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The Research of Ornamentally-Medicinally Useful Members of *Crassulaceae* D .C Family Spread in Caucasus Minor

Abstract

Irreplaceable ornamental plants in urbanization are used for aesthetic purposes in modern time. In connection with this, it is preferred to use ornamental plants in habitats and parks, gardens, streets, shopping centers, indoor and outdoor places. However, it is an important issue to choose and use the right ornamental plants in landscaping. Recently the succulents have become popular as the pot plants among the decoration plants. The tendency in the areas requiring less water and low maintenance increases the interest to succulents because of irrigation water limits and high costs. Succulents are the best choice for arid environments because they can tolerate drought for a long time. Moreover, these plants have interesting ornamental features. From this point of view the species of Crassulaceae family have more significance in decoration. In the framework of conducting research, the qualities of the Crassulaceae family species which naturally spread in Caucasus Minor are investigated as the medicinal and ornamental plants.

Keywords: *Caucasus Minor, Rosularia, Sedum, Sempervivum, Succulent*

Introduction

The succulents hold water in their stems and leaves, so they adapt extremal ecological environment with their way of living. However, viability in the minimal light makes them suitable (Bell, 2001). As the succulents globally spread and produced in all living areas, they are cultivated for the environmental benefit and aesthetic purposes (Oldfield, 1997). It has been investigated many species of Sedum which is suitable for "green roof" covering (Van Woert, Rowe, Andresen, Rugh, & Xiao, 2005; Kim, Huh, & Huh, 2010). On the other hand, the succulents draw attention in the field of medicine as they are a potential raw material in medicine (Cabahug, Nam, Lim, Jeon, Hwang, 2018). That's why it is desired fast spread of the succulents because of their impact on health and environment. 690 kinds and 12500 succulent species relating to Crassulaceae family have been described by Nyfeller and Eggly (2010). The members of the Crassulaceae family spread all over the world but they are widespread in the northern hemisphere (picture1). The species live typically in arid and cold places. The Crassulaceae family includes various kinds of plants from small sized annual plants to perennial grass, bush and trees. Many types have attractive flowers. The whole family consists of approximately 1410 members from 35 kinds. Sedum has most species typified by 428 sorts, Crassula (195 species), Kolonchoe (144species), (Sempervivum 63 species) (Lopez-Angulo, Montes-Avila, Díaz-Camacho, Vega-Aviña, Baez-Flores, & Delgado-Vargass, 2016). These are widely used as ornamental plants (Eid, Ezzat, Gonaid, & Choucry, 2018).

Research

The members of the family are commonly seen in the areas where monsoon rain and high humidity exist, some species (for example sempervivum) are mainly found in arid mountainous living areas and higher altitude. Fleshy leaves and "Crassulaceae Acid Metabolism" make them adapt to the changeable water environment, but they are not seen in the real desert areas. CAM is a type of photosynthesis observed in the plants such as pineapples and cacti living in the arid climate.

One of the useful features of Crassulaceae family is that some species are edible and important in treatment. Sedum acre and Sedum telephium are pharmaceutically significant (Akbarova, Mammadova, 2024).

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Different pharmaceutical investigations show that some members of the family have antioxidants, antimicrobial, anti-serogen, cytotoxic, anti-inflammatory and antiseptic activity, anti-malaria, antimutagen, myometrial, biological activity.

Picture 1. Distribution map of *Crassulaceae* D.C family in the world

Material and methods

The monitorings in the research, expeditions to Caucasus Minor, the literature data related to the Crassulaceae family are considered the main materials. Moreover, some bibliographical materials such as Flora of China, Flora of Irag, Flora of Tropical East Africa as well as flora of Azerbaijan and former SSR have been investigated. It has been used geographical, ecological, morphological-systematic methods during the investigation. The expeditions covering the various botanical-geographical regions of Azerbaijan have been carried out by route methods. Various diagnostically important bio-morphological indications of succulent plants have been encoded taking into account the available digital polytomous specification key while using the literal-digital polytomous specification key of studied species (Balkovsky, 1964; Qurbanov, 2011). Phenological observations have been conducted by Kuznetsov and Ruquzov's methods (Kuznetsov, 1976), evaluation of viability of the plants has been carried out by V. Alexeyeva's method (1990). R and JMP programs have been used in statistical analysis of data. The classification of species is based on herbarium fonds, SSR, Caucasus, Azerbaijani fundamental floras while naming of taxons have been carried out on the basis of Cherepanov (1998), "Caucasian Flora Conspectus" (2003-2006) and conspectus of A. Asgarov and the areological research have been conducted according to N.N Porteniyer's classifications (2006).

The result and its discussion

The members of Crassulaceae spread in Caucasus Minor are annual, biennial or perennial grass, but mostly succulent plants. Generally, these types have rosette-shaped, thick and fleshy leaves and cluster shaped, white, yellow and red flowers. Some of the species used as ornamental plants for their visual values are Sedum and Sempervivum.

Some taxons from the Crassulacaeae family naturally spread in Caucasus Minor are investigated according to their pharmaceutical and ornamental features. Four evergreen species from the kind of Rosularia, Sedum and Sempervivum which have leaf and flower aesthetics and their features have been shown in this framework.

Rosularia (STAPF, 2009)

Rosularia spread in semi-arid regions is a small kind consisting of 28 species (Mabberley 2008). Rosularia is rosette-shaped, perennial grass, while some sorts are a monocarp. The leaves of this

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kind are striped, spoon-shaped or rectangular spoon-shaped. The leaves are stalkless. The flowering is mono or multiflowered, cluster or cymose-shaped or cluster-shaped consisting of cymose. The flowers of species spread in Azerbaijan are yellow, white, pink or red. Some members of Rosularia are used for pharmaceutical purposes (Sarwar, Qaiser, 2012).

Some species are cultivated due to their flower and leaf structure. (R. alba, R. sempervivum, R. pallida, R. plathyphylla). These species are used in landscaping in the gardens and cities like pot plants as well.

Rosularia sempervivum (M. Bieb.) A. Berger. **(Syn.: Rosularia sempervivum subsp. sempervivum)**. Sempervivum is widespread in the areas up to the 900-3000 meters of altitude. Some subspecies are endemic. Its evergreen leaves have a stacked view (picture 2).

Picture 2. ***Rosularia sempervivum***

Rosularia has a floral structure that produces tall stalks (6-25 cm) bearing a compound cluster of flowers. It has small rosette-shaped flowers that typically are dark pink. Its ornamental aesthetics makes the succulents be cultivated in a large scaled places, roof and terrace gardens as well as rock gardens.

Sedum L

The species belonging to this kind are annual, biennial and perennial plants mostly branchy and succulent. The species of Sedum have a geographical widespread, mainly found in dry climate, shallow soils, stony or gravelly rocks, especially mild and subtropical regions. Sedum grows well in sunny or partially sunny places. Thanks to special photosynthesis, they are durable to humidity and high temperature. It has been revealed that some species (Sedum album, sedum acre, sedum spurium) of Sedum can survive for 88 days without water (Getter, Rowe, 2008). Some species are tolerant to windy conditions. The succulents are easily cultivated plants. The flowering period of Sedum lasts from the end of spring to autumn, they have star-shaped, yellow, white, red, pink, and golden shaded flowers. These plants have nectar-rich flowers. They are very attractive for the insects. At this point of view, Sedum L attaches importance for bees, butterflies, and the other pollinators. Their height reaches a few centimeters. The leaves have a soft structure and are easily

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crushed. Sedum L is not a water-loving plant. They can survive for a long time and gradually growing in waterless conditions while they grow fast where water exists (Carter, Butler, 2008, Nectarios, 2015). Demand and interest to this kind are linked to air pollution and urban heat island. They are used in steady and economical design – "green roof" in order to diminish the increasing economical problems in the cities. Nevertheless, the various Sedum taxons can differently adapt to the green roofs (Damas, Cite, Donvez, 2010; Nagase, Dunnett, 2010). They can be used as the technology of urban agriculture according to the decorational values and metabolic features. Majority of these taxons are ornamental plants and can be used in landscaping.

Sedum acre

It spreads in Europe, Caucasus, Georgia, Western Asia, Northern Africa. Known as Sedum acre the succulent has 5-10 cm of height in Azerbaijan. Being the perennial and evergreen grass, the plants are seen at the 800-2000 meters of altitude. They grow in rocky, stony areas, southern slopes and open spaces (Tubives, 2021). Its leaves are stalkless and opposite. The flowers of this succulent are yellow (picture 3).

Picture 3. *Sedum acre* L.

Inflorence of the succulents covers the months of May and July. They may grow in arid and shady places which can create a good ground cover. The succulents tolerate drought and need rare watering. Row or baked leaves can be used as food, but they have a bitter taste. The plants are used for medical purposes. The succulents propagate in a vegetative method. They are cultivated as ornamental plants at the moment. The aesthetics of leaves and flowers make a contribution to the visiual qualities of environment. They are used in the gardens, parks, cities, as well as a large scale of areas. It is also made a use of succulents as ground cover.

Sedum album L.

These are mainly specific to Europe, North-west of Iran, Caucasus, Lebanon, Near East, Anadolu. It is a taxon growing in sunny, sandy and rocky soils at the height of 2400 meters above the sea level. They are evergreen succulents growing at a medium speed (picture 4).

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Picture 4. *Sedum album* L.

The height of white flower receptacles flowering between June and September may reach 5-20 cm. This succulent is not a shade-loving plant which grow in undernourished soils and tolerate drought. Moreover, there are many investigations showing that this succulent can live without rain or watering for 100 days. These characteristic features make them a better alternative in the usage of "green roof" in the urban environment. It may improve the environment by insulating the building in this way and providing a good condition for living beings.

These may be used in the gardens, rocks, dry walls, pots, slopes, herbal compositions as ground cover.

Sempervivum L

It spreads to large areas through Europe to Asia. Approximately 40 main species of Sempervivum are found in the nature, generally mountainous areas as well as Iran, Armenia and Caucasus. They are evergreen perennial plants growing to 10-20 cm and have rosette-shaped, thick rhizoids. These plants develop in sandy soils and rocky surface. They grow better in sunny places than shady areas. The rosettes die after the inflorence period during some years, but the generations developing around them make the succulents vivid . In summer star-shaped flowers make a cluster and are white, yellow, red and purple. The flowers of species spreading to Azerbaijan consist of 8-15 parts. Sempervivum has enough viability in severe conditions. The leaves and young buds of these succulents are edible. They grow well in hot climate, as well as the plants can tolerate cold weather. Sempervivum are the succulents which have aesthetic leaves growing in the shape of rosette through the center to tips. During the growth of receptacle, the plant vertically grows and create a generation. For that reason, it makes an aesthetic tissue with these generations in various sizes and leaf colors. Many species exist naturally, while some are cultivated and used as ornamental plants indoor and outdoor places.

Sempervivum transcaucasicum muirhead

These species grow at the 550-2700 meters of altitude in volcanic rocks. They have stalks growing to 20-30 cm flowering in august and have yellow flowers. (picture 5).

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Picture 5. ***Sempervivum transcaucasicum***

This kind can grow in acid, neutral soils and mainland (slightly alkaline) especially in sunny areas. This succulent is suitable for drought not the shady places. While creating a receptacle only in summer, its invariable leaves, shape, texture, and color aesthetics draw attention. Many species of this kind are cultivated. In Alpine and rock gardens, dry walls, marginalia and containers can be cultivated as ornamental plants. The work on applying them in landscape is important due to increasing durability of these special kinds.

Conclusion

The frequency and intensity of drought period have significantly increased for last ten years in the Mediterranean basin including Azerbaijan (Giannakopoulos, Le Sager, Bindi, Moriondo, Kostopoulou, Goodess, 2009; Lopez-Nicolas, Pulido-Velazquez, Rouge, Harou, & Escriva-Bou, 2018; Ortega-Gomez, Perez-Martin, Estrela, 2018). According to the activity plan on climate change, Azerbaijan will be warmer, drier, and rainy, so it will cause indefinite climate change and loss of water as well. It is forecasted a significant decrease in terms of funds).

Drought is one of the most difficult stress factors that global ecosystems face and it affects the physiological and biochemical structure of the plants (Bartlett, Scoffoni, & Sack, 2012). So, it may have a negative impact on physiological processes (Osakabe, Osakabe, Shinozaki, & Tran, 2014; Mammadova, 2022). A cell as well as a small disbalance is linked to plant growth and productivity. It will affect the physiological processes as well (Mathur, Agrawal, & Jajoo, 2014; Nxele, Klein, & Ndimba, 2017). It has been revealed an effective adaptation for durability to drought, minimum-maximum temperature and precipitation change (Sari, Karashah, 2020). That's why this adaptation will empierce agriculture as well as cultivation of ornamental plants in the cities, gardens, and parks.

Protection of water reserve and its efficient use in all fields assume importance because of increasing effects of global warming. Some approaches have been accepted that support lasting use of natural reserves in planting of greenery. Regulatory conceptions such as "Effective use of water in Landscaping", "Use of water" (Wat-wise, Water Smart), and "Natural Landscape" under the general name of "A water-efficient landscape design". It includes planning principles providing the

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most rational use of these resources. Easiness and durability of adaptation in selecting the plant species which easily adapt to the ecological condition and have viability with natural rain water and limited watering.

The succulent plants are the best choice specially in landscape. The areas of use include not only open and green fields of the city but also roads, slopes and walking places. It can be used in the field demanding minimum technical service condition, airports, problematic places and rurals. Using of the succulents indoor places widely spread in order to contribute aesthetic, functional, and ecological value to the venues in green fields as being in outdoor areas. In the investigation conducted for outdoor places, it is preffered to cultivate 72,3 percent of succulents and cacti, 49,1 percent of ornamental species. Generally it is demanded decorational, aesthetics, leaf and flower and succulent-cacti kinds in the design of interiors. Durability of cacti and succulents to drought, easy care, prevention of radiation indoor places and easy carriage of the plants for its size are the main reasons to select these species.

Crassulaceae family, covering the majority of succulent species using in landscaping widely spreads to Caucasus Minor. Despite the great diversity of natural species in Caucasus Minor, cultivating of these species as ornamental plants is limited. That's why using of decoration plants draws more attention. It is reccomended to pay attention to the use of natural species and drought tolerant grass including succulent plants in order to lessen grass fields whether it is preffered to external species in designing of cities, parks and gardens.

It is a great demand to demonstrate people an increase of information, natural species, providing the permanence of their aesthetic features, and the succulents having the eatable, medicinal, and functional properties. In the framework of this investigation the aforesaid species are the succulents having a potential of being used indoor and outdoor places with aesthetical, ecological and functional features. It is considered that the investigation of landscaping properties of natural species will contribute to science in the point of view finding the most used field of ecosystem.

