Phyton-
International Journal of
Experimental Botany

Tech Science Press

http://doi.org/10.32604/phyton.2026.081637

ARTICLE

Exploring the Horticultural and Functional Diversity of Naturally Grown Sour Cherry Genotypes Coupled with Molecular Docking and DFT Analysis

Kerem Mertoğlu[1,*], Fatma Nur Senlik[1], İrem Yazıcı[2], Melekber Sülüşoğlu Durul[3], Levent Kırca[4], İbrahim Bulduk[5] and Erten Akbel[6]

[1]Department of Horticulture, Faculty of Agriculture, Usak University, Uşak, Türkiye
[2]Medical Promotion and Marketing Program, Pazaryeri Vocational School, Bilecik Seyh Edebali University, Bilecik, Türkiye
[3]Department of Horticulture, Faculty of Agriculture, Kocaeli University, İzmit, Kocaeli, Türkiye
[4]Department of Horticulture, Faculty of Agriculture, Pamukkale University, Denizli, Türkiye
[5]Department of Chemical Engineering, Afyon Kocatepe University, Afyon, Türkiye
[6]Department of Physiotherapy and Rehabilitation, Faculty of Health Sciences, Uşak University, Uşak, Türkiye
*Corresponding Author: Kerem Mertoğlu. Email: krmertoglum@gmail.com

Received: 06 March 2026; Accepted: 07 May 2026; Online first: 06 November 2026

ABSTRACT: This study evaluates 11 naturally grown sour cherry genotypes, focusing on their horticultural, functional, and antimicrobial properties, along with molecular docking (MD) and density functional theory (DFT) analyses. Genotypes showed significant diversity, with fruit weights ranging from 3.21 to 5.87 g and an average flesh-to-seed ratio of 90%, underlining their commercial and industrial potential. Biochemical analyses revealed rich bioactive profiles, including total phenolic (787.22–1898.10 mg GAE·kg^{-1}), flavonoid (564.73–947.11 mg QE·kg^{-1}), anthocyanin (75.74–204.08 mg cya-3-glu·kg^{-1}), and vitamin C (93.62–137.46 mg·kg^{-1}). These compounds contributed to strong antioxidant activity, with TEAC scavenging capacities ranging from 9.28 to 15.65 mmol Trolox·g^{-1}. Malic acid and *p*-coumaric acid emerged as the dominant organic acid and primary phenolic compound, respectively, with average concentrations of 1178.16 mg·100 g^{-1} and 28.80 mg·kg^{-1} across genotypes. Antimicrobial assays showed significant inhibition of bacteria and yeasts, with inhibition zones of up to 38.20 mm, surpassing standard antibiotics in certain cases. Molecular docking and DFT analyses revealed that key phenolic compounds such as *p*-coumaric and sinapic acids not only formed energetically favorable conformations but also exhibited strong binding affinities with essential bacterial enzymes, including DNA gyrase and dihydrofolate reductase, which are involved in DNA replication and folate metabolism, respectively. The inhibition of these critical enzymatic targets provides mechanistic insight into the antimicrobial potential of these compounds at both structural and electronic levels. Principal component analysis highlighted Genotype 8 for breeding due to its larger fruit size (4.99 g), while Genotype 10 was ideal for processing applications due to its higher acidity. These results demonstrate sour cherry's functional versatility and provide a scientific basis for breeding programs and health-focused industrial innovations.

KEYWORDS: DFT; antimicrobial activity; genetic diversity; molecular docking; selection; sour cherry

1 Introduction

Sour cherry is considered a species with relatively narrow genetic diversity, primarily due to its high self-fertility [1]. This limited variability poses significant challenges for breeding efforts aimed at improving agronomic traits and stress resilience. Furthermore, the impact of climate change is expected to constrain the cultivation range and genetic base of many crops, including sour cherry [2]. Consequently, targeted

Copyright © 2026 The Authors. Published by Tech Science Press. This work is licensed under a Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

breeding strategies have gained prominence, particularly those focused on developing genotypes that can withstand multiple environmental stresses while retaining high fruit quality [3]. A critical step in achieving such goals involves identifying parental genotypes with desirable attributes; however, the narrow genetic base of sour cherry complicates this selection, necessitating innovative strategies for expanding and utilizing available genetic resources [1].

Sour cherry is predominantly processed rather than consumed fresh, making it an important industrial fruit [4]. Its derivatives such as jam, compote, ice cream, liqueur, and juice are widely appreciated for their unique taste and versatility [5,6]. Notably, sour cherry juice is produced from high-quality fresh fruits, distinguishing it from many other fruit juices typically made from overripe or discarded fruits requiring preservatives and intensive processing [7]. These practices can negatively affect bioactive content, consumer preference, and product cost-efficiency [8,9].

Recognized as a functional food, sour cherry contains a rich diversity of bioactive compounds, including minerals, amino acids, vitamins, triterpenes, phytosterols, phenolics, and organic acids [10–13]. Its seeds are also valued for their unsaturated fatty acid and protein content [14]. Moreover, its capacity for phytoremediation makes it ecologically valuable, especially in mitigating pollution in industrialized environments [15,16]. Among its notable bioactives, phenolic compounds and anthocyanins possess strong antioxidant properties that reduce the risk of chronic diseases such as cancer and cardiovascular disorders [17–20], while also enhancing the plant's defense against environmental stresses [21,22]. With growing public awareness of nutritional health, consumer interest in foods rich in phytochemicals has increased significantly [23], pushing breeders to prioritize genotypes with superior phytochemical content [24,25].

Despite the documented health benefits of these compounds, their molecular mechanisms of action remain insufficiently characterized. This study addresses that gap by not only identifying the dominant bioactives in sour cherry but also evaluating their biofunctional potential through molecular docking (MD) and density functional theory (DFT) analyses.

MD is a computational tool used to explore interactions between bioactive ligands and protein targets based on binding affinity, steric complementarity, and molecular interactions such as hydrogen bonding and hydrophobic forces [26]. In plant systems, MD enables the prediction of how compounds like phenolics and flavonoids affect stress-related metabolic proteins, offering insight into both plant physiology and human health applications [27]. DFT complements this by offering accurate calculations of electronic structure, reactivity, and radical scavenging potential via HOMO-LUMO energy gaps and spin density distribution (SDD). DFT-based UV spectra also aid in interpreting light absorption features of phenolic acids [28,29].

Therefore, the main objectives of this work were (1) to determine and compare the basic horticultural and quality traits of 11 sour cherry genotypes that are naturally grown (2) to explore the interactions between the studied traits using correlation analysis to guide farming practices, (3) perform factor analysis to identify causes of variation for providing essential insights for breeding efforts, and (4) to analyze the protein interactions and chemical reactivity of key compounds in sour cherry, presenting as an initial study.

2 Materials and Methods

2.1 Plant Materials

The study was conducted with 11 (Genotype-1, Genotype-2, Genotype-3, Genotype-4, Genotype-5, Genotype-6, Genotype-7, Genotype-8, Genotype-9, Genotype-10, Genotype-11) self-grown sour cherry genotypes. For the preliminary selection, genotypes with dark fruit flesh color were preferred. The selection study was conducted in the districts of Merkez (37.74845776160336, 30.54576873779297) and Atabey (37.95053605143518, 30.64407250839912) in the province of Isparta, as well as in the districts of Odunpazarı

(39.74189134941596, 30.462180432781796) and Tepebaşı (39.804606505587394, 30.425631699790394) in the province of Eskişehir during 2022 and 2024. The geographic coordinates of each sampling site were recorded to enable spatial identification. Isparta is located in the northern part of Türkiye's Mediterranean Region and exhibits transitional characteristics between continental and Mediterranean climates. Eskişehir, situated in the northwestern part of the Central Anatolia Region, displays the distinct features of a continental climate (Fig. 1).

Figure 1: Selection areas of genotypes (yellow-marked).

Fruits were harvested at the stage of commercial ripeness by ensuring the uniform darkening of their upper color [27]. To ensure a representative sample, fruits were collected from all sides of the trees. Harvesting for all genotypes was conducted by the same person to maintain consistent maturity levels.

2.2 Determination of Pomological Characteristics, Soluble Solids, Titratable Acidity, and pH

Harvested fruit size was assessed using measurements of fruit, stalk, and stone weight (g), fruit length (mm), and equatorial diameter (mm). Fruit and stalk dimensions were measured with a digital Vernier caliper (VWR-6, Milan, Italy), whereas fruit and stone weights were determined using an electronic balance (CPA 16001S; Sartorius, Göttingen, Germany). Peel and flesh color were evaluated with a colorimeter (Minolta CR-400, Japan), and L*, C*, and h° values were recorded from two points, corresponding to the central and peripheral regions of each fruit [30]. For the determination of the flesh-to-peel ratio, fruits were cut into slices and the seeds were removed. Flesh and peel portions were then calculated relative to the total fruit weight, and the values were expressed as percentages (%) [13]. Juice samples were prepared by squeezing the fruits with a juice extractor (Arzum AR1060, Istanbul, Türkiye), followed by filtration through coarse filter paper. Soluble solid content (SSC) was measured in the filtered juice using a digital refractometer (Atago PR-32, Tokyo, Japan), and the results were expressed as percentages [10]. Juice pH was determined using a pH meter (Hach Co., Loveland, CO, USA) [31]. Titratable acidity (TA) was measured in the juice extract by titrating a mixture of 5 mL juice and 20 mL distilled water with 0.1 N NaOH until pH 8.1 was reached. The acidity values were calculated according to the equation reported by Korićanac et al. [32] and expressed as citric acid equivalent (%). Finally, the ripening index was calculated as the ratio of SSC to titratable acidity in the fruit juice [10].

