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Multielement Characterization and Chemometric Evaluation of Commercial Tomato Samples

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Abstract

Tomatoes are among the most widely consumed vegetables worldwide and represent an important dietary source of essential minerals. In this study, the concentrations of eleven chemical elements (boron, calcium, copper, iron, magnesium, manganese, sodium, phosphorus, strontium, sulfur, and zinc) were determined in 49 commercial tomato samples by inductively coupled plasma optical emission spectrometry (ICP-OES) following closed-block acid digestion. Element concentrations (mg kg^{-1}, fresh weight) ranged from 0.62–23.10 (B), 28.59–112.52 (Ca), 0.16–1.99 (Cu), 2.09–96.00 (Fe), 45.95–99.49 (Mg), 0.61–4.10 (Mn), 2.93–91.39 (Na), 95.48–365.41 (P), 0.02–0.76 (Sr), 70.87–199.91 (S), and 0.79–3.40 (Zn), revealing considerable variability in elemental composition among samples. Principal component analysis (PCA) of the autoscaled dataset showed that the first four principal components explained 69.09% of the total variance, revealing two major and largely independent patterns of elemental variation. The first was driven primarily by calcium, magnesium, phosphorus, zinc, manganese, and strontium, whereas the second was associated mainly with boron, sodium, iron, sulfur, and copper. Hierarchical cluster analysis (HCA) supported the PCA findings by separating both variables and samples into two principal groups while identifying several compositionally distinct samples characterized by unusually high concentrations of specific elements. Overall, the results demonstrate substantial variability in the mineral composition of commercial tomatoes and confirm the value of chemometric tools for interpreting complex multielement datasets.

1. Introduction

The tomato (*Solanum lycopersicum* L.), a fruit belonging to the Solanaceae family, originated in South America but is currently cultivated in virtually all regions of the world, representing one of the most important horticultural crops for both fresh consumption and the food-processing industry. In addition to being widely consumed raw, tomatoes constitute an essential ingredient in numerous culinary traditions and are extensively used in the production of sauces, pastes, juices, soups, ketchup, and other processed foods. Their global popularity is attributed not only to their versatility but also to their recognized nutritional value. Owing to their low energy density, high water content, and richness in bioactive compounds, tomatoes are frequently recommended in weight-management and healthy dietary programs. They are an important source of essential mineral nutrients C and E, and antioxidant phytochemicals, including carotenoids, phenolic compounds, vitamins, and amino acids (Ali et al., 2020; Bajon, Kidoń, & Kobus-Cisowska, 2026; Chabi et al., 2024). Comprehensive compositional studies have reported the presence of at least 17 amino acids in tomato fruits, including both essential and non-essential amino acids, which contribute to nutritional quality, flavor development, and several metabolic functions (Ali et al., 2020). Together, these characteristics make tomatoes an important functional food and justify continued investigations into their chemical composition, particularly their mineral nutrient profile, which directly influences both fruit quality and nutritional value (Ali et al., 2020; Bajon et al., 2026; Chabi et al., 2024).

Bressy et al. determined the concentrations of fifteen trace elements in tomatoes of different cultivars (Khaki, Cherry, and Italy). The study demonstrated that the mineral composition of the fruit is significantly influenced by the cultivar, the stage of maturity, and the cultivation system. In general, tomatoes at the final

stage of maturity exhibited higher concentrations of most of the elements evaluated. Among the elements determined in the study, the observed concentrations ranged from 2.44–9.19 mg kg^{-1} for Cu, 15.0–47.9 mg kg^{-1} for Fe, 5.64–18.2 mg kg^{-1} for Mn, 0.68–11.9 mg kg^{-1} for Sr, and 5.22–29.5 mg kg^{-1} for Zn, highlighting that agronomic factors exert a marked influence on the elemental composition of the fruit (Bressy, Brito, Barbosa, Teixeira, & Korn, 2013). Bonemann et al. investigated the elemental composition of different tomato cultivars and their derivatives (sauce and paste), determining the total concentrations and the bioaccessible fraction of essential and potentially toxic elements. The total concentrations found in fresh tomatoes ranged from 42–187 mg kg^{-1} for Ca, 0.26–0.72 mg kg^{-1} for Cu, 1.29–3.02 mg kg^{-1} for Fe, 80–108 mg kg^{-1} for Mg, 0.32–1.49 mg kg^{-1} for Mn, and 1.62–3.36 mg kg^{-1} for Zn (Bonemann et al., 2021). Ramesh et al. investigated the dynamics of mineral nutrients during the postharvest ripening of fruits from nine tomato cultivars stored after harvest. The authors determined the concentrations of phosphorus, potassium, iron, zinc, boron, copper, magnesium, calcium, and manganese in the outer pericarp and demonstrated that the mineral composition of tomatoes does not remain constant throughout the ripening process. Significant increases in the concentrations of phosphorus, potassium, iron, zinc, boron, and copper were observed during storage, whereas magnesium, calcium, and manganese remained essentially unchanged. These changes were attributed to the internal redistribution of nutrients within the fruit, highlighting that the stage of ripening is one of the major factors responsible for the variability in tomato mineral composition. Furthermore, the authors reported that lower potassium and calcium concentrations, combined with higher boron and copper contents, were associated with slower-ripening tomato cultivars (Ramesh, Paul, & Pandey, 2021). Caruso et al. evaluated the nutritional quality of "Piennolo del Vesuvio" tomatoes, a product with Protected Designation of Origin (PDO) status grown under conventional and organic systems, with or without the application of plant biostimulants. The authors demonstrated that, although the cultivation system had a limited effect on fruit mineral composition, the application of biostimulants significantly increased the concentrations of phosphorus, potassium, magnesium, sulfur, and sodium, while also improving various functional quality parameters, including phenolic compounds, ascorbic acid, lycopene, and antioxidant activity. The study also confirmed that potassium is the primary macronutrient in the fruit followed by calcium, phosphorus, magnesium, sulfur, and sodium demonstrating that agricultural management practices can alter the nutritional profile of tomatoes (Caruso et al., 2019). A study determined the concentrations of five major minerals (sodium, potassium, phosphorus, calcium, and magnesium) and nine trace elements (selenium, iron, zinc, copper, manganese, molybdenum, lead, cadmium, and arsenic) in 80 samples of fresh tomatoes and tomato-based products. Data evaluation was conducted using principal component analysis (PCA) and hierarchical cluster analysis (HCA). The results demonstrated that the samples could be grouped according to product type, revealing differences in their mineral composition and establishing nutritional relationships among the different tomato products (BUDAK & Aksahin, 2016).

