



ORIGINAL ARTICLE

Determination of volatile compounds in Andean berry (*Rubus glaucus* Benth) fruits to discriminate among commercial materials cultivated in Risaralda, Colombia

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Abstract

In Colombia, the cultivation of *Rubus glaucus* Benth. (Andean blackberry) is widespread. Commercial materials include fruits with and without thorns. In the present work, the volatile compounds in ripe mora de Castilla blackberry fruits from plants with and without thorns grown in two locations in the Department of Risaralda were compared. To obtain the volatile compounds, microextraction in the solid phase was used, and the volatile compounds were analyzed via gas chromatography coupled with mass spectrometry. A qualitative analysis of the identified compounds was performed, and a quantitative analysis was performed to compare the relative areas of those that were present in all the profiles. A maximum of 103 compounds were identified, of which 54 volatile compounds were present in all the profiles, corresponding to 18 terpenes, six fatty acid derivatives, 13 esters, 13 alcohols, and four aldehydes. Significant differences were found between the materials from plants with and without thorns and between the materials from plants cultivated in different locations, mainly with respect to the acid contents.

Keywords *Rubus glaucus* Benth. · Volatile compounds · Solid phase microextraction · Materials with and without thorns

Abbreviations

GC–MS Gas chromatography/mass spectrometry
VOCs Volatile organic compounds

Introduction

Berries are among the most consumed fruits in the human diet, including blackberries (*Rubus* spp.), strawberries (*Fragaria x ananassa*), raspberries (*Rubus occidentalis*), and blueberries (*Vaccinium corymbosum*), which are rich in minerals, vitamins, dietary fiber, and especially polyphenols and volatile compounds (Du and Qian 2010).

The genus *Rubus* comprises more than 1000 species and is distributed on six continents, including both blackberry and raspberry and their hybrids, and is especially cultivated in cold climates; however, most of these species originated on islands of the South Pacific (Hummer 2010). Since ancient times, species belonging to the genus *Rubus* have been associated with medicinal properties. Among other applications, they have been used in the treatment of colic pain, inflammation, diarrhea, wounds, and diabetes and as antimicrobial agents because of their content of phenolic compounds, tannins, flavonoids and anthocyanins (Rocabado et al. 2008), and they present a great variety of volatile compounds that give it organoleptic characteristics of great interest; thus, materials of the genus *Rubus* have great potential (Demir 2023).

Volatile organic compounds (VOCs) are of great interest in the perception of the sensory qualities of fruits and are directly related to their aroma. Volatiles are highly chemically diverse and include different functional groups, mainly esters, alcohols, aldehydes, ketones, lactones, and

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terpenoids, constituting specific profiles for each species (Apréa 2015). However, the concentration of these compounds can be affected by agronomic factors such as cultivar variation, weather conditions, soil conditions, and maturation stage and technological factors such as harvest and postharvest treatment (El Hadi 2013).

Volatile compounds have been widely studied in fruits such as apples (*Malus asiatica* var. Ruixue), in which transcriptomic and metabolomic studies have been carried out (Liu et al. 2021). Studies have also been carried out in grapes (*Vitis rotundifolia* Michx.) (Deng et al. 2021) to identify the profile of volatile compounds among cultivars and how these compounds vary during postharvest treatments. In blueberry crops (*Vaccinium angustifolium*), an attempt has been made to identify significant differences between shrubs in a cultivar with respect to the volatile profile of the fruit (Forney et al. 2022). In raspberry (*Rubus idaeus*), the entire volatilomic profile has been characterized (Farneti et al. 2023), and in blackberry (*Rubus* spp. Hyb), the entire volatilomic profile has been used to distinguish between two cultivated species (Klesk and Qian 2003).

In this manner, the importance of volatile compounds in the identification of cultivars of different types of fruit is noteworthy; however, volatile compounds have been used not only for the identification of cultivars but also to characterize fruits based on their place of origin. For example, in studies carried out in blackberry (*Rubus ulmifolius* Schott), the volatile profile provided a designation of origin to the crops in Calabria, Italy (D'Agostino et al. 2022). Goji berry (*Lycium barbarum*) has also been studied to identify differences in fruits grown in places outside its place of origin (Zhou et al. 2023).

The Andean blackberry (*Rubus glaucus* Benth.) is a fruit that belongs to the *Rubus* genus and the Rosacea family; it is native to the tropical Andean zone along with a great variety of species and is consumed fresh or minimally processed owing to its wide variety of bioactive compounds, which are mainly phenolic (Horvitz et al. 2017). In Colombia, this species is grown in 18 departments and is considered a competitive fruit because its production is permanent (SIOC 2021). It presents great morphological diversity, such as the presence or absence of thorns, the leaf shape, and the fruit number and color. With respect to the presence or absence of thorns, there are two types of cultivars: with thorns and without thorns.

The main studies on Andean blackberry have focused on efforts to reduce postharvest losses and the effects of storage (García Muñoz et al. 2020; Horvitz et al. 2017), along with the effects of soil micro- and macronutrients on fruit quality (Monroy Cárdenas et al. 2019) and the use of different coatings to preserve the fruit characteristics (Cortés Rodríguez et al. 2020; Gravier-Rodríguez et al. 2023). However,

few studies have characterized the bioactive compounds of interest for human consumption in mora de Castilla blackberry according to the origin of the fruit.

In Colombia, the volatile compound profile during the maturation process has been studied in *Rubus glaucus* Benth. (Sinuco 2013). Additionally, physicochemical and antioxidant characterization studies of *Rubus glaucus* Benth. (Andean blackberry) fruits from plants with and without thorns grown in Risaralda have been conducted (Guerrero 2023). However, no studies have been conducted that demonstrate differences related to volatile compounds in commercial materials attributed to the cultivated material and/or the place of origin.

