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Quantification and Chemometrics Characterisation of Nutritional Data of Selected Raw and Branded Tomatoes

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Abstract

Tomatoes offer great nutritional and health benefits to humans. The nutritional, physical, and chemical characteristics of tomatoes in raw and company processed forms were evaluated for their nutritional qualities. Three varieties of raw tomatoes and ten brands of processed tomatoes were sampled. The proximate, vitamins, and phenolic composition, as well as Physico-chemical parameters, were carried out using standard techniques. The datasets were subjected to both statistical and Chemometrics techniques.The proximate values (%) were in ranges of: Fat (0.29 – 11.31); Protein (6.65 – 20.15); Fibre (0.92 – 15.70) Ash 0.08 –3.18); Carbohydrate (53.07 – 80.53). The physicochemical parameters values are in ranges: pH (2.25–4.83); Conductivity (3.73 –12.97), Titratable acidity (0.11 –1.07); Total soluble solids (15.23–40.70). The vitamins and phenolic values are in ranges: Vitamin A (0.47 –8.20); vitamin C (1.31–18.49); Phenolic (0.041– 0.360). The raw tomatoes have a more prominent content of vitamin C. With the aid of biplot(loading/score) of the Principal Component Analysis (PCA), the Zaria and Minna varieties as well as processed brands (5, 7, and 10) are characterized by substantial carbohydrate content. The dendrogram of Hierarchical Cluster Analysis (HCA) revealed closed substitutability of Kano variety and brand 5, as a result of both samples having equivalence of nutritional content. This suggests that brand 5 got its raw tomato from Kano varieties and could therefore be used as a substitute of each other when consumption choice has to be made.

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Introduction

Tomatoes are valued vegetables that are widely consumed for their healthy and beneficial nutritional content (Eke-Ejiofor, 2015). Tomato (*Lycopersicon esculentum)* belongs to the *solanaceae,* tomatoes which are cultivated widely in home gardens and large farms for fresh consumption and commercial processing (Aditi*et al*., 2011). It is typically over 90% water and, once they are harvested, begins to undergo higher rates of respiration, resulting in moisture loss, quality deterioration, and potential microbial spoilage (Abdullahi*et al*., 2016).

Tomato has many nutrients with secondary metabolites that are important for human health (Demirbas, 2010 and Katırcı*et al*., 2018). Its consumption reduces the risk of certain types of cancer, cardiovascular, osteoporosis, and chronic degenerative diseases (Bhowmik*et al*., 2012; Hernández *et al*.2008 and Chang *et al*., 2006). The unique mineral contents are a pointer to the benefits offered by the tomatoes (Demirbas, 2010; Hernández *et al*., 2008 and Melø *et al*., 2008).

The proximate content of foods plays an important role in predicting their nutritional values. Fats, proteins, and carbohydrates constitute the major structural components of foods. Carbohydrates are a vital source of energy for most organisms, including humans. Moisture content information is a useful measurement in the storage, processing, and preservation of food. Proteins are organic compounds essential for body repair and health maintenance. Ash content is an inorganic residue remaining after the complete oxidation of organic matter. Ash value is an indication of mineral presence (Idris *et al*., 2019; Okello *et al*., 2018 and Salau *et al*., 2012).

The major quality perception of fruits is hinged upon the measures of the physicochemical properties such as pH, total soluble solids, and titratable acidity (Tehranifar *et al*., 2010). These values are indicators of maturity, storage capacity, spoilage, flavour, and taste (Zhao *et al*., 2020; Deng *et al.,* 2019 and Tehranifar *et al*., 2010).

Antioxidants are chemical agents that inhibit the destructive and pathogenic tendency of oxidation in the living system. In oxidation, free radicals are formed analogously to reactions of scavenging nature. Foods and other biological systems experience lipid pre-oxidation, autoxidation processes, and other types of oxidations. Food antioxidants in foodstuffs can protect them from these attacks, conserving their consumption safety properties organoleptic properties, and texture (Carocho *et al*., 2018).

