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Phenotypic yield-attributed traits, essential oil content and composition of Iranian *Grammosciadium platycarpum* (Apiaceae) populations: a rich source of (S)-(+)-linalool

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Abstract

(S)-(+)-linalool is a non-cyclic oxygenated monoterpene which is very useful and widely used in the cosmetic industries, especially in the production of perfume and cologne. Thus, due to the high commercial value and high demand, the search for new plant sources rich in (S)-(+)-linalool in agricultural systems to develop the business of this compound is of great interest. This investigation focused on the diversity of phenotypic yield and phytochemical traits in *Grammosciadium platycarpum* populations collected from fourteen geographical regions in Iran. The goal was to identify the essential compounds and select the best populations for domestication, cultivation, and future breeding programs. The highest coefficient of variation was observed in the umbrellas per plant, plant length, internode length, leaf width, number of lateral branches, and essential oil yield (EOY). The shoot dry weight ranged from 27.15 to 41.56 (g/plant) and the fruit dry weight from 9.23 to 20.80 (g/plant) among different populations, which was observed in the QOR population. The fruit of the plant was employed to extract and determine the content plus constituents of the essential oil. The essential oil content (EOC) exhibited a extend from 0.81 to 1.63%. MAQ population indicated the maximum and OSH population revealed the minimum EOC. The highest EOY (0.228 g/plant) was observed in the MAQ population and the lowest (0.083 g/plant) was related to the MAR population. Based on GC-MS and GC analysis, 91.97 to 99.93% of the essential compounds of different populations of *G. platycarpum* were identified. According to the results, linalool (65.90-81.62%) and limonene (9.73–15.34%) were the main ingredients of the essential oil profile. Rutin, ferulic acid, and chlorogenic acid were detected as the major phenolic compounds using HPLC. The high diversity observed among different populations of *G. platycarpum* provides good potential for selecting the best populations and using them in domestication projects, cultivation, and breeding programs.

Keywords Linalool, Diversity, Phenolic compounds, Multivariate analysis, Domestication

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Introduction

Essential oils (EOs) are the primary ingredients of natural perfumes and many food supplements that are produced in different organs of aromatic plants [23]. The EOs are made of hydrocarbons, which are classified into terpenes, esters, alcohols, ketones, aldehydes, and phenols based on their molecular structure [9, 14]. Terpenes are the broadest group of natural organic chemicals responsible

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for the odor of flowers and fruits [17]. Monoterpenes are a category of terpene compounds commonly utilized in the food and cosmetic sectors, as well as active pharmaceutical ingredients in various medicinal products, primarily owing to their anti-inflammatory, analgesic, and wound healing characteristics [10, 21].

(±)-Linalool (3,7-dimethyl-1,6-octadien-3-ol) is an acyclic monoterpene with a hydroxyl group, existing in two enantiomeric forms, R-(-) and S-(+), found in various plant essential oils [29]. It possesses numerous biological properties, including analgesic, anti-inflammatory, anti-depressant, anti-cancer, antimicrobial, anti-anxiety, and neuroprotective effects, making it useful in medicinal and cosmetic applications [3, 27]. Linalool is commonly used in products such as perfumes and cleaners for its pleasant aroma and as a flavoring agent in food as well as cosmetics [4]. Annually, around 1,000 metric tons of linalool are consumed globally, with its market value projected to rise from 529.32 million dollars in 2022 to 692.2 million dollars by 2030 [27]. More than 200 plant species contain linalool in their essential oils. This compound is contained in the Apiaceae family, *Coriandrum*, and *Grammosciadium* genera [4]. The genus *Grammosciadium* has nine species, of which three species, *G. pterocarpum*, *G. platycarpum*, and *G. scarbridu*, grow in Iran, and is found in most temperate or cold temperate regions as well as mountain pastures [26]. *G. platycarpum* is a perennial plant with a height of 40–100 cm, which is known in Iran as mountain parsley or mountain dill and is distributed in Turkey, Iran, Iraq, and Armenia. *G. platycarpum* is used as an infusion to reduce blood glucose plus lipids and it is consumed as food in some regions of Iran [5, 32, 35]. This variety is known for its appealing taste and fragrance is used as a vegetable and food additive in different regions in spring [24]. The fruit of *G. platycarpum* has an EOC ranging from 0.7 to 1.1%, with linalool (79–81.8%) and limonene (5.8–10%) being its primary components [32]. The analysis of *G. platycarpum* leaf and fruit essential oil revealed that 26.1% of the leaf essential oil and 53.9% of the fruit essential oil were linalool [25]. Considering the content of linalool in essential oil of the fruit of *G. platycarpum* and due to its commercial value plus high demand, the extraction and purification of S(-)-linalool from plant sources is of great interest and *G. platycarpum* can be a suitable option as a new source of linalool.

A literature review showed that no measures has been taken to cultivate and breed this plant; today the raw material of *G. platycarpum* needed by the food and perfumery industries is harvested from natural habitats, and excessive harvesting ultimately leads to the extinction of medicinal plant species [30]. The development and integration of medicinal plants in agricultural systems is one of the effective ways to preserving their genetic diversity, which requires breeding programs and production of improved cultivars [12]. The effectiveness of a plant breeding program relies on the level of diversity present. Thus, it is essential to examine the variation in morphological and yield traits, as well as the EOC and its components among different plant populations, to select superior genotypes in line with domestication and breeding programs [7, 13]. Given the significance and demand for *G. platycarpum* essential oil in the pharmaceutical, food, cosmetic, and fragrance industries, along with the necessity to incorporate its superior genotypes into cultivation and production systems, this study seeks to assess the diversity of agro-morphological and phytochemical attributes (particularly the EOC and its components) across various populations of *G. platycarpum*. The most promising populations, based on essential oil and linalool levels, were selected to initiate domestication, cultivation, and breeding programs to satisfy the requirements of the cosmetics, fragrance, and food sectors.

Materials and methods

Plant materials and evaluation of agro-morphological traits

The natural habitats of *G. platycarpum* were identified by Iranian Flora. From each habitat, ten plant samples in the flowering stage were selected, where quantitative and qualitative traits were measured including plant length, number of lateral branches, umbrellas per plant, umbels per umbrellas, number of fruits in the umbrella, number of internode, internode length, leaf length, and leaf width and recorded using a digital caliper plus meter at the natural habitat. A distance of 100 m was considered between the samples in each population. Then, the samples were labeled, taken during the fruit ripening stage, and transferred to the laboratory of Medicinal Plants and Drugs Research Institute. The samples were then allowed to air dry at room temperature (25 ± 2°C). The samples were identified by Prof. Ali Sonboli, and voucher specimens were deposited at the Shahid Beheshti University herbarium (Table 1). The authors confirm that the necessary permissions to collect and cultivate the samples have been obtained. Also, the present study complies with the IUCN Policy Statement on Research Involving Species at Risk of Extinction and the Convention on the Trade in Endangered Species of Wild Fauna and Flora. Climate data for each region were obtained from the nearest meteorological station. The climatic and geographical specifications of different collection regions are presented in Table 1 and Fig. 1.

Table 1 Geographical information for the collection regions of *Grammosciadium platycarpum* populations

No.	Province	City	Code	Voucher number	Longitude	Latitude	Altitude (m)	Mean annual temperature (°C)	Mean annual precipitation (mm)
1	Kurdistan	Saqqez, Tamgoogheh	SAQ	MPH-3245	46°08′	36°13′	1845	11.5	487
2	Kurdistan	Baneh, Qureh Darreh	QOR	MPH-3246	46°02′	37°07′	1641	14.2	565
3	Kurdistan	Baneh, Gardaneh Khan	GAR	MPH-3247	45°59′	36°05′	1832	14.0	684
4	West Azerbaijan	Mahabad, Qarah Bolagh	MAQ	MPH-3248	45°59′	36°37′	1894	12.0	387
5	West Azerbaijan	Mahabad, Gavmishan	MAG	MPH-3249	45°50′	36°23′	1840	12.5	392
6	West Azerbaijan	Urmia, Tergever	TAR	MPH-3250	45°03′	37°10′	2103	13.1	343
7	West Azerbaijan	Urmia, Silvaneh	SIL	MPH-3251	44°49′	37°25′	2059	13.5	300
8	West Azerbaijan	Oshnavieh, Ganj Abad	OSH	MPH-3252	45°09′	37°07′	1829	13.3	387
9	West Azerbaijan	Tekab, Pichaqchi	TAK	MPH-3253	46°47′	36°37′	1982	10.2	348
10	East Azerbaijan	Maragheh, Yayshahr	MAR	MPH-3254	46°20′	37°34′	2009	13.5	335
11	Zanjan	Abhar, Kalleh Khaneh	ABH	MPH-3255	49°20′	36°18′	1858	10.5	535
12	Qazvin	Qazvin, Razjerd	RAZ	MPH-3256	50°11′	36°22′	2199	13	323
13	Qazvin	Qazvin, Gostin Lar	QAS	MPH-3257	50°14′	36°24′	2234	13.5	340
14	Qazvin	Qazvin, Jolfadeh	JOL	MPH-3258	50°08′	36°28′	2026	13.2	362

Phytochemical analysis

Essential oil extraction

Following the procedure outlined in the British Pharmacopoeia, the essential oil content (EOC) was extracted from the samples. This involved hydrodistilling 50 g of dried fruit using a Clevenger apparatus over a 3-hour period. The essential oil yield (EOY) was determined based on 100 g of fruit after 180 min [32]. Subsequently, the extracted essential oils were analyzed through chemical profiling using targeted GC and GC-MS devices.

GC and GC-MS analysis and compound identification

The EOs analysis was conducted using a gas chromatograph equipped with a DB-5 column and a flame ionization detector (FID). The injector temperature was configured at 250°C, while the detector temperature was kept at 300°C. Nitrogen served as the carrier gas, flowing at a rate of 1.1 ml/min. The oven temperature initially started at 60°C and increased by 5°C per minute until reaching 250°C, where it remained constant for 10 min [32].

