Characterization by near infrared spectroscopy of seeds and oils of *Amaranthus* spp. as a function of cropping systems[1]

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ABSTRACT

Species of the *Amaranthus* genus are very versatile and have potential for the application in the development of commercial products. The near infrared spectroscopy (NIR) is an efficient tool that can help in the quality control of products, quickly and non-destructive to the sample. The goal of this study was to carry out the distinction of seed and oils of different *Amaranthus* species using the near infrared spectroscopy. Three species were used: *A. viridis* L., *A. hybridus* L. e *Amaranthus* sp. (commercial). The spectra acquired from the sample using the near infrared spectroscopy were submitted to the partial least squares discriminant analysis (PLS-DA) and to the principal component analysis (PCA). Through PCA, it was possible to differentiate the *Amaranthus* species both for seeds and oils. Through PLS-DA, it was possible to predict the classes of the species with high degree of correct classification, with 96.67% of correct classifications for seeds and 98.89% for oil. Thus, with the use of the near infrared spectroscopy associated with the multivariate statistical analysis, it is possible to classify the different *Amaranthus* species, especially when using the oil.

Keywords: non-conventional vegetable; partial least squares discriminant analysis; principal component analysis.

INTRODUCTION

With the increasing use of medicinal plants or plants that are considered functional foods, quality control has been of paramount importance when analyzing from the market perspective, to avoid adulteration and control quality according to current regulations (Gobbo-Neto & Lopes, 2007). Normally, chromatographic analysis is used to have absolute assurance that it really is the referenced species in terms of its chemical composition. Chromatography is an expensive technique and takes time to perform (Parys *et al.*, 2019). In this way, the identification of fast and preferably non-destructive techniques that can prove the presence and content of chemical compounds and, in turn, guarantee the quality and origin of the product are desirable.

Of the various techniques available, Near Infrared Spectroscopy (NIR) has shown promise in qualitative and quantitative analysis, being widely used in the area of chemistry of natural products and organic transformations (Lima & Bakker, 2011). It has advantages because it is a non-destructive technique, performed in a relatively short time (Agelet *et al.*, 2012), with wide acceptance in different fields. Vis-NIR spectroscopy is often used in combination with chemometric and multivariate analyzes that are selected based on the objectives of the study (Sohn *et al.*, 2021).

The genus *Amaranthus* contains about 70 species (Singh, 2017), widely known and consumed around the world. However, it is almost unknown in Brazil for food

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or medicinal use, it being recognized only as a weed, whose control significantly impacts the production cost of cultures (Jimoh *et al.*, 2022). The most commonly found species in most of the arable areas of Brazil, are *A. viridis, A.spinosus, A. deflexus, A. hybridus, A. retroflexus* and *A. lividus* (Bayón, 2022). However, studies with the species of widespread occurrence in Brazil are still incipient.

Species of the genus have shown great potential as a source of nutritional and medicinal compounds due to the chemical composition present in leaves, roots, inflorescences, grains and oils. It is rich in bioactive compounds such as phenolic acids, polyphenols, unsaturated fatty acids, glucosinolates, proteins, soluble peptides, flavonoids, squalene, beta-carotene and others (Parveen *et al.*, 2014; Silva *et al.*, 2018; Xavier *et al.*, 2018; Mir *et al.*, 2018; Xavier *et al.*, 2019a). Grains are rich in protein, essential amino acids, fiber, minerals and vitamins and oil (Sá *et al.*, 2020). When compared to oil seeds, the oil content in amaranth is low, however it has a high concentration of unsaturated fatty acids and squalene, a potent natural antioxidant, widely used in the cosmetics industry for skin hydration as an emollient in vaccines, in addition to having antitumor activity and cardioprotective (Srivastava, 2017). Amaranth seed oil has been suggested as an alternative to animals as a natural source of squalene.

