

SPECTRAL ANALYSIS OF TOXIC WEEDS: A CASE STUDY ON DATURA SPECIES

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Abstract

In this research work we focused on collection of the hyperspectral data library of cultivated Datura stramonium L. as a remote sensing training reference. During the study, 6 separated Datura stramonium L. plants were analysed. AvaSpec 2048 hyperspectral spectrometers were used under visible, near- and mid-infrared-calibrated measurement laboratory conditions.

The spectral data of maize as a cultivated crop were also determined with the same phenological time window. The chlorophyll content chemical analysis was performed, as well as detailed thermometric image recordings. The high resolution characteristic absorbance peaks of Datura stramonium L. were determined in visible and near-infrared electromagnetic spectrum.

We also measured and evaluated these data in the mid-infra range for soil, leaf and crop. The results allow the data collected for hyperspectral airborne data acquisition to be used as training data when classify images. The results of reference studies on leaves, diseased leaves, green and dry crops can also be used for field measurement of morphological and physiological plant properties influencing spectral properties and parameters.

When preparing precision weed control, it is recommended to calculate special hyperspectral vegetation indices and isolate management zones, mainly SWIR range by FFT processing. The Water and Environmental Management institute has several decades of references for the evaluation of hyperspectral data. Thermometric data processing also showed favorable results.

Key words: spectral analysis, *Datura stramonium*, hyperspectral, chlorophyll, toxic weeds, food safety

INTRODUCTION

Datura stramonium, commonly known as Jimson weed or thorn apple, belongs to the *Solanaceae* family and originates from Central and South America. Its high toxicity is due to alkaloids such as hyoscyamine, atropine, and scopolamine, which can cause fatal poisoning in humans and animals alike (Berkov et al., 2006; Klein-Schwartz and Oderda, 1984). Due to its hallucinogenic properties, this plant has been used historically in various cultures for ritualistic or recreational purposes (Glennon et al., 1987). In Hungary, *Datura stramonium* is the only representative of the *Datura* genus and is primarily recognized as a weed (Kiss et al., 2021).

Datura stramonium can grow up to one meter in height, with branching, smooth stems that may reach as tall as 180 cm under favorable

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conditions. Its oval leaves are large (up to 20–30 cm long) and serrated, allowing it to efficiently capture nutrients from the soil (Yockteng et al., 2013). The plant's large, white, trumpet-shaped flowers bloom primarily at night, attracting nocturnal pollinators such as moths (Motten, 1986). Its fruit capsule, containing the seeds, is covered with spiny projections and opens upon maturation, releasing seeds into the environment (Kiss et al., 2021).

Datura stramonium thrives in nutrient-rich, nitrogen-indicative soils and is frequently observed in Hungarian agricultural surveys. It poses significant challenges in crops like corn, sunflower, potato, and soybean, where it can cause considerable yield reductions (Vyskot et al., 1990; Kiss et al., 2021). The dense shading effect of its foliage, along with its woody stems, obstructs crop harvesting and may also contaminate forage, posing risks to livestock (Holm et al., 1991).

Effective weed management of *Datura stramonium* requires targeted control measures, especially during its early phenological stages. It is particularly susceptible to pigment biosynthesis inhibitors, and pre-emergence herbicide applications, as well as post-emergence treatments in the 2–4 leaf stage, are highly effective (Kudsk and Streibig, 2003; Zimdahl, 2007). Spectral analysis can also be instrumental in identifying *Datura stramonium* early in the season, enabling timely intervention with herbicidal treatments (Asner, 2008).

MATERIAL AND METHOD

Sampling and Spectral Analysis

During sampling, we collected specimens from healthy green leaves, yellowing leaves, dry leaves, soil, and both green and dry fruits. For spectral data collection on leaf samples, we utilized the AvaSpec 2048 spectrometer, covering the wavelength range of 400-1000 nm with an accuracy of 0.6 nm. Following calibration of the spectrometer to white and dark references, we placed each leaf sample under illumination, recording measurements in three repetitions. Reflectance values were then exported to MS Excel for organization. For investigations within the 1000-2500 nm range, the AvaSpec-NIR256-2.5-HSC spectrometer was used. This spectrometer comprises three components: a detector, 8 µm diameter fiber optics, and a halogen light source.