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The effect of a gluten-free diet on the biochemical parameters of patients with autoimmune thyroiditis

Abstract

The study of biochemical parameters after implementing a gluten-free diet in patients with autoimmune thyroiditis, a condition prevalent worldwide, holds significant practical and theoretical importance. The aim of the research is to determine how a gluten-free diet affects the progression dynamics of autoimmune thyroiditis by measuring the levels of triiodothyronine, thyroxine, thyroid-stimulating hormone and anti-thyroperoxidase antibodies in patients adhering to a gluten-free diet. The study were included 32 participants aged between 20 and 70 years, comprising 11 men and 21 women. The research was conducted using the enzyme-linked immunosorbent assay (ELISA) method on the "Mindray BA-88A" analyzer.

Keywords: *Autoimmune thyroiditis, Gluten-free diet, FT3, FT4, Anti-TPO*

Introduction

Autoimmune thyroiditis is an autoimmune disease of the thyroid gland. The disease was first described in 1912 by the Japanese scientist and physician Hakaru Hashimoto as an enlargement of the thyroid gland due to lymphoid infiltration, under the name lymphomatous hypertrophic goiter (Alimetov, Ibrahimova, 2014). Hakaru Hashimoto described four cases of the disease (Ihnatowicz, Wator, Drywien, Wojsiat, n.d.). Besides autoimmune thyroiditis, this condition is also known as lymphocytic thyroiditis, chronic autoimmune thyroiditis, lymphadenoid goiter, Hashimoto's thyroiditis or Hashimoto's disease (Alimetov, Ibrahimova, 2014; Mammadhasanov, 2019; Seed, 2024). the global prevalence of the disease is approximately 10-12%, while its occurrence among Caucasians is estimated to be around 5% (Kalaycı, Kamarlı, 2014; Aghayeva, Hasanguliyeva, Namazova, 2024). Autoimmune thyroiditis is 15-20 times more common in women than in men. The higher prevalence in women is associated with X chromosome abnormalities and the influence of estrogens on the lymphoid system (Saidova, Mirzazade, 2016). Age-related changes in the thyroid gland lead to an increased production of proteins associated with autoimmune processes, which is why autoimmune thyroiditis typically develops gradually. The risk of disease progression increases with age (Ihnatowicz, Wator, Drywien, Wojsiat, n.d.).

Research

In patients with autoimmune thyroiditis, an increase in TSH hormone and anti-TPO antithyroid antibodies, along with a decrease in FT3 and Ft4 hormone levels are key indicators of the disease (Imamoglu, Ozyardımcı Ersoy, 2019).

Thyroid-stimulating hormone – TSH is a glycoprotein complex protein synthesized in the basophilic cells of the adenohypophysis. The half-life of this hormone in the blood is between 50 and 60 minutes. The primary function of TSH is to stimulate the formation and function of the thyroid gland. The binding of TSH to the membrane receptors of thyroid cells accelerates the synthesis of cyclicAMP – cAMP in the gland.

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As a result of increased cAMP levels, the uptake of iodine by thyrocytes and the iodination of thyroglobulin are stimulated (Islamzade, Efendiyev, Islamzade, 2015). TSH influences the synthesis of thyroid hormones by stimulating the entry of iodine ions into thyrocytes and the iodination of tyrosyl residues (Islamzade, Efendiyev, Islamzade, 2015). The level of TSH is an important parameter that indicates the free values of thyroid hormone in the blood. As a result of reduced thyroid function, TSH synthesis increases. When thyroid hormone synthesis decreases, TSH synthesis rises and when it increases, TSH synthesis decreases. TSH is the first step in obtaining information about thyroid function (Imamoglu, Özyardımcı Ersoy, 2019).

Thyroid hormone – thyroxine – T4 and triiodothyronine – T3 are different from other hormones because they are iodinated compounds. These hormones are synthesized within the thyroglobulin, the colloidal protein substance found in the follicles of the thyroid gland. Thyroid hormones circulate in the blood bound to serum proteins. 99.97% of thyroxine and 99.7% of triiodothyronine circulate bound to proteins in the blood. 0.03% of thyroxine and 0.3% of triiodothyronine circulate freely in the blood, exerting biological effects on target cells. Thyroid hormones participate in a variety of biochemical changes in cells, including the metabolism of proteins, carbohydrates, lipids and nucleic acids, glucose and potassium into cells and the movement of calcium and phosphorus out of cells (Islamzade, Efendiyev, Islamzade, 2015).

Anti-thyroperoxidase – Anti-TPO antibodies play a crucial role in the diagnosis of autoimmune thyroiditis. The enzyme thyroperoxidase is located in the thyroid cytoplasm. Anti-TPO antibodies bind to the C-terminal part of the thyroperoxidase enzyme in the cytoplasm and induce apoptosis of thyrocytes (Imamoglu, Ozyardımcı Ersoy, 2019).

Several factors play a role in the etiology of autoimmune thyroiditis. These factors include genetic predisposition, infection, surgical intervention in the thyroid gland, inflammation of the gland, radiation, sedentary lifestyle, changes in dietary habits, psychological stress and the intake of foods that alter the composition of the gut microbiota (Mammadhasanov, 2019; Ulker, Aritici, Bash, Erdem, n.d.). Considering all these factors, a gluten-free diet has recently been recommended for patients with autoimmune thyroiditis. During a gluten-free diet, wheat, barley, rye and foods, beverages, medications and supplements containing these are removed from the diet. A gluten-free diet leads to a decrease in thyroid antibodies and prevents the progression of the autoimmune process. The mechanism by which this diet affects autoimmune thyroiditis is explained by a reduction in the levels of circulating proinflammatory cytokines, a decrease in intestinal permeability and an improvement in the absorption of selenium and vitamin D, which re essential thyroid gland health (Piticchio, Frasca, Malandrino, Trimboli, Carrubba, Tumminia, Vinciguerra, Frittitta, n.d.; Malanrini, Trimboli, Guzzaloni, Virili, Lucchini, n.d.; Krysiak, Szkrobka, & Okopieri, n.d.).

Conclusion

The participants in the study were classified into 3 groups. In the control group consisting of healthy individuals, among the 10 participants, 40% of men had an average FT3 level of 2.73pg/ml in their blood serum, while 60% of women had an average FT3 level of 2.95pg/ml in their blood serum. In the group 10 autoimmune thyroiditis patients unrelated to a gluten-free diet, 30% of men had an average FT3 level of 0.97pg/ml in their blood serum, while 705 of women had an average FT3 level of 1.14pg/ml in their blood serum. In the group of 12 autoimmune thyroiditis patients adhering to a gluten-free diet, 33.3% of men had an average FT3 level of 2.83pg/ml in their blood serum, while 66.7% of women had an average FT3 level of 2.73pg/ml in their blood serum.

In a control group of 10 participants, 40% of men had an average FT4 level of 1.63μg/dl in their blood serum, while 60% of women had an average FT4 level of 1.57μg/dl in their blood serum. In the group of 10 autoimmune thyroiditis patients nor adhering to a gluten-free diet, 30 of men had an average FT4 level of 1.13μg/dl in their blood serum, while 705 of women had an average FT4 level of 1.16μg/dl in their blood serum. In the group of 12 autoimmune thyroiditis patients adhering to a gluten-free diet, 33.3% of men had an average FT4 level of 1.53μg/dl in their blood serum, while 66.7% of women had an average FT4 level of 1.38μg/dl in their blood serum.

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In the control group consisting of 10 participants, 40% of men had an average TSH level of 2.93mIU/l in their blood serum, while 605 of women had an average TSH level of 2.92mIU/l in their blood serum. In the group of the 10 autoimmune thyroiditis patients not adhering to a gluten-free diet, 30% of men had an average TSH level of 5.74mIU/l in their blood serum, while 70% of women had an average TSH level of 4.99mIU/l in their blood serum. In the group of 12 autoimmune thyroiditis patients adhering to a gluten-free diet, 33.3% of men had an average TSH level 0f 3.18mIU/l in their blood serum, while 66.7% of women had an average TSH level of 2.66mIU/l in their blood serum.

In the control group consisting of participants, 40% of men had an average Anti-TPO antibody level of 19.4 IU/ml in their blood serum, while 60% of women had an average Anti-TPO antibody level of 16.8 IU/ml in their blood serum. In the group of autoimmune thyroiditis patients not adhering to a gluten-free diet, 30% of men had an average Anti-TPO antibody level of 758 IU/ml in their blood serum, while 70% of women had an average Anti-TPO antibody level of 745.6 IU/ml in their blood serum. In the group of 12 autoimmune thyroiditis patients adhering to a gluten-free diet 33.3% of men had an average Anti-TPO antibody level of 21.8 IU/ml in their blood serum, while 66.7% of women had an average Anti-TPO antibody level of 17.8 IU/ml in their blood serum.

Indicator		**Control group**		**Autoimmune thyroiditis patients group**			
		20-70 years		**20-70 years**			
		Group I		**Group II**		**Group III**	
	Gender	**M**	**F**	**M**	**F**	**M**	**F**
	Number	**4**	**6**	**3**	**7**	**4**	**8**
FT3	**M**	**2.73**	**2.95**	**0.97**	**1.14**	**2.83**	**2.73**
FT4	**M**	**1.63**	**1.57**	**1.13**	**1.16**	**1.53**	**1.38**
TSH	**M**	**2.93**	**2.92**	**5.74**	**4.99**	**3.18**	**2.66**
Anti-TPO	**M**	**19.4**	**16.8**	**758**	**745.6**	**21.8**	**17.8**

As shown by the results of the study, in autoimmune thyroiditis patients not adhering to a gluten-free diet, the levels of FT3 and FT4 hormones in their blood serum were lower compared to healthy individuals, while the levels of TSH hormone and Anti-TPO antibodies were higher compared to healthy individuals. In autoimmune thyroiditis patients adhering to a gluten-free diet, the levels of FT3, FT4, TSH hormones and Anti-TPO antibodies in their blood serum were similar to those of healthy individuals. Therefore, it is recommended a gluten-free diet to autoimmune thyroiditis patients can be considered.

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The Role of Calcium carboxylate in PVC Heat Stabilization: Mechanisms and Applications

Abstract

To replace heat stabilizers containing heavy metals in polyvinyl chloride (PVC), the effectiveness of calcium carboxylate synthesized from soybean wax—produced via the hydrogenation of soybean oil—as an environmentally friendly heat stabilizer was investigated. The thermal stability of PVC in the presence of this stabilizer was evaluated using thermogravimetric analysis (TGA) and differential thermal analysis (DTA). TGA curves obtained from polymer samples indicated that decomposition occurred in two distinct stages, with the initial stage dominated by dehydrochlorination, resulting in a mass loss of more than 50%. The thermal degradation behavior was further analyzed by examining the temperatures at which the polymer mass decreased by 5%, 10%, and 20%. In the absence of a stabilizer, these temperatures were recorded as 256.56°C, 270.71°C, and 279.25°C, respectively. However, after incorporating 5 phr (parts per hundred resin) of the synthesized calcium carboxylate, the corresponding degradation temperatures increased to 270.13°C, 279.68°C, and 295.21°C, respectively. Furthermore, the activation energy of the decomposition process was determined using the Coats-Redfern integral method. The analysis revealed that the activation energy in both decomposition stages increased following the addition of the stabilizer, indicating an improvement in thermal stability. These results demonstrate that the bio-based stabilizer effectively captures hydrogen chloride (HCl) released during the thermal degradation of PVC, exhibiting a strong suppressive effect on dehydrochlorination. The findings suggest that to combine this stabilizer with other compounds may further enhance its stabilizing performance.

Keywords: *heat stabilizer, polyvinyl chloride, poly(vinyl chloride), thermal stabilizer, calcium soap, calcium carboxylate, thermal degradation*

Introduction

The increasing role of polymers in modern life is undeniable, and their potential effects on human health have raised significant concerns (Meng, Wang, Chen, 2013).

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Among the polymers that individuals encounter daily, polyvinyl chloride (PVC) is particularly notable (Wen, Yang, Yan, 2015). In terms of annual production volume, PVC ranks as the third most widely manufactured polymer, following polyethylene and polypropylene. Due to the extensive range of products made from PVC, human exposure to this polymer is substantial. PVC is a versatile, cost-effective, and durable material used in applications spanning construction materials, food packaging, artificial leather, and cable insulation (Song, Huo, Zhang, 2022; Phomin, Deberdeev, 2012).

Despite these advantages, PVC is highly susceptible to thermal degradation. Above its glass transition temperature of approximately 70°C, PVC undergoes thermal decomposition, leading to the deterioration of its physical and mechanical properties (Patrick, 2007; Yu, Sun, Ma, 2016). To mitigate this instability, heat stabilizers are commonly employed (Folarin, Sadiku, 2011). The most widely used commercial heat stabilizers include lead salts, metal soaps, organic stabilizers, and organotin compounds (Yan, Yang, 2017). However, the use of toxic heavy metal-based stabilizers, particularly lead compounds, has been restricted in developed countries and Western regions due to environmental and health concerns (Guo, Leroux, Tian, 2021). In contrast, lead-based stabilizers remain prevalent in Eastern markets, where PVC demand is highest.

In response to these regulatory and environmental challenges, extensive research is being conducted to develop effective and eco-friendly alternatives to lead-based stabilizers in PVC processing (Egbuchunam, Okieimen, Balköse, 2010). The use of metal carboxylates synthesized from vegetable oils as thermal stabilizers presents an economically viable and environmentally sustainable solution (Putrawan, Indarto, Octavia, 2022). In line with this approach, the present study investigates the thermal stabilizing effects of calcium carboxylate synthesized from partially saturated soybean wax, obtained through the hydrogenation of soybean oil. Additionally, previous research on aluminum soap derived from sunflower oil has demonstrated its potential as an effective heat stabilizer for PVC, yielding promising results (Hasanov, Mammadova, Amirov, Aliyeva, 2025).

Research

The synthesis of calcium carboxylate involved the initial saponification of soybean wax in a water-ethanol mixture using a near-stoichiometric amount of alkali, followed by the precipitation of calcium carboxylate from the resulting soap. The percentage of carboxylic acids present in the glyceride esters of soybean wax used for calcium carboxylate synthesis, along with various physicochemical properties of soybean wax, are presented in Table.

The synthesized calcium carboxylate was dried, ground into a fine powder, and mechanically blended with 5 phr of Rusvinyl PVC-S (Russia). The mixture was then subjected to a pressure of 150 bar and a temperature of 180°C using an ECOPRESS 102 (Turkey) press to produce test samples. To facilitate a comparative analysis, a control sample was prepared under identical conditions using pure PVC without any stabilizer.

Table

Chemical Composition and Key Analytical Parameters of Soybean Wax.

