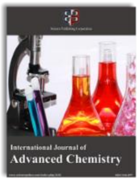
International Journal of Advanced Chemistry, 8 (1) (2020) 1-5

International Journal of Advanced Chemistry

Website: www.sciencepubco.com/index.php/IJAC

Research paper



Study on qualitative analysis in cosmetic takaout plant by multivariate statistical

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Abstract

This study examines the distributions and behavior of trace elements in five takaout plant samples. Multivariate statistical methods involving principal component analysis and hierarchical cluster analysis are applied. The measurements were performed using 21 elements (Al, B, Ba, Ca, Co, Cr, Cu, Er, Fe, K, La, Mg, Mn, Na, Ni, Sc, Sr, Ti, Y, Yb, Zn) at µg g^{-1} level determined by ICP-OES. The coefficients calculated for samples indicated a poorly negative correlation between the trace elements and Pr. A strong positive correlations among K, Na, Ca, Mg, Fe, Al, Sr, Ti, Er and Cr show a similarity in their change rules. Also, negative correlations between K and Na with Mn, Zn and Ba were showed, which indicates that these elements haven't a similarity in their behaviors, the increase of one (K and Na) conducting of decrease of others (Mn, Zn and Ba). The correlation matrix shows that Cr has good consistency with the trace elements in the sample. In particular, the correlation coefficient with Mg followed by Sr, Ca, and Fe correlations. These strong correlations between these variables show the similarity of the phenomena at the origin in takaout plant.

Keywords: *Takaout Plant; Multivariate Statistical; Trace Elements; Qualitative Study.*

1. Introduction

Takaout plant available from Moroccan herbalists, is a nontoxic natural product derived from galls of tamarix orientalis used traditionally by Moroccan women for dyeing and coloration of hairs and as adjuvant of henna [1-3], rich in aromatic amine. It is also used in the treatment of hypertension and heart disease for men and women [4], [5]. The same work reported that this plant was applied to detected of heavy metals in real samples by electrode modified [6], [7], but the research about this plant is not sufficient for determination of their properties.
Many people mixed various herbs or other substances like p-phenylenediamine in order to give it a stronger color, which can present a health risk due to the presence of toxic products such as trace elements.
Therefore, it is essential to develop sufficiently analytical methods for precise determination of trace metals in cosmetic products. Recently, several techniques, including Atomic Absorption Spectrometry (AAS) [8], [9], Energy dispersive X-ray Microanalysis [10], Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES) [11], and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) [12] have been used for the determination of elements like Pb and others in henna samples. At the same time, several analytical methods especially combined with chemometrics methods have been developed to study the characteristics and distribution of trace elements in different areas such as [13], [14] Food, [15], [16] soil, [17] groundwater and [18] agricultural soils, also the classification of essential oils and tea samples [19], [20].
In this study, we investigated for the first time the applied of different multivariate statistical for data interpretation of quality, distributions and behavior of trace elements in takaout plant.

2. Materials and methods

2.1. Sampling and analytical methods

Five samples of takaout plant were purchased from different Moroccan herbalists. Samples were stored in plastics flasks. The certified reference materials NIST 1573a Tomato Leaves (Gaithersburg, MD, USA) was analyzed in the same experimental conditions used for samples in order to evaluate the accuracy of the method. The blanks for the elements determined by ICP-AES were prepared by following all the analytical steps of the method in the absence of any sample or standard. As recommended in the respective certificate, the trace elemental concentration of the reference material was evaluated on a dry weight basis.

All teflon digestion vessels were previously cleaned in a bath of 10% (v/v) nitric acid solution for 48 hours to avoid cross-contamination. Samples were grounded with a mixer grinder and the obtained powdered samples were sieved through a 250 µm mesh before their digestion. For microwave digestion, 0.1 g of each powder sample was weighed inside the digestion reactor. After that 2 mL of concentrated nitric acid, 2 mL concentrated hydrochloric acid, 2 mL concentrated hydrogen peroxide and 4 mL of ultra-pure water were added to the samples, waiting for the elimination of foam for 5 min and the reactors were closed and installed inside the oven. All samples were digested according to the following program: step 1, 5 min to reach 180ºC; step 2, 15 min at 180ºC; step 3, cooling down. After cooling to ambient temperature, the reactors were opened and sonicated to eliminate the nitrous oxide vapors, nine samples and one blank were treated simultaneously. The resultant solutions were transferred to a plastic flask and made up to 25 mL with ultra-pure water. Finally, the solutions were centrifuged to eliminate silica and the supernatant was directly feed to the ICP-AES [21].

