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Effect of water stress on vegetative growth and leaf concentration of flavonoids in mint (mentha x piperita) under protected cultivation conditions

Tatiana Carolina Gavilanez BUÑAY *[1], Juan Pio Salazar ARIAS [1], Fabian Mauricio Santana ROMO [2], Diego Mauricio Quilumba MASAPANTA [1], Heydy Kym Carrillo GARCÍA [1]

[1] Universidad Tecnica de Cotopaxi, La Maná, Cotopaxi, Ecuador.
[2] Departamento de Ciencias Exactas, Universidad de Las Fuerzas Armadas ESPE, Sangolquí, Ecuador.
*E-mail: tatiana.gavilanez@utc.edu.ec

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ABSTRACT: Medicinal plants, such as mint, contain active ingredients, which, although they are responsible for the therapeutic properties attributed to them, are also responsible for poisoning and adverse reactions that can occur if they are used in inadequate doses, high doses, or for prolonged periods. Many of these plant species have survived for millions of years thanks to their ability to produce substances that protect them from predators or extreme conditions. Even though some of these compounds (condensed tannins, phenols, alkaloids, oligosaccharides, and saponins) can produce a violent and immediate reaction, in most cases, they have a subtle effect that manifests itself with prolonged ingestion. By applying computational chemistry, the structures of bioactive molecules were revealed, representing them three-dimensionally after virtual screening. Therefore, in the project's development, the effect of water stress on the production of flavonoids in the protected mint crop was studied, using the previously measured field capacity and ultimately controlling the irrigation. This was divided into four irrigation application treatments (each 3, 6, 9, and 12 days), evaluating different agronomic variables and through a foliar analysis of the content of flavonoids present in the four treatments under study. The findings of this study, with their significant implications for medicinal plant cultivation, underscore how water stress can affect the production of flavonoids in mint. This knowledge can be directly applied to optimize cultivation practices and enhance the quality of medicinal plants, thereby benefiting the agricultural and pharmaceutical industries.
Keywords: aromatic plants; computational chemistry; computational chemical structural study; secondary metabolites.

Efeito do estresse hídrico no crecimento vegetativo e na concentração foliar de flavonoides em hortelã (mentha x piperita) sob condições de cultivo protegido

RESUMO: As plantas medicinais, como a hortelã, contêm princípios ativos que, embora sejam responsáveis pelas propriedades terapêuticas que lhes são atribuídas, são também responsáveis por intoxicações e reações adversas que podem ocorrer se forem utilizadas em doses inadequadas, em doses elevadas ou por períodos prolongados. períodos. Muitas destas espécies de plantas sobreviveram durante milhões de anos graças à sua capacidade de produzir substâncias que as protegem de predadores ou de condições extremas. Embora alguns destes compostos (taninos condensados, fenóis, alcalóides, oligossacarídeos e saponinas) possam produzir uma reação violenta e imediata, na maioria dos casos, eles têm um efeito sutil que se manifesta com a ingestão prolongada. Através da aplicação da química computacional, foram reveladas as estruturas das moléculas bioativas, representando-as tridimensionalmente após triagem virtual. Portanto, no desenvolvimento do projeto foi estudado o efeito do estresse hídrico na produção de flavonóides na cultura protegida de hortelã, utilizando a capacidade de campo previamente medida, e em última instância controlando a irrigação. Este foi dividido em quatro tratamentos de aplicação de irrigação (cada um com 3, 6, 9 e 12 dias), avaliando diferentes variáveis agronômicas e através de uma análise foliar o teor de flavonóides presentes nos quatro tratamentos em estudo.
Palavras-chave: plantas aromáticas; química computacional; estudo estrutural químico computacional; metalólitos secundários.

1. INTRODUCTION

Aromatic plants are defined as those that can generate a product with a specific smell or flavor through some physicochemical process, regardless of its commercial or aesthetic quality. These plant species are used commercially or industrially as living, fresh, or dry matter or to obtain extracts and essential oils for their organoleptic characteristics, which give characteristic aromas, colors, and flavors to foods (ELANSARY et al., 2017).

Many species belonging to the Labiatae family are known as mints. Currently, 18 species and 11 hybrids are registered under the name mint2. The cultivation and use of these species date back several centuries. They are attributed to digestive, calming, anesthetic, culinary, and cosmetic properties (ELANSARY, 2017; ELANSARY et al., 2017).