Saturated fatty acid, %	Monounsaturated fatty acid, %	Others, %	Acid value, mg KOH/g	Iodine number, g I_2/100g	Saponification value, mg KOH/g
65	30	5	0.6	30	185

The thermal behavior of the polymer samples was examined through thermogravimetric and differential thermal analysis using a NETZSCH STA449F3 Jupiter (Germany) thermogravimeter. The samples were heated up to 900°C in a nitrogen (N_2) atmosphere at a controlled heating rate of 30°C/min. The results revealed that the pure PVC sample exhibited a 5% mass loss at 256.56°C, whereas the sample containing calcium carboxylate demonstrated greater thermal resistance, with the same level of degradation occurring at 270.13°C.

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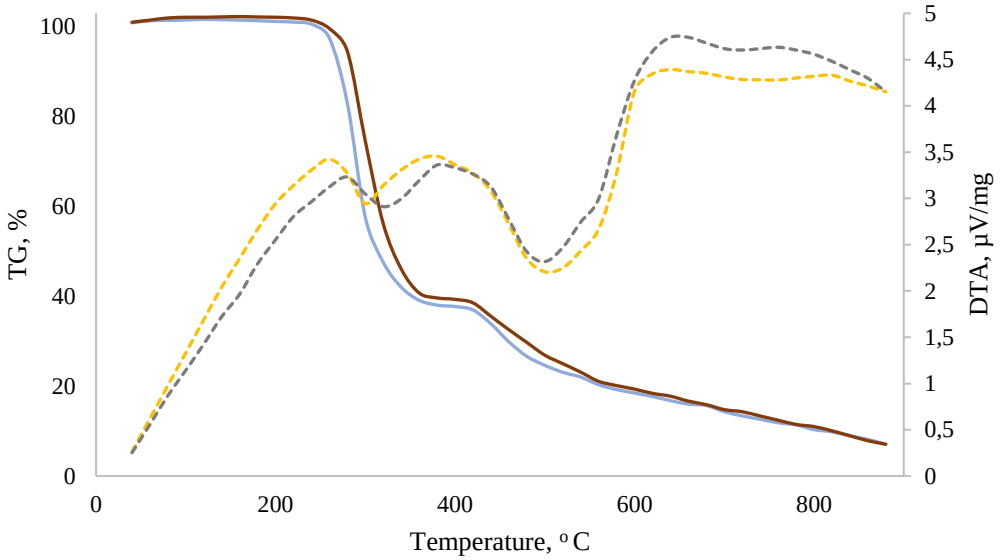
Figure 1
TG and DTA curves of polymer samples.



During the initial stage of degradation, which corresponds to PVC dehydrochlorination phase, occurred mass loss with significant fluctuations, reflecting the formation of conjugated double bonds within the polymer structure. As the temperature increased, decomposition progressed more rapidly, leading to 10% and 20% mass losses at 270.71°C and 279.25°C, respectively, for the pure polymer. In contrast, the stabilized polymer sample exhibited delayed degradation, with corresponding mass losses occurring at 279.68°C and 295.21°C. These findings indicate that the incorporation of the bio-based stabilizer enhances the thermal stability of PVC.

While the pure polymer exhibited a 50% mass loss at 313.14°C, the sample containing the heat stabilizer underwent the same degree of degradation at 328.96°C, demonstrating the effectiveness of the stabilizer. The significant increase in the decomposition temperature suggests that calcium carboxylate synthesized from soy wax efficiently neutralized the HCl released from the polymer chains during the initial thermal degradation of PVC. This stabilization mechanism effectively slowed down the decomposition process, preventing the release of chlorine (Cl) atoms, which constitute the bulk of the polymer matrix. The TG-DTA curves of the polymer samples are presented in Figure 1.

According to the DTA results, energy absorption associated with the decomposition of the pure polymer occurred at lower temperatures, whereas in the sample containing the thermal stabilizer, this process was observed at higher temperatures. This shift suggests that the presence of calcium carboxylate enhances the thermal stability of PVC by delaying decomposition. Additionally, since the neutralization of the released HCl by calcium carboxylate is an exothermic process, it is possible that partial compensation of the absorbed energy occurred.

To further analyze the thermal degradation behavior, the Coats-Redfern method was employed to calculate the activation energy of the decomposition stages based on thermogravimetric data. This calculation is derived from the Arrhenius equation:

$$k(T) = Ae^{-\frac{E_a}{RT}}$$

A – Pre-exponential factor (s^{-1} or min^{-1})
E_a – Activation energy of the reaction (J/mol)
R – Universal gas constant (8.314 J/(K·mol))
T – Absolute temperature (K)

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After incorporating the heating rate ($\beta = \frac{dT}{dt}$) into the Arrhenius equation, the resulting expression is:

$$\frac{d\alpha}{dT} = \frac{A}{\beta} e^{\left(-\frac{E_a}{RT}\right)} f(\alpha)$$

Integrating this equation using the Coats-Redfern method yields the following expression:

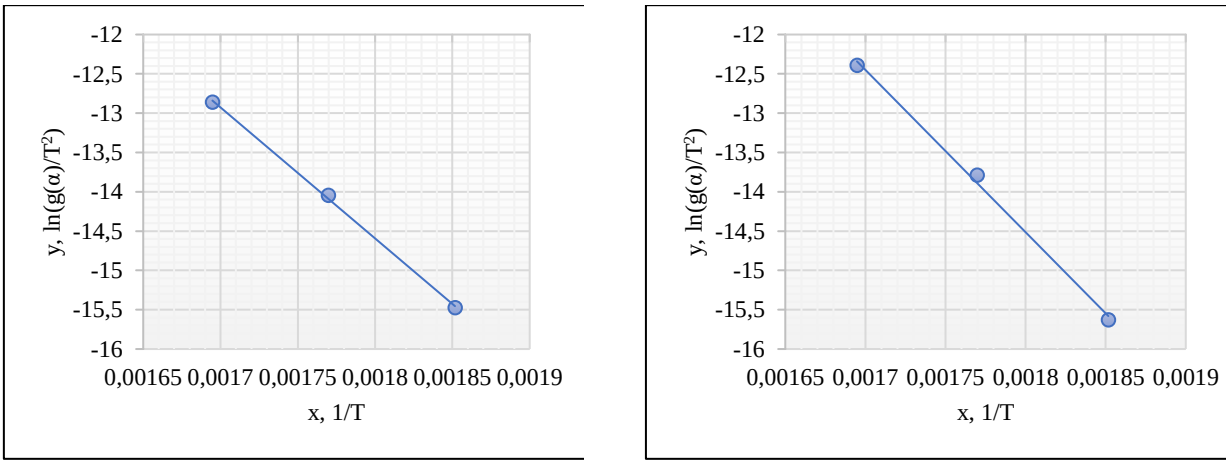
$$\ln\left(\frac{g(\alpha)}{T^2}\right) = \ln\left(\frac{AR}{\beta E_a}\right) - \frac{E_a}{RT}$$

The function g(α) in the equation represents the selected reaction model. For calculating the activation energy of PVC thermal decomposition using the Coats-Redfern method, three reaction models are commonly recommended:

$$\text{I. } g(\alpha) = -\ln(1-\alpha)$$
$$\text{II. } g(\alpha) = \frac{1}{(1-\alpha)} - 1$$
$$\text{III. } g(\alpha) = \left(1-(1-\alpha)^{1/3}\right)^2$$

Model I is applied to the initial stage of decomposition, specifically the dehydrochlorination process, while all three models are utilized for the second stage, where more complex chemical transformations occur.

Graphic 1.
The slopes of dehydrochlorination of PVC-pure (a) and PVC/CaSO (b) samples.



(a) (b)

To determine the activation energy, a corresponding point for each temperature is plotted in the coordinate system y = ln(g(α)/T²) versus x = 1/T. The activation energy (E_a) is then obtained by calculating the slope of the regression line fitted to these points.

$$m = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x^2 - \left(\sum x\right)^2}$$
$$E_a = -mR$$

m – slope

Based on the results obtained for the initial decomposition stage of the polymer samples using the aforementioned method (Graphic 1), the activation energy for the dehydrochlorination step was

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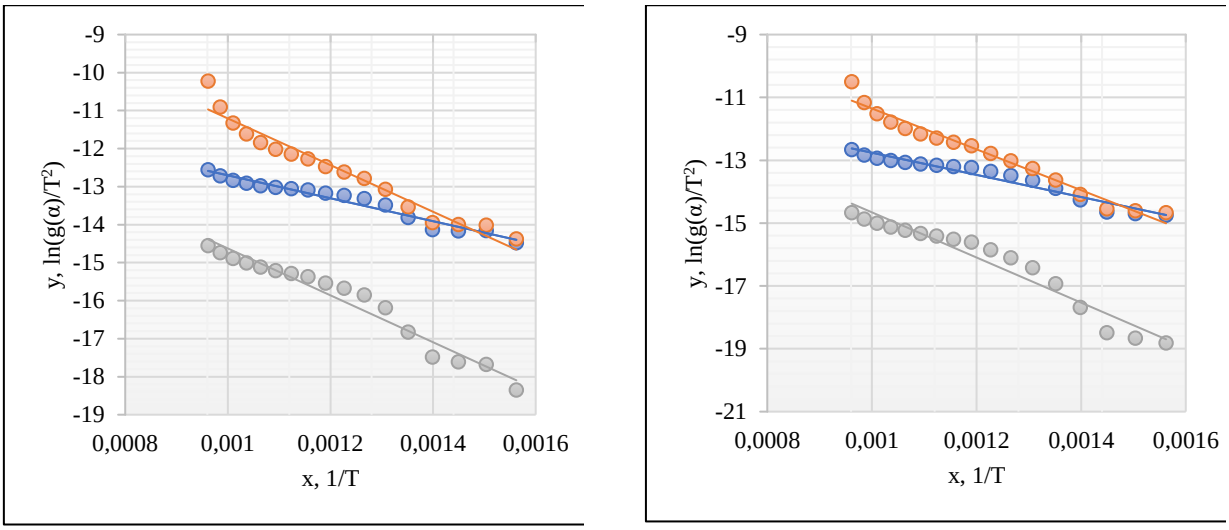
estimated to be approximately 62 kJ/mol for pure PVC and 65 kJ/mol for the PVC sample stabilized with a bio-based heat stabilizer. The relatively high heating rate in the thermogravimetric analysis resulted in a small difference between these values. However, the selected kinetic calculation method, which provides regression results based on a single heating rate, supports the general findings of the thermogravimetric analysis.

Graphic 2.
The slopes of polyene destruction of PVC-pure (a) and PVC/CaSO (b) samples.



(a) (b)

The results prove that the presence of the stabilizer increased the activation energy of initial decomposition stage of the polymer, indicating an improvement in thermal stability.

Following dehydrochlorination, the decomposition of the residual organic matrix occurred at a higher temperature. The degradation of the polyene structure required a greater amount of energy; however, due to the complexity of the chemical transformations occurring at this stage, the decomposition process exhibited fluctuations.

Since the degradation of the polyene structure involves complex interrelated transformations, multiple reaction models were employed to calculate the activation energy of this stage, as previously discussed. According to the calculation results (Graphic 2), the second stage of thermal decomposition exhibited a higher activation energy compared to the initial stage. Specifically, the activation energy for the second stage of thermal decomposition ranged from ≈ 83–106 kJ/mol for pure PVC and ≈ 87–110 kJ/mol for the PVC sample containing the stabilizer.

These results demonstrate that the addition of bio-derived calcium carboxylate significantly retarded the thermal decomposition of PVC. In addition to delaying the onset of polyene structure formation, the stabilizer also postponed the second stage of degradation.

Nevertheless, thermogravimetric analysis alone does not provide insight into the effects of stabilizer on other polymer properties. However, the findings indicate that calcium carboxylate synthesized from soybean wax holds promise as an effective suppressive heat stabilizer for use in the PVC processing industry.

Conclusion

The effectiveness of calcium carboxylate synthesized from soybean wax, a derivative of hydrogenated soybean oil, as an environmentally friendly heat stabilizer for polyvinyl chloride (PVC) was evaluated through thermogravimetric analysis. The results displayed that the bio-based stabilizer significantly slowed the thermal decomposition of the polymer. Notably, while the pure polymer exhibited 10% mass loss at 270.71°C, the introduction of the stabilizer increased the corresponding degradation temperature to 279.68°C. This is revealed that the HCl released during

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the initial decomposition of PVC was effectively neutralized by the stabilizer, thereby remaining within the total polymer mass and mitigating further degradation. Furthermore, based on the calculation of activation energies for different decomposition stages using the Coats-Redfern method, it was confirmed that calcium carboxylate positively influenced the thermal stability of PVC. However, the present study did not estimate effects of the stabilizer on other polymer properties. Despite this limitation, the thermal analysis results confirm the potential of calcium carboxylate synthesized from soybean wax as an effective suppressive heat stabilizer for PVC processing applications.

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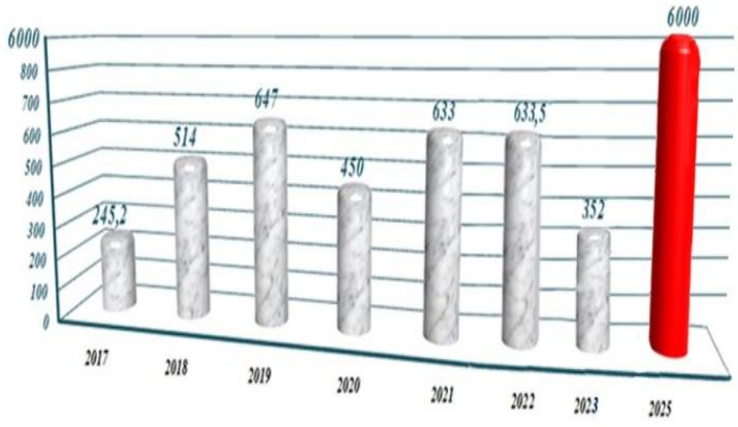
The Feeding and Development of Heat-Resistant Hybrids of Silkworms Under Adverse Conditions

Abstract

Decree of the President of the Republic of Azerbaijan dated November 27, 2017 on the approval of the "State Proqram for the development of cocooning and sericulture in the Respublic of Azerbaijan for 2018-2025"



For the further development of sericulture in the future, mechanization of all work in mulberry silkworm feeding and cocoon collection, creation of higher silky and productive breeds and hybrids, heavy varieties, etc. such directions have been taken into account.

In recent years, climate change is one of the global problems affecting the world. As it is known industrialization has had great negative effects on the Earth`s climate system along with other atmospheric wastes there has been a rapid increase in the scale of greenhouse effect gases.

In the lowland regions of our republic the fifth age of mulberry silkworm feeding falls on the temperature period of 28-30-32^{0}C.

