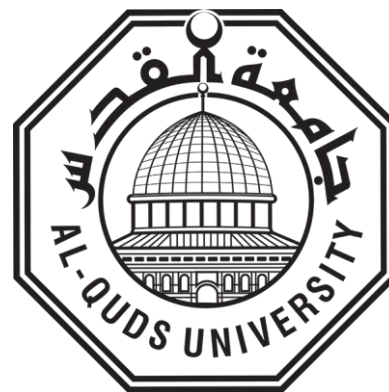


**Deanship of Graduate Studies
Al-Quds University**



Quantitative Analysis of Orange Juice by ATR-FTIR

Ayda Ayman Ahmad Abdallah

M.Sc. Thesis

Jerusalem – Palestine

2026/ 1447 هـ

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**Prepared By:
Ayda Ayman Ahmad Abdallah**

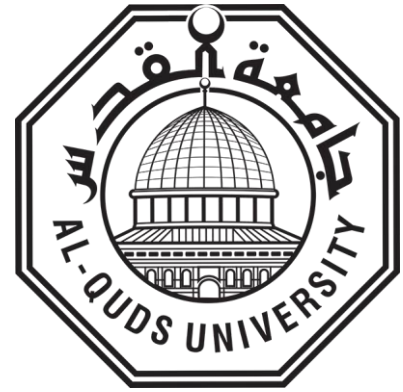
B.Sc. Industrial Chemistry, Bethlehem University, Bethlehem, Palestine

**Supervisor: Prof. Dr. Mutaz Qutob
Co-supervisor: Dr. Mahmoud Al-Khatib**

**A thesis submitted in Partial fulfillment of requirements for the degree of
Master of Applied Industrial Technology Program/ Deanship of
Graduate Studies/ Al-Quds University**

2026/1447 ♡

Al-Quds University
Deanship of Graduate Studies
Applied Industrial Technology Program



Thesis Approval

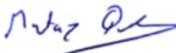



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Prepared By: Ayda Ayman Ahmad Abdallah
Registration No.: 22312035

Supervisor: Prof. Dr. Mutaz Qutob
Co-supervisor: Dr. Mahmoud Al-Khatib

Master Thesis submitted and accepted. Date: 17-1-2026

The names and signatures of the examining committee are as follows:

1. Prof. Dr. Mutaz Qutob, Supervisor, Signature: 
2. Dr. Mahmoud Al-Khatib, Co-Supervisor, Signature: 
3. Prof. Dr. Fuad Alrimawi, Internal examiner, Signature: 
4. Dr. Saleh Sawalha, External examiner, Signature: 


Jerusalem – Palestine

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Declaration

I certify that this thesis submitted for the degree of master in Applied and Industrial Technology Program, is the result of my own research, except where otherwise acknowledged, and that this thesis (or any part of the same material) has not been submitted for a higher degree to any other university or institution.

Ayda Ayman Ahmad Abdallah

Signed: 

Date: 17-1-2026

Acknowledgement

I want to sincerely thank Prof. Dr. Mutaz Qutob and Dr. Mahmoud Alkhatib, my supervisors, for their constant direction, constructive feedback, and continuous encouragement during this project. Their knowledge and support have been important for my academic and personal development. My family, whose love, tolerance, and unwavering support have been the cornerstone of my path, has my sincere gratitude. Through each challenge, their faith in me has inspired and supported me. I also want to express my gratitude to my friends, particularly Nareman Khallaf and Haneen Mubarak, for their support, understanding, and company. This trip was more pleasurable and meaningful because of them. Lastly, I would want to express my gratitude to Al-Quds University for providing the tools required to finish this job as well as a stimulating academic atmosphere.

Abstract

One way to adulterate orange juice is to dilute it with water and add sugars, acids, colorants, and flavor enhancers. These adulterants can cause an important decrease in the quality of the food and present a number of health hazards, particularly those associated with excessive sugar consumption. Therefore, it is crucial to assess the purity level of orange juice in commercial orange juice-based beverages utilizing a straightforward, quick, easy, cheap, safe, precise, and exact method that doesn't need sample preparation or chemometrics (multivariate statistical methods). The aim of this study is to quantify orange juice in drinks using attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy based on the simultaneous measurement of citric acid and sugar concentrations. It was discovered that the following equations, with an approximate error of 5%, may be used to determine the percentage of pure orange juice in commercial orange juice-based drinks; $Y = 0.0027x + 0.1734$, $R^2 = 0.9914$ where Y is the ratio of absorbance at 1064 cm^{-1} due to total sugar content divided by absorbance at 1635.9 cm^{-1} due to water. And the equation $Y = 0.0004x + 0.25$, $R^2 = 0.994$ where Y is the ratio of absorbance at 1177.7 cm^{-1} due to citric acid concentration divided by absorbance at 1635.9 cm^{-1} due to water.

Key words: Pure orange juice; adulteration; wavenumber; absorbance; ATR-FTIR.

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Chapter one:

Introduction

1.1. Background

Orange juice is commonly consumed because of its good taste and nutritional benefits. It supplies the body with important nutrients, including carbohydrates, proteins, fats, vitamins, and minerals. Vitamin C, also known as ascorbic acid, is one of the main vitamins present in orange juice. It plays an important role as an antioxidant by helping protect the immune system from oxidative stress through limiting the activity of pro-oxidant enzymes, reactive oxygen species, and metal ion catalysts (Aykas & Rodriguez-Saona, 2024). Since the human body is unable to produce vitamin C on its own, it must be obtained from food sources to prevent deficiency diseases such as scurvy. Oranges are considered one of the richest natural sources of this essential vitamin (Sánchez-Moreno et al., 2003). Additionally, orange fruits contain bioactive substances with anti-inflammatory and cardioprotective properties, such as flavonoids and carotenoids.

Despite its health properties, the nutritional composition of orange juice can differ due to factors such as maturity and storage conditions. It can affect nutrient, sugar compositions, taste, flavor, and quality.

Juice product adulteration for economic gain is a common activity that has been a significant economic issue for ages, and considerable economic challenges within the global food industry until now, by adding water, sugars, mixing with other processed juice fruit juices, the addition of colorants, organic acids, and amino acids. that causes a lower juice value. (Esteki et al., 2019). Such as blending orange juice with grapefruit juice is one way to indulge in adulteration, which is one of the most common food commodities (Varnasseri et al., 2022).

The term 100% natural, not from concentrate (NFC) describes freshly extracted fruit juices that are obtained directly from the edible portion of the fruit without adding water, sugars, or any other substances (Shen et al., 2016). These juices are valued for their ability to provide essential nutrients, including vitamins and dietary fiber (Ma et al., 2025; Shokri et al., 2024).

Oranges are regarded as one of the most significant citrus fruits due to their high nutritional importance and economic value. In recent years, various analytical techniques have been applied to detect different forms of fruit juice adulteration (Cuevas et al., 2017).

When vitamin C is intentionally added to fresh juice (FJ), laboratory testing is required to confirm that the actual nutritional content meets or exceeds the value declared on the product label. In contrast, if vitamin C is naturally present in the fresh juice, its measured concentration should be at least 80% of the labeled amount. Under proper manufacturing conditions, regulatory authorities such as the Food Drug Administration generally accept reasonable variations in vitamin C and total sugar levels. Nevertheless, the total sugar content of a fresh juice product must not be more than 20% higher than the value stated on the label (Aykas & Rodriguez-Saona, 2024).

For Quality Control and the identification of adulteration in juice products, juice composition evaluation is pivotal. Although they provide excellent accuracy, traditional analytical techniques including titrimetric and chromatographic procedures are sometimes time-consuming, reagent-intensive, and inappropriate for quick screening.

This study detected the orange juice by using ATR-FTIR for a study on both macronutrients and micronutrients, and the types of sugars in the orange juice, also to evaluate the nutritional quality of fresh versus commercial orange juice, and to evaluate the potential health consequences of regular consumption. This study will analyze the ability of ATR-FTIR to detect adulteration for quality control. The findings are expected to contribute to a better understanding of orange juice composition and adulteration, to support nutritional value and safety.

1.2.Problem Statement

Fresh juice is a natural and nutritious drink made from natural fruits or vegetables. contains important vitamins, minerals, and antioxidants to keep the body healthy. Orange juice is one of these important healthy juices. It has natural sugars, organic acids, and vitamin C content, but these components can lose their quality depending on fruit maturity, storage conditions, and time.

There is limited public awareness of its exact nutritional composition and its potential impact on health. Additionally, the high sugar content in orange juice raises concerns about its role in diets, particularly for individuals with conditions such as diabetes or obesity.

High-performance liquid chromatography (HPLC), gas chromatography-mass spectrometry (GC-MS), and ion chromatography are some of the conventional techniques used to assess the quality of fresh juices. These techniques are accurate but slow, requiring large equipment and time-consuming sample preparations, making them unsuitable for rapid on-site detection (Shen et al., 2016).

Therefore, there is a need for a rapid, reliable, and accurate method capable of quantifying key chemical constituents in fresh orange juice for adulteration detection, such as ATR-FTIR

spectroscopy. This study aims to analyze the nutritional profile of orange juice and evaluate its implications for dietary recommendations.

1.3. Research Objectives

- To compare the types of sugar in orange juice.
- To compare between processing methods of fresh juice and commercial orange juice (not natural) and how they affect the nutritional quality of orange juice.

1.4. Research Questions

- What are the types of sugars in orange juice?
- What are the possible health benefits and potential risks of regular orange juice consumption?
- How does the processing method (from fresh juice and commercial (non-natural)) affect the nutritional composition of orange juice?
- What macronutrients (fats, proteins, and carbohydrates) and micronutrients (vitamins and minerals) are present in orange juice?
- How do the types and levels of sugars differ in orange juice?
- How to detect or prevent the adulteration of orange juice?

1.5. Hypothesis

Excessive consumption of orange juice, despite its rich vitamin C and potassium source, may lead to excessive calorie intake because of its naturally high sugar levels, which reduces its nutritional benefits.

Chapter two:

Literature Review

2.1.Fruit juice

Fresh juice (FJ) is the natural liquid extracted from ripe fruits by hand, without heating or adding solvents (Aykas & Rodriguez-Saona, 2024). The goal of FJ producers is to enhance the taste and diversity of FJs while also developing new products and packaging. Beyond only one source of FJs, a multitude of unique juice blends have surfaced as a result of the juice industry's advances (Aykas & Rodriguez-Saona, 2024). Fruit juices are typically not marketed straight; instead, they are diluted with water and/or sweetened with sugar or another substance to lessen sourness and/or achieve the desired consistency for easier juice drinking (Aykas & Rodriguez-Saona, 2024).