The commercial value of this species is given by its essential oil, whose main component is menthol, used in the food industry, to produce liquors and sweets, to give the flavor known as “mint,” and in the perfume industry. Its dried leaves are also sold and used for infusions, and its fresh leaves are used for culinary applications. Its stimulant, antiseptic, and analgesic capacity stands out among its medicinal properties. The “mint” flavor is the third most crucial flavor worldwide, after vanilla and lemon (KUMAR et al., 2011).

In Ecuador, descriptive studies were carried out to determine the use of medicinal herbs in pregnancy and its relationship with beliefs about the effects on childbirth. In addition to the level of knowledge of the patients about the use of phytotherapy, a survey was used to verify the hypothesis. The results show that all the women surveyed use medicinal plants to relieve specific symptoms of pregnancy. The most practical method for the use of medicinal plants was the infusion; among the most used medicinal plants were Chamomile, Mint, Lemon Balm, Linseed, Cinnamon, Oregano, Anise, Yerbabuena, Aloe Vera, Rue, Avocado, Cherimoya, Fig. Family beliefs are what guide the other types, thus mediating the use of medicinal plants. Hence, it is crucial to evaluate the effect of water stress on vegetative growth, the concentration of flavonoids, and other active ingredients in mint cultivation (CONTRERAS et al., 2022).

Plants in regions with a tropical climate are subject to stress due to water deficit and high temperatures. Studies of the influence of different crop factors, such as the water-soil-plant relationship and its application to irrigation to increase plant productivity, are valuable and necessary for the productive and horticultural sector. Water use optimization is based on selecting plants with lower water demand. Aromatic plants are in high demand for their fragrance and resistance to certain species' drought conditions. The aromatic potential of these plants depends mainly on the production of essential oils and the production of secondary compounds, such as flavonoids, which are influenced by various environmental factors, such as water stress (CHOUDHURY et al., 2017).

Environmental stress limits the yield of crops and generates many changes in their molecular processes, such as variations in the profile of metabolites and the production of these compounds. Drought or water deficit constitutes one of the most important types of stress after the perception in plants leads to an unusual increase in the production of reactive oxygen species (ROS). There is a wide variety of free radical ROS, such as superoxide radicals, hydroxyl, perhydroxyl, and alkoxy radicals; non-radical forms include hydrogen peroxide. A part of the ROS produced participates in the transduction of drought tolerance signals. It impacts a biological process such as cell division and programmed cell death (PCD), caused by a change in the expression of the genes responsible for tolerance. to the drought. ROS can damage the cell membrane and increase the production of malondialdehyde (MDA) (CHOUDHURY et al., 2017). However, plants use enzymatic and non-enzymatic systems to handle the ROS produced. The enzymatic antioxidant processes involve the activity of enzymes such as catalase (CAT), the enzyme superoxide dismutase (SOD), ascorbate peroxidase (APX), and polyphenol oxidase (PPO) (RAHIMI et al., 2018).

However, in the climate and soil conditions of the province of Cotopaxi, Ecuador, there are few indications about the knowledge of the effect of water stress on mint cultivation and its productive response in biomass and substances such as essential oils and other compounds. It is obtained by the secondary metabolism of plants which, although they are generated as a defense mechanism against these conditions, are used in green medicine, cooking, and perfumery since flavonoids with natural pigments protect the body from damage caused by oxidizing agents, which are found in chemical substances present in the food.

For this reason, in the development of the project, the effect of water stress on the production of flavonoids in the protected mint crop was studied, using the previously measured field capacity and ultimately controlling the irrigation divided into four treatments of application of irrigation (every 3, 6, 9 and 12 days), evaluating different agronomic variables and through a foliar analysis the content of flavonoids presents in the four treatments under study. The results concerning the production of flavonoids were relevant because, with less irrigation frequency, a higher concentration of flavonoids was obtained, which did not occur with the agronomic variables under study. This demonstrates that for this type of trial, the efficient use of water can be a tool if the purpose of the crop is to use it as a therapeutic with its composition of secondary metabolites.

2. MATERIAL AND METHODS

2.1. Study site and experiment management

The experiment was carried out in the El Triunfo sector of the Cantón La Maná under protected cultivation conditions wholly covered because the treatments that were carried out were scheduled irrigation that was every 3, 6, 9, and 12 days with 380 mL of water that served to bring each plant to field capacity 11. Previously, soil corrections were performed to improve its quality to 5% organic matter and a pH of 6.5. The soil was disinfected, and the covers were prepared for transplanting with 60-day-old seedlings and a 15-day acclimatization treatment to start and control irrigation.