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Due to the effect of such high temperature at least 45-50% of the worms get sick and die due to the effect of heat. In addition, the weight of the cocoons is low. Taking into account all this the creation and testing of hybrids with high cocoon weight and resistance to disease and heat is especially relevant. That is if the heat tolerance of the newly created hybrids is high it is possible to increase the production of cocoons and raw silk by 1,5-2,0 times without incurring additional costs.

Keydwords: *breed, hybrid, heat, productivity, selection*

Introduction

Azerbaijan has been not remained unaffected by global climate change. Observations indicate that the agricultural sector is among the most climate-sensitive areas (Akhmedov, Murodov 1998). Therefore, taking preventive measures is crucial. In this regard, scientific research has been conducted to preserve the existing locally adapted silkworm breeds and to develop new heat-resistant hybrids.

Therefore, the development of new heat-resistant silkworm hybrids is a crucial issue of great practical and economic value for national agriculture (Abbasov 2010).

In the modern era, one of the primary tasks facing breeders and geneticists is the development of breeds, varieties, and hybrids that can better adapt to wide environmental fluctuations and ensure relatively high and stable productivity under various ecological conditions. Such breeds, varieties, and hybrids are highly valued by agricultural producers and are considered more economically viable (Khalilov, Gulubayova, Huseynova, 2012). Therefore, in recent years, the creation of highly ecologically resilient plant varieties and animal breeds has been regarded as a priority direction in selection breeding (Huseynov, Eminbayli, 1973). This issue is also relevant for sericulture. During the experimental testing of new hybrids created through crossbreeding of intensive silkworm breeds under optimal conditions, cocoon productivity per box reaches 90-100 kg, with a raw silk yield of 43-45%. However, in production conditions, these figures drop to 40-45 kg and 30-35%, respectively, which is well known to specialists (Mammadov, 2018). New Technology in Sericulture. As a result, more than half of the potential cocoon and raw silk yield is lost, reducing farmers' interest in sericulture and slowing down the development of both sericulture and the silk industry (Huseynova, Musayeva, 2020).

Research

The creation of new heat-resistant silkworm hybrids is an important issue of great practical and economic value with significant national economic importance (Huseynov, Eminbeyli, 1973).

For the implementation of the work, silkworms from the selection laboratory, including the Ughur, Ordubad-1, Ordubad-2, Mughan-1 and Mughan-2 breeds, as well as the Mizuri-1 and Mizuri-5 varieties introduced from the Georgian Sericulture Research Institute (GSRI), and the control varieties Mayak-2 and Mayak-3, were used. The following hybrid combinations were created: 1) Ordubad-1×Mughan-1; 2) Ordubad-1×Mughan-2; 3) Ordubad-1×Mizuri-1; 4) Ordubad-1×Mizuri-5; 5) Ordubad-1×Ughur; 6) Ordubad-2×Muğan-1; 7) Ordubad-2×Mughan-2; 8) Ordubad-2×Mizuri-1; 9) Ordubad-2×Mizuri-5; 10) Ordubad-2×Ughur; 11) Mayak-2×Mayak-3 (control variant). The Mayak-2×Mayak-3 hybrid was used for comparison. The experiments were conducted in two different environments (optimal and suboptimal).

Typically, in the lowland regions of our republic, the feeding periods of silkworms at the fourth and fifth instars coincide with hot and dry periods. Due to the high temperature and low humidity, the leaves wilt quickly and lose their quality. Considering these factors, a suboptimal environment was created for the fourth and fifth instar stages .

The crossbreeding of breeds was conducted in a suboptimal environment (Huseynova, Musaeva, 2024). The feeding of silkworms (hybrids) began in April. The feeding duration lasted for 27-28 days. The survival rate of the hybrids' larvae and the feeding duration are presented in the table below:

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Table 1
The survival rate of the hybrids' larvae and feeding duration.

№	Hybrid Name	Start Date		Survival Rate	Feeding Duration
		Incubation	Feeding		
1	Ordubad-1×Mughan-1	18.04	27.04	98.5%	28.0
2	Ordubad-1×Mughan-2	18.04	27.04	96.5%	28.0
3	Ordubad-1×Mizuri-1	18.04	27.04	96.0%	28.0
4	Ordubad-1×Mizuri-5	18.04	27.04	97.0%	28.0
5	Ordubad-1×Mayak-2	18.04	27.04	97.5%	27.0
6	Ordubad-1×Mayak-3	18.04	27.04	95.5%	27.0
7	Ordubad-1×Ughur	18.04	27.04	99.0%	27.0
8	Ordubad-2×Mughan-1	18.04	27.04	97.5%	28.0
9	Ordubad-2×Mughan-2	18.04	27.04	98.0%	28.0
10	Ordubad-2×Mizuri-1	18.04	27.04	96.5%	28.0
11	Ordubad-2×Mizuri-5	18.04	27.04	96.0%	28.0
12	Ordubad-2×Mayak-2	18.04	27.04	96.5%	28.0
13	Ordubad-2×Mayak-3	18.04	27.04	95.5%	28.0
14	Ordubad-2×Ughur	18.04	27.04	96.5%	28.0
15	Mayak-2×Mayak-3	18.04	27.04	98.5%	28.0

As seen in the table, the hybrid with the highest survival rate of larvae was Ordubad-1×Uğur, with a rate of 99.0% (Huseynova, Musaeva,

The biological indicators of the silkworm hybrids that were fed are presented in Table 2.

Table 2
The biological indicators of the hybrids are as follows.

№	**Hybrid Name**	**Average mass**		**Silkiness, %**
		Cocoon, g	**Silk thread, mg**	
1	Ordubad-1×Mugan-1	1,78	357	20,1
2	Ordubad-1×Mugan-2	1,67	328	19,4
3	Ordubad-1×Mizuri-1	1,78	384	21,5
4	Ordubad-1×Mizuri-5	1,75	331	18,7
5	Ordubad-1×Mayak-2	1,72	373	21,6
6	Ordubad-1×Mayak-3	1,62	340	21,0
7	Ordubad-1×Ughur	1,80	372	20,6
8	Ordubad-2×Mughan-1	1,66	362	21,9
9	Ordubad-2×Mughan-2	1,68	276	16,6
10	Ordubad-2×Mizuri-1	1,56	272	17,3
11	Ordubad-2×Mizuru-5	1,55	320	20,5
12	Ordubad-2×Mayak-2	1,66	319	19,1
13	Ordubad-2×Mayak-3	1,60	330	20,8
14	Ordubad-2×Ughur	1,66	314	18,9
15	Mayak-2×Mayak-3 (control)	1,79	369	20,6

As shown in Table 2, the average weight of the live cocoons in the hybrids ranges between 1.55g and 1.80g. The highest average weight of the live cocoon is observed in the Ordubad-1×Uğhur hybrid (1.80g), while the lowest is in the Ordubad-2×Mizuri-5 hybrid (1.55g). The average weight of the silk ranges between 272mg and 384mg across the hybrids. The best result is again observed in the Ordubad-

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1×Mizuri-1 hybrid (384mg), while the lowest result is in the Ordubad-2×Mizuri-1 hybrid (272mg). The silkiness of the hybrids fluctuates between 16.6% and 21.9%. The highest silkiness is found in the Ordubad-2×Muğan-1 hybrid (21.9%) (Huseynova, Musaeva, 2023; Huseynova, Bakirov, Shukurlu, Kuluntay, Rustamova, Yusifova, Mamadov, 2024).

Conclusion

1. The highest survival rate of larvae among the hybrids was observed in Ordubad-1×Ughur (99.0%).
2. The highest average weight of the live cocoon among the hybrids was in Ordubad-1×Ughur (1.80g).
3. The best result in terms of the average weight of the silk filament was in the Ordubad-1×Mizuri-1 hybrid (384mg).
4. Feeding was conducted in a suboptimal environment for 15 hybrids.

In the future, two hybrids selected for heat tolerance will be submitted to the Azerbaijan Patent Office (AXA) for getting patent. It is also recommended that these hybrids be fed in the lowland regions of our republic.

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The Impact of Fungal Diseases on Plants in Ecosystems and Ecological Control Methods

Abstract

Houseplants play an important role in modern life, not only in terms of aesthetics but also from ecological and psychological perspectives. As part of nature in residential and workspaces, they purify the air, improve microclimatic conditions, and enhance human well-being. However, houseplants are susceptible to various diseases, including fungal infections. These diseases threaten the healthy development of plants and their role in the ecosystem. Fungal diseases can lead to plant damage and, as a result, reduce their impact on the ecosystem. This situation can also disrupt the plants' interactions with the environment and alter the balance of various biological chains. The degree of focus on this topic has expanded in recent years, particularly with the application of ecological control approaches. Biological control and the use of natural fungicides, as well as soil health preservation, are key research areas in this field. However, the broader impact of fungal diseases on plants and other organisms at the ecosystem level is still underexplored. This indicates that the topic holds significant potential for further research and development.

Keywords: *fungal diseases, plant pathology, ecosystem impact, ecological control, plant disease resistance*

Introduction

The exploration of this topic has expanded in recent years, particularly with the application of ecological control approaches. Biological control and the use of natural fungicides, along with the preservation of soil health, have become key areas of focus in related research. However, the broader impact of fungal diseases on plants and other organisms at the ecosystem level is still insufficiently studied. This indicates that the topic holds significant potential for further research and development (Andrade, & Correa, 2018). At the same time, the application of ecological approaches in relation to houseplants is expanding. The implementation of ecological methods to enhance plants' resistance to diseases, both in natural and man-made environments, particularly in indoor settings and gardening environments, aligns with the demands of modern times. Using ecological approaches to combat fungal diseases, which are less harmful than chemical methods, has a significant impact on the development of modern ecological science, as well as on the formation of sustainable agricultural and horticultural practices (Ainsworth, & Bisby, 1995).

Research

Thus, it is necessary to conduct-in depth research in the impact of fungal diseases on houseplants and the application of ecological approaches to combat these diseases remain highly relevant. Research conducted on this topic will contribute significantly to both the preservation of plant health and the sustainable development of modern ecosystems. Fungal diseases in houseplants develop through the interaction of both physical and ecological factors. The progression of these diseases is typically linked to environmental conditions, the plant's vulnerability, and the source of infection. Fungal diseases can cause severe consequences by affecting the plant’s life cycle and the activities of other organisms within the microecosystem (Brown, & Pettitt, 2009). The impact of fungal diseases on houseplants affects not only the survival and growth of the plants but also extends to other organisms in the surrounding environment. The interactions between plants and microorganisms are often symbiotic, meaning both parties benefit from the relationship.

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However, fungal diseases can disrupt these interactions and alter the balance of the ecosystem (Cheng, Zhang, & Lin, 2020).

Fungal diseases interfere with the microbiomes in the root environments of plants. This damages the plant's relationships with beneficial microorganisms and creates favorable conditions for harmful microorganisms, particularly fungi, to proliferate. As a result, the plants face difficulties in processing nutrients, weaken their photosynthetic processes, and experience stunted growth. Many plants establish symbiotic relationships with fungi, such as mycorrhizal fungi that interact with plant roots, providing essential nutrients to the plants (Hoy, Boethel, 2014). However, pathogenic fungi can disrupt these symbiotic connections, leading to reduced nutrient uptake and poor plant development. Fungal diseases not only affect houseplants but also alter the development of other organisms associated with these plants, such as insects, microorganisms, and pests. Weakened plants become more vulnerable to harmful insects, which increases their populations. This, in turn, can disrupt a broader biological regulatory chain within the ecosystem (Gupta, & Verma, 2016).

The research examined in this paper focuses on the impact of fungal diseases related to houseplants on the ecosystem, as well as the application of ecological control methods, particularly in urban environments. These studies have been primarily conducted on plants grown in home and office settings. The research aims to explore the environmental conditions, plant characteristics, and the implementation of ecological approaches to combat fungal diseases, highlighting their broader impacts on ecosystems (Harris, & Dooley, 2014). The effects of fungal diseases on houseplants extend beyond the survival and growth of the plants, also impacting other organisms in the surrounding environment. The interactions between plants and microorganisms are often symbiotic, meaning both parties benefit from the relationship. However, fungal diseases can disrupt these interactions and alter the balance of the ecosystem (Hwang, & Liu, 2015).

Fungal infections disturb the microbiomes in the plant's root environment. This damages the plant's relationships with beneficial microorganisms and creates favorable conditions for harmful microorganisms, especially fungi, to thrive. As a result, plants face difficulties in processing nutrients, their photosynthetic processes weaken, and their growth slows down. Many plants form symbiotic relationships with fungi, such as mycorrhizal fungi that interact with plant roots and provide nutrients. However, pathogenic fungi can disrupt these symbiotic connections, leading to reduced nutrient uptake and poor plant development (Jeong, & Lee, 2018).

This article investigates the impact of fungal diseases associated with houseplants on the ecosystem and the application of ecological control methods, with research primarily conducted in urban environments, particularly in homes and office settings. The studies aim to explore the environmental conditions, plant characteristics, and the implementation of ecological approaches to combat fungal diseases and their broader effects on ecosystems. The research was carried out in various buildings and office environments located in urban areas (Smith, & Johnson, 2011). These spaces are the most common places where houseplants are found and regularly exposed to fungal diseases. The areas selected for the study are characterized by specific features. For example, research was conducted in the urban environment, a key location for houseplants. Homes, offices, and other building complexes in the urban environment reflect both internal microclimatic conditions and factors that are unfavorable for plant growth. The inherent characteristics of urban environments (such as low light, high humidity, ventilation issues, etc.) make houseplants more susceptible to fungal diseases (MacDonald, & Parker, 2017).

The areas where the research was conducted located in buildings with various climatic conditions. Houseplants in these buildings experience different growing conditions depending on the internal temperature and lighting. Lack of light, temperature fluctuations, and high humidity levels are among the factors that contribute to the increase in fungal diseases. Special attention was paid to the microclimatic conditions in the areas where the research was conducted. The watering, air circulation, temperature, and lighting conditions in the environments of houseplants can all influence the spread of fungal diseases. The following factors were particularly considered (Talbot, & Rispail, 2013):

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1. **Lighting**: The lighting conditions in the spaces where houseplants are located vary. In some areas, natural sunlight is insufficient, while in others, plants benefit optimally from either natural or artificial lighting. Lack of light is a contributing factor to the development of fungal diseases, as weakened light conditions diminish the plants' immunity.
2. **Humidity and Ventilation**: Humidity levels, especially high humidity and poor ventilation conditions, are important factors that increase the occurrence of fungal diseases. Therefore, humidity levels were regularly measured in the study areas, and the air circulation around the plants was also assessed.
3. **Soil and Watering**: The characteristics of the soil and the watering regimen directly affect the plants' resistance to fungal diseases. Attention was paid to the type of soil in the research areas, and the frequency and quality of watering were analyzed.