Excessive consumption of sugar-sweetened beverages (SSBs), including fruit juices, has been linked to various health issues such as weight gain in both children and adults, obesity, diabetes, cardiovascular diseases, and fatty liver syndrome (Malik et al., 2010). While high fructose corn syrup (HFCS) is considered the main contributor to these risks, replacing it with cane sugar or crystalline fructose does not eliminate concerns, as their high fructose and overall sugar content can still have negative effects (Melanson et al., 2008). High fructose intake has been associated with complications including insulin resistance, kidney stones, and an increased likelihood of obesity, diabetes, cardiovascular problems, and liver triglyceride accumulation (Aykas & Rodriguez-Saona, 2024).

The FDA checks that labeling rules are followed by setting nutrient standards and testing food products randomly. If vitamin C is added to a fresh juice, the product must provide at least the full amount listed on the label.

2.2. Adulteration of orange juice

Orange juice is a widely consumed and relatively expensive beverage. It is considered the most popular fruit juice worldwide due to its appealing taste and high nutritional value. Carbohydrates are the main macronutrients, mainly in the form of natural sugars such as glucose, fructose, and sucrose, which provide quick energy. Proteins and fats are present in smaller amounts but still contribute to flavor and the stability of bioactive compounds (Wang et al., 2012). This composition makes orange juice an excellent model for studying the balance between macronutrients and bioactive compounds in natural beverages.

The sugar naturally in orange juice affects both flavor and metabolic responses. These sugars, fructose, glucose, and sucrose, are the main sugars, and their relative ratios can change with fruit ripeness and processing methods. High levels of fructose sugar cause metabolic inferences, such as insulin resistance, if consumed in excess (Z. Li et al., 2025).

The nutritional value and quality of fresh orange juice are affected by processing techniques. Freshly squeezed juice generally keeps higher levels of vitamin C, flavonoids, and volatile compounds that contribute to aroma and flavor. Also, dilution of water storage may lead to changes in sugar content and minor nutrient losses. Some Comparative studies reveal that fresh juice provides higher antioxidant activity and better retention of bioactive compounds than commercially processed juice. (Roy et al., 2020).

Since orange juice is typically marketed in concentrate form, it is susceptible to adulteration by being substituted with other fruit liquids or additional sweeteners. With a 4% frequency, orange juice is frequently mentioned as one of the food categories with the most recorded occurrences of food fraud. These types of adulteration may have harmful effects on health, such as when orange juice is partially substituted with less expensive grapefruit juice, which can lead to harmful and dangerous pharmacological interactions. (Momtaz et al., 2023). Naringin, a common flavonoid glycoside found in grapefruit juice, is converted into naringenin in the human body. This conversion can influence the clinical regulation of drug transport, affect the bioavailability of certain medications and potentially alter their effectiveness (Ellis et al., 2016). In other words, drinking grapefruit juice could change how some medications work, which is important for patient safety. It was believed that the orange juice business alone in the US and Europe was worth over £4 billion (Róžańska et al., 2018). As a result, having suitable analytical methods for the quantitative examination of the main ingredients in orange juices becomes more and more crucial (Lanza & Li, 1984). Fruit juices that have lost their natural nutrients and fiber mainly serve as concentrated sources of sugar, lacking most of the components necessary for supporting digestion and metabolism. These juices typically contain more sugar than whole fruits, which can lead to a faster increase in blood glucose levels. It is also important to note that many commercial fruit juices include added sugars and only a small portion of actual fresh juice. Therefore, these liquids cause the body to consume a lot of calories without supplying any nutrients and vitamins (Rasekh & Karami, 2021). To differentiate between fresh and adulterated fruit juices, a range of traditional sensory assessments and advanced chromatographic methods are commonly used. These include high-performance liquid chromatography (HPLC), gas chromatography-mass

spectrometry (GC-MS), and ion chromatography (Shen et al., 2016). In my experience, combining sensory evaluation with these analytical techniques provides a more reliable assessment of juice quality. These methods require time-consuming sample preparations and large equipment, making them unsuitable for quick on-site detection. In contrast, there are some appealing aspects of Raman spectroscopy: it generates spectra rich in chemical information, is non-destructive, requires little to no sample preparation, and is water insensitive, allowing for direct measurement of the juice (Varnasseri et al., 2022). Juices that belong to a certain chemical class (such as sugars, flavonoids, organic acids, etc.) may have their chemical compositions identified and compared. Recently, electronic nose (E-nose) and Fourier transform infrared (FTIR) spectroscopy techniques have emerged as alternatives to traditional wet chemistry methods in the food and agricultural sectors, thanks to their low cost, rapid application, and non-destructive nature. FTIR, particularly using attenuated total reflectance (ATR), provides excellent opportunities for analyzing both liquid and solid samples. This well-established analytical method investigates the vibrational frequencies of chemical bonds in functional groups such as C-C, C-H, O-H, C=O, and N-H when absorbing light in the mid-infrared range ($400\text{--}4000\text{ cm}^{-1}$). Orange, melons, peaches, and other fruit juices are currently being analyzed using E-nose and IR in a number of studies for quality control, fresh and shelf-life assessment, process monitoring, and authenticity evaluation (Shen et al., 2016).

Near-infrared (near-IR) spectroscopy has proven to be a rapid and reliable method for a variety of analytical applications. It has also become a viable alternative to traditional wet chemistry techniques for analyzing and monitoring the quality of food and agricultural products. For example, Giangiacoimo et al. (1981) applied near-IR spectroscopy to identify specific sugars in dry fruit model systems. In practice, near-IR allows for quick assessments of sugar content without the need for extensive chemical preparation, which can save both time and resources. Fruit juice was analyzed using near-IR transmittance by Lanza and Li (1984); however, they only discovered total sugars (Lanza & Li, 1984). This study examines the effectiveness of near-IR spectroscopy in identifying specific sugars and acids. To enhance the method's sensitivity and accuracy, the procedure described by Meurens et al. (1982, 1990) for analyzing aqueous solutions can be applied, which involves placing the liquid sample on a fiberglass substrate and removing water to obtain a dry extract. Previous research has also utilized near-IR reflection of dry extracts on fiberglass filters to analyze artificial sugar solutions as well as selected fruit juice samples (Lanza & Li, 1984; Ravera et al., 2018). Experts in several sectors frequently use scent to assess quality. This approach has a number of disadvantages, including inaccurate olfactory matching, time requirements, uncertain responses from individuals, experts' subjective reactions to scents, and the inability to use this method to assess hazardous substances, in addition to being costly for the industries. The electronic nose is a recent and promising tool for evaluating food quality. Modeled after the human sense of smell, it has proven effective in assessing the freshness and composition of food products. The system comprises a sensor array, a signal processing unit, and a pattern recognition module. When the sensors detect odors such as high concentrations of volatile compounds in a sample's headspace, they generate outputs that represent a "fingerprint" of the sample's chemical composition. These fingerprints can then

be analyzed using appropriate algorithms to extract useful information. Thanks to its affordability, high sensitivity, and ease of use, the electronic nose has become a widely accepted, automated, non-destructive technology. Among its many applications, it has gained particular attention in quality control within the juice industry. For instance, this technology has been effective in classifying and forecasting various items, including orange juice. Fruit quality may be mostly determined by its morphological characteristics (color, firmness, and texture) and flavor (taste and fragrance). However, it is challenging to assess the quality when fruits are processed to form juice. For instance, it might be challenging to determine whether or not a bottle of juice is prepared from fresh fruit (Rasekh & Karami, 2021).

Many studies included the analysis of orange juice and its various components, whether these components are essential or rare, using different devices, including Raman, IR spectroscopy, and an electronic nose. In this review, I will discuss some of these studies.

The study aimed to test how E-nose and FTIR can differentiate fresh orange juice from samples mixed with 10–30% concentrated juice.

Three brands of 100% concentrated orange juice (Weiquan, Dahu, and Huiyuan) and one brand of freshly squeezed orange juice (Lingdu Guo fang) were sampled. A total of 54 adulterated samples (three levels \times six replicates \times three brands) and 18 control samples (six lots \times three repetitions) were collected for analysis. Before being blended, all juices were filtered through four layers of medical gauze. The samples were then shaken for half an hour on a shaking table and kept in a refrigerator between 0 and 4 degrees Celsius until analysis. Samples containing 0, 10, 20, and 30% (by volume) of adulteration were created (Shen et al., 2016).

A commercial FTIR spectrometer was used to obtain the samples' ATR-FTIR spectra.

A volume of 0.5 ml of juice was immediately placed on the ATR surface at a controlled room temperature of 20°C and scanned in the 800–4000 cm^{-1} range. Each sample was scanned three times, producing 32 scans at a resolution of 4 cm^{-1} . Before analyzing each replicate, a reference spectrum of air was recorded, and ultrapure water was used as a reference sample. After each measurement, the ATR crystal was rinsed with deionized water and gently dried with soft tissue to prevent cross-contamination (Shen et al., 2016).

Figure 1 presents the ATR-FTIR spectra of juice samples with varying levels of adulteration. The spectra are dominated by absorptions from sugars and water. For reference, the spectrum of ultrapure water was also recorded. The primary absorptions at 3200–3400 cm^{-1} and 1640 cm^{-1} are mainly due to the O-H vibrations in water. A notable difference between orange juice and ultrapure water appears in the 1500–950 cm^{-1} range, where strong bands from organic acids and sugars are observed. Specifically, the 1500–1000 cm^{-1} bands are primarily associated with $-\text{CH}_2$ deformations and the angular deformations of C–C–H and H–C–O groups, while the 1200–950 cm^{-1} region corresponds to the stretching vibrations of C–C and C–O bonds. Nevertheless, there were no visible distinctions between the four spectra upon eye check, and they were heavily overlapped. It was concluded that there was little difference in the chemical makeup of genuine and tampered samples.

Following careful analysis, minor variations between samples from various groups were found to exist in the 1200–950 cm^{-1} range. As the degrees of adulteration increased, the absorbance typically reduced, this might be used as a basis for discriminating using ATR-FTIR spectroscopy (Shen et al., 2016).