2.3 Extraction Protocols for Spectrophotometric and HPLC Analysis

Fruit extracts were prepared by extracting 100 g of fruit material from each genotype with 200 mL of 80% acetone containing 0.2% formic acid. The mixture was homogenized for 2 min and subsequently centrifuged at 20,000× *g* for 20 min at 4°C. The obtained extracts were used for spectrophotometric analyses, except for vitamin C determination. For vitamin C analysis, fresh fruit samples were homogenized with a threefold volume of 3% metaphosphoric acid (w/v), filtered, and the clear filtrate was used for further analysis [33]. For organic acid determination, 100 g of fruit sample from each replicate was weighed and homogenized at medium speed for 5 min with 100 mL of deionized water. For ascorbic acid analysis, only metaphosphoric acid was used at a volume corresponding to three times the fresh weight of the sample. The homogenized mixtures were then shaken for 30 min, followed by centrifugation at 20,000× *g* for 20 min at 30°C. The supernatants were collected and passed through 0.45 µm membrane filters prior to analysis [34]. Phenolic compounds were extracted according to the procedure reported by Singh et al. [35], with minor modifications. Briefly, fresh fruit samples were homogenized, and 50 g of the homogenate was combined with 200 mL of 80% methanol (v/v) acidified with 0.1% hydrochloric acid to improve phenolic stability. The mixture was vortexed for 2 min and then shaken for 2 h at room temperature under dark conditions to promote efficient extraction. After extraction, the samples were centrifuged at 8000 rpm for 15 min at 4°C. The resulting supernatant was carefully separated and filtered through a 0.45 µm membrane filter before analysis.

2.4 Spectrophotometric Analysis

The total phenolic content (TPC) of sour cherry samples was quantified using the Folin–Ciocalteu assay [27]. Briefly, fruit extract, Folin–Ciocalteu reagent, and distilled water were mixed at a ratio of 1:1:18 (v/v/v). The reaction mixture was allowed to stand for 8 min, after which 7% sodium carbonate solution was added. Samples were then kept in the dark for 2 h to enable complete color development. The absorbance of the blue-colored reaction product was recorded at 725 nm with a spectrophotometer (Varian, Cary 100 Bio; Melbourne, Australia). TPC values were calculated from a gallic acid calibration curve and expressed as mg gallic acid equivalent (GAE) per kg fresh weight (fw).

Total flavonoid content (TFC) was determined by the aluminum chloride colorimetric assay [35]. In a 10 mL test tube, 50 µL of fruit extract was mixed with 950 µL of methanol and 4 mL of distilled water. Subsequently, 300 µL of 5% sodium nitrite solution was added, followed by 300 µL of 10% aluminum chloride solution. After the mixture was allowed to react for 5 min, 2 mL of 1 M sodium hydroxide solution was incorporated, and the final volume was brought to 10 mL with distilled water. Following incubation for 15 min, absorbance was measured at 510 nm. Flavonoid concentration was estimated using a quercetin standard curve and expressed as mg quercetin equivalent (QE) per liter of juice.

Antioxidant activities: The antioxidant activity was evaluated using the DPPH radical scavenging assay. Five different sample concentrations (10, 50, 100, 250, and 500 µg/mL) were tested, with three replicate measurements performed for each concentration. The 50% inhibition concentration (IC_{50}) was calculated from the dose-response curve constructed from these five concentration points per sample, with an R^2 value higher than 0.99. Samples with concentrations up to the IC_{50} value were further analyzed to assess their capacity to neutralize DPPH radicals, following the method outlined by Çolak et al. [36]. Ascorbic acid at 500 µg/mL was used as the reference standard. The antioxidant activity of the samples was calculated relative to this reference and expressed as % DPPH inhibition, with ascorbic acid representing 100% inhibition. The antioxidant capacity was also assessed using the ABTS+ (2,2′-Azino-bis(3-ethylbenzothiazoline-6-sulfonic acid)) method as outlined by Tavallali et al. [33]. The ABTS+ solution (7 mM) was diluted with phosphate-

buffered saline (PBS, pH 7.4) to obtain an absorbance value of 0.70 ± 0.02 at 734 nm. Fruit extracts were prepared by diluting 100 µL of the sample with 900 µL of distilled water. Aliquots of 5 µL, 10 µL, or 15 µL of the diluted extracts were then combined with 1 mL of ABTS+ solution in a cuvette. Absorbance readings at 734 nm were taken at the initial time point (0 min) and after 6 min using a Shimadzu UV-1800 spectrophotometer. A Trolox standard curve was constructed using five concentrations (100, 200, 400, 600, and 800 µmol·L^{-1}), and the regression equation y = 0.0012x + 0.0426 (R^2 = 0.99) was used to convert the absorbance values into Trolox equivalents, where y is the change in absorbance and x is the Trolox concentration. Results were expressed as Trolox Equivalent in mmol·g^{-1} of fw.

Vitamin C content: Vitamin C, expressed as L-ascorbic acid, was determined using a spectrophotometric procedure [33]. The assay was based on the reaction with 2,6-dichlorophenolindophenol (2,6-D), which served as the coloring reagent. A calibration curve was prepared using standard solutions containing oxalic acid, ascorbic acid, and 2,6-D. For sample preparation, 10 mL of fruit extract was diluted tenfold with oxalic acid. The diluted extract was then transferred into two separate tubes, with 1 mL of sample placed in each tube. The first tube received 9 mL of distilled water, whereas the second was mixed with 9 mL of 2,6-D solution. Absorbance measurements were performed at 518 nm using a spectrophotometer. The vitamin C concentration was calculated from the standard curve and reported as mg kg^{-1} fresh weight (fw).

Total monomeric anthocyanin content: Total monomeric anthocyanins (TMA) were quantified using the pH differential method [24], which relies on the pH-dependent structural changes of anthocyanin molecules. Each extract was diluted separately with two buffer solutions: potassium chloride buffer at pH 1.0 (0.025 M) and sodium acetate buffer at pH 4.5 (0.4 M). The absorbance of both buffered solutions was recorded at 520 and 700 nm. Anthocyanin content was calculated from the absorbance difference obtained between the two pH conditions, using the molar extinction coefficient of cyanidin-3-glucoside. The final values were expressed as mg cyanidin-3-glucoside equivalents (cya-3-glu) per kg fw.

2.5 Quantification of Organic Acids and Phenolic Compounds by HPLC-UV

Quantitative analysis of organic acids and phenolic constituents in sour cherry samples was carried out using an Agilent 1260 high-performance liquid chromatography (HPLC) system (Agilent Technologies, CA, USA), equipped with ChemStation software, a quaternary pump, an autosampler, and a UV detector. Separation of organic acids was achieved on an ACE-C18 column (4 × 150 mm, 5 µm; Hichrom Ltd., Theale, UK) under isocratic conditions. The mobile phase consisted of a 10 mM potassium phosphate buffer solution, adjusted to pH 2.2 using orthophosphoric acid. The flow rate was fixed at 1.0 mL min^{-1}, and samples were introduced into the system with an injection volume of 20 µL. Detection was performed at 245 nm for ascorbic acid and at 210 nm for the remaining organic acids. The obtained results were expressed as mg per 100 g fw [36].

For phenolic profiling, the same chromatographic column (ACE-C18, 5 µm, 4.6 × 150 mm) was employed under gradient elution. The mobile phase consisted of solvent A (ultrapure water containing 0.02% trifluoroacetic acid) and solvent B (methanol with 0.02% trifluoroacetic acid). The gradient program was applied as follows: initial 8% B, increasing to 10% at 3.25 min, 12% at 8 min, 25% at 15 min, 30% at 15.8 min, 90% at 25 min, and reaching 100% at 25.4 min. The column temperature was maintained at 25°C, and an injection volume of 10 µL was used. Detection wavelengths were selected according to the maximum absorbance of each compound: syringic, protocatechuic, and gallic acids at 280 nm; vanillic acid at 225 nm; p-coumaric acid at 305 nm; and caffeic and chlorogenic acids at 330 nm. Quantification was based on calibration curves generated from authentic standards. Final concentrations were reported as mg kg^{-1} fw, and representative chromatograms are provided in Figs. S1 and S2 [27].

2.6 Microorganisms, Microbial Cultures, and Antimicrobial Activities

The antimicrobial potential of sour cherry extracts was evaluated against Gram-positive bacteria *Staphylococcus aureus* (ATCC 29213) and *Enterococcus faecalis* (ATCC 29212), the Gram-negative bacterium *Escherichia coli* (ATCC 25922), and the yeast species *Candida albicans* (ATCC 14053) and *Candida parapsilosis* (ATCC 22019). Antimicrobial activity was determined using the agar well diffusion assay in triplicate. Microbial suspensions were standardized before inoculation to ensure consistent distribution across Müller–Hinton agar plates. Wells of 11 mm diameter were aseptically formed in the agar medium, and 100 µL of each extract was carefully dispensed into the wells. Following application, bacterial plates were incubated at 37°C for 24 h, whereas yeast cultures were maintained at 25°C for 48 h to allow adequate growth [37]. Antimicrobial activity was quantified by measuring the diameter of the inhibition zones surrounding each well in millimeters (mm). The results were compared with those obtained from standard antibacterial (vancomycin, cefepime, and levofloxacin) and the antifungal (fluconazole) agents, which were used as positive controls.