2.2. Evaluation of vegetative growth variables in mint cultivation with water stress

The agronomic variables were evaluated on days 0 (transplant day), 15, 30, 45, and 60. These were plant height (cm), fresh weight of foliage, branches, and roots (g), weight dryness of foliage, branches and roots (g), growth rate (TAC), yield (kg/ha), and, finally, foliar concentration of flavonoids.

2.3. Determination of foliar flavonoid concentration in response to water stress

Samples of the aerial part were taken after 60 days to determine flavonoids using a BIOBASE BK-S360 UV-Vis spectrophotometer for quantitative determination. One gram of dry and pulverized aerial part was weighed in a 50 mL flask, adding 20 mL of 80% ethanol; it was placed on a heating plate at 60 °C; the result was filtered and completed to a volume of 25 mL with the same alcohol. 100µl of the resulting extract was placed in a 10ml vial, with 20µl of 1 M potassium acetate solution and 200µl of 10% aluminum nitrate and brought to volume with 80% ethanol. It was allowed to rest for 40 minutes, and the reading was taken at 415 nm, and the procedure was performed in duplicate. Analytical grade 12 quercetin was used to prepare the calibration curve.

2.4. Experimental design and statistical analysis

A completely randomized block design (DBCA) was used with four treatments, including control and five repetitions for all agronomic variables, except for the concentration of flavonoids, where a representative sample was taken from each treatment. For the statistical analysis, the SPSS program version 22 for Windows was used, and the difference in means was used using Tukey at 5%. The Kolmogorov-Smirnov test was used to determine the normality of the data, and the Bartlett test was used for the homogeneity of variances.

2.5. Computational chemical structural study

An exhaustive review of the state of the art concerning the bioactive compounds in mint plants. Thus, chemical structure graphing programs generated a library of compounds, which obtained their 2D representations, choosing the most representative ones. They optimized them spatially to obtain their 3D version, which is shown respecting their respective dihedral angles, bond lengths, and molecular geometry. A virtual screening was carried out to find out the most similar structures available from suppliers, using a Structure-Activity Relationship (SAR) with databases from the platform of the Swiss Bioinformatics Institute SwissADME (http://www.swissadme.ch/). Results will be obtained based on the three-dimensional comparison of a ligand and its structural form that considers electronic behaviors, such as electrophilicity and nucleophilicity, respectively 13,14,15.

3. RESULTS

3.1. Vegetative growth in cultivation under water stress conditions

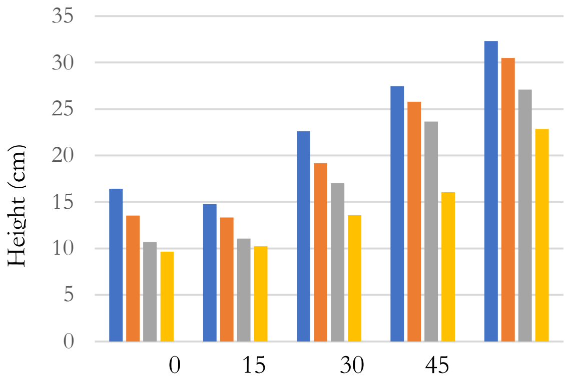
Vegetative growth in mint cultivation under water stress conditions. The most relevant results were the height of the plant at 60 days (32.36 cm) through irrigation intervals of 3 days; also, in this treatment, a higher yield of 1764.64 kg ha^{-1} was obtained. The best growth rate was also recorded at 60 days with irrigation intervals of every three days and 0.038g/day. The composition of metabolites of 0.33, 0.38, 0.42, and 0.46% increased as the irrigation days increased (3, 6, 9, and 12 days, respectively).

3.2. Plant Height

As can be seen, the height of the plants (Figure 1) experienced an increase with the days of irrigation up to 12 days with 32.33, 30.5, 27.1, and 22.85 cm for the 3, 6, 9, and 12-day irrigation intervals. While the lowest values were at 0 days with 16.41, 13.53, 10.68, and 9.65 cm for 0, 15, 30, 45, and 60 days of age, respectively, it is worth noting that the highest height was 32.33 cm at 60 days with a 3-day irrigation interval.