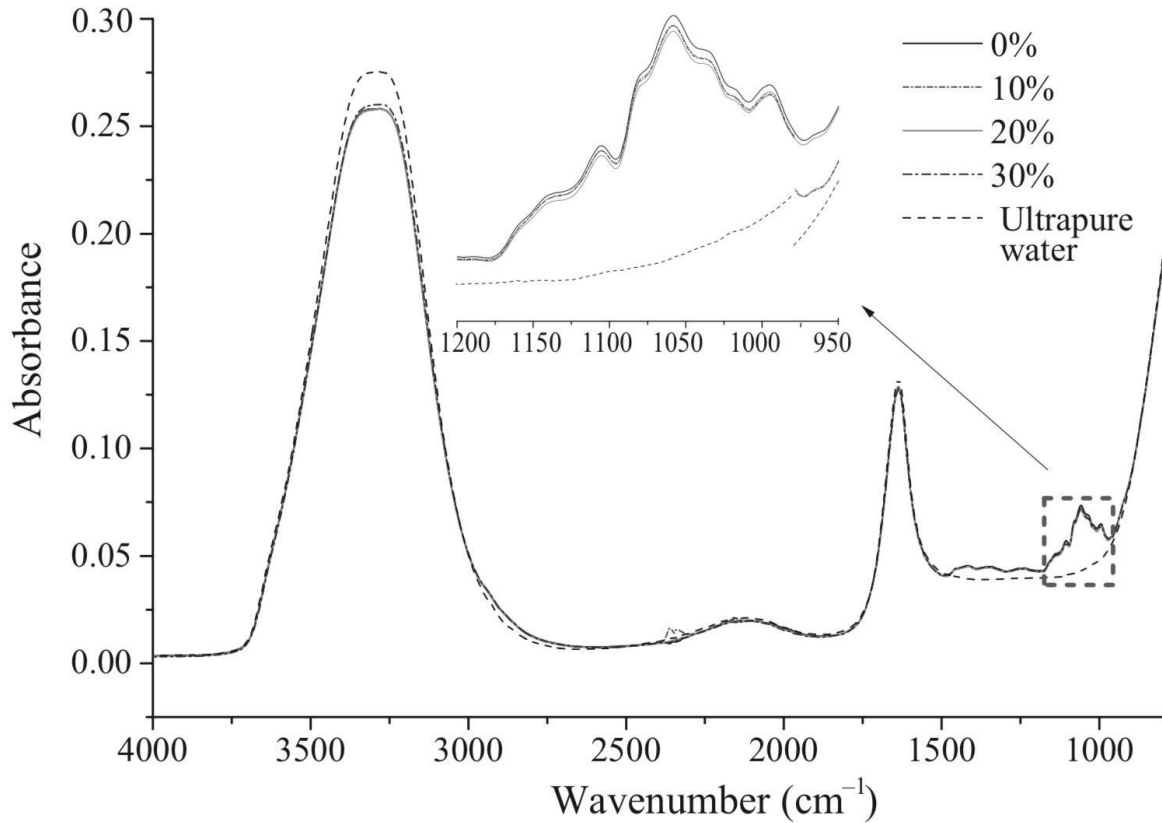


Figure 2.1 Spectra of samples with varying degrees of adulteration using attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) as described by Shen et al. (2016).

The aim of the second study was to simultaneously predict several quality parameters of fresh juices, including soluble solids, sucrose, glucose, fructose, total sugars, titratable acidity, citric acid, and ascorbic acid, using a portable FT-IR sensor that can be deployed in the field without any sample preparation (Aykas & Rodriguez-Saona, 2024).

A total of 68 fresh juice samples were analyzed in this study, including 28 single-fruit varieties such as apple, orange, lemon, grapefruit, pomegranate, and cranberry, and 40 mixed fruit juices. The samples were purchased from grocery stores in Columbus, Ohio, USA. Both spectral measurements and acid analyses (ascorbic and citric acids) were performed on the same day as purchase to minimize changes in the spectra and prevent loss of vitamin C. All samples were stored at 4°C to maintain their composition while subsequent analyses of soluble solids, sugars, and titratable acidity were conducted within two days of collection (Shen et al., 2016).

The sugar content, including fructose, glucose, and sucrose, was analyzed using high-performance liquid chromatography (HPLC). Prior to analysis, all juice samples were filtered. Ascorbic acid and citric acid levels were also measured using an Agilent HPLC system.

The stability of vitamin C during extraction and storage in the autosampler was improved by using a reducing agent. Ascorbic and citric acids were identified by comparing the retention times of their peaks with those of pure standards. Additionally, the spectra of the fresh juice samples were recorded using a portable FT-IR spectrometer (Shen et al., 2016).

Table 2.1. Results of reference analysis for the primary fruit juice quality indicators (Shen et al., 2016).

	Soluble solid (°Brix)	Total sugar (g/100g)	Titrateable acidity (mg/100g)	Citric acid (mg/100g)	Ascorbic acid (mg/100g)
Range	3.78-16.03	60.8-153.5	129.1-1139.1	18.6-1114.0	0.70-54.10
Mean ± SD	11.58±2.25	105.4±22.2	559.5±230.5	519.2±274.9	23.52±15.53

HPLC analysis revealed minor differences between the measured total sugar content and the amounts reported on commercial juice labels.

Fourteen (21%) of the 68 samples that were analyzed didn't match the reports of total sugar content. These non-compliant samples had a total sugar content that was more than 20% different from the amounts listed on the label. Two of the fourteen samples had lower sugar contents (<20%) than reported, whereas twelve of the fourteen samples had greater sugar contents (>20%). Additionally, we found variations in the FJs' ascorbic acid levels. In particular, 25 (37%) of the 68 samples that were examined did not match the nutritional fact label. Ten of them contained more ascorbic acid than what was listed on the label, while fifteen had lower ascorbic acid levels (Varnasseri et al., 2022).

The IR models and the key spectral bands in this region are shown in Figure 2a and 2b. The fingerprint region's most prominent bands were linked to C-C-H, C-O-H, and O-C-H vibrations (1470–1150 cm⁻¹), C-O and C-C stretching modes (1150–900 cm⁻¹), and O-H vibrations (1020–1060 cm⁻¹). Interestingly, as illustrated in Figure 2c, several fruit juice varieties exhibited distinct characteristics within this fingerprint region (Aykas & Rodriguez-Saona, 2024).

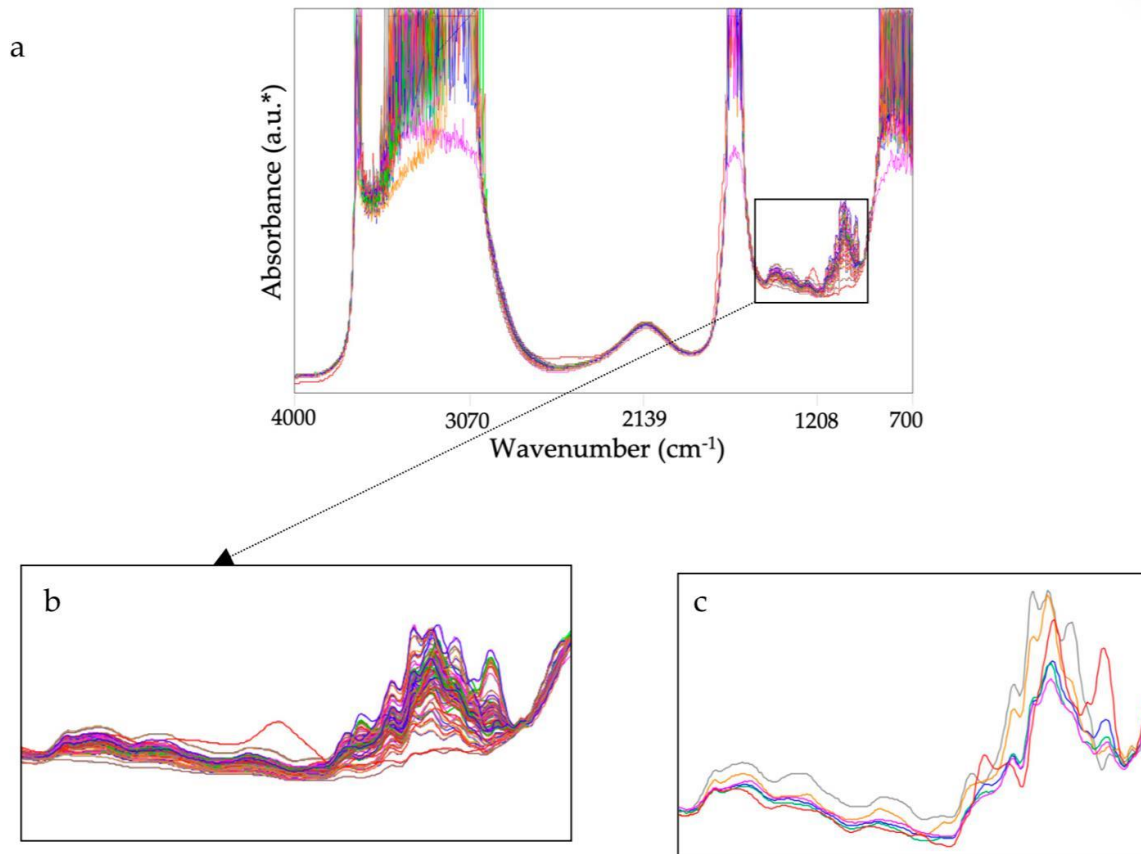


Figure 2.2

Illustrates: (a) representative raw mid-infrared spectra of fruit juice samples collected using a portable FT-IR sensor over the 4000–700 cm^{-1} range; (b) the fingerprint region of the spectra (1550–900 cm^{-1}); and (c) selected spectra in the fingerprint region corresponding to orange juice (blue), grapefruit juice (pink), pomegranate juice (grey), apple juice (orange), lemonade (red), and cranberry juice (green), presented in arbitrary units (a.u.*) (Aykas & Rodriguez-Saona, 2024).

The third goal is to measure fresh orange juices that have been contaminated with different amounts of grapefruit juice. Five distinct sources designated A, B, C, D, and E provided orange and grapefruit fruits. These sources are local businesses that are popular with the community (Varnasseri et al., 2022).

