



## Chemometric Approach to the Nutritive Value of Some Sorghum (*Sorghum Bicolor* L. Moench) Cultivars

Bazı Sorgum (*Sorghum Bicolor* L. Moench) Çeşitlerinin  
Besin Değerlerine Kemometrik Yaklaşım

Ferat UZUN<sup>1</sup>, Nuh OCAK<sup>2</sup>

<sup>1</sup> Department of Field Crops, Faculty of Agriculture, Ondokuz Mayıs University, Samsun, Turkey  
• [fuzun@omu.edu.tr](mailto:fuzun@omu.edu.tr) • ORCID > 0000-0001-7389-5835

<sup>2</sup> Department of Animal Science, Faculty of Agriculture, Ondokuz Mayıs University, 55139 Samsun, Turkey  
• [nuhocak@omu.edu.tr](mailto:nuhocak@omu.edu.tr) • ORCID > 0000-0001-7393-1373

### Makale Bilgisi / Article Information

**Makale Türü / Article Types:** Araştırma Makalesi / Research Article

**Geliş Tarihi / Received:** 8 Nisan / April 2021

**Kabul Tarihi / Accepted:** 13 Ekim / October 2021

**Yıl / Year: 2022 | Cilt – Volume: 37 | Sayı – Issue: 1 | Sayfa / Pages: 67-82**

**Atf/Cite as:** Uzun, F. ve Ocak, N. "Chemometric Approach to the Nutritive Value of Some Sorghum (*Sorghum Bicolor* L. Moench) Cultivars - Bazı Sorgum (*Sorghum Bicolor* L. Moench) Çeşitlerinin Besin Değerlerine Kemometrik Yaklaşım". Anadolu Tarım Bilimleri Dergisi - Anadolu Journal of Agricultural Sciences, 37(1), Şubat 2022: 67-82.

<https://doi.org/10.7161/omuanajas.911674>

**Sorumlu Yazar/Corresponding Author:** [fuzun@omu.edu.tr](mailto:fuzun@omu.edu.tr)



<https://doi.org/10.7161/omuanajas.911674>



## CHEMOMETRIC APPROACH TO THE NUTRITIVE VALUE OF SOME SORGHUM (*SORGHUM BICOLOR* L. MOENCH) CULTIVARS

### ABSTRACT:

This study aimed to determine which nutritional traits are a key to indicate the nutritive value of some sorghum cultivars by chemometric techniques such as principal component analysis (PCA) and cluster analysis (CA). Based on their genotype, seven sorghum (*Sorghum bicolor* L. Moench) cultivars (sorghum [Rox and Early Sumac], sudangrass [Gözde] and sorghum × sudangrass hybrid [Jumbo, Grazer, Hayday and El Rey]) were denoted. Nutritional traits used were comprised of neutral detergent fibre (NDF), acid detergent fibre (ADF), crude protein (CP), Ca, P, K and Mg that determined by near-infrared spectroscopy analysis and digestible dry matter (DDM), dry matter intake (DMI), metabolizable energy (ME) and relative feed value (RFV) calculated by empirical equations. The NDF and ADF contents showed a negative relationship with ME and RFV. The CP content was negatively correlated with NDF and ADF but positively correlated with ME and RFV. The PCA generated two significant principal components (PCs). PC1 (59.51%) and PC2 (20.31%) described 79.83% of the total variation with eigenvalues of 6.55 and 2.23 in the sorghum cultivars, respectively. The PC1 was more representatives of the cultivars (Grazer, Hayday, Early Sumac and Gözde) and the calculated traits (DDM, DMI, ME and RFV). PC2 was characterized by Ca and Mg, while ADF, NDF and K with negative loadings in each of the PCs were the most representatives of most cultivars. CA grouped cultivars and traits into two clusters. The P, DDM, DMI, ME and RFV were the most important among components, defining important traits of cultivars to improve feeding of ruminants.

**Keywords:** Cluster analysis, Feed value, Forage quality, Forage sorghum, Principal component analysis



## BAZI SORGUM (*SORGHUM BICOLOR* L. MOENCH) ÇEŞİTLERİNİN BESİN DEĞERLERİNE KEMOMETRİK YAKLAŞIM

### ÖZ:

Bu çalışma, temel bileşen analizi (TBA) ve kümeleme analizi (KA) gibi kemometrik tekniklerle, bazı sorgum çeşitlerinin besleyici değerini göstermede hangi besinsel özelliklerinin anahtar araç olduğunu belirlemeyi amaçlamıştır. Genotip bazında yedi sorgum (*Sorghum bicolor* L. Moench) (sorghum [Rox ve Early Sumac], sudanotu (Gözde) ve sorgum × sudanotu hibriti [Jumbo, Grazer, Hayday ve El

Rey]) çeşidi incelenmiştir. Numune setinde, yakın kızılötesi spektroskopi (NIR) ile belirlenen nötr deterjanda çözünmeyen lif (NDF), asit deterjanda çözünmeyen lif (ADF), ham protein (HP), Ca, P, K ve Mg ve ampirik denklemlerle hesaplanan sindirilebilir kuru madde (SKM), kuru madde tüketimi (KMT), metabolize edilebilir enerji (ME) ve nispi yem değerine (NYD) ait veriler incelenmiştir. NDF ve ADF içerikleri, ME ve NYD ile negatif ilişki göstermiştir. CP içeriği, NDF ve ADF ile negatif, ME ve RFV ile pozitif korelasyon göstermiştir. Veri kümesinin TBA, iki önemli temel bileşen (TB) üretmiştir. TB1 (%59.51) ve TB2 (%20.31), sorgum çeşitlerinde sırasıyla 6.55 ve 2.23 öz değerleri ile toplam varyasyonun %79.83'ünü tanımlamıştır. TB1, çeşitlerin (Grazer, Hayday, Early Sumac ve Gözde) HP ve P haricinde, hesaplanan özelliklerini (SKM, KMT, ME ve NYD) daha çok temsil etmiştir. TB2 ise Ca ve Mg ile karakterize edilirken, TB1 ve/veya TB2'de negatif yüklemelere sahip ADF, NDF ve K, çoğu çeşitleri daha fazla temsil etmiştir. KA, çeşitleri ve besinsel özellikleri iki gruba ayırmıştır. Geviş getiren hayvanların beslenmesini iyileştirme bakımından çeşitlerin özelliklerini tanımlayan bileşenler arasında en önemlileri P, DDM, DMI, ME ve RFV olmuştur.