For the GC-MS analysis, we utilized a Thermoquest-Finnigan gas chromatograph with a 60-meter long, 0.25 mm diameter fused silica capillary HP-5MS column, bearing a 0.25 µm thick film. This system was coupled with a TRACE mass spectrometer from Manchester, UK. We used helium as the carrier gas, with the ionization voltage set to 70 electron volts. The ion source and interface temperatures were maintained at 200°C and 250°C, respectively, while the mass spectrometer operated within a range of 40 to 460 atomic mass units. The oven temperature program was consistent with that used in the GC-FID analysis. To identify the essential oil components, we calculated retention indices through temperature-programmed analysis with n-alkanes (C6–C24) and compared these indices to those of the essential oil analyzed on a DB-5 column under the same chromatographic conditions. Compound identification was based on matching mass spectra with those found in an internal reference library (Adams and Wiley 7.0) or known standards. We confirmed identities by comparing retention indices with authenticated compounds or literature references. Quantification was conducted by analyzing the relative area percentages obtained from FID signals without applying any correction factors, as noted by Adams [1]. The enantiomer distribution of linalool was determined using a chiral column (Supplementary material).

Preparation of phenolic extracts

The powdered fruit samples (100 mg) were extracted with 80% methanol through ultrasonic assistance for 44 min. Following extraction, the mixtures were centrifuged at 4400×g for 15 min, where the supernatant obtained was used for phytochemical analysis [12].

Quantification of phenolic compounds by HPLC-DAD

The phenol compounds were isolated and measured using a Knauer HPLC (Germany) equipped with two Wellchron-K1001 pumps and a K2800 PDA detector.

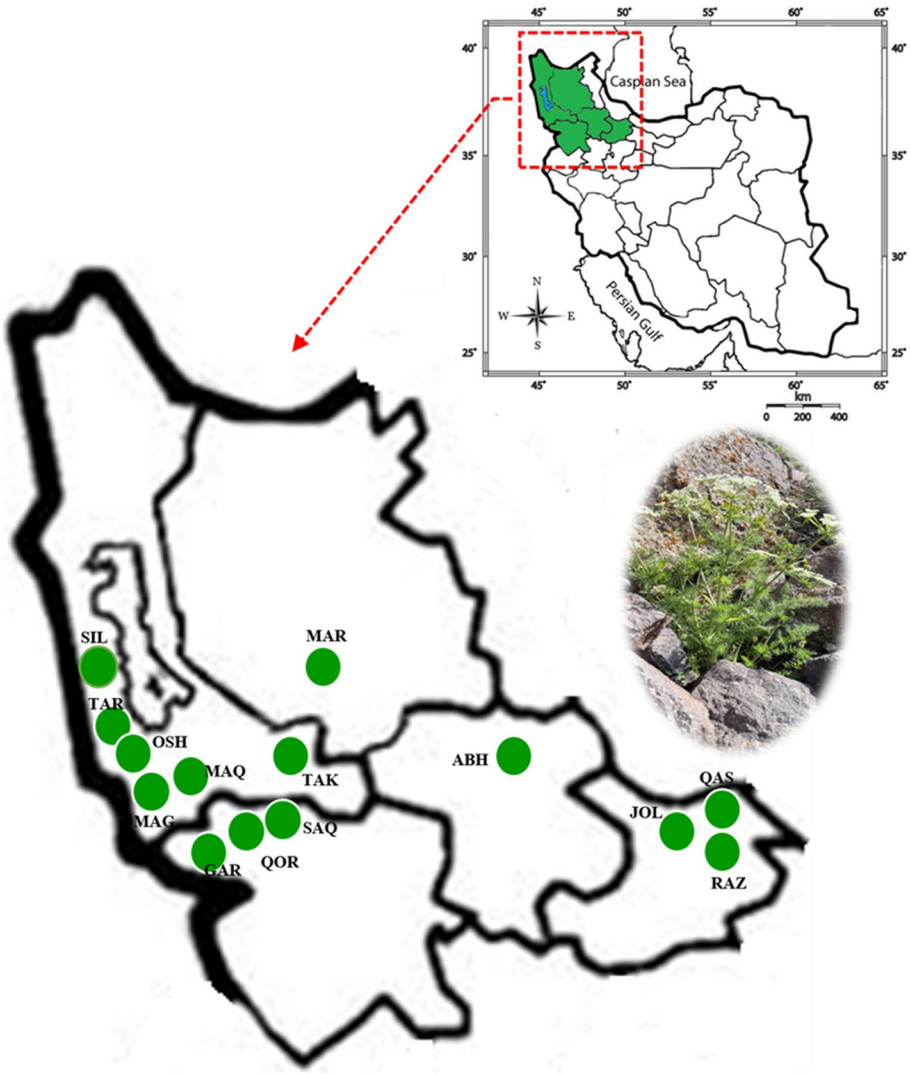

Fig. 1 Distribution map of the fourteen populations of *Grammosciadium platycarpum* collected across Iran

The column used was of the RP-C18 type with an internal diameter of 4.6 mm and a length of 250 mm (made by the Eurosphr company). The moving phase was composed of methanol solvent and HPLC-specific water. The peaks were checked at 200–600 nm. The injection volume was 20 µl, and the temperature was fixed at 25°C. The pure standard of the phenol compounds was procured from the Sigma Aldric company. The retention times and analysis of the spike oil extract with a standard solution were employed to identify phenolic acids. The calibration curves were obtained by injecting different concentrations (5, 10, 20, 40, 60, 80, 100, 150, and 200 ppm) of standard compounds to analyze the quantity of the phenolic acids. The compounds were expressed in mg/g DW [7].

Estimation of total phenol content (TPC) and flavonoid content (TFC)

TPC was quantified using the method described by Singleton et al., [2, 31], which involves the Folin-Ciocalteu reagent. TFC was measured based on the procedure outlined by Dewanto et al., [8, 11], utilizing aluminium chloride. The absorbance readings for TPC and TFC were taken at wavelengths of 765 nm and 510 nm, respectively.

Statistical analysis

The data was analyzed through multiple statistical techniques and software programs. One-way ANOVA (completely randomized design with ten replications) and Duncan's test at a significance level of $p < 0.05$ were performed using SAS software (Version 9.4). Statistical

descriptive parameters (including mean, maximum, minimum, standard deviation, and coefficient of variation) were estimated by SAS software. The correlation of the traits was determined using Pearson's coefficient of correlation in OriginLab 2021. Path coefficient analysis and factor analysis were performed on agro-morphological, EOC, and EOY traits using the R software package. For cluster analysis, the Euclidean distance coefficient by Ward's method in OriginLab 2021 was utilized. All graphs were created using the R and Excel (ver. 2016) software.

Results and discussion

Agro-morphological traits, EOC, and EOY

Significant diversity was observed among the *G. platycarpum* populations in the morphological and yield traits, providing the possibility of selection for these traits among different populations. The highest coefficient of variation (CV) was obtained in the traits number of inflorescence per plant (61.64%), plant height (47.03%), internode length (46.83%), leaf width (45.37%), number of lateral branches (32.86%) and the EOY (32.74%), while the lowest was related to the dry weight of aerial parts (16.57%) (Table 2). The high CV of the trait indicates the wide range of this trait quantitatively, which provides a wider range of selection for that trait for the breeder [12]. CV has been used for evaluating agro-morphological traits of many medicinal plants including *Equisetum arvense* [12], *Satureja rechingeri* [13], *Rosa canina* [7] and *Ruscus hyrcanus* [15].

The highest plant height was related to the SAQ population (50.50 cm) and the lowest to the JOL population (14.05 cm). QOR population (8.70) had the highest while SAQ population (3.10) had the lowest number of lateral branches. In terms of leaf length, the QOR population had the highest (16.65 cm) while the QAS population (6.56 cm) showed the lowest leaf length. The average leaf width among different populations varied from 2.60 to 7.50 cm, which was observed in ABH and OSH populations, respectively (Table 3). The shoot dry weight varied from 27.15 to 41.56 (g/plant) and the fruit dry weight from 9.23 to 20.80 (g/plant) among different populations, which was observed in the QOR population. The lowest shoot dry weight and fruit dry weight were observed in RAZ and MAR populations, respectively.

In this study, significant variation was observed among different populations of *G. platycarpum* in the morphological and yield traits. For programs of domestication, cultivation, and breeding of medicinal plants, the evaluation of intra- and inter-population diversity is very important. The assessment of the diversity of morphological traits provides useful information for plant breeders, which will lead to the development of new cultivars with desirable agricultural characteristics Gorbani [15]. The fruit EOC varied from 0.81 to 1.63%. The MAQ population had the maximum while the OSH population had the minimum EOC. The highest fruit EOY (0.228 g/plant) was observed in the MAQ population and the lowest EOY (0.083 g/plant) was linked to the population (Table 4). In the realm of medicinal and aromatic vegetation, a pivotal factor in assessing product quality is the quantity of essential oil present in the specific plant component intended for utilization [19]. Previous research endeavors have highlighted that the

Table 2 Statistical descriptive parameters for agro-morphological traits, essential oil content and yield of different *Grammosciadium platycarpum* populations

No.	Trait	Abbreviation	Unit	Mean	Max.	Min.	SD	CV (%)
1	Plant length	PL	cm	26.74	59.00	8.00	12.58	47.03
2	Number of lateral branches	NLB	-	5.75	15.00	2.00	1.88	32.86
3	Umbrellas per plant	UP	-	7.75	39.00	3.00	4.77	61.64
4	Umbels per umbrellas	UU	-	10.92	20.00	5.00	3.17	29.04
5	Number of fruits in the umbrella	NFU	-	9.12	21.00	3.00	2.36	25.94
6	Number of internode	NI	-	5.71	12.00	2.00	1.63	28.54
7	Internode length	IL	cm	3.71	8.00	1.00	1.74	46.83
8	Leaf length	LL	cm	11.15	21.00	3.00	3.64	32.65
9	Leaf width	LW	cm	7.51	12.50	1.50	2.05	45.37
10	Shoot dry weight	SDW	g/plant	29.93	63.12	26.11	4.96	16.57
11	Fruits dry weight	FDW	g/plant	13.89	24.00	8.10	3.79	27.31
12	Essential oil content	EOC	%	0.98	1.70	0.61	0.22	22.62
13	Essential oil yield	EOY	g/plant	0.135	0.272	0.068	0.044	32.74