2.2. Chemometric procedure for data analysis

Correlation, principal component analysis (PCA) and hierarchical cluster analysis (HCA) were carried out using STATISTICA 10 Software. Multivariate statistical methods are used to study the behavior, distribution and interrelationship of trace elements in takaout plant.
Correlations between trace elements are used almost in all related researches as it is simple and clear to optimize the information provided by the correlations matrix.
Principal component analyses (PCAs) can reduce the complexity of large-scale data sets and are broadly used to elucidate relations among variables. The number of significant principal components is selected on the basis of the Kaiser criterion of eigenvalues higher than 1 (Kaiser, 1960) and a total explained variance is equal to or higher than 85%. Similarities among different elements concentrations in the samples were explored with Factor Analysis (FA). The extraction of factors was done through principal component analysis (PCA) and rotation using unrotated method.
Cluster analysis (CA) is a group of multivariate technique, which allows the assembly of objects based on the characteristics. CA classifies objects, so that each object is similar to the others in the cluster with respect to a predetermined selection criterion. Hierarchical agglomerative clustering is the most common approach, which provides intuitive similarity relationships between any one variable and the entire data set and is typically illustrated by a dendrogram (tree diagram). The dendrogram provides a visual summary of the clustering processes, presenting a picture of the groups and their proximity with a dramatic reduction in dimensionality of the original data [22].

3. Results and discussions

3.1. Characteristics of trace elements in takaout samples

From the 42 studied elements, 21 elements (Al, B, Ba, Ca, Co, Cr, Cu, Er, Fe, K, La, Mg, Mn, Na, Ni, Sc, Sr, Ti, Y, Yb, Zn) were found in at least one of the Moroccan takaout plant samples. For the rest of the considered elements results found were, in all the samples, lower than the LOD values as reported by Ghanjaoui et al [21]. Table 1 summarises the concentration samples, minimum, maximum, mean, median, standard deviation, and skewness value of the trace element composition found in the takaout plant samples. Large standard deviations (SD) were found in all trace elements levels in all samples, which indicated a wide variation of contents in the study. From the data it can be seen that K, Na, Ca, Mg, Fe and Al are the main elements presented in takaout plant samples. For Cr, Ba, Er and Ti data show a high variability between samples with minimum and maximum values. The skewness values of Ca, Mg, Fe, Al, Sr, Pr, Ti, Er and Cr were positively, in accordance with the fact that their median concentrations were lower than their mean concentrations.

Table 1: Contents of Trace Elements (µg g^{-1}) Values in Takaout Plant Samples

	K	Na	Ca	Mg	Fe	Al	Mn	Sr	Zn	Pr	Ti	Er	Ba	Cr
S_1	12056	5434	3644	2109	478	627	14,3	17,3	26,4	21	4,4	7,2	1,3	4,2
S_2	12180	6098	6858	3976	3318	4622	66	34,4	31,5	14,1	57,8	41	31	56,2
S_3	6125	1623	978	801	2051	938	66	10	30	15	22	17	29	1,12
S_4	10735	5562	3587	1909	587	771	18,2	20,5	22,1	9,0	11,9	9,2	5,2	3,2
S_5	13395	5482	8966	4576	4919	2559	70	36	30	13	210	130	24	63
Min	6125	1623	978	801	478	627	14,3	22,1	10	9	4,4	7,2	1,3	1,12
Max	13395	6098	8966	4576	4919	4622	70	31,5	36	21	210	130	31	63
Median	12056	5482	3644	2109	2051	938	66	30	20,5	14,1	22	17	24	4,20
Mean	10898	4839,8	4806,6	2674,2	2270,6	1903,4	46,90	28,00	23,64	14,42	61,22	40,88	18,10	25,54
SD	2829,6	1817,8	3122,7	1559,2	1884,6	1707,6	28,06	3,8	11,23	4,33	85,66	51,60	13,86	31,20
Skewness	-1,65	-2,11	0,29	0,20	0,57	1,33	-0,6	-1,14	0,09	0,63	1,94	1,90	-0,50	0,63