Chemometrics is the use of mathematics and statistical method to improve the understanding of chemical information. It is applied to solve descriptive and predictive problems in chemistry (Brereton *et al*., 2018). Chemometrics is a veritable tool in the interpretation, analysis, and visual presentation of complex multivariate data (Munck *et al*., 1998). Its use in food chemistry has assisted in obtaining better information about the composition of a food product as well as its physical and chemical properties (Salau*et al*., 2020; Salau and Hasan, 2019, Hassan *et al.*, 2019, Salau and Hasan, 2018 and Salau *et al*., 2018).

The chemometrics methods involve the selection of data, the building of suitable models and adapting the model to give solutions to complex data problems (Munck *et al*., 1998). Unsupervised pattern recognition techniques of chemometrics such as the Cluster Analysis (CA) and Principal Component Analysis (PCA) are much revealing in terms of groupings and close neighborhood of the food sample respectively. Chemometrics has been extensively applied to varying categories of food samples (Salau and Hasan, 2019).

Materials and Methods

Sample collection

Three species of raw tomatoes which include Kano-India species, Minna-Gwari species, and Zaria species and ten brands of company processed tomatoes designated as Brand1 to 10 were sampled in triplicates across markets in Minna city.

Sample preparation

The raw tomatoes were cleaned, weighed, and then divided into two parts and their hardness and pH were determined using a durometer and potentiometer respectively. The one part was blended into a paste and moisture was determined while the other part on which vitamins analysis was to be carried out was then sliced using a sharp knife which was then dried. The dried tomato was crushed into a powder using a clean mortar and pestle. The powdered sample was then stored at room temperature before the analysis. For the processed tomato, the tomato paste was also divided into two parts; one part was used for moisture determination while the other part was dried for vitamin determination. The dried samples were stored at room temperature for analysis.

Proximate analysis

Proximate analysis for crude fat, crude protein, crude fiber, carbohydrate, and ash content were carried out according to the method described by Abdullahi *et al.* (2016) and Joel *et al.* (2020).

Analysis of phenolics and vitamins

The phenolic content was determined by the Folin-Ciocalteu method as described by Katırcı *et al.* (2018) while Vitamin A and C were determined according to the method described by Abdulahi *et al.*(2016).

Physico-chemical parameters

The pH and titratable acidity determinations were done using the method described by Joel *et al*. (2020), Total solid was obtained by difference (100-moisture content) as described by (Eke-Ejiofor, 2015), Moisture content was determined by the difference between the accurately weighed samples before and after drying in an oven at 105 °C as described by Abdullahi *et al.*(2016) while the determination of electrical conductivity of the tomato samples was carried out using a conductivity meter.

Statistical analysis

The statistical package of social sciences (SPSS) software version 21.0 was used. The results were evaluated using analysis of variance (ANOVA) and were presented as the mean value ± SD (standard deviation of the mean) for the samples. Differences among the means were assessed using Duncan's Multiple Range Test to determine which mean values were significantly different at $p<0.05$.

Chemometrics analysis

Chemometrics software package, The Math works Incorporations' MATLAB version 4.0 for windows, and the Eigenvectors Research Incorporations' PLS_ Toolbox version 6.2 were used for PCA and CA.

Results and Discussion

The physicochemical parameters

The nutritional, physical, and chemical parameters of three species of raw and ten brands of processed tomatoes differed significantly ($p<0.05$) due to different varieties and brands.

