

Article

What's in Your Fruit Juice?—Rapid Quality Screening Based on Infrared (FT-IR) Spectroscopy

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Featured Application: In this study, we introduce an approach for quickly profiling the nutritional content of fruit juices by using a portable Fourier transform mid-infrared (FT-IR) device. This method enables real-time prediction and simultaneous analysis of key components, such as sugars and acids in fruit juices, addressing concerns about obesity and other health risks. The portability of the FT-IR sensor makes it a valuable tool for food processors, providing a convenient out-of-the-laboratory solution. This application detects deviations in sugar and ascorbic acid levels compared to nutritional labels, helping consumers to make healthier decisions. Furthermore, applying portable FT-IR devices by the fruit juice industry will streamline quality control processes and represents a shift towards more efficient, non-destructive, and high-throughput analytical methods.

Abstract: Fruit juices (FJ) have gained widespread global consumption, driven by their perceived health benefits. The accuracy of nutrition information is essential for consumers assessing FJ quality, especially with increasing concerns about added sugars and obesity risk. Conversely, ascorbic acid (Vitamin C), found in nature in many fruits and vegetables, is often lost due to its susceptibility to light, air, and heat, and it undergoes fortification during FJ production. Current analytical methods for determining FJ components are time-consuming and labor-intensive, prompting the need for rapid analytical tools. This study employed a field-deployable portable FT-IR device, requiring no sample preparation, to simultaneously predict multiple quality traits in 68 FJ samples from US markets. Using partial least square regression (PLSR) models, a strong correlation ($R_{CV} \geq 0.93$) between FT-IR predictions and reference values was obtained, with a low standard error of prediction. Remarkably, 21% and 37% of FJs deviated from nutrition label values for sugars and ascorbic acid, respectively. Portable FT-IR devices offer non-destructive, simultaneous, simple, and high-throughput approaches for chemical profiling and real-time prediction of sugars and acid levels in FJs. Their handiness and ruggedness can provide food processors with a valuable “out-of-the-laboratory” analytical tool.

Keywords: fruit juice; sugar content; ascorbic acid; FT-IR; portable sensor; real-time prediction; chemical profiling; obesity risk



Citation: Aykas, D.P.; Rodriguez-Saona, L. What's in Your Fruit Juice?—Rapid Quality Screening Based on Infrared (FT-IR) Spectroscopy. *Appl. Sci.* **2024**, *14*, 1654. <https://doi.org/10.3390/app14041654>

Academic Editor: Daniel Cozzolino

Received: 2 February 2024

Revised: 16 February 2024

Accepted: 16 February 2024

Published: 19 February 2024



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1. Introduction

Fruit juice (FJ), defined as “the extract or the extractable fluid content of cells or tissues obtained through mechanical squeezing or pressing out the natural liquid contained in ripe fruits without the use of heat or solvent” [1], has witnessed a significant surge in global market growth. This growth is attributed to lifestyle changes and increasing consumer consciousness, driven by the desire for healthier food options. Furthermore, different health organizations across the world support the idea of consuming more fruit and vegetable products [2,3]. In 2022, the global juice market surpassed a market share of USD 147 billion and is anticipated to reach USD 190 billion by 2028, exhibiting a growth rate of 4.29% [4] and presenting its substantial contribution to the world economy. To fulfill the market

demand, FJ manufacturers are focused on enriching the flavor and variety of FJs, also introducing novel packaging and product development. Thanks to the innovations in the juice industry, a variety of new juice blends have emerged, going beyond a single source of FJs. These blends serve both commercial purposes, introducing new product lines with distinct organoleptic features, and technological purposes, allowing the industry to take advantage of specific properties of certain juices, such as antioxidants [5]. In most cases, juices obtained from fruit(s) are not sold directly, and dilution with water and/or the addition of sugar or sweetener may involve reducing the sourness and/or for ideal consistency to facilitate juice consumption [1,5]. In brief, the continuous innovations in the processing techniques of FJs and the blending of flavors have broadened the array of choices for consumers. In addition, ready-to-drink FJs provide convenience and portability, making them a popular choice for on-the-go consumption in busy lifestyles [4].

Ascorbic acid, also known as vitamin C, is naturally present in various fruits and vegetables and must be obtained from the diet to prevent scurvy, a clinical deficiency disease characterized by the deterioration of elastic tissues [6]. The recommended dietary allowance (RDA) for vitamin C is established at 60 mg. This recommendation is determined by considering the minimum amount of the vitamin excreted in the urine, aiming to ensure a safety margin against the development of scurvy [7]. Additionally, FJs are often supplemented with ascorbic acid for various purposes. This includes serving as an antioxidant to impede or slow down oxidation by suppressing oxidation promoters like transition metal ion catalysts, singlet oxygen, prooxidative enzymes, and other oxidants [8,9]. The fortification of juices with vitamin C is a common practice to replace the ascorbic acid lost during processing and storage [10–12]. As a readily reactive reducing agent and a swiftly operating antioxidant, the levels of ascorbic acid can experience a significant and rapid decrease [9]. A study by Piljac-Zegarac and others revealed that, during refrigerated storage, the ascorbic acid content in blueberry juice depleted entirely within 7 days and dropped to half of the initial value within the initial 74 h. Similar trends were observed for pomegranate and cranberry juices, with a complete loss within 9 days of refrigerated storage. Strawberry and cherry juices experienced 58% and 35% loss, respectively, after 28 days of refrigerated storage [13]. Talcott and others observed that the initial yellow passion fruit juice formulation had negligible ascorbic acid content (<5 mg/L). However, when the juice was fortified with 450 mg/L of ascorbic acid and subjected to pasteurization (85 °C for 30 min), a 25% ascorbic acid reduction occurred, leading to the complete loss of ascorbic acid after 14 days of storage at 37 °C [14]. On the other hand, citric acid, a naturally occurring weak organic acid that is concentrated in citrus fruits, serves as a common food additive to enhance acidity, improve the sour taste in foods and beverages, and ensure product stability [15].