The content and diversity of secondary metabolites present in plants show a strong interaction with the environment. Climatic conditions, the type of cultivation and the species are factors that can change the content and chemical composition of extracts and oils in plant species. In *Amaranthus*, the NIR technique associated with multivariate analysis was used to determine the chemical composition of leaves and extracts, on postharvest betacyanin degradation, on seed germination in the identification and classification of species (Matzrafi *et al.*, 2017, Silva *et al.*, 2018; Silva *et al.*, 2019; Xavier *et al.*, 2019b; Silva *et al.*, 2021, Sohn *et al.*, 2021). Studies using NIR to characterize Amaranth oil are scarce.

Therefore, the aim of this work was to evaluate the efficiency of near-infrared (NIR) spectroscopy in determining the chemical composition of oil and seed from different cultivation systems and the technical potential to distinguish *Amaranth* species.

MATERIAL AND METHODS

The experiment was performed with seeds of *Amaranthus* obtained from UFLA's (Federal University of Lavras) germplasm collection of non-conventional vegetables in Lavras, Minas Gerais (21º14'S, 45º00'W and altitude of 918 m). The climate of the region is Cwa (mesothermal) with dry winter and rainy summer, according to the Köppen classification (Álvares *et al.*, 2013).

The test was arranged in the field in a randomized block design (RBD) with three replications, in a factorial scheme 2x3, [planting systems (organic and conventional) *Amaranthus* species (*A. viridis* L., *A. hybridus* L. and *Amaranthus* sp. -commercial species)]. The materials were identified through exsicattes by EPAMIG (Agricultural Research Company of the State of Minas Gerais), being recorded and included in the EPAMIG Herbarium of Minas Gerais (PAMG) herbarium collection number 58002, 58003 and 57999, respectively.

The seeds were directly sown in the field in the spacing of 0.5m x 0.5m, and, later, the thinning was performed with density of 40,000 plants per hectare without the use of irrigation. Following soil analysis, the correction of acidity and the fertilizing were performed in accordance with the recommendation for the culture (Brasil, 2013).

In the organic cultivation system, dolomitic limestone, chicken manure (before seeding) and organic compost (40 days after seeding) were used. The application of plant extracts of *Ricinus communis* L., with insecticidal and fungicidal principles, was carried out for the phytosanitary control (Xavier *et al.*, 2018). In the conventional cultivation system, dolomitic limestone, urea, simple superphosphate and potassium chloride were used. The cultivation and the phytosanitary control were performed in accordance with the needs of the culture (Brasil, 2013).

The border effect was taken into consideration in order to avoid the influence of the neighbor portions on the treatments. Besides, a physical barrier was used with the maize culture to avoid crossing among species once polyploidy interspecific hyperbridization is common in these species, and hide their characteristics (Olusanya, 2017).

After harvesting, the drought and processing of seed was performed manually. Then, they were packed in multi-layer Kraft paper and stored in cold chamber (10 °C and 40% of relative air humidity). For the obtaining and quantification of oil, four replications were employed for each treatment. The oil was extracted from the seeds of different *Amaranthus* spp. species in accordance with the Vasconcelos *et al.* (2018) methodology. One hundred and fifty grams of dry and crushed seed were used per treatment.

The spectra of the seeds and oils were acquired in the near infrared (NIR) using a spectrometer based at the Fourier transform (Bruker, model MPA) alongside the OPUS_Spectroscopy software version 7.0. The spectra were collected from the range of 9.995 cm^{-1} and 4.000 cm^{-1} directly in the surface of each portion of the seed samples through optical fiber and oil in a cuvette. The spectra in NIR were registered in diffuse reflection mode with spectral resolution of 8 cm^{-1} using 32 sweeps for the background (reference spectrum) and 16 sweeps per sample. Thus, a spectrum was registered for each sample totaling 66 spectra from seed with conventional fertilizing (3 species x 22 replications), 34 from seeds with organic fertilizing (3 species x 15 replications), and 45 from organic oils (3 species x 15 repetitions).

The spectra collected from seeds and oils were selected in the wavelength in the range of 9.995 cm^{-1} and 4.000 cm^{-1} and submitted to the principal component analysis (PCA) and to the partial least squares discriminant analysis (PLS-DA). The analyzes were performed using Chemoface version 1.61 (Nunes *et al.*, 2012).