Min Minimum, *Max* Maximum, *SD* Standard deviation, *CV* Coefficient of variation

Table 3 Comparison of mean (± standard deviation) of morphological traits in different *Grammosciadium platycarpum* populations

Population	Plant length (cm)	Number of lateral branches	Umbrellas per plant	Umbels per umbrellas	Number of fruits in the umbrella	Number of internode	Internode length (cm)	Leaf length (cm)	Leaf width (cm)
TAK	22.40 ± 3.86^{d}	6.90 ± 1.44^{cb}	9.00 ± 3.12^{cb}	12.10 ± 3.07^{abc}	10.20 ± 1.39^{ab}	6.40 ± 1.77^{bc}	3.20 ± 0.95^{ef}	11.9 ± 2.96^{cde}	4.46 ± 1.37^{efg}
MAG	20.90 ± 5.62^{de}	4.70 ± 1.41^{e}	5.40 ± 1.57^{cd}	12.00 ± 3.36^{abc}	9.20 ± 1.22^{bc}	5.40 ± 1.50^{cd}	2.85 ± 0.95^{ef}	10.06 ± 0.91^{ef}	3.66 ± 0.60^{fgh}
MAR	16.25 ± 2.12^{fe}	5.10 ± 0.56^{de}	6.20 ± 0.63^{cd}	8.80 ± 1.13^{de}	9.00 ± 0.94^{bc}	5.40 ± 0.51^{cd}	2.21 ± 0.21^{f}	8.35 ± 1.87^{fg}	3.87 ± 0.87^{efgh}
TAR	21.50 ± 3.13^{d}	5.70 ± 0.82^{cde}	6.30 ± 0.94^{cd}	10.80 ± 2.20^{ab}	7.90 ± 1.66^{cd}	5.80 ± 0.63^{cbd}	3.77 ± 1.49^{de}	10.75 ± 2.23^{de}	3.48 ± 0.73^{gh}
QOR	32.60 ± 8.74^{c}	8.70 ± 3.19^{a}	19.00 ± 11.23^{a}	14.50 ± 3.92^{a}	10.60 ± 2.11^{ab}	6.70 ± 0.82^{b}	4.27 ± 1.57^{cd}	16.65 ± 3.02^{a}	5.77 ± 2.21^{cd}
GAR	31.10 ± 6.87^{c}	8.10 ± 1.79^{ab}	10.70 ± 2.66^{b}	14.40 ± 3.72^{a}	11.90 ± 3.69^{a}	8.00 ± 1.56^{a}	3.57 ± 1.15^{de}	14.58 ± 2.41^{b}	4.84 ± 1.54^{def}
JOL	14.05 ± 3.63^{f}	5.50 ± 0.7^{de}	6.80 ± 0.42^{cd}	10.95 ± 1.42^{cbd}	7.80 ± 2.04^{cd}	4.80 ± 1.03^{de}	2.15 ± 0.57^{f}	7.80 ± 1.35^{fg}	2.72 ± 0.84^{h}
RAZ	15.75 ± 3.02^{f}	5.10 ± 1.28^{de}	6.30 ± 2.00^{cd}	10.80 ± 1.87^{cbd}	9.60 ± 3.13^{bc}	4.20 ± 1.03^{ef}	2.40 ± 0.84^{f}	8.31 ± 3.12^{fg}	2.70 ± 0.58^{h}
MAQ	44.70 ± 5.07^{b}	5.00 ± 0.94^{de}	6.90 ± 1.52^{cd}	9.10 ± 0.99^{de}	9.80 ± 1.31^{bc}	6.80 ± 0.91^{b}	5.85 ± 0.81^{ab}	12.66 ± 2.03^{cbd}	6.20 ± 1.15^{bc}
QAS	15.00 ± 4.64^{f}	4.90 ± 1.10^{de}	6.30 ± 1.88^{cd}	9.60 ± 1.50^{cde}	7.90 ± 3.38^{cd}	3.90 ± 0.87^{ef}	2.55 ± 0.64^{f}	6.56 ± 1.63^{g}	2.59 ± 0.49^{h}
SAQ	50.50 ± 7.93^{a}	3.10 ± 0.73^{f}	3.90 ± 0.73^{d}	8.80 ± 1.75^{de}	8.80 ± 1.03^{cbd}	6.30 ± 1.25^{bc}	6.58 ± 1.16^{a}	13.77 ± 2.29^{bc}	7.32 ± 1.65^{ab}
OSH	42.10 ± 3.41^{b}	5.70 ± 0.82^{cde}	5.70 ± 0.82^{cde}	7.20 ± 1.93^{e}	8.70 ± 1.15^{cbd}	6.10 ± 0.73^{bc}	5.35 ± 1.15^{b}	12.45 ± 1.53^{cbd}	7.50 ± 2.08^{a}
SIL	29.60 ± 5.56^{c}	6.30 ± 0.94^{cd}	6.30 ± 0.94^{cd}	12.50 ± 2.59^{ab}	9.60 ± 2.27^{bc}	6.80 ± 1.03^{b}	4.92 ± 1.19^{bc}	13.84 ± 2.99^{bc}	5.03 ± 1.69^{cde}
ABH	18.00 ± 2.35^{fde}	5.70 ± 1.05^{cde}	5.70 ± 0.82^{cde}	11.40 ± 3.47^{cbd}	6.80 ± 1.31^{d}	3.30 ± 0.67^{f}	2.20 ± 0.91^{f}	8.51 ± 2.59^{fg}	2.60 ± 0.84^{h}

Values followed by the same letter within each column are significantly different ($p \leq 0.05$)

EOCs of *G. platycarpum* can fluctuate between 0.7% and 1.1% due to environmental conditions affecting the plant growth [5, 32]. Given these considerations, understanding the factor(s) influencing variations in EOY rate is of utmost importance [34].

Correlation between agro-morphological, EOC and EOY

Simple correlation coefficients between the measured agro-morphological features are displayed in Fig. 2. The results of simple correlation coefficients revealed that most of the evaluated traits have significant positive or negative correlations at different levels. The traits of internode length, number of internodes, leaf length, and leaf width exhibited a positive and statistically significant correlation with the plant height. The dry weight of fruit per plant, recognized as a significant economic trait, exhibited a positive and statistically significant correlation with several other traits, including the number of lateral branches, the number of umbrella, the number of umbellet per umbrella, the

Table 4 Comparison of mean (± standard deviation) of functional traits, essential oil content and yield in different *Grammosciadium platycarpum* populations

Population	Shoot dry weight (g/plant)	Fruits dry weight (g/plant)	Essential oil content (%)	Essential oil yield (%)
TAK	31.14 ± 2.56^{cbd}	13.62 ± 1.09^{de}	1.031 ± 0.04^{c}	0.140 ± 0.01^{d}
MAG	27.24 ± 0.90^{e}	14.52 ± 0.86^{d}	1.144 ± 0.01^{b}	0.166 ± 0.01^{c}
MAR	27.50 ± 0.86^{e}	9.23 ± 0.67^{h}	0.907 ± 0.06^{de}	0.083 ± 0.008^{f}
TAR	29.20 ± 1.54^{cde}	19.60 ± 1.42^{b}	0.870 ± 0.09^{ef}	0.170 ± 0.02^{c}
QOR	41.56 ± 10.71^{a}	20.80 ± 1.75^{a}	0.667 ± 0.03^{h}	0.138 ± 0.01^{d}
GAR	34.16 ± 3.75^{b}	17.82 ± 1.76^{c}	1.070 ± 0.04^{c}	0.190 ± 0.01^{b}
JOL	27.71 ± 0.91^{de}	9.27 ± 0.65^{h}	0.932 ± 0.04^{d}	0.086 ± 0.007^{f}
RAZ	27.15 ± 0.80^{e}	10.88 ± 0.51^{g}	0.851 ± 0.04^{fg}	0.092 ± 0.006^{f}
MAQ	28.94 ± 1.40^{cde}	14.05 ± 1.77^{d}	1.628 ± 0.07^{a}	0.228 ± 0.03^{a}
QAS	28.23 ± 1.33^{de}	11.63 ± 1.14^{fg}	0.949 ± 0.03^{d}	0.110 ± 0.01^{e}
SAQ	27.46 ± 0.86^{e}	11.46 ± 0.52^{g}	1.025 ± 0.08^{c}	0.117 ± 0.009^{e}
OSH	28.65 ± 2.68^{cde}	11.36 ± 0.86^{g}	0.809 ± 0.05^{g}	0.091 ± 0.009^{f}
SIL	31.90 ± 2.21^{cb}	17.70 ± 1.49^{c}	0.855 ± 0.02^{fg}	0.151 ± 0.01^{d}
ABH	28.20 ± 1.11^{de}	12.65 ± 1.15^{ef}	0.939 ± 0.04^{d}	0.118 ± 0.01^{e}

Values followed by the same letter within each column are significantly different ($p \leq 0.05$)