Table 1 shows the physical and chemical parameters (%). The physicochemical parameters values are in ranges. pH (2.25–4.83) with brand 4 having the least and brand 10 the highest. The pH (2.25–4.83) indicated the hygienic qualities of raw and processed tomato brands (CAC, 2011). Conductivity (3.73–12.97) with Kano-India species having the least and brand 5 the highest. The highest electrical conductivity was found with processed brands. This could be as a result of the processing mechanism. Titratable acids (0.11–1.07) with brand 9 having the least and brand 7 the highest. Titratable acidity (0.11–1.07) did not exceed the maximum acidity

(7%) recommended by Codex Alimentarius Commission (CAC, 2011). Total soluble solids (15.23–40.70) with brand6 having the least and brand7 the highest. The total soluble solid (15.23–40.70) of the samples were higher than the standard level of 20 to 22% required by the Codex Alimentarius Commission (CAC, 2011). The higher total soluble solid might be due to lower moisture content as reported by Eke-Ejiofor (2015).

Table 1: Physico-chemical properties of the tomato samples

S/N	Sample	pH	Conductivity uS/cm	Titratable Acids (%)	Total Soluble Solids
1	KI	4.79±0.01^{e}	3.73±0.01^{a}	0.41±0.01^{a}	28.42±0.01^{k}
2	MG	4.85±0.01^{h}	5.72±0.01^{d}	0.77±0.01^{b}	18.17±0.02^{h}
3	ZU	4.79±0.00^{f}	6.48±0.00^{f}	0.41±0.01^{a}	15.81±0.01^{d}
4	B1	4.78±0.01^{e}	8.87±0.01^{i}	0.18±0.00^{a}	17.53±0.01^{g}
5	B2	4.68±0.00^{c}	6.72±0.00^{g}	0.31±0.01^{a}	18.65±0.01^{i}
6	B3	4.86±0.01^{h}	8.34±0.00^{h}	1.02±0.01^{b}	15.21±0.01^{b}
7	B4	2.25±0.00^{a}	9.87±0.00^{k}	1.02±0.01^{b}	17.27±0.01^{e}
8	B5	4.72±0.00^{d}	12.97±0.00^{m}	1.04±0.00^{b}	15.23±0.03^{a}
9	B6	4.56±0.00^{b}	6.36±0.00^{e}	1.04±0.00^{b}	15.61±0.01^{c}
10	B7	4.86±0.01^{h}	5.25±0.00^{c}	1.07±0.00^{b}	40.61±0.01^{l}
11	B8	4.73±0.01^{d}	9.03±0.01^{j}	1.02±0.01^{b}	18.15±0.05^{h}
12	B9	4.88±0.01^{i}	9.92±0.00^{l}	0.11±0.01^{a}	19.01±0.01^{j}
13	B10	4.83±0.00^{g}	3.93±0.00^{b}	0.44±0.03^{a}	17.41±0.01^{f}

Values are reported as mean ± standard error of means. Values with the same letter on the column are not significant while values on the same column with different alphabetic superscripts are significant at $p \leq 0.05$ DMRT test. Key: KI = Kano-India variety, MG = Minna-Gwari variety, ZU= Zaria- UTC variety, B1–B10 are processed tomato brands 1-10

Proximate Composition

Table 2 shows proximate composition (%). The proximate values are in ranges: Moisture (0.74–11.84) with brand 7 having the least and brand 6 the highest. The moisture contents values (0.74 – 11.84) with brand 5 having the highest moisture. These were low compared to the values (69.00 – 84.85%) reported by Eke-Ejiofor (2015). These decreases in the moisture of the processed tomatoes increase the shelf life, hence being beneficial to the consumers (Joel *et al*., 2020). Crude fat (0.29–11.31) with brand 3 having the least fat and Minna-Gwari species the highest (11.31%). The fat content of the fresh tomato (Minna-Gwari species) is higher than all the processed brands and as well as its raw counterparts. The reason might be due to different geographical locations and differences in processing methods. Crude protein (6.66–20.15) with brand1 having the least and Minna-Gwari species the highest. The crude protein was higher in some of the raw than all the processed brands. The difference in crude protein contents could be attributed to species differences as well as differences in the processing conditions of the pastes. The higher protein content of the raw tomato in this study is at variance with the one reported by Abdullahi *et al*. (2016) as his study was based on processed tomato. Crude fiber (0.92–15.70) with brand 10 having the least and brand 8 the highest; Ash (0.08–3.18) with brand 10 having the least and brand 5 the highest. The ash content in both raw and processed brands differed significantly, however, one of the processed tomatoes has higher ash content than others. This might be as a result of the addition of salt to the processed and high water content of the raw. The crude fiber content of raw tomato is significantly lower than the processed brands' tomato. This could be a result of the high water content of the raw tomato. Abdullahi *et al.*(2016) reported a similar observation. Carbohydrate (53.07–80.53) with Kano-India species having the least and brand 3 the highest. The Carbohydrate percentage content in the raw tomato is lower than the processed brands. This might be as a result of high water contents in raw tomatoes.

