Science and Technology Publishing (SCI & TECH)
ISSN: 2632-1017
Vol. 8 Issue 1, January - 2024

The Physical and Chemical Properties of Some Albanian Fruit Juices Using Analytical and Statistical Methods

Ilirjan Malollari,
Department of Industrial Chemistry,
Faculty of Natural Sciences, University of Tirana, Tirana, Albania, ilirjan.malollari@fshn.edu.al

Terkida Prifti,
Department of Industrial Chemistry,
Faculty of Natural Sciences, University of Tirana, Tirana, Albania,

Gloria Kosova
Department of Industrial Chemistry,
Faculty of Natural Sciences,
University of Tirana, Tirana, Albania

I. ABSTRACT

It is believed that consuming fruits and vegetables keeps us away from hospitals and prolongs our existence while delaying the oxidation process through phyto antioxidants. Natural fruit juices are famous worldwide for their refreshing taste, nutritional value, and potential health benefits. Understanding the composition and properties of these juices is crucial for ensuring their quality and safety and enhancing consumer satisfaction. This essay explores experimental practices characterising natural fruit juices while utilising instrumental techniques alongside statistical analysis methods. The latest news and developments in science, especially in instrumental methods of analysis, have made it possible to know what exactly exists in plants and fruits and how to harmonise them. All these ingredients benefit the human body's health and meet its complex requirements. In addition, people are now more aware of the quality and composition of their consumption. As a result, increased attention is being paid and valued more and more consumption of minimally processed foods. Fruit juices must be treated appropriately, maintaining the essential physical, chemical, and organoleptic characteristics and nutritional value of the fruit from which it comes. The current selection of processing procedure or extraction will vary depending on the structure of the fruit and the type of juice provided.

Keywords—Natural Fruit Juices, Complex Properties, Statistical Analysis, Modelling the Nutrition Value

II. INTRODUCTION

This essay explores the experimental practice of natural fruit juice characterisation, highlighting the importance of instrumental and statistical analysis in assessing their quality [1]. There are a lot of instrumental analytical instruments, such as chromatographic, spectroscopic, and optical techniques, being used for raising awareness about the health benefits and toxicity of fruit phytochemicals, which make us more aware of the fate of the complex characteristics of fruit during extraction processing and liquid storage. Instrumental analysis is vital in determining various aspects of natural fruit juices [2], [3].

One commonly employed technique involves measuring the juice's acidity using pH meters or titration with indicators such as phenolphthalein or bromothymol blue [4] The acidity level provides valuable information about flavour balance and enables the identification of spoilage processes during storage [5],[6].

Natural fruit juices are consumed significantly due to their nutritional value and refreshing taste. However, the quality and composition of these juices can vary considerably depending on factors such as fruit variety, processing methods, and storage conditions. For customer satisfaction, it is essential to characterise and analyse these juices using instrumental and statistical techniques.

The further characterisation includes determining sugar content through refractometry or high-performance liquid chromatography (HPLC) coupled with a UV detector [7]. These approaches provide insights into sweetness levels that significantly contribute to sensory perception. Additionally, analysing vitamin C concentration is crucial due to its antioxidant properties [8], [9]. Spectrophotometric assays utilising dyes like DCPIP are frequently employed for this purpose [10]. By identifying variations in vitamin C levels across different samples or tracking changes over time, manufacturers can monitor product stability related to enzymatic browning reactions [11].

Fruit juices have a very complex composition with several hundreds of substances. In addition to water (80-90%) and common fruit metabolites (e.g.

Carbohydrates, organic acids, amino acids, minerals, vitamins, aromatic compounds) liquids, fruits are characterised by a large number of secondary plant metabolites (otherwise known as "phytochemicals") [12]. The two most prominent groups are polyphenols, including colourful anthocyanins and carotenoids. Therefore, some authors consider fruit juices natural "functional foods" without supplements [13]. Characterising natural fruit juices involves large datasets that can be challenging to interpret. Therefore, implementing appropriate statistical techniques is essential for drawing valid conclusions. Regression models enable relationships between different juice components or physicochemical parameters [14].

