysaccharides. Additional textural changes occur with protein breakdown which may be identified through C=O stretching at 1664 nm. Starches are also converted into sugar, sweetening the fruit, this increase in sugar presence may be indicated by peaks at 988 nm. Further sweetness is developed through acidity reduction, this occurs when organic acids like citric acid decreases, described by changes at 1398 nm. Fruit aroma and flavour profiles mature throughout ripening and subsequently degrade during post-harvest spoilage, these are contributed to by aromatic compounds comprising of esters, often associated with 1139 nm (Jiries *et al.*, 2022). Fruit deterioration and loss of structural integrity can be described by the appearance of peak wavenumbers 1509 nm and 1664 nm, associated with starches and volatiles that play a vital role in ripening fruit (Kapoor *et al.*, 2022).

LD2 showed peaks at 941 nm, 1124 nm, and 1395 nm, related to cell wall polysaccharides, fats and proteins metabolism and organic acids likely explaining significant changes in ripening processes in before-harvest fruit distinguishing these from all leaf phases and post-harvest fruit. 922 nm, 962 nm, 1139 nm, 1667 nm wavenumbers showed peak changes along LD3 axis, related to water, alkyl alcohols protein and fats pectins, cellulose, carbohydrates and proteins, changes in these are indicative of processes that occur in the plant during fruiting phases in both leaf and fruit, and the following post-harvest fruit spoilage. For example, Pectins play a role in cell wall structure providing rigidity and structural integrity, in ripening fruit softening of the fruit occurs associated with pectin degradation and subsequently, these cell wall components may experience enzyme-

driven changes in post-harvest fruit through spoilage processes and associated degradation

4.5.2 NIR Spectroscopy Combined with Chemometrics Does Not Provide a Specified Diagnostic Tool for Assessing the Quality and Shelf Life of Piccolo Tomatoes Throughout their Post-Harvest Journey

Despite visual interpretations from PCA-LDA revealing clustering and separation in time-series leaves and fruit, the application of SVM models for classification was not wholly successful. The varied range of classification accuracy rates rendered the time series SVM models unreliable suggesting that a more appropriate categorisation of the data would be using development phases.

The PCA-LDA analysis of plant development phases displayed significant clustering and separation. The temporally distributed leaf development phases support the hypothesis that distinct biochemical processes occur throughout development. Vegetative and post-harvest phases distinction was categorised by changes in carbohydrates, organic acids, lipids and proteins from loadings at 1139 nm, 1392 nm, 1422 nm, and 1686 nm (Figure 4.3 B), crucial for plant development (Arena *et al.*, 2023). Wavenumbers were drawn from PCA-LDA analysis of fruit ripening and post-harvest phases (Figure 4.3C) including 922 nm, 1135 nm, and 1664 nm suggesting these are indicative of stage differences and may provide critical markers relating to pectin and cellulose degradation, protein breakdown and sugar metabolism, 988 and 1398 nm indicative of softening and flavour development processes like sugar accumulation and acid reduction (Kanayama, 2017).

Fruit and leaf developmental and post-harvest phases displayed overlap between spectral features suggesting they shared some biochemical pathways, especially during fruiting phase, implying that certain metabolic processes are synchronised between leaves and plants as the plant progresses through its lifecycle (Perez-Fons et al., 2014). However there is the distinction between the phases suggesting during the plant development and as it matures and transitions into the ripening phase, divergence of the chemical pathways becomes more pronounced, leading to the unique characteristics of the post-harvest phase.The combination of fruit and leaf analysis provided some useful perspectives related to the separation between phases using LD1, LD2 and LD3 axes.

Biochemical signatures both connect and distinguish tomato phases from the leaf development phases. LD1 clearly separated post-harvest fruit from all other phases (Figure 4.3E), likely explained by wavenumbers 918 nm, 953 nm, 1139 nm, 1282 nm, 1380 nm, and 1667 nm which highlight cell wall components differences like cellulose, lignin and pectin and differences in metabolic compounds like sugars and proteins between leaves and fruits.

Sugar conversion, pectin breakdown, and lipid oxidation can be seen in changes at wavenumbers like 953 nm, 1139 nm, 1282 nm, and 1667 nm may represent the largest distinction, separating the post-harvest fruit stage group. LD2 instead separation before-harvest fruit from all other phases, 941 nm, 1124 nm with the development of pectins and structural polysaccharides in early fruit while LD3 separates all leaf phases and provides clustering of before and post-harvest fruit and ripening phases in leaves. There are similarities in wavenumbers that occur in neighbouring time-points in leaves and fruit. Between days 38-49 and 49-53, wavenumber nm occurred in both leaf and fruit, in addition to 1674 nm in fruit proteins. This same wavenumber range occurs again at 53-77 1683 nm in leaves and 1674 nm in fruit, again at 57-62, 1670 nm in both leaves and fruit, 62-65: 1674 nm in leaves and 1686 nm in fruit, 65-70: 1689 nm in leaves and 1686 in fruit and at 70-75 similar wavenumbers 941 nm in leaves and 945 nm in fruit which could be associated carbohydrates. SVM models were applied to developmental phases in leaves and fruit and were more highly successful in accurately classifying between phases than when applied to time series data.

4.5.3 Limitations and Future Work

The spectral profiles of NIR is limited in specificity in comparison to other techniques like ATR-FTIR spectroscopy due to the broader overtone output. Measurements using ATR-FTIR would provide a more detailed picture of the biochemical changes occurring in the plants tissues. Validation can be achieved by comparing spectral profiles with molecular analysis through targeting sets of key marker genes of leaf development, senescence and ripening of fruit that are well described in existing knowledge. A key research question omitted from this study asks whether key biomarkers could be characterised from spectral signatures of leaf tissue that indicate abscission of fruit. Achieving this

characterisation would be useful to growers for informing optimal harvesting time to extend product shelf life. There are a selection of useful genes that be used as markers to provide refeence for spectral analysis using chemometric tools and predictive models. Some examples of important genes including SISAG12 and SISAG113 expressing during leaf senescence especially when nutrients are reallocated from leaves to ripening or senescing fruit (Watanabe et al., 2013). Stay-Green 1 gene SISGR1 associated with leaf yellowing, may also be a useful marker for nutrient remobilisation supporting fruit maturation and abscission. Ethylene biosynthesis and signalling associated genes ACS and ACO are expressed driving ethylene rises during ripening, senescence and fruit abscission (Ahlawat and Liu, 2021). These genes are expressed in leaves in addition to fruit, the characterisation of these in leaves using spectra would provide useful biomarkers for development stages. These genes are sensitive to stresses further providing a useful indication of plant health, how the individual plant development might behave as a result and inform growers so appropriate treatment can be applied to improve quality. WRKY53 and WRKY70 are regulators of stress and senescence and modulate hormonal crosstalk and degradation of leaves (Besseau, Li and Palva, 2012).

It is unknown whether the characterisation of these genes would be possible using NIR spectroscopy, and very limited studies have explored a direct comparison of mid-infrared spectral signatures with marker genes, providing a significant research gap for future work.

4.6 Conclusions

NIR spectroscopy found it difficult overall to find distinguishing features in the spectral signatures at individual time points, however, it is evident that the spectral information is there due to the temporal spreading of the data when investigating it. It did well, however to distinguish between developmental phases, especially between fruit pre-harvest and post-harvest fruit, which suggests that these data classes were more powerful, due to there being more spectral information within them. The time points proved to not be distinct enough when using NIR. Future studies may see a more powerful distinction between time points with a larger sample set, allowing for a more reliable indication of the biochemical changes happening. This study would also benefit from

using MIR spectroscopy for increased specificity. The use of the handheld device did allow this data capture, simulating a similar environment in glasshouses that might be seen in the industry through the supply chain where they might find less portable systems like MIR spectroscopy to be more challenging to use. NIR could be a useful tool to read specific biomarkers, however, it does not seem powerful enough to achieve specificity in developmental time points. Correlation analysis and predictive models including regression analysis would be a useful next step to understand dependency of biochemical processes and to predict their occurrence, both useful for supply chain implementation to reduce food loss and waste.

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5. A Tool in the Toolkit: Can True Tost Accounting Remove Siloed Thinking About Food Loss and Waste?

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The findings of this report originate from a Global Food Security Policy Lab, and do not necessarily reflect the policy positions or views of GFS or its individual partners.

5.1 Food Loss and Waste, A Systemic Problem

The complex challenge of reducing food loss and waste is a deeply rooted systemic problem; therefore, it cannot be achieved with technological methods alone. Governmental policies and interventions are continuously evolving, focused on resolving the substantial problem. Simultaneously, other important actors and stakeholders are actively developing and implementing policies and processes that aim to reduce food loss and waste. These actions from individual organisations are critical to achieving this goal, however, there lies a lack of system functionality in the absence of communication and collaboration causing inconsistencies. These systemic issues occur within the national food system and are only exacerbated when observing the enormous and complex global food system. The lack of consistent definitions of food system elements between key organisations creates obstacles in formulating legislation and actions to alleviate systemic problems affecting everyone. An example of this is shown by the lack of consistency in food loss and waste definitions are defined inconsistently between UK government, the EU and food waste charities like WRAP, who all play significant roles in influencing action. While technical innovations, including spectroscopic tools are critical to targeted approaches, these are rarely implemented within a systemic governing framework. A variety of frameworks have been developed in theoretical proposals including True Cost Accounting (TCA). Correcting externalities associated with the food system that are often ignored has been identified as a promising method for improving food security on a global scale and more specifically to support the complex challenge of reducing food loss and waste. The conceptual basis of TCA assigns an economic value to environmental, societal, and health costs and benefits, which form a total value of food products. These assignments represent how costly an item is, intended to inform food system decision-making by food-system actors. Currently, there is a growing body of research and theory investigating TCA and its proposed methods of implementation however, there is a lack of consensus surrounding its feasibility and potential success. This chapter attempts to assemble insights from a diversity of perspectives representing all actors as stakeholders in the supply chain from position-influenced experiences. The perceived potential, TCA's feasibility in practice, and the barriers and limitations were explored and assessed to provide a deeper understanding of TCA framework and to form recommendations for systemic policy development.

This research was conducted collaboratively by multi-disciplinary researchers as part of the government organisation Global Food Security Network's scheme, encompassing contributions by early-career researchers to achieving global food security described by United Nations SDG goal 17. Programme participants are competitively selected and a final team is selected for their work design and awarded the role of conducting research and producing a policy think piece for publication, presentation to UK government and at the COP26 summit.

5.2 The Global Food Security Network Policy Lab

I was awarded the opportunity to participate in the Global Food Security Network's annual programme, which aims to establish early-career researcher contributions to influencing policy related to UN SDG Goal 17. Successful applicants were selected into the program that provided detailed knowledge from prominent figures and relevant stakeholders forming a basis for the design of a policy piece about the decided topic: reducing food loss and waste, The winning proposal formed the final team, to which I belonged, and was selected to conduct the work. The research was collaboratively conducted by my team consisting of early career researchers from multiple academic disciplines representing backgrounds of both STEM and social sciences. I was responsible for establishing contact and recruiting contributors that represented the spectrum of acting positions in the supply chain with the aim of obtaining diverse and balanced position-influenced experiences and perspectives. I was also responsible for the continuing engagement with these stakeholders and the conducting of data collection which was performed through focus groups. My role included the hosting of six focus groups that I introduced with a comprehensive presentation conveying our research topic and questions and subsequently stimulated discussion, ensuring equal opportunity for contribution from the participants. The discussion was directed by pre-prepared questions that we wanted to address in the work. I contributed to the literature review research and the writing of the final report in equal volume to my colleagues, including production of figures and appropriate images. I maintained continued contact with participating stakeholders with progress updates and presented them with the publication upon completion. We were invited to present the work to UK government representatives, to which I partially presented and was involved in discussion. A

significant achievement was the video presentation we created of the work that was presented at the COP26 climate summit.