Studies have shown a correlation between the excessive consumption of sugar-sweetened beverages (SSBs), including FJs, and weight gain in both adults and youth [16–20]. This excessive intake has also been associated with various health issues, such as obesity, diabetes, cardiovascular diseases, and fatty liver syndrome [21–26]. Even though the primary health risks are attributed to high fructose corn syrup (HFCS), beverages that substitute HFCS with cane sugar or the crystalline form of fructose, which may look like a healthier alternative and have a positive consumer perception, still raise concerns due to their high total sugar and fructose content [26]. Besides the risk of obesity, diabetes, cardiovascular diseases, and triglyceride deposition in the liver, fructose is linked to insulin resistance and kidney stones [26].

Despite the nutrition label on FJs requiring the disclosure of total sugar content in grams, complete information about the individual sugar content is not mandated. This lack of specificity allows for the potential substitution of fructose for glucose, given that an equivalent amount of fructose is sweeter than glucose [26]. Studies have also revealed that 100% fruit juices contain no fewer calories than SSBs, while they contain a limited amount of nutrients and carry a similar risk of obesity as SSBs [27–29].

The nutritional labels for pre-packed foods, mandatory and regulated by government agencies worldwide, are overseen by the Food and Drug Administration (FDA) in the US for food products other than meat and meat products, and in the European Union, the European Commission regulates the nutritional labels [30,31]. The FDA ensures compliance with labeling regulations by randomly analyzing collected food products and applying different criteria for different nutrients [32]. For instance, if vitamin C is added to an FJ for fortification, it must be present in the product at 100% or more of the declared value on the label. In other words, the laboratory analysis must confirm that the nutrient content is equal to or exceeds the value stated on the label when vitamin C is added to fortify an FJ. However, if vitamin C is a naturally occurring nutrient in the FJ, then it must be present at 80% or more of the declared value [32]. On the other hand, the total sugar content in an FJ product cannot exceed the declared value on the label by more than 20% [32]. The FDA generally tolerates reasonable excesses of vitamin C and reasonable deficiencies of total sugars within good manufacturing practices [32].

Our objective was to simultaneously predict multiple quality traits (soluble solids, sucrose, glucose, fructose, total sugars, titratable acidity, citric, and ascorbic acids) of FJs using a field-deployable portable FT-IR sensor that requires no sample preparation.

2. Materials and Methods

2.1. Materials and Reagents

In this study, a total of 68 FJ samples were used, comprising 28 samples from single fruit types, including apple, orange, lemon, grapefruit, pomegranate, and cranberry, and 40 samples representing a blend of various fruit juices (Table A1). Samples were collected from grocery stores in Columbus, OH, USA. Both spectral collection and acid analysis (ascorbic and citric acids) were performed on the same day of the purchase to prevent possible spectral changes and ascorbic acid (vitamin C) loss. Subsequent analyses for soluble solids, sugars, and titratable acidity were carried out within the next two days from the purchase; until then, samples were stored at 4 °C to prevent compositional changes.

The chemicals and reagents, including water, NaOH, H₂SO₄, and tris(2-carboxyethyl) phosphine (TCEP), utilized in the experiments were sourced from Fisher Scientific (Fair Lawn, NJ, USA) and Sigma Aldrich (St. Louis, MO, USA). They were of either ACS or HPLC grade quality. Additionally, for the individual sugar analysis, glucose, fructose, and sucrose were in >99% purity, purchased from Fisher Scientific (Fair Lawn, NJ, USA). Ascorbic and citric acid standards were ≥99% pure (Sigma Aldrich, St Louis, MO, USA).

2.2. Reference Analysis

The analysis of sugars (sucrose, glucose, and fructose) was conducted through high-performance liquid chromatography (HPLC). The juice samples underwent filtration using non-sterile 0.45 µm pore size filters (Phenomenex®, Torrance, CA, USA) into 2 mL amber colored HPLC vials. Subsequently, the vials were stored at −18 °C until the analysis. For the sugar analysis, a Shimadzu Prominence UFLC (Shimadzu, Columbia, MD, USA) system was utilized, featuring dual LC-6AD pumps, an SIL-20AHT auto-sampler, a CTO-20A column oven, and an RID-10A refractive index detector. The elution process involved passing the sugars through a 7.8 mm ID × 300 mm ion exclusion column (Rezex RCM-Monosaccharide column, Ca²⁺, 8 µm, Torrance, CA, USA) at a constant flow rate of 1 mL/min and a temperature of 80 °C, with the entire run lasting 30 min. The total sugar content in the analyzed FJ samples was determined by summing all three individual sugars. LC Solutions software version 3.0 (Shimadzu Scientific Instruments Inc., Columbia, MD, USA) was used to collect and analyze the chromatograms.

