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Multivariate discrimination of selected taxa of the Fabaceae family

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Abstract. *Abdulrahman MD. 2022. Multivariate discrimination of selected taxa of the Fabaceae family. Nusantara Bioscience 15: 227-232.* Nigeria is among the most interesting and diversified countries globally regarding tropical vegetation and medicinal plants. The taxonomy of the Fabaceae family is not entirely clear, to organize species into manageable groups that are helpful for taxonomical, conservational, or pharmacognostic study. This study aimed to discriminate the leaves of *Dialium guineense* Willd., *Detarium microcarpum* Guill. & Perr, *Tamarindus indica* L, *Acacia nilotica* (L.) Willd. ex Delile, *Abrus precatorius* L., *Senna occidentalis* (L.) Link, *Erythrina senegalensis* DC. and *Pterocarpus erinaceus* Poir. based on the mineral elements contents coupled with multivariate analysis. Three samples of each wild-growing species were collected. Unsupervised multivariate analysis using SIMCA-P (V.14.1, Umetrics Sweden) was employed. Five model groups were formed based on their mineral element contents. The species were fully discriminated along the PC1, accounting for 39.3% of the variation. Evidence from this study showed that a combination of mineral element analysis and chemometrics yielded a powerful classification method. Taxonomic identification of plants through biological research combined with chemometrics is an excellent method for preventing the adulteration or consumption of plants with excessive contents or harmful ingredients. However, a mix of molecular and developmental datasets is still necessary to explicitly examine their connections.

Keywords: Chemometrics, genera, medicinal plants, SIMCA, taxonomy

INTRODUCTION

The science of classifying, identifying, and describing different plant species into groups or classes is known as plant taxonomy (Cope et al. 2012). Although morpho-anatomical characteristics are fundamental to understanding the evolutionary relationship between plants, chemical and molecular identification are also necessary to classify plants correctly (Abdulrahman et al. 2018). Taxonomists have developed and employed biomarkers to help identify and categorize plants at the molecular and chemical levels (Abdulrahman et al. 2019). However, there is still a great deal of debate around the classification of plants concerning taxonomic identification of plants because of the significant variation in the chemical and molecular content of the plant, even among comparable species of plant. Therefore, the outcomes of the chemical studies on the plants will be a crucial piece of evidence to support the characterization and identification of these plants (Yunusa et al. 2018). Since the dawn of time, humanity has relied solely on plants to provide them with food, medicine, and oxygen for themselves and their domesticated animals (Abdulrahman and Abba 2021). Medicinal plants also serve food and contribute greatly to human health since they include all the important nutrients humans require. Without a doubt, the great civilizations of the ancient Chinese, Indians, and North Africans left written evidence of man's ingenuity in using plants to treat a wide range of ailments (Kankara et al. 2015). Furthermore, ethnobotany is becoming more prominent worldwide to satisfy the curiosity and willingness to understand how the environment and plants interact to help man survive (Abdulrahman and Abba 2021).

Due to extensive variation in plant chemical and molecular content, even among closely related species, there is still much controversy regarding the classification of plant species (Abdulrahman et al. 2018). Classification schemes were made because there is a lot of diversity between species and people wanted to learn more about it. As a result, numerous plant species exist, but the methods used to identify and categorize them are time-consuming and often inaccurate. Furthermore, the number of knowledgeable plant taxonomists is currently low and declining. This issue is so significant that it has been given the moniker "taxonomic obstacle" worldwide. Conversely, chemometrics can examine many plant samples simultaneously (Abdulrahman et al. 2021a).

The innovative methods developed in chemometrics have benefitted plant identification investigations for enhancing herbal and pharmaceutical compositions. Chemometrics is a useful method for identifying and classifying various plant parts (Yunusa et al. 2018). Multivariate analysis is used in computational systems to process numerical or metabolite data statistically. Finding the proper one will be simpler if they are grouped. Only a few of the approaches that fall under the category of "discrimination analysis" are Principal Component Analysis (PCA), Orthogonal Projections to Latent Structure Discriminant Analysis (OPLS-DA), and Hierarchical Cluster Analysis (HCA) (Yunusa et al. 2018). Score plots, loading plots, and even discrimination maps are produced by multivariate research for improved visualization and understanding of smaller datasets. In recent years, numerical taxonomy has substantially assisted taxonomic studies (Saric et al. 2009; Ningrum and Chasani 2021).