**Anahtar Kelimeler:** Kümeleme analizi, Temel bileşen analizi, Yem değeri, Yem kalitesi, Yemlik sorgum



## 1. INTRODUCTION

Sorghum (*Sorghum bicolor* L. Moench) is the most important food and feed crop after maize, wheat and barley and thus, is used for both the grain and forage to provide an important nutrient source to the human and animal population (Ritter et al., 2007; Singh et al., 2017). As such, it has conducted studies on the adaptability, stability, and nutritive value of forage sorghum cultivars (Farré and Faci, 2006; Jahansouz et al., 2014; Pinho et al., 2015; Singh et al., 2014, 2017; Uzun et al., 2017). Sorghum as a forage crop has received considerable attention in many regions of the world because their nutrient contents are well balanced in certain cultivars (Bean et al., 2013; Badigannavar et al., 2016; Uzun et al., 2017). Moreover, in the considerable studies, some forage sorghum cultivars have found to be more tolerant to abnormal growing conditions, and consequent higher in yield and quality (Farré and Faci, 2006; Kim et al., 2010a,b; Jahansouz et al., 2014; Pinho et al., 2015; Uzun et al., 2017). Therefore, cultivar choice is a very important management decision for forage production and animal operations (Ouda et al., 2005; Pinho et al., 2015; Uzun et al., 2017).

Multivariate or chemometric analyses such as principal component analysis (PCA) and cluster analysis (CA) concomitantly evaluate a set of characteristics

considering the correlations between variables, enabling better interpretations of the information extracted from a data set, which provided by analysing and/or calculating (Bro et al., 2012; Shin et al., 2012; Santos et al., 2019). While PCA shows relationships among groups of variables in a data set and/or relationships that exist between objects (Jolliffe and Cadima, 2016), CA detects groups of similar objects described by several qualitative and/or quantitative variables (Saraçlı et al., 2013; Drab and Daszykowski, 2014). Also, Drab and Daszykowski (2014) noted that the two-way clustering, extended with a colour map, enables a detailed interpretation of the studied treatments in terms of the variables that contribute most to the clustering tendency. In several studies that used one or both PCA and CA, some sorghum cultivars have been assessed in terms of agro-morphological diversity through quantitative and qualitative phenotypic traits (Chikuta et al., 2015; Mofokeng et al., 2017; Hamidou et al., 2018; Mulima et al., 2018; Martiwi et al., 2020). The evaluation of sorghum cultivars especially in terms of nutritive value is very important (Singh et al., 2014, 2017; Uzun et al., 2017) because farmers are interested in sorghum cultivars with higher nutritive value for domestic ruminants in many countries of the world, including Turkey. Forage quality indicators (FQI) such as crude protein (CP), acid detergent fibre (ADF), neutral detergent fibre (NDF), digestible dry matter (DDM), dry matter intake (DMI), metabolizable energy (ME) and relative feed value (RFV) as well as some mineral contents such as calcium (Ca), phosphorus (P), potassium (K) and magnesium (Mg), which are closely associated with animal productivity, are mainly considered in determining nutritional value of forages (Singh et al., 2014; Uzun et al., 2017; Aydin et al., 2019).

In the previous studies (Blümmel and Reddy, 2006; Singh et al., 2014, 2017), it has been reported that substantial variation in the feed value or nutritional quality of dual-purpose sorghum cultivars. Singh et al. (2014) have indicated that hybrids (686A x IS 697, 685A x ICSR 89 and 685A x GP 65072) are nutritionally superior in terms of CP, DDM, DMI and RFV. In our previous study, when some sorghum cultivars were compared for the yields of dry matter (DM), DDM and CP, they ranked in the following order: Rox = Early Sumac  $\leq$  Gözde = Grazer = Hayday = Jumbo = El Rey and also, the Jumbo and Grazer cultivars had higher ADF and NDF values, and lower DMI, ME and RFV compared to the other sorghum cultivars (Uzun et al., 2017). However, these variables evaluated by univariate analysis are considered limited for evaluating each of the variables individually compared with multivariate or chemometric analyses (Bro et al., 2012; Shin et al., 2012; Jolliffe and Cadima, 2016). Although the nutritional quality of forage crops is undoubtedly an important and widely debated topic, these FQI and minerals have yet to be extensively classified using PCA and CA. Because mutual correlations among many of the analysed nutritional traits generate redundant information and create difficulties in interpretation (Jolliffe, 2002; Jolliffe and Cadima, 2016), correlation analyses are essential for assessing the relationships among the studied traits (Mofokeng et al.,

2017). Therefore, this study aimed to determine which nutritional traits mentioned above can be a key means to indicate the nutritive value of some sorghum cultivars by chemometric techniques such as PCA and CA. Also, in this study, we examined the mutual relationships between the nutritional traits of the sorghum cultivars and thus, possible mechanisms behind the relationships.

## 2. Material and Methods

We have conducted a study, which evaluated some agronomic (plant height, the number of leaf and tiller, and dry matter yield) traits as well as nutrient contents (CP, NDF, ADF, Ca, P, K and Mg) and FQI (DDM, DMI, ME and RFV) responses to irrigation in two maize and seven sorghum cultivars (including sorghum, sudangrass and sorghum  $\times$  sudangrass) for two years (Uzun et al., 2017). In that study, we have presented a detailed description and the nutritional traits of seven sorghum cultivars. Therefore, the procedures to group the cultivars and nutritional traits were the same applied by Uzun et al. (2017). The database of this study was from the control treatment and comprised of NDF, ADF, CP, Ca, P, K and Mg and also, DDM, DMI, ME, and RFV calculated by empirical equations (Moore and Undersander, 2002). The analysis and calculation protocols performed in triplicate were described in detail by Uzun et al. (2017). Based on their genotypes, seven sorghum (sorghum [Rox and Early Sumac], sudangrass [Gözde] and sorghum  $\times$  sudangrass hybrid [Jumbo, Grazer, Hayday and El Rey]) cultivars grown in semi-humid climatic zone of Samsun, Turkey (Bölük, 2016) were denoted.