The measurement of soluble solids (°Brix) was conducted at 20 °C using a digital refractometer (Atago, Model RX-5000i, Bellevue, WA, USA), presenting results in percentage terms. The assessment of titratable acidity in the FJ samples was conducted using the official method specified by AOCS, employing an automatic titrator (Easy Plus Titration, Mettler Toledo, Greifensee, Switzerland).

Ascorbic and citric acids were quantified in juice samples using an Agilent HPLC system (1100 Series, Agilent Technologies, Santa Clara, CA, USA) equipped with a G1311A quaternary pump, G1322A degasser, G1313 ALS autosampler, G1316A column compartment, and G1315B diode array detector. After passing through non-sterile 0.45 μm filters into amber-colored 2 mL HPLC vials, 100 μL of TCEP was added and left overnight, acting as a reducing agent to convert oxidized dehydroascorbic acid back to ascorbic acid [33]. Adding a reducing agent enhanced the stability of vitamin C during the extraction and storage period in the autosampler during the HPLC analysis. The stability of ascorbic acid in sample extracts demonstrated stabilization for a minimum of 96 h. Additionally, the addition of TCEP as a reducing agent with an overnight incubation has proven to not induce any interference with the chromatographic system [33]. A total of 10 μL of a sample was injected into a stainless-steel HPLC-grade acidified water (pH 2.2, acidified with H_2SO_4) facilitated isocratic separation at a flow rate of 0.8 mL/min for 30 min on a stainless-steel, 4.6 mm ID $\times$ 150 mm Prevail organic acid column with 5 μm spherical packing (Hichrom Limited, Leicestershire, UK). Chemstation software (v B.04.03 Agilent, Santa Clara, CA, USA) was utilized for capturing and analyzing the chromatograms. Ascorbic and citric acids were discerned by matching their peak retention times with standards of pure ascorbic and citric acids. All the reference analyses were performed in duplicate.

2.3. FT-IR Analysis

The FJ samples underwent spectral analysis using a portable FT-IR spectrometer. The spectrometer was equipped with a dial-path transmittance accessory featuring a 50 μL pathlength selection, a zinc selenide (ZnSe) crystal, and a deuterated triglycine sulfate (dTGS) detector. Samples' mid-infrared spectra were gathered at ambient temperature, spanning a range of 4000–700 cm^{-1} with 4 cm^{-1} resolution. To enhance the signal-to-noise ratio, 64 co-scans were co-added. To initiate the spectral measurement, a 75 μL portion of the juice sample was directly deposited onto the opening of the dial path accessory. Before each spectral measurement, a background spectrum was acquired to mitigate potential environmental effects. Data collection was performed in duplicate, ensuring reliability and consistency. The spectral data, represented in absorbance, were examined using Resolutions Pro Software (Agilent, Santa Clara, CA, USA).

2.4. Multivariate Data Analysis

The spectral data, imported as GRAMS (.spc) files from the FT-IR instrument, underwent analysis using Pirouette[®] multivariate statistical analysis software (version 4.5, Infometrix Inc., Bothell, WA, USA). Partial least square regression (PLSR) models for soluble solids, sugars (sucrose, glucose, fructose, and total sugars), acids (ascorbic and citric acid), and titratable acidity were built using FT-IR-collected spectral data and reference values obtained through traditional methods. Following an evaluation of alternative pre-processing and transformation algorithms, the spectral data underwent mean-centering and second derivative transformation (Savitsky–Golay second-order polynomial filter with a 35-point window) prior to the PLSR analysis. Spectral data transformation techniques played a crucial role in enhancing the spectral features of the samples and extracting relevant information from the dataset. Specifically, the second derivative transformation can solve the scattering effect, separate overlapping peaks, and correct the baseline drifts [34].

PLSR is a quantitative technique for spectral decomposition that condenses spectral data into orthogonal structures referred to as latent variables or factors. These latent variables characterize the highest covariance between the spectral data and the reference values associated with the quality attributes of FJ [34,35]. PLSR analysis has demonstrated notable success in managing spectral data characterized by numerous, highly correlated, and noisy X-variables (spectra). This capability enables the simultaneous modeling of multiple dependent variables, such as sugars, acids, soluble solids, and titratable acidity [36]. Variable selection, a critical step in PLSR model generation, involves identifying and including informative band features in the spectral matrix while eliminating unnecessary variables [37].

The latent variables that elucidate the spectral data are organized through a cross-validation (leave-one-out) technique and are arranged in descending order according to their impact on the model [37]. It is also essential to select an ideal number of latent variables to prevent the overfitting or underfitting of the model.

Prior to conducting the multivariate analysis, the spectral data were randomly split into the two sub-groups calibration and external validation. The calibration samples, internally validated using the leave-one-out approach, comprised 80% of the total sample size. This subset was employed for constructing the training model, while the remaining 20% was reserved to assess the performance of the training model. Similar statistical performances between the training and test models, in terms of correlation coefficient (R) and standard error, indicated that the generated training model could successfully predict the tested quality trait parameters of the FJ for new samples in the future. Parameters, including latent variable (factor) numbers, the correlation coefficient of cross-validation (R_{cv}), the correlation coefficient of prediction for the external validation set (R_{pre}), the standard error of cross-validation (SECV), the standard error of prediction (SEP), the residual predictive deviation (RPD), and the range error ratio (RER), were employed to evaluate the PLSR models' performances. The RPD was determined by dividing the calibration set's standard deviation of reference data by the SEP. Similarly, the RER represents the ratio of the range of reference data in the validation set to the SEP. Higher values for both RPD and RER generally indicate a model that is more precise and robust [38,39].