The earth's second most popular medicinal plant belongs to the Fabaceae family (Da et al. 2018), with reports of over 490 species (Da et al. 2018). It is well known that the family has therapeutic benefits. More than 20 genera have been established within the family. Members of this family utilize a variety of environments. The food crops in the family are important economically because they are high in protein and other micronutrients that are good for livelihoods and health, especially in developing nations. However, because the Fabaceae family contains organisms well suited to the initial colonization and exploration of a variety of settings, such adaptations are brought about by the family's interaction with ectomycorrhizal fungi or with nitrogen-fixing bacteria (Da et al. 2018). Morphological characteristics will not provide sufficient data for the taxonomic characterization of Fabaceae species (Vižintin et al. 2012). Furthermore, due to flaws in traditional taxonomy, this technique cannot meet the complex demands of this species identification. The chemical components of all medicinal plants need to be assessed for identification and pharmacological research purposes to ensure dependability and repeatability. As a result, a reliable method of Fabaceae authentication is required (Al-Dabbagh and Fathulla 2022).

Trace elements are essential in the biosynthesis of active chemical compounds found in medicinal plants, which are responsible for their therapeutic and toxic properties. Furthermore, plants have both helpful and negative impacts on the human body due to their chemical components (Mat et al. 2006). Therefore, morphological observations and chemical content analysis are critical for proper authentication.

Moreover, Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) were used to distinguish between the species. The present study aims to determine the mineral content of the leaves of *Dialium guineense* Willd., *Detarium microcarpum* Guill. & Perr, *Tamarindus indica* L., *Acacia nilotica* (L.) Willd. ex Delile, *Abrus precatorius* L., *Senna occidentalis* (L.) Link, *Erythrina senegalensis* DC., and *Pterocarpus erinaceus* Poir. to be taxonomically identified. The plants mentioned above are known for their medicinal value in the northern part of Nigeria. The plant leaves, bark, roots, and fruits treat many ailments, including toothache, fever, cough, typhoid, and other diseases (Abdulrahman et al. 2020).

MATERIALS AND METHODS

Herbarium deposition and taxonomic identification

Each of the species under study was collected in triplicate in Kaduna State, Nigeria. For the collected samples, herbarium specimens were prepared. A botanist from Ahmadu Bello University Zaria (ABU), Sanusi Namadi, identified the collected plants which were later placed at the ABU herbarium (Table 1).

Table 1. Voucher number of the studied plant species

Species	Voucher number
Abrus precatorius L.	0917
Acacia nilotica (L.) Willd.ex Delile	0900266
Detarium microcarpum Guill. & Perr.	002346
Dialium guineense Willd.	007429
Erythrina senegalensis DC.	07095
Pterocarpus erinaceus Poir.	0751
Senna occidentalis (L.) Link	060125
Tamarindus indica L.	08961

Mineral element analysis

Samples of leaves were collected and dried in an oven at 60ºC for 24 hours before being ground into powder using a grinding machine. Then, between 0.15 and 0.20 grams of each sample and 100 microliters of standard solution were weighed into vials (polyethylene) and immediately subjected to neutron irradiation in a Triga MK-II reactor. Instrumental Neutron Activation Analysis (INAA) is used to identify the elements in the leaf. Short-lived radionuclides were used for element detection; for elements like V, Al, Ca, Mg, and V, this meant an irradiation time of 1 minute, followed by 20 minutes of cooling and 5 minutes of counting time. For elements like Na and K, this meant an irradiation time of 1 minute, followed by 24 hours of cooling and 20 minutes of counting time. Case in point elemental long-lived radionuclides for as, the process involved 7 hours of irradiation, followed by 3-5 days of cooling, and 2-4 hours of counting time; for Ba, Cr, Fe, Co, and Zn, the process involved 6 hours of irradiation, followed by 20-30 days of cooling, and 1-2 hours of counting time. Three identical sets of experiments were performed (Mat et al. 2006).

Multivariate analyses

Multivariate analyses with imputed data were performed using a SIMCA-P (V.14.1, Umetrics Sweden) to perform Hierarchical Cluster analysis (HCA) and Principal Component Analysis (PCA) (Morais et al. 2020).

Principal Component Analysis (PCA)

PCA focus on examining pairs of variables that are linearly connected. Also, the PCA can be used to tell apart closely related species and to pinpoint the specific states of characters that are responsible for the observed relationship (Nuez et al. 2004).