All multivariate studies were carried out in the region of 480 to 1200 cm^{-1} since it appears to contain the juices' most important Raman signal. Figure 3 presents the Raman spectra of pure orange and grapefruit juices. In this study, a total of 286 orange juice samples and 38 grapefruit juice samples collected from Florida, California, New Jersey, and Texas were analyzed. The results showed that although grapefruit juice had an average ratio of 1: 1: 1, orange juice had an average relative ratio of 1: 1: 2 for glucose, fructose, and sucrose

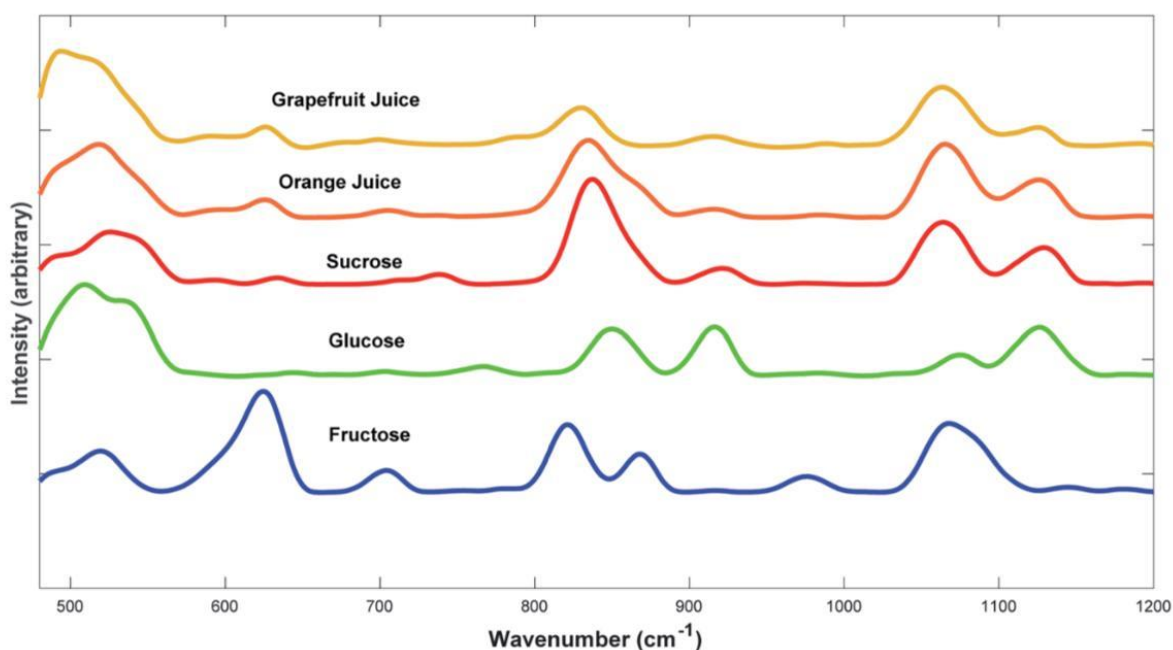


Figure 2.3

Shows typical Raman spectra of orange and grapefruit juices (both from source A), averaged over five repetitions, alongside the spectra of the three main sugars present in these juices: fructose, glucose, and sucrose. For better visual clarity, the y-axis has been offset (Varnasseri et al., 2022).

The fourth study presented Fourier-transform infrared (FT-IR) spectroscopy as a novel, rapid, cost-effective, and high-throughput method for quantitatively detecting sugar adulteration in orange juice. Juice was obtained by manually squeezing ten oranges using a portable juicer. The extracted juice was transferred to 10 mL centrifuge tubes, sieved to remove particles, and centrifuged for five minutes at 3080 g at 4 °C. Subsequently, 2 mL aliquots were further centrifuged at 15,871 g for three minutes, and the supernatant was stored at -80 °C until analysis. To examine adulteration with naturally occurring sugars (fructose, glucose, and sucrose), stock solutions (11.7% w/v) of each sugar were prepared by dissolving 10.5 g in 90 mL of water. Orange juice was then spiked with 0.5% of each stock solution. Samples were vortexed for 20 seconds, and 10 μ L aliquots were applied onto a 96-well silicon plate and oven-dried at 50 °C for 30 minutes to fix the sample and remove excess water. For simulating natural sugar composition, a stock solution reflecting the typical orange juice sugar profile was prepared by dissolving 2.45 g of glucose, 5.90 g of sucrose, and 1.90 g of fructose in 100 mL of water to yield a 10.25% (w/v) solution. Orange juice was then adulterated in 0.5% increments from 0% to 20%, generating 41 samples. The procedure was repeated twice to create three sets of samples. Gas chromatography-mass spectrometry (GC-MS) was used to determine the sugar content of the fresh orange juice (Ellis et al., 2016).

In the first experiment, pure orange juice was adulterated with 0.5–20.0% water, each portion pre-mixed with sucrose, fructose, or glucose. The sugar solutions were prepared at 11.7%

(w/v), reflecting the typical sugar content found in freshly squeezed orange juice, based on supermarket label information. Two observations are immediately evident: first, the procedure is highly reproducible; second, without applying chemometric analysis, accurately quantifying the amount of added water would be difficult. Slight visible differences are noticeable in the 1200–900 cm^{-1} range of the mid-infrared spectrum, which primarily corresponds to polysaccharide vibrations (Ellis et al., 2016).

Because the separate addition of sugars was easily detectable, the next phase aimed to make adulteration more challenging by adding water masked with a combination of sugars in appropriate ratios. Gas chromatography-mass spectrometry (GC-MS) was used to determine the sugar content. Accordingly, a stock solution was prepared containing 2.45 g of glucose, 5.90 g of sucrose, and 1.90 g of fructose per 100 mL. This solution was then used to create three series of adulterated orange juice samples, with final concentrations ranging from 0.5% to 20.0% in 0.5% increments (Ellis et al., 2016).

Table 2.2. A list of every important vibrational band together with the corresponding assignments. (W. Li et al., 1996).

Spectral region cm^{-1}	Dominant vibrational mode	Associated sugars
760-820	C-H / C-O deformation	Glucose, fructose
820-900	C-H deformation / C-C stretching	Fructose
900-980	C-C stretching	Sucrose
980-1040	C-O stretching	Glucose, sucrose
1040-1100	C-C / C-O stretching	Sucrose, fructose
1100-1140	C-O stretching	Sucrose

The current study aimed to present analytical results obtained from near-IR spectroscopy by evaluating the transmittance of dry extracts across a large set of orange juice samples. For accurate measurement of each component, the instrument was calibrated using a reference method, following standard laboratory procedures. Specific sugars and acids in the orange juice samples were determined using enzymatic techniques. Mathematical models, such as stepwise multiple linear regression (SMLR) and partial least squares regression (PLSR), were employed to establish correlations between the chemical reference values and spectral data for each component (W. Li et al., 1996).

Orange juice samples were collected from several European, African, and American countries, including 98 concentrates, 120 single-strength juices, and pulp washes. Prior to near-IR spectroscopy, the concentrates were diluted to 11.18° Brix (w/w) using distilled water, and a Kontes homogenizer was employed to homogenize the pulp washes and single-strength juices. For analysis, 0.6 mL of each juice sample was pipetted onto a fiberglass disc (Millipore AP40047) positioned in a centralizing device, then dried for four minutes in the DESIR (Dry Extract System for Infrared) unit at 45–50 °C. Once dried, the fiberglass filter was placed between two glass panes in a sample cup for near-IR scanning (W. Li et al., 1996).

Orange juice sample absorbances in transmission mode were calculated as $\log(1/T)$, where T represents the transmittance. The spectrum of each sample was obtained by averaging six spectra, which were recorded using two fiberglass discs and three rotational positions of the

sample cup inside the spectrometer (0° , 120° , and 240°). Each spectrum was measured ten times across the 1100–2500 nm range. Reference spectra were recorded by scanning a blank fiberglass disc (W. Li et al., 1996).

Near-IR spectra obtained from a set of calibration samples (the calibration set) were used to develop models linking spectral data to the chemical reference values of each component under study. These calibration models were then validated using a separate set of samples (the validation set), which were similar in component ranges, physical properties, and origin but not included in the calibration set. In this study, 218 orange juice samples were divided into two groups of 150 and 68 samples. The larger batch of 150 samples was used to build calibration models for glucose, fructose, sucrose, and citric and malic acids, while the remaining 68 samples were employed to validate these models (W. Li et al., 1996).

Derivative transformations of spectra are applied to extract additional information from the original data and to reduce band interference and overlap when multiple components are analyzed simultaneously. Multiplicative Signal Correction (MSC) can separate the additive contributions of chemical absorption from the multiplicative effects caused by light scattering and variations in sample thickness. The 1900–2000 nm wavelength range, corresponding to the main water absorption peak in this study, contains absorbances unrelated to the components of interest and therefore provides no useful information. As a result, the original spectra were adjusted to equalize absorption scatter levels, and the 1900–2000 nm region was selected as the basis for MSC standardization (W. Li et al., 1996).