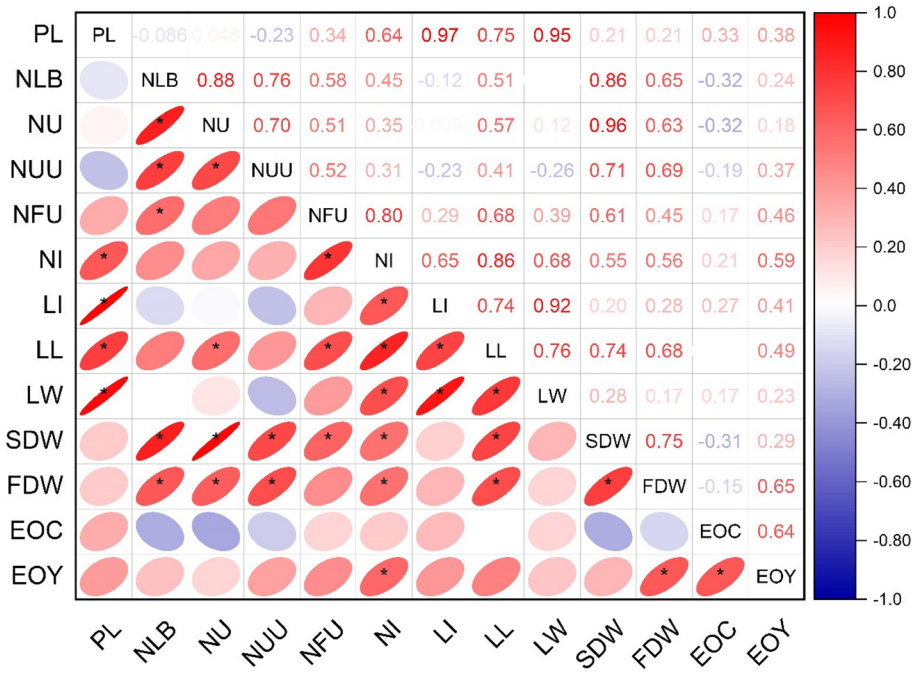

Fig. 2 Pearson correlation representation of agro-morphological traits, essential oil content and yield of *Grammosciadium platycarpum* populations

number of internodes, the shoot dry weight, and the EOY. The EOY showed a positive and significant correlation with the traits of internode number, fruit dry weight, and EOC. The ultimate efficacy of each medicinal plant, regarding the desired metabolites, is contingent upon the yield of the plant's medicinal organ. In the case of *G. platycarpum*, the primary site of metabolite (specifically essential oil) production is its fruit. Hence, any factor that increases the dry weight of the fruit in this plant can be effective on producing as many metabolites as possible. Thus, the traits that are effective on enhancing the dry weight of the fruit and the EOC can be considered by breeders [13].

Multivariate analyses based on agro-morphological traits, EOC, and EOY

Analysis into factors was done according to various agro-morphological parameters and essential oils of different populations of *G. platycarpum*. The first component (PC1) included the number of lateral branches, number of umbrellas, shoot dry weight, and fruit dry weight accounting for 48.42% of the total variance. The second component (PC2) with 27.86% of the total variation consisted of plant height, internode length, number of internodes, leaf length, and leaf width. The fruit dry weight, EOC, and EOY as the third component (PC3) explained 11.79% of the total variance (Table 5). In general, factor analysis was able to express the evaluated traits into three main factors. This analysis can clarify the main differentiating factors between the studied populations. In Eghlima et al. [21] study, PCA was employed to evaluate different ecotypes of *Equisetum arvense*, where the studied agro-morphological traits were categorized into three main components, which accounted for 96.77% of the total variance. In another study on *Rosa canina*, phytochemical and morphological characteristics were categorized into seven principal components using PCA, accounting for 93.53% of the total variance [7].

Cluster analysis was performed as a key approach for classifying different populations according to their agro-morphological traits, with the findings illustrated in Fig. 3. Based on the results, the populations were categorized into three main groups. Group I included five groups TAK, SIL, GAR, MAG, and TAR. MAQ, SAQ, and OSH populations were fallen in group II, and MAR, RAZ, JOL, QAS, and ABH populations were placed in group III. The influence of climatic and geographical conditions is well known on gene expression levels, as well as the diversity of morphological traits and phytochemical compounds among plant populations. Diversity among plants of a species is caused by environmental factors and the structure of genes, which is well shown in cluster analysis when similar populations are placed close to each other [28]. A 3D plot created using PC1, PC2, and PC3 indicated variations among populations and divided the populations into three main groups (Fig. 4). The 3D diagram based on agro-morphological features confirmed the results of cluster analysis.

Table 5 Eigenvalues of the principal component axes from the multiple regression analysis of the on morphophysiological and biochemical characteristics

Traits	Component		
	1	2	3
Plant length	−0.055	0.904	0.188
Number of lateral branches	0.865	0.019	0.129
Umbrellas per plant	0.885	0.092	−0.010
Umbels per umbrellas	0.419	−0.215	0.453
Number of fruits in the umbrella	0.241	0.219	0.369
Number of internode	0.313	0.528	0.446
Internode length	−0.019	0.882	0.130
Leaf length	0.444	0.673	0.308
Leaf width	0.129	0.879	−0.021
Shoot dry weight	0.889	0.246	0.071
Fruits dry weight	0.646	0.137	0.519
Essential oil content	−0.497	0.170	0.673
Essential oil yield	0.101	0.216	0.901
Eigenvalues	6.31	3.62	2.16
% of variance	48.42	27.86	11.79
Cumulative variance %	48.42	76.24	88.07

Path analysis

The path coefficient analysis was employed to further study the interaction of the agro-morphological and EOC traits of *G. platycarpum* as well as their effects on EOY (Fig. 5). The fruit dry weight (0.854), EOC (0.710), and plant length (0.253) had the strongest direct effect, while the number of umbrellas (−0.209), Internode length (−0.163), leaf width (−0.156), and number of umbrellas in the umbrella (−0.081) had the strongest negative effect on EOY. The strongest indirect effect on EOY was related to shoot dry weight (0.531) and the number of fruits in the umbrella (0.312) through fruit dry weight. The findings from the path analysis indicated that the dependent variables of fruit dry weight and EOC (as the first order) plus shoot dry weight and number of fruits in the umbrella (as the second order) influenced EOY significantly.

The path analysis diagram for all agro-morphological traits versus the EOC is depicted in Fig. 6. The EOC was most strongly influenced by the traits of EOY (1.410), number of umbrellas (0.298), internode length (0.230), and leaf length (0.218) positively and by fruit dry weight (−1.205), plant length (−0.355), and number of lateral branches (−0.188) negatively. The strong direct effect

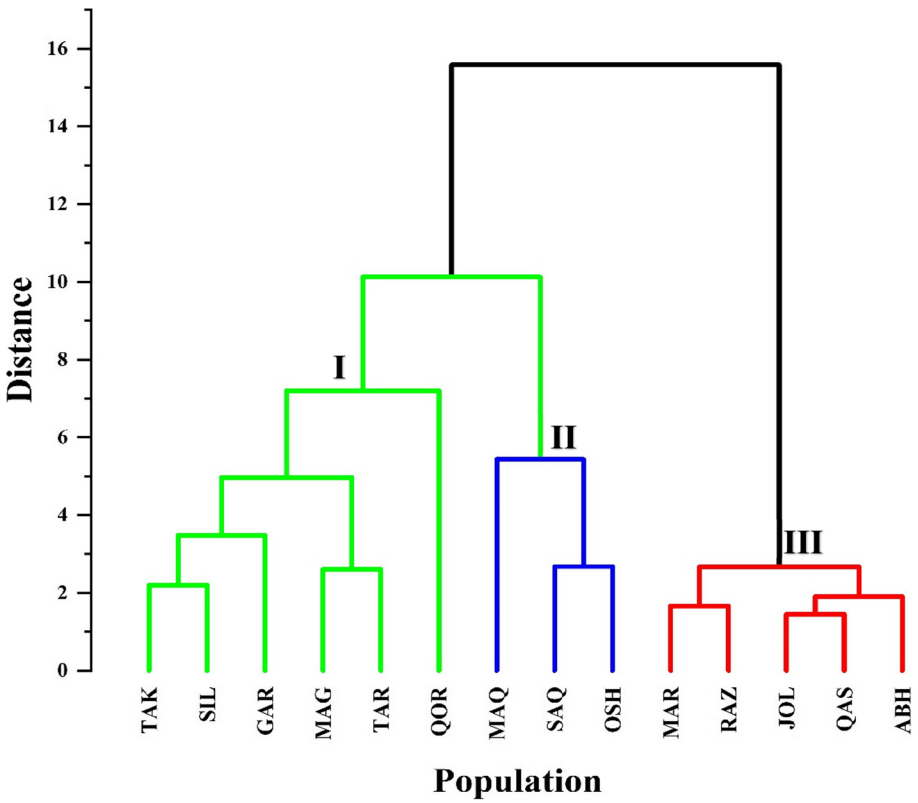

Fig. 3 Cluster analysis of *Grammosciadium platycarpum* populations based on agro-morphological traits, essential oil content and yield using Euclidean distances

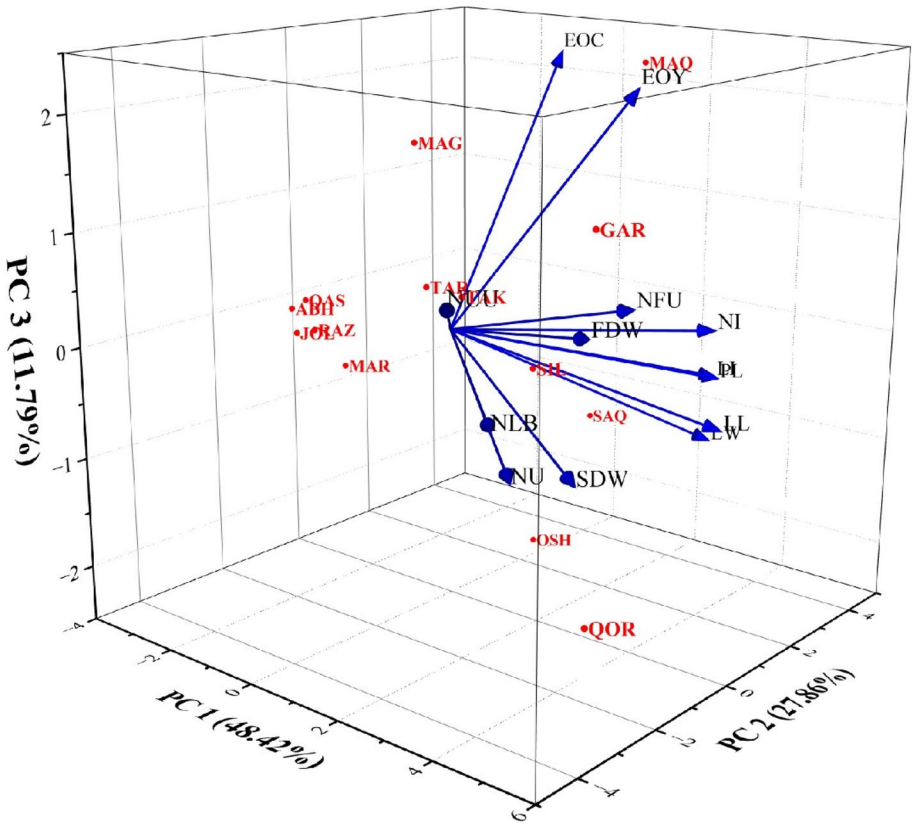

Fig. 4 3D-plot graph for the first, second and third principal components based on agro-morphological traits, essential oil content and yield for fourteen populations of *Grammosciadium platycarpum*