Eleven mineral nutrients were determined in 49 tomato samples purchased in Salvador, Brazil. Sample digestion was performed in a digester block, and the elements were quantified using ICP OES. Data characterization was performed using PCA and HCA.

2. Materials and Methods

2.1. Chemicals, Standards, and Materials

All reagents used in this study were of analytical grade. Working solutions and dilutions were prepared using deionized water with a resistivity of 18.2 MΩ cm obtained from an Arium Comfort water purification system (Sartorius, Göttingen, Germany). Nitric acid (HNO_3, 65%, Merck, Darmstadt, Germany) and hydrogen peroxide (H_2O_2, 30%, Merck, Darmstadt, Germany) were used for sample digestion. External calibration standards were prepared by appropriate dilution of stock standard solutions containing 1000 mg L^{-1} and 4000 mg L^{-1} of boron, barium, calcium, cadmium, copper, magnesium, manganese, sodium, phosphorus, sulfur, strontium, and zinc (Specsol, São Paulo, Brazil).

2.2. Instrumentation

Sample digestion was performed using a closed-block digestion system (model TE007-A, Tecnal, São Paulo, SP, Brazil) equipped with 15 polytetrafluoroethylene (PTFE) digestion vessels. Multielement determination was carried out using an inductively coupled plasma optical emission spectrometer (ICP-OES) with axial-view configuration (Agilent 720 Series, Mulgrave, Australia). The operating conditions of the ICP-OES spectrometer are presented in Table 1.

Table 1
The operating conditions of the ICP-OES spectrometer.

Chemical element	λ (nm)	Calibration range
P	213.618	10–100
S	182.034	5–50
Zn	206.200	0.1-1
B	249.678	0.1-1
Cu	324.754	0.1-1
Fe	238,204	0.1-1
Mn	257.610	0.1-1
Mg	285.213	5–50
Sr	407.771	0.1-1
Ca	422.673	5–50
Na	818.326	5–50

2.3. Sample Preparation

Tomato samples were prepared by acid digestion according to the methodology described by Bonemann et al. (2021), with minor modifications. Initially, approximately 1 kg of tomato was homogenized using a laboratory blender. A 5.0 g aliquot of the homogenized sample was transferred to a closed digestion

vessel, followed by the addition of 4 mL of nitric acid (HNO_3) and 1 mL of hydrogen peroxide (H_2O_2). The vessels were tightly sealed and subjected to closed-block digestion at 150°C for 3 h. After cooling, the digests were quantitatively transferred to 10 mL volumetric flasks and diluted to volume with ultrapure water. The resulting solutions were transferred to Falcon tubes and stored until elemental determination by ICP-OES.

2.4. Method Validation

2.4.1. Linearity

Calibration curves were prepared using multielement standard solutions. Concentration ranges were 0.1–1.0 mg L^{-1} for boron, copper, iron, manganese, and strontium; 5.0–50.0 mg L^{-1} for calcium, magnesium, and sodium; and 10–100 mg L^{-1} for phosphorus. All calibration standards contained a final nitric acid concentration of 1.0 mol L^{-1}. These calibration curves were used for quantitative determination by ICP-OES.

2.4.2. Limits of Detection (LOD) and Quantification (LOQ)

The method limits of detection (LOD) and limits of quantification (LOQ) were determined according to the recommendations of the *International Union of Pure and Applied Chemistry* (IUPAC), ensuring adequate analytical sensitivity and reliability for the elemental determinations. The limits found are shown in Table S2.

2.4.3. Accuracy study

Method accuracy was evaluated by analyzing 0.200 g of the certified reference material CRM-Agro C1004a (Tomato Pulp), which was subjected to the same sample preparation procedure and analytical conditions used for the tomato samples. Recovery percentages were calculated by comparing the experimentally determined concentrations with the certified values of the reference material. The results achieved are presented in Table 2.

Table 2
Validation parameters of the analytical method.

Chemical element		Detection limit (mg Kg^{-1})	Quantification limit (mg Kg^{-1})	Certified value (mg Kg^{-1})	Achieved value (mg Kg^{-1})	Recuperation (%)
P	15.46	51.53	3320 ± 220	2686 ± 35.6	86.64	
S	3.09	10.29	1570 ± 130	1489 ± 100	94.90	
Zn	0.07	0.23	16.42 ± 0.96	14.4 ± 0.60	92.90	
B	0.14	0.46	14.0 ± 2.5	10.04 ± 0.48	72.85	
Cd	0.01	0.04	1.23 ± 0.08	1.19 ± 0.08	96.75	
Cu	0.04	0.14	7.94 ± 0.67	8.27 ± 0.31	104.15	
Fe	0.27	0.91	30.9 ± 2.0	31.24 ± 1.15	101.10	
Mn	0.03	0.09	17.1 ± 1.3	14.55 ± 0.28	92.09	
Mg	0.15	0.50	1070 ± 100	952.46 ± 27.9	89.01	
Sr	1.84e-3	0.01	3.94 ± 0.42	3.06 ± 0.09	80.02	
Ca	0.65	2.16	876 ± 79	809.9 ± 45.4	92.14	