To ensure precise measurements and eliminate potential electromagnetic interference from fluorescent lights, we conducted the experiments within a closed, black darkroom laboratory cabinet. The AvaSpec-NIR256-2.5-HSC spectrometer has a precision of 6.0 nm. The WS-2 reference panel, made of white diffuse Teflon, which reflects 98% of light in the 350-1800 nm wavelength range, was used. For accuracy, the panel was positioned at a constant distance from the fiber optic head; any

variation between the sample-to-sensor and reference panel-to-sensor distances could lead to distorted reflectance values.

Prior to measurements, calibration was performed by first measuring the maximum intensity reflected from the white reference panel, followed by measuring the minimum intensity under dark conditions. For each plant and soil sample, we recorded three reflectance spectra, each calculated as an average of 30 measurements. This averaging was essential to minimize uncertainties arising from the heterogeneity of the material matrix. During the spectral analysis, we examined the following plant parts: healthy (green) leaves, yellow leaves, dry leaves, dry and green fruit, and soil (Fig. 1).



Fig. 1. Plant Parts Examined During Spectral Measurements

Pigment Content Analysis

In green plants, chloroplast concentration and intensity in reference bands significantly impact absorbance and reflectance ratios, warranting their assessment. To determine pigment content, fresh plant samples were macerated with 80% acetone and 1 g of quartz sand to ensure homogeneity. After extraction, suspensions were centrifuged for 3 minutes at 3000 rpm in a Hettich ROTOFIX 32A, and the clear solution was transferred into quartz cuvettes. Absorbance measurements of the solution were taken using a

SECOMAN Anthelie Light II spectrophotometer at 470 nm, 644 nm, and 663 nm. These wavelengths were selected for spectrophotometric measurements because, in an 80% acetone solution, chlorophyll *a* has a maximum absorbance at 663 nm, chlorophyll *b* at 645 nm, and carotenoids between 440-470 nm. Each measurement was preceded by zero calibration using 80% acetone.

Chlorophyll content in samples was calculated using the equation published by Droppa et al., 2003:

$$\text{Chlorophyll (a + b) } \mu\text{g/g fresh weight} = \frac{(20,2 * A_{644\text{nm}} + 8,02 * A_{663\text{nm}}) * V}{w}$$

The carotenoid values were determined based on the equation provided by Lichtenthaler and Wellburn, 1983:

$$\text{Carotenoid } \mu\text{g/g fresh weight} = (1000 * A_{470\text{nm}} - 3,27 (12,21 * A_{663\text{nm}} - 2,81 * A_{644\text{nm}}) - 104 * (20,13 A_{644\text{nm}} - 5,03 A_{663\text{nm}})) / 229 * V/w$$

where:

V = volume of the tissue extract (ml);

w = fresh weight of the tissue (g);

A = absorbance;

Thermal Imaging

During the thermal imaging sessions, we photographed all plants together and then individually captured images of the soil, dry leaves, yellowing leaves, healthy leaves, green fruit, and dry fruit. The images were processed using the IRSoft application, where we monitored the average temperature of the photographed sections and evaluated the results accordingly.

Statistical Evaluation

To analyze the results obtained from the investigations, we employed various statistical methods. The data for each measured parameter were entered into Microsoft Office Excel, where we created a database. Statistical analyses were conducted using R software within the R Studio user environment (R CORE TEAM, 2017).

RESULTS AND DISCUSSION

Results of Spectral Analysis Investigations in the 400-1000 nm Wavelength Range

The reflectance profiles of chlorophyll content were evaluated in the 400-1000 nm range. It was observed that healthy leaves exhibited reflectance values between 15-20% in the 600-670 nm range, while

yellowing leaves showed reflectance values between 30-50%, corresponding to a decrease in chlorophyll content. Completely dried leaves exhibited reflectance values between 30-40%. The reflectance maximum of carotenoids can be measured in the 520-580 nm wavelength range, where healthy plants showed reflectance values around 30%. As chlorophyll content decreases, the reflectance values for carotenoids increase proportionally, reaching approximately 60% for yellowing leaves, while around 40% was observed for dry leaves (Fig. 2).