The principal component analysis was performed with the objective of verifying the similarities among the samples analyzed. This analysis was performed with treated (first derivative, *multiplicative scatter correction,* standard normal variate and normalization) and non-treated spectra, and a two-dimensional graph was generated for score plot.

The PLS-DA was performed in order to generate predictive models for classification of the three species of seeds in the cultivation conditions (six classes) and its respective extracted oils (six classes). The adequate number of latent variables was defined by cross-validation. The models generated were evaluated by the number and percentage of hits in the predicted classes.

RESULTS

Near infrared spectroscopy

Spectruns collected in the NIR was registered for the seeds (Figure 1A) and for the oil (Figure 1B) of each *Amaranthus* species in the different cultivation systems with each spectrum representing the average of various samples**.** There was a similar spectrum pattern regarding absorbance peaks. In the entire wavelength range adopted, the spectra of oil and seed showed similar absorption bands among species and different among seeds and oils, regardless of the cultivation system.

In the seeds, the absorbance peaks were concentrated in the range between 7044 and 5077 cm^{-1} (Figure 1A). The spectra of the species from the organic cultivation system showed higher absorbance peaks when compared to the conventional system, except for A. hybridus. In the oil, the absorbance peaks were concentrated in the range between 6060 and 4000 cm^{-1}. In this case, the species A. viridis and A. hybridus presented the highest absorbance peaks in the conventional system while *Amaranthus* sp. (commercial) showed more intense bands in the organic system. However, evidencing the greater interaction between the near infrared radiation and the probable functional groups of the *A.* species (Figure 1B) making evident the greater interaction between the near infrared radiation and the probable functional groups of the *A.* species (Figure 1B).

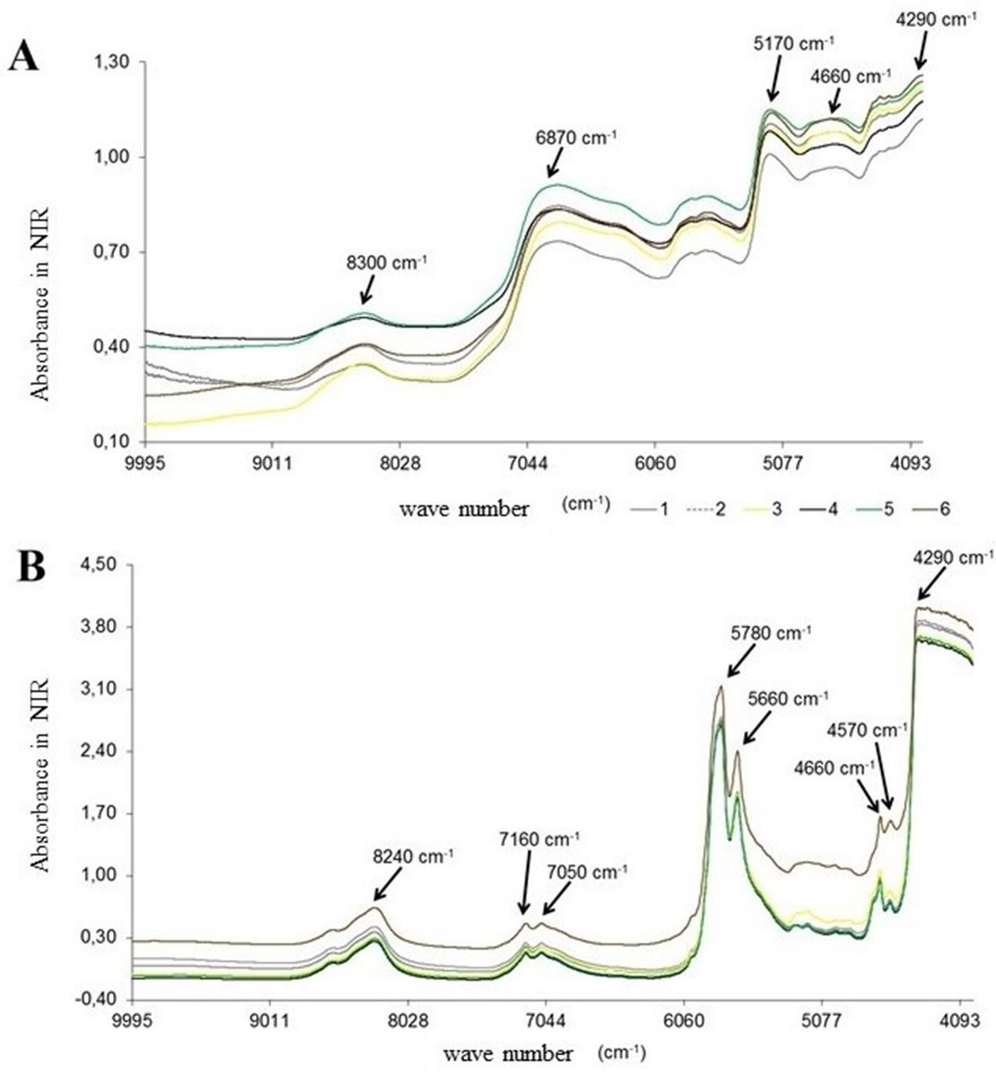
Using the *Practical Guide and Spectral Atlas for Interpretive Near-Infrared Spectroscopy* (Workman Júnior & Weyer, 2012), it was possible to infer about the identification of chemical functional groups (Table 1) present in the grains and oils of the species in the different cultivation systems. There was a specific absorption band at certain wavelengths corresponding to compounds such as aliphatic hydrocarbons, polysaccharides, water and lipids in addition to aromatic hydrocarbons and proteins in the oil.