In this context, the objective of this study was to analyze and compare the profiles of volatile organic compounds present in mature *Rubus glaucus* Benth. fruits from plants with and without thorns by gas chromatography coupled with mass spectrometry (GC–MS) from crops from the Department of Risaralda, Colombia.

Materials and methodology

Plant material

A completely randomized block design was used. The sampling was carried out in two municipalities of the department of Risaralda located between 1600 and 1900 m a.s.l. In the municipality of Guática, the farm “Santa Teresita” is in Vereda La Unión, with geographic coordinates N 05° 19' 7.41" and W 075° 47' 29.72". Meanwhile, in Santa Rosa de Cabal, the farm “El Rubí” is situated in the area known as Sidewalk Potrereros, with coordinates N 04° 53' 24.1" and W 075° 33' 44.0". Ripe *Rubus glaucus* Benth. (Andean blackberry) fruits were collected from plants with and without thorns at maturity stages 5 and 6 according to the classification established in the NTC 4106 standard (ICONTEC 1997). The fruits were stored in Ziploc-type plastic bags at a temperature of 4 °C for later analysis.

Extraction of volatile compounds

The experiments were carried out using the solid-phase microextraction (SPME) method in headspace mode, using 85 µm polydimethylsiloxane (PDMS) fiber, following the methodology described previously (D'Agostino 2014) with some modifications. Three grams of frozen and macerated mora de Castilla blackberries was placed in a 10 mL vial, which was sealed with a screw cap containing a predrilled Teflon rubber septum. The vial was placed in a container at 45 °C in a water bath with a magnetic stirrer and allowed to

equilibrate for 5 min, after which the fiber was exposed to the headspace to adsorb the analytes for 30 min.

Analysis of volatile compounds by GC–MS

Chromatographic analysis was carried out with a gas chromatograph (GC-2010 Plus) coupled to a mass spectrometer (QP-2020) equipped with a Shimadzu SH-Rxi-5MS capillary column 30 m in length and with an internal diameter of 0.25 mm and a 0.25 μm film thickness. Helium was used as the carrier gas at a linear speed of 1.0 ml min^{-1} . The oven temperature was set at 40 $^{\circ}\text{C}$ (2 min) and then increased by 8 $^{\circ}\text{C/min}$ until it reached 200 $^{\circ}\text{C}$ (8 min), which was maintained for 5 min. Then, the oven temperature was increased by 10 $^{\circ}\text{C/min}$ until it reached 250 $^{\circ}\text{C}$ as the final temperature, which was maintained for 10 min. The mass spectrometer was operated in electron impact (EI) mode at 70 eV within the mass range of m/z 35–450. The transfer line temperature and ionization source were set at 280 and 230 $^{\circ}\text{C}$, respectively (D'Agostino et al. 2015), respectively. Qualitative analysis was performed by comparison with spectra from the NIST mass spectral library.

Statistical analysis

The data for the evaluated plant material were the averages of three repetitions. Multivariate analysis of variance (MANOVA) was used in STATISTICA version 9.0 2020 software to determine the significant differences in other volatiles between the sampled municipalities. For the comparison of means, the Tukey test was used with a significance level of 5% ($p \leq 0.05$).

Results

Figures 1 and 2 show the chromatographic profiles identified in the *Rubus glaucus* material evaluated. And the names of the identified compounds can be seen in Table 1.

A quantitative analysis was carried out with the compounds present in all the study materials; a total of 54 volatile compounds were quantified, including 18 terpenes, six fatty acid derivatives, 13 esters, 13 alcohols, and four aldehydes, like those reported in other studies on volatiles in mora de Castilla blackberry (Meret et al. 2011). Differences were found mainly in the acid contents. According to the multivariate analysis, with a significance of 95%, the place of cultivation and the type of material clearly had significant effects on the volatile compounds evaluated. Among the 54 compounds identified by GC-MS, only 36 presented sufficiently significant differences to distinguish among materials.

Discussion

The chromatographic profiles revealed differences in the volatile compounds identified in the *Rubus glaucus* Benth. materials studied. The profile of the Andean blackberry fruits from plants with thorns cultivated in Guática presented a total of 85 compounds, whereas that of the fruits from plants without thorns cultivated in Guática presented 103 compounds (Fig. 1). With respect to the chromatographic profile of the fruits from plants with thorns from the municipality of Santa Rosa, 78 compounds were found, whereas the profile of fruits from plants without thorns grown in the same location presented a total of 103 compounds (Fig. 2). Statistical analysis revealed significant differences ($p\text{-value} < 0.05$) between the materials from plants with and without thorns, with the number of volatile compounds being greater for the fruits from plants without thorns, and between cultivation locations, with the fruits from the Guática crops presenting a greater number of volatile compounds than those grown in Santa Rosa.

These results are in line with those of previous studies, where differences in the content of total phenols and total anthocyanins were observed between the materials from plants with and without thorns (Álvarez et al. 2021, 2023), as were differences in the content of ascorbic acid and the antioxidant activity between materials cultured in different locations (Álvarez et al. 2023). These differences can be attributed to the type of material grown, harvest maturity, environmental factors, and crop management, among other factors (Farg et al. 2022; Horvitz et al. 2017; Samaniego et al. 2020; Schulz and Chim 2019).

According to Fig. 3, a total of 20 statistically significant compounds were identified in mora de Castilla blackberry fruits from plants with thorns grown in the municipality of Guática, whereas a total of 14 compounds were identified in fruits from plants without thorns. The compounds identified in both materials were 2-heptanol, 2-nonanol, ethyl acetate, terpinen-4-ol, β -myrcene, β -pinene and α -pinene.

Figure 4 shows that for fruits from plants with thorns grown in Santa Rosa de Cabal, there are 14 volatile compounds that enable differentiation between materials, and for fruits from plants without thorns, there are 18 statistically significant compounds, including 2-nonanol, camphene, ethyl acetate, ethyl benzoate, terpinen-4-ol, terpinolene, β -myrcene and α -pinene.