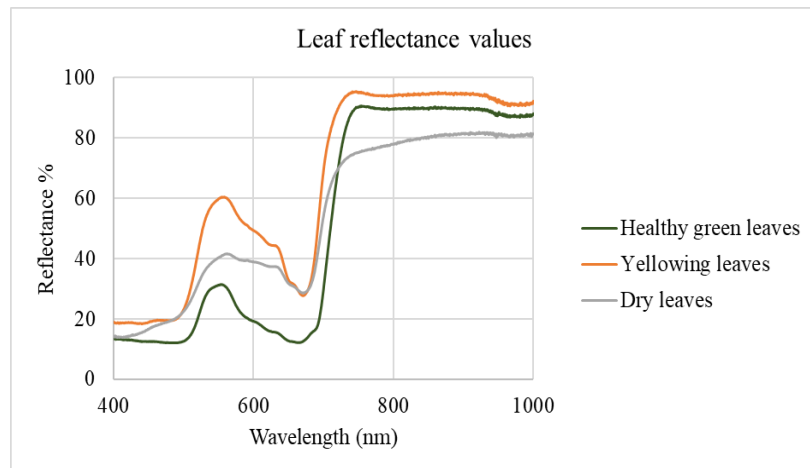


Fig. 2. Reflectance of Leaves in the 400-1000 nm Wavelength Range

The reflectance profile of soils was evaluated in the 400-1000 nm range. For the soil, a reflectance value close to 0% was observed. The soils were loess soils with a humus content of 2-3% and were irrigated up to field capacity (Fp 2.2), appearing nearly black in the visible range. This low reflectance was characteristic due to the spectral absorbance of soil moisture.

The reflectance profiles of fruits were also assessed in the 400-1000 nm range (Fig. 3). It was noted that green fruits exhibited reflectance values between 2-5% in the 600-670 nm range. The reflectance maximum for carotenoids can be measured in the 520-580 nm wavelength range, where green fruits showed reflectance values around 5%. In contrast, dried fruits exhibited reflectance values between 1-5%.

In Hungary, *Datura stramonium L.* is most commonly found in maize (*Zea mays*) fields, particularly in well-drained soils rich in nitrogen and organic matter. During the condition assessment with precision agriculture drones, it is essential to know the spectrum of the cultivated crop for object segmentation. As a reference measurement, we observed the reflectance values of maize leaves. The reflectance profiles of chlorophyll content were evaluated in the 400-1000 nm range (Fig. 4).

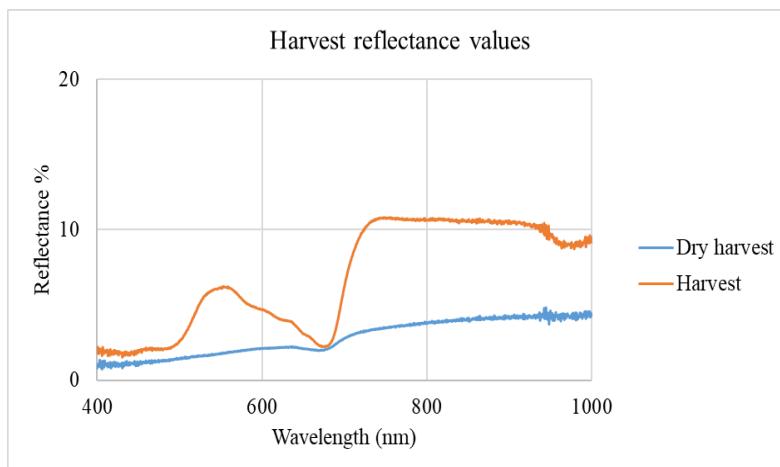


Fig. 3. Reflectance of Fruits (harvest) in the 400-1000 nm Wavelength Range

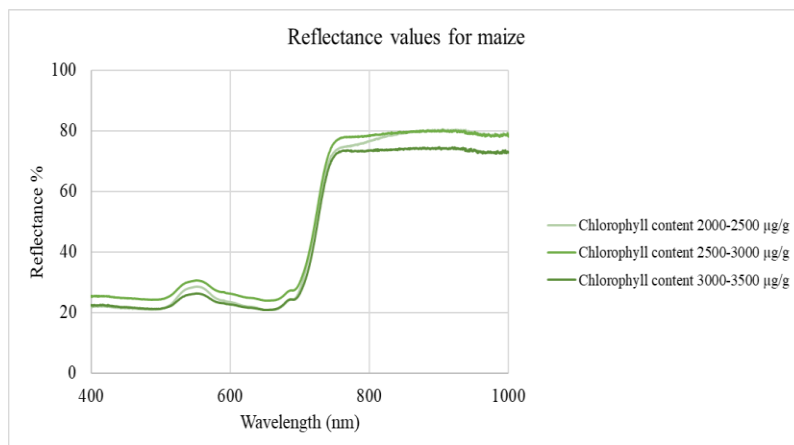


Fig. 4. Reflectance of Maize and Total Chlorophyll Content ($\mu\text{g/g}$) in the 400-1000 nm Wavelength Range