Principal Components Analysis – PCA

After the construction of the calibration models, the factorial distribution of the spectra through NIR was carried out based on the PCA analysis in order to detect differences among the species and cultivation systems.

The principal components analysis (PCA) was carried out starting from the seeds spectra (Figure 1) aiming at evaluating the spectral similarity in the behavior of the species and the similarities among the cultivation systems of the materials studies. In order to focus on the most interesting answers, only the results of the analyzes with the spectra without treatments were presented.

The PCA scores for the three species of *Amaranthus* seeds in the organic and conventional systems were plotted in the two-dimensional graph (Figure 2A) in which the sum of the principal component 1 (PC1) and principal component 2 (PC2) explain 99.95% of the data variation. In the PCA that only used the conventional (Figure 2B) and the organic (Figure 2C) cultivation system, the sum of PC1 and PC2 obtained explanation of 99.99% and 99.97% of the data variation, respectively.



1: *A. viridis* (conventional*)*; 2: *A. hybridus* (conventional); 3: *Amaranthus* sp. (conventional); 4: *A. viridis* (organic); 5: *A. hybridus* (organic); 6: *Amaranthus* sp. (organic).

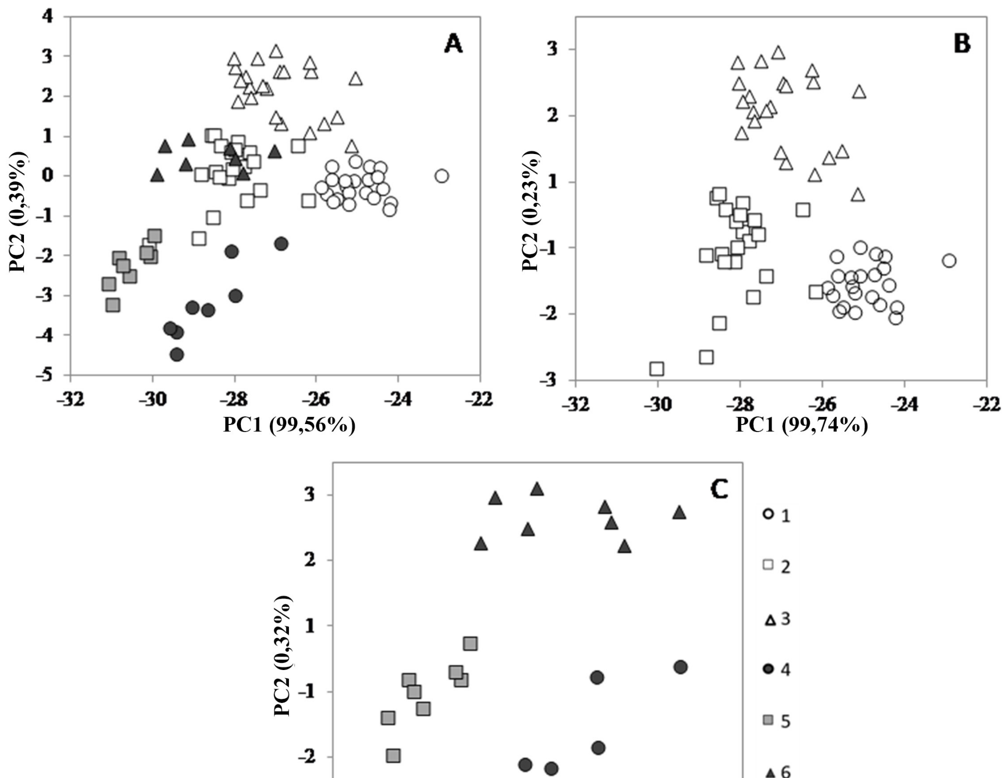