2.7 Computational Details for Molecular Docking and DFT

AutoDock Vina was utilized to investigate the interaction between the selected ligands (Citric acid–Compound CID: 311-, Malic acid–Compound CID: 525-, *p*-coumaric acid–Compound CID: 637542-, Sinapinic acid–Compound CID: 637775-) and their receptors (DNA Gyrase B (Topoisomerase II-4URM), Dihydrofolate reductase (6E4E), Gyrase B (4PRX), Rhomboid Protease (3ZMI), Sterol 14α-Demethylase (5TZ1) and Aspartic Proteinase Sapp2 (4YBF)). RCSB PDB and PubChem were used for receptor and ligand selection, respectively [38]. Vancomycin (Compound CID: 14969) and Fluconazole (Compound CID: 3365) were used as positive controls. The minimization process was performed, and the grid box dimensions adjusted. The control ligands' binding affinity was evaluated. The results were prepared using YASARA to display the bound ligands [38].

All calculations were performed with the DFT method on the B3LYP/6–311++G(d)(p) basis set in ethanol solvent using Gaussian16 and GaussView6.0.16. Theoretical UV–VIS excitation energies for the first singlet states were calculated using the TD-SCF and TD-DFT/CAMB3LYP/6–311++G(d)(p) theoretical methods [39].

2.8 Statistical Analysis

This study was carried out using a randomized plot experimental design. Pomological traits were measured from 25 fruits collected from each of the four sides of the plants, resulting in a total of 100 fruits per genotype, while spectrophotometric, chromatographic, and antimicrobial analyses were performed in triplicate. Differences in these traits among the genotypes were analyzed using one-way ANOVA in Minitab (Version 17, Minitab Inc., State College, PA, USA). To compare genotypes, Tukey's HSD multiple comparison test was applied. Normality and homogeneity of variance were assessed using the Smirnov ($p > 0.05$) and Levene ($p > 0.05$) tests, respectively. Correlation analysis was conducted to determine relations among the traits using Pearson correlation coefficients. Principal component analysis (PCA) was utilized to explore the interconnections among the variables, identifying similarities and variations in the traits. Scatter plots were created using the first two principal components (PC1 and PC2) in R (v. 4.0.3) [40].

3 Results and Discussion

The results of the physicochemical characteristics belonging to sour cherry genotypes are detailed in Table 1. The fruit width, length, and weight of the genotypes varied within ranges of 14.77–21.09 mm,

12.13–18.46 mm, and 1.95–4.99 g, respectively, while the stalk length and width ranged between 36.78–64.31 mm and 0.82–1.10 mm. Among these traits, the coefficient of variation for fruit weight (29.71%) was notably higher compared to fruit width (12.71%) and fruit length (14.92%). This discrepancy is likely attributable to the cordate shape of cherries [41], which results in greater variability in weight compared to dimensions. Selection studies conducted in regions with diverse ecological characteristics have similarly reported a broad range of variation in sour cherry genotypes, with fruit width, length, weight, seed weight, stalk length, and stalk width ranged between 12.56–25.44 mm, 11.17–28.45 mm, 1.36–8.14 g, 0.15–0.61 g, 25.75–54.48 mm, and 0.77–1.96 mm, respectively [30,32,41–44]. The current study's findings align well with these reports, highlighting the reliability of the observed data. Stone weight was consistently measured at relatively low levels (0.18–0.35 g) compared to the whole fruit. The flesh-to-seed ratio is a critical parameter for assessing consumer appeal and industrial usability, as a higher ratio signifies a greater proportion of edible parts, enhancing its market value. In this study, the average flesh-to-seed ratio across genotypes was approximately 90%, closely in agreement with previously reported values from Lithuanian (92.50%) and Iranian (88.81%) sour cherry germplasm [31,45]. Notably, the high flesh-to-seed ratio exhibited low variability across all genotypes (Table 1), combined with the favorable size and weight traits, underscores the commercial potential of sour cherries for diverse uses, including fresh market sales, juicing, and other value-added processed products.

The coloration of cherries is largely determined by their phenolic compounds, particularly the total and type of anthocyanins [46]. The distribution and concentration of anthocyanins vary not only between different cultivars/genotypes but also between the skin and flesh of the fruit. Typically, the pigment concentration is higher in the skin compared to the flesh [47]. The findings of this study align with this perspective, as sour cherry was found to exhibit high anthocyanin content in both the peel (20.00) and flesh (18.46), as indicated by the a* values. In red-toned fruits like sour cherry, the low L* (peel: 16.77, flesh: 27.73) and b* (peel: 6.27, flesh: 2.02) values reflect the dominance of anthocyanins and the minimal presence of carotenoids, which are key factors defining the fruit's color profile [48,49].

Crops' flavor at maturity is predominantly determined by soluble solid content and acidity, which are critical factors influencing consumer preferences in cherries [50]. Higher Brix offers a significant advantage in processing, especially in the production of sour cherry juice concentrate. Thus, genotypes with elevated soluble solid content as the raw material reduce processing time and energy consumption, leading to lower production costs and greater efficiency [51]. Moreover, organic acids play a vital role in preserving the stability of processed products by suppressing microbial growth and preventing spoilage [52]. As a result, the accumulation and conservation of these molecules are essential for maintaining product integrity, yield, and market value. Assessment of these metrics including SSC (mean: 19.82%, CV: 4.63%), TA (mean: 1.95%, CV: 8.06%), and RI (mean: 10.24, CV: 8.65%) reveals that sour cherries exhibit low variation in these traits, reflecting a consistent and balanced chemical profile in line with Koricanac et al. [32] and Najafzadeh et al. [44]. The harmonious balance of sweetness and tartness is a defining feature of sour cherries, offering a unique and highly appealing flavor profile. This synergy not only distinguishes sour cherries in the market but also solidifies their role as a preferred choice among consumers, aligning with both sensory expectations and functional requirements in food applications.

Previously, researchers have consistently highlighted the significant levels of biochemicals with antioxidant effects found in different organs of the sour cherry, including fruits, leaves, and seeds [12–14,53]. Due to their rich and diverse biochemical composition, different parts of sour cherry are widely utilized for product enhancement in the food industry [4,54]. Moreover, the abundance of these antioxidant compounds has made sour cherry a focal point in numerous medical and cosmetic studies, facilitating the development

of functional products with added health benefits [55]. The findings of this study align with the current literature, demonstrating high phenolic content and strong antioxidant activities in sour cherries. Significant statistical differences were identified among genotypes in TPC, TFC, and TMA. Average values were measured respectively as 1102.62 mg GAE·kg^{-1} fw, 732.45 mg QE·kg^{-1} fw, and 134.11 mg cya-3-glu·kg^{-1} fw (Table 1). The variation coefficient for TPC (CV: 28.92%) was particularly notable, underscoring the genetic diversity and potential for selecting superior genotypes with enhanced bioactive properties. In addition, substantial vitamin C content (115.39 mg·kg^{-1} fw) reinforces the nutritional value of sour cherry as a significant natural source of essential nutrients. Elevated concentrations of bioactive compounds played a pivotal role in enhancing the antioxidant activity. Both DPPH (mean: 73.58%) and TEAC (mean: 12.19 mmol Trolox·g^{-1} fw) assays demonstrated robust antioxidant potential, highlighting sour cherry as an excellent candidate for use in health-focused food products and innovative industrial formulations.

Table 1: Phenotypic diversity of sour cherry Genotypes regarding the investigated characteristics.

Variable	Abbreviation	Unit	Min.	Max.	Mean	±SD	CV (%)
Fruit Weight	FWe	g	1.95	4.99	3.60*	1.07	29.71
Fruit Width	FWi	mm	14.77	21.09	17.93*	2.28	12.71
Fruit Length	FL	mm	12.13	18.46	15.64*	2.33	14.92
Stalk Length	SL	mm	36.78	64.31	52.32*	9.22	17.61
Stalk Width	SWi	mm	0.82	1.10	0.92*	0.10	10.83
Pulp/Stone	P/S	%	86.60	92.00	89.35^{NS}	1.62	1.81
Stone Weight	SWe	g	0.18	0.35	0.27*	0.06	23.45
Flesh L*	FL*	-	26.84	28.56	27.73^{NS}	0.68	2.47
Flesh a*	Fa*	-	13.24	22.35	18.46*	3.29	17.81
Flesh b*	Fb*	-	0.53	3.26	2.02*	0.90	44.58
Peel L*	PL*	-	12.95	21.91	16.77*	2.25	13.44
Peel a*	Pa*	-	16.27	26.23	20.00*	2.93	14.65
Peel b*	Pb*	-	2.83	9.65	6.27*	1.92	30.59
SSC	SSC	%	18.60	21.70	19.82^{NS}	0.92	4.63
TA	TA	%	1.67	2.26	1.95*	0.16	8.06
Ripening Index	RI	-	8.76	11.90	10.24*	0.89	8.65
pH	pH	-	2.90	3.25	3.03^{NS}	0.09	3.11
Anthocyanin	TMA	Mg cya-3-glu·kg^{-1} fw	75.74	204.08	134.11*	38.28	28.55
Total Flavonoids	TFC	mg QE·kg^{-1} fw	564.73	947.11	732.45*	122.26	16.69
Total Phenolics	TPC	mg GAE·kg^{-1} fw	787.22	1898.10	1102.62*	318.84	28.92
Vitamin C	VitC	mg·kg^{-1} fw	93.62	137.46	115.39*	13.92	12.06
Antioxidant Activity	TEAC	mmol Trolox·g^{-1} fw	9.28	15.65	12.19*	1.88	15.46
Antioxidant Activity	DPPH	%	68.26	80.13	73.58^{NS}	3.88	5.28
Malic Acid	MA	mg·100 g^{-1} fw	861.40	1486.90	1178.16*	222.46	18.88
Oxalic Acid	OA	mg·100 g^{-1} fw	2.60	5.60	3.67*	0.97	26.51
Citric Acid	CiA	mg·100 g^{-1} fw	40.00	88.00	63.91*	16.13	25.23
Ascorbic Acid	AA	mg·100g^{-1} fw	2.90	6.90	4.62*	1.29	27.83
Chlorogenic Acid	ChlA	mg·kg^{-1} fw	7.60	9.40	8.51^{NS}	0.54	6.29
Vanilic Acid	VA	mg·kg^{-1} fw	16.30	22.60	18.77*	1.78	9.48
Syringic Acid	SA	mg·kg^{-1} fw	12.90	19.00	14.87*	1.76	11.82
Caffeic Acid	CA	mg·kg^{-1} fw	14.70	28.50	23.24*	4.64	19.98
p-coumaric Acid	*p*-CA	mg·kg^{-1} fw	24.70	34.40	28.80*	3.18	11.05
Ferrulic Acid	FA	mg·kg^{-1} fw	4.00	8.20	5.32*	1.14	21.40
Sinapinic Acid	SiA	mg·kg^{-1} fw	15.90	41.60	25.25*	8.56	33.88
Ellagic Acid	EA	mg·kg^{-1} fw	8.40	10.10	9.27^{NS}	0.53	5.75
Quercetin	Que	mg·kg^{-1} fw	1.30	3.20	1.87*	0.53	28.57

* indicates significant differences among genotypes at $p < 0.05$; NS indicates non-significant differences.