Conclusion

Fungal diseases in houseplants are a significant problem that seriously affects both plant health and the integrity of the ecosystem. This research analyzed the spread of fungal diseases in houseplants and proposed new approaches to combat them using ecological methods. Based on the results of the study, it is clear that using chemical methods alone is insufficient to ensure the sustainability of ecosystems and the healthy development of plants. The application of ecological control methods, such as natural fungicides, microorganisms, and plant extracts, presents an effective alternative for maintaining both plant health and environmental protection. Additionally, it has been found that integrated pest management approaches for fungal diseases have a positive impact on preserving both the environment and plant health. This research encourages the application of more ecological and sustainable approaches to combating fungal diseases in houseplants and demonstrates how these methods can help maintain the overall balance of ecosystems. At the same time, the findings provide plant growers and ecology experts with new, healthier, and more environmentally suitable methods for dealing with fungal diseases. Future research should be focused on further developing, expanding, and testing these approaches on other plant species. This is crucial for supporting the healthy growth of houseplants and ensuring environmental protection.

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What Should We Know About Bioavailability and Bioequivalence?

Abstract

Bioequivalence studies a crucial role in the development and approval of generic drugs, requiring input from multiple disciplines, including regulatory affairs, pharmacokinetics, and statistics. These studies assess whether the test (T) and reference (R) formulations exhibit similar bioavailability, ensuring therapeutic equivalence. Typically, they involve well-established study designs, such as parallel or crossover approaches, which help compare the pharmacokinetic parameters of both formulations. The bioanalytical methods used in these studies must be highly accurate, precise, selective, sensitive, and reproducible to generate reliable data. Peripheral blood, including plasma, serum, or whole blood, is the most commonly used biological matrix for evaluating a drug's systemic availability. The collection and analysis of biological fluid samples allow for the quantification of the active drug ingredient, its active moiety, and, when necessary, its active metabolites. These measurements are essential for determining the pharmacokinetic properties of the drug and ensuring compliance with regulatory bioequivalence criteria, ultimately supporting safe and effective drug substitution.

Keywords: *bioequivalence, bioavailability, biological fluid, dosage form*

Introduction

Pharmaceuticals have become an indispensable consumption item today. In order to increase their market share, pharmaceutical companies produce, licence and offer for sale over-sold drug products under different names. Thus, the number of similar preparations containing the same active substance in the same amounts is increasing rapidly. One of the most important factors affecting the success of medication applications is the bioavailability of the drug, that is, the amount that can reach the target area from the application site. The fact that the effectiveness of drugs containing the same active substance at the same rate in treatment is close to each other indicates that their bioavailability is equal. Whether the expected therapeutic response can be obtained from systemically effective drugs is determined by bioavailability studies. Bioavailability, which is important in the development of both new and generic drugs, can be investigated in two different ways, absolute and relative bioavailability, and these two concepts give us different information about the active substance and the preparation containing it. Similar preparations containing the same active substances in the same ratio must be pharmaceutically bioequivalent in order to be equivalent (Canbolat, 2002).

Research

The efficacy, safety, quality, control and supervision of drugs are primarily performed by bioequivalence and bioavailability studies. Bioavailability and/or bioequivalence studies are among the documents required for the licensing of pharmaceutical products.

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In particular, proving the therapeutic equivalence between the drug of the company that first discovered the drug and a drug produced as a pharmaceutical equivalent that is not under patent protection is considered as the most important factor showing that this drug can be used clinically instead of the other. Therefore, in the licensing of drugs, it is as important for the health and safety of the patient whether they can be used interchangeably (equivalence) as quality, efficacy and safety. Bioequivalence tests play an important role in the evaluation of drug formulations with similar clinical and pharmacological effects and similar plasma drug concentration-time curves (Mehta, 2023). Bioequivalence tests are the most important tests in demonstrating therapeutic equivalence, especially for active substances and/or pharmaceutical dosage forms that are used orally and show bioavailability problems. Drugs with proven therapeutic equivalence are interchangeable drugs. In other words, they can be used interchangeably. In a broad sense, bioavailability is the rate and degree to which the active substance is absorbed from its pharmaceutical form (except iv) and passes into the systemic circulation and is thus present at the site of action in the body or in biological fluids (usually serum and plasma) that reflect it. These two parameters determine the 'bioavailability' of a drug (Feng, 2008).

Compared to the solid pharmaceutical form of a drug with a liquid, it is absorbed from the gastrointestinal tract faster and sometimes more. The drug effect starts earlier. Drugs in solid form such as tablets undergo disintegration and dissolution in gastrointestinal fluids after oral administration and are absorbed. An undispersed or slowly disintegrating tablet may result in inadequate absorption or, in the best case, a further delay in the clinical response. Depending on the pharmaceutical form of the drug, bioavailability is in the order of solution > capsule > tablet > coated tablet.

Source of Raw Material; Purity and quality differences that may arise due to the supply of both the active substance and the excipients in the composition of the preparation from different sources may lead to significant bioavailability and bioequivalence problems (Lee, 2008).

Particle Size of Active Substance; The smaller the drug molecule, the faster it is absorbed. As the particles become smaller, the dissolution rate increases as the surface area increases. In studies, it has been observed that the dissolution rate and absorption of griseofulvin increases as the particle size decreases (Dortunç, 2007).

Crystal Shape of the Active Substance; The solubility of a drug with polymorphous structure in water and therefore in the gastrointestinal system varies according to its crystal shape. Amorphous shapes are better soluble than crystallised shapes. Differences in bioavailability may occur as a result of the use of a different crystal form of the active substance, the transformation of an unstable crystal form into another form in the preparation or the use of an amorphous form of the active substance. The amorphous form of novobiocin has at least 10 times more solubility than the crystalline form. In studies in dogs, the amorphous form was rapidly absorbed by oral administration, whereas the crystalline form could not be absorbed.

Formation of Complex with Active Substance; The formation of a drug complex in the gastrointestinal reduces the rate and amount of absorption. For example, the polysaccharide called mucin in the intestine can bind streptomycin and dihydrostreptomycin to a high degree. This binding may cause poor absorption of antibiotics. Similarly, bile salts in the small intestine can form insoluble complexes with some drugs including neomycin and kanamycin. Sometimes bioavailability of drugs that cause bioavailability problems due to their slow and low solubility in water can be increased by complexing them with other drugs or substances (Traş, 2005).

Ionisation Degree of the Active Substance: The degree of ionisation affects the solubility of drugs in oil or water. Since it is determined by the pH of the environment in which the drug is administered and absorbed, even small changes in the pH of the digestive system affect the bioavailability of some drugs. As the environment becomes more acidic, the proportion of non-ionised parts of weakly acidic substances increases and their absorption becomes easier. The ionisation of weak basic substances increases and their absorption rate decreases. When the environment becomes alkaline, ionisation of weak acidic substances is encouraged and absorption

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rates decrease, while the ratio of non-ionised parts of weak basic substances increases and absorption becomes easier (Güç, 2008).

Interaction; Drugs are mixed with excipients (fillers, dyes, binders, binders, lubricants, surfactants) during their production while forming solid pharmaceutical forms. These substances may change the disintegration and dissolution rate of the active substance.

Patient Related Factors Stomach Emptying Rate; Rapid emptying of the stomach increases the absorption rate and rate of drugs absorbed from the small intestine. Absorption rate of many drugs decreases in the presence of food. Digoxin, cephalexin and various sulphonamides can be given as examples. Drugs that are broken down as a result of acid hydrolysis in the stomach are absorbed at a higher rate. In general, absorption is better when the stomach is empty. However, absorption of some drugs increases when they are taken after a meal. For example, absorption of riboflavin is higher than normal after a standard breakfast. In general, weakly acidic drugs are better absorbed from the stomach than from the intestine.

In the small intestine; absorption increases due to the length of the transit time and the fact that the surface area suitable for absorption in the small intestine is much larger than in the stomach. Intestinal Motility; Slowing of intestinal motility prolongs the transit time through the intestine. Some drugs, which are absorbed difficultly because they are hardly soluble in the intestine, remain in the intestine for a long time, increasing their solubility and allowing them to be absorbed at a high rate.

Perfusion of the gastrointestinal tract; Blood flow in the digestive tract is generally important for lipophilic drugs absorbed by simple diffusion. Acceleration of blood flow here is important for absorption rate and clearance, especially for drugs with high presystemic elimination (FDA, 2002).

Individual Differences; A small genetic variation in each enzymatic step involved in the CT of drugs may cause intra-individual or inter-individual differences in the effect of the drug. Bioavailability is the genetic polymorphism shown by liver enzymes. In vitro and in vivo (clinical) trials in the determination of bioavailability In Vitro Trials In vitro tests, which require less expense, are performed in a short time and with simple techniques, have practical and economic importance. In vitro tests can actually provide an indication of bioavailability. These tests are applied to solid pharmaceutical forms.

Disintegration Test; It is a test applied to tablets other than chewable and slow-release tablets. It is performed with the help of hanging basket system and discs. The purpose of the test is to compare the level of disintegration of the tablets in the appropriate liquid with the limits of disintegration determined in the monographs. Usually at least 16 out of 18 tablets should be completely disintegrated.

Dissolution Test; The dissolution rate of the drug in solid pharmaceutical form in a certain environment, such as artificial gastric or intestinal juice, under certain test conditions (370C) is determined. At the end of this test, the dissolution of 50% of the amount of the drug in the pharmaceutical form is evaluated.

Determination of Plasma Concentration Profile; The drug is administered to patients or volunteers and the drug concentration in blood samples is measured at certain intervals and the drug concentration-time curve is drawn. As a rule, the total sampling time should be the half-life of the drug. If the Cmax and tmax of the two preparations analysed are equal, they are considered equivalent in terms of absorption rates.

Measurement of Cumulative Drug Amount in Urine; After the drug is given to the patient, the urine of the subject is collected at certain intervals for a certain period of time (5-10 times the half-life) and the curve of the cumulative amount of the drug excreted in the urine is drawn according to time. These curves are evaluated in terms of the maximum amount reached and their slope, i.e. the rate at which they reach the maximum (FDA, 2003).

Bioequivalence can be defined as the bioavailability (the rate and extent to which the active ingredient in the pharmaceutical alternatives reaches the site of action) of two pharmaceutically equivalent preparations (one test and one reference) after administration of the same molar dose,

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within accepted limits (±20%), so that their therapeutic effects are similar enough to be identical in terms of both efficacy and safety (Armando, Serra, Porta, Koono, Kano, 2009).

Therapeutic Equivalence: A preparation is therapeutically equivalent if it contains the same active substance or therapeutically effective molecule part with another preparation whose efficacy and safety have been previously determined and if it shows the same efficacy and safety clinically with that (Gozzo, 2022).

Pharmacological equivalence is the situation where molecules that are chemically different but produce the same active molecules in the body and cause the same pharmacological effect are added into two different pharmaceutical forms.

Pharmaceutical Alternatives; Pharmaceutical products are pharmaceutical alternatives if they contain the same active molecule part, but differ in chemical form, dosage form or quantity (Novakovic, 2019).

Pharmacokinetic Properties of the Active Substance; Non-linear (dose-dependent) kinetics of the drug within the therapeutic dose range, presystemic elimination of more than 70%, absorption of less than 70%, absorption and elimination rate of the preparation showing high variability between individuals (Kaya, 2006).

Conclusions

In ***in vivo*** bioequivalence studies, bioavailability is typically evaluated based on the rate and extent of drug absorption into the bloodstream of human subjects. However, for certain locally acting drug products, such as nasal aerosols and nasal, which are not meant to enter the bloodstream, bioavailability is instead assessed using measurements that indicate how efficiently the active ingredient or moiety reaches the site of action.

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The Impact of Quercetin Glycosides on ACE2, AT1R, and AT2R: The Molecular Docking and in Silico Analysis

Abstract

The renin-angiotensin-aldosterone system (RAAS) plays a critical role in cardiovascular homeostasis, and its dysregulation is associated with hypertension and thrombotic disorders. In this study, we performed a comparative molecular docking analysis of four quercetin glycoside derivatives against three key RAAS-related targets: angiotensin-converting enzyme 2 (ACE2), angiotensin II type 1 receptor (AT1R), and angiotensin II type 2 receptor (AT2R). The aim is to identify ligands that inhibit AT1R to lower blood pressure, without antagonizing ACE2 and AT2R functions which are protective against thrombosis and endothelial dysfunction. The results showed quercetin 5-glucoside and 7-glucoside are promising dual-function ligands with selective AT1R inhibition and peripheral, non-blocking interaction with ACE2 and AT2R.

Keywords: *RAAS, ACE2, AT1R, AT2R, quercetin glycosides, molecular docking*

Introduction

The renin–angiotensin system (RAS) is a key regulatory pathway involved in cardiovascular homeostasis, fluid balance, and vascular tone. It has become increasingly evident in recent years that beyond its classical roles, RAS also exerts profound effects on inflammation, fibrosis, and thrombosis. The dual axis system –comprising the classical ACE1/angiotensin II/AT1R pathway and the counter-regulatory ACE2/Angiotensin-(1–7)/MasR pathway – has attracted significant attention in the pathophysiology of cardiovascular and thrombo-inflammatory disorders (Santos, Sampaio, Alzamora, Motta-Santos, Alenina, Bader, & Campagnole-Santos, 2018; Patel, Zhong, Grant, & Oudit, 2019).

Both ACE1 and ACE2 are endothelium-associated carboxypeptidases that are widely distributed in various organs, including the heart, kidneys, brain, and blood vessels. Additionally, ACE2 is present in vascular smooth muscle cells of coronary arteries and intrarenal blood vessels (Wang, Bodiga, Das, Lo, Patel, Oudit, 2012); Hikmet, Méar, Edvinsson, Micke, Uhlén, Lindskog, 2020). ACE, a highly glycosylated transmembrane protein, exists in two isoforms due to alternative splicing: somatic ACE, which consists of two domains (N- and C-domains) with distinct but overlapping substrate preferences (Turner, 2015).

Research

ACE1 converts angiotensin I into angiotensin II, a peptide that promotes vasoconstriction, oxidative stress, platelet aggregation, and pro-thrombotic responses via AT1R activation. Conversely, ACE2 plays a crucial role in the RAS by converting angiotensin II (Ang II) into angiotensin-(1-7) [Ang-(1-7)], a peptide with vasodilatory and cardioprotective effects primarily through the Mas receptor (Gheblawi, Wang, Viveiros, Nguyen, Zhong, Turner, Raizada, Grant, & Oudit, 2020).