Figure 1: Average of the spectra obtained through spectroscopy in the near infrared in the different *Amaranthus* species and cultivation systems using (A) seeds and (B) oils.

After the analyzes with all the treatments in different cultivation systems (Figure 2A), PCA clearly separated the species *A. viridis* in the conventional system, *A. viridis* in the organic system and *A. hybridus* in the organic system. These results showed that the spectral range allowed the separation of species in their respective cultivation systems. An exception can be observed in the overlapping of the spectra of *A. hybridus* cultivated in the conventional system and *Amaranthus* sp. (commercial) in the organic cultivation. This shows that there is a spectral similarity between these two materials.

For the oil, the principal components analysis (PCA) of the spectra was carried out without treatment (Figure 3A) and treated (Figure 3B). In the graph of the scores (Figure 3A) of the PCA using spectra without treatment of the oils of different species of *Amaranthus*, the first principal component (PC1) explained 97.97% of the total data variation. The second principal component (PC2) explained only 1.84% of the variation, and the sum of both explains 99.74% of the data variation.

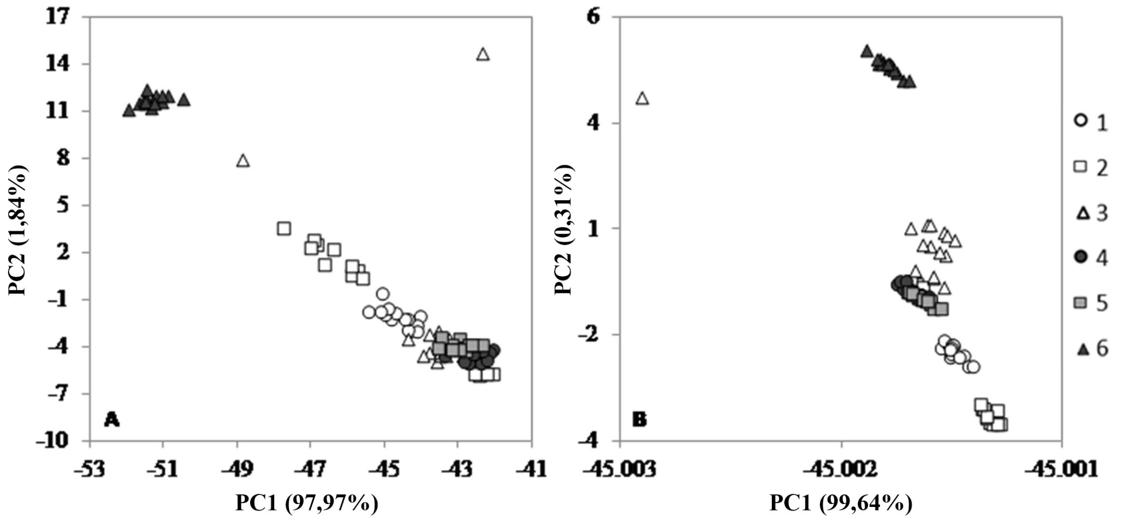
Table 1: Correlation spectrum-structure by near infrared spectroscopy for the different cultivation seeds of *Amaranthus* seed and oil