3.3. Fresh weight and dry weight

For the fresh weight of roots, branches, and leaves, there were significant differences for all the indicators evaluated, with the best results for the root weight at 0, 15, 30, and 45 days, except for 60 days of age when there were no statistical differences between the intervals every 3 and 6 days of irrigation, with 16.95 and 17.52 g. For the leaves, a similar behavior was observed (0, 15, 30, and 45 days), without significant differences at 60 days of age for the vegetable, with 9.37 and 9.95 g in the irrigation intervals every 3 and 6 days. In the case of the branches, the highest values were every three days of irrigation (Table 1).



3 days	16,41a	14,78a	22,6a	27,47a	32,33a
6 days	13,53b	13,31a	19,17b	25,77b	30,5b
9 days	10,68c	11,04b	16,99c	23,63c	27,1c
12 days	9,65d	10,24b	13,56d	16,04d	22,85d

Figure 1. Effect of irrigation interval and water stress on plant height.
Figura 1. Efeito do interval de irrigação e do estresse hídrico na altura das plantas.

Table 1. Fresh weight of roots, shoots and leaves according to experimental methods.
Tabela 1. Peso fresco das raízes, galohos e folhas de acrodo com métodos experimentais.

Irrigation Interval (days)	Age of plant (days) 0	15	30	45	60
	Root weight (g)				
3	6.76a	11.74a	14.98a	17.02a	16.95a
6	4.86b	11.12a	13.50b	15.57b	17.52a
9	4.39c	10.97b	14.44a	13.28c	15.51b
12	4.34c	9.89c	9.74c	10.60d	15.10b
EE±	0.023	0.953	1.023	1.345	0.856
P	0.001	0.001	0.001	0.0001	0.001
	Leaf weight (g)				
3	3.86a	6.49a	9.31a	10.13a	9.37a
6	2.58b	6.27a	8.59b	7.60b	9.95a
9	1.98c	5.06b	7.72c	6.54c	7.18b
12	1.38c	4.99c	5.60d	5.29d	7.21b
EE±	0.678	0.234	0.785	0.756	0.997
P	0.001	0.001	0.0001	0.0001	0.012
	Branches weight (g)				
3	2.94a	7.54a	11.54a	13.37a	10.49a
6	1.71b	6.81b	9.46b	7.62b	7.66b
9	0.85c	4.25c	9.22b	7.32b	6.02c
12	0.75c	3.82d	6.50c	4.33c	4.11d
EE±	0.123	0.0324	1.005	1.349	0.894
P	0.001	0.0001	0.001	0.001	0.0001

Values with unequal letters differ for P<0.05 (Tukey)

For dry weight (Table 2), there were significant differences with the best values for roots and branches at 0, 45, and 60 days with irrigation every three days and 15 and 30 days with irrigation every six days. For the leaves, the dry weight was greater every three days of irrigation for 0 and 45 days and 60 days for irrigation every six days with 1.54, 1.75, and 2.10g.

Table 2. Dry weight of roots, shoots and leaves according to experimental methods.
Tabela 2. Peso seco das raízes, galohos e folhas de acrodo com métodos experimentais.

Irrigation Interval (days)	Age of plant (days)				
	0	15	30	45	60
	Root weight (g)				
3	2.62a	3.25a	3.56b	7.30a	5.47a
6	1.78d	3.39a	4.58a	6.35b	4.70b
9	1.91d	2.92b	4.56a	6.21b	4.35b
12	1.16c	2.84b	2.87c	4.73c	4.15b
EE±	0.045	0.067	0.0567	0.456	0.035
P	0.001	0.023	0.001	0.001	0.01
	Leaf weight (g)				
3	1.91a	1.32b	1.42b	2.18a	1.83b
6	1.25b	1.54a	1.75a	1.69b	2.10a
9	0.51c	1.37b	1.38b	1.74b	1.75b
12	0.35c	1.44b	1.30b	1.18c	1.74b
EE±	0.0239	0.003	0.012	0.067	0.0113
P	0.001	0.01	0.01	0.001	0.01
	Branches weight (g)				
3	1.56a	1.15b	2.15b	2.88a	1.89a
6	1.02b	1.53a	2.25a	2.48b	1.66b
9	0.14c	0.89c	2.05b	2.10c	1.29c
12	0.12c	0.93c	1.35c	1.29d	0.98d
EE±	0.035	0.023	0.05	0.0256	0.023
P	0.001	0.001	0.001	0.001	0.0001

Values with unequal letters differ for P<0.05 (Tukey)

3.4. Growth rate

The absolute growth rate increased with the maturity of the plant by 0.038 g/day at 60 days, while it was affected to the extent that the irrigation interval increased, with the lowest values with irrigation every 12 days with 0.016, 0.024; 0.021 and 0.017 0 g/day, for 15, 30, 45 and 60 days of the age of the vegetable, respectively.