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Additionally, AT2R, mentioned in some articles as another receptor for Ang II, counteracts AT1R by inducing nitric oxide production, vasodilation, and anti-fibrotic responses (Carey, Wang, Siragy, 2017). It can also hydrolyze Angiotensin I (Ang I) to generate Angiotensin-(1-9) [Ang-(1-9)], although the latter is primarily produced by carboxypeptidase A in the heart (Kuriakose, Montezano, Touyz, 2021, 2021). Beyond its role in angiotensin metabolism, ACE2 functions as a multifunctional enzyme, breaking down various bioactive peptides such as Apelin-13, Apelin-17, Apelin-36, and [des-Arg9]-bradykinin, thereby influencing multiple physiological pathways (Turner, 2015) (Fig. 1).

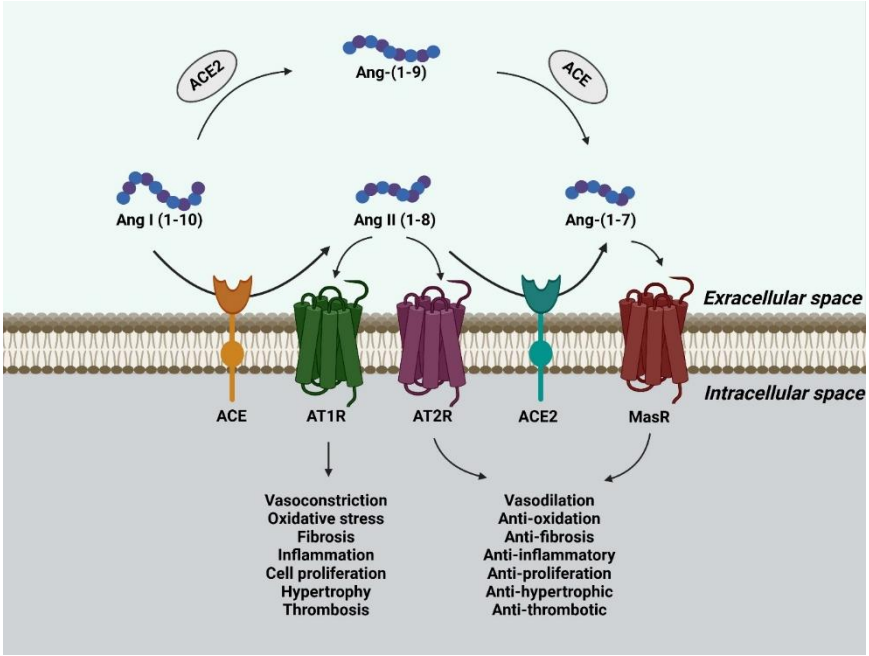

Fig. 1. Simplified illustration of RAS axis – ACE/Ang II/AT1R and ACE2/Ang-(1-7)/MasR. ACE converts Ang I (1-10) to Ang II (1-8), which activates the ACE/Ang II/AT1R signaling pathway, driving associated physiological responses. On the other hand, ACE2 catalyzes the conversion of Ang-(1-7) either directly or through the intermediate Ang-(1-9), initiating antagonist processes through the ACE2/Ang-(1-7)/MasR pathway.

The imbalance between these axes – often characterized by ACE1/AT1R overactivation and ACE-2/AT2R downregulation – has been implicated in a range of disorders including hypertension, thrombosis, acute lung injury, and cardiovascular complications (South, Brady, & Flynn, 2020). In addition, ACE2 plays a crucial role in kidney health by reducing tubulointerstitial fibrosis and protecting against diabetic renal injury (Hardenberg, Luft, 2020). Furthermore, ACE2 gained increased attention as the entry receptor for SARS-CoV-2, which also resulted in endothelial dysfunction and coagulation abnormalities, highlighting the potential of ACE2-targeted interventions (Verdecchia, Cavallini, Spanevello, & Angeli, 2020).

Several natural polyphenols, including quercetin and its analogues, have been reported to modulate RAS components by inhibiting ACE1 or influencing receptor activity. However, the direct binding affinity and molecular interaction of these compounds with ACE2, AT1R, and AT2R remain insufficiently studied. Structure-based drug design and molecular docking tools provide a powerful approach to explore these interactions in silico before proceeding to in vitro or in vivo validations (Samavati & Uhal, 2020; Galandarli, Mollayeva, Javadzade, Mammadova, & Amrahov, 2022).

In this study, we aim to investigate the binding potential of selected quercetin-derived compounds to ACE2, AT1R, and AT2R through molecular docking and binding site analysis. The ultimate objective is to identify molecules that may enhance ACE2 and AT2R activity while

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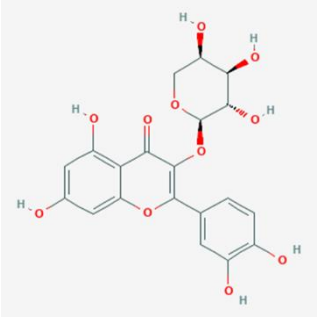
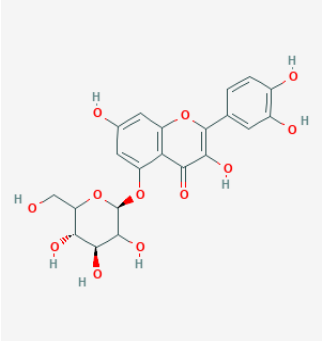
antagonizing AT1R, thus shifting the RAS equilibrium toward a vasoprotective and antithrombotic profile.

Material and method

Structure search and preparation of proteins and ligands. The coordinates for the ACE2, AT1R and AT2R were obtained from the PDB database (https://www.rcsb.org/). Quercetin glucosides (Fig. 2) were obtained from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). Ligands for molecular docking were prepared using Chimera (V:1.18; https://www.cgl.ucsf.edu/chimera/download.html) and AutoDock Vina (V:1.5.7; https://vina.scripps.edu/downloads/). The preparation of proteins was performed using the AutoDock software suite. Heteroatoms, including water molecules, were removed, polar hydrogens were added, non-polar hydrogens were merged, and Kollman and Gasteiger charges were assigned, as well as the conversion into.pdbqt format (Afriza, Suriyah, Ichwan, 2018). The file conversion into.pdbqt format was done to allow the file to be loaded in Autodock Vina for molecular docking simulation (Huey, Morris, Forli, 2012). Ligands downloaded from PubChem in .sdf format were converted to.pdb format using Open Babel (http://openbabel.org/wiki/Main_Page). The charges of the ligands were set to neutral, Gasteiger charges were added, and the number of torsions was kept at the default setting and conversion into.pdbqt format.

№	Compounds	Molecular formula	Molecular weight g/mol	2-Dimensional structure
1	12309865	$C_{20}H_{18}O_{11}$	434.3	 Quercetin 3-O-arabinoside
2	44259222	$C_{21}H_{20}O_{12}$	464.4	 Quercetin 5-glucoside

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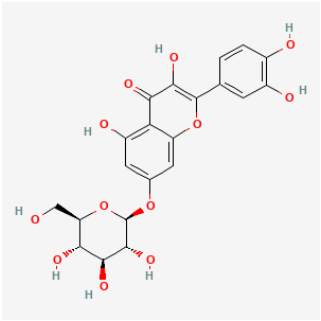
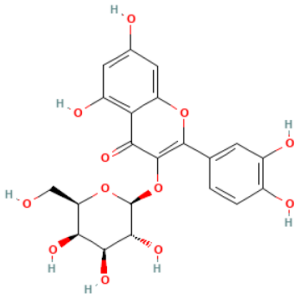
3	5282160	$C_{21}H_{20}O_{12}$	464.4	 Quercetin 7-glucoside
4	5281643	$C_{21}H_{20}O_{12}$	464.4	 Quercetin-3-O-galactoside

Fig. 2. Quercetin glucosides

Protein-ligand docking. Molecular docking was carried out using the AutoDock Vina tool (V: 1.5.7; https://vina.scripps.edu/downloads/). First, blind docking was performed, followed by precision docking. The spacing value was set to 1 angstrom, and the grid box was manually adjusted to cover the active regions of the receptor. The grid box dimensions were set to X = 20, Y = 20, Z = 20 for three proteins. The exhaustiveness value was set to 8 for the proteins. The center coordinates of the grid box were defined as shown in Table 1. All docking experiments were repeated three times to ensure reliability. Discovery Studio Visualizer (https://discover.3ds.com/discovery-studio-visualizer-download) was used to generate two-dimensional (2D) representations of protein-ligand interactions (Laskowski & Swindells, 2011). The three-dimensional (3D) images of protein-ligand complexes were created using the Chimera software (https://www.cgl.ucsf.edu/chimera/download.html) (Pettersen et al., 2004).

Table 1. Central coordinates of the Grid box

ACE2	**X**	**Y**	**Z**
1R42	39.409556	30.548984	9.472548
AT1R	X	Y	Z
6DO1	40.636558	37.312950	43.571732
AT2R	X	Y	Z
5UNG	4.839429	6.950571	-18.760843

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Molecular docking analysis of four quercetin glycoside derivatives against ACE2 (PDB ID: 1R42), AT1R (PDB ID: 4YAY), and AT2R (PDB ID: 5UNG) was conducted to evaluate their binding affinities and interaction profiles. The results provide key insights into the potential of these ligands to modulate RAAS components relevant to hypertension and coagulation regulation.

Among the tested compounds (Fig.3), quercetin 5-glucoside exhibited the strongest binding affinity toward ACE2 (-9.0 kcal/mol), AT1R (-8.4 kcal/mol), and AT2R (-8.1 kcal/mol), followed closely by quercetin 7-glucoside (-8.8 kcal/mol, -8.6 kcal/mol, -8.6 kcal/mol, respectively). The remaining derivatives, such as quercetin 3-O-arabinoside and quercetin 3-O-galactoside, also displayed moderate-to-high affinities ranging from -8.0 to -8.7 kcal/mol.

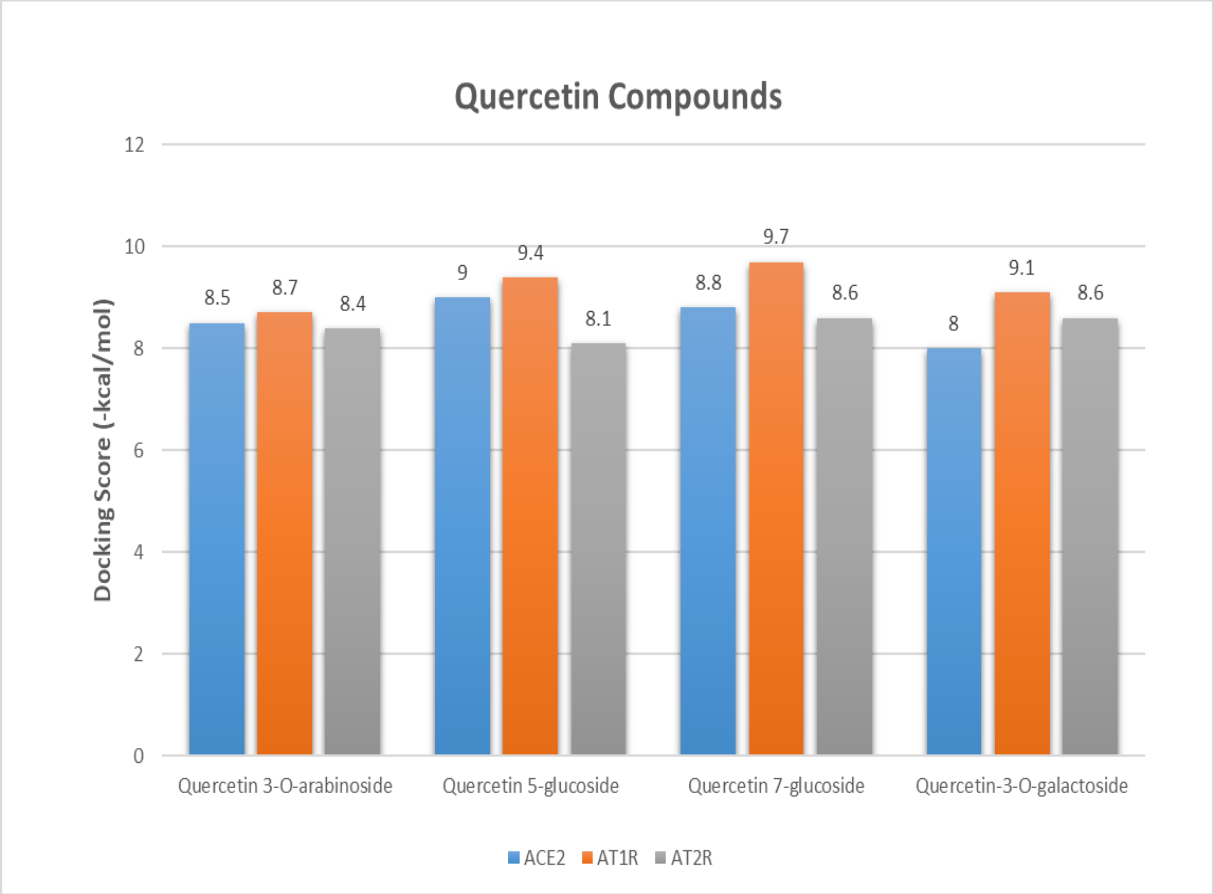

Fig. 3. Docking score between the test ligands and ACE2, AT1R, AT2R

Molecular interaction analysis revealed that (Fig. 4) quercetin 5-glucoside and quercetin 7-glucoside consistently interacted with key residues in the catalytic site of ACE2, including HIS374, GLU375, GLU402, and ASN290, which are known to play vital roles in substrate recognition and enzymatic function (Towler et al., 2004) (Table 2). However, based on the binding mode and absence of deep catalytic blockage, these interactions may result in modulatory effects rather than full inhibition (Pettersen, Goddard, Huang, Couch, Greenblatt, Meng, & Ferrin, 2004).