Spectral Range (cm^{-1})	Functional Group	Material Type
	Seed	
4297	C-H (.C-H & CH2)	Polysaccharide
4668	C-H/C = O associated lipid (.RC = CH & RC = O)	Lipids
5173	O-H (.O-H & HOH)	Polysaccharide
5675	C-H Methylene (.CH2) (Symmetric)	Aliphatic Hydrocarbons
6874	O-H of water	Water
8309	C-H Methyl (.CH3)	Aliphatic Hydrocarbons
	Oil	
4378	C-H Starch (.C-H & CH2)	Polysaccharide
4571	N-H/C-N/C = O	Proteins
4664	C-H/C = O associated lipid (.RC = CH & RC = O)	Lipid
5667	C-H Methylene (.CH2) (Symmetric)	Aliphatic Hydrocarbons
5786	C-H Methylene (.CH2)	Methylene Hydrocarbons
7052	C-H Aromatic C-H	Aromatic Hydrocarbons
7167	C-H Methyl C-H, linear associated aliphatic CH3 (CH2)N CH3	Aliphatic Hydrocarbons
8240	C-H Methylene (.CH2)	Aliphatic Hydrocarbons



1: *A. viridis* (conventional); 2: *A. hybridus* (conventional); 3: *Amaranthus* sp. (conventional); 4: *A. viridis* (organic); 5: *A. hybridus* (organic); 6: *Amaranthus* sp. (organic).

Figure 2: Principal Components Analysis (PCA) of the spectra without treatment in seeds of different *Amaranthus* species in different cultivation systems: conventional and organic (A), conventional cultivation (B) and organic (C).



1: *A. viridis* (conventional*)*; 2: *A. Hybridus* (conventional); 3: *Amaranthus* sp. (conventional); 4: *A. viridis* (organic); 5: *A. Hybridus* (organic); 6: *Amaranthus* sp. (organic).

Figure 3: Principal component analyzes of the spectra without treatment (A) and treated by the Multiplicative Scatter Correction (B) of oils of different *Amaranthus* species and cultivation systems.

For the oil samples of the different *Amaranthus* species with treated data (Figure 3B), PC1 explained 99.64% of the total data variation. PC2 explained only 0.31% of the variation in a total of 99.95% of total data variation.

According to the PCA results for the spectra not treated (Figure 3A) for the oils extracted from the seeds, it was not possible to distinguish the species clearly. Therefore, it was possible verify a grouping of almost all the species in the different cultivation systems except *Amaranthus* sp. (commercial) with grouped separately. However, with the spectra treatment through the Multiplicative Scatter Correction (Figure 3B) it was possible to increase the visualization and distinguish the species in the conventional cultivation system more prominently.

Classification of the different Amaranthus species by PLS-DA

The spectra obtained from the seeds of the different species of *Amaranthus* were also differentiated when associated with PLS-DA, proving the efficiency of the technique. The validated models generated by the PLS-DA were presented through the number and hit percentage (Table 2).

Table 2: Classification of the different *Amaranthus* species and cultivation system through PLS-DA starting from the spectra without treatments measured in the seeds

Treatment	NIR Prediction						Total number	Total hits	% Correct
	1	2	3	4	5	6			
1	22	-	-	-	-	-	22	22	100,00
2		20	1		1		22	20	90,91
3			22				22	22	100,00
4	1			7			8	7	87,50
5					8		8	8	100,00
6						8	8	8	100,00
Total							90	87	96,67

1: *A. viridis* (conventional*)*; 2: *A. Hybridus* (conventional); 3: *Amaranthus* sp. (conventional); 4: *A. viridis* (organic); 5: *A. Hybridus* (organic); 6: *Amaranthus* sp. (organic).