Leaves with high chlorophyll content exhibited reflectance values between 20-22%, which showed an increasing reflection proportional to the decrease in chlorophyll values. The reflectance maximum of carotenoids can be measured in the 520-580 nm wavelength range, where high chlorophyll content resulted in reflectance values around 25%. It was observed that as chlorophyll content decreases, the reflectance values for carotenoids increase proportionally.

Investigations in the 1000-2500 nm Wavelength Range

The 1000-2500 nm wavelength range encompasses the near-infrared (NIR) and shortwave infrared (SWIR) spectrum. This range is particularly useful for measuring and analyzing plants, as different components of plants absorb and reflect these wavelengths differently. This data provides crucial

information for precision weed management during the evaluation of the n-dimensional hyperspectral data cube.

Measurements taken in the near and shortwave infrared range carry important information from several perspectives, which can be observed during the study of various plant parts of *Datura stramonium*. During the measurements, we examined healthy green leaves, dry leaves (or diseased leaves), yellow leaves, dry and green fruits, and soil within this electromagnetic range (Fig. 5).

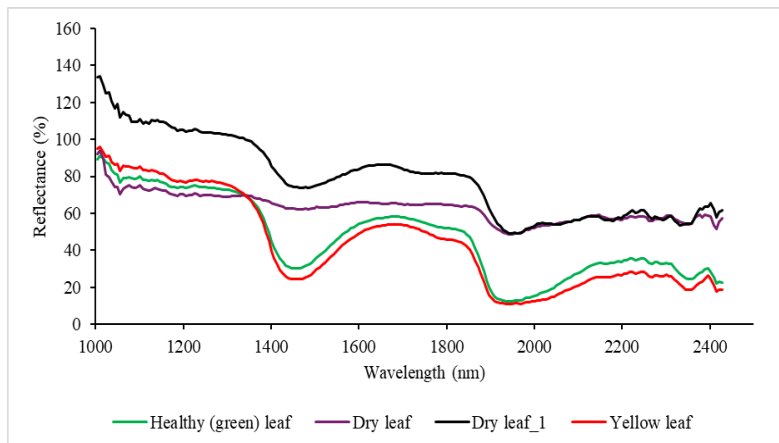


Fig. 5. Reflectance of Healthy, Dry, Dry1, Yellow Leaves in the 1000-2500 nm Wavelength Range

The spectral characteristics of plant leaves indicate that the reflectance of healthy and yellowing (yellow) leaves differs minimally, yet their shape remains consistent. Both healthy green leaves and yellowing leaves exhibit a reflectance of 90% at 1100 nm. However, significant reductions occur at two local minima: between 1300-1400 nm, where reflectance drops to 30% for healthy leaves and 24% for yellow leaves, and again at 1900 nm, where both types of leaves show a reflectance of 11%.

Two valleys can be identified in the spectral curve, located in the wavelength ranges of 1430-1510 nm and 1890-1980 nm. The water content of plants significantly affects spectral reflectance in the 1000-2500 nm range (Fig. 6). Water strongly absorbs light at certain wavelengths (e.g., 1450 nm and 1950 nm), making these wavelengths sensitive to changes in plant water content.

Therefore, the two local minima observed for both healthy and yellow leaves correlate with the water content of the plant. This is further supported by the observation that in the two dry leaves (where the dry leaf_1 sample was infected with *Phytophthora infestans* and *Alternaria* sp. fungi), these two minima are absent. Both fungal species are typical of the Solanaceae

family, but *Phytophthora infestans* prefers wetter conditions, while *Alternaria* sp. favors drier growing environments.



Fig. 6. Evolution of reflectance of dry and green crops in the wavelength range 1000-2500 nm

Structural properties of plants, such as leaf thickness and cell wall structure, influence light reflectance and transmittance in this spectral range. These structural differences can assist in identifying the condition and type of plants. Plant stress, such as water deficiency or disease, alters the spectral reflectance of plants. In the NIR and SWIR ranges, these changes are often detectable earlier than in the visible light range. For dry leaves, we did not obtain a uniform spectrum. Nearly 100% reflectance indicates that a significant portion of the leaf reflects light in this spectral range, which is typical for dry and dead plant material.