Most of the volatile compounds found, especially those that are common to both cultivation sites, have been reported as volatile compounds in other cultivars of the *Rubus* genus (D'Agostino et al. 2015), except for β -myrcene, β -pinene and α -pinene; however, these compounds have been reported in the cultivar *Rubus glaucus* Benth. (Meret et al.

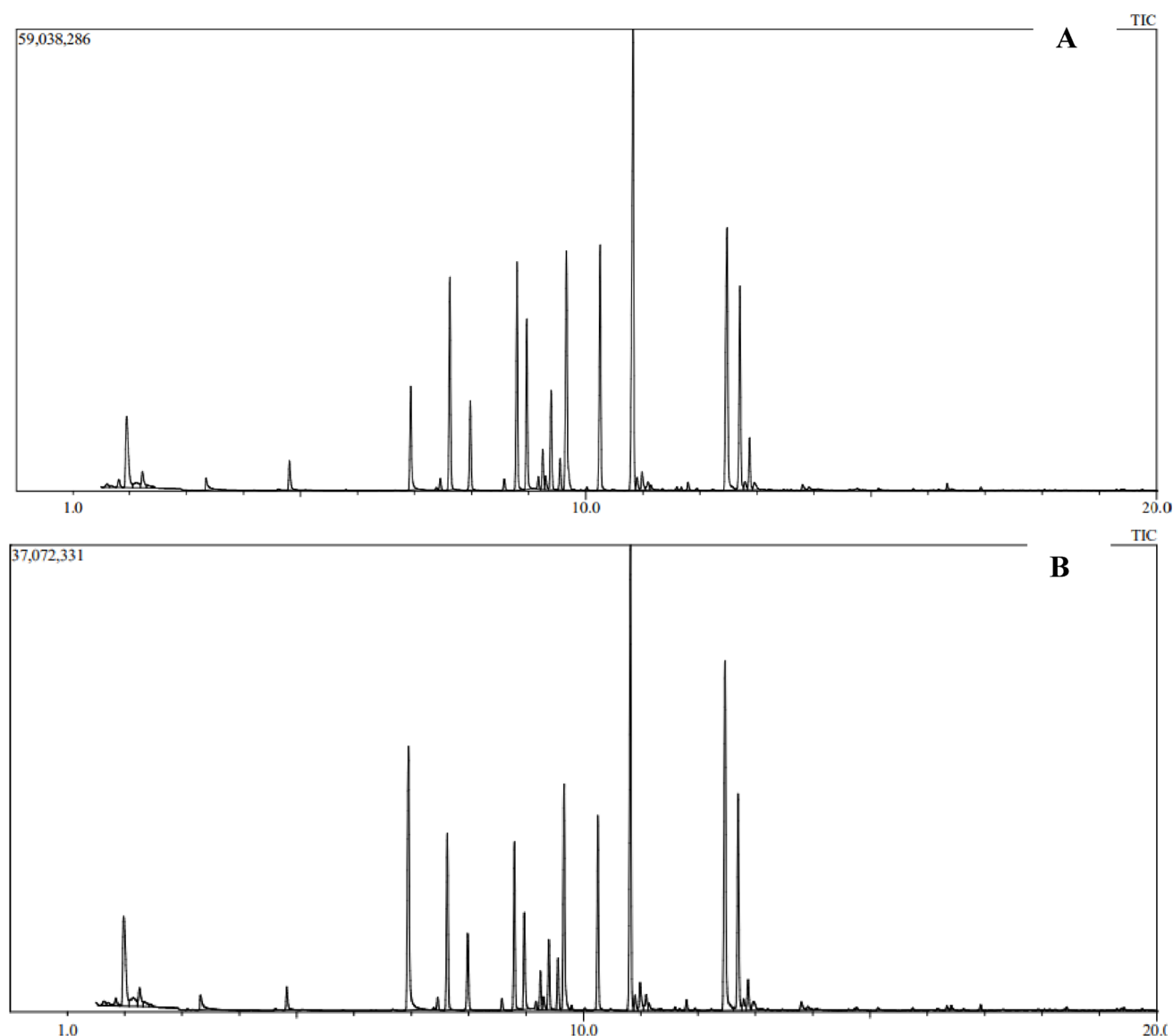


Fig. 1 Chromatogram of mora de Castilla blackberry fruits from plants **A** with thorns and **B** without thorns from the municipality of Guática

2011), indicating differences in the volatile profiles between mora de Castilla blackberries and other cultivars.

According to the heatmap of correlations (Fig. 5), the compounds that had the highest positive correlation and that allowed association with Guática mora de Castilla with thorns were borneol, dodecanal, caryophyllene, and limonene. In relation to Guática mora de Castilla without thorns, the compounds with a positive correlation were methyl benzoate, tricycline, and β -pinene. For plants from Santa Rosa de Cabal with thorns, compounds such as trans-3-carene-2-ol, none-1-ol, and α -pinene were strongly positively correlated. Finally, mora de Castilla blackberries produced in Santa Rosa de Cabal from plants with thorns presented positive correlations with the compounds terpinolene, β -cymene, geraniol, hexyl benzoate, and nonanal.

Finally, the heatmap allowed us to observe that there is variability in the volatile compounds of the fruits collected in the different municipalities, and each material and each place of cultivation presents unique compounds that allow differentiation between these factors.

Conclusion

The SPME technique for the extraction of volatiles using PDMS fiber and the use of gas chromatography coupled with mass spectrometry constitute a valuable route for the analysis of volatile profiles in the mora de Castilla blackberry (*Rubus glaucus* Benth.), presenting reproducible results.