Fig. 4. Visualization of the molecular interactions of ACE2 with various ligands. (a) quercetin 3-O-arabinoside, (b) quercetin 5-glucoside, (c) quercetin 7-glucoside, (d) quercetin 3-O-galactoside

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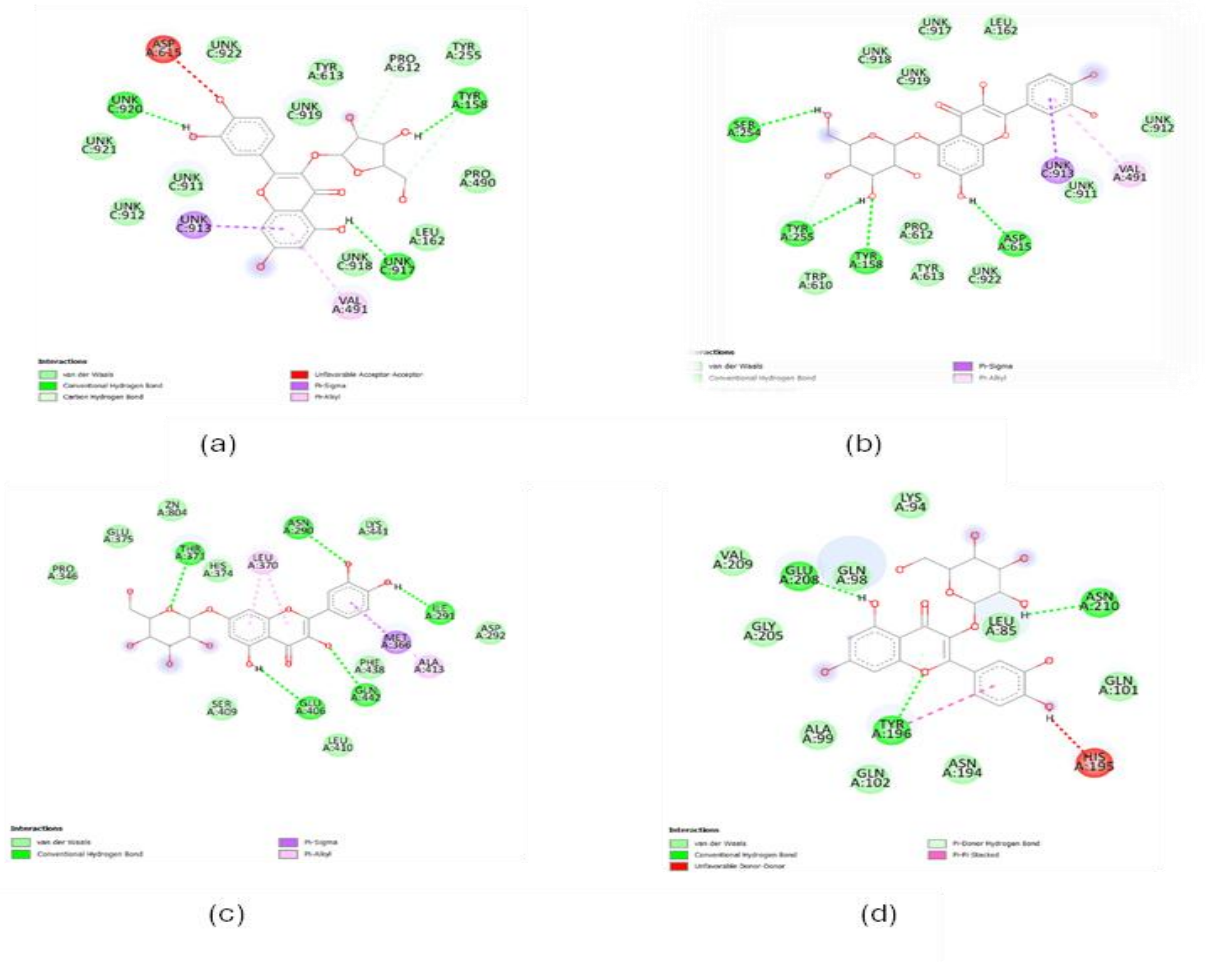
Table 2. Interaction profiles between ACE-2 and test ligands.



	Compounds	Hydrogen bonds	Hydrophobic interactions	Number of interactions
	Quercetin 3-O-arabinoside	Trp^{158}, Unk^{920}, Unk^{917}	Unk^{918}, Val^{491}, Tyr^{613}, Leu^{162}, Pro^{490}, Tyr^{255}, Pro^{612}, Unk^{919}, Unk^{922}, Unk^{921}, Unk^{911}, Unk^{912}, Unk^{913}	16
	Quercetin 5-glucoside	Ser^{254}, Tyr^{255}, Tyr^{158}, Asp^{615}	Trp^{610}, Pro^{612}, Tyr^{613}, Unk^{922}, Unk^{911}, Unk^{912}, Unk913, Val491, Leu162, Unk^{917}, Unk^{918}, Unk^{919}	16
	Quercetin 7-glucoside	Thr^{371}, Asn^{290}, Ile^{291}, Gln^{442}, Gln^{406}	Pro^{346}, Glu^{375}, Zn^{804}, His^{374}, Leu^{370}, Lys^{441}, Asp^{292}, Ala^{413}, Met^{366}, Phe^{438}, Leu^{410}, Ser^{409}	17
	Quercetin 3-O-galactoside	Glu^{208}, Asn^{210}, Tyr^{196}	Lys^{94}, Leu^{85}, Gln^{101}, Asn^{194}, Gln^{102}, Ala^{99}, Gyl^{205}, Val^{209}, Gln^{98}	12

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Conversely, both ligands showed robust interactions with AT1R active site residues, particularly ARG167, VAL108, TYR35, and TRP84, which are central to the orthosteric binding pocket of angiotensin II (Table 3 and Fig.5). These interactions suggest competitive inhibition potential of AT1R, potentially contributing to vasodilation and blood pressure reduction mechanisms, consistent with prior reports on flavonoid-AT1R interactions. Regarding AT2R (Table 4), binding profiles of the ligands showed lower binding depths compared to AT1R, further confirming the preservation of AT2R activity rather than antagonism. Ligands such as quercetin 3-O-arabinoside and quercetin 3-O-galactoside, while showing comparable scores (-8.4 and -8.6 kcal/mol, respectively), demonstrated fewer key residue interactions, reducing their therapeutic priority (Fig.6).

Taken together, quercetin 5-glucoside emerges as the most promising dual-acting ligand due to strong AT1R inhibition and ACE2/AT2R modulation without antagonism. Quercetin 7-glucoside follows closely with a similar favorable binding pattern (Towler, Staker, Prasad, Menon, Tang, Parsons, Ryan, Fisher, Williams, Dales, Patane, & Pantoliano, 2004).

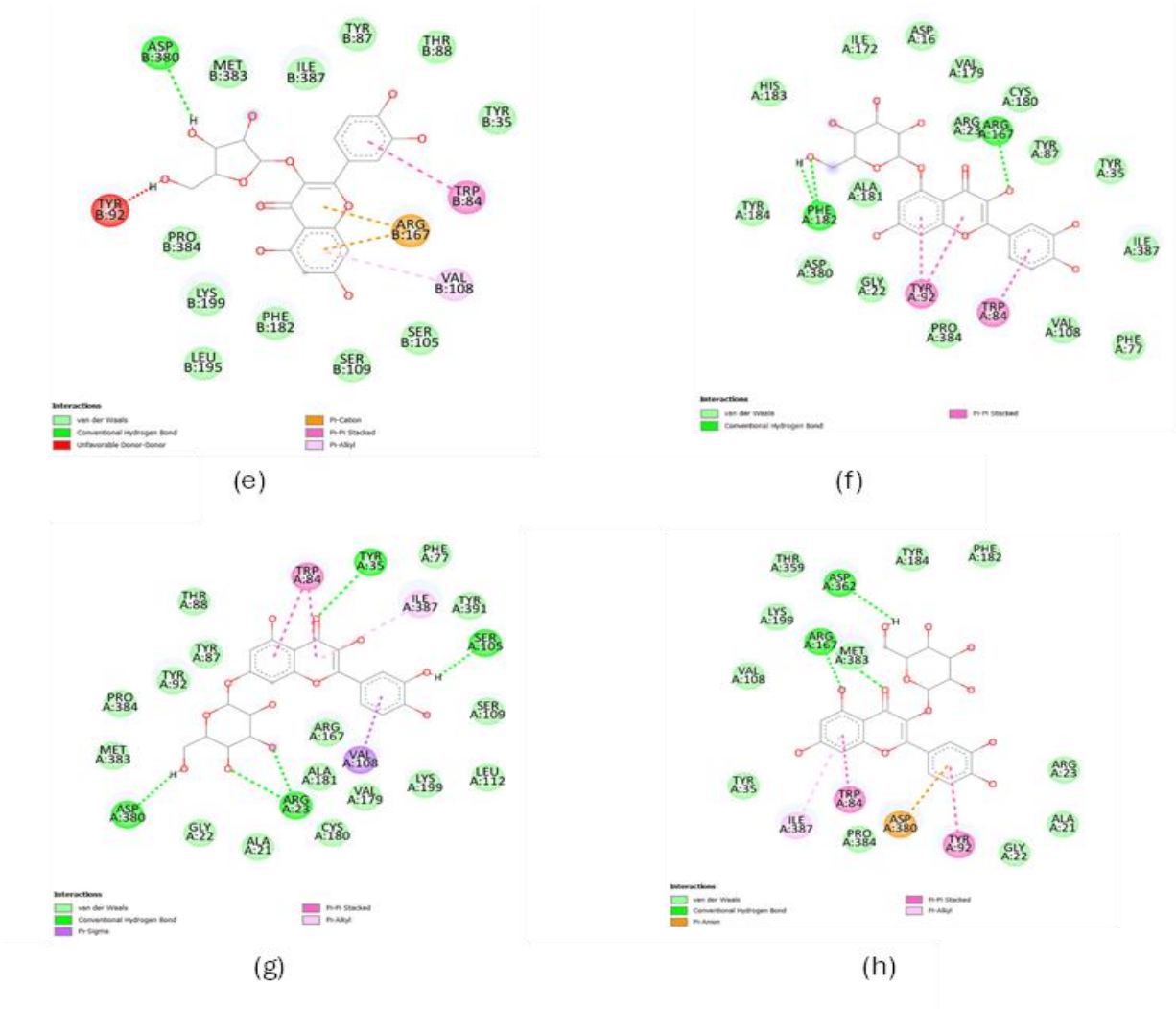

Fig. 5. Visualization of the molecular interactions of AT1R with various ligands. (e) quercetin 3-O-arabinoside, (f) quercetin 5-glucoside, (g) quercetin 7-glucoside, (h) quercetin 3-O-galactoside

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Table 3. Interaction profiles between AT1R and test ligands.

	Compounds	Hydrogen bonds	Hydrophobic interactions	Number of interactions
	Quercetin 3-O-arabinoside	Asp^{380}	Met^{383}, Ile^{387}, Tyr^{87}, Thr^{88}, Tyr^{35}, Trp^{84}, Arg^{167}, Val^{108}, Ser^{105}, Ser^{109}, Phe^{182}, Ley^{195}, Lys^{199}, Pro^{384},	15
	Quercetin 5-glucoside	Arg^{167}, Phe^{182}	His^{183}, Ile^{172}, Asp^{16}, Val^{179}, Arg^{23}, Cys^{180}, Tyr^{87}, Tyr^{35}, Ile^{387}, Phe^{77}, Val^{108}, Trp^{84}, Pro^{384}, Tyr^{92}, Gly^{22}, Asp^{380}, Tyr184, Ala^{181},	20
	Quercetin 7-glucoside	Tyr^{35},Ser^{105} Arg23, Asp^{380}	Trp^{84}, Phe^{77}, Ile^{387}, Tyr^{391}, Ser^{109}, Leu^{112}, Lys^{199}, Val^{179}, Cys^{180}, Ala^{181}, Arg^{167}, Ala^{21}, Gly^{22}, Met^{383}, Pro^{384}, Tyr^{92}, Tyr^{87}, Thr^{88}	22
	Quercetin 3-O-galactoside	Arg^{167}, Asp^{362}	Arg^{23}, Ala^{21}, Gly^{22}, Tyr^{92}, Asp^{380}, Pro^{384}, Trp^{84}, Ile^{387}, Tyr^{35}, Val^{108}, Lys^{199}, Met^{383}, Thr^{359}, Tyr^{184}, Phe^{182}	17

Table 4. Interaction profiles between AT2R and test ligands.

	Compounds	Hydrogen bonds	Hydrophobic interactions	Number of interactions
	Quercetin 3-O-arabinoside	Tyr^{189}, Ser^{1108},	Tyr^{108}, Gln^{37}, Lys^{38}, Ser^{36}, Leu^{190}, Gly^{1109}	8
	Quercetin 5-glucoside	Tyr^{108}	Asp^{297}, Leu^{190}	3
	Quercetin 7-glucoside	Arg^{182}	Tyr^{108}, Tyr^{103}, Ile^{196}	4
	Quercetin 3-O-galactoside	Tyr^{189}	Tyr^{108}, Gln^{37}, Lys^{38}, Leu^{190}, Ser^{36}, Asp^{297}, Gly^{1109}	8

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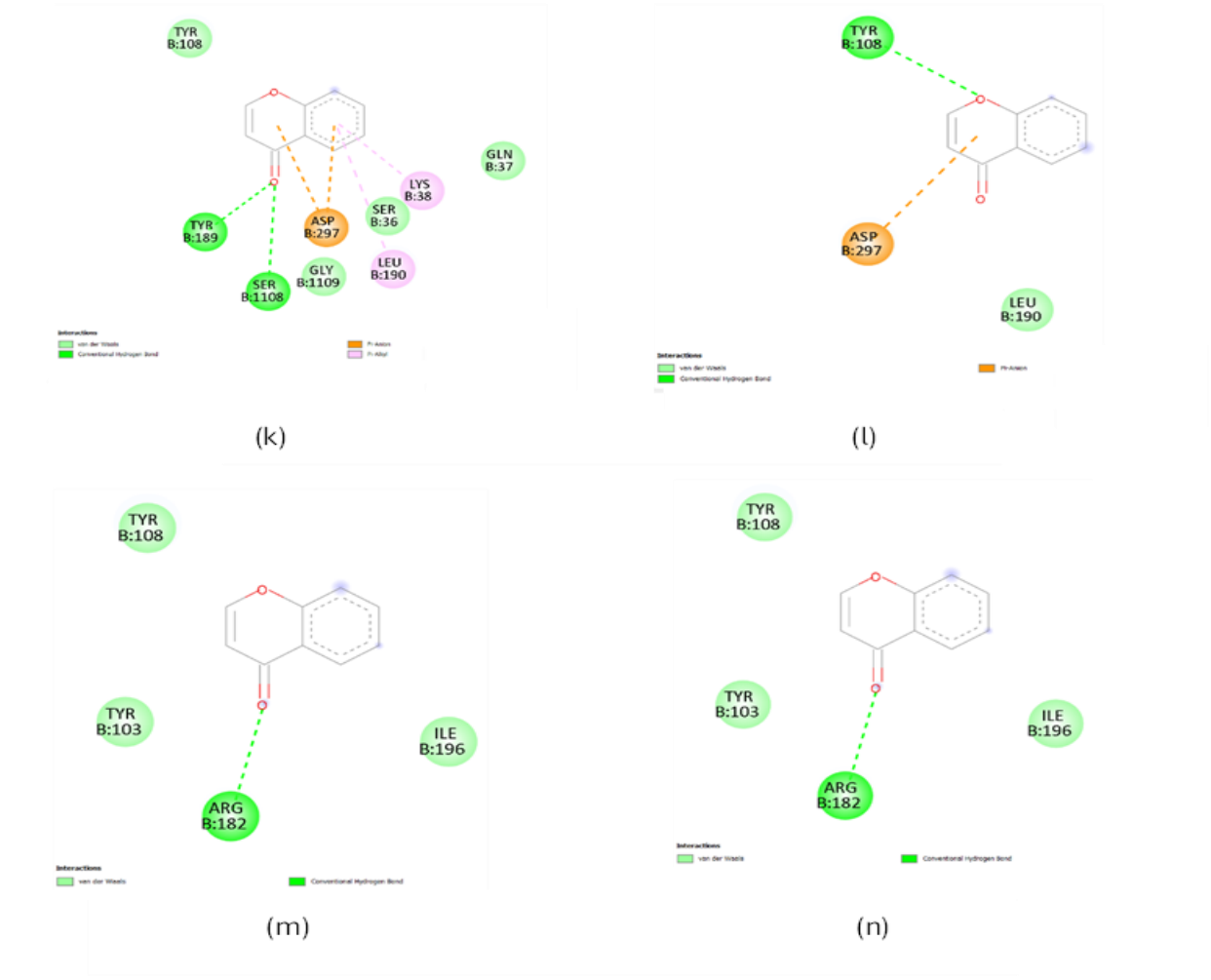

Fig. 6. Visualization of the molecular interactions of AT2R with various ligands. (k) quercetin 3-O-arabinoside, (l) quercetin 5-glucoside, (m) quercetin 7-glucoside, (n) quercetin 3-O-galactoside.