2.4.4. Principal Component Analysis (PCA)

Principal Component Analysis (PCA) is an unsupervised multivariate statistical technique for dimensionality reduction that transforms a set of correlated variables into a smaller number of orthogonal principal components (PCs), while retaining most of the variability present in the original dataset. This approach enables the identification of patterns, clusters, trends, and outlying samples, as well as the variables that contribute most to the observed variability. The principal components are linear combinations of the original variables and are ordered according to the proportion of explained variance, with the first component accounting for the largest fraction of the total variability. Loadings represent the contribution of each variable to the formation of the principal components, allowing the identification of the variables with the greatest influence on each PC, whereas scores correspond to the coordinates of the samples in the new multivariate space and are used to evaluate similarities, clustering patterns, and differences among observations. The main advantages of PCA include the simplification of complex datasets, the reduction of redundancy among correlated variables, and the facilitation of data interpretation. However, PCA assumes linear relationships among variables and may be influenced by data scaling, making mean-centering and autoscaling essential when variables are expressed in different units

or exhibit substantially different variances (Bro & Smilde, 2014; M. M. C. Ferreira, 2015; S. L. C. Ferreira et al., 2025; Jolliffe & Cadima, 2016).

2.4.5. Hierarchical Cluster Analysis (HCA)

Hierarchical Cluster Analysis (HCA) is an unsupervised multivariate statistical technique used to explore the structure of datasets by identifying groups of samples or variables with high similarity. HCA is based on the calculation of a distance or dissimilarity matrix followed by the application of a linkage method, which hierarchically organizes the objects without requiring the number of groups to be defined in advance. This approach enables the identification of patterns, associations, trends, and outlying samples, while also revealing relationships among variables that exhibit similar behavior. The results are displayed as a dendrogram, in which the branches represent the sequence of cluster formation and their height reflects the degree of dissimilarity between objects. In the sample dendrogram, samples joined at lower distances exhibit more similar chemical profiles, whereas clusters formed at greater distances indicate more pronounced compositional differences. In the variable dendrogram, elements or parameters belonging to the same cluster tend to vary similarly across the samples, suggesting possible common physiological functions, geochemical origins, or accumulation mechanisms. The main advantages of HCA include its intuitive graphical representation of hierarchical relationships, the identification of natural clusters, and its complementary application alongside other exploratory techniques such as Principal Component Analysis (PCA). However, the interpretation of HCA results depends on the selected distance metric, the linkage algorithm, and the preprocessing of the data; therefore, autoscaling is generally recommended when variables differ substantially in magnitude or measurement units (Correia & Ferreira, 2007; M. M. C. Ferreira, 2015).

3. Results and discussions

3.1. Determination of the mineral composition of the tomato samples

The elemental composition of 49 commercial tomato samples was investigated to characterize their mineral nutritional profile and evaluate the variability of essential and trace elements. The concentrations of boron, calcium, copper, iron, magnesium, manganese, sodium, phosphorus, strontium, sulfur, and zinc, expressed as mg kg^{-1} (fresh weight), are presented in Table 3. Descriptive statistics, including the mean ± 95% confidence interval, median, and concentration range, are summarized below. In addition to describing elemental occurrence, the following discussion emphasizes the nutritional importance of these elements for human consumption and, where appropriate, their physiological roles in tomato growth, fruit development, and crop productivity. Overall, the results revealed considerable differences in mineral composition among commercial tomatoes, suggesting the influence of multiple agronomic and environmental factors on elemental accumulation.

Table 3

Determination of the chemical elements in tomato samples (mg Kg^{-1})

Sample	P	S	Zn	B	Cu	Fe	Mn	Mg	Sr	Ca	Na
1	185.73	95.20	2.96	1.73	0.54	4.45	1.62	79.72	0.33	75.99	6.38
2	162.59	80.53	1.22	1.29	0.16	3.60	2.18	66.53	0.48	99.93	10.67
3	216.12	95.41	3.40	2.54	1.07	2.80	4.10	70.81	0.17	53.98	6.72
4	118.65	70.87	3.17	0.90	0.67	4.64	1.08	70.89	0.48	65.51	3.47
5	212.88	104.64	2.91	1.29	0.35	4.87	1.74	86.57	0.15	65.05	4.50
6	156.80	86.12	1.73	1.33	0.74	3.75	1.26	68.88	0.15	81.48	26.43
7	122.38	75.77	1.71	1.53	0.93	3.17	0.96	46.92	0.12	56.96	8.63
8	365.41	161.80	2.78	0.76	0.30	8.61	1.88	99.49	0.09	111.66	11.85
9	155.44	82.38	2.18	1.38	0.60	3.06	1.68	75.72	0.09	84.52	10.24
10	180.90	91.42	3.01	1.33	0.88	4.01	1.46	70.47	0.10	47.78	4.59
11	179.54	123.48	2.75	1.90	0.20	2.91	2.50	72.33	0.39	82.59	2.93
12	219.42	106.5	2.82	1.06	0.94	5.38	1.90	79.61	0.73	94.90	43.52
13	155.13	99.39	2.68	2.44	0.28	4.51	3.33	76.01	0.54	102.51	3.69
14	230.76	101.99	2.59	1.10	0.40	4.50	3.41	66.69	0.76	106.89	41.27
15	166.14	93.33	1.68	1.24	0.49	2.09	1.37	67.28	0.06	34.81	8.62
16	125.51	91.05	2.07	1.39	1.05	6.85	1.73	69.59	0.31	70.66	13.96
17	117.22	114.00	2.52	1.30	0.30	5.41	1.05	75.91	0.52	112.52	4.97
18	235.15	114.32	2.97	2.07	0.21	5.20	1.87	77.45	0.37	82.87	58.11
19	124.17	112.21	2.61	1.53	0.35	5.50	3.69	92.93	0.57	90.26	48.02
20	211.21	122.33	2.55	23.1	0.50	7.43	2.57	81.99	0.35	74.85	91.39
21	127.55	93.26	1.10	0.90	0.72	5.16	1.74	60.72	0.03	40.42	14.63
22	139.18	99.75	1.20	0.69	0.68	5.73	0.92	53.12	0.06	43.57	9.94
23	145.97	150.42	1.26	1.05	0.72	7.11	1.17	69.26	0.32	46.64	19.20
24	115.06	130.01	1.71	1.66	0.81	3.45	0.87	58.54	0.10	43.53	8.24
25	139.94	120.71	1.74	1.39	0.46	3.26	0.94	54.89	0.07	38.64	7.60
26	159.04	133.78	1.84	0.96	1.99	2.76	0.85	61.14	0.09	47.52	17.01
27	95.48	124.48	1.53	0.82	1.34	5.11	3.03	56.43	0.10	64.56	11.88