5.3 Contributions

The work was produced by Bernd Bonfert (Cardiff University), Miranda Burke (Lancaster University), Aoife Caffrey (Ulster University), Siobhan Maderson (Aberystwyth University), Amy Molotoks (Stockholm Environment Institute, University of York), Justine Pearce (Royal Veterinary College), Mehroosh Tak (Royal Veterinary College)

Written contributions from: Bernd Bonfert, Miranda Burke, Aoife Caffrey, Siobhan Maderson, Amy Molotoks,, Justine Pearce, Mehroosh Tak

Qualitative analysis contributions from: Bernd Bonfert and Siobhan Maderson

Stakeholder Contact contributions from: Miranda Burke
Focus Group contributions (hosting and facilitating): Miranda Burke, Justine Pearce, and Amy Molotoks

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Maryam Rezaei (Food and Agriculture Organization)
Pete Belk (Business in the Community)
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Some participants who participated in the Focus Groups decided to remain anonymous and are not listed

This chapter presents a proposal for a system-wide framework approach that seeks to address the complex challenge of reducing food loss and waste. While technological innovations are critical in targeting direct supply chain optimisations, these approaches are not sufficient alone. Reformations are necessary to eradicate the deeper systemic issues that facilitate and exacerbate food insecurity and specifically food loss and waste. This chapter seeks to bridge the gap between technological methods and holistic approaches for complementary application.

5.4 Executive summary

Food loss and waste (FLW) is a global economic, environmental, and ethical problem which has been specifically targeted within the United Nations Sustainable Development Goals (SDG's); Goal 12.3 aims to "halve per capita global food waste at the retail and consumer level, and reduce food losses along production and supply chains by 2030". While most efforts to decrease FLW focus on the individual consumer or householder, FLW is generated at all points throughout the food system, including production, processing, distribution and consumption. Since FLW is exacerbated by long and complex supply chains with many different stakeholders throughout the food system, efforts to decrease it must engage with all stakeholders and all of their impacts on FLW, rather than simply focussing on individual stakeholders or processes. In this think-piece, True Cost Accounting (TCA), a method for measuring and quantifying the true social, economic, and environmental impacts of different food production systems, was explored to assess how it could help to overcome siloed thinking and support collaborative efforts to reduce FLW throughout the whole food system. To do this, a literature review was conducted, followed by a series of focus groups leading to the formation of six policy recommendations that could support stakeholder collaboration across the food system to reduce FLW.

5.5 Key Findings

Barriers to reducing food waste at the household level include a lack of time, knowledge, and skills for purchasing and preparing food. Use-by dates on packaging and large portion sizes exacerbated this issue. Almost unlimited accessibility to inexpensive, globally produced food disconnects consumers from the true value and impact of their food, and the value lost when wasting it. The barriers to food loss from producers and suppliers include large, complex supply chains resulting in overproduction and overstocking. Unavoidable waste, as well as spoiled or damaged food is usually sent to landfill, due to current regulations on repurposing FLW.

Collaboration across the food system was demonstrated to be a vital solution in reducing FLW as responsibility for food waste is frequently passed between stakeholders and no single actor is held responsible for FLW, although it is most frequently measured at the

end of the supply chain. To encourage a collaborative approach, changes to supplier-retailer contracts, shorter, localised supply chains, closed-loop systems and communal storage facilities within food systems are discussed.

Benefits and opportunities of TCA included providing a wider system-level and collaborative perspective for decision makers and using TCA as a tool within a toolkit of other initiatives to reduce FLW. TCA could aid the co-production of policies between policy-makers and other stakeholders, making them more widely accepted and effective.

Challenges of TCA included the complexity and impracticality of applying TCA to the complex food system and how TCA metrics would be accurately measured, collated, and analysed across the many processes involved within the food system.

5.6 Policy Recommendations

1) Ensure supplier-retailer contracts address FLW at all points of the supply chain and mandate stakeholders to measure, state and reduce FLW in their contracts.
2) Hospitality, supermarkets, and local authorities should be required to disclose all FLW and set mandatory annual targets to decrease FLW.
3) Review current rules and regulations regarding use and processing of FLW, and consider options for repurposing of FLW, for example as animal feed.
4) Address supply chain inefficiency: supporting public procurement directly from suppliers could decrease FLW, while simultaneously strengthening local economies.
5) Incentivise suppliers, retailers, and hospitality to address social, economic and environmental food system externalities potentially offering incentives and rewards to do so via lower business rates.
6) Clear definitions of terminology including: food loss, food waste, surplus, inedible parts and destinations of food loss and waste. Development of government recognised language for system-wide standardisation of data recording

5.7 Further Research and Development

There are several areas that we feel need further development and research that will support our policy recommendations. We have emphasised the need for effective measures of data reporting, especially in FLW. Currently, there is more focus on recording and reporting food waste, which has led to an underrepresentation of food loss. To support our policy recommendations surrounding data reporting, we suggest that data on FLW should be measured across the whole food chain to represent a balanced and more accurate view of the FLW issue.

The infrastructure for FLW can be strengthened and supply chains supplemented through support for centralised FLW distribution hubs within local areas, so that surplus food and food not fit for sale, can be stored, managed, and distributed appropriately within local food systems.

The simplification of information could be addressed with the creation of a central database that contains sustainability, health and environmental schemes and metrics. This would help provide consistency and be used to inform when used in application throughout the food system. For example; a simple labelling system encompassing metrics within the SDGs could be developed to incentivise positive change throughout the food system.

Further research is needed to explore if food pricing could reflect external social and environmental costs and what the implications on food poverty and affordability would be. There should be further work employing TCA to investigate if healthy food produced with low environmental impact is ultimately more economical overall, compared to foods that have negative public and environmental health impacts.

5.8 The Challenge of Food Loss and Waste

Globally, nearly 40% of all food produced for human consumption is lost or wasted (WWF, 2021). According to the Food and Agriculture Organization of the United Nations (FAO, 2011), food loss is *"the decrease in the quantity or quality of food resulting from decisions and actions by food suppliers in the chain, excluding retailers, food service*

providers and consumers", and food waste refers to "*the decrease in the quantity or quality of food resulting from decisions and actions by retailers, food service providers and consumers"* (FAO, 2011). Therefore, food loss includes estimates from post-harvest up to, but not including, the retail stage, whereas food waste includes estimates at the retail and consumption level. According to the FAO's food loss index, globally, 14% of all food produced is lost from the post-harvest stage before reaching retail level (FAO, 2019). Food waste is most commonly addressed at the individual level (Canali *et al.,* 2017). An estimated 931 million tonnes of food waste is generated from retail, food service and households annually, this is 17% of all food produced globally. 11% of all food waste, or 570 million tonnes is from the household level (UNEP, 2021) . Solutions typically focus on the household, as this is where the majority of food waste is typically recorded. As awareness around the impacts of food waste increases, and other parts of the food chain begin to be measured, food loss on farms is now emerging as a significant cause of food wastage (WWF, 2021). Current solutions to reducing food loss and waste (FLW) include recycling, recovery and disposal, however, to more effectively address the issue of FLW, a greater focus on *preventative* measures and reducing FLW at all points of the food system is required. This necessitates all stakeholders recognising that the current, siloed approach to reducing FLW at individual stages of the food system is a barrier that must be overcome, and emphasises the need to work collaboratively across the supply chain.

FLW is an ethical, economic and environmental issue. On the 25th September 2015, the 193 Member States of the United Nations adopted the 17 Sustainable Development Goals (SDG) of the 2030 Agenda for Sustainable Development, global objectives with major outcomes including the Paris Climate Agreement (a global treaty to limit climate change). However, it is estimated that if FLW were a country, it would be the third largest source of greenhouse gases (UNEP, 2021). The commitment to the Sustainable Development Goal included target 12.3; to halve per capita global food waste at the retailer and consumer levels and reduce food losses along production and supply chains, including post-harvest losses by 2030. Furthermore, reducing FLW is critical to creating a Zero Hunger world (SDG 2), and ensuring responsible consumption and production (SDG 12). The positive impacts could also extend to sustainable water management (SDG 6), climate action (SDG 13), life below water (SDG 14) and life on land (SDG 15) (Figure 5.1). Understanding, therefore, how to implement policy action to efficiently reduce FLW

across supply chains is intrinsically important not only for reducing production costs and improving efficiency, but for contributing towards social and environmental sustainability.

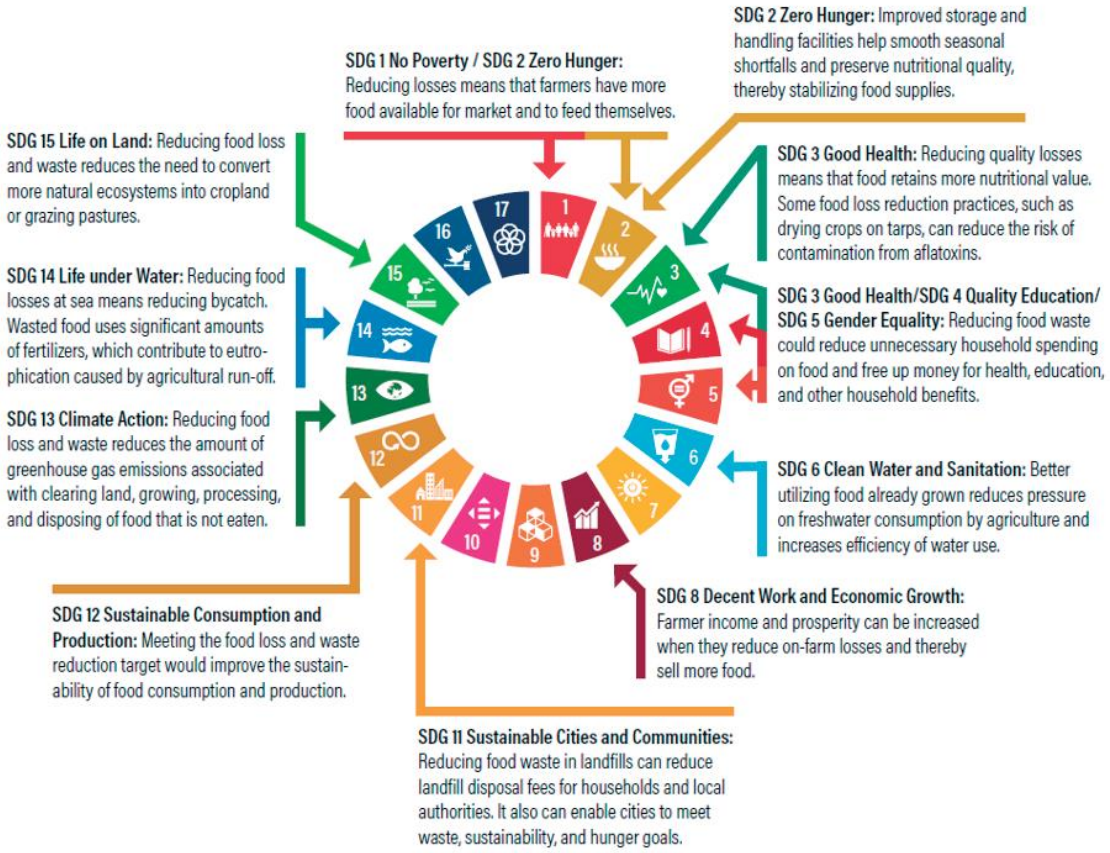

Figure 5.1: Food loss and waste is an important issue for the Sustainable Development Goals (SDG) as reducing food loss and waste can help achieve multiple SDGs (Source: WRI, 2019 : Flanagan *et al*., 2019).

5.9 Definitions

True Cost Accounting (TCA): TCA is a systemic approach to assess, measure, and value all externalities involved in the production and consumption of a product or service. In this report, TCA is used in context of, but is not limited to, the UK food-system. This can take the form of effective data recording and reporting. The use of TCA as a tool and its associated metrics, provide a holistic understanding of the relationships that form the food system, including: agriculture, food, the environment, and human well-being. The

application of TCA principles by stakeholders within the food system provides transparency and being accountable for externalities (Global Alliance for the Future of Food, 2021)

Externality: A positive or negative external cost or benefit that is not financially incurred by the producer or consumer, but has an impact on a third party that has not consented to the cost. Externalities are normally environmental costs, societal or costs to public health (Khemani, et al., 1993). Examples include water pollution from agricultural practices, low wages to food system workers, and the public health costs resulting from dietary illnesses, such as diabetes and cardiovascular disease.