Discussion

The results of this docking investigation offer important new information about the therapeutic potential of quercetin glycoside derivatives in modifying thrombosis and hypertension by targeting RAAS components. For RAAS regulation, blocking AT1R while maintaining ACE2 and AT2R activity is the optimal pharmacological strategy. According to Santos et al. (2018), AT1R inhibition is a proven method of lowering hypertension and averting harmful cardiovascular effects associated with excessive angiotensin II signaling. According to the docking data, quercetin 5-glucoside and quercetin 7-glucoside interact with important active site residues like ARG167, VAL108, TYR35, and TRP84, making them the most potent AT1R inhibitors (Verdecchia, Cavallini, Spanevello, & Angeli, 2020).

In contrast, ACE2 and AT2R are critical for vasodilation and anti-thrombotic mechanisms (Gheblawi, Wang, Viveiros, Nguyen, Zhong, Turner, Raizada, Grant, & Oudit, 2020). While some quercetin glycosides exhibited high docking scores against ACE2, interaction mapping revealed that binding was largely to peripheral or semi-catalytic regions rather than to the enzymatic active site. This is an important finding, as the full inhibition of ACE2 could disrupt its protective functions, particularly in counteracting angiotensin II-driven vasoconstriction and thrombosis (Wang, Bodiga, Das, Lo, Patel, Oudit, 2012).

AT2R plays a protective role in vascular homeostasis, counterbalancing AT1R-induced effects (Carey, Wang, Siragy, 2017). The docking analysis confirms that quercetin derivatives, particularly quercetin 5-glucoside and 7-glucoside, interact favorably with AT2R without deep binding into the

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core active site. This suggests a modulatory role rather than antagonism, which aligns with the therapeutic goal of preserving AT2R function.

It's interesting to note that quercetin 3-O-arabinoside and quercetin 3-O-galactoside had similar binding scores but weaker interactions at important AT1R residues, suggesting a lesser inhibitory potential. As a result, these substances might not be as effective AT1R antagonists. These results provide compelling evidence for the choice of quercetin 5-glucoside as the most promising dual-function ligand, with quercetin 7-glucoside coming in second. By potently inhibiting AT1R while maintaining ACE2 and AT2R function, these drugs have a desired pharmacological profile that is in line with treatment approaches for hypertension and thrombotic risk reduction.

Conclusion

This molecular docking study provides a structural basis for the potential therapeutic effects of quercetin glycosides in RAAS modulation. Among the tested compounds:

1. Quercetin 5-glucoside demonstrated the strongest binding affinity to AT1R (-8.4 kcal/mol), while maintaining non-inhibitory interactions with ACE2 (-9.0 kcal/mol) and AT2R (-8.1 kcal/mol).
2. Quercetin 7-glucoside followed closely with high docking scores (-8.6 kcal/mol for AT1R, -8.8 kcal/mol for ACE2, and -8.6 kcal/mol for AT2R).
3. These two ligands emerged as the most promising candidates for selective AT1R inhibition while preserving ACE2 and AT2R functionality, contributing to antihypertensive and potential antithrombotic effects.
4. Quercetin 3-O-arabinoside and quercetin 3-O-galactoside showed moderate binding scores but had fewer interactions with AT1R, making them less ideal for targeted inhibition.
5. The study confirms that quercetin glycosides may serve as potential dual-targeting ligands that shift RAAS balance toward a vasodilatory and anti-thrombotic profile.

Future research should include in vitro and in vivo validation to confirm these molecular interactions and functional effects in biological systems.

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Application of Chemical Control in Corn Crops

Abstract

In Azerbaijan, corn is considered the most cultivated crop after winter cereals. Corn is widely used both as food and as animal feed in agriculture. In modern economy, the use of ecologically sound seeds plays a leading role and optimizes the cultivation process. The use of high-quality, certified seeds with low disease and high yield potential is considered an important production factor and is the main criterion for achieving high performance in agricultural enterprises. The Azerbaijani government aims to meet the country's need for agricultural products, especially rice, through domestic production, and thereby strives to become free from imports. As a cover crop, corn is a good predecessor that clears the soil of weeds for subsequent crops. Compared to other cereals, corn is less damaged by pests and does not fall asleep during harvest. However, various diseases and pests observed in corn crops lead to reduced yield. Among the most common diseases affecting corn in the country are helminthosporiosis, common smut, and loose smut.

Keywords: *corn, disease, common smut, loose smut, stalk*

Introduction

FAO, (2020) defines nutrition as one of the most important needs of humanity and as the consumption of sufficient amounts of nutrients necessary for long-term growth, development, healthy and sustainable life, and is becoming a problem with the increase in the world population. The fact that a large part of the world's population, which is increasing irreversibly, is struggling with severe hunger is discussed all over the world and solutions are proposed in each case (FAOSTAT, 2020).

Corn is a valuable crop that yields high grain and silage yields under good agrotechnical conditions. It yields even higher yields under irrigated conditions. In areas where there are no natural pastures, corn plays a key role in strengthening the feed base of livestock. Corn occupies a leading place among crops grown under irrigated conditions (Seyidaliyev, Gurbanov, Mammadova, 2013).

In our republic, this plant is sown on 100-110 thousand hectares for fodder purposes, and on 10-12 thousand hectares for grain purposes. In the Sheki-Zagatala zone of Azerbaijan, specialized in corn cultivation, under irrigation conditions, 80-90 tons of grain and more are obtained per hectare, and 800-1000 tons of silage and more are obtained from fodder crops (Ismayilov, Mammadov, 2012).

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Increasing the productivity of corn, which is used as a fodder and technical crop, is of great importance in the implementation of the program for the rapid development of agriculture (Gurbanov, 2017; Gurbanov, Ibrahimov, Huseynov, 2017; Mammadov, 2017)

Thanks to the phytochemical content of corn kernels, its health benefits have been the subject of many scientific studies (Hagiwara, Miyashita, Nakanishi, Sano, Tamano, Kadota, Koda, Nakamura, Imaida, Ito, Shirai, 2001). Due to the anthocyanin pigments in the composition of corn, colon cancer is prevented by corn; Breeding Techniques and Cultivation helps to reduce the risk, purple corn extract is rich in anthocyanin content, helps to improve diabetes complications, helps in the treatment of diabetes, obesity, and heart diseases, supports aging and various diseases thanks to its antioxidant activity was determined (Simla, Boontang, Harakotr, 2016).

Research

In the experimental fields of ADAU, we encountered common smut and loose smut diseases in the cultivated varieties “ADAU-80,” “Ganja,” and “Mahsuldar.” To combat these diseases, we applied Shansli EC at a rate of 0.75 L/ha by spraying, achieving high effectiveness. Additionally, we observed damage caused by the corn stalk borer, cotton bollworm, and winter cutworm. To control these pests, we applied Karate pesticide through spraying.

Corn Cultivation and Its Importance (Sadigov, 1974) corn is one of the main agricultural crops in the global farming system and is the second most cultivated crop in Azerbaijan after winter cereals.

Although corn is most widely grown in South America, its origin is believed to be Mexico. Due to its high demand for heat and moisture, it is primarily cultivated in Azerbaijan’s Sheki-Zagatala, Balakan, Gazakh, and Lankaran regions. Globally, 20% of corn production is used as food, 20% for industrial purposes, and 60% as livestock feed. This highlights its crucial role in livestock development (Gurbanov, 2017).

Given Azerbaijan’s favorable conditions for corn cultivation, it is possible to harvest crops twice a year. Corn is a nutritious food source, containing essential nutrients in its kernels, silk, and leaves. The corn stalk is rich in calcium (Ca), B vitamins, PP, E, A, and C vitamins, amino acids, sugars, and other beneficial compounds.

Diseases and Pests Affecting Corn Yield. Several diseases and pests significantly impact corn productivity. The most common diseases include:

• Leaf Spot Disease, is caused by the fungus Cochliobolus carbonum. It leads to spot formation on leaves, which eventually dry out. The pathogen overwinters in plant residues in the soil. When temperatures rise in spring, the overwintered spores reactivate, infecting the plant and damaging the leaves.

• Helminthosporiosis, is caused by the fungus Cochliobolus heterostrophus. This disease manifests as brown spots on the leaves, primarily damaging them. The fungus overwinters in plant residues in the soil and can sometimes spread through contaminated seeds (Jafarov, 2024).

• Common Smut and Loose Smut, which primarily affect corn ears.

• Common smut can also develop on the stems, causing them to break. The stem form of the disease is considered highly dangerous.

• Infected ears develop blister-like swellings, which initially appear firm and covered with a grayish-white layer. As the disease progresses, cracks form on the swellings, releasing chlamydospores in the form of dust. These spores spread to healthy plants and overwinter in plant residues, maintaining their viability for 7-8 years.

Common Smut and Loose Smut in Corn

• Common Smut Disease is caused by the fungi Ustilago zeae. These fungi do not infect the root system.

• This disease is more severe in dense plantings (Jafarov, 2024).

• Young corn seedlings are resistant to infection, but chlamydospores infect the plants when they develop 3-4 leaves.

• The ideal conditions for disease development are temperatures of 18-20°C and rainfall, which accelerates its spread.

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• In Azerbaijan, common smut is most prevalent in the Sheki-Zagatala and Quba-Khachmaz regions.

Loose Smut Disease

• Loose smut is one of the most widespread diseases in corn.
• Unlike common smut, it only affects the ears and tassels.
• Infected ears turn into black, oval, cone-shaped masses, while infected tassels blacken, wither, and fall off.
• The disease is caused by the fungus Sorosporium reilianium (Jafarov, 2001).
• Black powdery spores develop on the ears and tassels, which then disperse and infect healthy plants.
• Loose smut can reduce corn yield by up to 20%.
• Both diseases' pathogens overwinter in plant residues in the soil, enabling them to survive and spread in future growing seasons.

Disease Control Measures in Experimental Corn Fields. In the ADAU experimental nursery, we cultivated the corn varieties "ADAU-80," "Ganja," and "Mehsuldar". Despite treating the seeds with 75% Vitavax before sowing and strictly following all agrotechnical guidelines, we still observed common smut and loose smut infections in our corn fields. Since environmental conditions were favorable for disease development, the infection spread rapidly. To combat this, we treated our experimental field with the Shansli EC systemic fungicide. This fungicide has both curative and preventive effects, targeting multiple diseases.

For application, we prepared a solution of 75 ml of Shansli EC in 30 liters of water and sprayed it across the affected area. The results of this treatment are presented in the following table.

Table 1. Results of Fungicide Treatment in Corn Fields Application Details.

Fungicide Name	Application Rate	Crop	Disease	Application Time	Number of Application
Shansli	0.750L/ha	Corn	Common Smut	During Vegetation	1 time
			Loose Smut		

After spraying,we monitored the field every three days and observed that the disease progression had stopped. During the growing season, the pests of corn primarily damage the ears, which leads to a reduction in yield. Among these pests are the field moth, corn stem borer, cotton bollworm, rodents, and others that damage the corn plant (Khalilova, Ismayilzadeh 2016). The field moth (Loxostege sticticalis) produces 3–4 generations in Azerbaijan and is polyphagous, with the caterpillars of the third generation being the main culprits damaging the corn ears.

Table 2.

Crop	Disease	Fungicide Name	Infected Plants Treatment
Corn	Common Smut	Shansli	55
Corn	Loose Smut	Shansli	40

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The corn stem borer (Pyrausta nubilalis Hb.), as its name suggests, damages the stem. In Azerbaijan, it produces two generations, and the moths are active at night. The first generation of moths flies at the end of May and the beginning of June, after which they lay fertilized eggs on the lower part of the corn plant. The larvae that hatch feed on and damage the stem. The cotton bollworm (Helicoverpa armigera) is widely spread across all regions of Azerbaijan. It produces 3 to 4 generations and damages many plants. It primarily feeds on the ears of corn, causing harm. The autumn grain moth (Agrotis segetum Schiff.) is a dark brown-colored moth. The larvae that hatch from the eggs are grayish-brown in color and mostly damage the lower parts of corn plants, gnawing on the stems near the soil and the root collar, which harms the plant.

To combat these pests, all agro-technical measures must be followed. In autumn, deep plowing should be carried out because these pests overwinter in the soil on plant residues. Deep plowing helps destroy some of them. Before sowing in early spring, seeds should be treated with pesticides. During the vegetation period, if these pests are observed, spraying should be carried out using the following pesticides: Pharaoh (1.5 kg/ha), Resonance (1.5 kg/ha), Karate (0.2 kg/ha), or Desis (0.6 kg/ha). In our experimental field, we conducted spraying with Karate to combat these pests in corn plants. The results of the Karate treatment are shown in the table below

Table 3.

Pest name	Pesticide Name	Spraying Count	Number of Damaged Plant	5days after spraying	10 days after spraying
The corn stem borer	Karate	1 Time	38	3	-
The cotton bollworm	Karate	1 Time	75	6	-
The autumn grain moth	Karate	1 Time	112	28	2

This table shows the effectiveness of Karate treatment against different pests, with a noticeable reduction in the number of damaged plants over time. Let me know if you need any further refinements! As seen from the table, we applied Karate pesticide once, and the results are satisfactory.

Conclusion

Firstly agrotechnical measures should be implemented for combating all these diseases. Deep freezing of crop stubble should be carried out, crop rotation must be used, fields should be cleared of weeds, resistant varieties should be employed, and seeds should be treated before sowing. It is advisable to apply fungicides (such as Shansli EC) during the vegetation period in fields already infected.

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