Genotype acted as the dominant factor in determining the main traits, strongly supported by previous research [27,44]. Results of the current study demonstrate a high level of consistency with prior investigations, further reinforcing the validity and reliability of the results [10–13,32,53]. The observed variations across traits can be attributed to a complex interplay of factors, including the discrepancies in cultural treatments, analytical methods, ecological and geographical conditions of the selection/cultivation region, variations in harvesting practices and timing, differences in post-harvest storage and processing, etc. [7,9,46,48,56,57].

Examining organic acids and phenolics provides valuable information about the chemical profile of sour cherry genotypes, and all the organic acids investigated were found statistically significant among genotypes (Table 1). In agreement with previous findings by Sokół-Łętowska et al. [12] and Najafzadeh et al. [44], malic acid was identified as the dominant organic acid in cherries. The distribution of organic acids persisted consistently across all genotypes, with malic acid being the most abundant (1178.16 mg·100 g^{-1} fw), followed by citric acid (63.91 mg·100 g^{-1} fw), ascorbic acid (4.62 mg·100 g^{-1} fw), and oxalic acid (3.67 mg·100 g^{-1} fw). Organic acids significantly influence the sensory properties of cherries, particularly taste, which is a critical aspect of consumer preference. Their breakdown is strongly associated with the diminishment of flavor, as noted by Zhang et al. [58]. Beyond enhancing taste, organic acids contribute to preserving fruit quality by maintaining a low pH, which suppresses the growth of spoilage microorganisms [52]. Consequently, sustaining adequate levels of organic acids is essential for maintaining both the flavor and overall quality of cherries.

Although a consistent ranking of phenolic components could not be established, sour cherry genotypes exhibit diverse phenolic compositions (Table 1). The majority of phenolic cycles in fruits are formed by chlorogenic acid. Chlorogenic acid gives rise to more than forty phenolic compounds, a number that is notably higher than that of other phenolic compounds in cherries [59]. In the study, chlorogenic acid was detected at similar levels (7.60–9.40 mg·kg^{-1} fw) across all genotypes, with a low coefficient of variation (CV: 6.29%), while quercetin, known for its anti-inflammatory effects, was measured at lower levels (1.30–3.20 mg·kg^{-1} fw). Phenolic compounds are essential for enhancing antioxidant activity, contributing to stress resistance, influencing color, flavor, and shelf life by participating in various physiological processes [27,48]. Based on their average concentrations, the rest phenolics contributing to these properties were ranked in the following order: *p*-coumaric acid (28.80 mg·kg^{-1} fw) > sinapinic acid (25.25 mg·kg^{-1} fw) > caffeic acid (23.24 mg·kg^{-1} fw) > vanillic acid (18.77 mg·kg^{-1} fw) > syringic acid (14.87 mg·kg^{-1} fw) > ellagic acid (9.27 mg·kg^{-1} fw) > ferulic acid (5.32 mg·kg^{-1} fw) and results are comparable reported by [11,17,37].

The antimicrobial activity of sour cherry genotypes against various bacterial strains and yeasts is summarized in Table 2. The results emphasize the potent antimicrobial properties of sour cherry, with significant differences observed between genotypes in their ability to inhibit microbial growth. Among the antibiotics tested as controls, vancomycin was the most effective across all bacterial strains. However, certain genotypes exhibited greater efficacy compared to vancomycin against specific microorganisms. For instance, Genotype 10 (34.50 mm) demonstrated superior activity against *Enterococcus faecalis*, while Genotype 1 (33.60 mm), Genotype 4 (38.20 mm), and Genotype 8 (37.50 mm) outperformed vancomycin against *Staphylococcus aureus.* Additionally, Genotype 7 (14.90 mm) showed enhanced activity against *Escherichia coli* in comparison to vancomycin. Similarly, some genotypes displayed significant antifungal activity. Genotype 5 (14.40 mm) and Genotype 6 (14.30 mm) exhibited antifungal activity against *Candida albicans*, showing comparable results to the reference fungicide used in the study. Furthermore, Genotype 3 (14.40 mm), Genotype 6 (14.40 mm), Genotype 7 (14.40 mm), Genotype 9 (14.40 mm), and Genotype 11 (14.40 mm) demonstrated equivalent effectiveness against *Candida parapsilosis* as the tested fungicide.

These findings suggest that sour cherry genotypes possess significant antimicrobial potential against a wide range of microorganisms, with certain genotypes showing particularly strong activity against both bacterial and fungal pathogens. It is scientifically established how different sour cherries exhibit antimicrobial effects to varying degrees [60–62]. This activity is attributed to their rich and diverse bioactive compounds, as well as their low pH levels, which inhibit microbial growth. Additionally, these compounds are reported to cause protein denaturation, disruption of DNA synthesis, prevention of biofilm formation, impairment of cell membrane integrity, and interference with energy metabolism [63,64]. The results suggest sour cherry additives could be a significant alternative for combating microorganism-induced spoilage in foods.

Table 2: Anti-microbial activities of sour cherry genotypes on chosen bacteria and yeasts (mm).

	Enterococcus faecalis*	***Staphylococcus aureus****	***Escherichia coli****	***Candida albicans****	***Candida parapsilosis****
Genotype-1	6.60	33.60	9.20	12.60	7.90
Genotype-2	13.90	13.50	7.20	8.30	6.60
Genotype-3	14.10	6.70	6.30	6.80	9.30
Genotype-4	28.20	38.20	ineffective	7.80	8.20
Genotype-5	7.10	7.40	ineffective	14.40	7.90
Genotype-6	10.50	12.80	8.80	14.30	9.60
Genotype-7	22.60	9.90	14.90	12.50	8.80
Genotype-8	7.20	37.50	6.90	13.00	8.10
Genotype-9	11.90	11.80	5.90	12.90	14.80
Genotype-10	34.50	8.30	8.60	8.80	5.80
Genotype-11	14.80	7.50	9.30	7.20	9.40
Vancomycin	30.80	32.90	14.10	-	-
Cefepime	13.70	12.90	12.60	-	-
Levofloxacin	28.80	14.70	13.90	-	-
Fluconazole	-	-	-	14.40	8.40

* indicates significant differences among genotypes at $p < 0.05$, while ineffective means no inhibition zone was observed (0 mm) under the tested conditions.

Analyzing the relations among different traits is vital in minimizing the time and cost associated with cultivation and breeding efforts. The correlation coefficients observed among the examined traits are illustrated in Fig. 2. Fruit width and fruit length exhibited a very strong positive correlation (0.97). Following fertilization, cell division occurs initially in fruits, followed by cell expansion [65]. The simultaneous transverse and longitudinal growth of cells during the expansion phase accounts for the close relation between these traits. The enlargement of cells that make up the fruit contributes to an increase in fruit weight. Accordingly, significant positive correlations were observed between fruit weight and fruit width (0.95) and fruit length (0.98). Literature supports our findings, confirming robust and affirmative correlations among fruit weight and size [65,66].

The acidic environment in fruits not only limits the activity of microbes that cause spoilage but also allows for higher levels of accumulation of phenolic compounds with antioxidant effects [34,67]. The main contributors to creating an acidic environment, organic acids and titratable acidity, have generally positive relations with DPPH and TEAC, while these traits were discovered to be inversely correlated with pH and microorganism growth (Fig. 2). As expected, rising amounts of individual phenolics that are respected for their antioxidant effect increased the TPC, TFC, and contributed to antioxidant activity (Fig. 2) previously confirmed by Lachowicz et al. [47] and Kurnaz et al. [68] as well.