True Price: The true price consists of the market value of a product, in addition to the social and environmental externalities or 'hidden' costs that make up the true price gap. The true price gap is defined to remediate the harm caused by the externalities of production and consumption, and so now included in the price of the product. The extra money must be used to repair the damages for it to be considered a 'true price' (De Groot Ruiz, 2021).

True Pricing: True pricing is the application of the true price to products within the consumer market. This application must additionally include providing transparency about the associated true costs and prices, preventing external costs through the transformation of products, and remediating external costs through transaction or taxation which creates a sustainable economy (De Groot Ruiz, 2021).

Food System: A complex system of actors and activities that contribute to, or are directly or indirectly involved in feeding a population. This can include, but is not limited to the; growing, harvesting, processing, packaging, transporting, marketing, consumption, distribution and disposal of food and food-related items. There are further economic, political, environmental, health and social interactions with the food supply chain which influence and are influenced by it, that are considered parts of the food system, see Figure 5.2. (Parsons, *et al.,* 2019).

Food Loss: Food Loss is the decrease in the quantity or quality of food resulting from decisions and actions by food suppliers in the chain, excluding retailers, food service providers and consumers. Empirically, it refers to any food, including spoiled or

deteriorated food, that is discarded, incinerated or otherwise disposed of along the food supply chain from harvest/slaughter/catch up to, but excluding, the retail level, and does not re-enter in any other productive utilisation, such as feed or seed. (FAO. 2011)

Food Waste: Food Waste refers to the decrease in the quantity or quality of food resulting from decisions and actions by retailers, food service providers, and consumers. This refers to any food, including spoiled or deteriorated food, that is discarded, incinerated, or otherwise disposed of by retailers, food service providers, or consumers that is not otherwise repurposed (FAO. 2011).

Figure 5.2: The food system. The food supply chain at the core of the food system, has interdependencies with politics, health, environment, society and economy. Source: Centre for Food Policy, City, University of London 2019 (Parsons, *et al.,* 2019).

5.10 True Cost Accounting (TCA) – What is it?

One of the tools available for helping to address detrimental practices, and support healthy, resilient, equitable and sustainable food systems is True Cost Accounting (TCA). TCA aims to acknowledge and assess the economic, environmental, and social impacts of food production and food waste. TCA can inform decision-makers (i.e. producers, governments, institutions, businesses) to make better decisions which reflect the full range of impacts of the food system (Global Alliance for the Future of Food, 2021). It is important to note that TCA includes multiple assessments and metrics for assessing value, and is not a solely monetary analysis (Scialabba *et al.,* 2021). Societal impacts, local contexts and full supply chain analyses are addressed via TCA. Significant work has been done on developing and collating such metrics including; 'The Economics of Ecosystems & Biodiversity for Agriculture and Food programme' (TEEBAgriFood; De Groot Ruiz, 2021) The United Nations Food and Agriculture Organisation (FAO), has estimated the true cost of FLW as that of economic costs (US$ 2.6 trillion/year), environmental costs (US$ 700 billion/year), and social costs (US$ 900 billion/year) (FAO, 2014). These TCA figures include the carbon impact (3.5 gigatons CO_2e or US$ 294 billion/year), water impact (250 Km^3 or US$ 164 billion/year), and biodiversity impacts (e.g. pesticides, nitrate & phosphorus eutrophication, pollinator loss etc.), at US$ 32 billion/year.

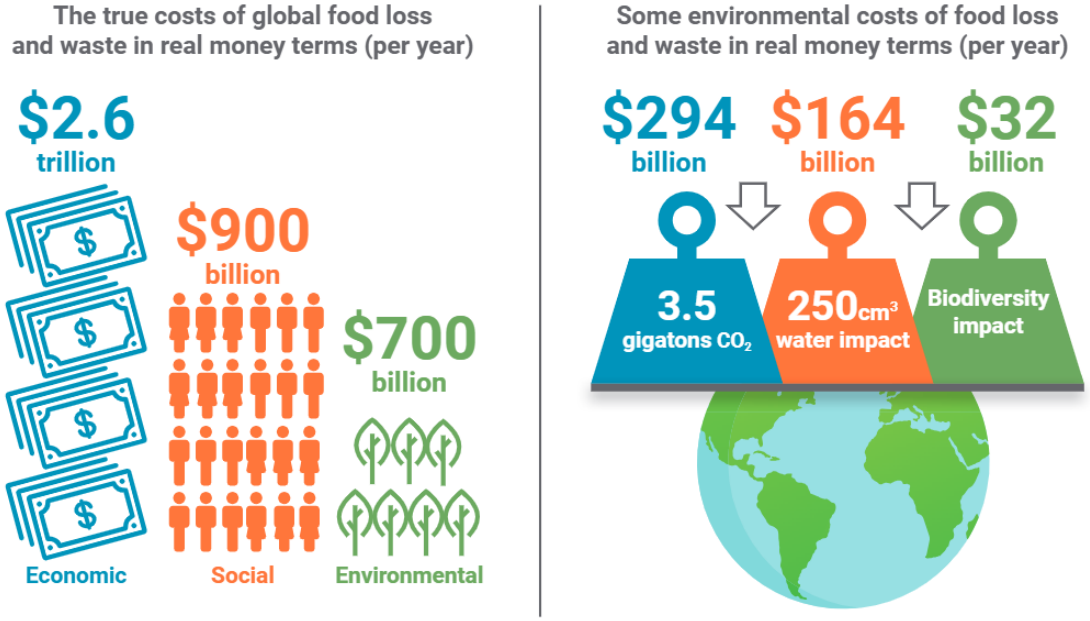

Figure 5.3 The true costs of global food loss and waste in real money terms

Sustainable diets that ensure healthy nutrition have been proposed as drivers for food system transformation. In the UK, the National Food Strategy set out ambitious proposals based on the current food system and its true cost on human and planetary health (NFS, 2021). The EAT-Lancet Planetary Health Diet report reviewed global targets for healthy diets and proposed that a diet rich in plant-based foods and with fewer animal source foods confers both improved health and environmental impacts (EAT Lancet, 2019). The Commission developed a sustainable diet that would provide adequate adult reference intakes of energy, macro- and micronutrients; compared to typical UK diets, the EAT-Lancet diet contains more fruit and vegetables, more wholegrain starchy foods and more plant based proteins, but less meat and dairy, starchy tubers, sugars and processed foods, a diet that is supported by the British Dietetic Association (British Dietetic Association, 2021).

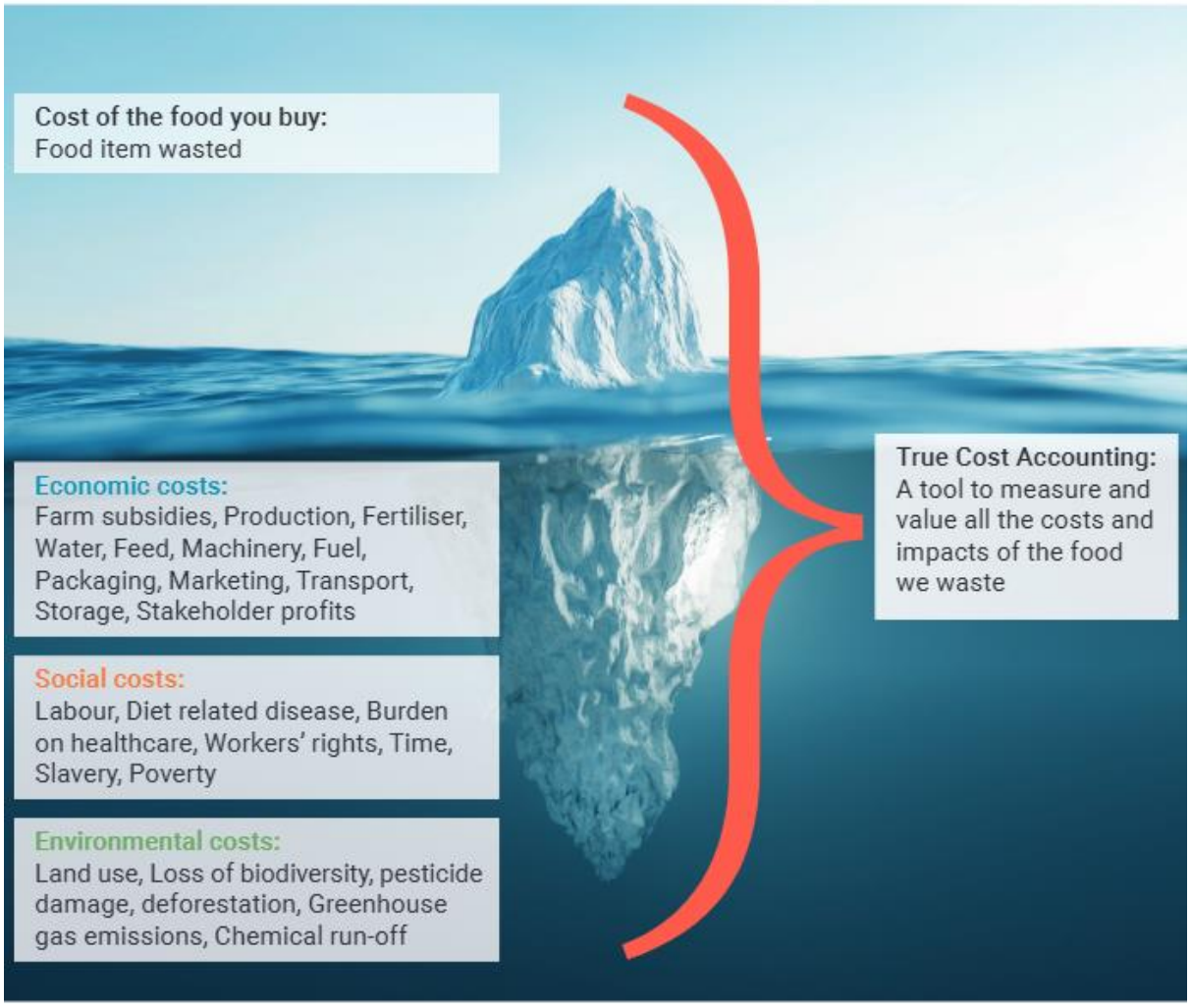

Figure 5.4 What we really waste when we waste food and how True Cost Accounting can measure this

5.11 Case Study: True Cost of Food Waste from the UK Hospitality and Food Service Sector, WRAP, UK

The Waste Resources Action Programme (WRAP) has explored the true cost of food waste within the UK's hospitality and food service sector (Parfitt and Freyer, 2013), identifying the true cost of food waste from a financial perspective and estimating the costs associated with food purchase, waste management, energy, water, labour, administration and transport. Whilst these sectors serve over 8 billion UK meals, they also produce over 2.87 million tonnes of food and associated packaging waste. Of total food purchased by

the UK's hospitality and food service sector industry by weight 17.8% is wasted, of which 13.2% is avoidable and the remaining 4.6% is unavoidable. The true cost of food waste generated within this UK sector was estimated at £2.5 billion/year, and a true cost figure that is *double* the costs of the food purchased.

5.12 Case Study: Subsidising Healthy School Meals, Food Policy for Public and Economic Health, USA

Healthy diets with a high level of fresh fruit and vegetables are commonly seen as prohibitively expensive. At the same time, there is a public health crisis, with poor diet linked to 18-25% of all deaths. Diet-related chronic diseases such as obesity, cardiovascular disease, and diabetes; devastate communities, particularly people of colour and/or those experiencing poverty. Healthy eating needs to be affordable and accessible to all. The Supplemental Nutrition Assistance Programme (SNAP) subsidises increased fruit and vegetable purchases amongst low income consumers. The Good Food Purchasing Program promotes public procurement directly from farms, and has increased the amount of organic and fair-trade foods included in school meals. Direct procurement has multiple True Cost benefits, and is also associated with lower levels of food waste (Gemmill-Herren *et al.,* 2021).