A commonly raised question is whether the bio-availability and bio-activity of substances from fruit juice are comparable to those from fruit. It is a significant task of modern technology to transfer the valuable components of the fruit into the fluid and produce sustainable products through physical methods. For some substances, especially plant secondary metabolites, such as carotenoids, bioavailability from liquids is significantly better than from fruits [14]. Fruit juices contain essential vitamins, minerals, and bioactive compounds with many health benefits. In most cases, the mode of action of these fruit juice components is the modulation of gene activity. The health benefits of minerals, vitamins, and micronutrients have been well-characterised. However, many potential beneficial properties of juices have been shown to result from phytochemicals, mainly polyphenols, carotenoids, and limonoids.

III. MATERIALS AND METHODS

The juices were analysed using instrumental techniques such as spectrophotometry, gas chromatography, and HPLC. Gas chromatography analysis identified volatile compounds responsible for each juice's characteristic aroma and flavour. HPLC analysis revealed significant differences in the four juices' sugar and organic acid profiles. For the fruit juice characterisation, a study was performed on four popular fruit juices: Plum Juice (Sample 1), Peach Juice (Sample 2), Apple Juice (Sample 3), and Smothie Carrot + Apple + Peach Juice (Sample 4).
That is why it has been carried out statistical analysis. Statistical analysis is indispensable for interpreting and drawing meaningful conclusions from experimental data. It helps identify significant differences between samples, establish correlations between variables, and predict the behaviour of fruit juices under different conditions (Devolli A, Stafasani M, Shahinasi E, Dara F, Hamiti H., 2021). Techniques such as analysis of variance (ANOVA), principal component analysis (PCA), and regression analysis are commonly employed in fruit juice characterisation studies. ANOVA allows the comparison of means between multiple samples, while PCA helps visualise patterns and relationships among different variables. Regression analysis aids in predicting the concentration of specific compounds based on known variables.

In due course, the involvement of sophisticated fruit selectors and the modelling of their mixture will play a vital role in improving quality assurance and increasing the shelf life of fruit juices.
Moreover, principal component analysis (PCA) aids in identifying patterns and grouping similar samples based on multiple variables simultaneously. PCA provides a comprehensive overview by reducing multidimensional data into lower dimensions while maximising variance representation.
Characterising natural fruit juices using instrumental and statistical analysis methods is critical for ensuring consistent quality standards within the industry. Techniques such as pH measurement, sugar determination, vitamin C quantification, and sensory evaluation provide valuable insights into their composition and complex properties. Manufacturers gain substantial knowledge regarding variations across batches or the effects of different processing techniques on final products' characteristics by employing regression models and PCA analyses.

A. Experimental Practice:

For the study, the objective has considered four samples of cold-pressed fruit juices.
The characterisation of the complex properties of these food liquids has been performed through the following instrumental laboratory analysis:
a. *Free Total Acidity*: Among the four samples, Plum juice has the highest acidity percentage, while apple juice has the lowest acidity. Meanwhile, the acidity values of the apple and the carrot + apple + peach mixture fall in between.
b. *Reducing Sugars*: Comparing the experimental results, sample 3, which is apple juice, has the highest amount of reducing sugars, while sample 2, which is plum juice, has the lowest amount. Meanwhile, apple juice and the carrot + apple + peach mixture have intermediate values. Usually, apples have high sugar content, and the low amount of sugar in the apple juice may be because the fruit might not have reached full maturity at harvest.
c. *Sucrose content*: Based on the results, the carrot + apple + peach mixture has the highest sucrose content, followed by apple juice, and finally, plum juice and apple juice have the same sucrose content. Plum juice has the highest formaldehyde units, while apple juice has the lowest. This means that the number of free carboxylic acid groups of amino acids present is higher in apple juice and lower in plum juice. A high amount of free carboxylic acid groups is also found in the carrot + apple + peach mixture, while a lower amount is found in plum juice.
d. *Formol Number:* Plum juice has the highest specific gravity, while apple juice has the lowest. The carrot + apple + peach mixture and apple juice have intermediate values, with the carrot + apple + peach mixture having a lower specific gravity. Plum juice has

the lowest pH, which its high acidity can explain. The carrot + apple + peach blend has the highest pH, likely due to the generally higher pH of carrot juice, which can go up to 6, unlike the other juices that range up to 4.5. The other two juices have intermediate values, with apple juice having a higher pH than plum juice (see Fig. 2).

e. *Refraction Index and C vitamin*

The analytical results show that plum juice has the highest vitamin C content, followed by the carrot + apple + peach mixture, apple juice, and peach juice with the lowest vitamin C content. Another interpretation could be that plum juice has the highest antioxidant activity while apple juice has the lowest.

f. *Microbiological content of fruit juices:* After a 2-day incubation in the thermostat, the PCA and Mac Conkey media resulted in no growth, indicating no different microorganisms were found. This implies that the treatment of fruit juices before packaging was done appropriately.