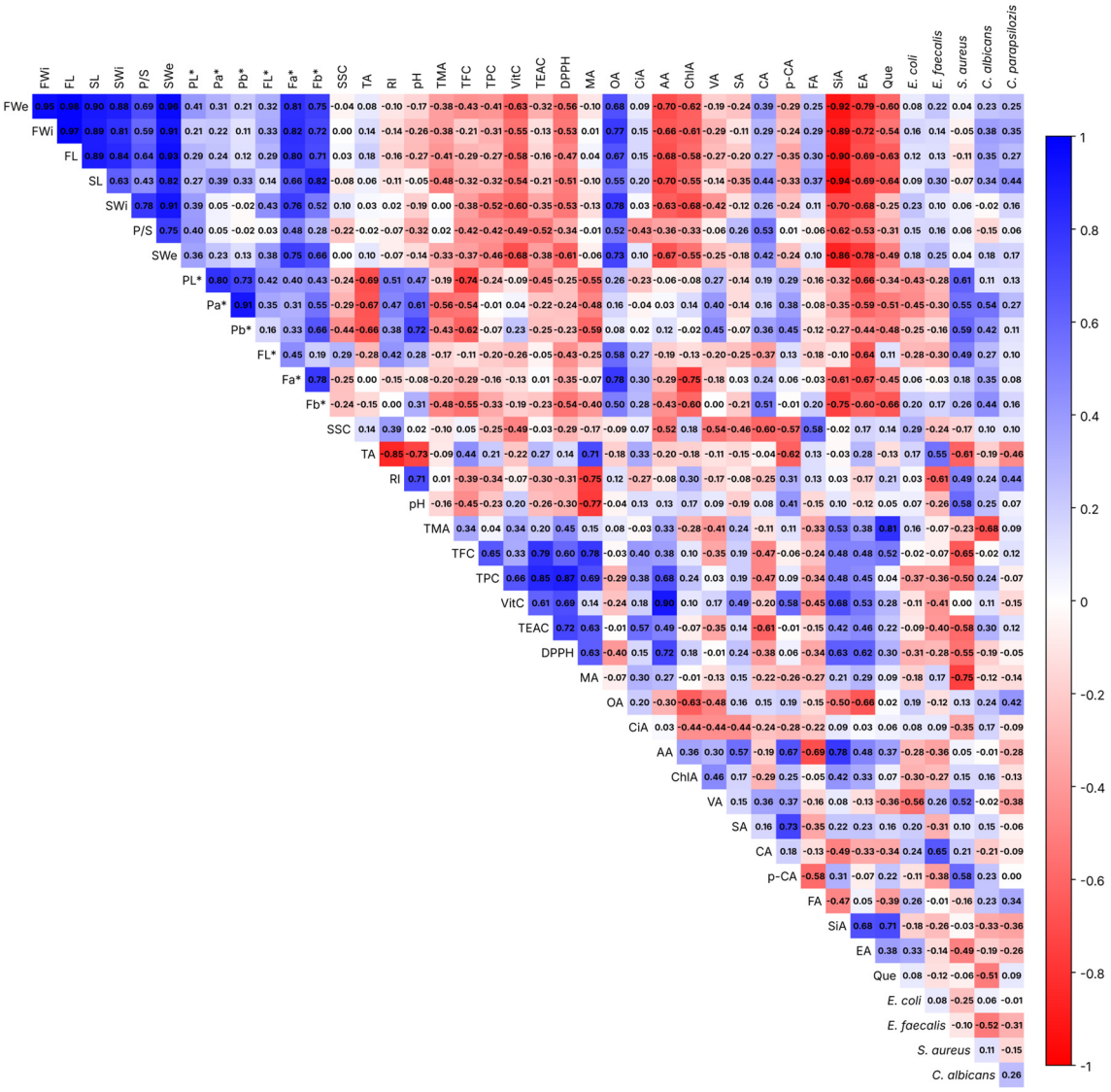

Figure 2: Visualization of characteristic correlations and strengths (Larger, darker circles represent stronger correlations. Blue denotes positive correlations, while red highlights negative correlations. Look at Table 1 for abbreviations).

PCA was conducted to examine the distribution patterns of traits associated with various genotypes, as depicted in Fig. 3. This technique has been extensively employed in selection studies for horticultural crops such as loquats [68], strawberries [69], and cherries [1,30,59]. In this study, the first two principal components explained 50.68% of the total variation, with PC1 contributing 32.58% and PC2 accounting for 18.10%. Furthermore, detailed information has been presented in Fig. S3 regarding which traits exhibit a strong relationship with which components. The placement of genotypes across distinct planes underscores the potential for sour cherry genotypes to be utilized in diverse applications, including breeding, processing, or fresh consumption. This highlights the critical importance of selecting the appropriate genotypes to achieve specific targeted outcomes.

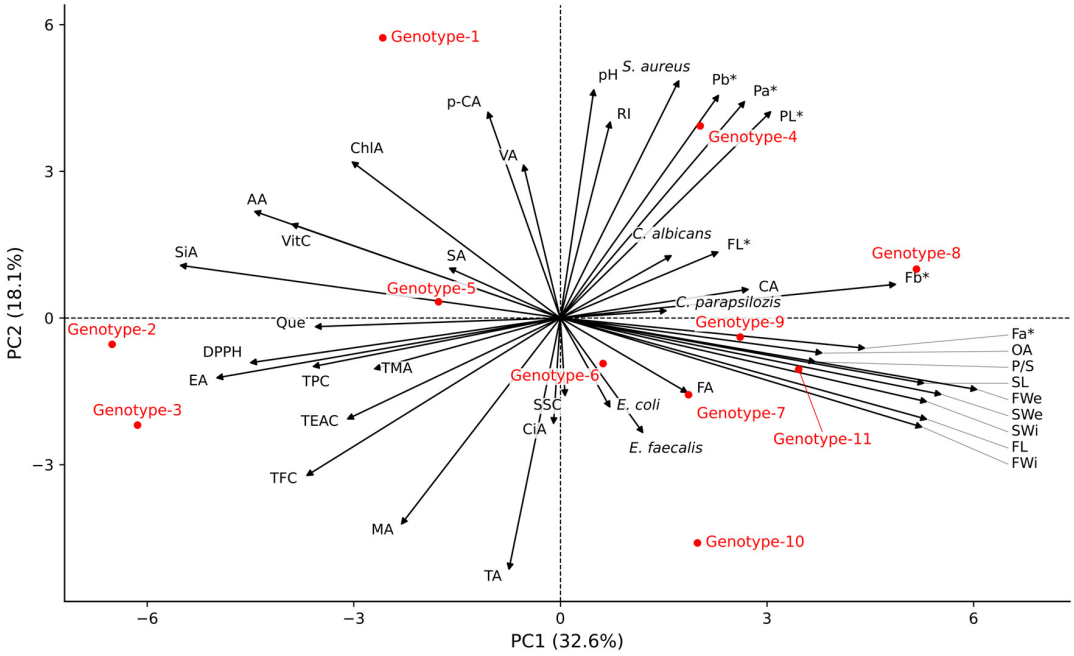

Figure 3: Bi-plot distribution of characteristics according to genotypes.

Genotype 8 came to the fore with its large fruit size (Fig. 3 and Table S1), making it suitable as a parental variety in breeding programs to develop new genotypes with larger fruits. For many fruit species, including cherries, the combination of large fruit size and a high ratio of soluble solid content to titratable acidity is a primary breeding goal [70,71]. Similarly, Genotypes 2, 3, and 5 demonstrated potential for enhancing phytochemical content with antioxidant properties in future breeding efforts. These genotypes are also suitable for fresh consumption due to their high levels of antioxidant activity, as indicated by Table S1. Given its high flavonoid content, Genotype 3 holds additional promise for wine production. Flavonoids contribute to the astringent and bitter flavors desired in wine, offering unique sensory characteristics [72]. On the other hand, Genotype 10 was identified as particularly suitable for industrial processing due to its high acidity (Table S2). Organic acids are essential in maintaining product stability by inhibiting microbial activity, which helps reduce spoilage and extends product shelf life [67]. Furthermore, studies on both major and minor fruit species have demonstrated that high organic acid content and low pH are critical factors for improving antioxidant activity and ensuring long-term product preservation [27,67]. The ability to tailor genotypes for specific purposes, such as breeding programs, fresh consumption, wine-making, or industrial processing, demonstrates the versatility and value of selection studies. By identifying genotypes with desirable traits, immediate cultivation and targeted crop production can be achieved, providing opportunities to address market demands and expand agricultural production.

Binding affinities measure the strength of ligand interactions with target proteins, with more negative values indicating stronger binding [26,27,36]. The binding interactions of the major compounds with target proteins are summarized in Table S3. Among the ligands analyzed, *p*-coumaric acid exhibited the highest binding energy to the *Staphylococcus aureus* gyrase enzyme (4URM) at −6.9 kcal·mol^{-1}, whereas sinapinic acid showed the strongest binding to the *Escherichia coli* gyrase enzyme (4PRX) with an energy of −6.7 kcal·mol^{-1}. As illustrated in Fig. 4B,C, these compounds act by binding to the active sites of the 4URM and 4PRX proteins, effectively disrupting DNA synthesis and cell division, thereby exhibiting notable antibacterial effects. In addition to its activity against gyrase enzymes, sinapinic acid also demonstrated

high binding affinity for the *Staphylococcus aureus* dihydrofolate reductase enzyme (6E4E), with a binding energy of −7.2 kcal·mol^{-1}. This interaction significantly inhibits folate metabolism, an essential pathway for bacterial growth and survival, and prevents the synthesis of nucleic acids, as visualized in Fig. 4D. Such potent inhibition underscores the broad-spectrum antibacterial potential of sinapinic acid. For *Escherichia coli*, citric acid demonstrated the most effective antibacterial activity via its interaction with the Rhomboid protease enzyme (3ZMI), showing a binding energy of −7.2 kcal·mol^{-1}. This inhibition likely interferes with the protease's ability to process substrates, leading to disruption of proteolytic activity, cellular signaling pathways, and bacterial membrane stability. Consequently, this results in bacterial growth arrest, as depicted in Fig. 4A.