Table 2: Proximate composition of tomato samples

Samples	Moisture (%)	Crude Fat (%)	Crude Protein (%)	Crude Fibre (%)	Ash (%)	Carbohydrate (%)
KI	4.77±0.01^{b}	9.08±0.00^{f}	19.26±0.01^{k}	11.57±0.01^{i}	2.28±0.00^{j}	53.07±0.00^{a}
MG	5.68±0.01^{d}	11.31±0.00^{m}	20.15±0.01^{l}	3.91±0.01^{e}	2.26±0.05^{j}	56.68±0.00^{c}

ZU	5.78±0.01^{e}	9.81±0.00^{l}	13.35±0.05^{i}	1.03±0.01^{b}	1.43±0.00^{f}	68.58±0.00^{i}
B1	7.93±0.01^{j}	9.11±0.00^{g}	6.66±0.01^{a}	2.92±0.01^{d}	2.01±0.00^{i}	71.39±0.00^{k}
B2	8.18±0.01^{k}	9.67±0.00^{i}	11.39±0.01^{g}	11.68±0.01^{j}	1.54±0.00^{g}	68.96±0.00^{j}
B3	5.47±0.01^{c}	0.29±0.00^{a}	10.07±0.01^{d}	2.60±0.00^{c}	1.07±0.00^{d}	80.53±0.00^{m}
B4	7.03±0.01^{h}	8.57±0.00^{d}	9.19±0.01^{c}	6.75±0.01^{h}	1.46±0.00^{f}	66.91±0.00^{h}
B5	8.37±0.01^{l}	9.73±0.00^{k}	10.07±0.01^{d}	11.94±0.01^{k}	3.18±0.00^{k}	56.73±0.00^{d}
B6	11.84±0.01^{m}	6.82±0.00^{b}	8.32±0.01^{b}	11.94±0.01^{k}	0.86±0.00^{c}	60.25±0.00^{e}
B7	0.74±0.01^{a}	8.58±0.00^{e}	10.51±0.01^{e}	3.94±0.01^{f}	0.52±0.00^{b}	75.74±0.01^{l}
B8	7.52±0.01^{i}	9.73±0.00^{j}	10.94±0.01^{f}	15.61±0.01^{l}	1.69±0.00^{h}	54.45±0.00^{b}
B9	5.99±0.01^{f}	9.19±0.00^{h}	12.26±0.01^{h}	4.23±0.01^{g}	1.39±0.01^{e}	66.98±0.00^{g}
B10	6.52±0.01^{g}	7.76±0.00^{c}	17.93±0.01^{j}	0.92±0.01^{a}	0.08±0.00^{a}	66.79±0.01^{f}

Values are reported as mean ± standard error of means. Values with the same letter on the column are not significant while values on the same column with different alphabetic superscripts are significant at p≤0.05 DMRT test

Key: Kano = Kano-India variety, Minna =Minna-Gwari variety, Zaria= Zaria UTC variety

Anti-oxidant vitamins and phenolic compounds

Phenolic and vitamins (antioxidants) are shown in Table 3. The highest value of vitamin A, C, and Phenolic were found in Brand 9, Kano-India species, and Brand 7 respectively. Vitamin A, C, and Phenolic are important quality parameters used in assessing tomato paste. They act as antioxidants, preventing the oxidation of some fatty acid components, and play an important vital role in the body's metabolism.