IV. RESULTS AND DISCUSSION

Table 1 shows a Summary of statistics for all parameters considered and experimentally practised. In Table 2, there are all complex datasets profiled by all series of analyses for characterised fruit juices.

Table 1 Summary statistics for all parameters considered and experimentally practised

Variable	Obser-vations	Minimum	Maximum	Mean	Std. deviation
Refraction Index (%)	4	11.700	13.200	12.308	0.708
Total Free Acidity (%)	4	0.350	0.630	0.508	0.116
pH	4	2.900	4.300	3.765	0.605
Specific Gravity	4	1.050	1.058	1.055	0.004
Reducing Sugars (mg)	4	52.400	207.800	146.675	72.344
Sucrose (%)	4	6.530	11.090	7.968	2.156
Formole Number	4	7.000	12.000	9.250	2.217
C Vitamine (mg)	4	8.980	13.700	10.800	2.073

Table 2 Complex dataset that profited from all analyses of fruit juices' characterisation.

Fruit Juice	Refraction Index (%)	Total Free Acidity (%)	pH	Specific Gravity	Reducing Sugars (mg)	Saharoze (%)	Formole Number	C Vitamine (mg)
Plum	13.2	0.63	2.9	1.0579	198.8	6.53	8	15.85
Peach	11.7	0.525	3.8	1.0548	52.4	7.72	12	10.6
Apple	12.5	0.35	4	1.0497	207.8	6.53	7	9.72
Mixture	11.8	0.49	4.3	1.0562	127.7	11.09	10	10.8

A. ***Statistical processing:*** PCA (Principal Component Analysis)

Principal Component Analysis is a dimensional reduction method often used to reduce the dimensionality of a large data group by transforming a large group of variables into a smaller one while retaining most of the information from the original dataset. Reducing the number of variables comes with some loss of accuracy, but the trade-off in dimensional reduction is to sacrifice some accuracy for simplicity. The idea behind PCA is simple - reduce the number of variables in a dataset while preserving as much information as possible. Discriminant Analysis - Methods, Types and Examples. https://researchmethod.net/discriminant-analysis/

The first step of PCA analysis is *standardisation,* which means that if there are significant differences between the values of the original variables within the same variable or even concerning other variables, they will dominate over those with slight differences. Therefore, transforming the data into comparable data makes the comparison problem easier. Once standardisation is done, all variables will be converted to the same scale.

Calculating the Covariance Matrix means that if it is positive, two variables increase or decrease together (a positive correlation). If negative, one increases when the other decreases (a negative correlation). The covariance matrix is nothing more than a table that summarises the correlations between all possible combinations of variables.

Calculation of Eigenvectors and Eigenvalues of the Covariance Matrix to Identify Principal Components. Eigenvectors and eigenvalues are the magic of principal components because the covariance matrix's eigenvectors are essentially the axes' directions where there is more variance (information), which we call principal components. Moreover, eigenvalues are just coefficients attached to eigenvectors, giving the variance retained in each principal component. By arranging the eigenvectors according to the eigenvalues, from highest to lowest, we take the principal components according to their significance.

Principal components are new variables constructed as linear combinations or mixtures of the original values. These combinations are made so that the new variables (principal components) are uncorrelated, and most of the information within the original variables is placed in the first components. The idea is that the 10-dimensional data gives ten principal components. However, PCA tries to put the maximum possible information in the first component, then the maximum of the remaining information in the second component, and so on. Organising the information into principal components allows us to reduce dimensionality without losing much information by eliminating components with low details and considering the remaining components as new variables. Principal components are less interpretable and have no real meaning since they are constructed as a linear combination of the original values. Geometrically, principal components represent the

Science and Technology Publishing (SCI & TECH)
ISSN: 2632-1017
Vol. 8 Issue 1, January - 2024

directions of the data and explain a maximum amount of variance, which means that the lines capture more data information. The relationship between variance and information is that the higher the variance retained by a line, the more spread of data points along it, and the more spread along a line, the more information it has.