3.2. Multivariate statistical analysis

3.2.1. Correlation analysis

The results of the correlations between trace elements (Table 2) illustrate the distribution and behaviors of trace elements in the samples. The coefficients calculated for samples indicated a poorly negative correlation between the trace elements and Pr. The strong positive correlations among the main elements K, Na, Ca, Mg, Fe, Al, Sr, Ti, Er and Cr shows a similarity in their change rules. Also negative correlations between K and Na with Mn, Zn and Ba were showed, which indicates that these elements haven't a similarity in their behaviors, the increase of one (K and Na) conducting of decrease of others (Mn, Zn and Ba). The correlation matrix shows that Cr has good consistency with the trace elements in the sample. In particular, the correlation coefficient with Mg followed by Sr, Ca, and Fe correlations. These strong correlations between these variables show the similarity of the phenomena at the origin in takaout plant.

Table 2: Correlation Matrix for Trace Elements in the Samples

	K	Na	Ca	Mg	Fe	Al	Mn	Zn	Sr	Pr	Ti	Er	Ba	Cr
K	1													
Na	0,930	1												
Ca	0,853	0,704	1											
Mg	0,840	0,705	0,993	1										

Fe	0,338	0,105	0,771	0,775	1									
Al	0,436	0,433	0,697	0,768	0,698	1								
Mn	-0,132	-0,307	0,385	0,419	0,869	0,640	1							
Zn	-0,022	-0,216	0,356	0,424	0,745	0,680	0,875	1						
Sr	0,810	0,726	0,976	0,986	0,752	0,810	0,418	0,374	1					
Pr	0,036	-0,101	-0,181	-0,140	-0,211	-0,156	-0,178	0,283	-0,275	1				
Ti	0,512	0,238	0,830	0,790	0,904	0,435	0,613	0,453	0,741	-0,229	1			
Er	0,518	0,243	0,838	0,801	0,913	0,456	0,624	0,474	0,751	-0,213	0,999	1		
Ba	-0,243	-0,341	0,257	0,312	0,752	0,681	0,970	0,864	0,337	-0,195	0,420	0,434	1	
Cr	0,647	0,495	0,935	0,956	0,904	0,863	0,663	0,632	0,950	-0,178	0,818	0,831	0,576	1

3.2.2. Principal component analysis

We used a PCA to identify the distribution. of trace elements and their intrinsic relations, thus we analyzed the concentrations of trace elements from takaout plant samples. The results are shown in below.
Table 3 shows the results of the PCA applied to the trace elements. This multivariable analysis indicates that three principal components (PC) were significant with eigenvalues higher than 1, contributing 93% of the observed variance. Thus, PC1 and PC2 show major contributions, whereas PC3 has a relatively lower effect.

Table 3: Total Variance of Trace Elements in Takaout Plant by PCA

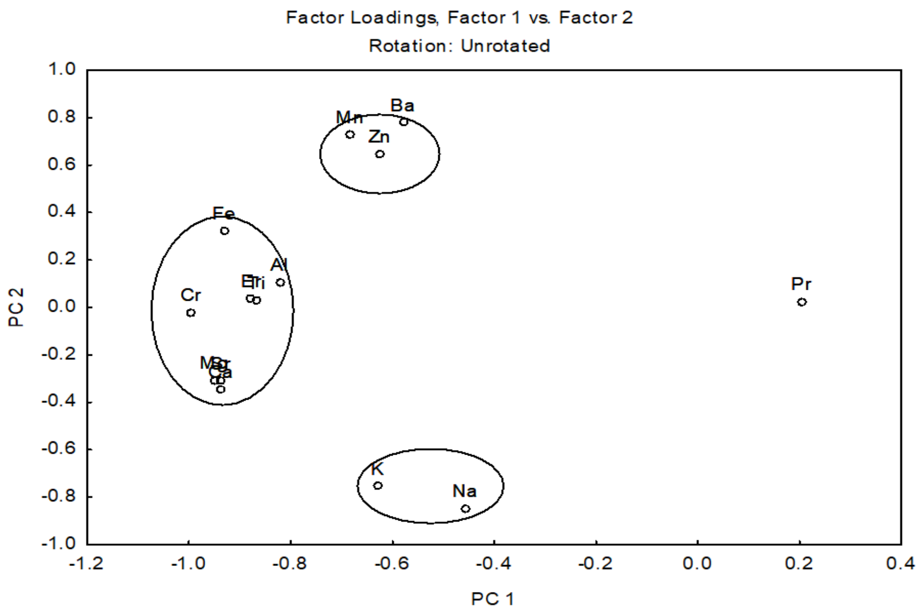
	Eigenvalue	Percentage of variance %	Cumulative %
PC1	8,539761	61	61
PC2	3,277661	23,41	84,41
PC3	1,225940	8,75	93,16
PC4	0,956637	6,83	100,0000