Sample	P	S	Zn	B	Cu	Fe	Mn	Mg	Sr	Ca	Na
28	202.97	152.48	2.02	1.38	0.80	4.39	1.48	69.86	0.50	80.75	11.00
29	156.28	108.37	1.76	0.78	0.72	4.52	0.79	49.68	0.36	50.75	5.82
30	148.65	141.40	1.26	1.17	0.74	96.0	1.30	67.86	0.07	40.79	14.45
31	151.06	138.82	1.92	0.62	0.58	5.26	0.61	61.39	0.13	28.59	10.30
32	151.54	124.64	1.22	0.65	0.61	3.84	1.27	59.28	0.10	53.40	12.31
33	165.20	172.96	1.34	1.26	0.78	6.12	1.70	75.43	0.10	60.57	13.40
34	226.56	156.88	3.07	1.84	0.56	4.50	1.58	61.70	0.68	53.40	7.59
35	142.51	116.50	1.35	0.90	0.29	4.26	2.56	47.81	0.12	44.52	9.88
36	116.62	113.90	1.40	0.70	0.55	3.19	0.86	70.43	0.09	29.80	11.41
37	129.95	132.36	1.71	1.62	0.25	3.12	0.98	54.13	0.04	48.84	6.37
38	152.31	106.38	1.14	1.04	0.24	2.77	0.80	45.95	0.08	34.23	5.26
39	101.80	105.19	1.02	0.90	0.34	2.82	1.26	53.75	0.02	40.59	13.76
40	167.68	151.63	2.19	1.59	0.60	3.48	0.98	64.27	0.14	40.57	8.03
41	130.60	126.33	1.18	0.74	0.25	3.14	1.06	49.86	0.08	52.88	12.23
42	161.38	123.74	0.79	0.71	0.24	3.81	0.86	52.32	0.10	54.86	14.75
43	126.17	124.55	1.64	0.62	0.51	3.81	1.12	64.31	0.13	34.44	12.54
44	196.64	112.88	1.46	0.78	0.46	2.74	0.90	60.32	0.14	53.96	20.14
45	177.94	199.91	1.74	1.01	0.56	5.87	2.36	79.45	0.19	49.10	10.03
46	123.11	129.18	1.73	1.52	0.53	2.49	1.27	55.16	0.08	48.07	9.78
47	136.02	117.27	0.93	0.84	0.19	2.42	0.83	53.35	0.07	47.10	13.44
48	199.53	152.31	2.07	1.07	0.61	4.37	3.55	68.98	0.13	68.65	5.81
49	207.43	156.31	2.30	1.14	0.70	4.67	3.92	65.64	0.16	62.13	12.07

Boron concentrations ranged from 0.62 to 23.10 mg kg^{-1}, with a mean concentration of 1.66 ± 0.91 mg kg^{-1} and a median of 1.17 mg kg^{-1}, indicating substantial variability among the analyzed tomatoes. Such variability probably reflects differences in soil boron availability, fertilization practices, cultivar, and environmental conditions. Boron plays fundamental roles in tomato physiology, including cell wall formation, membrane integrity, pollen germination, fruit set, and seed development. Adequate boron nutrition improves fruit quality and reduces physiological disorders such as fruit cracking and hollow fruit. Although not currently recognized as an essential nutrient for humans, increasing evidence suggests that boron contributes to bone metabolism, cognitive function, and regulation of inflammatory processes. (Brdar-Jokanović, 2020; Mehri, 2020; Nielsen, 2014, 2026). Unlike boron, calcium is required in much larger