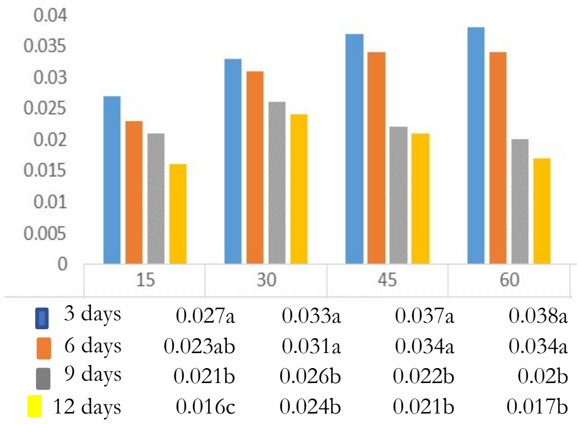


Figure 2. Taxas de crescimento.
Figure 2. Growth rates.

3.5. Foliage production, plant weight, and yield

Foliage production, plant weight per plot, and total yield were affected by irrigation intervals on days with the highest values in the control treatment with 35.29, 564.64 g, and 1764.46 kg/ha. The P significance values for all cases were 0.0001 (Table 1).

Table 3. Foliage, plant weight and total yield according to experimental methods.
Tabela 3. Peso da folhagem, planta e rendimento total de acrodo com métodos experimentais.

Variable parcel g	Irrigation interval, days				EE±
F.W.	35.29a	34.51a	29.31b	26.99c	1.89
P.W.	564.64a	552.23b	469.03c	431.86d	9.57
Yield kg/ha	1764.46a	1725.72b	1465.71c	1349.56d	12.76

Values with unequal letters differ for P<0.05 (Tukey)
F.W: foliage weight, Weight of plants per plot, Total yield

3.6. Leaf concentration of flavonoids produced in response to water stress.

The flavonoid contents increased with the days without irrigation, with the highest values at 12 days with 0.46%, followed by 0.42%, 0.38, and 0.33 in descending order (9, 6, and 3 days, respectively).

3.7. Computational chemical screening

Through an in-depth search of secondary metabolites produced by mint plants, a library of 12 flavonoid-type compounds was obtained, and they are shown in Figure 4. Five polyphenolic compounds were found (Figure 5), the most referenced by authors highlighting mint plants' bioactivity. It is emphasized that all preliminary renderings are shown in their 2D conformation.

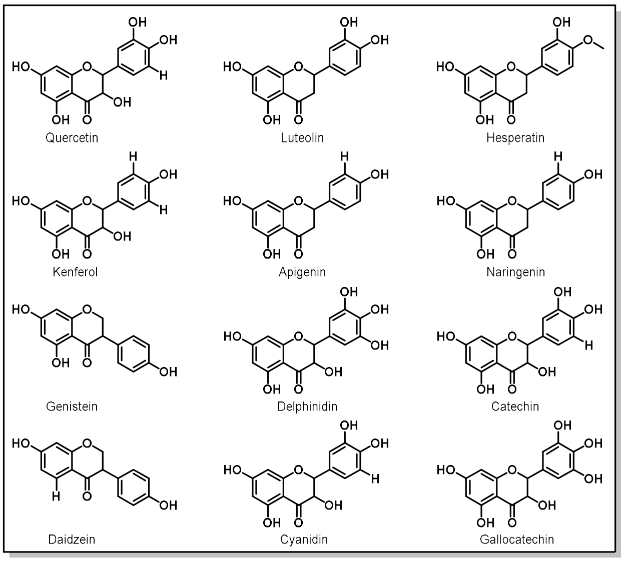


Figura 3. Compostos mais comuns do tipo flavonóide.
Figure 3. Most common flavonoid compounds.