Hierarchical cluster analysis

Using the information that has been given, hierarchical cluster analysis attempts to classify the data. Hierarchical Cluster Analysis (HCA) creates a similarity matrix between the plant species under study, then highly similar clusters, highlighting similarities and contrasts between and among the clusters (Abdulrahman et al. 2021c). The cophenetic correlation coefficient between the distance matrix and the tree matrix was calculated to assess the closeness of the cluster analysis to the distance matrix.

RESULTS AND DISCUSSION

In many regions of the world, the use of medicinal plants in conventional medicine is becoming more widespread. However, a well-established and strict quality evaluation system must be implemented before medicinal plants can be trusted for their alleged benefits, authenticity, and safety. Computational techniques are used in metabolomics, specifically, multivariate analysis to statistically process the chemical content based on numerical values to assign known metabolites to specific species for identification (Okada et al. 2010; Saito and Matsuda 2010; Tokalıoğlu 2012; Xia and Wishart 2016). Through multivariate analysis, the concept of mineral element analysis combined with chemometrics shows potential as a rapid method to discriminate between plant species. The concept was employed in studying some medicinal or cultivated plant species (Tokalıoğlu 2012; Kumar et al. 2019). An unsupervised analysis was used to discriminate and classify plant species based on multivariate analysis. A summary of the fit plot for the Principal Component Analysis (PCA) is shown in Figure 1.

The R2 value represents the percentage of variation in the training data set with the PCA. R2 is a fit metric that indicates how well the model fits the data. A large R2 (nearing 1) is required to show how well the data set fits the model. According to cross-validation, Q2 is the percentage of the variance of the data set predicted by the model. The model's ability to forecast fresh data is measured in Q2. A high Q2 shows a high level of predictability of 0.998 (Figure 1). The model is, therefore, fit for further analysis of the PCA and HCA models. A similar pattern of fitness and predictive model (FT-NIR: R^2X (cum): 0.956, Q^2 (cum) = 0.952. FT-NIR: R^2X (cum): 0.753, Q^2 (cum) = 0.731) (Maree and Viljoen 2011). PCA offers a wide variety of methods for better-representing data categorization and grouping instances into clusters with common characteristics. For any two groups to be truly distinguishable from one another, they must share certain similarities along the same dimensions that set them apart (Tokalıoğlu 2012).

Multivariate statistical analysis can significantly augment more conventional ways of investigating mineral chemistry by uncovering connections between elements and grouping geochemical results into pertinent and understandable groupings (Dmitrijeva et al. 2020). Principal Component Analysis (PCA) is a window that shows how the observations are related. These graphics display similarities, dissimilarities, and other patterns in the data. The score plot is a map of the observations.

Along the PC 1 X axis, there was clear, distinct discrimination of the examined species (Figure 2). The *D. guineense*, *D. microcarpum*, *T. indica*, *A. nilotica*, and *A. precatorius* were found along the left side of the PC1 while along the right side of the PC1 *S. occidentalis*, *E. senegalensis* and *P. erinaceus* were found with the variation accounting to 39. 3% (Figure 2 to 6). Along the Y-axis PC2, had no clear discrimination of *T. indica* and *P. erinaceus* (Figure 2). However, intra-species variation was seen in *T. indica* and *P. erinaceus* in the X-axis of the PC2 (Figures 2-6). The variation in PC 2 accounts for 21.5 % (Figures 2-6). The PCA revealed *D. guineense*, *D. microcarpum*, *T. indica*, *A. nilotica*, and *A. precatorius* are closely related in terms of calcium, potassium, magnesium, and sodium. Calcium is solely responsible for nerve and muscle maintenance. It is also reported to serve as an engine for activating enzymes in the body, absorption of dietary vitamin B, and synthesis of the neurotransmitter acetylcholine (Mat et al. 2006). Potassium is also necessary for activating enzymes, particularly coenzymes, which are necessary for muscle function and appropriate body growth (Abdulrahman et al. 2021b). Magnesium is a key cofactor in transporting glucose and enzymes involved in carbohydrate oxidation mechanisms in cell membranes (Mat et al. 2006). Sodium is one of the most important elements for maintaining life, and a lack of it causes physiological function to be impaired.