amounts and represents one of the principal macronutrients in tomato fruits. Calcium concentrations varied from 28.59 to 112.52 mg kg^{-1}, with a mean of 61.20 ± 6.47 mg kg^{-1}. Besides its well-established importance in human nutrition, calcium is indispensable for maintaining cell wall stability and membrane integrity in tomato plants. Insufficient calcium transport to developing fruits is the principal cause of blossom-end rot, one of the most economically important physiological disorders affecting tomato production. The relatively broad concentration range observed among samples suggests considerable differences in calcium accumulation under commercial production conditions (Mehri, 2020; Nielsen, 2026). Copper contents varied from 0.16 to 1.99 mg kg^{-1}, with a mean of 0.59 ± 0.10 mg kg^{-1} and a median of 0.56 mg kg^{-1}. Copper is an essential trace element for humans, acting as a cofactor for enzymes involved in iron metabolism, antioxidant defense, connective tissue formation, and cellular respiration. In tomato plants, copper participates in photosynthesis, lignin biosynthesis, respiration, and disease resistance. However, both copper deficiency and excessive accumulation may impair plant development and fruit quality (Mehri, 2020; Nielsen, 2026). Iron concentrations were found within 2.09 to 96.00 mg kg^{-1}, with a mean of 6.18 ± 3.79 mg kg^{-1} and a median of 4.37 mg kg^{-1}, indicating considerable variability among samples. Iron is an essential micronutrient for humans because of its role in hemoglobin synthesis, oxygen transport, cellular respiration, and immune function. In tomato plants, iron is required for chlorophyll synthesis and photosynthetic electron transport, and deficiency commonly results in interveinal chlorosis and reduced plant productivity (Mehri, 2020; Nielsen, 2026). Among all micronutrients, iron exhibited one of the widest concentration ranges, indicating pronounced heterogeneity among commercial tomatoes. Such variability is consistent with the influence of cultivar, soil characteristics, and agronomic management on iron uptake and accumulation. Magnesium concentrations varied between 45.95 and 99.49 mg kg^{-1}, with a mean of 66.14 ± 3.41 mg kg^{-1} and a median of 66.69 mg kg^{-1}. Magnesium is an essential macronutrient for both plants and humans. In humans, it participates in more than 300 enzymatic reactions involved in energy metabolism, protein synthesis, neuromuscular function, and cardiovascular health. In tomato plants, magnesium occupies the central position of the chlorophyll molecule and is therefore indispensable for photosynthesis, carbohydrate metabolism, and normal vegetative growth (Mehri, 2020; Nielsen, 2026). In contrast to iron, magnesium exhibited comparatively limited variability, suggesting tighter physiological regulation of this essential macronutrient during fruit development. Manganese concentrations ranged from 0.61 to 4.10 mg kg^{-1}, with a mean of 1.69 ± 0.27 mg kg^{-1} and a median of 1.37 mg kg^{-1}. Manganese is an essential trace element involved in antioxidant defense, bone formation, and carbohydrate metabolism in humans. In tomato cultivation, manganese functions as an activator of numerous enzymes and is particularly important in photosynthetic oxygen evolution, nitrogen metabolism, and resistance to oxidative stress (Mehri, 2020; Nielsen, 2026). Sodium was detected over the range from 2.93 to 91.39 mg kg^{-1}, with a mean of 15.08 ± 4.58 mg kg^{-1} and a median of 10.67 mg kg^{-1}, demonstrating marked variability among the analyzed tomatoes. Sodium is an essential electrolyte in humans, regulating extracellular fluid balance, nerve impulse transmission, and muscle contraction (Noda & Matsuda, 2022). However, excessive dietary sodium intake is associated with hypertension and cardiovascular disease. In tomato plants, sodium is not considered essential, although limited amounts may partially substitute for potassium in some physiological processes, whereas excessive sodium causes salinity stress and reduced crop productivity (Julkowska & Testerink, 2015; Van Zelm, Zhang, & Testerink, 2020). Phosphorus exhibited values of 95.48 to 365.41 mg kg^{-1}, with a mean of 163.99 ± 13.38 mg kg^{-1} and a median of 155.44 mg kg^{-1}, representing

one of the highest concentrations among the analyzed elements. Phosphorus is an essential macronutrient in humans, where it is required for bone formation, ATP synthesis, nucleic acids, and phospholipid metabolism (Fukumoto, 2014). In tomato cultivation, phosphorus is indispensable for root development, flowering, fruit set, and energy transfer, thereby contributing directly to plant establishment and fruit yield (Chen, Wang, & Wu, 2008). Strontium concentrations varied of 0.02 to 0.76 mg kg^{-1}, with a mean of 0.23 ± 0.06 mg kg^{-1} and a median of 0.13 mg kg^{-1}. Strontium has no recognized essential biological function in either humans or tomato plants. Nevertheless, because of its chemical similarity to calcium, strontium can accumulate in bone tissue in humans and has been investigated for therapeutic applications in bone disorders. In plant sciences, strontium is frequently used as a tracer to study calcium transport and nutrient uptake mechanisms (Coelho, Castanheira, Bordado, Donard, & Silva, 2017; Sarian et al., 2022). Sulfur concentrations ranged from 70.87 to 199.91 mg kg^{-1}, with a mean of 119.17 ± 7.67 mg kg^{-1} and a median of 116.50 mg kg^{-1}. Sulfur is an essential nutrient for both humans and plants (Li, Gao, & Yang, 2020). In humans, it is supplied mainly through sulfur-containing amino acids, including methionine and cysteine, which are fundamental for protein synthesis and antioxidant metabolism (Ali et al., 2020; Bajon et al., 2026). In tomato plants, sulfur is required for amino acid synthesis, chlorophyll formation, enzyme activity, and the production of defense compounds, contributing to fruit quality and stress tolerance (Kumar et al., 2026). Zinc concentrations varied between 0.79 to 3.40 mg kg^{-1}, with a mean of 1.96 ± 0.20 mg kg^{-1} and a median of 1.74 mg kg^{-1}. Zinc is an essential trace element for humans, participating in immune function, DNA synthesis, wound healing, growth, and the activity of hundreds of enzymes. Zinc deficiency remains one of the most common micronutrient deficiencies worldwide (Cunha et al., 2021). In tomato plants, zinc is required for enzyme activation, auxin biosynthesis, photosynthesis, and protein metabolism, and its deficiency reduces vegetative growth and fruit production (Mehri, 2020; Nielsen, 2026). The high concentrations observed for phosphorus, together with calcium, magnesium, and sulfur, confirm that these macronutrients constitute the principal mineral fraction of tomato fruits and largely determine their nutritional composition.