Of the 90 samples of *Amaranthus* seeds, 87 were correctly classified, with 96.67% of correct classifications (Table 2). For the species *A. viridis* and *Amaranthus* sp. originating from conventional cultivation and *A. hybridus* and *Amaranthus* sp from the organic system, 100% accuracy was obtained in the classifications, which corroborates the results of PCA (Figure 3), where most of these species do not mixed with each other in the different systems. In the other species the error observed was only two. Therefore, such models are considered satisfactory. These results corroborate with the PCA (Figure 2).

Regarding the oil, the classification of species according to the cultivation system by PLS-DA and cross-validation, obtained 98.89% success (Table 3). Almost all species obtained 100% hits.

Table 3: Classification of the different *Amaranthus* species in different convention (c) and organic (o) cultivation systems through PLS-DA starting from spectra without treatments measured in oil

Treatment	NIR Prediction						Total number	Total hits	% Correct
	1	2	3	4	5	6			
1	15	-	-	-	-	-	15	15	100,00
2		15					15	15	100,00
3			14				15	14	93,33
4				15			15	15	100,00
5					15		15	15	100,00
6						15	15	15	100,00
Total							90	89	98,89

1: *A. viridis* (conventional*)*; 2: *A. Hybridus* (conventional); 3: *Amaranthus* sp. (conventional); 4: *A. viridis* (organic); 5: *A. Hybridus* (organic); 6: *Amaranthus* sp. (organic).

DISCUSSION

Near infrared spectroscopy

As observed (Figure 1), both the grains and the oil of the different species, regardless of the cultivation system, showed a similar spectral pattern in relation to the absorbance peaks, but different between the grains and the oil (Figures 1A, 1B), that is, along the adopted wavelength range, both the oil and grain spectra showed different absorption bands in the NIR, however similar among the species.

Using the *Practical Guide and Spectral Atlas for Interpretive Near-Infrared Spectroscopy* (Workman Júnior & Weyer, 2012), it was possible to infer about the chemical functional groups of the different treatments. According to the spectral correlation, absorption bands were verified in the number of waves corresponding to aliphatic hydrocarbons, polysaccharides, water and lipids, in the grains. Similar compounds were identified in the oil, in addition to aromatic hydrocarbons, proteins and methylene hydrocarbons. Xavier *et al.* (2019b) identified in seeds of the same species, in addition to the groups observed in this study, aromatic amines and ovalbumin. These differences may be due to the degree of absorption is proportional to the concentration of functional groups in the sample (Curran *et al.*, 1992) or to sound noise from the device itself or from the environment (Sohn *et al.*, 2021).

Amaranth seed is composed of aliphatic hydrocarbons, lipids, present in the form of triglycerides constituted by unsaturated fatty acids (Marzzoco & Torres, 2017). They are present in the embryo, endosperm and reserve tissue (Carvalho & Nakagawa, 2012). Among the substances belonging to this group is squalene. Studies have proven the beneficial effect of squalene in the cosmetics and pharmaceutical industry (Lozano-Grande *et al.*, 2018). Rats fed with *Amaranthus* showed reduced cholesterol and this effect was attributed to the presence of squalene (Shin *et al.*, 2004). The aromatic hydrocarbons identified in the oil are the chemical group of antioxidant substances such as complex phenolic compounds such as anthocyanins, flavonoids (flavones and flavonols), isoflavonoids (isoflavones) and tannins. In the oil, the chemical group related to proteins was detected, an important food reserve of the seeds, they constitute important components of the protoplasm and are essential for the formation of new tissues. Polysaccharides were also detected, which belong to carbohydrates that are reserve substances. Amaranth is considered a pseudocereal rich in carbohydrates and low in lipids (Marcos Filho, 2015). Vasconcelos *et al.* (2018), correlated the different wavelengths of the spectra to functional groups and, finally, types of compounds in sunflower seeds and oil, as performed in this study.