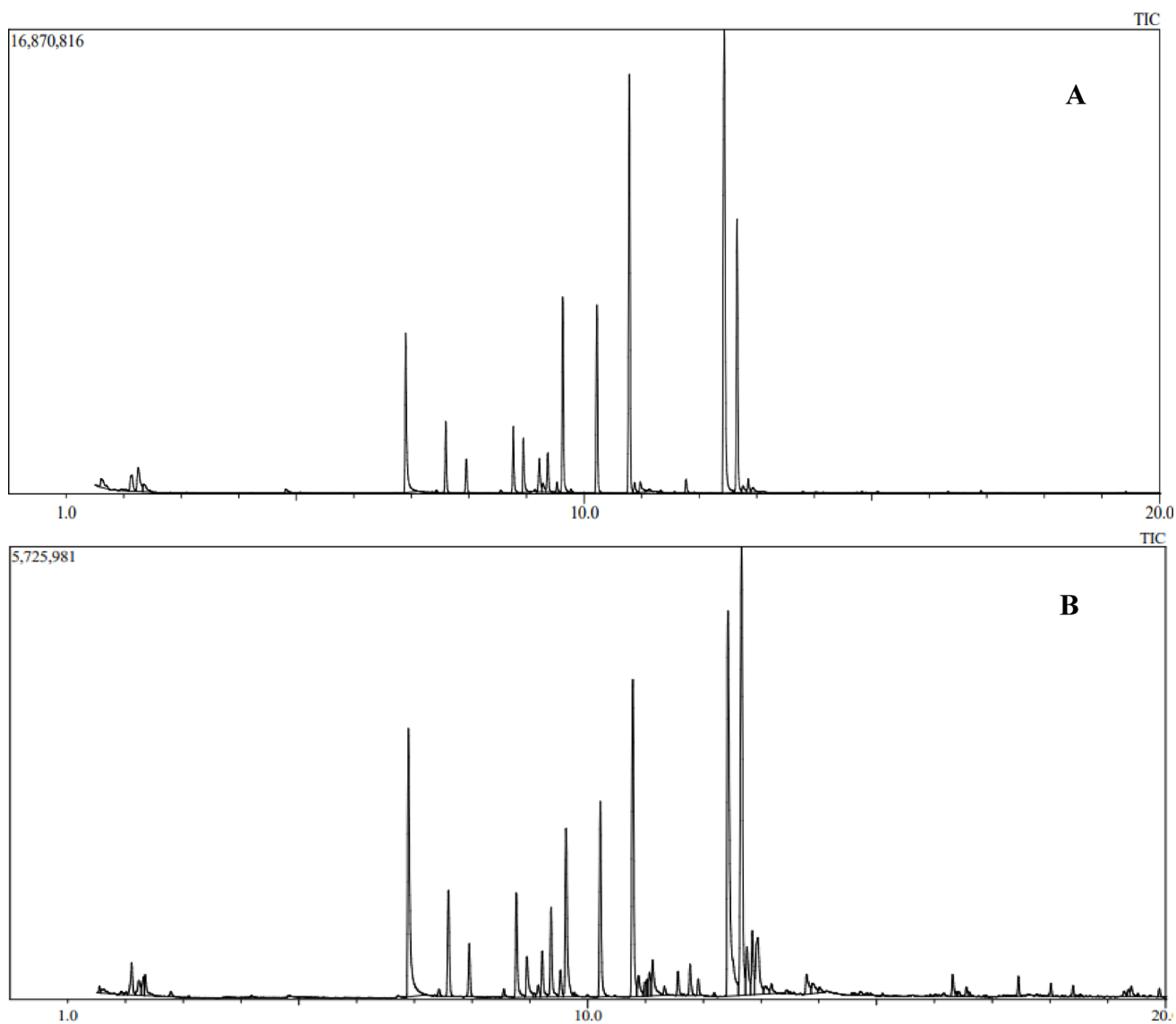


Fig. 2 Chromatogram of mora de Castilla blackberry fruits from plants **A** with thorns and **B** without thorns from the municipality of Santa Rosa de Cabal

Differentiation is possible both between planting material types (with and without thorns) and between different places of cultivation via the volatile compounds present in mora de Castilla blackberry, with specific compounds for each group of characteristics, such as the place of cultivation and the type of material shown.

Table 1 Compounds identified in the chromatographic profiles from the *Rubus glaucus* material evaluated