5.13 True Cost Accounting Does Not Mean True Pricing

Two concepts that are often conflated are: 'TCA' and 'True Pricing'. TCA is a tool using a universal currency for valuing externalities without the application in real monetary terms. True pricing is the application of the true price to real product pricing. True pricing has been proposed as a possible method of reconciling the true costs for products and services . True pricing would internalise the externalities into product prices to support a sustainable food system. A similar concept of taxing market activity to include externalities: 'Pigovian Taxes' was first suggested by Pigou, Sigdwick and Marshall (1920) but has always been considered an impossibility (Pigou, A. C, 1920).

To consider the implementation of a systemic price realignment for all food products with a range of externalities would be complex, particularly when accurately measuring the precise value of true prices. In the last decade, the development of sophisticated data

collection and reporting could make true pricing a legitimate possibility for the future (De Groot Ruiz, A. *et al* 2021). The True Price Foundation (2012) have now created frameworks for true pricing using a rights-based approach that takes the market value of the product, and fills the 'true price gap', reconciling the external social and environmental costs resulting from production and consumption that breach basic rights (True Price Foundation, 2020). These recuperated funds are then used to remediate these externalities.

In theory, true pricing in the food system could influence consumer behaviour into considering the types of diets they have, based on environmental impact, health or at least financial choices. It has been noted that true pricing may be too expensive and exclusionary to some consumers. Alleviation of this could be through subsidisation, however, there is a significant risk that this would not be implemented fairly and the financial burden would inevitably fall to the consumer (De Groot Ruiz, A. *et al* 2021). There is much debate surrounding the efficacy of true pricing, but it is important to note that this is not the aim of TCA, and they should be considered separate concepts.

5.14 Exploring the Potential of TCA in Reducing FLW with Food System Stakeholders

To explore the potential of using TCA in reducing FLW across the whole food system and reducing siloed approaches, a series of stakeholder focus groups were held. Stakeholders from across the food system were invited to participate in a series of 5 focus groups, which were held in July-August 2021. The 25 participants included food producers, wholesalers, retailers, researchers, restaurant owners, policy-makers, civil society organisations (CSOs) and consumers. Participants were encouraged to consider their multiple roles and identities within the food system – e.g., retailer and consumer - as well as engage with the reality of climate change impacting everyone, and reaching net zero emissions being a challenge for all of us. These multi-stakeholder dialogues provided a breadth of insights, generating a clear picture of TCA's potential to support effective stakeholder collaboration for the reduction of FLW and thus ensuring the proposed policy recommendations had the best chance of being accepted by all stakeholders. The results of these focus groups are summarised below:

5.15 What are the Personal and Professional Barriers to Reducing FLW

Stakeholders acknowledged that there is often a conflict between their professional knowledge about food waste issues and their personal capacity to act, both domestically and professionally. Personal barriers to reducing FLW included a lack of time, knowledge and skills for purchasing and preparing food effectively, which is often exacerbated by misleading use-by dates on packaging, advertising schemes and large portion sizes in supermarkets and restaurants. The importance of household food provisioning routines e.g. shopping, reuse of leftovers, etc., have been highlighted as major drivers of food waste (Stancu, 2016). Recent research notes how COVID-19 lockdowns increased time at home which supported better food management and planning of meals, resulting in a decrease in food waste (WRAP, 2020). Many stakeholders also emphasised that difficulties in agreeing on meals due to changing schedules and accommodating different dietary restrictions or preferences contributes to the amount of food wasted.

"People want consistent supply – even of waste. Transport costs are also an important factor. In order to collect everyone's waste, and do something with it, we need to know what's coming, and what can be done with it" – (Wholesaler)

Age and cultural backgrounds were also mentioned as factors influencing attitudes and behaviours surrounding FLW, with those who have experienced food scarcity being less prone to wasting food. This has also been shown in recent research with 18-34 year olds being consistently more likely to report higher levels of food waste, as well as those under higher time pressure on a daily basis (WRAP, 2020).

Beyond barriers in their personal lives, all focus group participants noted systemic barriers affecting them on both a personal and professional level, challenging their capacity to reduce FLW in their organisations. Stakeholders across all status groups agreed that the large, complex supply chains throughout the food system made it difficult to disrupt the status quo of business-as-usual. These supply chains are often focused on industrial production and distribution methods that require stakeholders to overproduce or overstock in order to guarantee they meet demand and avoid financial risks (Isakson, 2014). Producers face extremely tight profit margins and need to fulfil contracts with

narrow product specifications that retailers can unilaterally opt out of. This leads to high levels of overproduction and food waste, as not being able to meet demands currently poses a much more serious financial risk than wasting food (Stuart, 2009). In order to stay profitable and competitive, retailers are also pressured to overstock and use certain packaging and aesthetic standards to cater for consumer tastes and demand. Retailers and restaurant owners perceived that consumers had negative views of their businesses when not offering bountiful portions or full shelves, thus driving overstocking and food waste in hospitality and retail. Some literature sources suggest responding to this problem by encouraging customers to adjust portions based on how hungry they are or charging lower prices for smaller portions (Reynolds, *et al.,* 2019). There was also a suggestion that over or excessive consumption of food should be classed as food waste.

Results from the focus groups corroborated findings in the wider literature, noting that targeting consumer behaviour alone is unlikely to significantly reduce FLW (Willersinn, *et al.,* 2019), and that increasing all stakeholders' understanding of the significance of FLW was a key factor driving any potential reductions (Bandel, 2021). The requirements for fresh produce (producing and direct sales) are narrow and can fluctuate suddenly e.g. in response to changes in the weather. This is exacerbated by a lack of adequate storage facilities, short windows for shipping certain harvests and little funding for scaling up innovations for repurposing or redistributing surplus food to avoid waste. There are also often hidden costs and logistical challenges for the third sector and those involved in initiatives for reducing and redistributing food waste. More resources and stakeholder support are needed for these initiatives, as well as enhanced shelf life, and better storage and distribution technologies. Food waste from spoiled or damaged foods, or inedible portions of foods, is usually sent to landfill; in the past, it was repurposed as animal feed (Stuart, 2009). Policy-makers and CSO representatives also noted a lack of regulation around repurposing and distribution of excess food, particularly for larger supply chains, and an inflexibility among public procurers, as well as a hesitancy from the government to restrict consumer choice. Conversely, they felt constrained in their ability to repurpose FLW as animal feed, due to legal restrictions enacted in 2001 in response to an outbreak of Foot and Mouth Disease.

5.16 Opportunities for Stakeholder Collaboration to Reduce FLW Across the Food System

Identifying and managing the ultimate responsibility for FLW between multiple stakeholders is difficult. Positive interventions that a siloed-working stakeholder might make to reduce their personal or organisational levels of FLW may inadvertently and unknowingly move the problem to another point in the food system, negating efforts to achieve an overall waste reduction. One example of this is poorly managed stock in a retail organisation. Overstocking followed by extreme reduction in price to the consumer at the end of the product shelf life can cause a shift of food waste to the consumer (Stuart, T., 2009). Therefore focus group participants widely agreed that no single actor could be blamed for food waste or loss. As there are many factors and reasons for waste creation throughout the food system, including differences between food products, it is important to increase cross-system collaboration through improved communication about shared responsibilities (Göbel, C*, et al*., 2015). Thus, more collaborative action is necessary to reduce FLW in the food system for which TCA can be a useful tool to eliminate harmful practices (Aspenson, 2020).

Multiple stakeholders (policy-makers, CSOs, researchers) noted that small-scale innovative efforts, such as direct sales from farmers are useful and effective, but lack the means to scale up (Mert-Cakal, 2020). As such, local collaboration for community initiatives working to decrease FLW and engage directly with consumers has great potential, but are resource-intensive. In part, this is because grassroots organisations that reduce FLW are often unaware of each other. This can lead to some efforts being replicated, while others are not addressed. Various civil society organisations serve as FLW redistribution centres, but these are often disconnected and lack the infrastructure to receive, process, store, and distribute variable quantities and content of FLW. The example was given of organisations being informed by a wholesaler that 500 kg of tomatoes were available for collection by the charity, and if not, they would go to landfill. These are large, awkward, and potentially expensive quantities for small voluntary organisations to manage without infrastructural support.

'That's the only way that we're going to be able to effectively decrease food waste. Working with the grower, seeing what they have and then following that all the way through into retail and into the household.' - (Retailer)

Agro-ecological producers suggest that direct sales and shorter supply chains, as well as using communal storage, can be part of the solution to reduce FLW (SUSTAIN & RSPB, 2021). Yet, they often see such efforts sidelined by a more dominant research and policy focus on lowering production costs and using high-tech solutions to automate farming, neither of which are feasible options for small-scale producers, who tend to waste less food than larger producers. Planning for cropping and transport is highly complex and difficult to manage on a small, local level. Hence the need for collaboration across the system. Furthermore, CSOs highlighted that shortening supply chains requires institutional support from the existing retailers.

The role of managing demand in reducing FLW was also discussed. In its current form, the food system is focused on "meeting demand", a phrase that is vague and ill-defined. Stakeholders agreed that this demand-driven, productionist paradigm needs to be challenged by questioning the vested interests of organisations and businesses that profit from the current system.

5.17 Challenges and Shortcomings of TCA as a tool to reduce FLW

Stakeholders noted that the main challenges of TCA related to the logistics of implementation and adaptation across all food system processes. As an example, one wholesaler described the extreme difficulties of a decade's work on trying to assess and apply carbon footprinting. These sentiments were echoed by an academic researcher who had studied the carbon footprint of tomatoes, and highlighted the inconsistency in values due to producers residing in different countries and using different production systems. Similarly, one retailer was concerned that the complexity of TCA was a shortcoming of the initiative, stating their own lack of capacity and expertise for incorporating TCA:

"I think it is an interesting concept, but I can't see it yet on the retail side, how we would make it work." (Retailer)

This lack of consensus about TCA and what it should account for across the food system was another challenge that stakeholders identified. Many stakeholders saw shortcomings with creating valid and reliable TCA metrics, which could be consistently measured, collated and analysed (Scialabba, 2021). Researchers suggest that TCA metrics and policies need to be co-produced with stakeholders to garner collective agreement. There is concern about how governments and other stakeholders will act upon receiving TCA data, since it does not suggest specific interventions:

"I struggle to see how TCA could be communicated to the people who make decisions about food waste. I don't think it will change behaviours, practices. How we communicate the true cost to decision-makers is too complex." (Researcher)

"It's a tool and method being used by some organisations, for various goals – but its potential depends on who is using it, for what purpose. Some stakeholders will lose out as they are just a part of the process." (Researcher)

One potential unintended outcome of TCA could be public 'naming and shaming' based on the data surrounding FLW. Researchers and wholesalers were sceptical about whether this would positively impact consumer behaviour, as they considered regulation a more effective method for driving decreases in FLW. Agro-ecological producers were especially concerned about whether TCA can successfully address the power imbalances within the food system that underpin wasteful behaviours (Marsden, 2019), or merely reproduce dominant paradigms. Another unintended outcome could be that some stakeholders (particularly international farmers) may lose out if there is an increased emphasis on localising food systems and shortening supply chains due to TCA. Our current system is driven by the lowest cost of production. Cheap food comes at the cost of exploitation of workers, land-use and resources (WRAP, 2020). Furthermore, of the 1/3 of global GHG from the food system, the largest contribution (71%) is from agriculture and land-use (Marsden, 2019). TCA has the potential to capture these external costs. However, farming communities, including internationally, should not be expected

to absorb the cost of negative externalities; it is imperative that international policy is carefully negotiated to protect vulnerable suppliers (Gemmill-Herren, 2021).