The statistical methods as PCA and CA are common applied in the evaluation of the nutritional quality of forage sources to enhance the interpretation and validity of results (Aydin et al., 2019; Santos et al., 2019). Based on the objective of this study, these statistical methods were selected and applied. As such, in the present study, the data (Table 1) belong to the nutritional traits of each sorghum cultivar were used for the chemometric approach to the nutritive value by PCA and CA. Multivariate analysis was done for the classification and discrimination of the sorghum cultivars based on PCA and CA in which sorghum cultivars were combined. Also, these data were subjected to Pearson's correlation analysis. While PCA was to determine the relatedness of traits, hierarchical CA was performed according to similarity measures to simultaneously identify the associations between cultivars and the studied nutritional traits (defined as nutrient content and FQI).

Pearson correlation analysis for all nutritional traits was used to study the relationship between the variables. PCA was also used to indicate the sources of variation differentiating the sorghum cultivars in terms of the studied nutritional traits. Before performing PCA, the suitability of data for PCA was assumed using the Kaiser-Meyer-Olkin (KMO) test and Bartlett's test. Thus, a new set of seven orthogo-

nal variables was generated by PCA (Jolliffe, 2002). The correlation and PCA were performed using the Correlate and Dimension Reduction, respectively of a statistical package program (IBM SPSS Statistics version 21, SPSS Inc., Chicago, IL). The mean of six repetitions ( $n=12$ ) of each sorghum cultivars at two years ( $N=84$ ) was used as the cases. In the present study, two-way clustering that assumed a hierarchical clustering applied independently to data objects and variables using the selected linkage approach and similarity measure was used (Drab and Daszykowski, 2014). As such, the replication values of each trait for each cultivar were subjected to hierarchical two-way clustering analysis (unweighted pair-group) using the JMP statistical program (SAS Institute Inc. USA). Thus, both the sorghum cultivars and the nutritional traits (defined as nutrient content and FQI) were clustered according to similarity measures to simultaneously identify the associations between the species and the nutritional traits. The clustering method, distance type, and scale type used in the cluster analysis (Saraçlı et al., 2013) were group average (unweighted pair-group), euclidean and none or if any, standard deviation (SD), respectively computed by the cophenetic correlation coefficient (CCC). The CCC is the Pearson correlation between the actual distances and the predicted distances based on a particular hierarchical configuration. When CCC had a value of 0.75 or above, the clustering was considered useful.

### 3. Results and Discussion

We reported previously that seven cultivars of sorghum exhibited significant differences in terms of some nutritional and chemical parameters (Uzun et al., 2017). This study examined the mutual relationships between nutritional traits in the same sorghum cultivars and also, interpreted via the PCA and CA analysis the possible mechanisms behind the relationships. Therefore, the data matrix of the studied nutritional traits (CP, NDF, ADF, Ca, P, K and Mg determined by NIR and DDM, DMI, ME and RFV calculated by empirical equations) of these sorghum cultivars were subjected to PCA and CA, a chemometric approach (Shin et al., 2012).

Correlations displaying the relationship among these variables are presented in Table 2. The CP was negatively correlated with NDF ( $r = -0.598$ ) and ADF ( $r = -0.625$ ) while positively correlated with ME ( $r = 0.625$ ) and RFV ( $r = 0.625$ ). However, there was a strong relationship between the CP with these parameters ( $P < 0.01$ ). The relationships between the ADF and NDF, ME ( $r = -1.000$  and  $r = -0.872$ , respectively) and RFV ( $r = -0.945$  and  $r = -0.978$ , respectively) were very strong and negative ( $P < 0.001$ ). The ME value had a positive and strong correlation with RFV ( $r = 0.945$ ;  $P < 0.001$ ). There was a strong and positive relationship between the DDM with DMI, ME and RFV ( $r = 0.858$ ,  $r = 1.000$  and  $r = 0.945$ , respectively;  $P < 0.001$ ).

**Table 1.** The nutritional traits (defined as nutrient content and forage quality indicator) of the sorghum cultivars and the overall mean of the variables evaluated in these sorghum cultivars (% of DM, except for ME, Mj kg-1 DM)

Traits <sup>1</sup>	Jumbo	Grazer	Hayday	Gözde	El Rey	Rox	Early Sumac	Overall
ADF	44.2±4.87	40.8±3.46	39.9±4.14	40.5±4.17	42.5±3.62	36.7±2.92	36.9±2.67	40.2± 4.44
NDF	71.3±6.03	68.4±3.49	66.9±6.23	67.9±6.01	71.1±4.78	63.4±3.38	63.6±3.30	67.5±5.58
CP	6.7±2.08	7.2±1.67	7.2±1.16	6.3±0.99	6.4±1.23	7.8±1.02	8.0±1.16	7.1±1.48
DDM	54.4±3.79	57.1±2.70	57.8±3.23	57.4±3.25	55.8±2.82	60.3±2.28	60.2±2.08	57.6±3.46
DMI	1.7±0.16	1.8±0.09	1.8±0.18	1.8±0.16	1.7±0.13	1.9±0.10	1.9±0.10	1.8±0.15
ME	7.3±0.65	7.7±0.46	7.8±0.55	7.8±0.55	7.5±0.48	8.3±0.39	8.2±0.35	7.8±0.59
RFV	71.9±11.80	78.0±7.20	81.4±12.47	79.5±11.56	73.5±8.75	88.9±7.59	88.3±7.16	80.2±11.23
Ca	0.5±0.14	0.6±0.18	0.5±0.27	0.5±0.13	0.5±0.19	0.7±0.08	0.6±0.20	0.6±0.18
P	0.3±0.05	0.2±0.02	0.2±0.03	0.2±0.03	0.2±0.03	0.3±0.03	0.3±0.03	0.2±0.04
K	1.7±0.39	1.0±0.32	1.3±0.25	1.1±0.28	1.1±0.46	0.8±0.23	1.1±0.35	1.1±0.40
Mg	0.2±0.04	0.2±0.08	0.2±0.06	0.2±0.07	0.2±0.11	0.3±0.05	0.2±0.06	0.2±0.08

<sup>1</sup>Values represent the mean ± standard deviation (n= 12 for each sorghum cultivars and n= 84 for overall mean) of each sample analysed in duplicate. ADF: Acid detergent fibre, NDF: Neutral detergent fibre, CP: Crude protein, DDM: Digestible dry matter, DMI: Dry matter intake, ME: Metabolizable energy, RFV: Relative feed value, Ca: Calcium, P: Phosphorus, K: Potassium, Mg: Magnesium