The relationship of the score plots resulted from the fingerprint (Figure 3). The score loading plot represents the weights combining variables to form the score units. They are proportional to the correlations between the scores and the assessed variables. For example, the scores on the X axis result from the following variables (Figures 3 and 4) while the Y axis (Figures 3-5).

The Biplot goal is to co-chart scores and loadings so that they may be displayed and interpreted simultaneously (Abdulrahman et al. 2021c). As a result, this plot better displays similarities and differences between observations to better understand the observations in relation to the study variables.

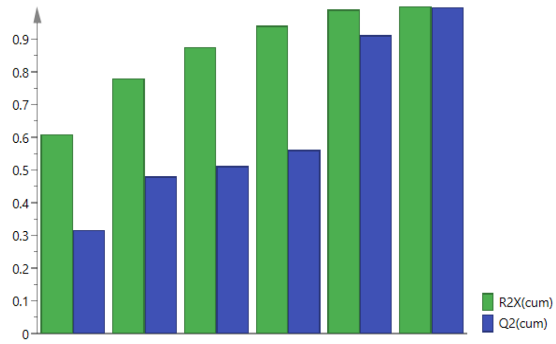

Figure 1. Summary of fit model

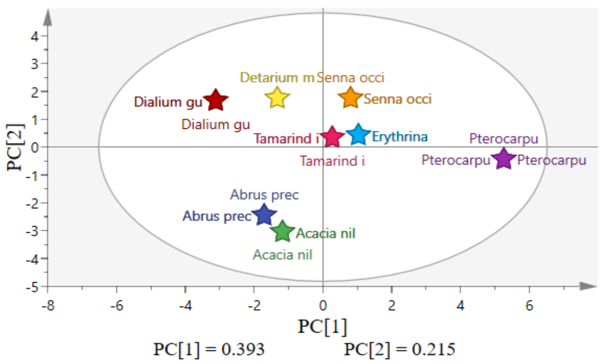

Figure 2. PCA score plot of *D. guineense, D. microcarpum, T. indica, A. nilotica, A. precatorius, S. occidentalis, E. senegalensis* and *P. erinaceus*

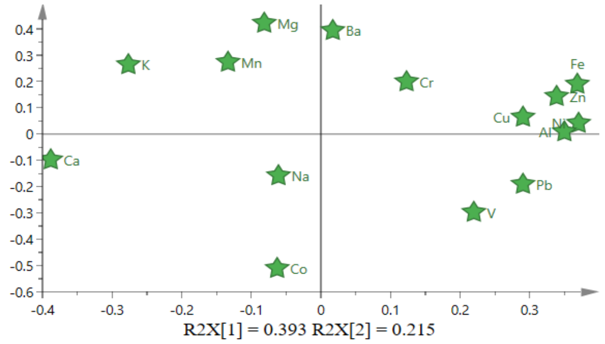

Figure 3. PCA score plot of the mineral analysis responsible for the discrimination

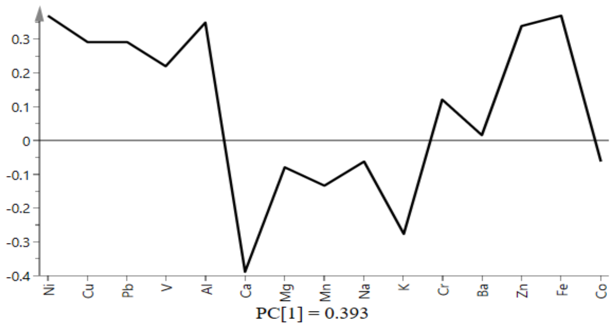

Figure 4. Loading score plot of the mineral analysis responsible for the discrimination of the PC1

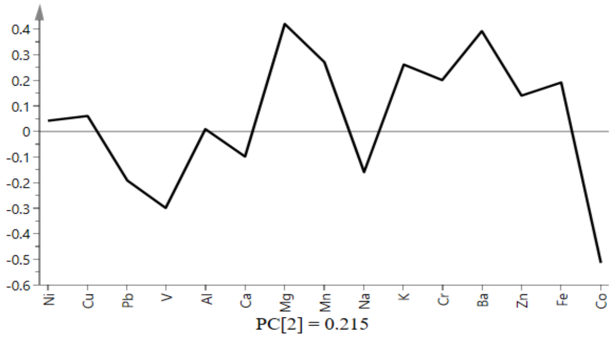

Figure 5. Loading score plot of the mineral analysis responsible for the discrimination of the PC1