In relation to true pricing, there should be a focus on ensuring consumers are not also expected to absorb extra costs associated with TCA. Regardless of feasibility, most stakeholders emphasised that TCA must not be used to change food pricing as this is considered a potential risk to healthy diets, particularly for low-income consumers. Food prices have already been on the rise over the past year (ONS 2021), and the surge in food insecurity caused by the pandemic has only partially receded (Food Foundation, 2021). Those consumers facing food poverty and injustice – local, national and global – risk being negatively impacted by true pricing. However, one researcher suggested that this is not the aim of TCA:

"...this is not supposed to, in principle, trickle down to the consumers [...] I don't think by any means it should really be the price that people start to pay, because I think it will only decrease the interest of people in [making] better food choices." (Researcher)

However, understanding the value of food and its associated costs and externalities (costs, benefits, risks, opportunities) could influence attitudes towards waste throughout the food system by, in part, informing consumers. There have been several examples in recent years displaying responses to 'sin taxes'. In 2015, the UK government implemented a £0.05 charge for plastic bags to reduce single use plastic which caused an overwhelming change to consumer behaviour with an 86% decrease in plastic bag use (Sutherland, 2020). Conversely, consumer buying behaviour did not significantly change immediately after the UK introduced the Soft Drinks Industry Levy (SDIL) in 2016. However, manufacturers diversified the range of low-sugar alternatives, and adjusted the sugar levels to fall below the threshold for the levy which in turn created a consumer shift toward low-sugar and sugar-free alternatives, potentially exposing consumers to less sugars and associated health risks (Scarborough*, et al* 2020) These are examples of very simple taxes or levies associated with one specific externality.

Finally, it was suggested in focus groups that TCA is not actually a *true* account of associated costs. It is difficult or almost impossible to precisely and accurately quantify the many factors TCA claims to address and apply them to a wide range of stakeholders

across the food system. Nonetheless, providing an approximate numerical value for social impacts, global inequalities, nutrition, toxicity, etc., to report on FLW from the food system may be a good starting place to make stakeholders accountable.

5.18 The Benefits of Using TCA for FLW and Opportunities for Stakeholder Collaboration

Given these challenges and limitations, there was widespread agreement in the focus groups that TCA could not reduce FLW alone, but that it could be used to inform further interventions. TCA was perceived as 'one tool in the toolbox' that could help encourage greater understanding and appreciation of food, as well as raise awareness of the various negative impacts of FLW. While various hidden costs are already being reported throughout the supply chain, TCA could provide a more holistic perspective to account for a wider range of impacts. For instance, some retailers measure the financial burden of their waste, and other businesses apply life-cycle assessments and extended input-output analyses to measure some of their externalities (De Menna, 2018). However, all businesses would benefit from having access to more nuanced and accurate data, in particular with regard to social and ecological impacts (Willersinn, 2017) TCA could provide that data, not only for individual stakeholders but at a systemic level by highlighting externalities that are produced and transmitted across the whole supply chain. TCA both requires and encourages stakeholders to adopt a wider system-level perspective and engage in collaboration, first to generate the necessary wealth of data and then to reduce FLW collectively.

Participants suggested that TCA could help inform a more holistic government approach to re-valuing the food system (Dasgupta, 2021). Through its integrated engagement with the economic, social, environmental, and health impacts of FLW (Sandhu, 2021), TCA could encourage waste reduction across government ministries. Additionally, TCA could aid policy-makers in implementing more precise sustainability measures, including sanctioning FLW, subsidising reduction initiatives, creating fairer producer-retailer relations, and rebalancing disposal costs. It could also encourage public-private partnerships and other forms of stakeholder collaboration, especially in the form of waste and surplus distribution, public procurement, planning new waste reduction measures,

and introducing novel food certification. Stakeholders noted the confusion generated by the disparity in clear definitions when describing FLW. Recognised definitions and a common language would support collaborative efforts to reduce FLW.

'I think at policy level [TCA] will help bring different ministries and authorities together around a common shared vision – that we are producing this much waste, let's not point fingers at each other, we are all in this together, we are all responsible.' - (Policy Campaigner)

5.19 Policy Recommendations that Employ TCA Principles to Reduce FLW

Based on current literature and stakeholder input, we make the following policy recommendations. Overall, we advise that the underlying principles of TCA should be used to guide all stakeholders in the food system, as well as policy-makers, to acknowledge and assess the multiple impacts of the food system on society, the environment, and public health. When taken together as a suite of policy changes, our recommendations combine to create a culture shift towards stakeholder cooperation and shared responsibility in reducing FLW, whilst simultaneously ensuring our food system maximises environmental and wider benefits. Diverse metrics assessing the underlying socio-ecological and economic principles of TCA, combined with regulation, incentives, and education, can support efforts to decrease FLW throughout the food system. These recommendations focus on creating culture change for efficient and transparent data reporting, opening opportunities for a collaborative workforce towards significantly reducing FLW and the application of TCA principles throughout the food system.

1. **Ensure supplier-retailer contracts address FLW at all points, and make it mandatory for all stakeholders to measure and state FLW in contracts.**

A significant share of FLW occurs during production, as suppliers are pressured to overproduce in order to guarantee fulfilling their contracts with retailers. To prevent this, contracts need to ensure a level playing field between stakeholders. They should include requirements for suppliers and retailers to measure and limit the FLW created through

their transactions, as well as narrowly limit the option for retailers to opt out of contracts. This would also encourage better communication and collaboration between stakeholders by requiring them to more closely align their supply and demand to each other.

2. **Require transparency in hospitality, supermarkets and local authorities to disclose all FLW and set mandatory reduction targets annually.**

Currently, reporting and publishing of FLW data is completed on a voluntary basis. We propose that this should be mandatory for all stakeholders; comprehensive FLW data is to be reported and published with additional encouragement for full disclosure of non-financial data reporting (NFR). NFR includes environmental and social impact data which is in line with the principles of TCA. The UK government wants to keep "*the UK at the leading edge of international developments in sustainability reporting"* (HM Government. 2018). Mandatory reporting of FLW data could help stakeholders to become aware of their FLW, whilst enabling the identification of parts of the food system that generate a lot of food loss and waste, and increasing the focus on these. We recommend support for those organisations that require it, both financially and by providing the tools to infrom and encourage the value of data reporting for developing, improving and re-risking (HM Government. 2018).

3. **Review current rules and regulations and consider options for repurposing of FLW (e.g. as animal feed).**

Opportunities for a more efficient food system are currently being missed. An example of this is through historic legislation enacted in 2001 in response to the outbreak of Foot and Mouth Disease, which prohibits the recycling of catering waste to pigs. A review of legislation such as this should be undertaken to enable the safe recycling of food waste and reduction of the primary production and importation of feed that has large-scale impacts environmentally.

4. **Support public procurement directly from suppliers: this will decrease FLW, while simultaneously strengthening local economies**

There needs to be more support for public procurement through interventions and innovation to shorten supply chains. We recommend interventions for creating circular, closed-loop networks, incorporating redistribution, reuse, and recycling. Creating a regenerative system will aid in the reduction of FLW throughout the food system, and help to reduce externalities. We recommend that special attention should be paid to using locally based resources and organisations. There should be tighter regulations around food recovery and distribution. There should also be investment into the way food is reused and recycled, improving flexibility, with a focus on the local setting, needs and infrastructure and upscaling to a national level. There should be a focus amongst hospitality stakeholders to encourage consumers to adjust their portion sizes to avoid food waste.

5. **Incentivise suppliers, retailers, and hospitality to use TCA's emphasis on food system externalities (social / economic / environmental): reward with potential lower business rates.**

'Sin Taxes' have a propensity for penalising the consumer, especially affecting the most vulnerable in society if not properly implemented. Instead, we recommend focusing on rewarding stakeholders throughout the food system including suppliers, retailers and hospitality for embedding TCA principles within their business model and practices. A suggested incentive scheme could offer the reward of lower business rates for participants who report TCA data and show clear evidence of incorporating social and environmental metrics into business practice.

6. **Clear definitions of food loss, food waste, surplus, inedible parts and destinations of food loss and waste, and development of government recognised language for system-wide standardisation of data recording**

There is a clear disparity in the use of food-system-associated terminology which creates distortion of data, confusion in protocol, and provides a method for passing FLW to another stakeholder. Clear, government recognised definitions should be established to form a 'common language' for continuity and collective action towards reducing FLW. Having this common language would enable the creation of standardised FLW measurements and the accurate quantification of sustainability data, thus building a foundation for the future widespread implementation of TCA.

5.15 Further Research and Development

Current FLW data predominantly focuses on food waste due to the increased availability of this data. Current food loss data needs to be updated to present a balanced view between food loss and food waste. The recommendations of mandatory measuring and reporting of food loss will support this need for updated data.

There is a need for further development of infrastructure support for FLW distribution hubs. This includes a database and network of relevant schemes and metrics that can be used to generate and encourage TCA principles and practise. Metrics could include, but not be exclusive to carbon footprinting, socio-economic values and animal welfare parameters that could be linked to current animal welfare assurance schemes. Metrics and schemes for sustainable development should be recognised in one place. Research and development to combine these metrics to create a simple, holistic labelling system encompassing the 17 UN SDGs would be beneficial and could also be used to incentivise behavioural change across all stakeholders. Using the SDGs within labelling for food products acts as a standardised key for buyer choice. Additionally it becomes recognised in the public forum for the progression of sustainability both within, and outside the context of food. Foundation Earth are currently trialling environmental rating labelling for food packaging in collaboration with several major UK retail organisations (Foundation Earth, 2021). This type of labelling could provide consumers a method for making environmental and ethical choices. Our recommendations will support these areas through stronger measuring of data, and the defining of FLW.

Further research is required to determine whether food pricing can not only reflect market activity, but whether prices can also reflect the external costs and what

implications these price changes might have on socio-economic groups. Lastly, further investigation into whether healthy food with low environmental costs is more economically viable compared to ultra-processed, 'unhealthy' foods that are bad for the environment when all external costs are accounted for. This could support the introduction of dynamic costs into the food system, however 'unhealthy' would need to be strictly and consistently defined.

5.20 Conclusions

Systemic change is a difficult problem to address. According to the focus groups we conducted, opinion is divided on whether a whole system shake-up is necessary, as opposed to small incremental changes. True Cost Accounting can be perceived, and is described in many formats, ranging from; entirely repurposing the food system and using externalities to inform real-time product pricing (true pricing). Other stakeholders suggested that TCA should only be used as an informative tool without price changes, and small incremental changes should be made to implement TCA principles. After discussing with stakeholders and based on literature, we suggest that TCA should not be disregarded; but to implement TCA may require a simplified supply-system. We have made our recommendations to provide a pathway to a functioning True Cost Accounted, sustainable food system.

TCA's principles and frameworks are useful tools for increasing understanding and engagement with the social, economic and environmental aspects of sustainability, and of how the food system impacts these. By emphasising the diverse, and often overlooked externalities of the food system, TCA can be informative to all stakeholder groups: It should be used to influence and positively change culture through all points of the food system. We propose that collaboration is key to making a systemic impact. These changes should be approached by all organisations within the food system, but also supported by the government in educational support and financial aid, using policy to incorporate the principles of TCA and the UN sustainability goals.

5.21 Future work

The complexity of TCA is limiting and poses a significant challenge for system-wide implementation on a national scale or global scale. However, there are important elements of TCA that could be realistically implemented and effectively used. Large scale companies involved in the food supply chain have opportunities to apply monitoring of important TCA costs associated with their business practices, forming vital environmental data, and informing decision-making to improve practices and reduce externalities including social and environmental costs. Powerful organisations can have significant influence on government policy and the propensity to make significant positive change, aiding climate change mitigation, improving national and global society and contributing to strengthening public health (Batawalage, Williams and Wijegoonewardene, 2023). Some organisations have initiated environmental monitoring, however the societal costs, a key element of TCA is often not accounted for due to the complexity of obtaining the associated data and accurately quantifying it. This should be a focus for future work, through the design of feasible metrics, researching methods for data accessibility and robust formulae for quantification. An important intervention to provide data accessibility could be addressed through the design of a central open-access database that collects socially associated data, this should be a shared global system that allows for collaboration and sharing of information with the aim of transparency and the enrichment of global societies. There are a range of technologies that are rapidly advancing that would be useful to support the implementation of TCA elements. Blockchain tracking would secure data, removing risk for hacking or data adulteration (Dutta et al., 2020). Blockchain uses a decentralised data management, encouraging shared usage, responsibility and collaboration, and negates ownership. Predictive modelling, machine learning and AI could play important roles in forecasting future costs, consolidating complex data, automation to improve accessibility and extracting and interpreting vital elements from the data.