3.2. Data evaluation using Principal Component Analysis (PCA)

A Principal Component Analysis was applied to the dataset comprising 49 tomato samples and the concentrations of 11 chemical elements after mean-centering and autoscaling (unit variance). The percentages of explained and cumulative variance, as well as the variable loading values, are presented in Table 4.

Table 4
Results obtained by PCA.

Chemical element	Factor 1	Factor 2	Factor 3	Factor 4
P	-0.6672	-0.0549	-0.4342	0.1877
S	-0.0053	-0.3812	-0.7395	0.2130
Zn	-0.7794	0.2640	-0.0743	-0.2503
B	-0.4261	-0.7058	0.3999	-0.0126
Cu	0.1211	-0.0885	-0.1540	-0.9308
Fe	0.0617	-0.4027	-0.3826	-0.1369
Mn	-0.6354	0.0495	-0.1110	-0.1520
Mg	-0.7972	-0.0150	-0.2688	-0.0211
Sr	-0.7113	0.2620	0.1952	-0.0178
Ca	-0.8041	0.2948	0.0834	0.0932
Na	-0.5526	-0.6240	0.3941	0.0071
Eigenvalue	3.75	1.43	1.36	1.06
Explained variance (%)	34.09	13.03	12.33	9.65
Cumulative variance (%)	34.09	47.12	59.45	69.09

The first four principal components accounted for 69.09% of the total variance, indicating that they adequately summarize the main sources of variability in the elemental composition of the tomato samples.

PC1, which explained 35.25% of the total variance, was primarily associated with calcium (loading = − 0.8136), magnesium (− 0.8025), zinc (− 0.8003), strontium (− 0.6916), manganese (− 0.6897), and phosphorus (− 0.6148). The similar magnitude and sign of these loadings indicate a strong positive correlation among these elements, suggesting that they tend to vary simultaneously across the analyzed samples. Consequently, samples with negative PC1 scores are characterized by relatively high concentrations of this elemental group. This behavior is clearly illustrated by samples 8, 12, and 14, which exhibited elevated concentrations of calcium, magnesium, and phosphorus, with samples 12 and 14 also showing high strontium contents. Sample 20 was also positioned in the negative region of PC1 because of its comparatively high boron and sodium concentrations, accompanied by an elevated phosphorus level. Therefore, PC1 essentially describes a nutritional gradient dominated by the major mineral constituents and associated trace elements of tomato fruits. The score plot of PC1 versus PC2 is shown in Fig. 1a.

PC2 explained 13.03% of the total variance and was mainly influenced by boron (− 0.7058), sodium (− 0.6240), iron (− 0.4027), and sulfur (− 0.3812). These negative loadings indicate that samples with negative PC2 scores tend to present higher concentrations of these elements simultaneously. In the PC1 × PC2 score plot, sample 45 stands out because of its exceptionally high sulfur concentration. Sample 20 is

distinguished by its high sodium and boron contents, whereas sample 30 is distinguished by its markedly elevated iron content. On the other hand, samples 2 and 4 have low concentrations of these four elements. Thus, PC2 represents an independent source of variability associated primarily with sulfur and boron, while also reflecting the influence of iron in specific samples. Figure 1b presents the scores plot of PC1 versus PC3.

PC3, accounting for 12.32% of the total variance, was characterized by sulfur (− 0.7395), phosphorus (− 0.4341), iron (− 0.3826), boron (0.3998), and sodium (0.3940). The negative loadings of sulfur, phosphorus, and iron indicate that samples with negative PC3 scores are relatively enriched in these elements. Accordingly, samples 8, 30, and 45 displayed the most negative scores and were distinguished by their comparatively high concentrations of sulfur, phosphorus, and iron. Sample 20 was differentiated by its high boron concentration, whereas sample 7 exhibited the lowest levels of phosphorus and sulfur. These results indicate that PC3 captures compositional variations associated with sulfur, phosphorus, iron, and sodium that are largely independent of the mineral pattern described by PC1.

PC4 explained an additional 9.65% of the total variance and was predominantly influenced by copper (− 0.9308), zinc (− 0.2502), and sulfur (0.2130). In this context, samples 26 and 27 are distinguished by higher copper contents. In contrast, samples 38, 41, 42, and 47 exhibited the lowest copper concentrations. Therefore, although PC4 explained a smaller proportion of the total variance, it provided additional discrimination among samples with distinctive copper profiles. The scores plot of PC1 versus PC4 is shown in Fig. 1c.

Overall, the PCA demonstrated that the variability in the elemental composition of the tomato samples was mainly governed by two independent chemical patterns. The first, represented by PC1, was associated with the coordinated accumulation of calcium, magnesium, phosphorus, zinc, manganese, and strontium, reflecting differences in the mineral nutritional composition of the fruits. The second pattern, represented by PC2 and complemented by PC3 and PC4, was related primarily to sulfur, copper, iron, sodium, and boron, allowing the identification of specific samples with unusually high concentrations of individual elements, particularly samples 8, 20, 30, 34, and 45, which consistently appeared as the most compositionally distinct samples in the dataset.

3.3. Data evaluation using Hierarchical cluster analysis (HCA)

Hierarchical cluster analysis (HCA), performed using Ward's method and Euclidean distance, corroborated the compositional patterns identified by PCA. At the selected cut-off level, the dendrogram of the variables separated the eleven determined elements into two main clusters. The first cluster comprised sodium, iron, strontium, copper, boron, manganese, and zinc, whereas the second included calcium, magnesium, sulfur, and phosphorus. This result indicates that the latter four elements exhibit similar variation among the tomato samples and represent the principal compositional pattern governing the mineral profile, while the remaining elements constitute a second group characterized by a different distribution pattern.