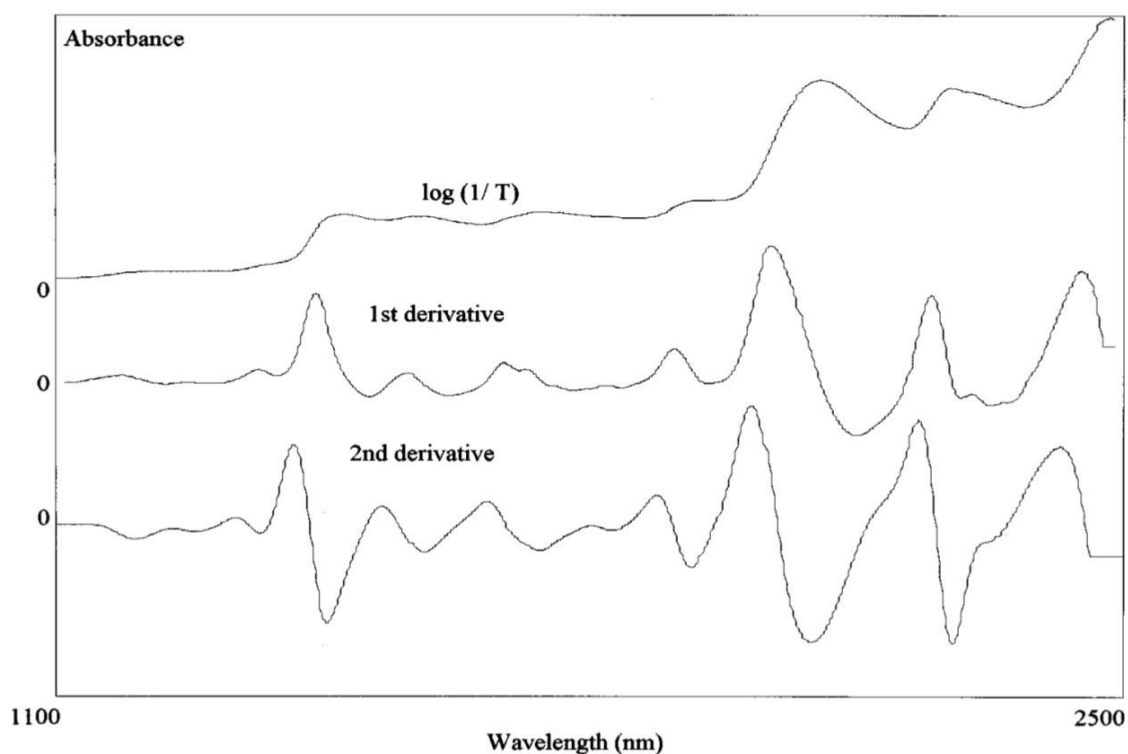


Figure 2.4

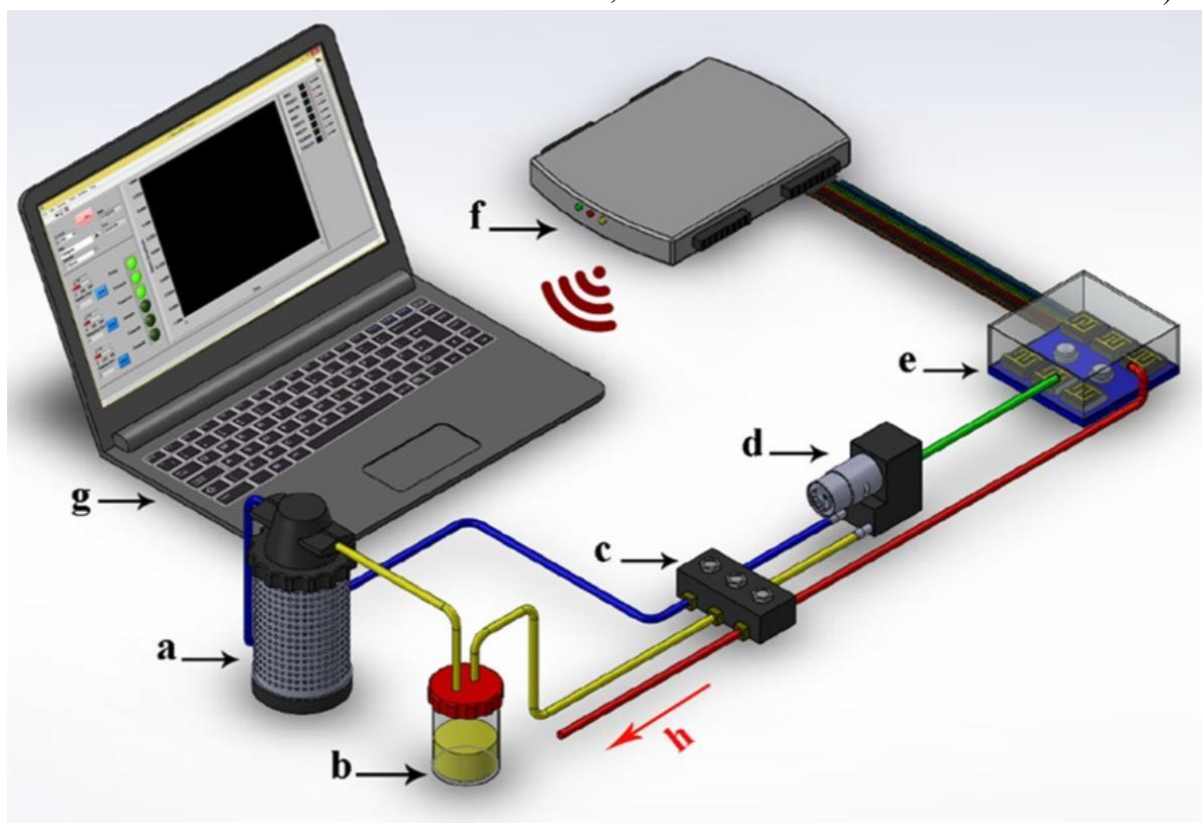
Orange juice sample's dry extract spectrum before and after derivative conversions.

The final study employed an electronic nose to assess adulteration in both natural and industrially produced juices. Four types of natural juices from the industrial line strawberry, lemon, orange, and mango were analyzed (Rasekh & Karami, 2021).

First, four types of fresh fruits, including oranges, were purchased from the fruit market in Kermanshah, Iran. The samples were refrigerated until the experiments began. The fruits were then washed and juiced using a juice extractor, while the room temperature was maintained at 20 ± 0.5 °C during sample preparation and analysis. A total of 120 samples were prepared (15 replicates \times 8 fruit juice groups), consisting of 15 pure and 15 industrial samples for each fruit type. For the experiments, 20 mL of each sample was placed in a 50 mL glass jar at room temperature (23 ± 2 °C). The samples were sealed and allowed to equilibrate for 10 minutes to stabilize the headspace (Rasekh & Karami, 2021).

Assessing the quality of fresh fruits is relatively straightforward because of their observable morphological characteristics, such as color, texture, and firmness, as well as flavor attributes like taste and aroma. However, evaluating quality becomes more challenging once the fruits are processed into juice, as it can be difficult to determine whether a juice bottle was made from fresh fruit or not (Rasekh & Karami, 2021).

Principal component analysis (PCA) was used to identify patterns and extract information from the data collected by the electronic nose. PCA reduces a multidimensional dataset into fewer dimensions while retaining the essential information necessary for analysis (Rasekh & Karami, 2021).



Instead of differentiating between juice types, the electronic nose likely detected the general aroma profile of the fruit juices (Rasekh & Karami, 2021).

Chapter three:

Materials and methods

3.1.Chemicals

Fresh orange juice, industrial orange juice, citric acid, sugars (glucose, fructose and sucrose), distilled water.

3.2.Instruments

Analytical balance, Bruker tensor II spectrophotometer equipped with an attenuated total reflectance ATR .

3.3.Fresh orange juice preparation

Three distinct types of fresh orange juice Abu-sora, Shamote, and Yousufi were gathered from the area market. After giving the oranges a thorough cleaning, they were juiced in a home juicer. Test tubes were filled with the extracted juice. For additional examination, the clear supernatant (pure orange juice) was carefully collected. To prevent the breakdown of sugars and organic acids, the clear juice was examined by Mid-FTIR within a few hours following extraction.

We bought ACS-grade glucose, fructose, sucrose, and citric acid from Fluks. Mili-Q water was used to prepare all aqueous solutions. The pure orange juice was blended with water to produce a range of diluted juices with V/V concentrations ranging from 10% to 100% in order to replicate various dilution levels of fresh orange juice.

3.4.Commercial orange juice preparation in Palestinian markets

The most common four orange juice brands in Palestinian markets were studied in this work. Code numbers from 1 to 4 were given to them. The concentration of orange juice in them was estimated using ATR-FTIR, based on determining sugar and citric acid contents.

3.5. Citric acid and sugar mixture solutions preparation

An FTIR spectrometer was used to evaluate the transmission values after an aqueous solution containing 1.8% glucose, 2.1% fructose, and 4.5% sucrose was produced. Plotting the spectrum according to the connection between transmission and wavelength was done using the transmission values. This made it possible to determine the special wavelength of sugar absorption as well as the precise peaks at which sugar absorbs. From the spectrum (fig.4.1D) we can see that the 1064 cm^{-1} is the distinguishing wavenumber of sugar. As well as 1% aqueous citric acid solution. These solutions were used to assign the absorption peak characteristic for sugar and citric acid in aqueous solutions (fig.4.1B). we can see that the 1177.7 cm^{-1} is the distinguishing wavenumber of citric acid.

3.6. FTIR instrument and method specifications

The Bruker Tensor II FTIR spectrometer, fitted with a Platinum ATR attachment with a diamond crystal, was the tool utilized in this investigation. The $4000\text{-}400\text{ cm}^{-1}$ measurement parameters were retained. Every sample (solid citric acid, juice sample, and aqueous solution of sugars and citric acid) was tested 7 times while it was on the ATR crystal.



Figure 3.1

Bruker Tensor II FTIR spectrometer.

Chapter four:

Results and discussion

4.1. IR spectra of fresh orange juice, aqueous sugars mixture, water and pure citric acid

Fig. 4.1A shows the IR transmittance spectrums of water. It has a broad strong absorption peak ranging between $3720 - 2820 \text{ cm}^{-1}$ with maximum absorption at 3262 cm^{-1} , an acute medium peak at 1635.9 cm^{-1} and a broad peak below 900 cm^{-1} with maximum absorption at 480 cm^{-1} . The IR spectrum of water looks similar to that of both abo-sora pure orange juice Fig. 4.1C and that of aqueous solution of the sugar's mixture Fig. 4.1D. The water IR spectrum does not contain the weak broad peak $1180 - 988 \text{ cm}^{-1}$ with maximum absorption at 1064 cm^{-1} which refers to sugar molecules that appear in both Fig. 4.1C and Fig. 4.1D. Orange juice and sugar solution appear to have the same infrared spectra. Citric acid's infrared spectrum is seen in Fig. 4.1B. O-H alcohol stretching causes a sharp, faint peak at 3437 cm^{-1} . O-H carboxylic acid causes a wide peak that stretches to 2900 cm^{-1} . a wide, faint peak caused by C-H stretching at 2873 cm^{-1} . The C-O stretching causes a strong peak at 1170 cm^{-1} . This absorption peak is important, but since it overlaps with the sugar peak at 1064 cm^{-1} , we did not utilize it for the quantitative study of orange juice. Since all other components of orange juice exhibit low absorbance at this wavenumber, we instead chose the peak caused by C-O stretching at 1177.7 cm^{-1} . In this work the absorbance due to sugar mixture at 1064 cm^{-1} and due to citric acid 1177.7 cm^{-1} are used for quantitative analysis of orange juice, since both chemicals are the major constituents after water in the orange juice. Each sample was measured 7 times. The IR spectrums of all samples were collected as data points. absorbance then was calculated by taking $(-\log \text{ transmittance})$.