Table 3; Antioxidants content of the tomato samples

Samples	Vitamins A (mg/100g)	Vitamins C (mg/100g)	Phenolic content (mg/100g)
KI	0.47±0.00^{a}	18.49±0.01^{j}	0.25±0.01^{f}
MG	1.28±0.02^{d}	10.60±0.10^{h}	0.11±0.00^{d}
ZU	1.93±0.00^{g}	15.89±0.01^{i}	0.16±0.00^{c}
B1	1.89±0.00^{f}	2.61±0.01^{b}	0.20±0.00^{d}
B2	3.57±0.00^{i}	1.31±0.01^{a}	0.46±0.00^{j}
B3	1.06±0.00^{c}	7.81±0.01^{f}	0.04±0.00^{a}
B4	4.28±0.00^{j}	7.91±0.01^{f}	0.24±0.00^{f}
B5	5.62±0.00^{k}	8.51±0.01^{g}	0.12±0.00^{b}
B6	0.76±0.00^{b}	5.31±0.01^{e}	0.22±0.02^{e}
B7	1.81±0.00^{e}	4.62±0.02^{d}	0.36±0.00^{i}
B8	6.55±0.00^{l}	5.35±0.05^{e}	0.32±0.00^{g}
B9	8.20±0.00^{m}	3.81±0.00^{c}	0.34±0.00^{h}
B10	2.32±0.00^{h}	2.65±0.05^{b}	0.32±0.00^{g}

Values are reported as mean ± standard error of means. Values with the same letter on the column are not significant while values on the same column with different alphabetic superscript are significant at p≤0.05 DMRT test.

Key: KI = Kano-India variety, MG = Minna-Gwari variety, ZU= Zaria UTC variety, zB1–B10 are processed tomato brands 1-10.

Principal component analysis

PCA Biplot for physicochemical parameters

The studied physicochemical parameters data has a computational matrix of dimension (13 X 4). It was auto-scaled before applying the PCA procedure. Ward’s method was followed (Salau and Hasan, 2019). Two principal components resulted from the pre-processed data. These two principal components retained the maximum variability of the food samples. The PCA biplot in Figure 1 is a simultaneous loading and score plot. The biplot reveals the correlation of the physicochemical parameters with tomato samples. It is revealed in Figure 1 that samples 13 and 8 are characterized by acidity and conductivity respectively.