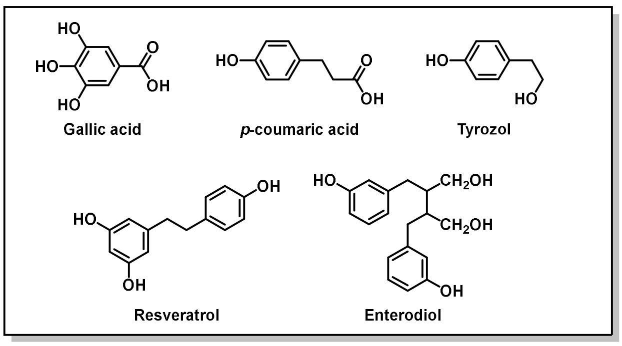


Figura 4. Principais compostos do tipo polifenol.
Figure 4. Main polyphenol-type compounds.

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In this way, bibliographic contrast determined that the flavonoid quercetin is one of the most bioactive. It is shown that it can also be considered an adjuvant agent in the presence of other flavonoids, increasing the antioxidant activity and the effects of different types of stress on plants, both wild and controlled greenhouse production. Thus, it is chosen to represent this group for virtual screening, as shown in Figure 6, with its 2D structural representation and similar electronic compounds.

The compound (3R,4S,6S)-3,10,13-trihydroxy-6-methyl-5-oxapentacyclo [9.7.0.02,8.04,6,012,17] octadeca-1,8,10,12(17),13,15-hexaene-7,18-dione, showed the highest electronic affinity, since after the application of the filters for virtual screening, as a ligand in biological reactions, it was determined that it has 85.0% similarity, that says that it can act as a bioisostere of the flavonoid quercetin, and have only a 15% probability of not acting favorably.

Consecutively, gallic acid became the most referenced polyphenol since it is one of the smallest and has the steric capacity to facilitate its entry into the catalytic sites. Also, having several oxydryl groups in its primary structure makes it quite soluble compared to other polyphenols with longer chains and, therefore, greater molecular mass. Figure 7 shows the most similar compounds by virtual screening, showing the electronically similar compounds compared to the stated computational hypothesis.

The compound (2R,3E)-2-hydroxy-3-imino-2,3-dihydrooxepin-4 carboxylic acid showed electronic affinity in the virtual screenings, the comparison was carried out as a ligand, 86.7% was obtained of similarity as a bioisostere, and that in the case of using it as a substitute for the polyphenol gallic acid, approximately 13% of the cases could not function as a bioactive molecule or adjuvant.

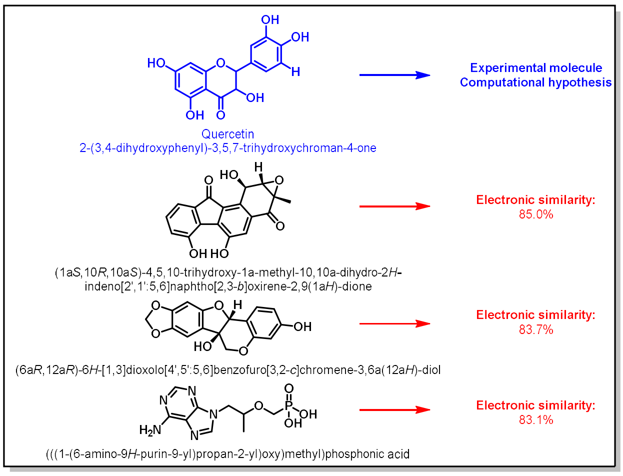

Figure 5. Result of the REA computational comparison of quercetin.
Figura 5. Resultado da comparação computacional REA da quercetina.

Finally, a three-dimensional structure comparison was carried out to corroborate whether the previous structures, without optimization, are similar or equal to the optimized ones when assigning electronic components and force fields to each heteroatom. The spatial coordinates, direction of the dipole moment, dihedral angles, and bond lengths have different values, so the optimization allows us to understand the structures of the molecules as possible donors or acceptors of hydrogen atoms in Van der Waals intermolecular interactions such as hydrogen and London bonds. In Figure 7, you can see the achievement of the optimized 2D to 3D structures.

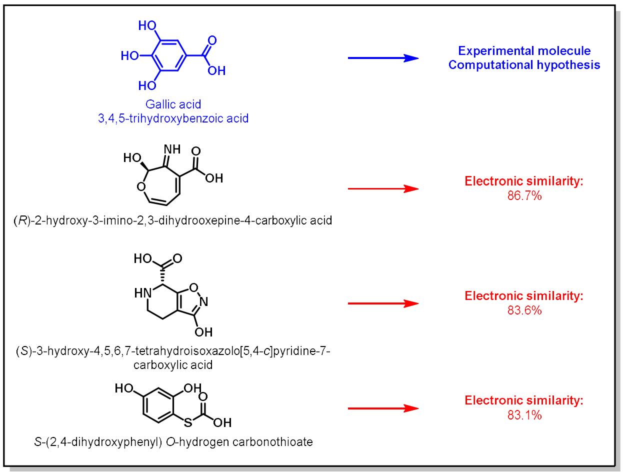

Figure 6. Result of the REA computational comparison of gallic acid.
Figura 6. Resultado da comparação computacional REA da ácido gálico.