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6 Discussion and Conclusions

20-50% of all fruit and vegetables produced are lost or wasted before reaching the consumer level globally and represent the food items that are most wasted in the UK (Alfie, 2024). This presents an important opportunity for achieving a significant impact to FLW reduction. Among the wider category of fresh fruit and vegetables that are key contributors to human nutrition and represent cultural importance are tomatoes, peppers and lettuce, all highly perishable products (Donhouedé *et al.*, 2023). Several factors that contribute to the waste of these items is the inappropriate handling of postharvest produce which inhibits the maximisation of shelf-life and compromises quality. The inappropriate handling can be attributed to a lack of knowledge of postharvest spoilage processes, and insufficient detection methods (Rajapaksha *et al.*, 2021). Additionally, food items that enter the supply chain fraudulently can heavily contribute to FLW if not effectively identified and dealt with. A wider knowledge on developmental processes that may contribute to FLW later is needed (Lindley, 2021).

The research that forms this thesis used MIR and NIR paired with chemometric analysis to better understand the processes and mechanisms involved in postharvest spoilage and storage conditions, fraudulent food identification and the developmental processes in tomato plants and fruit, in addition to suggestions for a more system-wide holistic approach to standardise practices. Food loss and waste is a significant challenge that must be addressed from all angles (Ma, Yin and Liu, 2017). The work in this thesis focuses on technological methods for tightening the gaps in the food system. The technology involved, although robust, high-throughput and allows for highly specific analysis in some cases, holds its own limitations that may provide barriers to its applied use (Ferrari, Mottola and Quaresima, 2004). There is a wide variety of IR spectrometers available which vary in capabilities. MIR spectrometers are often less portable than NIR spectrometers, but the NIR spectrum is more restrictive on the specificity of information it can obtain. Spectrometers will require software that isn't standardised and may require proficiency for use (Crocombe, 2018). There are financial considerations as well, despite the low-cost use of a spectrometer, the equipment itself can have significant financial outlay making the technology inaccessible to some organisations wishing to use it,

especially small businesses (J. Wang *et al.*, 2022; Kumar and Alamgir, 2024). In addition, the analysis of acquired data requires chemometric analytical skills for accurate outputs and interpretation. For the successful application of these techniques for wide use in the supply chain, there would need to be additional interventions. These might include the use of AI tools that are able to perform the chemometric analysis instead of a human. Furthermore, for uses described in this research, there is a requirement for the building of archival data resources related to spectral signatures related to food products, including post-harvest spoilage phases in commercially popular fruit and vegetables, especially highly perishable items (Kayikci *et al.*, 2022). Additionally, archives of fraudulent ingredients, and signatures from regions that are known fraudsters. This would also require access to shared data repositories to allow these to be useful (Hueni *et al.*, 2011).

IR spectroscopy is widely used to test the quality of fruit in academic work and in some instances in the supply chain. NIR is more commonly used than MIR (Amirvaresi *et al.*, 2021). There are very few studies that incorporate a detailed time series analysis of spectral biochemical processes. Chapter 2 utilised chemometric analytic techniques to visualise spectral features indicative to postharvest spoilage in tomatoes, peppers and lettuces, and the influences from a variety of storage temperatures. Key compounds were found to be impacted by the temperature at which they were stored, this included changes in cellulose, an important polysaccharide in cell structure and key to maintaining structural integrity (Alberts *et al.*, 2002). The loss of integrity reduces the characteristic firm aesthetic influencing consumer purchasing decisions. This plays a significant role in FLW as perceived poor quality results in items not being purchased and potentially wasted at the retail level. Fruit structure also plays an important role in defence against pathogen infection (Nevo *et al.*, 2017), infection presents health risks if the product is consumed, additionally pathogen infection accelerates spoilage processes further reducing shelf life (Akinsemolu and Onyeaka, 2024) and opportunity to be used.

Biochemical and molecular processes in fruit ripening and senescence are well understood, how pre-harvest processes connect with post-harvest processes is less well known (Pott, Vallarino and Osorio, 2020). The changing climate and increasing environmental pressures, in addition to other variables that might include chemical exposure, microbial evolution, changes to biodiversity and the development of new fruit

varieties may all have unknown influences on these biochemical processes in the future (Araya *et al.*, 2021). It is important that we are continuing to broaden our scientific knowledge into these aspects in order to succeed in successful production and reduce food losses and waste. Bio-spectroscopy may be a useful method for providing insights into these important processes with rigorous test approaches.

6.1 Neighbouring time points were isolated and key wavenumbers identified

Analysis of the fruit and vegetables as an overall dataset allowed for the identification of key biochemical changes and differences in storage condition, however lacked the specificity to locate when these changes occurred. Exploring the key biochemical changes between neighbouring time points was useful to understanding this temporal categorisation and was able to identify changes that were not strong enough to be a key variance overall but were present at specific times. This allows for a more nuanced understanding provision of biomarkers.

One of the biggest hurdles that we are faced with, not only for food waste reduction, but the wider climate crisis is societal perception. This is reflected in food system. Market trends and consumer buying habits dictate the system as a whole, which often can become reductive to positive efforts for mitigation of these issues (Shah and Asghar, 2023).

6.2 The Food System Requires Holistic Approaches to Remove Vulnerabilities and Improve Resilience

Optimising the supply chain to facilitate the most efficient and effective utilisation of food products, especially highly perishable goods like fruit and vegetables also remains a complex challenge. This challenge must be overcome to achieve the United Nations target 12.3 of reducing FLW globally by 50% (FAO, 2023). Numerous aspects must be considered and addressed with a holistic approach. The wider supply chain is in need of standardisation in relation to regulatory standards, applied methods conducted by industry actors and the availability and accessibility of modern technology to allow companies to be optimally efficient (Chauhan *et al.*, 2022). Policy recommendations were

made that aim to provide metrics for standardised reporting of impacts associated with food system processes, these encompassed a multifaceted approach that included social, economic and environmental costs. It was found that key stakeholders in the supply chain supported the need for these to be addressed in tandem. This was further supported by evidence that a healthy society, economy and environment are reliant on each other. It was recognised that work needs to be done to simplify the supply chain to strengthen current vulnerabilities and improve resilience against outside influences like geopolitical events, threats to human health like disease epidemics or pandemics like seen in COVID-19, or climate-related impacts that may present challenges to food production (Guo *et al.*, 2024). Food loss and waste (FLW) has significant impacts that effect society, economy and the environment and addressing the issue will have global benefits.

6.3 Aesthetics are an important driver to FLW

Aesthetic characteristics influence consumer purchasing decisions, market trends and standards have cascading effects that are exhibited earlier in the supply chain. Fruit and vegetable products undergo grading which is determined by shape, size, colour and freshness(Akter *et al.*, 2024). There are certain retailers that will only accept produce categorised by high quality grades, although the aim of this is to provide quality products for their customers, and to maintain an aspired reputation, these restrictive practices have knock-on effects and can drive waste in earlier stages in the supply chain (Litt *et al.*, 2011). These decisions can also drive up prices, as producers lose profitability on crop yields, to recoup losses, sale prices may increase which ultimately falls on increased pricing in store (Kopalle *et al.*, 2009). Key aesthetic quality is the colour of fruit, determined by biochemical components forming pigmentation. Pigments were identified in spectral signatures as key changes in post-harvest fruit, these biochemical changes occurred before they visibly presented on the fruit. The visual discolouration appeared around 10 days after detection in some cases. This was also observed in fruit softening, with key wavenumbers attributed to structural components including cell wall compounds that were observed earlier than in visual or textural observations. These serve as important indicators of spoilage initiation and provide a quantifiable window before degradation is relevant to the buyer or consumer. Not only could these serve as biomarkers for the detection of spoilage in individual batches, but may provide a more

dynamic approach to assigning shelf-life of food products (Wen *et al.*, 2022). A significant driver of food waste at the consumer level is the misunderstanding of shelf-life labelling or inaccurate shelf-life assignments (Barone and Aschemann-Witzel, 2022), normally based on standardised time-frames for certain products based on how long they take to present spoilage through texture or visual appearance. These assignments are often flawed as they neglect to consider the variety of factors that contribute to quality.

A wider problem is the perception and association that consumers base food-related decisions on. Aside from the general perception of minor degradation or abnormalities being associated with poor quality or inedible food (Hartmann, Jahnke and Hamm, 2021), there is a lack of understanding of the seriousness of food waste impacts (Richter, 2017). There has been a drive in social awareness around packaging (Brennan *et al.*, 2023), especially plastic, and while this is an important issue, there is a need for a similar movement for social awareness to be driven around food waste. Obstacles to social awareness often arise alongside wider societal issues. The UK has been experiencing substantial financial strain which has affected most of the population. Personal and immediate problems will always be prioritised over wider and long-term issues(Karanikolos *et al.*, 2013). The cost of living crisis will no doubt have had an impact on the progress the UK has made towards environmental repair (Jenkins, 1998), the responsibility is held by organisations and governments with the propensity to make positive social and environmental impact.

Social media has been an important place for raising awareness of environmental issues, and there has been an increase in online movements with a food waste reduction focus. This has led to a rise in companies that have designed their business model around reducing food waste. Companies who ‘save’ wonky food products by redirecting them from the supply chain before disposal (Gollnhofer and Boller, 2020), have then created platforms for these food items to be delivered to customers’ homes. Food items include wonky fruit and veg and coffee and are bought in the form of a regular subscription. Other schemes include free food-sharing apps, and apps for food service vendors to supply mystery bags of food reaching the end of shelf life for a heavily reduced price. These movements are highly beneficial but often are only accessible to certain people who means of travel and can afford monthly subscriptions (Eom, Kim and Sherman, 2018). A movement is needed that will be accessible to everyone, avoids exploitation and provide

a much-needed social awareness for the severity of the problem but also provides the tools for people to become involved.

In conclusion, technological advances and advanced tools like IR spectroscopy has been shown to be an important tool, and accompanied with high accuracy analytical techniques including chemometrics, they can provide a highly beneficial contribution to reducing food loss and waste. It is important that approaches like these are not conceived to be a magic fix and holistic approaches must be employed in all areas in order to achieve the ultimate target of global food security and climate change mitigation. The involvement of government organisations is fundamental to the facilitation of these approaches through subsidisation, policy and education directives. The development of methods that bridge the gap allowing for widespread application of technologies like IR spectroscopy, for example through AI tools, may be achieved with the proper investments in place.

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8. Appendix

Provenance Future Forensics Ltd Stable Isotopes: The Netherlands

Food Forensics Ltd,
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Food Forensics

Certificate of Analysis

Report No :	FFSIRA0923-EU10069	Report Date:	12/09/2023
Customer:	Suncrop, Chilterns Commonside Road, Harlow, CM18 7EZ		
Date Received:	29/08/2023	Sample Type:	Tomato
Analysis Requested:	Origin	Analyte/Test:	$\delta^{13}C_{VPDB}$, $\delta^{15}N_{Air}$, $\delta^{2}H_{VSMOW}$, $\delta^{18}O_{VSMOW}$
Technical Procedure:	TP001	Test Method:	AM06-01 V220121

Sample Information			
Laboratory ID	EU10069	Customer ID	ST2483
Product Description	Conventional Classic Vine Tomatoes		
Supplied by	Suncrop		
Other details on packaging			
BB/UB/Other Date:	N/A	Other Information:	051704 Supplier: Combilo, Schenkeneld De Lier Town: Westland/De Lier Country: Netherlands County: Zuiol Holland Collected By: Martyna Company: Suncrop Raw material ref: CLVT1447 which arrived on 19/08/23 PO669
Barcode:	N/A		
Health Mark:	N/A		
Supplier Code:	N/A		
Lot Number:	N/A		

Results: Origin						
Target Population (X):				**Netherlands**		
ANOVA				**Test 1: DA**		
P($\delta^{13}C$)	**P($\delta^{15}N$)**	**P($\delta^{2}H$)**	**P($\delta^{18}O$)**	**Prob. X (%)**	**Prob. Non X (%)**	**Conclusion**
0.35	**0.78**	**0.69**	**0.78**	**74.0**	**26.0**	**PASS**

Supporting Figures or Interpretation:
N/A

Conclusion
The test sample has been classified as a PASS test for consistency with Netherlands origin.