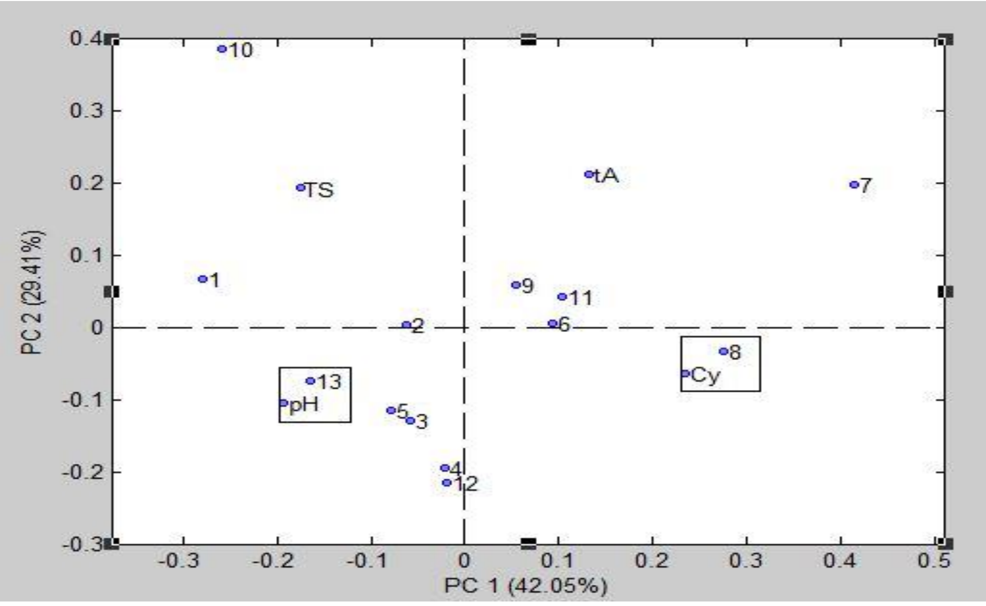

Figure 1: PCA Biplot (Score/Loading) of physico-chemical properties of tomato samples
Key ; 1 : Kano variety, 2 : Minna variety, 3 : Zaria variety, 4 : Brand 1, 5 : Brand 2, 6 : Brand 3, 7 : Brand 4, 8 : Brand 5, 9 : Brand 6, 10 : Brand 7, 11 : Brand 8, 12 : Brand 9, 13 Brand 10 and TS : Total soluble, tA : titratable acidity, Cy : vitamin C.

PCA Biplot for antioxidant and proximate composition

The antioxidant and proximate Compositiondata has a computational matrix of dimension (13 X 9) and 2PCs are retained. In Figure 2, it is observed that brand 4 and brand 9 are characterized by high Crude fat, Ash, Vitamin A and Moisture are at the positive plane (0.0 to 0.5 weighting values) of the PC1. Similarly, Brand 8 is characterized by Crude fiber which is crowed at the negative and opposite plane of the biplot. The brand displays anti-correlation behaviour relative to other samples

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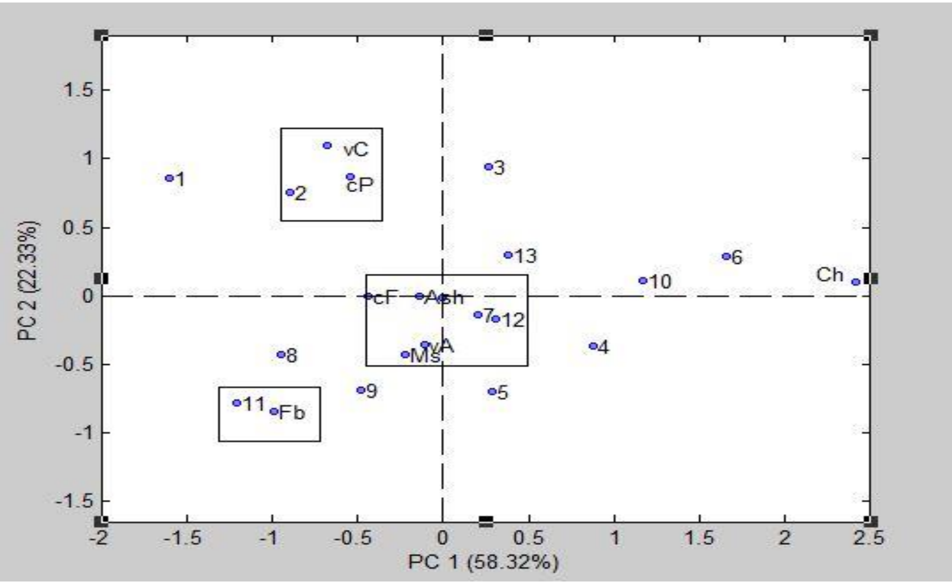

Figure 2: PCA Biplot (Score/Loading) for Antioxidant and Proximate Composition of tomato samples
Minna variety is characterized by Vitamin C and Crude protein. while samples (1, 3, 4, 5, 6, 8, 9, 10, and 13) have moderate content as they could not be correlated with any of the nutritional contents.