The increase in reflectance in dry leaves can be attributed to several factors:

1. Degradation of Chlorophyll and Other Plant Pigments:

Chlorophyll and other pigments decompose or significantly decrease, leading to reduced absorption and increased reflectance. Since green pigments absorb light during photosynthesis, their absence enhances the amount of reflected light.

2. The water content of dry leaves significantly decreases, which also increases reflectance. The presence of water in leaves generally absorbs light at certain wavelengths (e.g., 1450 nm and 1950 nm), so the absence of water enhances the amount of reflected light.

3. The cellular structure of dry leaves changes, and the air spaces between the cells may enlarge, which also contributes to increased

reflectance. Due to these structural changes, the leaf surface reflects more light.

4. The surface of dry leaves is often rougher and drier, resulting in increased scattered light. This scattered light contributes to the increased reflectance.

5. In addition to the leaves, we also examined the reflectance changes of dry and still-green fruits.

The reflectance of green fruits (18.61% at 1000 nm) is higher compared to that of dry fruits (11.25% at 1000 nm). The two water absorption wavelength sections can also be observed in the spectral curves in this case.

The differences in reflectance between green and dry fruits primarily arise from variations in water and pigment content. Green fruits contain more water and pigments, which absorb light, while dry fruits have lost these components. Green fruits are in an active physiological state, whereas dry fruits are not. This significantly affects their spectral characteristics. The reflectance spectrum of green fruits shows multiple absorption peaks due to chlorophyll and water, whereas the spectrum of dry fruits is smoother and exhibits higher reflectance.

The spectral characteristics of the soil in the 1000-2500 nm wavelength range provide numerous important insights into the soil's composition, texture, and condition. This range is particularly effective at detecting the mineral components, organic matter, and moisture content of the soil (Fig. 7).

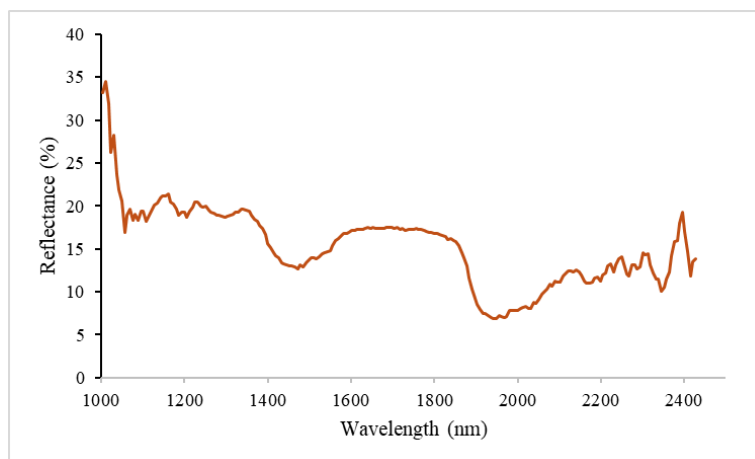


Fig. 7. The development of the spectral characteristics of the soil in the 1000-2500 nm wavelength range

Two distinct water absorption points can also be observed in this spectral curve, similar to those seen in the examined plant parts. The water

present in the soil results in strong absorption peaks in the 1400-1450 nm, 1900-1950 nm, and 2200-2500 nm ranges. These peaks arise from the vibrational and rotational modes of the water's OH groups. As the moisture content of the soil increases, reflectance decreases since water absorbs near-infrared and short-wave infrared light.

Soil particle size and texture also influence spectral characteristics. Finer-grained soils typically show lower reflectance, while coarser-grained soils exhibit higher reflectance. The moisture content of the obtained soil was high, which may account for its dark color and result in lower reflectance values in the 1000-2500 nm wavelength range.

Results of Pigment Content Investigations

The results obtained from destructive pigment content investigations are presented in the following table and figure (Table 1, Fig. 8).