Prepared By:	MCADuffy	Matt Duffy, SIRA Analyst
Approved By:	ESt	Ethan Strak, Senior SIRA Analyst
Date:	12/09/2023	

Provenance Future Forensics Ltd Stable Isotopes:
The Norfolk

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Food Forensics

Certificate of Analysis

Report No :	FFSIRA0923-EU10070 addendum 1	Report Date:	10/10/2023
Customer:	Suncrop, Chilterns Commonside Road, Harlow, CM18 7EZ		
Date Received:	29/08/2023	Sample Type:	Tomato
Analysis Requested:	Origin	Analyte/Test:	$\delta^{13}C_{VPDB}$, $\delta^{15}N_{Air}$, $\delta^{2}H_{VSMOW}$, $\delta^{18}O_{VSMOW}$
Technical Procedure:	TP001	Test Method:	AM06-01 V220121

Sample Information			
Laboratory ID	EU10070	Customer ID	ST2484
Product Description	Conventional Classic Vine Tomatoes		
Supplied by	Suncrop		
Other details on packaging			
BB/UB/Other Date:	N/A	Other Information:	051705 Supplier: The Green House, Norwich Country: UK County: Norfolk Collected By: Martyna Company: Suncrop Raw material ref: MLV606 which arrived on 21/08/2023 PO669
Barcode:	N/A		
Health Mark:	N/A		
Supplier Code:	N/A		
Lot Number:	N/A		

Results: Origin						
Target Population (X):				**UK**		
ANOVA				**Test 1: DA**		
P($\delta^{13}C$)	**P($\delta^{15}N$)**	**P($\delta^{2}H$)**	**P($\delta^{18}O$)**	**Prob. X (%)**	**Prob. Non X (%)**	**Conclusion**
0.03	**0.99**	**0.48**	**0.09**	**11.1**	**88.9**	**WARNING**

Supporting Figures or Interpretation (Origin):

The multi-isotope discriminant analysis prediction model predicts that there is a 11.1 % probability of this sample originating in the UK.

Conclusion (Origin)

The test sample has been classified as a WARNING test for consistency with UK origin.

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Results: Direct Comparison					
Target Population (X):				Reference samples collected from Greenhouse Grower Norwich	
Test 1: ANOVA				Test 2: PCA	
P($\delta^{13}C$)	P($\delta^{15}N$)	P($\delta^{2}H$)	P($\delta^{18}O$)	Figure 1	Conclusion
0.71	0.09	0.73	0.38	PASS	PASS

Supporting Figures or Interpretation (Direct Comparison):

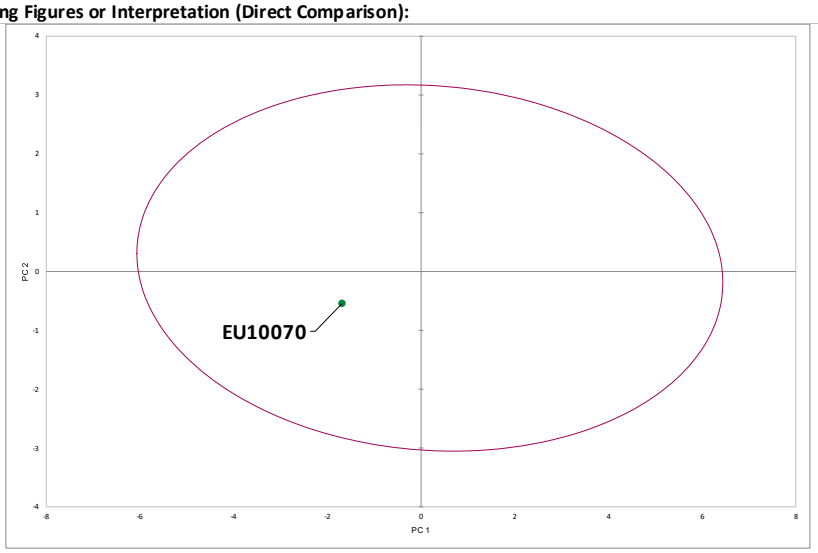

Figure 1: PCA plot showing the tomato reference sample population (red ellipse = 95 % confidence interval) in comparison to the test sample (green point).

The test sample was compared directly to the reference samples that were collected from the same site as stated on the original test sample. There were no significant differences between the test sample and these reference samples for any of the elements measured. Therefore, in the opinion of the analyst, the test sample is consistent with the reference samples collected from the same site.

Conclusion (Direct Comparison)

In the opinion of the analyst, the test sample is consistent with the reference samples collected from the same site.

Prepared By:	ESt	Ethan Strak, Senior SIRA Analyst
Approved By:	M Abigail	Megan Abigail, Senior Laboratory Analyst
Date:	10/10/2023	

Food Forensics Ltd,
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Test Definitions
Origin
PASS: Test 1, probability of target origin is >60%
MONITOR: Test 1, Probability of target origin is between 40% - 60%
WARNING: Test 1, Probability of target origin is <40%

Great Britain, GB: England, Scotland & Wales
United Kingdom, UK: England, Scotland, Wales & Northern Ireland
British Isles, BI: England, Scotland, Wales, Northern Ireland & Republic of Ireland

Direct Comparison
PASS: Test 1, all isotopic compositions are consistent with the Food Forensics reference population at the 95% confidence interval (i.e. P>0.05). Test 2, sample falls within 95% confidence interval of the multi isotope PCA model.
MONITOR: One of the 2 statistical tests has resulted in a WARNING.
WARNING: Two of the statistical tests has resulted in a WARNING.

Addendum to include direct comparison to recently collected reference samples

Provenance Future Forensics Ltd Stable Isotopes:
Cambridgeshire

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Food Forensics

Certificate of Analysis

Report No :	FFSIRA0923-EU10071 addendum 1	Report Date:	10/10/2023
Customer:	Suncrop, Chilterns Commonside Road, Harlow, CM18 7EZ		
Date Received:	29/08/2023	Sample Type:	Tomato
Analysis Requested:	Origin	Analyte/Test:	$\delta^{13}C_{VPDB}$, $\delta^{15}N_{Air}$, $\delta^{2}H_{VSMOW}$, $\delta^{18}O_{VSMOW}$
Technical Procedure:	TP001	Test Method:	AM06-01 V220121

Sample Information			
Laboratory ID	EU10071	Customer ID	ST2485
Product Description	Conventional Classic Vine Tomatoes		
Supplied by	Suncrop		
Other details on packaging			
BB/UB/Other Date:	N/A	Other Information:	051706 Supplier: Comarket - Stubbins Town: Fen Drayton Country: UK County: Cambridgeshire Collected By: Martyna Raw material ref: MBLV367 which arrived on 18/08/2023 PO669
Barcode:	N/A		
Health Mark:	N/A		
Supplier Code:	N/A		
Lot Number:	N/A		

Results: Origin						
Target Population (X):				**UK**		
ANOVA				**Test 1: DA**		
P($\delta^{13}C$)	**P($\delta^{15}N$)**	**P($\delta^{2}H$)**	**P($\delta^{18}O$)**	**Prob. X (%)**	**Prob. Non X (%)**	**Conclusion**
0.15	**0.53**	**0.94**	**0.09**	**17.4**	**82.6**	**WARNING**

Supporting Figures or Interpretation (Origin):

The multi-isotope discriminant analysis prediction model predicts that there is a 17.4 % probability of this sample originating in the UK.

Conclusion (Origin)

The test sample has been classified as a WARNING test for consistency with UK origin.

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Results: Direct Comparison					
Target Population (X):				Reference samples collected from Fen Drayton, Cambridgeshire	
Test 1: ANOVA				Test 2: PCA	
P($\delta^{13}C$)	P($\delta^{15}N$)	P($\delta^{2}H$)	P($\delta^{18}O$)	Figure 1	Conclusion
0.41	0.30	0.07	0.07	PASS	PASS

Supporting Figures or Interpretation (Direct Comparison):

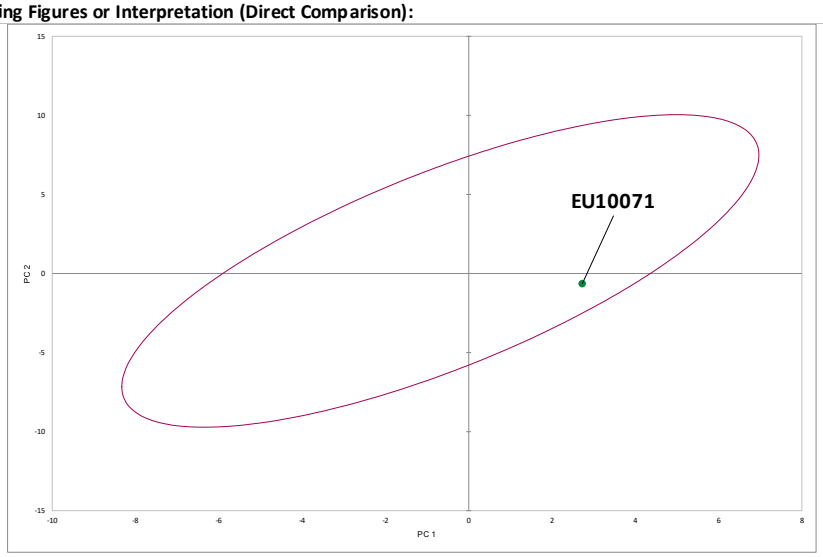

Figure 1: PCA plot showing the tomato reference sample population (red ellipse = 95 % confidence interval) in comparison to the test sample (green point).

The test sample was compared directly to the reference samples that were collected from the same site as stated on the original test sample. There were no significant differences between the test sample and these reference samples for any of the elements measured. Therefore, in the opinion of the analyst, the test sample is consistent with the reference samples collected from the same site.

Conclusion (Direct Comparison)

In the opinion of the analyst, the test sample is consistent with the reference samples collected from the same site.

Prepared By:	ESt	Ethan Strak, Senior SIRA Analyst
Approved By:	M.Abigail.	Megan Abigail, Senior Laboratory Analyst
Date:	10/10/2023	

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Test Definitions
Origin
PASS: Test 1, probability of target origin is >60%
MONITOR: Test 1, Probability of target origin is between 40% - 60%
WARNING: Test 1, Probability of target origin is <40%

Great Britain, GB: England, Scotland & Wales
United Kingdom, UK: England, Scotland, Wales & Northern Ireland
British Isles, BI: England, Scotland, Wales, Northern Ireland & Republic of Ireland

Direct Comparison
PASS: Test 1, all isotopic compositions are consistent with the Food Forensics reference population at the 95% confidence interval (i.e. P>0.05). Test 2, sample falls within 95% confidence interval of the multi isotope PCA model.
MONITOR: One of the 2 statistical tests has resulted in a WARNING.
WARNING: Two of the statistical tests has resulted in a WARNING.