3. Results and Discussion

3.1. Quality Parameters of Fruit Juices

The reference compositional ranges for various quality parameters in tested FJs are outlined in Table 1. Based on these findings, it was observed that employing a diverse array of FJ samples led to a broad spectrum of compositional levels (Table 1). Similar compositional quality parameter levels have been reported for commercially available FJs [40–43]. Examination of the sugar content of orange juices included in our study was found to align with the findings of Zhang and Ritenour [33], demonstrating consistency in sucrose, glucose, fructose, and total sugar content for most samples. Interestingly, two samples (out of 12) of 100% orange juice in our study deviated from this trend, exhibiting higher levels of sucrose, fructose, and total sugar compared to the corresponding samples in Zhang and Ritenour's investigation.

Table 1. Reference analysis results for the main quality parameters of fruit juices.

	Soluble Solid (°Brix)	Glucose (g/100 g)	Fructose (g/100 g)	Sucrose (g/100 g)	Total Sugar (g/100 g)	Titrateable Acidity (mg/100 g)	Citric Acid (mg/100 g)	Ascorbic Acid (mg/100 g)
range	3.78–16.03	13.7–66.0	6.6–73.1	11.9–125.4	60.8–153.5	129.1–1139.1	18.6–1114.0	0.70–54.10
avg $\pm$ stdev	11.58 $\pm$ 2.25	26.9 $\pm$ 9.6	36.2 $\pm$ 17.9	54.7 $\pm$ 30.8	105.4 $\pm$ 22.2	559.5 $\pm$ 230.5	519.2 $\pm$ 274.9	23.52 $\pm$ 15.53

A comparison between the total sugar content indicated on the nutrition fact labels of commercially available FJ samples and our HPLC analyses revealed some discrepancies. Among the 68 samples examined, 14 (21%) did not align with the total sugar content declarations. These non-compliant samples exhibited a difference of more than 20% in total sugar content compared to the declared label values. Twelve out of fourteen samples showed higher sugar content (>20%), while the remaining two showed lower (<20%) sugar content, than declared.

Moreover, we identified discrepancies in the ascorbic acid levels of the FJs. Specifically, out of the 68 samples tested, 25 (37%) did not conform with the nutritional fact label. Among these, 15 exhibited lower ascorbic acid levels, while 10 had higher ascorbic acid content than indicated on the label.

3.2. IR Spectral Analysis of the Samples

The FT-IR spectra of fruit juice samples were collected using a dial path accessory, and a representative absorption spectrum of selected samples is visually depicted in Figure 1. The spectral composition of the juices was prominently dominated by water absorption bands within the ranges of 3600–2900 and 1700–1500 cm^{-1} [44,45]. Given their dominating presence, these regions were omitted during model generation because they saturated the detector signal. This exclusion was particularly driven by the inherent high water content in fruit juices, saturating the signal within the mentioned ranges due to the strong infrared absorptivity of water. The fingerprint region (1550–900 cm^{-1}) that contains rich information was used to generate the IR models, and the significant bands in this region are given in Figure 1a,b. The most important bands in the fingerprint region were associated with C-C-H, C-O-H, O-C-H (1470–1150 cm^{-1}), C-O, and C-C stretching modes (1150–900 cm^{-1}) and O-H vibrations (1020–1060 cm^{-1}) [46]. Notably, different types of fruit juices exhibited distinct characteristics in the fingerprint region, as visually represented in Figure 1c.