Table 1

The development of total chlorophyll and carotenoid content in healthy and yellow leaves

Pot	Condition of leaves	Total chlorophyll content ($\mu\text{g/g}$)	Total carotenoid content ($\mu\text{g/g}$)
1	healthy green leaves	1745,96	300,29
2	healthy green leaves	1059,51	177,15
3	healthy green leaves	1260,31	222,01
4	healthy green leaves	1864,82	337,59
5	healthy green leaves	693,11	152,45
6	healthy green leaves	1776,80	340,84
	mean	1400,08	255,05
	standard deviation	471,776	82,348
4	yellow leaves	875,65	148,27
5	yellow leaves	920,81	220,64
	mean	898,23	184,46
	standard deviation	31,933	51,168

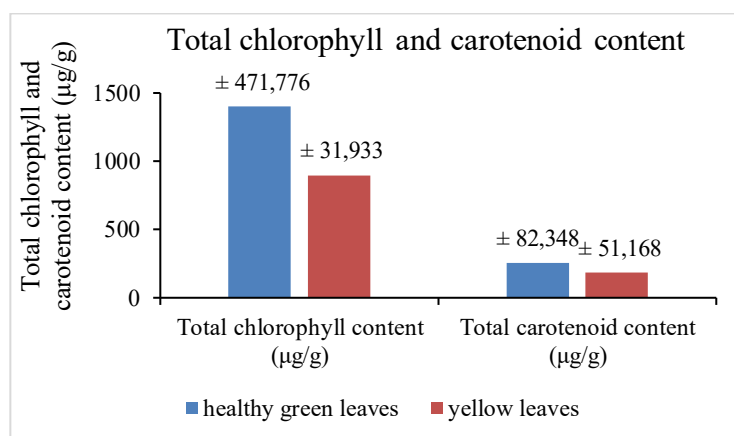


Fig. 8. Summary diagram of total chlorophyll and carotenoid content

The average chlorophyll content in healthy green leaves (1400.08 $\mu\text{g/g}$) is significantly higher than that in yellow leaves (898.23 $\mu\text{g/g}$); however, no significant difference was observed in the statistical analysis performed. The variability, as indicated by the standard deviation, is also significantly greater in healthy green leaves (471.776 $\mu\text{g/g}$) compared to yellow leaves (31.933 $\mu\text{g/g}$), suggesting that the chlorophyll content shows greater variability among healthy leaves. Similarly, the average carotenoid content in healthy green leaves (255.05 $\mu\text{g/g}$) is higher than in yellow leaves (184.46 $\mu\text{g/g}$), but, like chlorophyll content, no significant difference was noted for this parameter either. The standard deviation is also higher in healthy green leaves (82.348 $\mu\text{g/g}$) compared to yellow leaves (51.168 $\mu\text{g/g}$).

CONCLUSIONS

This study investigated the spectral characteristics, pigment content, and thermal properties of various plant parts, including healthy, yellowing, and dry leaves, as well as soil and fruits.

In the spectral analysis conducted within the 400-1000 nm range, the reflectance of healthy leaves was observed to be between 15-20% in the 600-670 nm range. In contrast, yellowing leaves displayed a higher reflectance of 30-50%, while dried leaves showed reflectance values of 30-40%. The reflectance peak for carotenoids was measured at 520-580 nm, with yellowing leaves exhibiting a significant increase to 60%, compared to approximately 30% in healthy leaves. For the soil, a reflectance value of nearly 0% was noted, attributed to its low humus content and moisture levels. Green fruits demonstrated a reflectance of 2-5% within the 600-670 nm range, whereas dry fruits had lower reflectance values of 1-5%.

Further analysis in the infrared measurements within the 1000-2500 nm range revealed that healthy and yellow leaves exhibited similar reflectance at 90% at 1100 nm. However, significant dips in reflectance were observed at 1300-1400 nm (30% for healthy leaves and 24% for yellow leaves) and at 1900 nm (11% for both). Absorption peaks corresponding to water content were identified, particularly at 1450 nm and 1950 nm, indicating correlations with plant water stress and health conditions.

Regarding pigment content, the average chlorophyll content in healthy leaves was found to be 1400.08 $\mu\text{g/g}$, significantly higher than that of yellow leaves, which measured 898.23 $\mu\text{g/g}$. The variability, as indicated by the standard deviation, was also notably greater in healthy leaves, suggesting a wider range of health status. Additionally, the average carotenoid content in healthy leaves was 255.05 $\mu\text{g/g}$, compared to 184.46

µg/g in yellow leaves; however, no statistically significant differences were detected between the two groups.

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