Guática with thorns	Guática without thorns	Santa Rosa de Cabal with thorns	Santa Rosa de Cabal without thorns
(+)-4-Carene	(+)-4-Carene	(1R,2R,3R,5S)-(-)-Isopinocampheol	(-)-Myrtenol
alpha.-Pinene	alpha-Cadinol	(1R,2R,3R,5S)-(-)-Isopinocampheol	(+)-4-Carene
beta.-Myrcene	alpha-Pinene	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	(+)-5-Methyl-2-hexanol
beta.-Pinene	beta-copaene	alpha.-Pinene	alpha.-Phellandrene
gamma.-Terpinene	beta-Myrcene	beta.-Myrcene	alpha.-Phellandrene
1,3,8-p-Menthatriene	beta-Pinene	beta.-Pinene	alpha.-Pinene
1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane	gamma-Terpinene	gamma-Terpinene	beta-Longipinene
1-Oxaspiro[4.5]dec-6-ene, 2,6,10,10-tetramethyl-	1,2,4-Methenoazulene, decahydro-1,5,5,8a-tetramethyl-, [1S-(1.alpha.,2.alpha.,3a.beta.,4.alpha.,8a.beta.,9R*)]-	1,4-Methano-1H-cyclopenta[d]pyridazine, 4,4a,5,7a-tetrahydro-8,8-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,7a.alpha.)-	.beta.-Myrcene
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	1,3,5,7-Cyclooctatetraene	1,5-Anhydro-d-altritol	.beta.-ylangene
2,4-Decadienal	1,3,5-Benzenetriol, 3TMS derivative	1-Hexene, 4-methyl-	.gamma.-Terpinene
2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-	1,3,8-p-Menthatriene	1-Propenylaziridine	1,3,5,7-Cyclooctatetraene
2-Heptanol	1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane	2-Bromononane	1,3,5-Cycloheptatriene
2-Hexen-1-ol, acetate, (E)-	11-Hexadecynal	2-Cyclohexen-1-one, 2-methyl-	1,4-Methanophthalazine, 1,4,4a,5,6,7,8,8a-octahydro-9,9-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,8a.alpha.)-
2-Nonanol	11-Octadecenoic acid, methyl ester	2-Decen-1-ol	1-Butanol, 3-methyl-, benzoate
3,7,11,Trimethyl-8,10-dodecadienyl-acetate	13-Methyltetradecanal	2-Heptanol	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	1-Heptanol, 4-methyl-	2-Hexen-1-ol, acetate	2,4-Decadienoic acid, ethyl ester, (E,Z)-
4-Isopropyl-1-methylcyclohex-2-enol	1-Isopropyl-4,7-dimethyl-1,2,3,5,6,8a-hexahydronaphthalene	2-Pentanol	2-Bromotetradecane
4-Isopropyl-1-methylcyclohex-2-enol	1-Oxaspiro[4.5]dec-6-ene, 2,6,10,10-tetramethyl-	2-Pentanone, 5-hydroxy-	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, cis-
6,7-Dibromo-Z-11-tetradecene-1-ol acetate	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	2-Pentenoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, trans-
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethenyl)-	2,4-Decadienal	3-Hepten-1-ol	2-Cyclohexen-1-ol, 3-methyl-
9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, trans-	3-Hexanone, 2,5-dimethyl-4-nitro-	2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, trans-

Table 1 (continued)

Guática with thorns	Guática without thorns	Santa Rosa de Cabal with thorns	Santa Rosa de Cabal without thorns
9,17-Octadecadienal, (Z)-	2-Heptanol	3-Undecen-1-yne, (Z)-	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-
Acetic acid, 5-methylhex-2-yl ester	2-Heptanone	5,5-Diethyl-2-(methylthio)-4,6(1H,5H)-pyrimidinedione	2-Decen-1-ol, (E)-
Acetonitrile	2-Hexen-1-ol, acetate, (E)-	6,6-Dimethyl-2-(3-oxobutyl)bicyclo[3.1.1]heptan-3-one	2-Hexanone, 4-hydroxy-3-propyl-
Benzene, 1-methyl-3-(1-methylethenyl)-	2H-Pyran, 2-(7-heptadecynyloxy) tetrahydro-	7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethenyl)-	2-Nonanol
Benzenemethanol, .alpha.,.alpha.,4-trimethyl-	2-Nonanol	Benzene, 1-methyl-4-(1-methylethenyl)-	2-Oxatricyclo[4.3.1.0(3,8)]decane
Benzenemethanol, alpha, alpha.,4-trimethyl-	3,7,11, Tri-methyl-8,10-dodecedienylacetate	Benzenemethanol, .alpha.,.alpha.,4-trimethyl-	2-Propenoic acid, 3-phenyl-, ethyl ester
Benzoic acid, ethyl ester	3-Hexen-1-ol, acetate, (E)-	Benzoic acid N'-(2-bromo-butyl)-hydrazide	3,4-Dimethyl-2,5-diprop-2-enyl-2,5-dihydrothiophene 1,1-dioxide
Benzoic acid, hexyl ester	4-Isopropyl-1-methylcyclohex-2-enol	Benzoic acid, ethyl ester	3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy) tetrasiloxane
Benzoic acid, methyl ester	4-Isopropyl-1-methylcyclohex-2-enol	Bicyclo[3.2.1]oct-2-ene, 3-methyl-4-methylene-	3-Cyclohexene-1-ethanol
Benzyl Benzoate	4-Methyl-exo-tricyclo[6.2.1.0(2,7)]undecane	Butane, 1-isocyanato-	4-tert-Butylcyclohexyl acetate
Bicyclo[2.2.1]heptan-2-ol, 2,3,3-trimethyl-	6,7-Dibromo-Z-11-tetradecene-1-ol acetate	Butane, 1-nitro-	5,8,11-Eicosatriynoic acid, methyl ester
Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-	7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethenyl)-	Camphene	5,9-Undecadien-2-one, 6,10-dimethyl-
Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-	7-Tetradecenal, (Z)-	cis-.beta.-Farnesene	9,12-Octadecadienoic acid (Z,Z)-
Butanoic acid, 1-methylhexyl ester	9,12-Octadecadienoic acid, methyl ester	Cyclodecene	9-Octadecenoic acid (Z)-, methyl ester
Butanoic acid, 2-methyl-, ethyl ester	9,17-Octadecadienal, (Z)-	Cyclohexasiloxane, dodecamethyl-	Acetic acid, 5-methylhex-2-yl ester
Butanoic acid, ethyl ester	Acetic acid, 5-methylhex-2-yl ester	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-	Acetic acid, nonyl ester
Camphene	Acetonitrile	Cyclohexene, 3-methyl-6-(1-methylethylidene)-	Benzene, 1-methyl-3-(1-methylethenyl)-
Caryophyllene	Benzene, 1,2,4-trimethyl-	Cyclohexene, 4-methyl-3-(1-methylethylidene)-	Benzene, 2-methoxy-1-methyl-4-(1-methylethyl)-
Cyclohexasiloxane, dodecamethyl-	Benzene, 1-methyl-3-(1-methylethenyl)-	Cyclopentane, methyl-	Benzenemethanol, .alpha.,.alpha.,4-trimethyl-
Cyclohexene, 3-methyl-6-(1-methylethylidene)-	Benzenemethanol, .alpha.- (1-aminoethyl)-, [R-(R*,R*)]-	Cyclopentane, methyl-	Benzenemethanol, .alpha.,.alpha.,4-trimethyl-