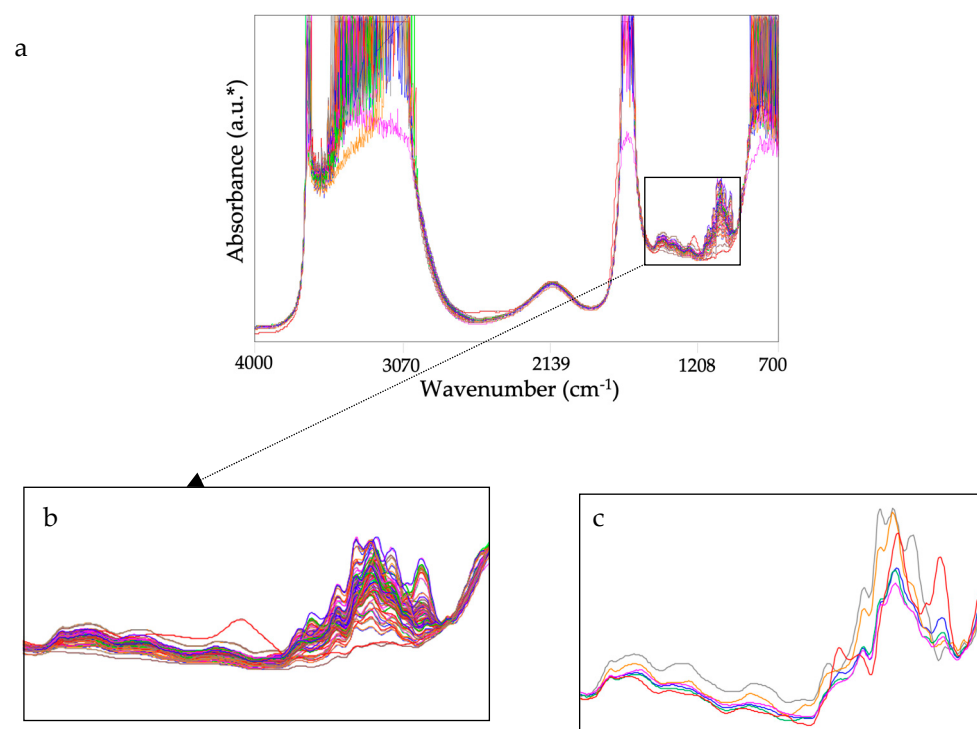


Figure 1. (a) Representative raw mid-infrared spectra of fruit juice samples in the wavelength range 4000–700 cm^{-1} , obtained using a portable FT-IR sensor. (b) The fingerprint region (1550–900 cm^{-1}) of spectra. (c) Selected samples of spectra in the fingerprint region representing pomegranate juice (gray line), apple juice (orange line), lemonade (red line), orange juice (blue line), grapefruit juice (pink line), and cranberry juice (green line). a.u.*: Arbitrary units.

3.3. Quantification of Main Quality Attributes in Fruit Juices Using Partial Least Squares Regression (PLSR)

The PLSR was used to develop models for key quality traits in fruit juices, including soluble solids, sucrose, glucose, fructose, total sugar, titratable acidity (TA), and citric and ascorbic acid content. PLSR analysis was carried out by combining the FT-IR spectral data from the portable infrared sensor with reference data obtained from the traditional analytical equipment. Statistical performances for each quality parameter are presented in Table 2. Discrepancies in sample numbers for specific quality parameters are attributed to the exclusion of outliers identified through high leverage and/or studentized residual criteria, and not all samples contain each individual sugar.

Table 2. Statistical performances of the fruit juice PLSR models developed during the calibration and external validation steps.

Parameter	Range	Calibration Model				Range	External Validation Model				
		N ^a	Factor	SECV ^b	R _{CV} ^c		N ^d	SEP ^e	R _{Pre} ^f	RPD ^g	RER ^h
Soluble solid (°Brix)	3.78–15.99	53	5	0.23	1	7.56–16.03	14	0.26	0.99	8.84	32.38
Glucose (g/100 g)	13.90–57.34	51	5	3.01	0.93	13.69–33.43	13	3.49	0.93	3.49	5.66
Fructose (g/100 g)	7.52–73.08	53	2	3.52	0.98	6.65–70.81	13	3.06	0.99	5.91	20.94
Sucrose (g/100 g)	11.93–123.78	46	6	5.75	0.98	18.33–125.36	12	6.03	0.99	6.11	17.74
Total sugar (g/100 g)	60.84–151.87	53	5	6.32	0.95	67.61–153.50	14	8.96	0.95	3.10	9.59
Titrateable acidity (mg/100 g)	129.15–1139.12	53	5	59.42	0.97	180.09–891.04	14	54.22	0.97	4.43	13.11
Citric acid (mg/100 g)	18.6–1114.0	53	5	55.35	0.98	178.1–1056.9	14	66.04	0.96	4.31	13.31
Ascorbic acid (mg/100 g)	1.04–50.90	50	5	4.37	0.95	0.70–54.10	12	4.53	0.97	3.17	11.79

^a Number of samples used in calibration models; ^b standard error of cross-validation; ^c correlation coefficient of cross-validation; ^d number of samples used in external validation models; ^e standard error of prediction; ^f correlation coefficient of prediction for external validation. ^g Residual predictive deviation. ^h Range error ratio. SECV and SEP are in units of the predicted parameters.

The PLSR calibration models demonstrated a robust correlation between the measured reference values and the predicted values obtained from the FT-IR sensor, as illustrated in Figure 2a–h. In the process of model generation, two to six latent variables were employed, as given in Table 2, explaining 93.53 to 99.85% of the total variance. The determination of the optimum number of latent variables, crucial for minimizing prediction error [47], was executed through a cross-validation (leave-one-out) procedure, with a focus on fulfilling the minimum standard error of cross-validation (SECV) criteria, which involved plotting the SECV against PLSR factors. In order to generate accurate and robust prediction models, it was crucial to choose the optimal number of latent variables in calibration models. While incorporating more factors enhances prediction accuracy by capturing relevant variation, an excess can introduce random noise and over-fitting. Conversely, using too few factors may result in under-fitting, failing to explain essential data variation. Finding this balance is critical, as under-fitted models exhibit high bias and low variance, while over-fitted models show low bias and high variance [48].

The models for the main quality traits of fruit juice exhibit strong correlations ($R_{CV} \geq 0.93$) and low errors ($SECV \leq 59.42$ mg/100 g), as detailed in Table 2. Lower SECV values indicate good predictive performance, while R_{CV} values close to 1, especially above 0.8, are considered excellent for accurate predictions [49]. Using an independent data set to externally validate the model is the most robust method to ensure the model accuracy, as the data set in external validation is not part of the model development process [50]. A comparison of statistical performances between calibration and external validation models, including correlation coefficients (R_{CV} and R_{Pre}) and errors (SECV and SEP), revealed similar results (Table 2), confirming the robustness of the calibration model. This suggests that, when the models encounter new samples within the tested range, they will predict with comparable performance. Figure 2a–h depict the correlation plots between reference values and predicted values for various parameters, including soluble solids, sucrose, glucose, fructose, total sugars, TA, citric acid, and ascorbic acid, obtained using FT-IR spectra. The figures also illustrate the distribution of external validation set samples within the range of the calibration set. The correlation plots revealed a pronounced linearity, signifying the models' capability to precisely predict FJ quality attributes using the FT-IR spectral data. Our models demonstrated similar or better performances in estimating

the quality parameters of fruit juices, including a lower R_{Pre} and SEP, compared to those reported by other researchers for fruit juices using a benchtop FT-IR sensor [51–53].