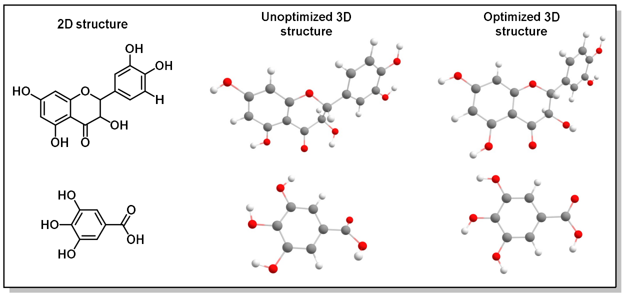

Figure 7. Contrast of non-optimized and spatially optimized biomolecules.
Figura 7. Contraste de biomoléculas não otimizadas e otimizadas espacialmente.

4. DISCUSSION

The research carried out to determine the effect of irrigation intervals in the cultivation of mint in protected cover concerning the impact of agronomic variables and the production of flavonoids is evident, as demonstrated below.

As you can see, the height of the plants experienced an increase with the days of irrigation up to 12 days with 32.33, 30.5, 27.1, and 22.85 cm for the 3, 6, 9, and 12-day irrigation intervals. While the lowest values were at 0 days with 16.41, 13.53, 10.68, and 9.65 cm for 0, 15, 30, 45, and 60 days of age, respectively, it is worth noting that the highest height was 32.33 cm at 60 days with a 3-day irrigation interval. The literature reports that when evaluating the interactions between the application of organic fertilization and water stress, adequate adaptability was found to counteract the harmful effects caused by exposure to water deficit in mint. The variable length that expresses the plant's growth maintained a progressive increase of 2% with the sampling time, while as the days without irrigation increased, they gradually decreased. This behavior occurred due to the strategies of physiological behaviors presented by plants under stress (GARCÍA, 2018).

The literature highlights that the use of organic fertilizers plays an essential role in increasing the efficiency of water use, fundamentally due to the presence of phosphorus in its composition; this element increases the expansion of the leaves, the growth of the axillary buds and the canopy of the shoots, improving photosynthetic activity (VÁZQUEZ et al., 2018), aspects to be taken into account depending on the irrigation interval to which the plants are subjected. Furthermore, these authors report how soil moisture can be retained using organic fertilizers, which is necessary for the productivity of plants in drier climates and more advanced vegetative states18. Thus, edaphic water deficiencies severely decrease the water content of the plant, causing high levels of stress and substantial reductions in seed yield, aboveground biomass, number of pods and average seeds, and seed weight when drought coincides with flowering and seed formation (BARRIOS et al., 2011; VILLALOBOS et al., 2018).

The absolute growth rate increased with the maturity of the plant at 0.038 g/day at 60 days, while it was affected to the extent that the irrigation interval increased with the lowest values with irrigation every 12 days with 0.016; 0.024, 0.021 and 0.017 0 g/day, for 15, 30, 45 and 60 days of age of the vegetable, respectively. Lower results than those obtained in another investigation with 1 and 0.22 g/days in aquaponic and contained bed systems (CÁRDENAS et al., 2022). However, it is assumed that, in previous studies, the absolute growth rate was lower than that obtained in another study where two g/day was shown (ESPINOSA et al., 2018). This is possible because we worked with larger and older plants, so they increased more grams per day, in addition to the aspects discussed in the previous paragraph.

The literature highlights that water limitation is one of the conditions that most affect the photosynthesis and productivity of plants, especially when the days of water deficit increase, which brings with it a decrease in soil humidity, which can be associated with high temperatures and poor drainage, among other aspects. This can cause a direct effect on photosynthesis through diffusive limitations through the stomata and the mesophyll or alterations in photosynthetic metabolism (CAMPOS et al., 2014; ESPINOSA et al., 2018). The above is reflected in the closure of the stomata in response to the decrease in leaf turgor, the increase in the vapor pressure deficit in the atmosphere, or the chemical signals generated in the root28. This decreases the photosynthetic rate due to the proportional increase in inactive reaction centers (RCs) and the consequent inhibition of electron transfer (CAMPOS et al., 2024).