**Table 2.** Pearson correlation coefficients between the nutritional traits (defined as nutrient content and forage quality indicator) sorghum cultivars

	ADF	NDF	CP	DDM	DMI	ME	RFV	Ca	P	K	Mg
ADF	1										
NDF	0.872***	1									
CP	-0.625**	-0.598**	1								
DDM	-1.000***	-0.872***	0.625**	1							
DMI	-0.858***	-0.996***	0.591**	0.858***	1						
ME	-1.000***	-0.872***	0.625**	1.000***	0.858***	1					
RFV	-0.945***	-0.978***	0.625**	0.945***	0.978***	0.945***	1				
Ca	-0.062 <sup>ns</sup>	-0.038 <sup>ns</sup>	0.317*	0.062 <sup>ns</sup>	-0.013 <sup>ns</sup>	0.062 <sup>ns</sup>	0.002 <sup>ns</sup>	1			
P	-0.144 <sup>ns</sup>	-0.207*	0.139 <sup>ns</sup>	0.144 <sup>ns</sup>	0.241*	0.144 <sup>ns</sup>	0.221*	-0.516**	1		
K	0.134 <sup>ns</sup>	0.080 <sup>ns</sup>	0.128 <sup>ns</sup>	-0.134 <sup>ns</sup>	-0.047 <sup>ns</sup>	-0.134 <sup>ns</sup>	-0.077 <sup>ns</sup>	-0.485*	0.395*	1	
Mg	-0.650**	-0.475*	0.408*	0.650**	0.435*	0.650**	0.531**	0.552**	-0.159	-0.451*	1

ADF: Acid detergent fibre, NDF: Neutral detergent fibre, CP: Crude protein, DDM: Digestible dry matter, DMI: Dry matter intake, ME: Metabolizable energy, RFV: Relative feed value, Ca: Calcium, P: Phosphorus, K: Potassium, Mg: Magnesium, ns: Nonsignificant; \*, P < 0.05, \*\*, P < 0.01, \*\*\*, P < 0.001 (Two-tailed test)

The relationship between the ADF or DDM and Mg was negative and strong ( $r = -0.650$ ;  $P < 0.01$ ), whereas NDF showed a negative and weak correlation with P and Mg ( $r = -0.475$ ;  $P < 0.05$ ). The CP content of the cultivars exhibited a negative and weak correlation with Ca ( $r = 0.317$ ) and Mg ( $r = 0.408$ ;  $P < 0.05$ ). The DMI level was positively and strongly correlated with ME and RFV ( $r = 0.858$  and  $r = 0.978$ , respectively;  $P < 0.001$ ), while positively and weakly correlated with P and Mg ( $r = 0.241$  and  $r = 0.435$ , respectively;  $P < 0.05$ ). The Mg level exhibited a positive and strong correlation with ME, RFV and Ca ( $r = 0.650$ ,  $r = 1.531$  and  $r = 0.552$ , respectively;  $P < 0.01$ ) but a negative and weak correlation with the K content ( $r = -0.451$ ;  $P < 0.05$ ). The Ca content showed a negative correlation with P ( $r = -0.485$ ;  $P < 0.01$ ) and K ( $r = -0.485$ ;  $P < 0.05$ ). The P content was positively correlated with K ( $r = 0.375$ ;  $P < 0.05$ ).

The correlation analysis indicated that the relationship between some of the studied nutritional traits was mutual and complicated. The ME and RFV of forages are complex nutritional traits, which have many components contributing to its totality (Aydin et al., 2019) because there was a positive and strong correlation between these quality indicators. The NDF, ADF and Ca contents of the cultivars played an important role in the relation between the analysed and calculated traits with the highest-value correlation coefficient among the nutritional parameters (Muir et al., 2007; Moreas et al., 2015; Aydin et al., 2019). As predictors of forage quality, the RFV is calculated using NDF and ADF correlated with intake and the digestibility of the forages, respectively (Muir et al., 2007). The nutritional traits correlated positively with ME and RFV may be attributed to the positive correlation between carbohydrates with total calories and fat with fibre in some sorghum varieties (Moreas et al., 2015). The results of the correlation analysis supported the idea that higher CP and low cell wall contents (NDF and ADF) are indicative of good fodder quality (Singh et al., 2017). The negative correlation between NDF and ME or RFV may be related to the variation noted in the DMI (% body weight) of the sorghum varieties due to variability in their NDF contents (Singh et al., 2017; Aydin et al., 2019).

The results of PCA and CA suggested that significant diversity existed among sorghum cultivars for the nutritional traits studied. Indeed, the results that indicated differences among the cultivars for the nutritional traits and clustering based on these traits classified the sorghum cultivars into two main clusters. PCA of the dataset generated two significant PCs. The statistical loadings (or scores) of these PCs are presented in Table 3. In Figure 1, different locations are used to represent the positive and negative correlations, respectively between the analysed characteristics within a component (Table 3). The PCs having only eigenvalues of  $>1.0$  were considered significant to describe most of the total variations of data (Jolliffe, 2002). The loadings corresponding to the PCs indicate that it has high contributi-



ons from three groups. PC1 (59.51%) and PC2 (20.31%) described 79.83% of the total variation with eigenvalues of 6.55 and 2.23 in the sorghum cultivars, respectively (Figure 1). These variables were closely related to each other, characterizing PC1 as an index for determining FQI. Based on the correlation matrix loadings ( $\geq 0.75$  and positive factor loadings) of the variables (Table 3), DDM, DMI, ME and RFV contributed most strongly to PC1, while CP and P contributed less strongly.