PCA Data Processing

In the Observations/variables table, we select the variables we want to analyse, in this case, all of them, starting from refractive index to vitamin C. In the data format, we choose the Observations/variables table, and for the type of PCA, we select Correlation (Plumson). The type of PCA to be used during calculations will be the correlation matrix, which corresponds to the Plumson correlation coefficient. There is an analysis output we select to activate the option to display significant correlations in bold (Test significance). Here, we need to determine which axes will represent the Graph. In this case (see Table 3), we notice that the Variability presented by the first and third factors has a low percentage (63.29%). To avoid misinterpretation, we plot the results using the first two factors with higher rates (89.62%).

Table 3 Squared cosines of the variables:

	F1	F2	F3
Refraction Index (%)	**0.934**	0.060	0.007
Total Free Acidity (%)	0.001	**0.991**	0.008
pH	0.421	**0.461**	0.118
Specific Gravity	0.012	**0.917**	0.070
Reducing Sugars (mg)	**0.887**	0.042	0.071
Sucrose (%)	0.428	0.002	**0.570**
Formol Number	**0.848**	0.111	0.040
C Vitamin (mg)	**0.808**	0.000	0.192

Significant correlations are shown in bold. The correlation coefficients range from -1 to 1. The closer to 1 or -1, the stronger the relationship between the two variables. Negative values indicate a negative correlation, and positive values indicate a positive correlation. Values close to 0 indicate no correlation between variables. In this case, we have positive correlations between refractive index and reducing sugars, free total acidity, and specific gravity. We can mention formaldehyde and reducing sugars, refractive index, and pH in negative correlations.

Table 4. Eigenvalues, % of Variability, Cumulative % through Principal Component Analysis

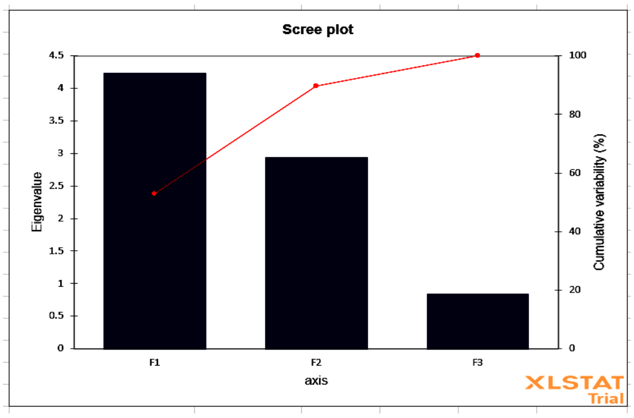
	F1	F2	F3
Eigenvalue	4.233	2.937	0.830
Variability (%)	52.910	36.713	10.377
Cumulative %	52.910	89.623	100.000

Table 4 contains eigenvalues, which reflect the projection quality from an N-dimensional original table to a smaller number of variables. Eigenvalues can also be used to determine the number of principal components. For example, only those principal components with eigenvalues greater than one are selected using the Kaiser criterion.

The first eigenvalue, equal to 4.233, represents 52.910% of the total variance. This means that if we define the data only on one axis, we can still see 52.910% of the total variance of the data. Each eigenvalue corresponds to a factor, and each element corresponds to a dimension. A factor is a linear combination of the original variables; all factors are uncorrelated.

Eigenvalues and corresponding factors are ranked according to a descending rule representing how much of the original variance they explain.

Variability expresses the proportion of Variability in each principal component's data (as seen in Graph 1). The higher the ratio, the more Variability that the principal component expresses. The magnitude of the ratio helps determine if the principal part is significant enough to retain. The cumulative balance helps determine the number of principal components to be used. The first two axes represent approximately 90% of the original Variability.