Addendum to include direct comparison to recently collected reference samples

Provenance Future Forensics Ltd Stable Isotopes:
West Sussex

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Food Forensics

Certificate of Analysis

Report No :	FFSIRA0923-EU10072 addendum 1	Report Date:	10/10/2023
Customer:	Suncrop, Chilterns Commonside Road, Harlow, CM18 7EZ		
Date Received:	29/08/2023	Sample Type:	Tomato
Analysis Requested:	Origin	Analyte/Test:	$\delta^{13}C_{VPDB}$, $\delta^{15}N_{Air}$, $\delta^{2}H_{VSMOW}$, $\delta^{18}O_{VSMOW}$
Technical Procedure:	TP001	Test Method:	AM06-01 V220121

Sample Information			
Laboratory ID	EU10072	Customer ID	ST2486
Product Description	Conventional Classic Vine Tomatoes		
Supplied by	Suncrop		
Other details on packaging			
BB/UB/Other Date:	N/A	Other Information:	051709 Supplier: The Green House, Sussex Town: Barnham Country: UK County: West Sussex Collected By: Martyna Taken from arrived samples which arrived on 22/08/2023 PO669
Barcode:	N/A		
Health Mark:	N/A		
Supplier Code:	N/A		
Lot Number:	N/A		

Results: Origin						
Target Population (X):				**UK**		
ANOVA				**Test 1: DA**		
P($\delta^{13}C$)	**P($\delta^{15}N$)**	**P($\delta^{2}H$)**	**P($\delta^{18}O$)**	**Prob. X (%)**	**Prob. Non X (%)**	**Conclusion**
0.22	**0.32**	**0.39**	**0.05**	**31.2**	**68.8**	**WARNING**

Supporting Figures or Interpretation:

The multi-isotope discriminant analysis prediction model predicts that there is a 31.2 % probability of this sample originating in the UK.

Conclusion

The test sample has been classified as a WARNING test for consistency with UK origin.

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Results: Direct Comparison					
Target Population (X):				Reference samples collected from Greenhouse Grower Sussex	
Test 1: ANOVA				Test 2: PCA	
P($\delta^{13}C$)	P($\delta^{15}N$)	P($\delta^{2}H$)	P($\delta^{18}O$)	Figure 1	Conclusion
0.10	0.15	0.68	0.35	PASS	PASS

Supporting Figures or Interpretation (Direct Comparison):

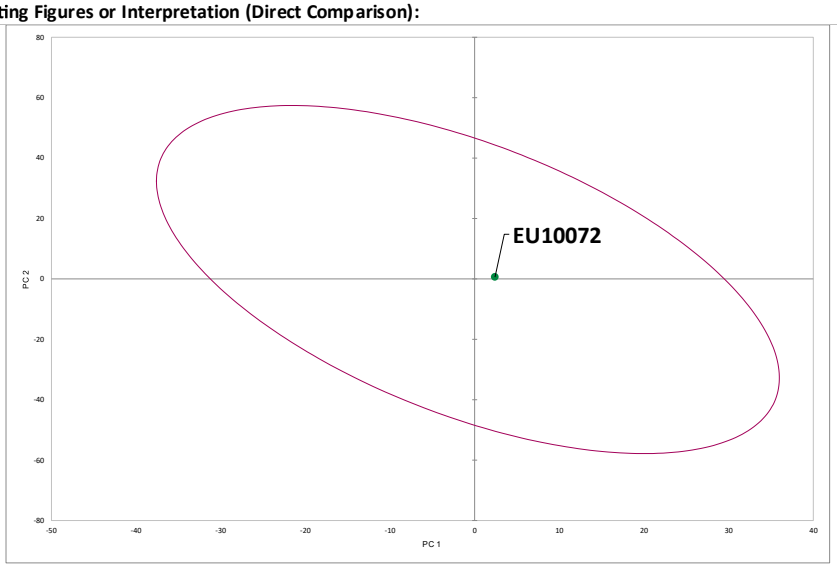

Figure 1: PCA plot showing the tomato reference sample population (red ellipse = 95 % confidence interval) in comparison to the test sample (green point).

The test sample was compared directly to the reference samples that were collected from the same site as stated on the original test sample. There were no significant differences between the test sample and these reference samples for any of the elements measured. Therefore, in the opinion of the analyst, the test sample is consistent with the reference samples collected from the same site.

Conclusion (Direct Comparison)

In the opinion of the analyst, the test sample is consistent with the reference samples collected from the same site.

Prepared By:	ESt	Ethan Strak, Senior SIRA Analyst
Approved By:	M.Abigail	Megan Abigail, Senior Laboratory Analyst
Date:	10/10/2023	

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Test Definitions
Origin
PASS: Test 1, probability of target origin is >60%
MONITOR: Test 1, Probability of target origin is between 40% - 60%
WARNING: Test 1, Probability of target origin is <40%

Great Britain, GB: England, Scotland & Wales
United Kingdom, UK: England, Scotland, Wales & Northern Ireland
British Isles, BI: England, Scotland, Wales, Northern Ireland & Republic of Ireland

Direct Comparison
PASS: Test 1, all isotopic compositions are consistent with the Food Forensics reference population at the 95% confidence interval (i.e. P>0.05). Test 2, sample falls within 95% confidence interval of the multi isotope PCA model.
MONITOR: One of the 2 statistical tests has resulted in a WARNING.
WARNING: Two of the statistical tests has resulted in a WARNING.

Addendum to include direct comparison to recently collected reference samples

Organic Status Future Forensics Ltd Stable Isotopes: Conventional

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Food Forensics

Certificate of Analysis

Report No :	FFSIRA1022-EU10064	Report Date:	13/10/2022
Customer:	Suncrop, Chilterns Commonside Road, Harlow, CM18 7EZ		
Date Received:	29/09/2022	Sample Type:	Tomato
Analysis Requested:	Organic	Analyte/Test:	$\delta^{15}N_{Air}$
Technical Procedure:	TP001	Test Method:	AM06-03

Sample Information			
Laboratory ID	EU10064	Customer ID	ST2214
Product Description	Conventional Vine Cocktail Tomatoes		
Supplied by	Suncrop, Ronald House, Chatters, PE166UP		
Other details on packaging			
BB/UB/Other Date:	N/A	Other Information:	PO No: PO600 SUNCROP Security bag no: 055314 Supplier: Suncrop Growers Origin: UK Grower: Kevin Wolfe Variety: Brioso Sample taken from Block D2 on 21/09/2022
Barcode:	N/A		
Health Mark:	N/A		
Supplier Code:	N/A		
Lot Number:	N/A		

Results: Production system	
Target Population (X):	**Organic**
$\delta^{15}N_{AIR} \pm \sigma$* (‰) (Figure 1)	**Conclusion**
0.56 ± 0.05	**WARNING**

** σ = 1 standard deviation of triplicate measurement. Expanded uncertainty of measurement (U) for $\delta^{15}N_{AIR}$ = ± 1.67‰*

Supporting Figures or Interpretation:

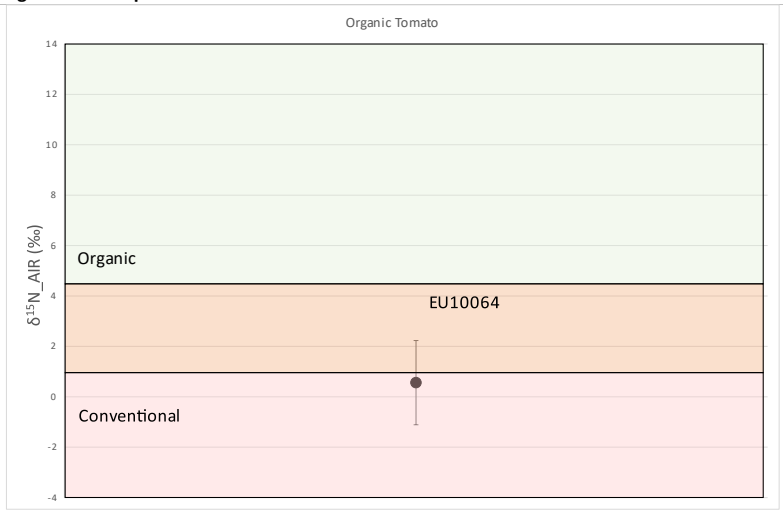

Figure 1: The nitrogen isotopic composition of the test sample (blue point). Error bars represent the expanded uncertainty of measurement. The green region represents the range of nitrogen isotopic composition for organic tomatoes previously observed in the Food Forensics database.

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Supporting Figures or Interpretation:
The test sample has a nitrogen isotopic that falls within the range observed for conventional produce. Therefore, the test sample has been classified as a WARNING test for consistency with organic production system.

Conclusion
The test sample has been classified as a WARNING test for consistency with organic production system.

Prepared By:	MCADuffy	Matt Duffy, SIRA Analyst
Approved By:	M.Abigail	Megan Abigail, Senior Laboratory Analyst
Date:	13/10/2022	

Test Definitions
Organic Tomato
PASS: δ15NAIR(‰) ≥ +4.48‰
MONITOR: +1.00 ‰≤ δ15NAIR(‰) < +4.48 ‰
WARNING: δ15NAIR(‰) < +1.00‰

Organic Status Future Forensics Ltd Stable Isotopes: Organic

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Food Forensics

Certificate of Analysis

Report No :	FFSIRA1022-EU10064	Report Date:	13/10/2022
Customer:	Suncrop, Chilterns Commonside Road, Harlow, CM18 7EZ		
Date Received:	29/09/2022	Sample Type:	Tomato
Analysis Requested:	Organic	Analyte/Test:	$\delta^{15}N_{Air}$
Technical Procedure:	TP001	Test Method:	AM06-03

Sample Information			
Laboratory ID	EU10064	Customer ID	ST2214
Product Description	Conventional Vine Cocktail Tomatoes		
Supplied by	Suncrop, Ronald House, Chatters, PE166UP		
Other details on packaging			
BB/UB/Other Date:	N/A	Other Information:	PO No: PO600 SUNCROP Security bag no: 055314 Supplier: Suncrop Growers Origin: UK Grower: Kevin Wolfe Variety: Brioso Sample taken from Block D2 on 21/09/2022
Barcode:	N/A		
Health Mark:	N/A		
Supplier Code:	N/A		
Lot Number:	N/A		

Results: Production system	
Target Population (X):	**Organic**
$\delta^{15}N_{AIR} \pm \sigma$* (‰) (Figure 1)	**Conclusion**
0.56 ± 0.05	**WARNING**

** σ = 1 standard deviation of triplicate measurement. Expanded uncertainty of measurement (U) for $\delta^{15}N_{AIR}$ = ± 1.67‰*

Supporting Figures or Interpretation:

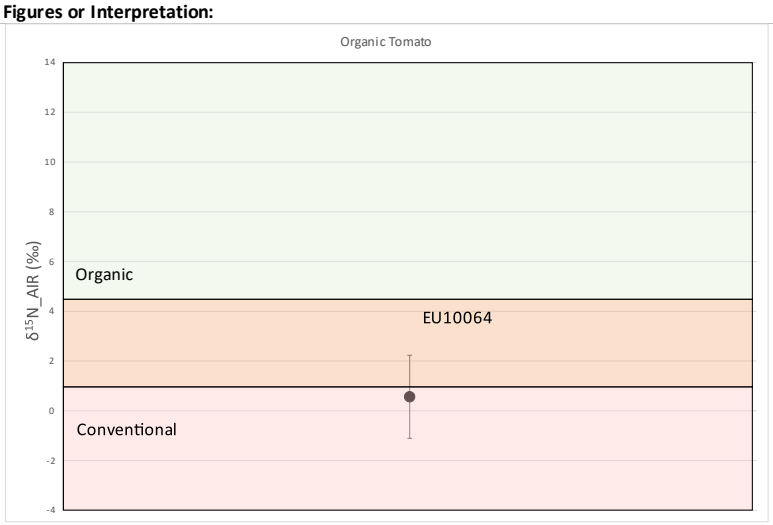

Figure 1: The nitrogen isotopic composition of the test sample (blue point). Error bars represent the expanded uncertainty of measurement. The green region represents the range of nitrogen isotopic composition for organic tomatoes previously observed in the Food Forensics database.

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Food Forensics

Supporting Figures or Interpretation:
The test sample has a nitrogen isotopic that falls within the range observed for conventional produce. Therefore, the test sample has been classified as a WARNING test for consistency with organic production system.

Conclusion
The test sample has been classified as a WARNING test for consistency with organic production system.

Prepared By:	MCADuffy	Matt Duffy, SIRA Analyst
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Date:	13/10/2022	

Test Definitions
Organic Tomato
PASS: δ15NAIR(‰) ≥ +4.48‰
MONITOR: +1.00 ‰≤ δ15NAIR(‰) < +4.48 ‰
WARNING: δ15NAIR(‰) < +1.00‰