Table 4 shows the factor loadings of the principal components. The first component (PC1) explained 61% of the total variance and displayed loadings on Ca, Mg, Fe, Al, Sr, Ti, Er and Cr but the factor loadings of Al, Ti and Er were lower than those of Ca, Mg, Fe, Sr and Cr; therefore, the behavior of elements in this group may be relatively independent. PC2 is composed mostly of K, Na, Mn, Zn and Ba, contributes 23% of the variance. PC3 only involves a single major element, Pr.

Table 4: Factor Loadings of Trace Elements in Takaout Plant Samples

	Factor 1	Factor 2	Factor 3	Factor 4
K	-0,628918	-0,754781	-0,171360	-0,073510
Na	-0,456211	-0,849416	-0,115507	0,238792
Ca	-0,936292	-0,345390	0,008110	-0,063225
Mg	-0,948735	-0,307469	-0,072192	0,012370
Fe	-0,930336	0,320308	0,097396	-0,149637
Al	-0,820358	0,106715	-0,226919	0,513937
Mn	-0,681917	0,728968	0,052325	0,029253
Zn	-0,623580	0,648311	-0,436852	-0,000494
Sr	-0,937658	-0,311031	0,020641	0,153722
Pr	0,202694	0,024896	-0,900822	-0,383165
Ti	-0,866245	0,030001	0,244587	-0,434623
Er	-0,877676	0,035700	0,220155	-0,424195
Ba	-0,578387	0,779081	0,004764	0,241824
Cr	-0,995721	-0,020943	-0,056400	0,070137

In Fig. 1, the graphical projection of the PCA results shows that the first component (PC1), accounts for 61% of the total variance and has loadings on Ca, Mg, Fe, Al, Sr, Ti, Er and Cr, reveals an association of strongly correlated elements, can be explained that these elements are mainly symmetric matrix. The second component (PC2), which describes 23.41% of the total variance shows that is K close to Na, whereas Ba and Mn are close to Zn. The third component (PC3) accounts for 8.7% of the total variance and has loadings on Pr.



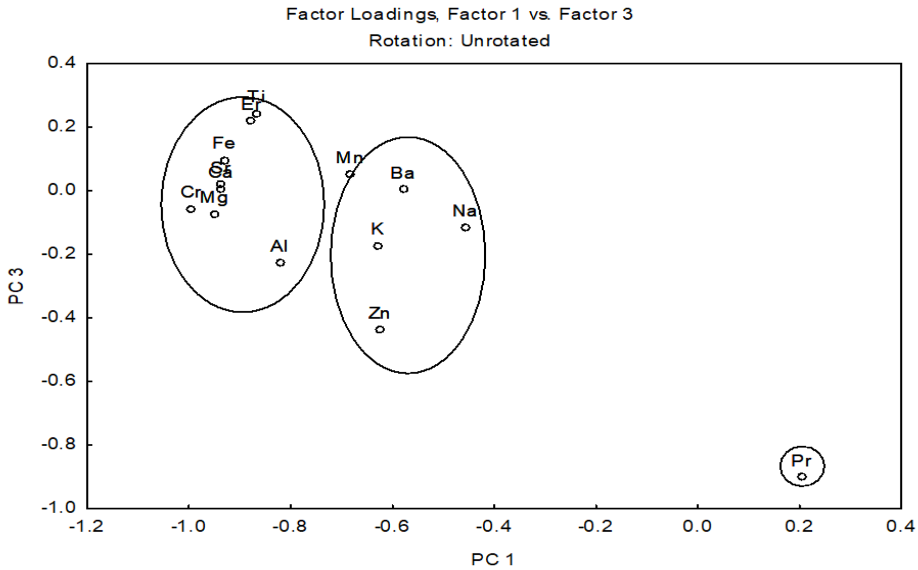


Fig. 1: Loading Plots of Trace Elements in the Space Defined by Two Components.