Compared to the control compound vancomycin, these ligands, especially *p*-coumaric acid, sinapinic acid, and citric acid, exhibited comparable or superior binding affinities to the target proteins. This suggests their potential as promising antibacterial agents. These findings not only highlight the inhibitory mechanisms of these ligands on key bacterial enzymes but also emphasize their potential applications in designing new therapeutic strategies for combating resistant bacterial strains. On the other hand, although the major compounds were also found to exhibit antifungal activity, they were not as effective as fluconazole, which was used as a reference indicator.

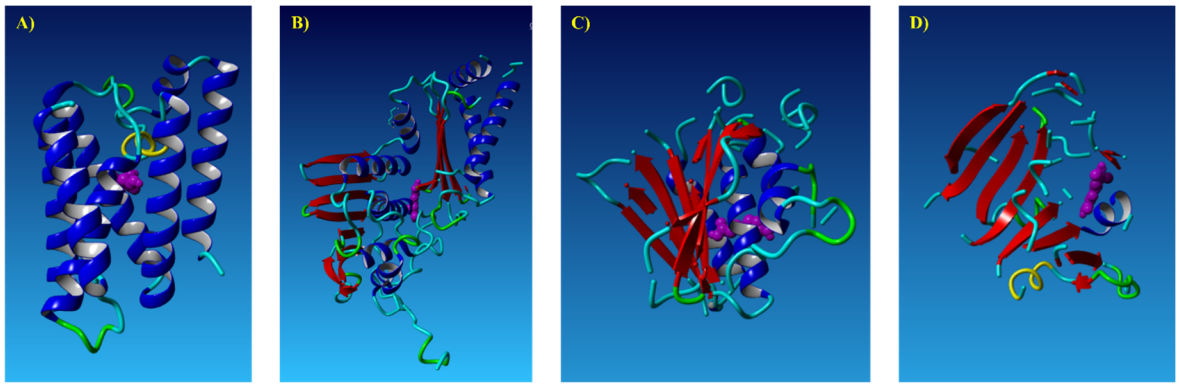

Figure 4: 3D view of docked ligands (purples) with related receptors. (**A**) Rhomboid protease (PDB ID: 3ZMI) with citric acid, (**B**) Gyrase B (PDB ID: 4PRX) with sinapinic acid, (**C**) DNA gyrase B (PDB ID: 4URM) with *p*-coumaric acid, (**D**) Dihydrofolate reductase (PDB ID: 6E4E) with sinapinic acid.

The optical and electronic properties of caffeic acid, Sinapinic acid, and *p*-coumaric acid molecules were investigated in detail via maximum absorbance wavelengths (λ_{max}), energy gaps, and oscillator strengths. Molecule structures and the HOMO-LUMO orbitals showed the effect of functional groups on chemical reactivity and electron distribution [28,37,38]. The methoxy group in Sinapinic acid and the dihydroxyphenyl group in caffeic acid significantly affect the electronic transitions and energy levels of these molecules. Sinapinic acid has the highest λ_{max} value with a wavelength of 307 nm, while *p*-coumaric acid has the lowest value with 299 nm. Energy gaps were calculated as the lowest in Sinapinic acid with 13.85 kJ/mol and the highest in *p*-coumaric acid with 14.60 kJ/mol. These data show that the chemical reactivity of Sinapinic acid is higher (Table S4).

HOMO-LUMO orbitals shed light on the chemical reactivity of molecules. HOMO indicates that electron density is concentrated in phenolic groups, while LUMO indicates that electron-accepting regions are around carbonyl groups and aromatic rings. The energy gap between molecules is directly related to the orbital arrangements. The similarity of energy gaps between caffeic acid (−0.22672 a.u.), Sinapinic acid (−0.22520 a.u.), and *p*-coumaric acid (−0.23198 a.u.) is remarkable (Fig. 5). In particular, the methoxy

group in Sinapinic acid keeps the energy gap at a level close to caffeic acid, while the wider energy gap in *p*-coumaric acid indicates low chemical reactivity.

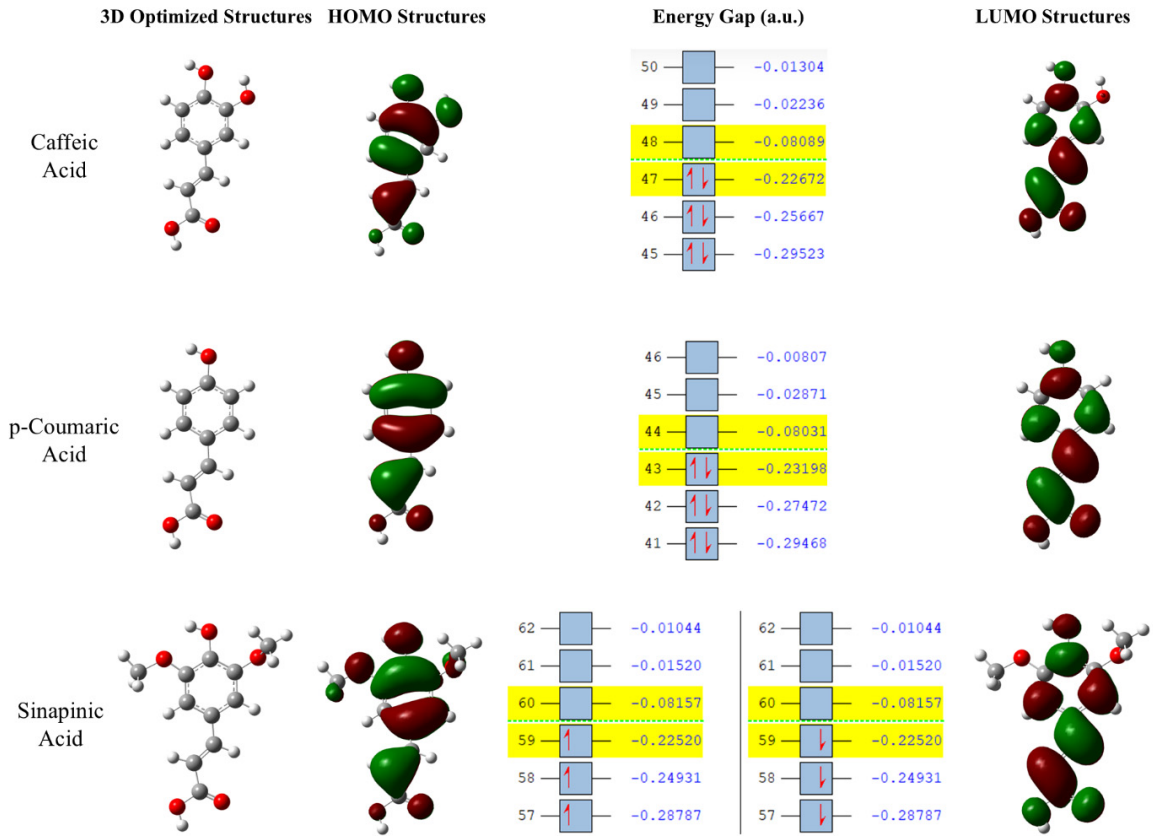

Figure 5: 3D optimized, HOMO, LUMO structures and energy gaps of major phenolics.

In terms of oscillatory strengths, *p*-coumaric acid exhibits the highest value with 0.83, while Sinapinic acid and caffeic acid have values of 0.78 and 0.65, respectively. This indicates that *p*-coumaric acid exhibits a stronger absorbance and electron transition density. In addition, it has been stated in the literature that Sinapinic and caffeic acids, which have lower energy gaps, are more effective in photochemical processes and antioxidant activities.

As a result, the examination of the optical and electronic properties of these molecules provides important information in terms of evaluating their potential in biological and industrial applications. HOMO-LUMO analyses contribute to the understanding of the chemical reactivity and photochemical properties of such molecules for pharmaceutical use. These data reveal that the antioxidant activities of the molecules are directly related to their energy gaps and electronic properties.

4 Conclusion and Future Recommendations

This study provides a comprehensive assessment of eleven naturally grown sour cherry genotypes by integrating pomological evaluation with phytochemical profiling, antioxidant analysis, and molecular-level bioactivity assessments. Substantial genotypic variation was recorded in fruit weight (1.95–4.99 g), pulp-to-stone ratio (86.60–92.00%), and titratable acidity (up to 2.72%), highlighting the horticultural potential of certain accessions, particularly Genotype 8 for fresh consumption and Genotype 10 for processing. Biochemically, *p*-coumaric acid (28.80 mg·kg^{-1} fw) and malic acid (1178.16 mg·100 g^{-1} fw) were

identified as the dominant phenolic and organic acids, respectively. The highest total phenolic content (1898.10 mg GAE·kg^{-1} fw), flavonoid content (947.11 mg QE·kg^{-1} fw), and anthocyanin levels (204.08 mg cya-3-glu·kg^{-1} fw) were associated with strong antioxidant activities (up to 15.65 mmol Trolox·g^{-1} fw), particularly in genotypes 3, 5, and 10. Molecular docking and DFT analyses revealed that key compounds such as *p*-coumaric and sinapic acids formed energetically favorable interactions with bacterial enzymes like DNA gyrase and DHFR, providing mechanistic support for their antimicrobial potential. Results obtained demonstrate how certain sour cherry genotypes combine high fruit quality with strong functional properties, making them promising candidates for cultivar development, functional food design, and nutraceutical applications. Nevertheless, the current study has some limitations, as the docking and DFT results have not yet been validated through *in vitro* or *in vivo* assays. To strengthen the application potential of the identified genotypes, antimicrobial interactions observed *in silico* should be validated through *in vitro* and *in vivo* assays to confirm the pharmacological relevance of the identified compounds. Finally, expanding the genotypic pool with wild relatives and underutilized sour cherry resources may enrich genetic diversity and support future breeding efforts aimed at enhancing both fruit quality and bioactive content.

Acknowledgement: Not applicable.