4.2. Constructing calibration curves for quantitative analysis of orange juice depending on sugar and citric acid quantities

In this study, absorbance ratios $1064/1635.9$ (due to sugar mixture concentration normalized with absorption due to water) and $1177.7/1635.9$ (due to citric acid concentration normalized

with absorption due to water), were employed as a method to evaluate orange juice's purity. Absolute absorbance values at specific wavenumbers can vary slightly due to factors such as measurement timing, instrument differences, and the method employed for obtaining the IR spectrum such as Attenuated Total Reflectance (ATR). To reduce these variations, absorbance ratios were adopted as a form of normalization. Tables 4.1,4.2 and 4.3 show the absorbance ratios at selected wavenumbers for a series of diluted orange juice of the three selected varieties of oranges: abu-sora, shamote and yousufi, respectively.

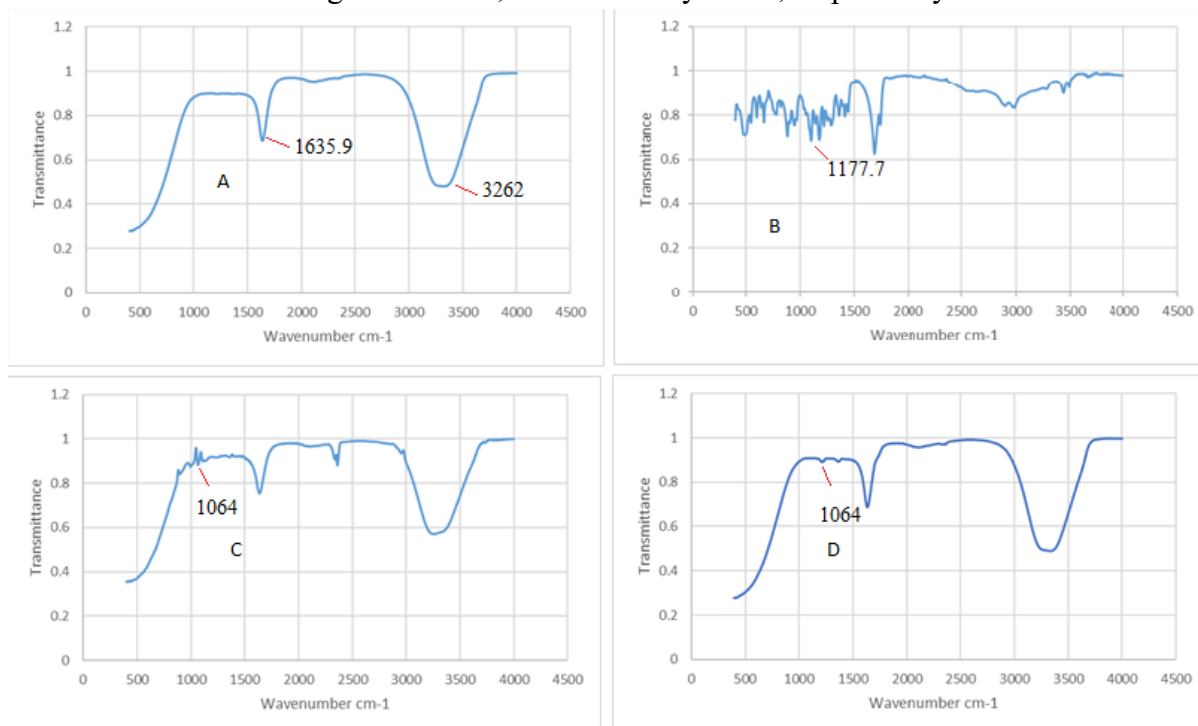


Figure 4.1 IR spectrums of water A, pure citric acid B, abu-sora orange juice C and sugar mixture aqueous solution D.

The absorbance ratio 1064/1635.9 of aqueous solution of sugar mixture, with mean value was measured to be 0.3180 ± 0.014 . It can be seen from tables 4.1-4.3 that the sugar concentration in all oranges studied in this work are slightly around the mean value found, since for all pure orange juices their ratios are higher than the mean value. It can be seen from tables 4.1-4.3, the sweetest oranges are abu-sora and very close to yousufi oranges. The concentration of sugar in shamote oranges are slightly less than the previous two oranges. While the absorbance ratio 1177.7/1635.9 that determines the concentration of citric acid, was found to be 0.27643 ± 0.002 . According to tables 4.1-4.3, the citric acid concentration is around the mean value found. Very close results were found in all orange juice variety. IR spectrum depends on the composition of orange juice as well as the concentration of each component. We can see that IR spectrum of orange varieties is not completely identical. As result, using simple calibration curves for quantitative analysis of orange juice involve some risks in terms of the accuracy of the results. This risk is greatly reduced when using two independent variables (sugar and citric acid). We can see this fact when we analyze real samples in the next section. Calibration curves obtained from tables 4.1-4.3 are shown in Fig.4.2 (depending on sugar analysis) and in Fig.4.3 (depending on citric acid analysis). The

formulae for quantitatively estimating pure orange juice in commercial orange juice-based drinks are shown in Table 4.4 and are obtained from Figures 4.2 and 4.3.

Table 4.1: absorbance and absorbance ratios at various wavenumbers (cm^{-1}) of various abu-sora orange juice dilutions in order to create curves for the quantity of pure juice in the aqueous solution.

Concentration of Abu-sora orange juice V/V	Absorbance at 1635.9 cm^{-1}	SEM	Absorbance at 1064 cm^{-1}	SEM2	Absorbance at 1177.7 cm^{-1}	SEM3	Absorbance ratio 1064/1635.9	Absorbance ratio 1177.7/1635.9
1	2	3	4	5	6	7	8	9
10	0.1201	0.0006	0.0235	0.0004	0.0315	0.0003	0.1962	0.2624
20	0.1204	0.0007	0.0274	0.0002	0.0323	0.0004	0.2280	0.2683
30	0.1209	0.0005	0.0311	0.0005	0.0328	0.0002	0.2571	0.2719
40	0.1214	0.0005	0.0341	0.0001	0.0332	0.0006	0.2811	0.2741
50	0.1213	0.0004	0.0374	0.0002	0.0337	0.0004	0.3089	0.2785
60	0.1216	0.0004	0.0415	0.0001	0.0346	0.0005	0.3415	0.2844
70	0.1216	0.0006	0.0415	0.0001	0.0346	0.0005	0.3415	0.2844
80	0.1220	0.0004	0.0481	0.0002	0.0359	0.0005	0.3946	0.2944
90	0.1222	0.0003	0.0508	0.0001	0.0363	0.0003	0.4159	0.2975
100	0.1230	0.0004	0.0541	0.0006	0.0364	0.0008	0.4402	0.2965

Notes: 3 separate oranges of the same kind were used to figure the mean value, and each orange's juice was sampled 7 times. SEM is the standard deviation from the mean value. Column 8 values are obtained by dividing column 4 values / column 2 values. Column 9 values are obtained by dividing column 6 values / column 2 values.

Table 4.2: absorbance and absorbance ratios at various wavenumbers (cm^{-1}) of various shamote orange juice dilutions to create curves for the quantity of pure juice in the aqueous solution.

Concentration of Shamote orange juice V/V	Absorbance at 1635.9 cm^{-1}	SEM	Absorbance at 1064 cm^{-1}	SEM2	Absorbance at 1177.7 cm^{-1}	SEM3	Absorbance ratio 1064/1635.9	Absorbance ratio 1177.7/1635.9
1	2	3	4	5	6	7	8	9
10	0.1220	0.0006	0.0236	0.0001	0.0314	0.0005	0.1940	0.2572
20	0.1222	0.0002	0.0268	0.0009	0.0318	0.0003	0.2198	0.2609
30	0.1225	0.0009	0.0296	0.0008	0.0326	0.0006	0.2418	0.2662
40	0.1225	0.0001	0.0325	0.0001	0.0331	0.0001	0.2655	0.2701
50	0.1235	0.0005	0.0366	0.0002	0.0336	0.0009	0.2963	0.2725
60	0.1235	0.0001	0.0403	0.0002	0.0342	0.0002	0.3267	0.2775
70	0.1241	0.0004	0.0436	0.0002	0.0349	0.0004	0.3513	0.2813
80	0.1241	0.0005	0.0465	0.0002	0.0355	0.0005	0.3751	0.2862
90	0.1240	0.0005	0.0504	0.0001	0.0364	0.0006	0.4066	0.2942
100	0.1241	0.0007	0.0534	0.0002	0.0369	0.0005	0.4304	0.2976

Notes: Column 8 values are obtained by dividing column 4 values / column 2 values, and column 9 values are obtained by dividing column 6 values / column 2 values.

Table 4.3: absorbance and absorbance ratios at various wavenumbers (cm^{-1}) of various yousufi orange juice dilutions in order to create curves for the quantity of pure juice in the aqueous solution.

Concentration of Yousufi orange juice V/V	Absorbance at 1635.9 cm^{-1}	SEM	Absorbance at 1064 cm^{-1}	SEM2	Absorbance at 1177.7 cm^{-1}	SEM3	Absorbance ratio 1064/1635.9	Absorbance ratio 1177.7/1635.9
1	2	3	4	5	6	7	8	9
10	0.1232	0.0002	0.0247	0.0004	0.0314	0.0001	0.2012	0.2548
20	0.1240	0.0004	0.0280	0.0007	0.0319	0.0001	0.2260	0.2573
30	0.1241	0.0001	0.0314	0.0008	0.0325	0.0008	0.2529	0.2625
40	0.1244	0.0006	0.0344	0.0002	0.0328	0.0005	0.2768	0.2640
50	0.1241	0.0008	0.0387	0.0001	0.0334	0.0007	0.3124	0.2695
60	0.1245	0.0006	0.0420	0.0001	0.0341	0.0002	0.3376	0.2738
70	0.1247	0.0001	0.0451	0.0002	0.0345	0.0007	0.3618	0.2768
80	0.1250	0.0006	0.0493	0.0004	0.0353	0.0001	0.3944	0.2825
90	0.1255	0.0003	0.0524	0.0092	0.0357	0.0002	0.4174	0.2843
100	0.1252	0.0005	0.0560	0.0004	0.0363	0.0008	0.4471	0.2900

Notes: Column 8 values are obtained by dividing column 4 values / column 2 values, and column 9 values are obtained by dividing column 6 values / column 2 values.