3.2.3. Cluster analysis

The trace element was used to examine the similarity of takaout plant by means of hierarchical cluster analysis. The dendogram obtained applying the 1-Pearson r and Ward's method defines four different groups (Fig. 2). By using the Ward method the production of small clusters is favored in our studies.

Pr is alone in cluster 1. It is remarkably different from the other elements in terms of 1–Pearson r, which implies a poorly effect from the other elements. Zn, Ba and Mn form cluster 2, mainly under the influence of K and Na. Er, Ti, Fe, Al, Cr, Sr, Mg, and Ca form cluster 3. Finally, Na and K form cluster 4, which result is in accord with the PCA.

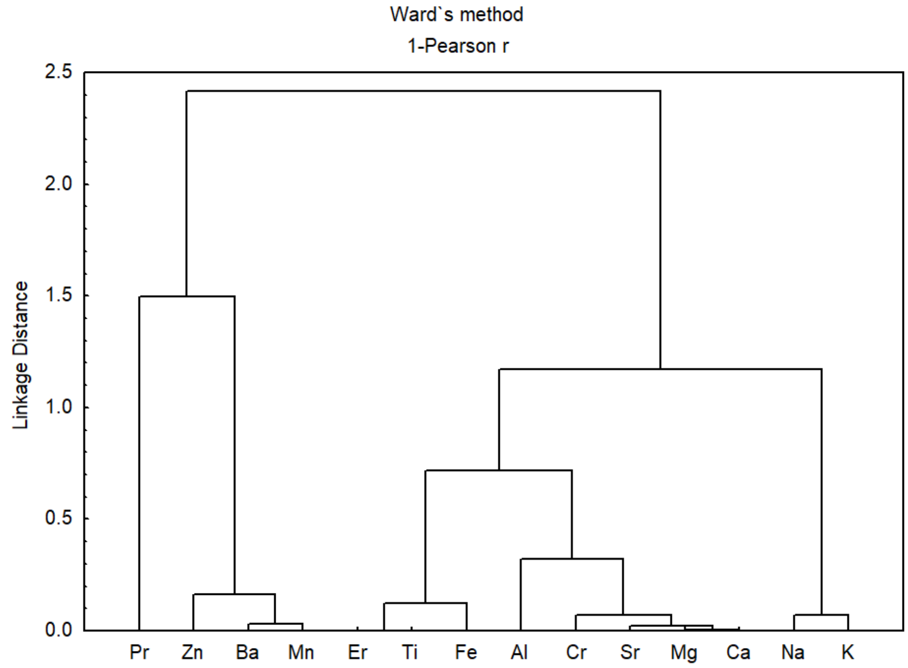


Fig. 2: Hierarchical Dendrograms From the Hierarchical Clustering Method.

4. Conclusions

In this study, trace elements were used as input data for identification of the differentiating characteristics of takaout plant samples. The strong positive correlations among K, Na, Ca, Mg, Fe, Al, Sr, Ti, Er and Cr shows a similarity in their change rules. Also negative correlations between K and Na with Mn, Zn and Ba were showed, which indicates that these elements haven't a similarity in their behaviors, the increase of one (K and Na) conducting of decrease of others (Mn, Zn and Ba). A principal component analysis performed in these data allowed a reduction in the data matrix to three principal components. The PC1 showed a strong relation between some trace elements such as Ca, Mg, Fe, Al, Sr, Ti, Er and Cr, indicating that these elements have similar behavior. The PC2 composed mostly of K, Na, Mn, Zn and Ba indicates that these elements haven't similar behavior. Finally, the PC3 consist only Pr. The same results found by hierarchical cluster. In resume, the results obtained by multivariate statistical analysis shows that the takaout plant samples have a three groups of trace elements, and cannot affected the quality of this product.

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