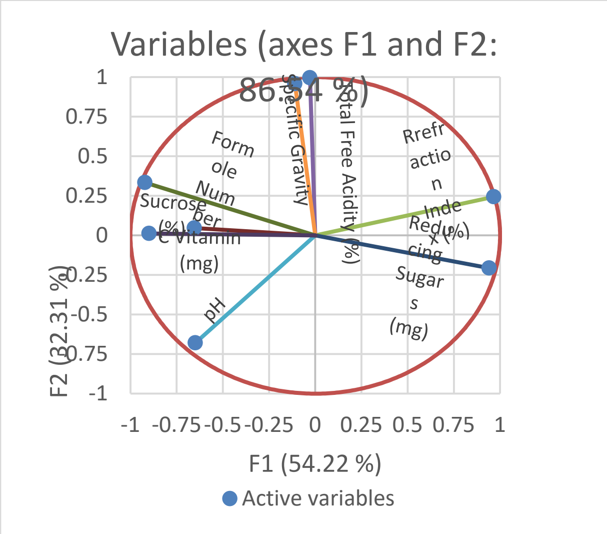
Graph 1. Eigenvalue Variance vs. Cumulative % of Variability

Ideally, the first two eigenvalues correspond to a high % of the variance, assuring us that the Graph based on the first two principal components is a good-quality projection of the multidimensional original table. In this case, the first two factors represent 89.623% of the original Variability of the data.

The magnitude and direction of the original variables' coefficients are determined to interpret each principal component. The larger the absolute value of the coefficient, the more critical the corresponding variable is in the calculation of the element. In the case of the first principal component, we see that it has a significant positive relationship with refractive

index and reducing sugars and a negative relationship with pH.
At the same time, the second principal component has a largely positive relationship with total free acidity, specific gravity, and formal number.

Factor loadings represent the coordinates of the correlation circle (as seen in Graph 2). The correlation coefficients are equivalent to the factor loadings in the case of a classic PCA analysis.



Graph 1. Correlation Circle

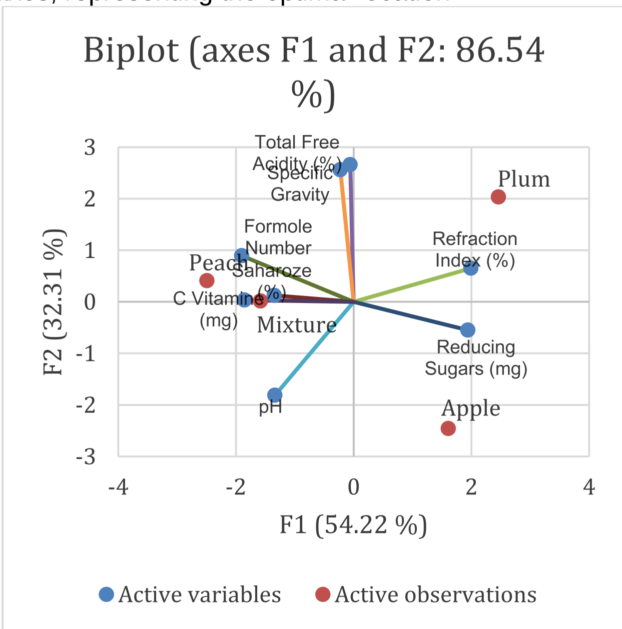
The first Graph is called the correlation circle. It represents the projection of the original variables into the space of the principal components. The horizontal axis is the first dimension of PCA, and the vertical axis is the second dimension of PCA. The red vectors represent the studied variables. The length of the vectors represents the representativeness in the dimensions of PCA. If a variable has a short vector length in sizes F1 and F2, then its information is likely better represented in other dimensions of PCA, possibly F3. In our case, the information about sucrose might be better represented in dimension F3. The interpretation here is done using the terms of angles:

- An acute angle represents positively related variables. In this case, we have total free acidity and specific gravity, formol number and sucrose, refractive index and reducing sugars.
- A right angle represents variables that are not related to each other. In this case, we have specific gravity with reducing sugars and sucrose with total free acidity.
- An obtuse angle represents negative relationships. We have pH and invert sugars, pH and refractive index, vitamin C and invert sugars, and formol number with vitamin C.

To confirm that a variable is well related to an axis, we consider the results of squared cosines (as seen in the respective Graph, the more significant the cosine squared, the greater the relationship with the corresponding axis. About the first axis, we find that the refractive index, pH, and vitamin C are well related to this axis. (see Graph 3). In contrast, the second axis is well associated with total free acidity, specific gravity, reducing sugars, and formal number.

V. CONCLUSIONS

The last comprehensive and determining Graph is essential for evaluating samples and their indicating parameters. It can be concluded that:
The bi-dimensional representation within the two axes (F1 and F2) shows scattered points, and at first glance, they are almost close to the centre of the axes, representing the optimal location.