Table 1 (continued)

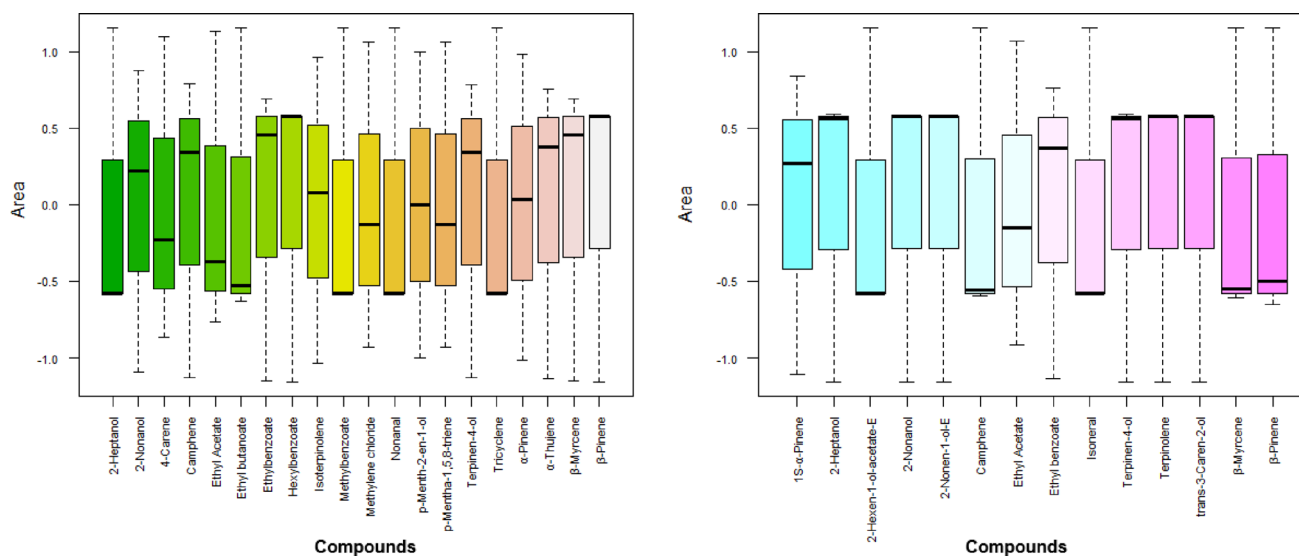
Guática with thorns	Guática without thorns	Santa Rosa de Cabal with thorns	Santa Rosa de Cabal without thorns
Cyclopentasiloxane, decamethyl-	Benzen- emethanol,. alpha.,.alpha.,4- trimethyl-	Cyclotrisiloxane, hexamethyl-	Benzoic acid, ethyl ester
Cyclopentene, 3-isopropenyl-5,5-dimethyl-	Benzoic acid, ethyl ester	Decanoic acid, ethyl ester	Benzoic acid, hexyl ester
Decanoic acid, ethyl ester	Benzoic acid, hexyl ester	Disulfide, dipropyl	Benzoic acid, methyl ester
Decanoic acid, TMS derivative	Benzoic acid, methyl ester	Ethanol	Bicyclo[2.2.1]heptan-2-ol, 2,3,3-trimethyl-
D-Limonene	Benzoic Acid, TMS derivative	Ethanone, 2-amino-1-phenyl-	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-
Dodecanal	Benzyl Benzoate	Ethyl Acetate	Butanoic acid, ethyl ester
Dodecanal	Bicyclo[2.2.1] heptan-2-ol, 2,3,3-trimethyl-	Germacrene D	Camphene
Dodecanoic acid, ethyl ester	Bicyclo[3.1.0] hex-2-ene, 2-methyl-5-(1- methylethyl)-	Glycolaldehyde dimethyl acetal	Caryophyllene
endo-Borneol	Bicyclo[3.1.0] hex-2-ene, 2-methyl-5-(1- methylethyl)-	Hexanoic acid, 2-methylpropyl ester	Cyclohexasiloxane, dodecamethyl-
Ethanol	Butanoic acid, 1-methylhexyl ester	Hexanoic acid, ethyl ester	Cyclohexene, 1-methyl-4-(1-methylethylidene)-
Ethyl (E)-2-octenoate	Butanoic acid, 2-methyl-, ethyl ester	Malic Acid	Cyclooctyl alcohol
Ethyl Acetate	Butanoic acid, ethyl ester	Methylene chloride	Cyclopentane, methyl-
Geraniol	Camphene	Mexiletine	Cyclopentene, 3-isopropenyl-5,5-dimethyl-
Hexanoic acid, 2-hexenyl ester, (E)-	Caryophyllene	Naphthalene, decahydro-, cis-	Cyclopropane, 1-bromo-2,2,3,3- tetramethyl-1-prop-1-ynyl-
Hexanoic acid, 2-methylpropyl ester	Cetene	n-Hexane	Decanoic acid, ethyl ester
Hexanoic acid, ethyl ester	Cyclohep- tasiloxane, tetradecamethyl-	n-Hexane	Dimethyl ether
Hexanoic acid, hexyl ester	Cyclohex- asiloxane, dodecamethyl-	n-Hexane	Di-n-octyl phthalate
Hexanoic acid, TMS derivative	Cyclohexene, 3-methyl-6-(1- methylethylidene)-	Nonane	Disulfide, bis(1-methylethyl)
Methyl 2-hydroxystearate, TMS derivative	Cyclonon- asiloxane, octadecamethyl-	Octanal	D-Limonene
Methylene chloride	Cyclopent- tasiloxane, decamethyl-	Octane, 1-azido-	Eicosanoic acid, ethyl ester
Myristic acid, TMS derivative	Cyclopentene, 3-isopropenyl- 5,5-dimethyl-	Octane, 2,7-dimethyl-	Ethanol
n-Hexane	Decanal	Octane, 3,4,5,6-tetramethyl-	Ethyl (E)-2-octenoate