**Table 3.** Eigen analysis of the correlation matrix loadings of the experimental variables on the significant principal components (PCs)

Traits	PC1	PC2
Crude protein	0.697	0.002
Acid detergent fibre	<b>-0.975*</b>	-0.018
Neutral detergent fibre	<b>-0.940</b>	-0.127
Digestible dry matter	<b>0.975</b>	0.018
Dry matter intake	<b>0.928</b>	0.179
Metabolizable energy	<b>0.975</b>	0.018
Relative feed value	<b>0.978</b>	0.133
Calcium	0.140	<b>-0.853</b>
Phosphorus	0.165	<b>0.755</b>
Potassium	-0.144	<b>0.750</b>
Magnesium	0.662	-0.554

*Bold values represent strong ( $\geq 0.75$ ) and positive factor loadings \*, negative correlation*

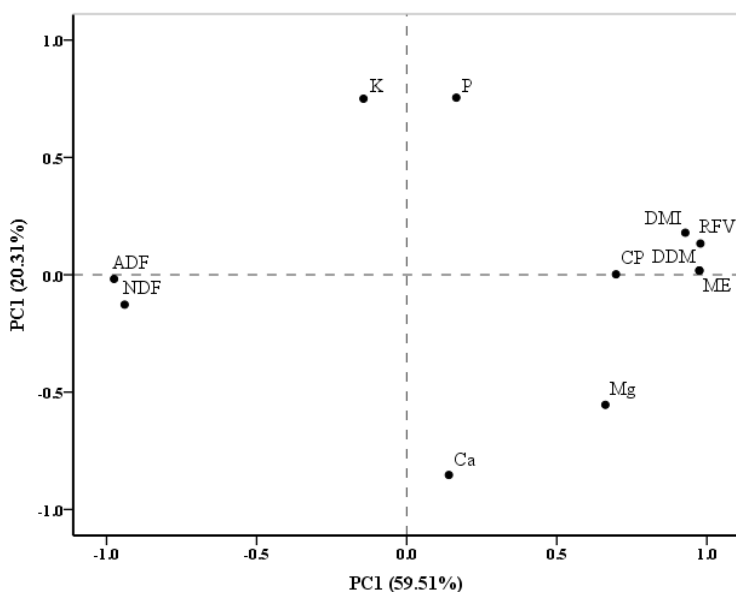


Figure 1. Scatter diagram based on loading plots of principal components (PC1 and PC2) for the nutritional traits (defined as nutrient content and forage quality indicator) sorghum cultivars. ADF: Acid detergent fiber, NDF: Neutral detergent fiber, CP: Crude protein, DDM: Digestible dry matter, DMI: Dry matter intake, ME: Metabolizable energy, RFV: Relative feed value, Ca: Calcium, P: Phosphorus, K: Potassium, Mg: Magnesium.

Figure 2 depicts the score plots of nutritional traits generated from comparing the sorghum cultivars based on PC1 and PC2. Based on scores, group I was composed of nutritional traits with positive loadings for PC1 and PC2 (CP, DDM, DMI, ME, RFV and P), group II included nutritional traits with positive loadings for PC1 and negative loadings for PC2 (Ca and Mg) and group III was composed of nutritional traits with negative loadings for PC1 (ADF, NDF and K). The results with relation to correlation confirmed the idea that the plots in PCA depicted the correlation of variables and objectives (Shin et al., 2012). The PCA results indicate that the PC1 were fewer representative of the cultivars and the calculated FQI (DDM, DMI, ME and RFV), except for CP and P, while PC2 was characterized by Ca and Mg and that the ADF, NDF and K with negative loadings in the PC1 and/or PC2 were more representatives of most cultivars. Although high values for the calculated FQI characterized the Early sumac, Hayday, Jumbo and El Rey cultivars, the other cultivars were somewhat in the middle and less tightly clustered than either group. Therefore, either PC1 or PC2 did not enable the Early sumac, Hayday, Jumbo, and El Rey cultivars to be separated from the other cultivars associated with nutritional traits from groups 1 and 2, respectively.

Differently to PC1, in the PC2, no mutual relationship was observed between the K content and other nutritional traits while Ca and Mg were related to opposite quadrants, indicating the negative association between the K content. This relationship may represent a decrease in the K content when Ca and Mg increase. Indeed, an imbalanced intake of Ca, Mg, P and K is common in forage crops and consequently in ruminants (Masters, 2018) due to a mechanism called nutrient antagonism (Senbayram et al., 2016). For example, when K or Ca concentration in the soil-root interface is high, the plant's ability to take up sufficient Mg is limited even if its concentration in the soil solution is high (Senbayram et al., 2016; Masters, 2018). This result suggested that the sorghum cultivars were important and enough since they described the current variation for the nutritional traits. Our PCA results shows that the variations among the cultivars resulted from especially quality indicators because the ME, RFV and RFQ were dominated an important part of the total variance. These notions are a significant forage species effect, as also revealed previously (Aydin et al., 2019).

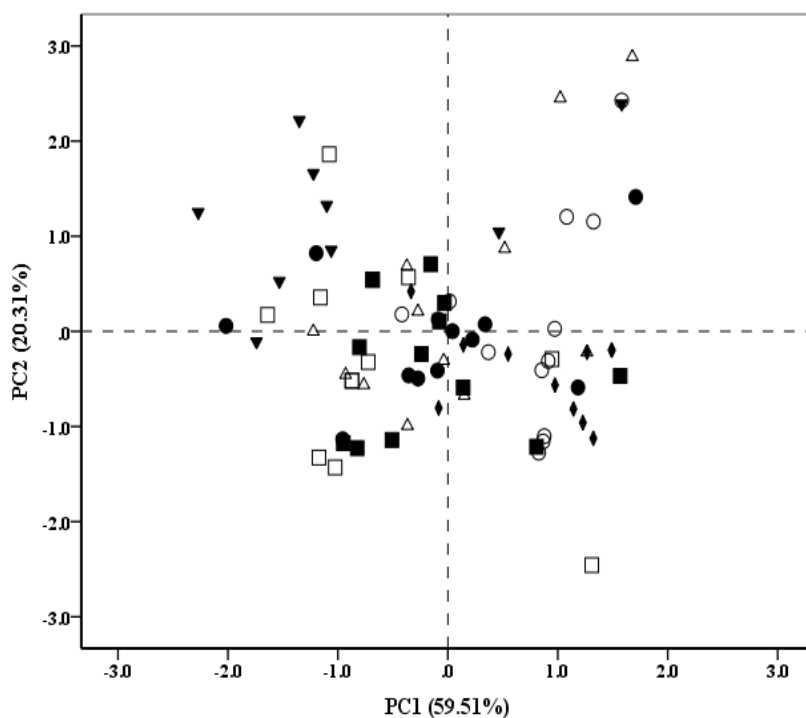


Figure 2. Score plots of principal components (PC1 and PC2) for the nutritional traits (defined as nutrient content and forage quality indicator) sorghum cultivars. ▼: Jumbo; ■: Grazer △: Hayday; □: Gözde; ●: El Rey; ◆: Rox; ○: Early sumac.