The dendrogram of the samples also revealed two major clusters, indicating the existence of two predominant elemental composition profiles among the 49 tomato samples. The first cluster was composed mainly of samples presenting comparatively lower concentrations of calcium, magnesium, zinc, and phosphorus, whereas the second included samples relatively enriched in these elements, particularly calcium, magnesium, phosphorus, and strontium. This separation is fully consistent with the PCA results, where calcium, magnesium, zinc, phosphorus, manganese, and strontium were the variables with the greatest contribution to PC1, demonstrating that these nutrients are the main drivers of the compositional variability observed among the commercial tomato samples.

Although two major groups were identified, several samples occupied isolated positions within the dendrogram, reflecting distinctive elemental compositions. Sample 8 was one of the most differentiated samples because it exhibited the highest phosphorus concentration, together with among the highest calcium and magnesium contents, resulting in a markedly enriched mineral profile. Sample 20 also displayed an atypical behavior, primarily due to its exceptionally high boron (23.10 mg kg^{-1}) and sodium (91.39 mg kg^{-1}) concentrations, which clearly distinguished it from the remaining samples. Likewise, sample 30 appeared as an outlier owing to its extremely elevated iron concentration (96.00 mg kg^{-1}), approximately one order of magnitude higher than that found in most tomatoes analyzed. These observations indicate that, although the majority of the samples share similar mineral composition patterns, a limited number of tomatoes exhibited unique elemental profiles that substantially contributed to the overall multivariate variability. The dendrograms of the variables and samples are presented in Fig. 2.

The high similarity between the HCA and PCA results demonstrates the robustness of the multivariate analysis. Both techniques consistently indicated that the variability among commercial tomatoes is primarily controlled by differences in the concentrations of the major mineral nutrients, while the presence of a few chemically distinctive samples further contributes to the heterogeneity of the dataset. Such differences are likely associated with variations in cultivar, cultivation practices, soil characteristics, fertilization regimes, or geographical origin, factors known to influence mineral accumulation in tomato fruits.

4. Conclusion

This study provides a comprehensive characterization of the elemental composition of commercial tomato samples through the determination of eleven essential and trace elements by inductively coupled plasma optical emission spectrometry (ICP-OES) following closed-block acid digestion. The results demonstrated that commercial tomatoes constitute an important dietary source of essential mineral nutrients, with phosphorus, sulfur, magnesium, and calcium occurring at the highest concentrations, whereas boron, iron, and sodium exhibited the greatest variability among samples. This marked compositional heterogeneity indicates that mineral accumulation in tomato fruits is strongly influenced by factors such as cultivar, soil characteristics, fertilization practices, and crop management.

The application of complementary chemometric techniques substantially improved the interpretation of the analytical dataset. Principal component analysis demonstrated that the first four principal components

explained 69.09% of the total variance and revealed that the elemental composition of commercial tomatoes is governed primarily by two independent compositional patterns rather than by isolated variations in individual elements. The first pattern reflected the coordinated accumulation of calcium, magnesium, phosphorus, zinc, manganese, and strontium, whereas the second was associated mainly with boron, sodium, iron, sulfur, and copper. Hierarchical cluster analysis independently confirmed these relationships by resolving both variables and samples into two major compositional groups, demonstrating excellent agreement with the PCA results and reinforcing the robustness of the multivariate interpretation.

Both PCA and HCA consistently identified a limited number of compositionally distinct tomatoes. In particular, sample 8 was characterized by enrichment in phosphorus, calcium, and magnesium, sample 20 by exceptionally high boron and sodium concentrations, and sample 30 by an unusually elevated iron content. These samples contributed disproportionately to the overall multivariate variability while illustrating the natural heterogeneity of commercial tomatoes.

Overall, this study demonstrates that the combination of ICP-OES with chemometric analysis provides a robust and informative strategy for investigating complex multielement datasets. Beyond characterizing the mineral composition of tomatoes commercialized in Salvador, Bahia, Brazil, this integrated analytical approach offers valuable support for studies involving nutritional quality, authenticity, geographical origin, agricultural practices, and food quality assessment. The excellent agreement between PCA and HCA further highlights the importance of combining complementary multivariate techniques to obtain a more comprehensive understanding of compositional variability in food matrices.

Declarations

Conflicts of interest

The authors have declared no conflict of interest.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contribution

Rafael F. Jesus: conceptualization, performed experiments, collected data, and prepared the manuscrip; Adriana S. Lima: performed experiments, collected data; Caio S.A. Felix: performed experiments, collected data; Icaro S.A. Porto: performed experiments, collected data;Francisco A.S. Cunha: supervision, review and editting; Sergio L.C. Ferreira: visualization, funding acquisition, supervision, resources.