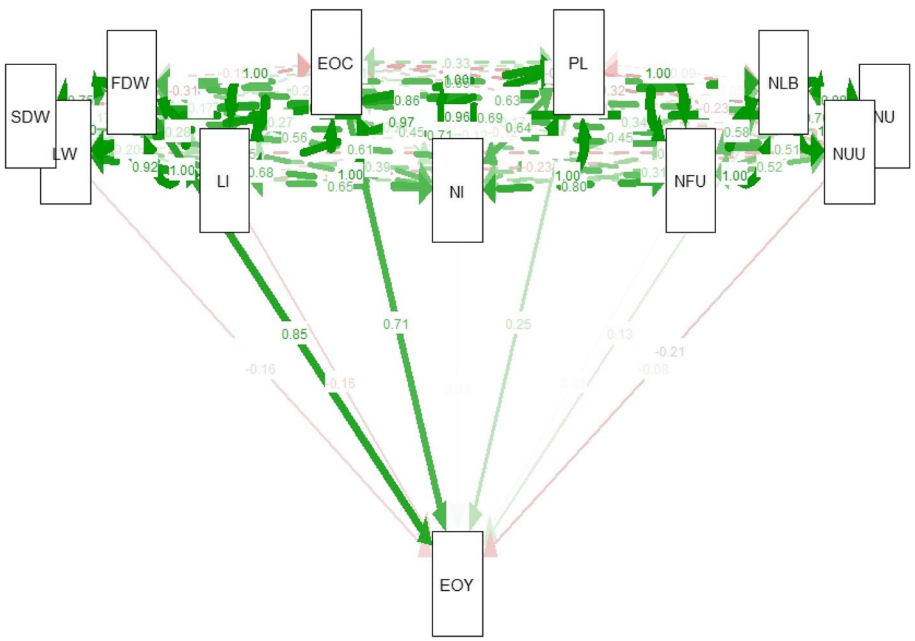

Fig. 5 Path coefficient analysis of essential oil yield (EOY) with all the agro-morphological and essential oil content of the studied *Grammosciadium platycarpum* populations. For a detailed description of the codes, cf. Table 2

of EOY, number of umbrellas, internode length, and leaf length on the EOC implies that these traits can be selected for breeding programs to improve the EOC content of *G. platycarpum* plants.

Essential oil compositions

EOs were extracted from the fruit of *G. platycarpum*, sourced from various regions of Iran, using a Clevenger apparatus. The composition of these EOs was analyzed through GC and GC-MS techniques. Based on GC-MS and GC data analysis, approximately 97.91–99.93% of essential oil compounds were recognized in different populations of *G. platycarpum* (Table 6; Fig. 7). The main chemical groups identified in the essential oil of different *G. platycarpum* populations included hydrocarbon monoterpenes (14.78–22.14%), oxygenated monoterpenes (67.54–81.75%), hydrocarbon sesquiterpenes (1.88–10.15%), and oxygenated sesquiterpenes (0.10–1.46%). Based on the results, linalool (65.90–81.62%), limonene (9.73–15.34%), and β-pinene (3.04–6.45%) were the major compounds in the essential oil of different *G. platycarpum* populations. Sonboli et al. [32] found that linalool (79–81.8%) and limonene (5.8–10%) were the principal components of *G. platycarpum* fruit essential oil. In Nickavar et al. [25] study, the most abundant compounds of *G. platycarpum* fruit essential oil were reported β-santanol (10.9%), α-farnesene (20.4%), and linalool (53.9%).

Babashpour-Asl et al. [5] identified 31 chemical components from *G. platycarpum* fruit essential oil, the main components of which were linalool (61.05%) and α-humulene (5.62%). In this study, the highest content of linalool (81.62%) was observed in the QOR population while the lowest content (65.90%) was found in the MAR population. The maximum (15.34%) and minimum (9.73%) limonene contents were found in MAR and TAR populations, respectively. Also, the MAR population had the highest content of β-pinene, while the lowest was related to the MAG population (Table 6). The amounts of the dominant compounds of the essential oil were very variable due to the geographical diversity of the collected samples. This attribute underscores a beneficial feature of plants sourced from their native habitats, as it helps identify useful chemotypes for breeding and cultivation. Different studies suggest that the quantitative and qualitative characteristics of essential oil components produced in different organs of medicinal plants are different and are influenced by the environmental factors of growing place, harvest time, and genetic characteristics [22]. The concentration of linalool in different plant species can fluctuate based on various factors, such as the specific plant part, the timing of the harvest, local climate conditions, the method of extraction, and abiotic factors affecting the plant's chemotype [16, 18, 33].

The Simple correlation coefficients of geographical and climatic characteristics with the EOC and composition of essential oil is shown in Fig. 8. Gamma-terpinene exhibited a negative and statistically significant correlation

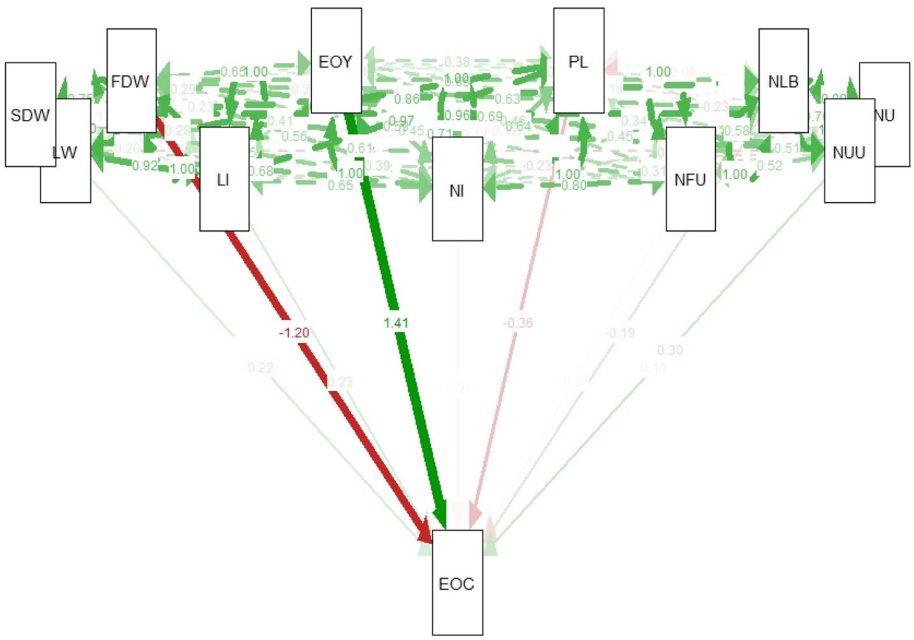

Fig. 6 Path coefficient analysis of essential oil content (EOC) with all the agro-morphological and essential oil yield of the studied *Grammosciadium platycarpum* populations. For a detailed description of the codes, cf. Table 2

Table 6 Chemical variability in the essential oils of *Grammosciadium platycarpum* populations