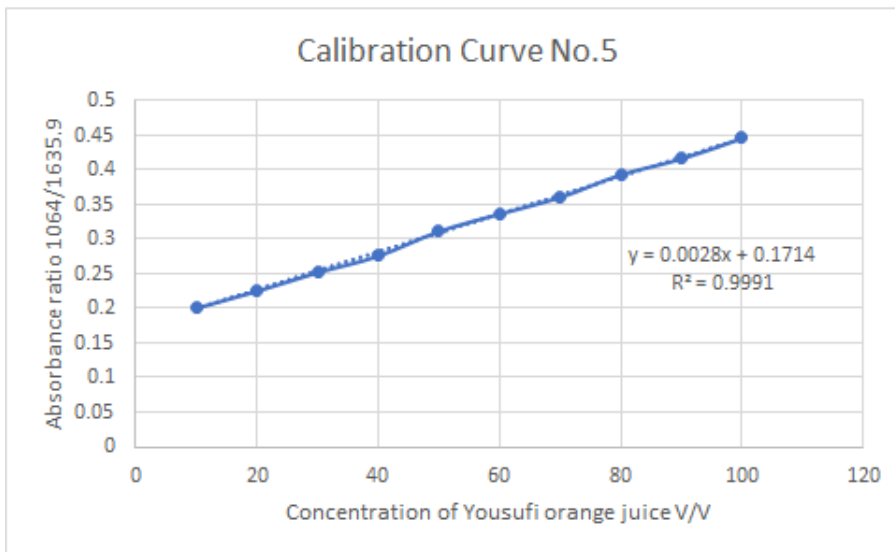
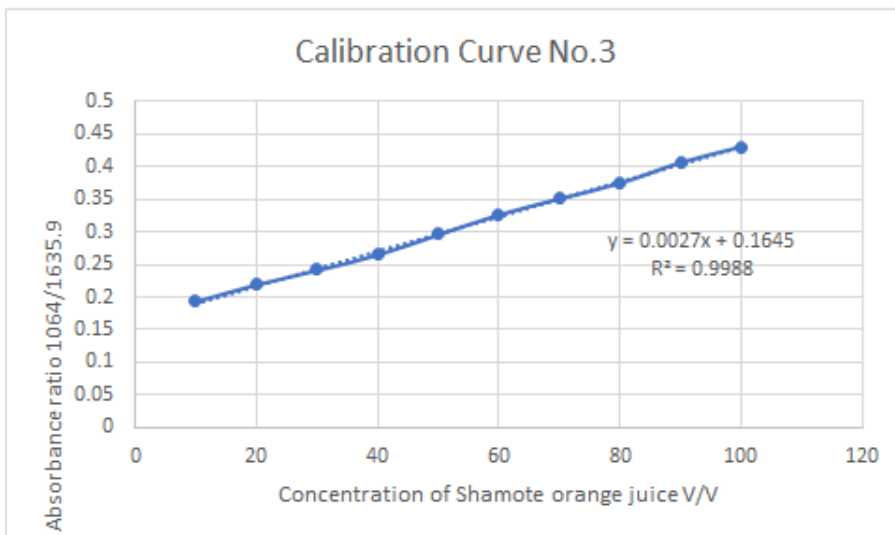
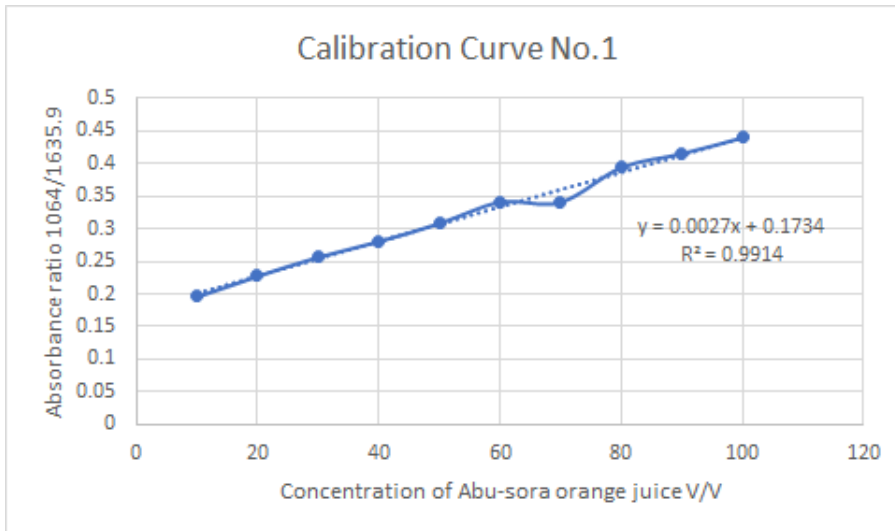


Figure 4.2 calibration curves based on the sugar content of 3 distinct types for the quantitative assessment of pure orange juice in commercial orange juice-based drinks.

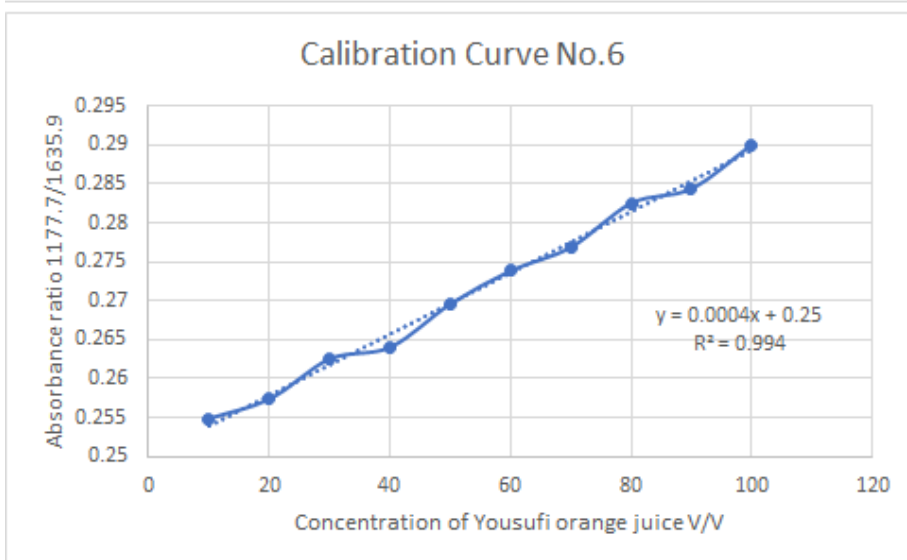
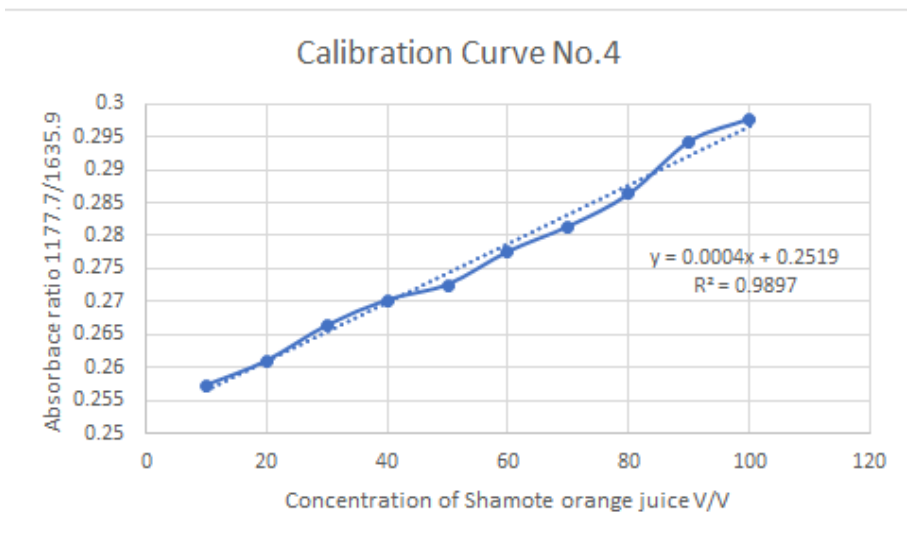
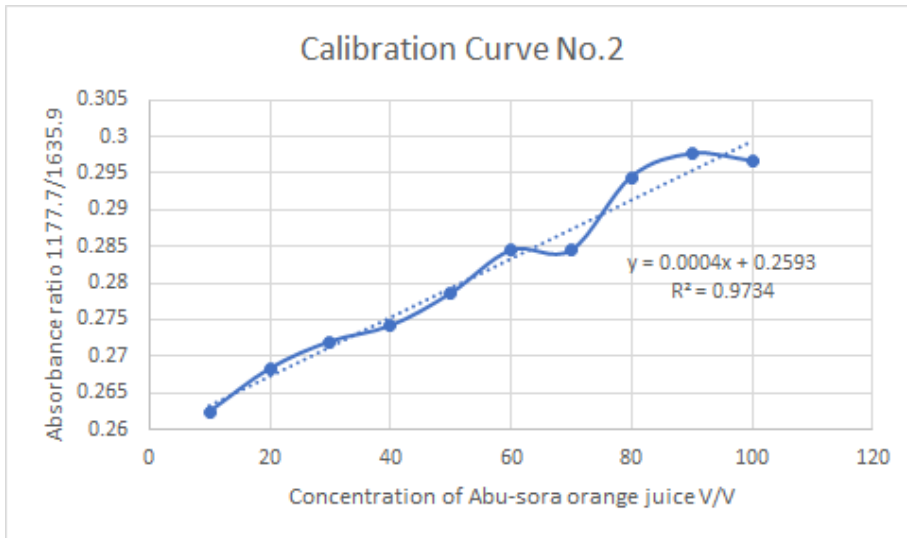


Figure 4.3 calibration curves based on the quantity of citric acid in 3 distinct types for the quantitative measurement of pure orange juice in commercial orange juice-based drinks.

Table 4.4: Equations for calibration curves that allow for the quantitative measurement of pure orange juice in commercial orange juice-based drinks.