The variables that had a high correlation with one or more variables increased the commonality, and thus the PCs extracted explained much of the variable variance, as also noted by Santos et al. (2019), who used PCA in nutritional epidemiology studies. Figure 2 depicts the score plots of nutritional traits in the cultivars generated from comparing the groups based on PC1 and PC2. The traits of groups I and II were strongly related to the Early sumac, El Rey and Rox cultivars, while group II was related to the other cultivars. Also, groups I and II were weekly related to the Grazer, Hayday and Jumbo cultivars. The position of the nutritional traits in the score plot was consistent with the cultivars clustering in the CA and also, demonstrates that PC1 described the calculated traits, except for P, distribution between the cultivars. PC2 does not enable to be separated all the cultivars, which were associated with the variables from group II.

The CA and dendrogram are presented hierarchical relationships between the species in the dataset in terms of similarity or dissimilarity of their attributes represented by the parameters (Figure 3). CA grouped (CCC = 0.924) genotypes into two clusters (A and B) based on 11 nutritional traits. The cultivars in Cluster A (Jumbo, Grazer, El Rey, Hayday and Gözde) and Cluster B (Rox and Early Sumac) had no similarity. Also, the cultivars in two sub-groups of Cluster A, (Jumbo in the sub-group I and Grazer, El Rey, Hayday and Gözde in the sub-group II) had differences. The nutritional traits were grouped (CCC = 0.808) into two main Clusters (I and II) with two sub-groups, respectively. While Cluster I was included NDF, DDM, RFV and ADF, Cluster II was composed of CP, DMI, ME, Ca, P, K and Mg. The CP and ME contents of the cultivars included in Cluster I differed the studied minerals and DMI. Based on the colour intensity of the dendrogram, the similarity between Cluster I and Cluster II in terms of the nutritional traits is reduced. This may be related to the association between the calculated traits and the analysed traits (Mofokeng et al., 2017).

The CA results and dendrogram suggests this separation can provide a visual idea about variability presented in the seven cultivars. Accordingly, this confirmed that the accumulation of nutrients in fodder crops is influenced by certain factors such as plant species and variety (Singh et al., 2017; Aydin et al., 2019). Our results are consistent with the findings of Mulima et al. (2018) who reported that promising sorghum genotypes can be identified from cluster means recorded for each trait. Classification of these cultivars revealed large variation for the studied nutritional traits in the entire set as well as among the different pure and hybrid cultivars, as also noted by Upadhyaya et al. (2010) and Chikuta et al. (2015). It has been suggested that sorghum cultivars from different clusters would provide a generation of different purpose sorghum genotypes or availability of genetic variability for efficient selection (Abdel-Fatah et al., 2013; Chikuta et al., 2015; Mulima et al., 2018). Such a notion might also be suggested based on the CA results of our study. Therefore, the present study might play a significant role in filling up the gaps on these sorghum cultivars and in providing the trait-specific cultivars for use by the breeders because *Sorghum bicolor* comprises of weedy and cultivated annual forms that are fully inter-fertile (Upadhyaya et al., 2010; Chikuta et al., 2015; Martiwi et al., 2020). Thus, the evaluation and use of these new cultivars in their breeding program may contribute the sorghum improvement activities across the globe (Burow et al., 2012). Santos et al. (2019) noted that, based on that the theoretical rationale and assumptions for using chemometric and univariate methods as well as the interpretation of results are different, these techniques should not be equal statistical methods. The results of the previous study, which the data analysed as univariate (Uzun et al., 2017), and our current study, was confirmed this notion.