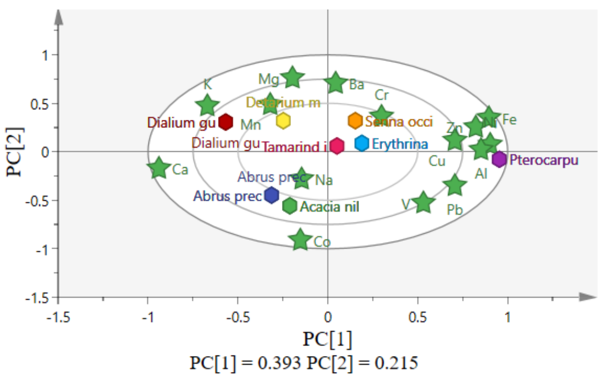

Figure 6. Bi-plots of the score and loading plots showing variables responsible for the formation of scores

Species near the variables have high levels of these variables and low levels of variables located opposite. Variables near the plot origin do not affect the formation of the scores in the plots. The bi-plots along the Y-axis revealed that the species are high in terms of calcium, potassium, cobalt, magnesium, manganese, and sodium. While along with the X-axis, Aluminum, Iron, Zinc, and Vanadium (Figure 6). The PCA score plot of the mineral analysis also shows a high relation in terms of baron, cranium, iron, copper, aluminum, nickel, and vanadium from *S. occidentalis*, *E. senegalensis*, and *P. erinaceus*. Principal Component Analysis (PCA) score plots are a good model for identifying species based on their chemical contents in their studies, quality control, and discrimination of three *Curcuma* species with the aid of metabolomics (Xiang et al. 2011). Moreover, in agreement with the findings on *Ficus deltoidea* discrimination in Peninsular Malaysia, they report variation (Intra and inter) among similar species of the same cultivar (Fatihah et al. 2014).

The HCA was constructed to further determine the relationships and dissimilarities and categorize them into various classes (Fatihah et al. 2013). The model was used to create Hierarchical Cluster Analysis (HCA) to classify them into various groups. The Dendrogram (Tree plot) displays the results of HCA. The number of clusters formed is shown in the tree plot (Figure 7). The tree plots are divided into two major groups, with the first group having only species of *P. erinaceus* with *a* 92% bootstrap value. While the other main groups divide into two main groups, with the first group from the left side accommodating *S. occidentalis, T. indica, and E. senegalensis* and the other subgroups accommodating *D. guineense, D. microcarpum, A. nilotica*, and *A. precatorius* at 81% bootstrap value (Figure 7).

The HCA dendrogram further confirmed the relationship (similarities and differences) that the PCA had already established. The HCA model showed a similar pattern in the score plot. The dendrogram was split into different groups based on the trace element contents. Interestingly, the correlation table revealed that the parameters used to distinguish plant species were very good and accurate in identifying them based on their mineral contents. The mean and standard deviation of the variable is shown in Table 2.

The correlation table shows that all variables used in the study positively impact the formation of scores along the Y and X axes of the score plot (Table 3). Table 3 reveals the correlation matrix of the variables used to discriminate the medicinal-importance plants from the family Fabaceae. The models showed a clear separation of the species concerning their mineral contents. The findings of the studies using mineral element analysis combined with chemometrics have provided an efficient way of discriminating plant species that are closely related. Biological investigations combined with chemometrics are a great tool for the taxonomic identification of plants to avoid adulteration and consumption of plants with high contents and dangerous ingredients.

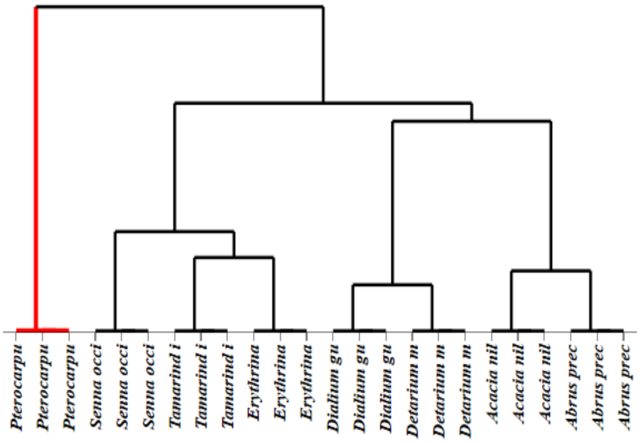

Figure 7. Hierarchical cluster analysis of *D. guineense, D. microcarpum, T. indica, A. nilotica, A. precatorius, S. occidentalis, E. senegalensis,* and *P. erinaceus*