Funding Statement: The authors received no specific funding for this study.

Author Contributions: Kerem Mertoğlu: Supervision, Conceptualization, Investigation, Visualization, Resources, Formal Analysis, Data Curation, Methodology, Writing—Original Draft, Review & Editing. Fatma Nur Senlik: Writing—Original Draft, Review & Editing. İrem Yazıcı: Investigation, Resources, Writing—Original Draft, Review & Editing. Melekber Sülüşoğlu Durul: Review & Editing. Levent Kırca: Visualization, Formal Analysis, Methodology, Software, Writing—Original Draft, Review & Editing. İbrahim Bulduk: Formal Analysis, Validation, Methodology. Erten Akbel: Formal Analysis, Validation, Methodology, Writing—Original Draft. All authors reviewed and approved the final version of the manuscript.

Availability of Data and Materials: The data that support the findings of the study are available from the corresponding author upon reasonable request.

Ethics Approval: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

Supplementary Materials: The supplementary material is available online at https://www.techscience.com/doi/10.32604/phyton.2026.081637/s1.

References

1. Antonius K, Aaltonen M, Uosukainen M, Hurme T. Genotypic and phenotypic diversity in Finnish cultivated sour cherry (*Prunus cerasus* L.). Genet Resour Crop Evol. 2012;59(3):375–88. [CrossRef].
2. Paltineanu C, Chitu E. Climate change impact on phenological stages of sweet and sour cherry trees in a continental climate environment. Sci Hortic. 2020;261:109011. [CrossRef].
3. Debnath P, Chakma K, Bhuiyan MSU, Thapa R, Pan R, Akhter D. A novel multi trait genotype ideotype distance index (MGIDI) for genotype selection in plant breeding: application, prospects, and limitations. Crop Des. 2024;3(4):100074. [CrossRef].
4. Yılmaz FM, Görgüç A, Karaaslan M, Vardin H, Ersus Bilek S, Uygun Ö, et al. Sour cherry by-products: compositions, functional properties and recovery potentials—a review. Crit Rev Food Sci Nutr. 2019;59(22):3549–63. [CrossRef].

5. Özen M, Özdemir N, Ertekin Filiz B, Budak NH, Kök-Taş T. Sour cherry (*Prunus cerasus* L.) vinegars produced from fresh fruit or juice concentrate: bioactive compounds, volatile aroma compounds and antioxidant capacities. Food Chem. 2020;309:125664. [CrossRef].
6. Teslić N, Kojić J, Đermanović B, Šarić L, Maravić N, Pestorić M, et al. Sour cherry pomace valorization as a bakery fruit filling: chemical composition, bioactivity, quality and sensory properties. Antioxidants. 2023;12(6):1234. [CrossRef].
7. Lan T, Wang J, Bao S, Zhao Q, Sun X, Fang Y, et al. Effects and impacts of technical processing units on the nutrients and functional components of fruit and vegetable juice. Food Res Int. 2023;168:112784. [CrossRef].
8. Silva A, Rocha C, Ribeiro JC, Aganovic K, Lima RC, Methven L, et al. Consumer perception of risk towards new sustainable non-thermal food processing technologies: a cross-cultural study between Portugal, Germany, and the UK. Innov Food Sci Emerg Technol. 2024;96:103772. [CrossRef].
9. Toydemir G, Gultekin Subasi B, Hall RD, Beekwilder J, Boyacioglu D, Capanoglu E. Effect of food processing on antioxidants, their bioavailability and potential relevance to human health. Food Chem X. 2022;14:100334. [CrossRef].
10. Grafe C, Schuster M. Physicochemical characterization of fruit quality traits in a German sour cherry collection. Sci Hortic. 2014;180:24–31. [CrossRef].
11. Serradilla MJ, Hernández A, López-Corrales M, Ruiz-Moyano S, de Guía Córdoba M, Martín A. Composition of the cherry (*Prunus avium* L. and *Prunus cerasus* L.; Rosaceae). In: Simmonds MSJ, Preedy VR, editors. Nutritional composition of fruit cultivars. London, UK: Academic Press; 2016. p. 127–47. [CrossRef].
12. Sokół-Łętowska A, Kucharska AZ, Hodun G, Gołba M. Chemical composition of 21 cultivars of sour cherry (*Prunus cerasus*) fruit cultivated in Poland. Molecules. 2020;25(19):4587. [CrossRef].
13. Bozhuyuk MR. Morphological and biochemical characterization of wild sour cherry (*Prunus cerasus* L.) germplasm. Erwerbs Obstbau. 2022;64(3):357–63. [CrossRef].
14. Başyiğit B, Görgüç A, Gençdağ E, Cansu Ü, Yılmaz FM, Karaaslan M. Functional characterization of high-yield plant protein powder valorized from de-oiled sour cherry seed using microwave-assisted enzymatic extraction followed by spray- and freeze-drying. Biomass Convers Biorefin. 2023;13(16):14657–71. [CrossRef].
15. Soceanu A. Presence of heavy metals in fruits from prunus genera. Ovidius Univ Ann Chem. 2009;20(1):108–10.
16. Milošević T, Moreno MÁ, Milošević N, Milinković M. Regulation of yield, fruit size, and leaf mineral nutrients of the 'šumadinka' sour cherry cultivar with help of rootstocks. J Plant Growth Regul. 2023;42(9):5587–99. [CrossRef].
17. Blando F, Oomah BD. Sweet and sour cherries: origin, distribution, nutritional composition and health benefits. Trends Food Sci Technol. 2019;86:517–29. [CrossRef].
18. Han B, Srikanth Bhagavathula A, Rashid M, Chhabra M, Clark C, Abdulazeem HM, et al. The effect of sour cherry consumption on blood pressure, IL-6, CRP, and TNF-α levels: a systematic review and meta-analysis of randomized controlled trials sour cherry consumption and blood pressure. J King Saud Univ Sci. 2020;32(2):1687–93. [CrossRef].
19. Gholami A, Amirkalali B, Baradaran HR, Hariri M. The beneficial effect of tart cherry on plasma levels of inflammatory mediators (not recovery after exercise): a systematic review and meta-analysis on randomized clinical trials. Complement Ther Med. 2022;68:102842. [CrossRef].
20. Ghane-Sharbaf F, Reza-Jafar Z, Bakhtiari E, Saadat S. Effect of *Prunus cerasus* (sour cherry) on nephrolithiasis in children: the first noninferiority two-arm randomized clinical trial. Urol Res Pract. 2024;50(2):134–8. [CrossRef].
21. Salunke P, Koche D. Role of phenolic compounds in plant defense mechanism: an updated review. Indian J Appl Pure Bio. 2023;38(3):1199–215.
22. Zhang X, Gao X, Liu B, Wang J, Shan J, Wang J, et al. Transcriptome and metabolome reveal the primary and secondary metabolism changes in *Larix gmelinii* seedlings under abiotic stress. BMC Plant Biol. 2024;24(1):1128. [CrossRef].
23. Demir G, Aktaş N. A research on functional food knowledge, preference and consumption of unıversity students. J Hum Sci. 2018;15(4):2387–97. [CrossRef].
24. Ozturk Erdem S, Cekic C, Uysal D. Determination of the quality and phytochemical content of F1 strawberry genotypes selected in Bilecik province ecological conditions. Acta Sci Pol Hortorum Cultus. 2023;22(1):19–26. [CrossRef].