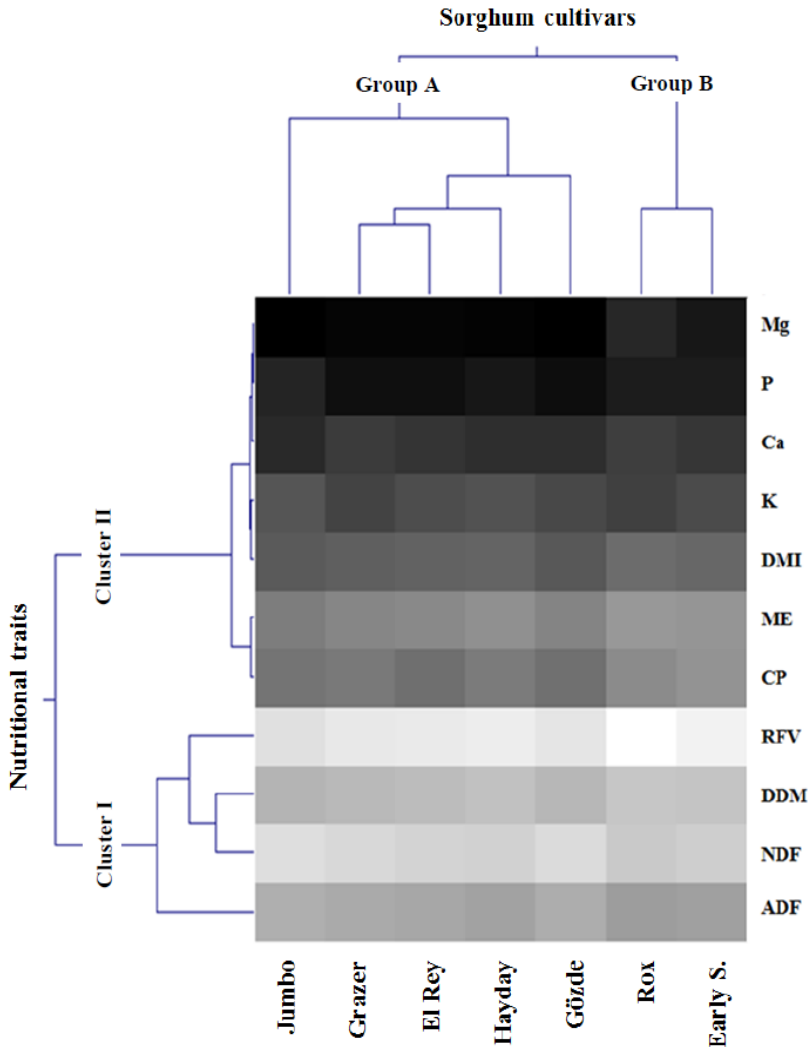


Figure 3. Dendrogram that derived from hierarchical clustering analysis of the nutritional traits (defined as nutrient content and forage quality indicator) of the sorghum cultivars. The horizontal and vertical dendrogram are the clusters of nutritional traits (CCC = 0.808; Delta = 0.186; Distance value = 0.504 – 1.701) and sorghum cultivars (CCC = 0.924; Delta = 0.209; Distance value = 0.002 – 1.885), respectively, according to similarities in the studied parameters. The intensity of colour histogram indicates the highest (light white, amount = 88.93) and the lowest (dark black, amount = 0.16) strength of similarity. ADF: Acid detergent fibre, NDF: Neutral detergent fibre, CP: Crude protein, DDM: Digestible dry matter, DMI: Dry matter intake, ME: Metabo-

lizable energy, RFV: Relative feed value, Ca: Calcium, P: Phosphorus, K: Potassium, Mg: Magnesium, Early S.: Early Sumac.

#### 4. CONCLUSIONS

The present study reports on the employment of PCA and CA as chemometric approaches, to discriminate and classify field-grown sorghum cultivars based upon their nutritive value (FQI and mineral contents). The techniques used in the study proved useful in obtaining effective characteristics, with two PCs and two clusters considered important in explaining the relationship and similarity among the nutritional traits and cultivars, respectively. The variables such as DDM, DMI, ME and RFV were the most important traits among the selected components, defining as important characteristics in the selection of cultivars to improve the feeding of the domestic ruminants. Because very significant and strong positive correlations were observed among the calculated nutritional traits, these traits should be selected for strategic improvement in breeding programs. From the result of this study, it can be suggested that a combination of analysed and calculated traits may be useful in studying the genetic diversity of sorghum for conservation, breeding and other crop improvement activities. Moreover, the presence of vast diversity among the studied cultivars clearly shown by the distant relationships among the genotypes may be appealing to researchers, farmers and end-users.

#### Acknowledgments

The authors thank Dr. H.S. Abacı for her invaluable contribution to clustering analysis.

#### REFERENCES

- Abdel-Fatah, B.E., Ali, E.A., El-Din, A.A.T., Hessein, E.M., 2013. Genetic diversity among Egyptian sorghum (*Sorghum bicolor* L. Moench) landraces in agro-morphological traits and molecular markers. *Asian Journal of Crop Science*, 5: 106-124. doi: 10.3923/ajcs.2013.106.124.
- Aydın, I., Algan, D., Pak, B., Ocak, N., 2019. Similarity analysis with respect to some quality indicators and quality categories based on relative forage quality ranges of desirable rangeland forages. *Fresenius Environmental Bulletin*, 28: 5926-5936.
- Badigannavar, A., Girish, G., Ramachandran, V., Ganapathi, T.R., 2016. Genotypic variation for seed protein and mineral content among post-rainy season-grown sorghum genotypes. *Crop Journal*, 4(1): 61-67. doi: 10.1016/j.cj.2015.07.002.
- Bean, B.W., Baumhardt, R.L., McCollum, F.T., McCuistion, K.C., 2013. Comparison of sorghum classes for grain and forage yield and forage nutritive value. *Field Crops Research*, 142: 20-26. doi: 10.1016/j.fcr.2012. 11.014.
- Blümmel, M., Reddy, B.V.S., 2006. Stover fodder quality traits for dual-purpose sorghum genetic improvement. *Journal of SAT Agricultural Research*, 2:74-77.
- Bölük, H., 2016. The climate of Turkey according to Thornthwaite climate classification (in Turkish). [https://www.mgm.gov.tr/FILES/iklim/iklim\\_siniflandirmalari/Thornthwaite.pdf](https://www.mgm.gov.tr/FILES/iklim/iklim_siniflandirmalari/Thornthwaite.pdf) (Access: 02.04.2021).
- Bro, R., Papalexakis, E.E., Acar, E., Sidiropoulos, N.D., 2012. Coclustering-a useful tool for chemometrics. *Journal of Chemometrics*, 26(6): 256-263. doi: 10.1002/cem.1424.