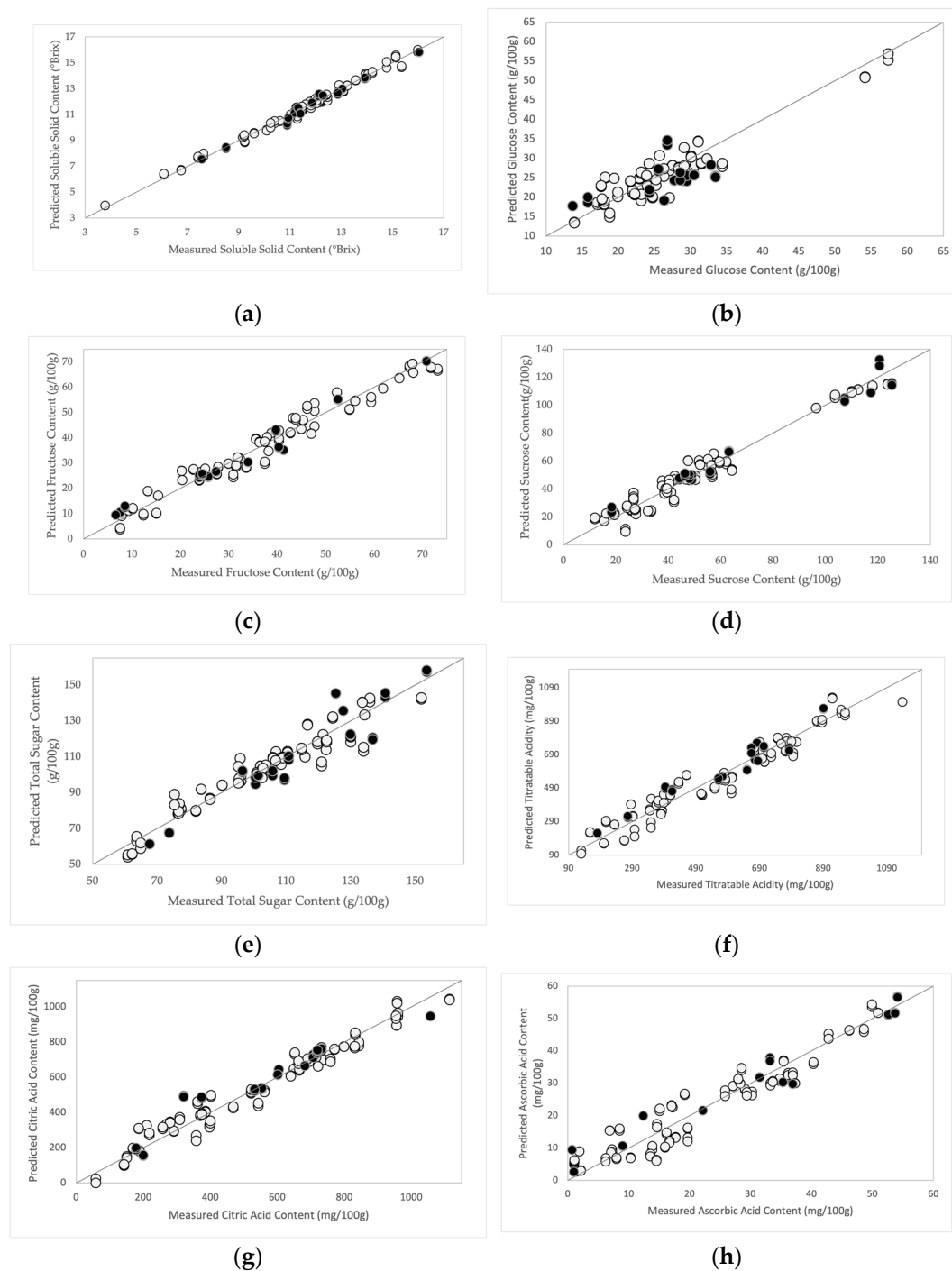


Figure 2. Partial least squares regression (PLSR) calibration and external validation plots for soluble solids (a), glucose (b), fructose (c), sucrose (d), total sugar (e), titratable acidity (f), citric acid (g), and ascorbic acid (h) contents in fruit juice samples using the portable FT-IR sensor. Gray circles represent samples in the calibration set; black circles represent samples in the external validation set.

Model accuracy was further evaluated using RPD and RER values, with RPDs ranging from 3.49 to 8.84 and RERs ranging from 5.66 to 32.38 (Table 2). According to the RPD and RER results, all generated models, except for the glucose prediction model, are suitable

for quality control purposes. Conversely, the glucose model is considered suitable for screening applications based on its RER results [38,39].