No.	Composition	RI	Population						
			QOR	MAG	QAS	TAR	MAQ	SIL	TAK
1	α -pinene	0987.0	-	t	0.12 ± 0.01	0.10 ± 0.02	0.19 ± 0.04	0.14 ± 0.01	0.17 ± 0.02
2	β-pinene	1008.0	3.44 ± 0.12	3.04 ± 0.34	5.15 ± 1.37	3.85 ± 0.87	4.53 ± 0.82	5.94 ± 0.95	4.18 ± 0.82
3	octanal	1027.5	0.24 ± 0.09	0.22 ± 0.07	0.39 ± 0.09	0.24 ± 0.06	0.29 ± 0.06	0.38 ± 0.09	0.26 ± 0.07
4	limonene	1055.0	12.43 ± 1.62	15.25 ± 1.37	10.51 ± 2.26	9.73 ± 0.09	11.94 ± 1.87	13.33 ± 1.91	11.91 ± 1.65
5	myrcene	1063.2	-	-	-	0.11 ± 0.01	-	t	t
6	gamma-terpinene	1084.5	-	0.96 ± 0.11	1.44 ± 0.18	0.99 ± 0.13	0.74 ± 0.12	1.09 ± 0.30	1.08 ± 0.17
7	linalool	1125.2	81.62 ± 5.26	71.98 ± 2.71	71.88 ± 3.64	80.68 ± 4.69	75.56 ± 5.89	70.09 ± 4.76	73.45 ± 3.93
8	α-Terpineol	1180.0	t	t	t	t	0.12 ± 0.01	-	0.19 ± 0.05
9	geraniol	1225.7	0.13 ± 0.01	0.15 ± 0.02	0.21 ± 0.01	t	t	0.12 ± 0.02	0.15 ± 0.01
10	bornyl acetate	1274.0	-	1.87 ± 0.82	0.62 ± 0.10	-	-	-	t
11	α-copaene	1348.1	-	0.38 ± 0.06	0.10 ± 0.00	-	0.12 ± 0.01	-	-
12	caryophyllene	1439.1	0.10 ± 0.01	0.93 ± 0.03	2.45 ± 0.37	0.93 ± 0.25	0.75 ± 0.03	1.71 ± 0.56	2.01 ± 0.12
13	(Z, E)-α-farnesene	1510.0	1.05 ± 0.24	1.31 ± 0.11	2.40 ± 0.33	1.34 ± 0.36	1.98 ± 0.47	2.59 ± 0.70	1.85 ± 0.16
14	bicylogermacrene	1517.3	0.31 ± 0.04	1.34 ± 0.09	0.46 ± 0.07	0.36 ± 0.05	0.71 ± 0.14	t	0.34 ± 0.02
15	α-farnesene	1522.8	0.42 ± 0.03	1.57 ± 0.13	2.16 ± 0.35	1.42 ± 0.18	1.84 ± 0.49	2.01 ± 0.38	2.12 ± 0.37
16	spatulenol	1595.3	t	0.25 ± 0.02	0.34 ± 0.09	0.18 ± 0.02	0.13 ± 0.01	t	t
17	caryophyllene oxide	1601.1	0.10 ± 0.00	0.54 ± 0.05	t	t	0.29 ± 0.03	0.32 ± 0.08	0.41 ± 0.08
18	caryophyllenol-II	1658.9	-	t	0.38 ± 0.05	-	0.15 ± 0.01	0.19 ± 0.02	0.25 ± 0.04
	Monoterpene hydrocarbons		15.78	19.25	17.22	14.78	17.40	20.50	17.34
	Oxygenated monoterpenes		81.75	74.22	73.10	80.92	75.97	70.59	74.05
	Sesquiterpene hydrocarbons		1.88	5.53	7.75	4.05	5.40	6.31	6.32
	Oxygenated sesquiterpenes		0.10	0.79	0.72	0.18	0.57	0.51	1.46
	Total identified		99.51	99.79	98.79	99.93	99.34	97.91	99.17
No.	Composition	RI	Population						
			MAR	GAR	JOL	RAZ	SAQ	OSH	ABH
1	α -pinene	0987.0	0.23±0.07	0.13±0.01	0.27±0.04	0.15±0.03	0.11±0.01	0.18±0.05	0.19±0.04
2	β-pinene	1008.0	6.45±0.52	3.05±0.39	3.19±0.41	4.83±0.75	3.92±0.38	4.21±0.36	3.91±0.29
3	octanal	1027.5	0.21±0.05	0.19±0.04	0.29±0.09	0.31±0.11	0.37±0.10	0.28±0.07	0.41±0.13
4	limonene	1055.0	15.34±2.73	12.61±2.29	11.84±1.97	10.74±1.64	10.39±1.58	11.48±1.43	13.92±3.46
5	myrcene	1063.2	0.12±0.01	0.14±0.01	0.18±0.02	-	t	t	0.21±0.03
6	gamma-terpinene	1084.5	t	t	t	1.04±0.14	1.23±0.17	1.02±0.09	1.32±0.14
7	linalool	1125.2	65.90±2.81	73.46±3.10	72.43±2.92	72.84±2.63	77.19±2.95	76.61±2.01	68.79±2.31
8	α-Terpineol	1180.0	0.53±0.21	t	-	t	t	-	0.23±0.08
9	geraniol	1225.7	0.45±0.13	0.34±0.17	t	0.21±0.10	0.16±0.05	0.18±0.11	0.21±0.05
10	bornyl acetate	1274.0	0.45±0.07	0.51±0.14	0.41±0.09	1.53±0.37	-	-	1.32±0.25
11	α-copaene	1348.1	0.12±0.01	0.19±0.03	t	0.12±0.01	-	t	0.21±0.06
12	caryophyllene	1439.1	1.95±0.44	2.12±0.51	1.63±0.26	1.49±0.20	1.08±0.15	1.85±0.17	2.19±0.31
13	(Z,E)-α-farnesene	1510.0	2.20±0.38	2.33±0.27	3.51±0.49	1.81±0.15	1.83±0.13	1.34±0.10	2.41±0.19
14	bicylogermacrene	1517.3	1.45±0.15	1.61±0.19	1.82±0.24	0.43±0.08	0.94±0.05	0.84±0.07	1.63±0.12
15	α-farnesene	1522.8	2.16±0.31	1.85±0.27	3.19±0.45	1.74±0.11	1.41±0.17	1.01±0.14	2.13±0.31
16	spatulenol	1595.3	0.38±0.02	t	0.22±0.01	0.33±0.04	t	0.23±0.02	t
17	caryophyllene oxide	1601.1	0.37±0.04	0.53±0.09	0.34±0.03	0.51±0.07	0.41±0.05	t	0.41±0.02
18	caryophyllenol-II	1658.9	0.41±0.06	0.28±0.01	t	-	0.12±0.03	0.21±0.02	0.16±0.01
	Monoterpene hydrocarbons		22.14	15.93	15.48	16.76	15.65	16.89	19.55
	Oxygenated monoterpenes		67.54	74.50	73.13	74.89	77.72	77.07	70.96
	Sesquiterpene hydrocarbons		7.88	8.10	10.15	5.59	5.24	5.04	8.57
	Oxygenated sesquiterpenes		1.16	0.81	0.56	0.84	0.53	0.44	0.57
	Total identified		98.72	99.34	99.32	98.08	99.14	99.44	99.65

RI: Retention index

t: trace < 0.10%

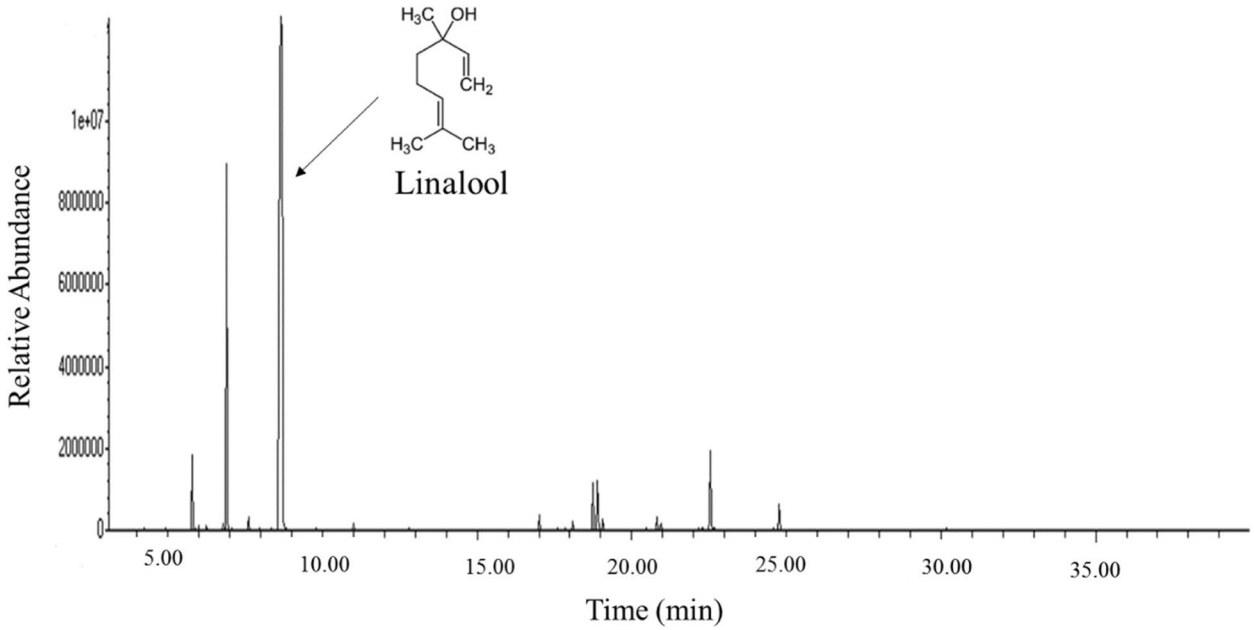

Fig. 7 The GC–MS chromatogram of *Grammosciadium platycarpum* essential oil

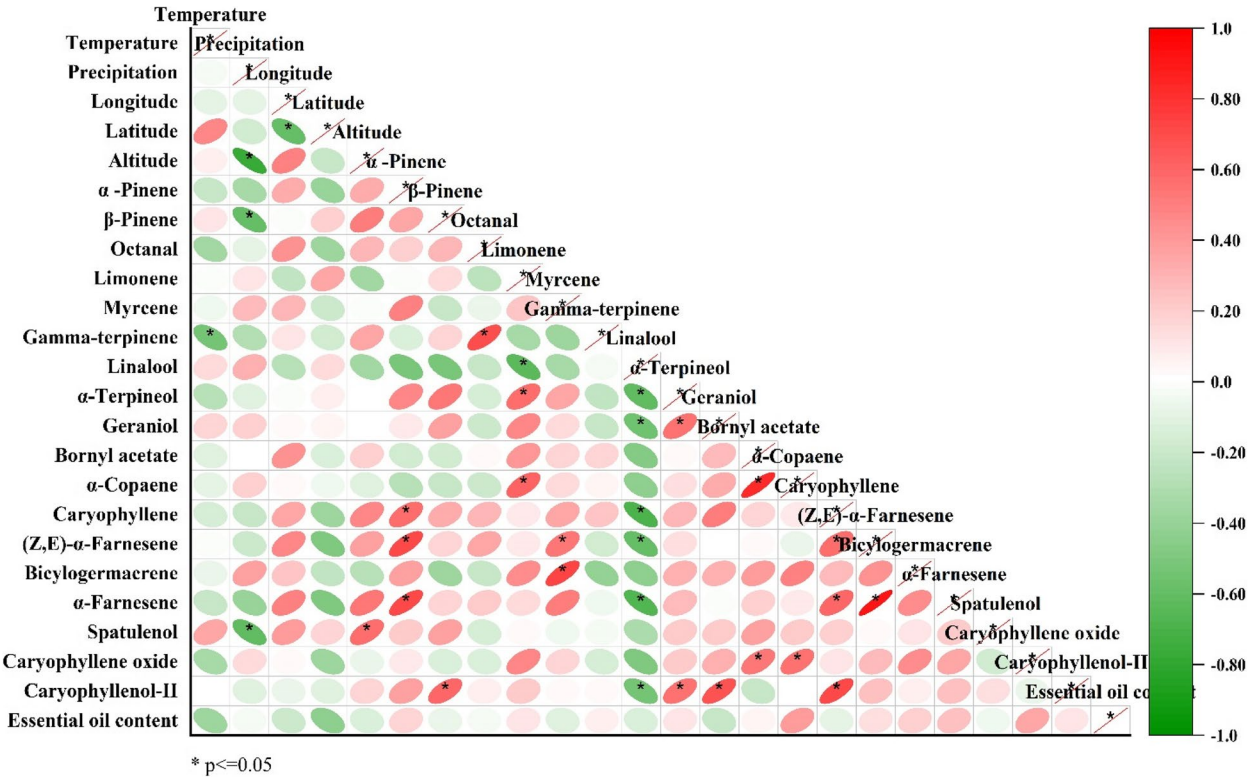

Fig. 8 Pearson correlation representation of geographical and climatic characteristics with essential oil content and compounds of *Grammosciadium platycarpum* populations