- Burow, G., Franks, C.D., Xin, Z., Burke, J.J., 2012. Genetic diversity in a collection of Chinese sorghum landraces assessed by microsatellites. *American Journal of Plant Sciences*, 3(12): 1722. doi:10.4236/ajps. 2012.312210.
- Chikuta, S., Odong, T., Kabi, F., Rubaihayo, P., 2015. Phenotypic diversity of selected dual purpose forage and grain sorghum genotypes. *Journal of Experimental Agriculture International*, 9(6): 1-9. doi: 10.9734/AJEA/2015/20577.
- Drab, K., Daszykowski, M., 2014. Clustering in analytical chemistry. *Journal of AOAC International*, 97(1): 29-38. doi: 10.5740/jaoacint.SGEDrab.
- Pinho, R.M.A., Santos, E.M., Oliveira, J.S.D., Bezerra, H.F.C., Freitas, P.M.D.D., Perazzo, A.F., Ramos R.C.D.S., Silva, A.P.G.D., 2015. Sorghum cultivars of different purposes silage. *Ciência Rural*, 45(2): 298-303. doi: 10.1590/0103-8478cr20131532.
- Farré, I., Faci, J.M., 2006. Comparative response of maize (*Zea mays* L.) and sorghum (*Sorghum bicolor* L. Moench) to deficit irrigation in a Mediterranean environment. *Agricultural Water Management*, 83(1): 135-143. doi: 10.1016/j.agwat.2005.11.001.
- Hamidou, M., Souleymane, O., Ba, M., Danquah, E., Kapran, I., Gracen, V., Ofori, K., 2018. Principal component analysis of early generation sorghum lines for yield-contributing traits and resistance to midge. *Journal of Crop Improvement*, 32(6): 757-765. doi: 10.1080/15427528.2018.1498423.
- Jahansouz, M.R., Keshavarz, A.R., Heidari, H., Hashemi, M., 2014. Evaluation of yield and quality of sorghum and millet as alternative forage crops to corn under normal and deficit irrigation regimes. *Jordan Journal of Agricultural Sciences*, 10(4): 699-715. doi: 10.5897/AJAR2018.13316.
- Jolliffe, I.T., Cadima, J., 2016. Principal component analysis: a review and recent developments. *Phil. Trans. R. Soc. A* 374:20150202. doi:10.1098/rsta.2015.0202.
- Jolliffe I.T., 2002. *Principal component analysis*, 2nd edn. 487 p., New York, NY: Springer-Verlag.
- Kim, H.K., Luquet, D., van Oosterom, E., Dingkuhn, M., Hammer, G., 2010a. Regulation of tillering in sorghum, genotypic effects. *Annual Botanical*, 106(1): 69-78. doi.org/10.1093/aob/mcq080.
- Kim, H.K., van Oosterom, E., Dingkuhn, M., Luquet, D., Hammer, G., 2010b. Regulation of tillering in sorghum, environmental effects. *Annual Botanical*, 106(1): 57-67. doi.org/10.1093/aob/mcq079.
- Martwi, I.N.A., Nugroho, L.H., Daryono, B.S., Susandarini, R. 2020. Morphological variability and taxonomic relationship of *Sorghum bicolor* (L.) Moench accessions based on qualitative characters. *Annual Research & Review in Biology*, 35(6): 40-52. doi: 10.9734/ARRB/2020/v35i630234.
- Masters, D.G., 2018. Practical implications of mineral and vitamin imbalance in grazing sheep. *Animal Production Science*, 58(8): 1438-1450. doi: 10.1071/AN17761.
- Mofokeng, A.M., Shimelis, H.A., Laing, M.D., 2017. Agromorphological diversity of South African sorghum genotypes assessed through quantitative and qualitative phenotypic traits. *South African Journal of Plant and Soil*, 34(5): 361-370. doi: 10.1080/02571862.2017.1319504.
- Moraes, É.A., da Silva Marineli, R., Lenquiste, S.A., Steel, C.J., de Menezes, C.B., Queiroz, V.A.V., Júnior, M.R.M., 2015. Sorghum flour fractions: Correlations among polysaccharides, phenolic compounds, antioxidant activity and glycemic index. *Food chemistry*, 180, 116-123. doi: 10.1016/j.foodchem.2015.02. 023.
- Moore, J.E., Undersander, D.J., 2002. Relative forage quality: An alternative to relative feed value and quality index. *Proc 13th Annual Florida Ruminant Nutrition Symposium*, 16-32, January 10-11, University of Florida, USA.
- Muir, J., Lambert, B., Newman, Y., 2007. Defining Forage Quality. <http://hdl.handle.net/19691/87461>. (Accessed: 20.03.2021)
- Mulima, E., Sibiya, J., Cousin Musvosvi, C., Egas Nhamucho, E., 2018. Identification of important morphological traits in Mozambican sorghum [*Sorghum bicolor* (L.) Moench] germplasm using multivariate analysis. *African Journal of Agricultural Research*, 13(34): 1796-1810. doi: 10.5897/AJAR2018.13316.
- Ouda, J.O., Njehia, G.K., Moss, A.R., Omed, H.M., Nsahlai, I.V., 2005. The nutritive value of forage sorghum genotypes developed for the dry tropical highlands of Kenya as feed source for ruminants. *South African Journal of Animal Science*, 35(1): 55-60.
- Ritter, K.B., McIntyre, C.L., Godwin, I.D., Jordan, D.R., Chapman, S.C., 2007. An assessment of the genetic relationship between sweet and grain sorghums, within *Sorghum bicolor* ssp. *bicolor* (L.) Moench, using AFLP markers. *Euphytica*, 157(1): 161-176. doi: 10.1007/s10681-007-9408-4.
- Santos, R.D.O., Gorgulho, B.M., Castro, M.A.D., Fisberg, R.M., Marchioni, D.M., Baltar, V.T., 2019. Principal component analysis and factor analysis: Differences and similarities in nutritional epidemiology application. *Revista Brasileira de Epidemiologia*, 22, e190041. doi: 10.1590/1980-549720190041.

- Saraçlı, S., Doğan, N., Doğan, İ., 2013. Comparison of hierarchical cluster analysis methods by cophenetic correlation. *Journal of Inequalities and Applications*, 2013(1): 1-8.
- Senbayram, M., Gransee, A., Wahle, V., Thiel, H., 2016. Role of magnesium fertilisers in agriculture: plant-soil continuum. *Crop and Pasture Science*, 66(12): 1219-1229. doi: 10.1071/CP15104.
- Shin, E.C., Hwang, C.E., Lee, B.W., Kim, H.T., Ko, J.M., Baek, I.Y., Lee, Y., Choi, J., Cho, J.S., Cho, E.J., Seo, W.T., Cho, K.M., 2012. Chemometric approach to fatty acid profiles in soybean cultivars by principal component analysis (PCA). *Preventive Nutrition and Food Science*, 17(3): 184-191. doi: 0.3746/pnf.2012.17.3.184
- Singh, S., Shukla, G.P., Joshi, D.C., 2014. Evaluation of dual-purpose sorghum hybrids for nutritional quality, energetic efficiency and methane emission. *Animal Nutrition and Feed Technology*, 14(3): 535-548. doi : 10.5958/0974-181X.2014.01356.0
- Singh, S., Bhat, B.V., Shukla, G.P., Gaharana, D., Anele, U.Y., 2017. Nutritional evaluation of different varieties of sorghum stovers in sheep. *Animal Feed Science and Technology*, 227: 42-51. doi: 10.1016/j.anifeedsci.2017.03.011.
- Upadhyaya, H.D., Sharma, S., Ramulu, B., Bhattacharjee, R., Gowda, C.L.L., Reddy, V.G., Singh, S., 2010. Variation for qualitative and quantitative traits and identification of trait-specific sources in new sorghum germplasm. *Crop Pasture Science*, 61: 609-618.
- Uzun, F., Garipoğlu, A.V., Ocak, N., 2017. Water use efficiency, yield, and nutritional quality of maize and sorghum cultivars as influenced by irrigation in a shallow soil. *Anadolu Journal of Agricultural Sciences*, 32: 358-366. doi: 10.7161/omuanajas.293642.