Regression vector plots were employed to identify functional groups responsible for the highest variation in explaining the relationship between FTIR spectral data and reference data. For sugars, including sucrose, glucose, fructose, and total sugars, the PLSR models were dominated by the region of 1200–1000 cm^{-1} (Figure 3a). This region is linked to the vibrations of C-C rings, which overlap with the stretching vibrations of C-OH side groups and the glycosidic band vibrations of C-O-C in carbohydrates [51], while the regression vector plots related to acids exhibited prominent absorption bands within the range of 1500–1000 cm^{-1} (Figure 3b). These bands correspond to the absorption features of C-O-H, C-C-H, and O-C-H bending modes present in the acids found in the juice samples [54].

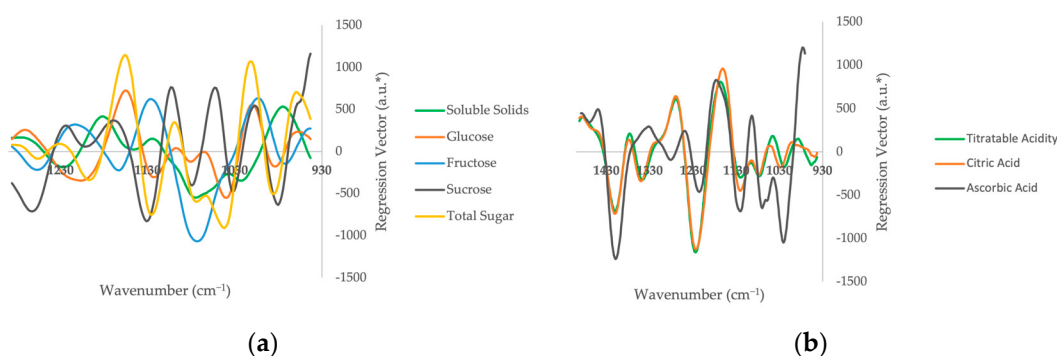


Figure 3. PLS regression vector plots for soluble solids, glucose, fructose, sucrose, total sugars (a), titratable acidity, citric acid, and ascorbic acid (b). a.u.*: arbitrary units.

4. Conclusions

In this study, a field-deployable portable FT-IR sensor, requiring no sample preparation, was utilized to simultaneously predict multiple quality traits in 68 fruit juice samples from the USA markets. Employing partial least square regression (PLSR) models, our results demonstrated a robust correlation ($R_{CV} \geq 0.93$) between FT-IR predictions and reference values, accompanied by a low standard error of cross-validation ($SECV \leq 59.42 \text{ mg}/100 \text{ g}$). Notably, our findings revealed discrepancies of 21% and 37% in fruit juices deviating from the nutritional label values for sugars and ascorbic acid, respectively. Utilizing portable FT-IR devices offers a non-destructive, simultaneous, straightforward, and high-throughput method for the chemical profiling and real-time prediction of sugars and acid levels in fruit juices. The handiness and ruggedness of the FT-IR sensor make it a crucial “out-of-the-laboratory” analytical tool, particularly beneficial for fruit juice processors seeking efficient quality control measures.

Author Contributions: Conceptualization, D.P.A. and L.R.-S.; methodology, D.P.A. and L.R.-S.; validation, D.P.A. and L.R.-S.; formal analysis, D.P.A.; investigation, D.P.A.; resources, L.R.-S.; data curation, D.P.A.; writing—original draft preparation, D.P.A.; writing—review and editing, L.R.-S.; visualization, D.P.A.; supervision, L.R.-S.; project administration, L.R.-S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Acknowledgments: The authors thank Monica M. Giusti (The Ohio State University) for her technical support rendered during this study.

Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A

Table A1. The ingredient list of the analyzed fruit juice samples.

Sample	Ingredients
1	Apples, Fuji apples, ascorbic acid
2	Water, cane sugar, citric acid, green tea, ascorbic acid, natural flavor, ginseng extract
3	Apples, raspberries, ascorbic acid
4	Organic orange juice
5	Water, cane sugar, lemon/orange juice concentrate blend, citric acid, lemon pulp, natural flavors
6	Apples, strawberry, ascorbic acid
7	Mango puree, apple juice, orange juice, banana puree, lemon juice, natural flavor, modified corn starch, sugar, medium chain triglycerides, beta carotene, tocopherols, rosemary extract
8	Organic orange juice
9	Organic unfiltered apple juice
10	Carrot juice, apple juice, lemon juice, cucumber juice, orange juice, vanilla bean, turmeric
11	Water, orange juice concentrate, coconut water concentrate, apple puree concentrate, banana puree, lemon juice concentrate, carrot juice concentrate, peach puree, dextrin, inulin, pectin, natural flavor, vitamins (A, D3, E, B7, B9, B3, B5, B1, B12, B2, B6, C, K1)
12	Organic beet juice, organic carrot juice, organic orange juice, organic lemon juice
13	Pineapple juice, cucumber juice, filtered water, lemon juice, lemon oil
14	Pure filtered water, apple juice concentrate, purple carrot juice from concentrate, strawberry juice from concentrate, pure filtered water, strawberry juice from concentrate, strawberry puree, lemon juice concentrate, natural flavor, apple pectin
15	Pure filtered water, apple juice concentrate, pineapple juice from concentrate, cucumber puree, lemon juice, natural flavor, apple pectin
16	Organic carrot juice, organic apple juice, organic lemon juice
17	Filtered water, unpasteurized lemon juice, cane sugar
18	Mango puree from concentrate, apple juice from concentrate, orange juice from concentrate, banana puree, pineapple juice from concentrate, lemon juice, natural flavors
19	Apple juice, mango puree, orange juice, guava puree, peach puree, strawberry puree, ascorbic acid, natural flavors, acerola juice powder, rosehips powder, zinc oxide
20	Orange juice
21	Unpasteurized grapefruit juice
22	Apple juice, pineapple juice, yellow pepper juice, cucumber juice, lime juice, mint juice
23	Orange and apple juice from concentrate, mango puree, banana puree, natural flavors, lemon juice concentrate, vitamin E, vitamin C, beta carotene, pectin, gellan gum
24	Orange and apple juices from concentrate, peach puree from concentrate, passionfruit, raspberry and pineapple juices from concentrate, guava puree, vitamin C, natural flavors, rose hips, fruit and vegetable juice (for color), lemon juice concentrate, pectin, gellan gum
25	Pomegranate juice from concentrate
26	Organic apple juice, organic carrot juice, organic red beet juice, organic banana puree, organic orange juice, organic pineapple juice, organic lemon juice, organic ground turmeric
27	Apple juice, celery juice, cucumber juice, kale juice, collard greens juice, lemon juice, ginger juice, spinach juice, chlorella powder, spirulina powder
28	Purified water, organic strawberry puree, organic raspberry puree, organic lemon juice, organic honey, organic tart cherry juice from concentrate, probiotic <i>Bacillus coagulans</i> GBI-30 6086, organic stevia leaf extract powder