Foliage production, plant weight per plot, and total yield were affected by irrigation intervals on days with the highest values in the control treatment with 35.29, 564.64 g, and 1764.46 kg/ha. Plant growth is strongly affected by water deficit, salinity, and extreme temperatures. Water availability is the factor that most affect plant growth and yield. Plant responses to water deficit are influenced by the period, intensity, duration, and frequency of stress and the interactions between plants, soil, and atmosphere. Crop yield is reduced more when water stress occurs during the heading or flowering stages 30. It is highlighted that the possibility of measuring the relative water content in the plant (an aspect not evaluated in this work) would help know precisely the plant's water content under conditions of stress due to water deficiency since this is related to the water potential. Its components, pressure and osmotic potential, are a function of the volume of water. In the protoplasm, elements to consider when temperature increases and soil humidity decreases can cause water stress (BACARRILLO et al., 2021).

The flavonoid contents increased with the days without irrigation, with the highest values at 12 days at 0.46% (Figure 5). Results that coincide with those reported by other authors Abdel et al. (2018) and Wani; Basis (2018) with values of 0.41 to 0.49% in aqueous and methanolic extracts. Phenolic compounds and flavonoids are the most widely distributed secondary metabolites in plants. They have an essential role in physiological and ecological processes and are involved in the resistance of plants to different types of stress. These metabolites have several defense functions. Therefore, their biosynthesis in plants is generally induced in response to abiotic and biotic stimuli such as drought, ozone, UV radiation, heavy metals or pathogen attacks. Aspects that explain its increase in response to the effect of stress caused by water deficit. Hence, plants can respond to water stress conditions with various mechanisms (PAGARE et al., 2015).

On the other hand, it is noted that the increase in secondary metabolites may be due to different aspects, which must be considered to achieve better use of the crop or plant (SAXENA et al., 2013). Thus, another report states that the management system can influence the synthesis of secondary metabolites with potential for biological activity or aromatic properties, which is associated with the stage of plant development and growth conditions, among others. Aspects. Thus, a high concentration of secondary metabolites can be associated with more excellent protection of the plant or a particular condition, given as an adaptive strategy to the climatic conditions of the environment in which the crop is grown, such as soil humidity, high temperatures, days without water, among others (PAGARE et al., 2015).

Likewise, it was reported that the difference in the environmental condition of each management system could influence the concentration of secondary metabolites, such as flavonoids, phenolic compounds, tannins, and terpenes, present in different plant structures (IBARRA et al., 2018). Therefore, a particular set of secondary metabolites produced by a population of plants or crops may reflect the specific characteristics of a given environment or species (MOORE et al., 2014). Thus, the changes that occur in the secondary metabolism of a plant are a response to changes in the environment since its metabolic mechanisms are modified to keep its routes in optimal conditions, aspects that can explain what happened in this investigation.

Both 2D and mainly 3D images respect the dihedral angles, bond lengths, and molecular geometry. For a correct understanding of bioactive molecules, theoretical and computational chemistry must generate structural representations that respect the spatial coordinates of each functional group in organic compounds.

5. CONCLUSIONS

Vegetative growth in mint cultivation under conditions of water stress produced by controlled irrigation intervals directly influenced morphological indicators, decreasing height, production of fresh and dry mass of roots, branches, and leaves, as well as the growth rate and biomass production per unit area.

The foliar concentration of flavonoids had a direct effect due to water deficit since it is the plant's first defense against the stress response in the treatments under study, with increases in its concentration as the days without irrigation progressed.

The application of computational chemistry contributed favorably by highlighting that the difference between the representative bioactive compounds, gallic acid and quercetin, is significant when comparing the percentages obtained by REA, thus determining that there are similar structures and that they may have biological activity, considered bioisosteres by having structurally and spatially electronic characteristics related to their reactivity, electrophilicity and nucleophilicity.

Three-dimensionally, it was proven that the charge assignment in the structural optimization appropriately directs the location of the substituents and functional groups of the secondary metabolites analyzed; it also considers the steric volumes and the final molecular geometry. All of this provided vital information to predict the possible intermolecular interactions, such as hydrogen bonds that these molecules will generate to have their antioxidant action in plants and foods.

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