Equation No.	Equation	Details
1	$Y = 0.0027x + 0.1734$ $R^2 = 0.9914$	Obtained by plotting concentration of pure abu-sora orange juice in aqueous preparation x verses absorbance ratio (absorbance at 1064 cm ⁻¹ (sugar content) / absorbance at 1635.9 cm ⁻¹ (water)), as shown in Fig. 4.2A.
2	$Y = 0.0004x + 0.2593$ $R^2 = 0.9734$	Obtained by plotting concentration of pure abu-sora orange juice in aqueous preparation x verses absorbance ratio (absorbance at 1177.7 cm ⁻¹ (citric acid content) / absorbance at 1635.9 cm ⁻¹ (water)), as shown in Fig. 4.3A.
3	$Y = 0.0027x + 0.1645$ $R^2 = 0.9988$	Obtained by plotting concentration of pure shamote orange juice in aqueous preparation x verses absorbance ratio (absorbance at 1064 cm ⁻¹ (sugar content) / absorbance at 1635.9 cm ⁻¹ (water)), as shown in Fig. 4.2B.
4	$Y = 0.0004x + 0.2519$ $R^2 = 0.9897$	Obtained by plotting concentration of pure shamote orange juice in aqueous preparation x verses absorbance ratio (absorbance at 1177.7 cm ⁻¹ (citric acid content) / absorbance at 1635.9 cm ⁻¹ (water)), as shown in Fig. 4.3B.
5	$Y = 0.0028x + 0.1714$ $R^2 = 0.9991$	Obtained by plotting concentration of pure yousufi orange juice in aqueous preparation x verses absorbance ratio (absorbance at 1064 cm ⁻¹ (sugar content) / absorbance at 1635.9 cm ⁻¹ (water)), as shown in Fig. 4.2C.

6	$Y = 0.0004x + 0.25$ $R^2 = 0.994$	<p>Obtained by plotting concentration of pure yousufi orange juice in aqueous preparation x verses absorbance ratio (absorbance at 1177.7 cm⁻¹ (citric acid content) / absorbance at 1635.9 cm⁻¹ (water)), as shown in Fig. 4.3C.</p>
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4.3. Calculating of the amount of pure orange juice in commercial orange juice-based drinks using table's 4.4 equations 1-6

Table 4.5 displays the findings of an analysis of the quantity of pure orange juice in four commercial orange juice brands in the Palestinian market. In general, Brand No. 1's claim that its juice is 100% pure aligns with our developed formulas for determining orange juice purity. The purity of orange juice was not mentioned by the other companies. We observe excellent agreement between the findings from equations 1, 2, 3, 4, and 5. This shows that orange juice was made from either shamote orange, abu-sora orange, or a combination of the two in every brand under investigation. If not, youсуfi oranges are either not used at all or are utilized in very limited quantities to make orange juice. Also, there must be a good agreement between the equations derived from sugar quantity with that derived from citric acid concentration for any variety of orange used for producing orange juice. If there is no agreement between these equations, we can judge that the orange juice isn't pure and appreciable quantities of additive were used in producing the juice. We can also conclude that if the results of equation No.6 are in a good agreement with the results obtained from all other equations but largely different than the result obtained from equation 5, this means that a large quantity of sugar was added to the orange juice, as we can see from the results of brands in table 4.5.

Finally, we conclude that, we can use the 6 equations derived in this work for rapid estimation for the purity of orange juice in commercial orange juice-based beverages, without sample preparation and without using any statistical mathematical method combined with IR measurements. This method is very fast, very easy and cheap.

Table 4.5: employing formulas developed in this work (table 4.4) based on the concentrations of sugar and citric acid to analyze the purity of four brands of orange juice on the Palestinian market.

Code no. of orange juice brands	Absorbance at 1635.9 cm ⁻¹	SEM	Absorbance at 1064 cm ⁻¹	SEM	Absorbance at 1177.7 cm ⁻¹	SEM	Absorbance ratio 1064/1635.9	Absorbance ratio 1177.7/1635.9	Conc. of Orange juice using equation 1	Conc. of Orange juice using equation 2	Conc. of Orange juice using equation 3	Conc. of Orange juice using equation 4	Conc. of Orange juice using equation 5	Conc. of Orange juice using equation 6
1	0.1590	0.0003	0.0920	0.0012	0.0506	0.0002	0.5787	0.3185	150.14	148.11	153.43	166.61	145.49	171.36
2	0.1605	0.0001	0.0812	0.0012	0.0500	0.0002	0.5062	0.3115	123.27	130.54	126.56	149.04	119.58	153.79
3	0.1592	0.0003	0.0872	0.0009	0.0513	0.0002	0.5477	0.3225	138.65	158.05	141.95	176.55	134.41	181.30
4	0.1610	0.0003	0.0604	0.0007	0.0467	0.0002	0.3753	0.2905	74.807	78.042	78.103	96.542	72.849	101.29

4.4. Estimation of adulteration percentage based on FTIR calibration

This study used FTIR spectroscopy to determine the amount of sugar and citric acid in commercial orange juices to identify adulteration. The concentration of sugar was estimated as a first indicator, due to its low-cost, availability and popular ingredient used in commercial juice manufacturing. And the concentration of citric acid as a second indicator, because it's the main organic acid found in oranges.

The following actions were done in order to calculate the proportion of adulteration in each commercial orange juice:

First of all, for each juice sample the sugar and citric acid content were measured using three types of oranges. Then, the average sugar percentage and the average citric acid percentage were calculated for each sample (avg. sugar = mean (sugar from abu-sora, sugar from shamote and sugar from yousufi)) (avg. citric = mean (citric from abu-sora, citric from shamote and citric from yousufi)). Then, the average pure juice content was estimated as the mean of both average (avg. pure juice content = (avg. sugar + avg. malic) / 2). Finally, the percentage of adulteration calculated as: adulteration % = 100 – avg. pure juice content.

Table 4.6: results of adulteration analysis in commercial orange juices.

Code no. of orange juice brands	Avg. sugar	Avg. citric acid	Avg. pure juice content	% Adulteration
1	149.69	162.03	155.86	-55.86
2	123.14	144.45	133.79	-33.79
3	138.34	171.97	155.15	-55.15
4	75.253	91.959	83.60	16.39

4.5. Interpretation of adulteration results

Brand no.1 has a 155.86% natural juice content and a -55.86% adulteration percentage. Brand no.2 has a 133.79% natural juice content and a -33.79% adulteration percentage. Whereas brand no.3 has a 155.15% natural juice content and a -55.15% adulteration percentage. All of them have a value above 100% (high sugar content and high citric acid content), which could mean that either extremely concentrated apple extract was used in excess of the usual juice levels, or isolated orange components (such as sugar fractions or refined citric acid) were added to improve flavor profiles. Knowing that adding sugar will enhance the sweetness or will mask the taste of added water or low-quality juice. Instead of only dilution, this artificial elevation above natural composition raises the possibility of technological processing. However, brand no.4 has an 83.60% and a 16.39% adulteration percentage, this indicates that citric acid was added for many reasons, to enhance flavors, as a preservative, restore the natural acidity (due to dilution) and as antioxidant.

Chapter five:

Conclusion and Recommendations

This study successfully shown that attenuated total reflection. Pure orange juice in commercial orange juice-based drinks may be measured quickly, simply, and affordably using Fourier transform infrared (ATR-FTIR) spectroscopy. Reliable calibration curves were created for three different orange varieties: abu-sora, shamote, and yousufi, by concentrating on the two main components of orange juice, total sugars and citric acid, and normalizing their absorbance values against a specific water peak at 1635.9 cm^{-1} . The effectiveness of this analytical method is shown by the calibration curves' good linearity (R^2 values greater than 0.97). In conclusion, without the need for sample preparation or expensive statistical techniques, the equations created in this study allow for the rapid and precise calculation of juice purity. This method's practical use for identifying dilution and sugar addition was demonstrated when it was applied to commercial brands, showing various differences in purity. All things considered, ATR-FTIR is a reliable and efficient technique for routinely assessing the authenticity and quality of orange juice.

Based on the findings and results of this research, it is recommended that regulatory authorities require food and beverage manufactures to clearly label the percentage of pure orange juice contained in their products. Such labeling would enhance transparency, support consumer awareness, and enable informed purchasing decisions. Implementing this practice, as adopted in countries such as Germany, would contribute to improving product quality control and ensuring compliance with international food labeling standards. Additionally, this measure may help reduce competition among commercial brands.

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التحليل الكمي لعصير البرتقال باستخدام جهاز قياس طيف الأشعة تحت الحمراء

اعداد: عايدة ايمن احمد عبدالله

اشراف: الاستاذ البروفيسور معتز القطب والدكتور محمود الخطيب

ملخص

إحدى الطرق الشائعة لغش عصير البرتقال هي تخفيفه بالماء وإضافة السكريات والأحماض والملونات ومحسنات النكهة. يمكن أن تؤدي هذه المواد المغشوشة إلى انخفاض كبير في جودة الغذاء، كما قد تشكل عددًا من المخاطر الصحية، خاصة تلك المرتبطة بالاستهلاك المفرط للسكر. لذلك، من المهم للغاية تقييم مستوى نقاء عصير البرتقال في المشروبات التجارية المعتمدة على عصير البرتقال باستخدام طريقة بسيطة وسريعة وسهلة ورخيصة وآمنة ودقيقة، ولا تحتاج إلى تحضير للعينات أو إلى الأساليب الإحصائية المتقدمة (التحليل متعدد المتغيرات). يهدف هذا البحث إلى تقدير كمية عصير البرتقال في المشروبات باستخدام جهاز قياس طيف الأشعة تحت الحمراء وذلك بالاعتماد على القياس المتزامن لتركيزات حمض الستريك والسكريات. وقد تبين أن المعادلتين التاليتين، بنسبة خطأ تقارب 5٪، يمكن استخدامهما لتحديد نسبة عصير البرتقال النقي في المشروبات التجارية المبنية على عصير البرتقال:

$$R^2 = 0.9914 \text{ ، } Y = 0.0027x + 0.1734$$

حيث يمثل Y نسبة الامتصاص عند 1064 cm^{-1} الناتجة عن السكريات الكلية مقسومة على الامتصاص عند 1635.9 cm^{-1} الناتج عن الماء.

$$R^2 = 0.994 \text{ ، } Y = 0.0004x + 0.25$$

حيث يمثل Y نسبة الامتصاص عند 1177.7 cm^{-1} الناتجة عن حمض الستريك مقسومة على الامتصاص عند 1635.9 cm^{-1} الناتج عن الماء.

الكلمات المفتاحية: عصير البرتقال النقي، الغش/ التلاعب، العدد الموجي، الامتصاصية، مطافية الأشعة تحت الحمراء.