Hierarchical Cluster Analysis

The similarity and closeness of the foods are illustrated by cluster analysis (Brereton *et al*., 2018). Hierarchical Cluster Analysis was performed on all the nutritional datasets. The output is illustrated in form of a dendrogram which is presented in Figure 2. The similarities or closeness of the foods are measured by the variances of the weighted distance between the centers of clusters. Ward's method was adopted (Salau and Hasan, 2019).

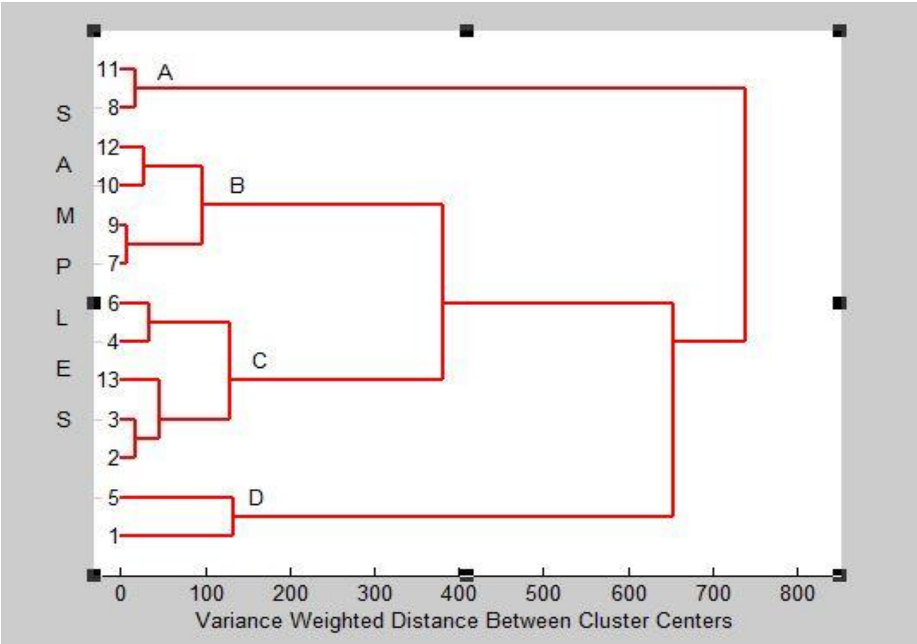

Figure 3: HCA dendrogram for all the studied nutritional datasets of tomato samples
Key ; 1 : kano variety, 2 : Minna variety, 3 : Zaria variety, 4 : Brand 1, 5 : Brand 2, 6 : Brand3, 7 : Brand 4, 8 : Brand 5, 9 : Brand 6, 10 : Brand 7, 11 : Brand 8, 12 : Brand 9, 13 Brand 10.

Four major groupings A, B, C, and D of 2, 4, 5 and 2 membership sizes respectively, can be observed based on the similarity of foods in each grouping. Cluster analysis on the samples reveals information about closely related foods which can be predicted as a substitute. Three close substitute pairs revealed are (9 and 7) > (8 and 11) > (2 and 3). Each of the pairs is equivalent in terms of nutritional content. Consumption of Minna variety (2) is of the same quality as consuming Zaria (3) variety. In cases of non-availability or dislike for one tomato, the similar tomato in terms of nutrients value can still serve the same purpose and provides a similar level of nourishment.

Conclusion

The physicochemical parameters are all within the range of acceptable value. The moisture content of the studied raw and processed brands is low. Hence, the total solids are conversely high. Both raw and processed have similar values in most parameters. However, the antioxidant content showed a significant difference. The presence of antioxidant vitamin C is more pronounced in raw samples. This implies that they could protect the body cell against cancer and heart disease.

Hierarchical Cluster Analysis (HCA) in raw and processed tomato brands reveals established close neighborhood of Kano variety and brand 5. This close substitutability implies that the company may have sourced their raw tomatoes from the Kano variety. Principal Component Analysis (PCA) revealed the unique characterizations of brands 10, 5, Minna variety, and brand 8 respectively with pH, conductivity, protein, and fibres.

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