Table A1. Cont.

Sample	Ingredients
29	Orange juice, pineapple juice, mango puree, apple juice, acerola cherry juice
30	Apple, cucumber, kale, spinach and blueberry juices from concentrate, strawberry puree from concentrate, lemon juice concentrate, natural flavors, fruit and vegetable juice (for color)
31	Pure filtered water, organic cane sugar, organic lemon juice
32	Organic unfiltered apple juice
33	Organic orange juice
34	Filtered water, organic cane sugar, organic lemon juice from concentrate, natural lemon flavor, ascorbic acid
35	Organic orange juice
36	Pomegranate juice from concentrate
37	Organic watermelon juice, organic strawberry juice, organic lime juice
38	Organic pineapple juice, organic cucumber juice, organic raspberry juice, organic lime juice, organic mint juice
39	Organic cucumber juice, organic pineapple juice, organic turmeric root juice, organic lemon juice
40	Orange juice
41	Water, orange juice concentrate
42	Unpasteurized grapefruit juice
43	Filtered water, unpasteurized lemon juice, cane sugar
44	Unpasteurized lemon juice
45	Organic orange juice, organic carrot juice, organic pineapple juice, organic apple juice, organic lime juice
46	Orange juice
47	Filtered water and concentrated apple juice, ascorbic acid, malic acid
48	Pure filtered water, sugar, lemon juice, natural flavors
49	Pure filtered water, cranberry juice, sugar, natural flavors
50	Orange juice
51	Pure filtered water, sugar, lemon juice, raspberry juice, natural flavors
52	Unpasteurized orange juice
53	Fresh pressed apple juice
54	Filtered water, organic evaporated cane juice, organic strawberry puree, organic lemon juice concentrate, organic lemon juice, organic natural lemon flavor, organic fruit and vegetable juices (for color)
55	Filtered water, pineapple juice concentrate, apple juice concentrate, clarified pineapple juice concentrate, orange juice concentrate, banana puree, citric acid, ascorbic acid, natural flavors
56	Filtered water, apple juice concentrate, orange juice concentrate, clarified pineapple juice concentrate, peach puree concentrate, grape juice concentrate, mango puree concentrate, citric acid, beta-carotene (color), natural flavors, ascorbic acid
57	Filtered water, organic orange juice concentrate, organic apple juice concentrate, organic pineapple juice concentrate, organic peach puree, organic grape juice concentrate, organic mango puree, ascorbic acid, natural flavors
58	Orange juice
59	Unpasteurized grapefruit juice
60	Filtered water, white grape juice concentrate, sugar, white cranberry juice concentrate, strawberry juice from concentrate (filtered water, strawberry juice concentrate), fruit and vegetable juice concentrate (for color), citric acid, natural flavors, sodium citrate, ascorbic acid
61	Water, sugar, apple juice concentrate, cranberry juice concentrate, raspberry juice concentrate, grape juice concentrate, fumaric acid, natural flavor, ascorbic acid, vegetable juice concentrate (for color), citric acid, sodium citrate
62	Water, cranberry juice concentrate, grape juice concentrate, apple juice concentrate, pear juice concentrate, natural flavors, ascorbic acid, pectin

Table A1. Cont.

Sample	Ingredients
63	Orange juice
64	Water, apple puree concentrate, apple juice concentrate, blackberry puree, banana puree, strawberry puree, raspberry puree, lemon juice concentrate, blueberry puree, natural flavor
65	Filtered water, mango puree, apple and peach juice concentrates, peach puree, natural flavors, ascorbic acid (for color), beta carotene (for color)
66	Filtered water, organic apple, organic cranberry, and organic pomegranate juice concentrates, organic natural flavor
67	Filtered water, grape, strawberry, peach puree and pineapple juices from concentrate, sugar, citric acid, ascorbic acid, natural flavors, pectin, ester gum, fruit and vegetable juices (color)
68	Filtered water, pineapple, orange and coconut juice concentrates, sugar, natural flavors, citric acid, ascorbic acid, pectin, fruit and vegetable juices (for color)

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