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Figures

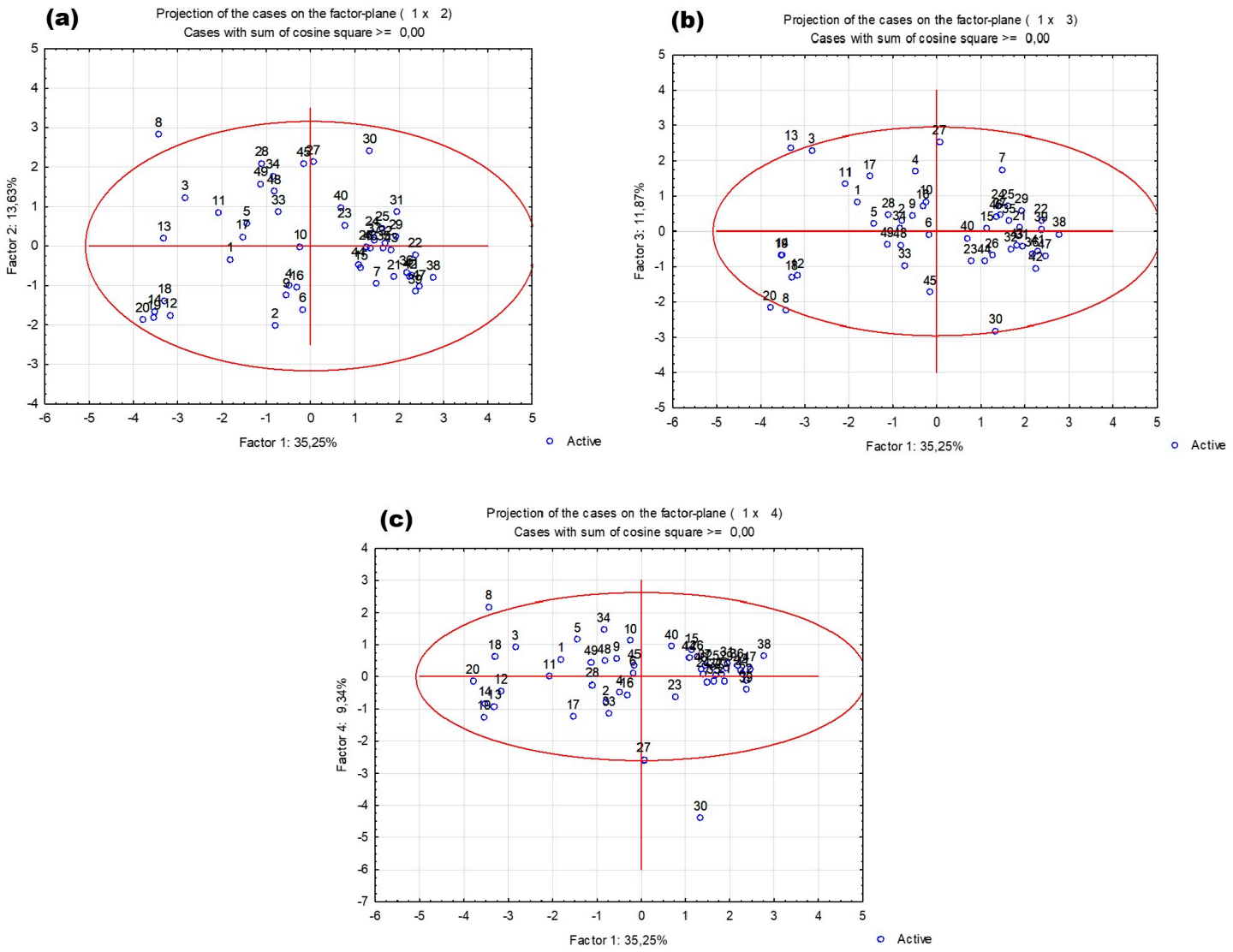


Figure 1

Scores plot. PC1 versus PC2 (Fig.1a). PC1 versus PC3 (Fig1b), and PC1 versus PC4 (Fig1.c).

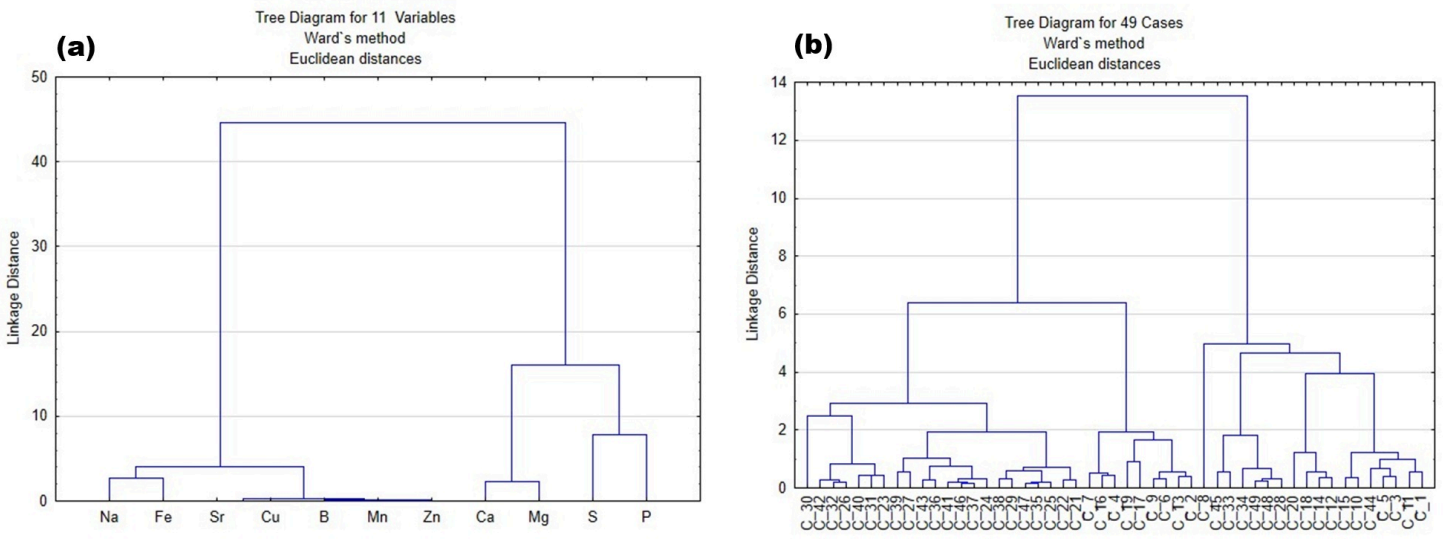


Figure 2

Dendrogram for the variables (2a). Dendrogram for the cases (2b).