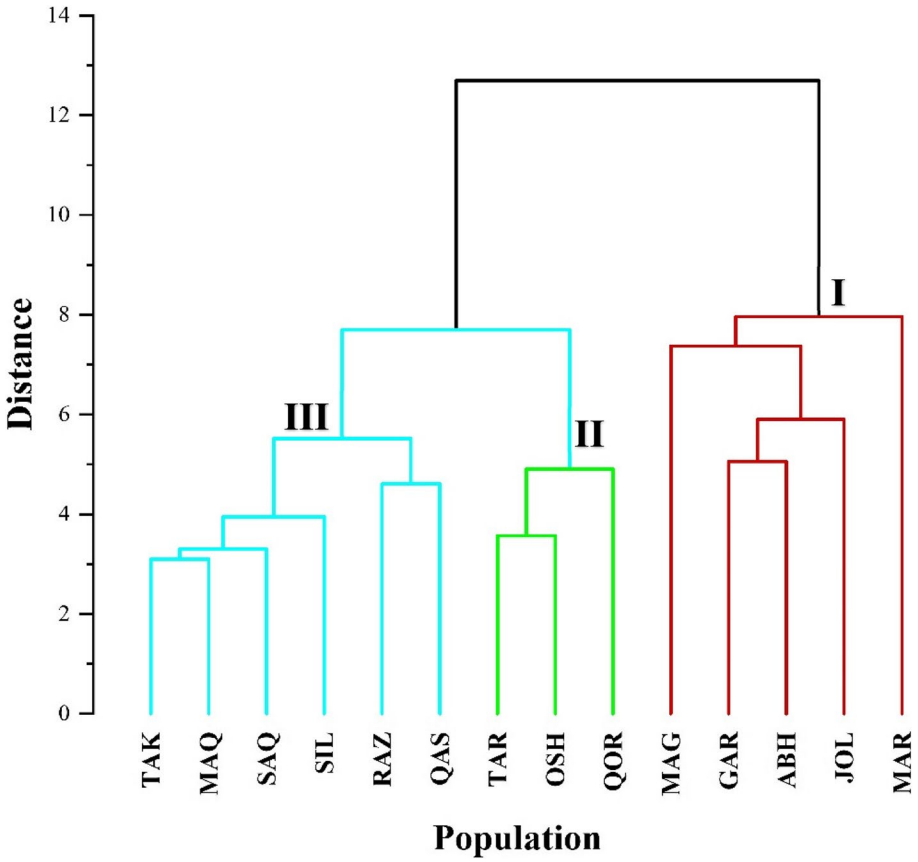

Fig. 9 Cluster analysis of *Grammosciadium platycarpum* populations based on essential oil compounds using Euclidean distances

with the temperature. In addition, β-pinene and spatulenol had a negative and significant correlation with precipitation. The linalool showed a negative and significant correlation with the limonene, α-terpineol, geranol, caryophyllene, (Z, E)-α-farnesene, α-farnesene, and caryophyllenol-II. There was a positive and significant correlation between caryophyllenol-II with bronyl acetate and α-copaene. The α-Farnesene had a positive and significant correlation with α-pinene, caryophyllene, and (Z, E)-α-farnesene, and had a negative correlation with linalool.

Cluster analysis of different populations based on essential oil compositions is depicted in Fig. 9. The findings from the cluster analysis indicated that the populations were categorized into three main groups. The first group (I) includes populations MAR, JOL, ABH, GAR, and MAG. In addition to having a high level of linalool (65.90–73.46%) as the main compound, this group was superior in terms of limonene content compared to other populations. Populations of the second group (II) were superior in terms of linalool content compared to other populations, and QOR, TAR, and OSH populations were placed in this group with 81.62, 80.68 and 76.61% of linalool, respectively. TAK, MAQ, SAQ, SIL, RAZ, and QAS populations were placed in the third group (III), which was average in terms of essential oil compounds. The bi-plot (Fig. 10) presents the relationship between populations and essential oil compounds. The PC1 and PC2 accounted for 32.10 and 12.24% of the total variance, respectively. Additionally, this graph categorized the populations into three main groups, aligning with the findings from the cluster analysis.

Phenolic compounds profiles

Phenolic compounds are commonly utilized for treatment of human diseases thanks to their many biological attributes including anti-inflammatory, anti-cancer, and antioxidant effects [28]. The content of phenolic acids of different populations of *G. platycarpum* was analyzed by HPLC. The main phenolic compounds identified in *G. platycarpum* extract included rutin, chlorogenic acid, and ferulic acid (Figs. 11 and 12). Rutin is one of the most important flavonoids that has medicinal activities such as anti-inflammatory, antiradical, antiproliferative, and antimetastatic [36]. The amount of rutin varied from 0.85 to 2.26 mg/g of dry weight among different populations of *G.*

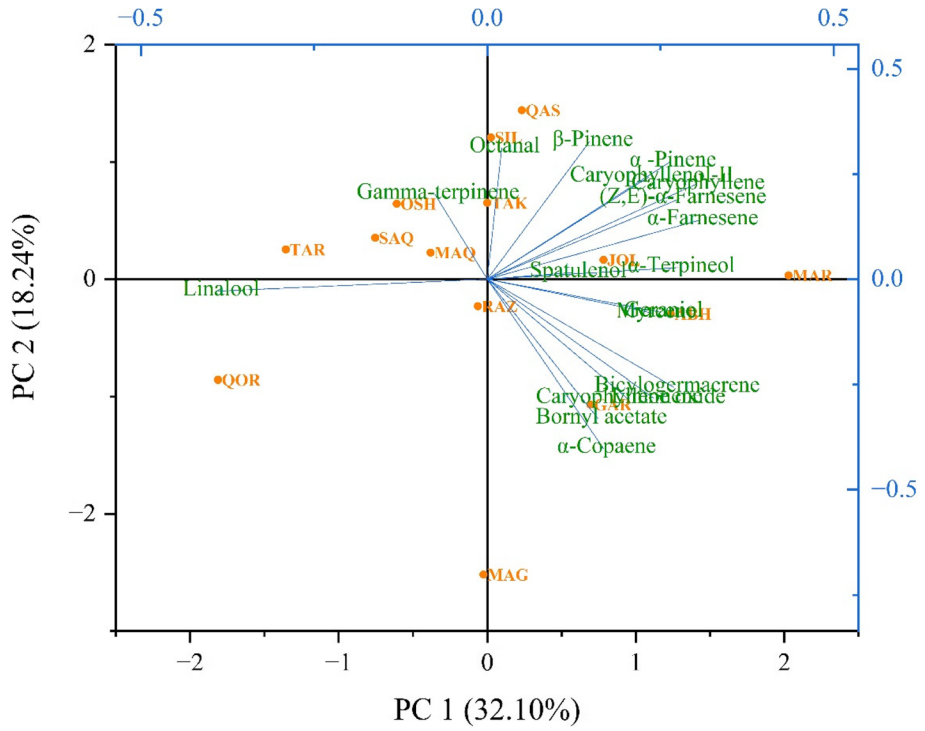

Fig. 10 Bi-plot graph for the first and second principal components based on the essential oil compounds for fourteen populations of *Grammosciadium platycarpum*

platycarpum, which was the most populous in QAS and the least populous in MAR. Chlorogenic acid is the most important and available polyphenol among phenolic acid compounds, which has antibacterial, anti-inflammatory, antioxidant activity, anti-hypertension, cardioprotective, neuroprotective, and central nervous system stimulator properties [36]. The amount of chlorogenic acid varied from 0.032 to 0.429 mg/g of dry weight among different populations of *G. platycarpum*. The highest amount of chlorogenic acid was related to the population of QAS. Ferulic acid is one of the phenolic compounds that have therapeutic properties such as anti-diabetic, anti-cancer,