25. Titirică I, Roman IA, Nicola C, Sturzeanu M, Iurea E, Botu M, et al. The main morphological characteristics and chemical components of fruits and the possibilities of their improvement in raspberry breeding. Horticulturae. 2023;9(1):50. [CrossRef].
26. Fan J, Fu A, Zhang L. Progress in molecular docking. Quant Biol. 2019;7(2):83–9. [CrossRef].
27. Mertoğlu K. Sweet cherry fruit nutritional profile modulation and molecular docking studies of major compounds. Food Chem. 2025;465(Pt 2):142153. [CrossRef].
28. Becke AD. Density-functional thermochemistry. III. The role of exact exchange. J Chem Phys. 1993;98(7):5648–52. [CrossRef].
29. Li Y, Zhao S, Hu D, Ragauskas AJ, Cao D, Liu W, et al. Role evaluation of active groups in lignin on UV-shielding performance. ACS Sustain Chem Eng. 2022;10(36):11856–66. [CrossRef].
30. Desiderio F, Szilagyi S, Békefi Z, Boronkay G, Usenik V, Milić B, et al. Polyphenolic and fruit colorimetric analysis of Hungarian sour cherry genebank accessions. Agriculture. 2023;13(7):1287. [CrossRef].
31. Momeni H, Bouzari N, Zeinolabedini M, Jahromi MG. Genetic diversity in a core collection of Iranian sour cherry. Braz J Biol. 2023;84:e273386. [CrossRef].
32. Korićanac A, Radičević S, Marić S, Glišić I, Milošević N, Mitrović O, et al. Evaluation of sour cherry (*Prunus cerasus* L.) landraces originated from the west Serbia region. Voćarstvo. 2023;57(215–216):17–26. [CrossRef].
33. Tavallali V, Alhavi N, Gholami H, Mirazimi Abarghuei F. Developmental and phytochemical changes in pot marigold (*Calendula officinalis* L.) using exogenous application of polyamines. Plant Physiol Biochem. 2022;183:128–37. [CrossRef].
34. Selçuk N, Erkan M. Impact of passive modified atmosphere packaging on physicochemical properties, bioactive compounds, and quality attributes of sweet pomegranates. Turk J Agric For. 2016;40:475–88. [CrossRef].
35. Singh B, Singh JP, Kaur A, Singh N. Phenolic compounds as beneficial phytochemicals in pomegranate (*Punica granatum* L.) peel: a review. Food Chem. 2018;261:75–86. [CrossRef].
36. Çolak AM, Mertoğlu K, Alan F, Esatbeyoglu T, Bulduk İ, Akbel E, et al. Screening of naturally grown European cranberrybush (*Viburnum opulus* L.) genotypes based on physico-chemical characteristics. Foods. 2022;11(11):1614. [CrossRef].
37. Aytaç Z, Gülbandılar A, Kürkçüoğlu M. Humic acid improves plant yield, antimicrobial activity and essential oil composition of oregano (*Origanum vulgare* L. subsp. *hirtum* (link.) ietswaart). Agronomy. 2022;12(9):2086. [CrossRef].
38. Burley SK, Bhatt R, Bhikadiya C, Bi C, Biester A, Biswas P, et al. Updated resources for exploring experimentally-determined PDB structures and computed structure models at the RCSB protein data bank. Nucleic Acids Res. 2025;53(D1):D564–74. [CrossRef].
39. Dennington R, Keith TA, Millam JM. GaussView 6.0. 16. Shawnee Mission, KS, USA: Semichem Inc.; 2016.
40. Zar JH. Biostatistical analysis. 4th ed. Upper Saddle River, NJ, USA: Prentice-Hall; 1999.
41. Khadivi A, Mohammadi M, Asgari K. Morphological and pomological characterizations of sweet cherry (*Prunus avium* L.), sour cherry (*Prunus cerasus* L.) and duke cherry (*Prunus* × *gondouinii* Rehd.) to choose the promising selections. Sci Hortic. 2019;257:108719. [CrossRef].
42. Rakonjac V, Akšić MF, Nikolić D, Milatović D, Čolić S. Morphological characterization of 'Oblačinska' sour cherry by multivariate analysis. Sci Hortic. 2010;125(4):679–84. [CrossRef].
43. Usenik V, Fabčič J, Štampar F. Sugars, organic acids, phenolic composition and antioxidant activity of sweet cherry (*Prunus avium* L.). Food Chem. 2008;107(1):185–92. [CrossRef].
44. Najafzadeh R, Arzani K, Bouzari N, Hashemi J. Identification of new Iranian sour cherry genotypes with enhanced fruit quality parameters and high antioxidant properties. N Z J Crop Hortic Sci. 2014;42(4):275–87. [CrossRef].
45. Feldmane D, Dēķena D, Cirša E. Frost tolerance of flower buds, self-pollination and fruit quality traits in local sour cherries of Latvia. Proc Latv Acad Sci Sect B Nat Exact Appl Sci. 2022;76(4):469–76. [CrossRef].
46. Pedisić S, Dragović-Uzelac V, Levaj B, Škevin D. Effect of maturity and geographical region on anthocyanin content of sour cherries (*Prunus cerasus* var. marasca). Food Technol Biotechnol. 2010;48:86–93.
47. Lachowicz S, Seliga Ł, Pluta S. Distribution of phytochemicals and antioxidative potency in fruit peel, flesh, and seeds of Saskatoon berry. Food Chem. 2020;305:125430. [CrossRef].

48. Kapoor L, Simkin AJ, George Priya Doss C, Siva R. Fruit ripening: dynamics and integrated analysis of carotenoids and anthocyanins. BMC Plant Biol. 2022;22(1):27. [CrossRef].
49. Sharma S, Tripathi A, Baran C, Awasthi A, Tiwari A, Sharma S, et al. Monitoring pigment dynamics involved in the ripening of sweet cherries non-destructively using confocal micro Raman spectroscopy. Anal Lett. 2023;56(11):1826–42. [CrossRef].
50. Paunović G, Hajder Đ, Korićanac A, Pašalić B, Glišić I, Jovanović-Cvetković T, et al. Preferences in sweet cherry fruits among consumers in Serbia and Bosnia and Herzegovina. Hortic Sci. 2022;49(4):189–96. [CrossRef].
51. Habiba U, Alam ANMI, Aunsary L, Jubayer MF, Karmoker P, Alim MA, et al. Exploring the potential of wild date palm (*Phoenix Sylvestris* L. Roxb) fruits for vinegar production in Bangladesh. Appl Food Res. 2024;4(2):100628. [CrossRef].
52. Adamczak A, Ożarowski M, Karpiński TM. Antibacterial activity of some flavonoids and organic acids widely distributed in plants. J Clin Med. 2019;9(1):109. [CrossRef].
53. Zymonė K, Liaudanskas M, Lanauskas J, Nagelytė M, Janulis V. Variability in the qualitative and quantitative composition of phenolic compounds and the *in vitro* antioxidant activity of sour cherry (*Prunus cerasus* L.) leaves. Antioxidants. 2024;13(5):553. [CrossRef].
54. Göncü A. The effect of using sour cherry (*Prunus cerasus* L.) puree in tarhana formulations on nutritional value and functional properties of tarhana. Food Sci Nutr. 2024;12(8):5412–25. [CrossRef].
55. García-Villegas A, Fernández-Ochoa Á, Alañón ME, Rojas-García A, Arráez-Román D, de la Luz Cádiz-Gurrea M, et al. Bioactive compounds and potential health benefits through cosmetic applications of cherry stem extract. Int J Mol Sci. 2024;25(7):3723. [CrossRef].
56. Mertoğlu K. Investigation of genetic parameters and phytochemical characteristics in plum under altitude change. Genetika. 2022;54(1):73–89. [CrossRef].
57. Ozkan G, Oner ME, Tas D, Esatbeyoglu T, Capanoglu E. Effect of various food processing techniques on the retention of loquat phenolics and their antioxidant capacity during *in vitro* digestion. J Food Meas Charact. 2024;18(1):428–36. [CrossRef].
58. Zhang W, Jiang Y, Zhang Z. The role of different natural organic acids in postharvest fruit quality management and its mechanism. Food Front. 2023;4(3):1127–43. [CrossRef].
59. Martini S, Conte A, Tagliazucchi D. Phenolic compounds profile and antioxidant properties of six sweet cherry (*Prunus avium*) cultivars. Food Res Int. 2017;97:15–26. [CrossRef].
60. Hanbali L, Almor R, Teen D, Ghadieh R, Hasan H, Nakhal Y, et al. The antimicrobial activity and MICs of black/red sour cherry (*Prunus cerasus* L.) extracts: III. measurement of sensitivity and attenuation of gram-positive and gram-negative bacteria and C. albicans in culture. Curr Nutr Food Sci. 2013;9(3):233–48. [CrossRef].
61. Tomar O, Akarca G, Gök V, İstek Ö. Chemical composition and antifungal potential of apricot, sour cherry, and cherry tree bio-products (resins) against food-borne molds. Food Biosci. 2022;47:101627. [CrossRef].
62. Erbil N, Murathan ZT, Arslan M. Comparison of biochemical, microbiological, and toxicological properties of wild and cultivated sour cherry genotypes (*Prunus cerasus* L.). KSU J Agric Nat. 2024;27(5):1137–47. [CrossRef].
63. Angane M, Swift S, Huang K, Butts CA, Quek SY. Essential oils and their major components: an updated review on antimicrobial activities, mechanism of action and their potential application in the food industry. Foods. 2022;11(3):464. [CrossRef].
64. Zhou P, Zheng M, Li X, Zhou J, Shang Y, Li Z, et al. A consecutive extraction of pectin and hesperidin from *Citrus aurantium* L.: process optimization, extract mechanism, characterization and bio-activity analysis. Ind Crops Prod. 2022;182:114849. [CrossRef].
65. Guardiola JL, García-Luis A. Increasing fruit size in Citrus. Thinning and stimulation of fruit growth. Plant Growth Regul. 2000;31(1):121–32. [CrossRef].
66. Akkurt E, Mertoğlu K, Evrenosoğlu Y, Alpu Ö. Pollinizer potentials of reciprocally crossed summer apple varieties by using ANOVA and resampling based MANOVA. Appl Fruit Sci. 2024;66(1):25–34. [CrossRef].
67. Tejero-Sariñena S, Barlow J, Costabile A, Gibson GR, Rowland I. *In vitro* evaluation of the antimicrobial activity of a range of probiotics against pathogens: evidence for the effects of organic acids. Anaerobe. 2012;18(5):530–8. [CrossRef].

68. Kurnaz OC, Ozturk A, Ahmad Faizi Z, Ates U, Ozturk B. Pomological, bioactive compounds, and antioxidant activity of selected superior genotypes from a highly diversified loquat population. Genet Resour Crop Evol. 2024;71(4):1507–20. [CrossRef].
69. Ali Sarıdaş M, Ağçam E, Akbaş FC, Akyıldiz A, Paydaş Kargı S. Comparison of superior bred strawberry genotypes with popular cultivars in terms of fruit bioactive compounds over the full range of harvest dates. S Afr J Bot. 2022;147:142–52. [CrossRef].
70. Huang Z, Hu H, Shen F, Wu B, Wang X, Zhang B, et al. Relatively high acidity is an important breeding objective for fresh juice-specific apple cultivars. Sci Hortic. 2018;233:29–37. [CrossRef].
71. Mertoğlu K, Durul MS, Korkmaz N, Polat M, Bulduk I, Esatbeyoglu T. Screening and classification of rosehip (*Rosa canina* L.) genotypes based on horticultural characteristics. BMC Plant Biol. 2024;24(1):345. [CrossRef].
72. Nishiyama S, Onoue N, Kono A, Sato A, Yonemori K, Tao R. Characterization of a gene regulatory network underlying astringency loss in persimmon fruit. Planta. 2018;247(3):733–43. [CrossRef].