Table 1 (continued)

Guática with thorns	Guática without thorns	Santa Rosa de Cabal with thorns	Santa Rosa de Cabal without thorns
n-Nonadecanol-1	Decanoic acid, ethyl ester	Octanoic acid, ethyl ester	Ethyl Acetate
Nonanal	Decanoic acid, TMS derivative	o-Cymene	Ethylene glycol, 2TMS derivative
Nonanoic acid, TMS derivative	Diisooctyl phthalate	Pentadecanoic acid, 2,6,10,14-tetramethyl-, methyl ester	Farnesene epoxide, E-
Octanoic acid, ethyl ester	D-Limonene	Propan-2-ol, 1-(2-isopropyl-5-methylcyclohexyloxy)-3-(4-morpholyl)-	Fenchol
Octanoic acid, TMS derivative	Dodecanoic acid, ethyl ester	Propane, 1-(ethenyloxy)-2-methyl-	Geraniol
p-Cymene	Ethanol	Propanoic acid, 2-methyl-, ethyl ester	Heptadecane, 2,6,10,15-tetramethyl-
Pentadecane	Ethyl Acetate	Salicylic acid, 2TMS derivative	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Pentadecane	exo-2,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	sec-Butyl acetate	Hexanoic acid, 3-pentyl ester
p-Mentha-1,5,8-triene	Geraniol	Spiro (6,6-dimethyl-2,3-diazobicyclo [3.1.0] hex-2-ene-4,1'-cyclopropane)	Hexanoic acid, ethyl ester
Silanediol, dimethyl-	Heptasiloxane, hexadecamethyl-	Spiro[2.2]pentane-1-carboxylic acid, 2-cyclopropyl-2-methyl-	Hexanoic acid, hexyl ester
Silanol, trimethyl-	Hexadecane	Terpinen-4-ol	Isoneral
Silanol, trimethyl-	Hexanoic acid, 2-hexenyl ester, (E)-	trans-beta-Ocimene	Linalool
Terpinen-4-ol	Hexanoic acid, 2-methylpropyl ester		Methylene chloride
Terpineol	Hexanoic acid, ethyl ester		Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-
Tetradecanal	Hexanoic acid, TMS derivative		Naphthalene, decahydro-, cis-
Tetradecanal	Ibuprofen, TMS derivative		n-Hexane
Trichloromethane	Methyl 2-hydroxysearate, TMS derivative		Nonanal
Tricyclo[2.2.1.0(2,6)]heptane, 1,7,7-trimethyl-	Methylene chloride		Octadecane, 1-chloro-
Tridecane	Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-		Octanoic acid, ethyl ester
	Nonanal		Oxirane, tetradecyl-
	Nonanoic acid, TMS derivative		p-Cymene
	Octadecane		Pentadecanoic acid, 14-methyl-, methyl ester
	Octanoic acid, ethyl ester		Pentane, 3-methyl-

Table 1 (continued)

Guática with thorns	Guática without thorns	Santa Rosa de Cabal with thorns	Santa Rosa de Cabal without thorns
	Octanoic acid, TMS derivative		Pentane, 3-methyl-
	p-Cymene		p-Mentha-1,5,8-triene
	p-Mentha-1,5,8-triene		p-Mentha-1,5,8-triene
	Silanediol, dimethyl-		Propanoic acid, 2-methyl-, 3-hydroxy-2,2,4-trimethylpentyl ester
	Silanol, trimethyl-		Salicylic acid, 2TMS derivative
	Silanol, trimethyl-		Silanol, trimethyl-
	Spiro[androst-5-ene-17,1'-cyclobutan]-2'-one, 3-hydroxy-, (3.beta.,17.beta.)-		Sulfurous acid, 2-ethylhexyl hexyl ester
	Terpinen-4-ol		Terpinen-4-ol
	tert-Butyldimethylsilanol		Terpinen-4-ol
	Tetradecanal		Thujone
	Tetradecane		Trichloromethane
	Tetradecane		Undecane, 2-cyclohexyl-
	Trichloromethane		Undecanoic acid, ethyl ester
	Tricyclo[2.2.1.0(2,6)]heptane, 1,7,7-trimethyl-		Z,Z,Z-1,4,6,9-Nonadecatetraene

**Fig. 3** Volatile compounds that allow the differentiation of materials from plants with and without thorns in mora de Castilla blackberries produced in the municipality of Guática