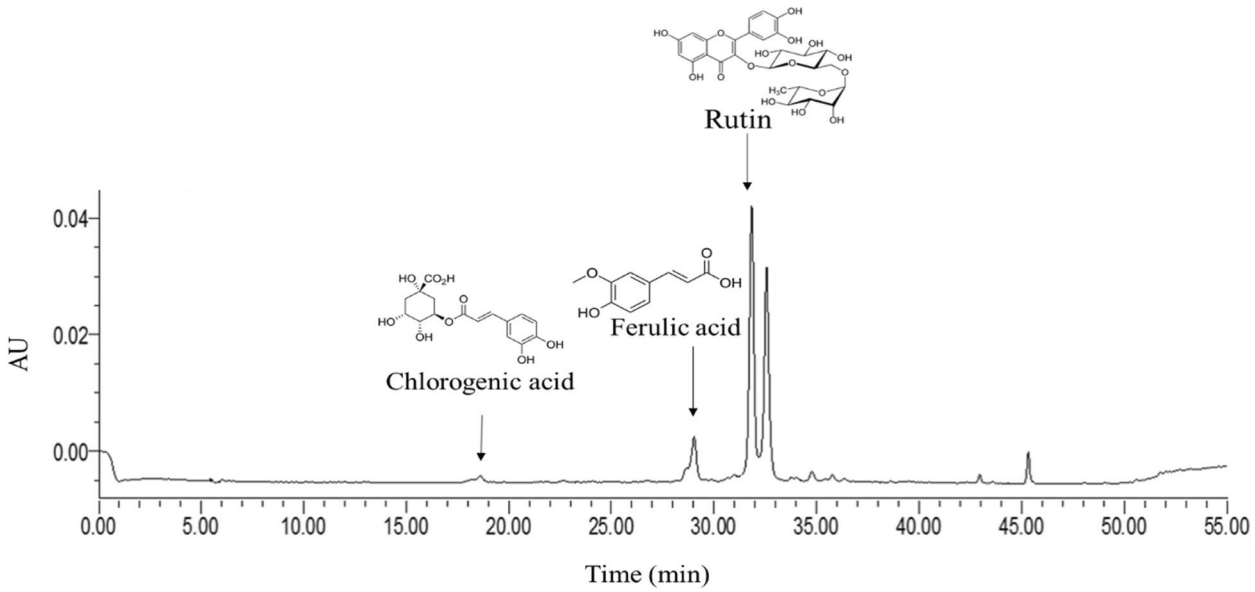

Fig. 11 The HPLC–PDA chromatogram of *Grammosciadium platycarpum* extract

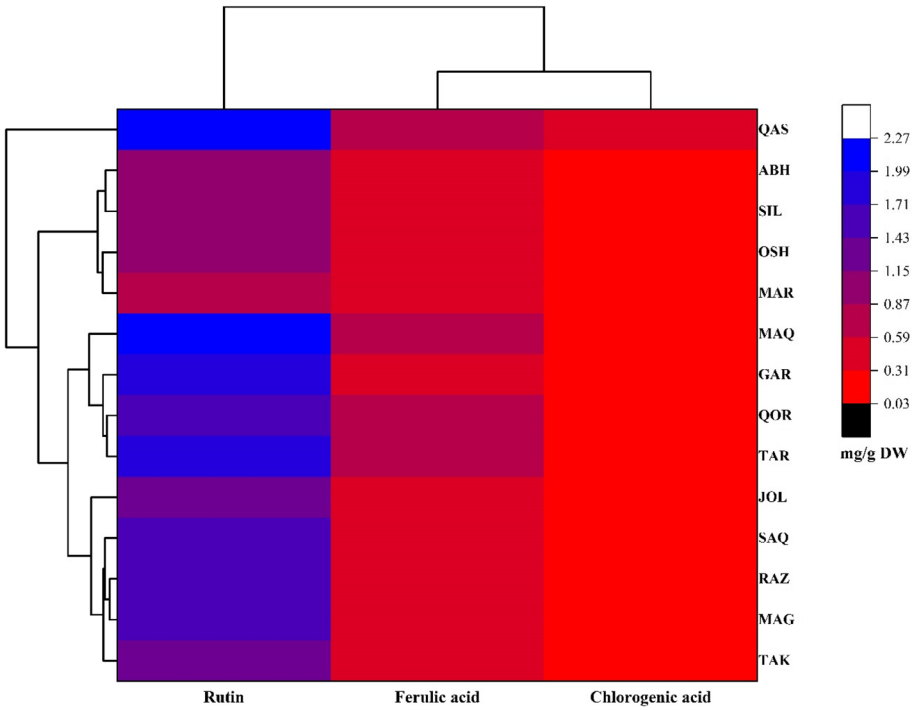

Fig. 12 Heat map of the phenolic compound profiles of *Grammosciadium platycarpum* populations

anti-inflammatory, neuroprotective, and antioxidant. The maximum amounts of ferulic acid 0.662, 0.599, and 0.596 mg/g DW were related to the QOR, TAR and MAQ populations, respectively.

TPC and TFC

A statistically significant disparity ($p < 0.01$) was identified among various populations of *G. platycarpum* concerning the aggregate content of phenolic compounds and flavonoids. The TPC within *G. platycarpum* fruit exhibited a range from 1.46 to 19.22 mg GAE/g DW. The QAS (19.22 mg GAE/g DW), TAR (18.30 mg GAE/g DW), and JOL (18.14 mg GAE/g DW) populations demonstrated the most elevated levels of TPC, whereas the MAR population exhibited the lowest concentration, measured at 1.46 mg GAE/g DW (Fig. 13a). Based on the obtained results, the TFC of the fruit extract across different populations of *G. platycarpum* was observed to range from 11.66 to 27.1 (mg RE/g DW), the lowest of which was related to the population of OSH and the highest in the population of QAS (Fig. 13b). The variation among different populations of *G. platycarpum* in TPC, TFC, and antioxidant activity can be caused by climatic factors, geographical conditions, and genetics [6]. Furthermore, the type of solvent, environmental factors and climatic conditions are paramount variables influencing the quantity of phenolic and flavonoid compounds obtained from botanical sources [28]. Phenolic compounds have been documented in the literature for their antimicrobial and antioxidant activities, playing a crucial role in plants defense mechanisms by warding off infections caused by pathogens and pathogenic microorganisms. Further, the existence of these compounds within plant tissues serves as a shield against the detrimental impacts of reactive oxygen species [20].

Conclusion

Linalool is a non-cyclic oxygenated monoterpene. It has extensive uses in the food and cosmetic fields, particularly for perfume and cologne production. Due to its commercial value and high demand, it is essential to find new plant sources rich in linalool to support its extraction as well as purification. The demand for products derived from linalool is increasing, necessitating the improvement and cultivation of the plant to meet demands in the food, cosmetic, and perfumery industries. A recent study investigated the diversity of agro-morphological and phytochemical attributes, essential oil content, and compounds in fourteen populations of *G. platycarpum*. The findings revealed significant diversity among the different populations of *G. platycarpum*, particularly in terms of agro-morphological characteristics, phytochemical properties, as well as EOC and composition. This research provided valuable preliminary information on the characteristics of various

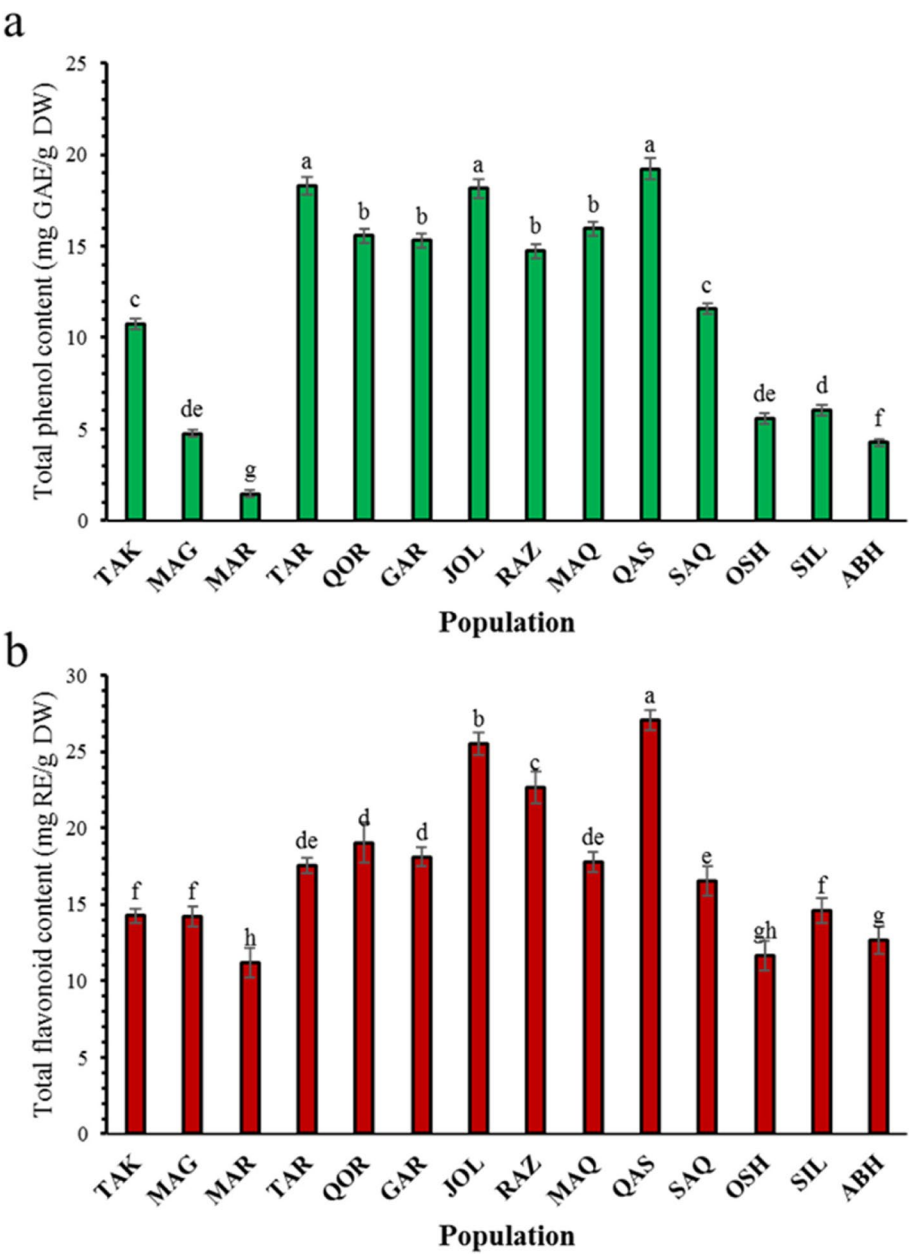

Fig. 13 Total phenol (**a**) and flavonoids content (**b**) among the populations of *Grammosciadium platycarpum*

G. platycarpum populations, especially pertaining to agro-morphological traits, essential oil content, linalool content, and phenolic compounds. The considerable genetic variability within these populations facilitates the selection of superior populations for domestication and breeding programs, aimed at developing cultivars with beneficial growth traits, adaptability, and a high concentration of linalool.

Supplementary Information

The online version contains supplementary material available at https://doi.org/10.1186/s12870-025-06231-4.

Supplementary Material 1.

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Ethical review
This study does not involve any human or animal testing.

Authors' contributions
GE: methodology, sample collection, conceptualization, supervision, data curation, data analysis and writing-original draft, BSA: lab work, analysis data; AS: reviewing, and editing; H.R: methodology and editing; MHM: methodology, conceptualization, data curation, reviewing, and editing.

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Data availability
All data generated or analyzed during this study are included in this article. Further enquiries can be directed to the corresponding author.

Declarations

Ethics approval and consent to participate
This manuscript is an original research and has not been published or submitted in other journals.

Consent for publication
Not applicable.

Competing interests
The authors declare no competing interests.

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