Graph 3 Biplot Correlation Circle with two axes, F1 and F2, the distribution of the samples and studied variables.

1. The spatial comparison between the studied samples (blue dots) is done about axes F1 and F2, where the values of the squared cosines determine the weight of each sample in the corresponding axes. The derived tables and graphs found that apple juice, peach juice, and carrot + apple + peach mixture juice have the largest share of distributed information along axis F1, while apple juice has the largest share along axis F2. Among the four fruit juices, apple and apple + peach have the most significant values, which means that the importance of the studied variables of these samples has the most weight toward optimal values.

2. The variables' information distribution is also done along axes F1 and F2. Along axis F1, the highest information weight is concentrated in the refractive index, pH, and vitamin C variables. In contrast, along axis F2, we have total free acidity, specific gravity, reducing sugars, and formal number variables. Values close to the optimal value are better represented along axis F1 for refractive index, pH, specific gravity, total free acidity, and vitamin C.

3. The reference and determining values for both axes (F1 and F2) for samples and variables should have the highest cosine squared values.

Therefore, the conclusions from the analysis of the comprehensive Graph are as follows: The determining parameters for modelling and obtaining an optimal mixture of fruit juice are refractive index, pH, and vitamin C for apple juice, and total free acidity and specific gravity for apple + peach juice since these have the most significant values.

VI. REFERENCES

[1] Build your beverage empire (2020) https://newloadslaiw.firebaseapp.com/wubbel22955ru/103405.html

[2] Anon (2003b). *Fruit Juice and fruit nectars (England) regulations 2003*. 2003 SI 1564.Drinks and Beverages | Artisan Food Law. https://artisanfood.law/blog/drinks-and-beverages

[3] Anon (2006b). EU regulation 2006, 1924 Nutrition and health claims regulations.

[4] Anon (2010a). *IFU Compendium of Analytical Methods for Fruit Juices and Nectars*. International Fruit Juice Union, France. (http://www.ifu-fruitjuice.com).

[5] Anon (2011b). *AIJN Code of Practice for fruit juices*. Available for a fee from AIJN, Rue de la Loi 221, boîte 5, B- 1040, Brussels or from their website (http://www.aijn.org).

[6] Clark A.C., Ferruzzi M.G.(Eds.) (2018). Nutritional Composition of Fruit Juices.

[7] Smith K.M., Johnson L.D., Clark (Khachatoorian), García.-D.&W.Y.ZANSARY, M (Taylor and Mimi (Mersch) (2020)). Handbook for Sensory Evaluation: Identification Methods

[8] Williams JW, Cooper D, Wallace T(2019). "Fruit and Vegetable Phytochemicals: Chemistry and Human Health.

[9] Wu, Yinggeng, et al. "Rapid Discrimination of Organic and Non-Organic Leafy Vegetables (Water Spinach, Amaranth, Lettuce, and Pakchoi) Using VIS-NIR Spectroscopy, Selective Wavelengths, and Linear Discriminant Analysis." Applied Sciences, vol. 13, no. 21, 2023, p. 11830.

[10] George MJ, Moiloa LV: Determination and Comparison of Physico-chemical Properties of Home-made Juices in Lesotho and Commercial Juice Available in the Local Markets. American Chemical Science Journal, 2015; 5(3), 247-252

[11] Leahu A, Damian C, Oroian M, Ropciuc S: Physico-Chemical Parameters of Fruit Juices - Evolution During Storage. Lucrari Stiintifice-Seria Zootehnie 2013, 59, 213-217.

[12] Devolli A, Stafasani M, Shahinasi E, Dara F, Hamiti H: Determination of vitamin C content in commercial fruit juices by volumetric and spectrophotometric methods. Journal of Hygienic Engineering and Design, 2021, Vol. 34, 124–131.

[13] Hashemi, Seyed M. B., and Dornoush Jafarpour. "Ultrasound and Malic Acid Treatment of Sweet Lemon Juice: Microbial Inactivation and Quality Changes." Journal of Food Processing and Preservation, 2020, https://doi.org/10.1111/jfpp.14866.

[14] Ujan, Sahar, et al. "Hierarchical Classification Method for Radio Frequency Interference Recognition and Characterization in Satcom." Applied Sciences, vol. 10, no. 13, 2020, p. 4608.