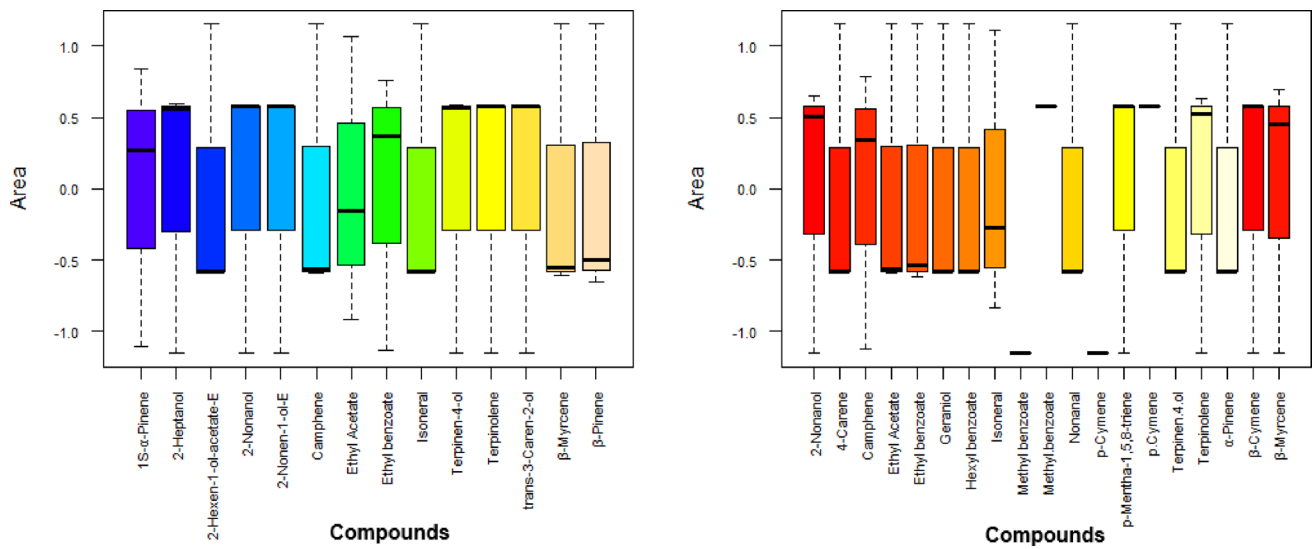


Fig. 4 Volatile compounds that allow the differentiation of mora de Castilla blackberry materials from plants with and without thorns produced in the municipality of Santa Rosa

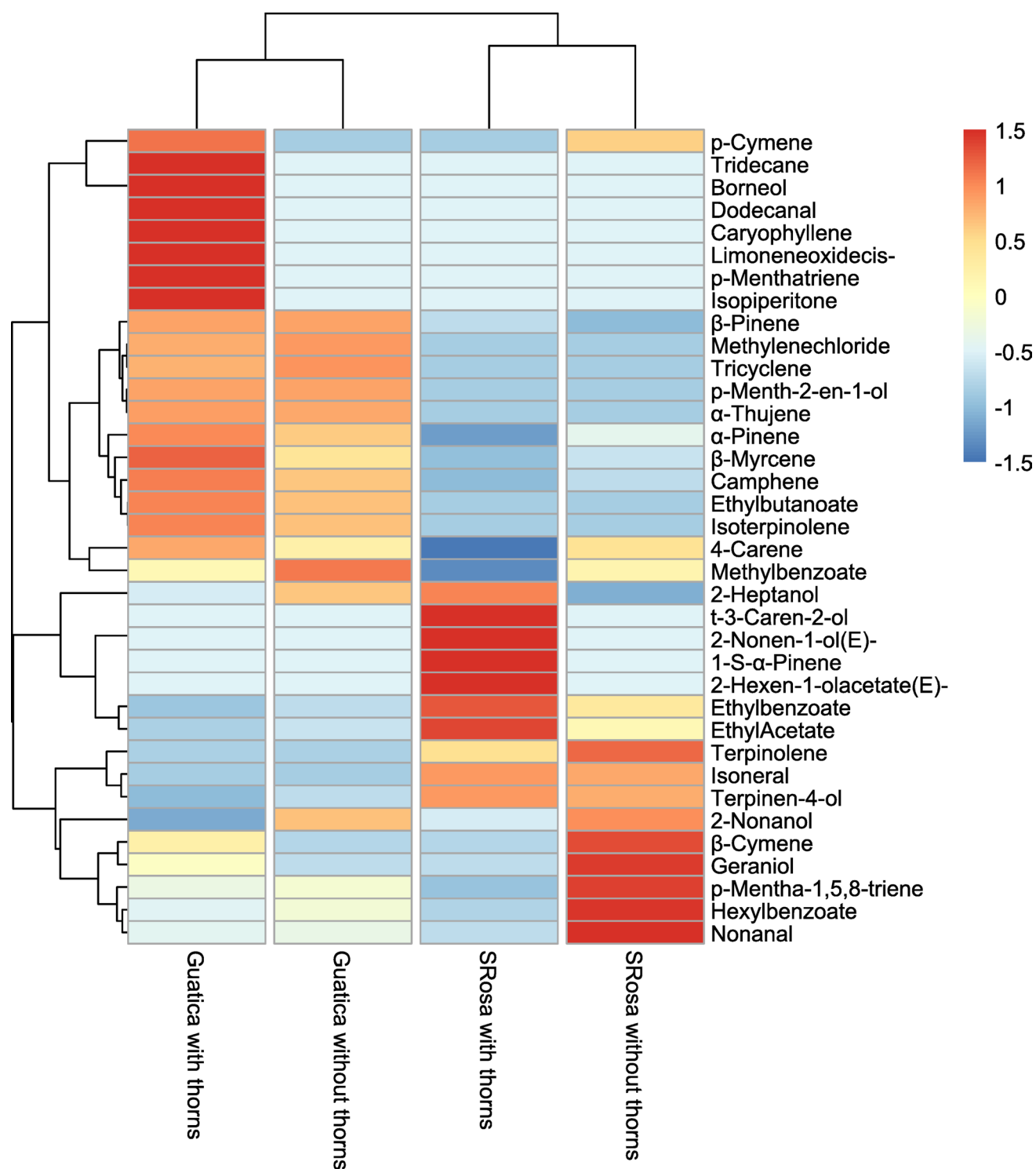


Fig. 5 Heatmap of the correlations for statistically significant volatile compounds in mora de Castilla fruits from plants with and without thorns in the municipalities of Guática and Santa Rosa de Cabal

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Declarations:

Authors' contributions Gloria Edith Guerrero: Conceptualization, Investigation, Supervision Writing- Reviewing and Editing. Daniel Steven Fernandez: Formal analysis, Investigation, Writing- Original draft. Nathalia Cardona Hurtado: Investigation, Writing- Original draft

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Data availability - (data transparency) The data and materials supporting the findings of this study are available upon request and will be provided upon reasonable request.

Code availability - (software application or custom code) Not applicable.

Declarations

Competing interests (include appropriate disclosures) Not applicable for that section.

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