Table 2. Mean and standard deviation of the study variables

Variables	Mean	Standard deviation
Ni	3.36	2.44
Cu	47.51	45.79
Pb	2.357	1.24
V	0.19	0.08
Al	97.01	111.18
Ca	0.76	0.20
Mg	0.10	0.02
Mn	27.93	10.61
Na	343.64	206.84
K	0.83	0.39
Cr	1.18	0.98
Ba	22.66	11.70
Zn	39.43	25.75
Fe	98.88	64.73
Co	0.37	0.35

Table 3. Correlation matrix of the study variable

	Ni	Cu	Pb	V	Al	Ca	Mg	Mn	Na	K	Cr	Ba	Zn	Fe	Co
Ni	1	0.4308	0.6194	0.6704	0.9759	-0.7810	0.0497	0.0538	0.0941	-0.5376	0.2130	0.1189	0.6479	0.9112	-0.1224
Cu		1	0.4627	-0.1008	0.4022	-0.8178	-0.3256	-0.5551	-0.4409	-0.5148	-0.0220	0.1857	0.6552	0.4718	-0.3925
Pb			1	0.5449	0.6703	-0.5545	-0.1967	-0.4359	0.3725	-0.3471	-0.1901	-0.3439	0.5526	0.5130	0.0586
V				1	0.6599	-0.3258	-0.2313	-0.1028	0.4773	-0.5610	0.1074	-0.2401	0.1275	0.4546	0.5818
Al					1	-0.7045	0.0938	0.1127	0.1903	-0.5145	0.0287	0.0342	0.5773	0.8331	-0.0996
Ca						1	0.1313	0.4047	0.2626	0.6352	-0.3391	-0.2973	-0.7686	-0.8424	0.3284
Mg							1	0.7048	0.3129	0.5994	0.0540	0.5092	-0.1011	0.1701	-0.6441
Mn								1	0.1401	0.4542	-0.0216	0.1824	-0.2298	0.0223	-0.2506
Na									1	0.2575	-0.4676	-0.0274	-0.4398	-0.1220	0.2679
K										1	-0.0931	0.1592	-0.3147	-0.3827	-0.4113
Cr											1	0.2047	0.4759	0.5167	-0.1746
Ba												1	-0.0861	0.2357	-0.6075
Zn													1	0.8221	-0.4163
Fe														1	-0.3771

Note**:** Ni: Nickel, Cu: Copper, Pb: Iron, V: Vanadium, Ca: Calcium, Mg: Magnesium, Na: Sodium, K: Potassium, Cr: Cranium, Ba: Baron, Zn: Zinc Fe: Iron, Co: Cobalt

For the first time, we have attempted to propose a chemometrics phylogenetic framework for a subset of the Nigerian Fabaceae family, which will serve as a foundation for future phytochemical and pharmacological studies. Moreover, gaining a more comprehensive knowledge of the systematic links between the varieties will facilitate these plants' rapid exploitation and long-term sustainability.

The common bean, pea, and legume are among the edible and economically significant species of flowering plants in the Fabaceae family. In all, they comprise the second-largest family of plants. Despite being tamed by humans, they are significant commercially. Differentiating *D. guineense*, *D. microcarpum*, *T. indica*, *A. nilotica*, *A. precatorius*, *S. occidentalis*, *E. senegalensis*, and *P. erinaceus* from one another was done using the fingerprints left by mineral elements in the leaves. The formation of five models based on mineral composition led to the discovery of a significant relationship between the species. Furthermore, it is discovered that species from the same region differ. The discrimination was explained using PCA, and HCA supported the produced dendrogram. The multivariate analysis will be crucial for the delimitation and authentication of plant species. The results would be of great value to support the classical taxonomy.

However, a mix of molecular and developmental datasets is still necessary to explicitly examine their connections. That is the first attempt at proposing a chemometrics phylogenetic framework for a subset of the Nigerian Fabaceae family; it will provide the basis for future taxonomic research. Understanding the systematic relationships between the variations is crucial for quick commercialization and long-term viability.

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