Principal Components Analysis – PCA

Changes in NIR spectra are often too small to be noticed by the human eye, hence it is often used in combination with various chemometric and multivariate analysis (Sohn *et al.*, 2021). Pre-processing techniques are proposed as one of the initial steps in data analysis with the aim of optimizing the results obtained by spectroscopy. For grains, PCA performed with untreated data (Figures 2A, 2b and 2C) considering the two cropping systems together, allowed the separation of species within each cropping system, except for *A. Hybridus* (conventional) and *Amaranthus* sp. (organic) (Figure 2A). Considering each system individually, the technique was more efficient in separating the species in the organic system (Figures 2B and 2C). This makes evident that the NIR was sensitive to differences among *Amaranthus* species.

For oil, considering the untreated data, there was an overlap of groups among some species in the PCA. According to Souza *et al.* (2017) this overlap may indicate, at first, a similarity in the chemical composition of the species. For the data treated in both cropping systems, the species were grouped separately, clearly demonstrating the difference in the chemical composition of the species as a function of the cropping system. In the organic cropping system (Figure 2B), it was possible to observe that oil *Amaranthus* sp. differed from the others, which may be related to the typical presence of specific chemical structures in this region. This fact is proven in a conventional system with the same species in which some scores migrated to the same region of the graph (Figure 3B). In *Amaranthus* the near infrared (NIR) has been successfully used in determination of the chemical composition, in the germination of seeds, in the response to herbicides and in the discrimination of species, where the spectra were obtained from leaves and seeds. However, studies with obtaining NIR spectra in oil are scarce. However, the use of NIR has provided promising results in the analysis of oils from other oilseed species. Monferrere *et al.* (2012) were successful in differentiating among sunflower species based on oil content by applying PCA in NIR spectra. Souza *et al.* (2017) applied this analysis in the spectra obtained by NIR generating a model that allowed the detection of differences in the composition of phenolic and flavonoid compounds in *Raphanus sativus* L., *Secale cereale* L. and *Avena strigosa* L. The technique of near infrared spectroscopy was sufficiently accurate to determine the moisture content and protein content of rice and wheat grain (Li *et al.*, 2013), biochemical evaluation of sorghum grains for food, feed and fuel without destruction, and complex chemical analysis (Ejaz *et al.*, 2021); On the other hand, the PCA scores of first 2 main components showed that none of the spectral pre-processing treatment (SNV, 1st and 2nd derivative) provided discrimination between soybean cultivars and detection of physicochemical changes of stored soybean (Bazoni *et al.*, 2017).

Classification of the different Amaranthus species by PLS-DA

This technique was efficient to separate the different species according to the cultivation system, with a high percentage of correct answers. These results agree with Xiaobo *et al.* (2010) who stated that the NIR-PLS-DA technique allows a faster analysis of spectral variations, in the prediction of the chemical composition of each sample. Vasconcelos *et al.* (2018) were successful using NIR-PLS-DA spectra in the separation of sunflower seeds. This technique was efficient to classify viable and nonviable soybean seeds (Kusumaningrum *et al.*, 2017).

In all analyzes carried out, the effect of the cropping system was clear. The composition of the oil and the grain generated different spectra depending on the cultivation systems, as verified in the PCA clusters. Passion fruit cultivation in the organic system increased the content of chemical compounds in this plant (Ramaiya *et al.*, 2021). Organic fertilizers increased the production of active compounds in rice (Siavoshi & Laware, 2013).

CONCLUSION

Through the analysis of principal components, it is possible to differentiate the different species of *Amaranthus* when using the spectra oil and seeds, in function of the different cultivation systems.

The PLS-DA model provided, with a high percentage of correct answers, the classification of species according to the oils and seeds of the different species. With the use of NIR, the oil showed more expressive results than the seed.

Near infrared spectroscopy of oils and seeds can be used to quick identify the different species of *Amaranthus* in different cropping systems.

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