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SHORT COMMUNICATION

The Volatile Compounds of Elderberries (*Sambucus nigra* L.)

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Abstract

This study reports the volatile compounds of elderberries - *Sambucus nigra* L. (Caprifoliaceae), which are used in food and medicinal industry. The air-dried and crushed mature elderberries were subjected to microdistillation by using an Eppendorf MicroDistiller. The sample was analysed by gas chromatography (GC) and gas chromatography-mass spectroscopy (GC-MS), simultenaously. According to our results, 34 volatile compounds were identified by yielding 86.1% of the sample. Phenylacetaldehyde (32.3%) and benzaldehyde (7.9%) were observed as main constituents in elderberries.

KEYWORDS: Elderberry, Microdistillation, Gas Chromatography, Gas Chromatography-Mass Spectroscopy, Phenyl acetaldehyde

Introduction

Elderberry is widely used as both food and medicinal plant in Europe. It has been used to colour jams, jellies, juices and wines (Inami, Tamura, Kikuzaki, & Nakatani, 1996). Elderberries are used traditionally to make elderberry wine, liqueurs, marmalade, juice, tea, jam and pies. The berry infusion is consumed as diuretic, laxative, diaphoretic, and anti-inflammatory. The berries are used to treat flu and to stimulate the immune system. The elderberry juice or tea is suggested to drink for several times per day for well-being (Vlachojannis, Cameron, & Chrubasik, 2010). The aroma composition of elderberries are very important because of their uses as food stuff. The characteristic aroma of elderberries is due to (*E*)-β-damascenone, dihydroedulan, ethyl-9-decenoate, 2-phenyl ethanol, phenylacetaldehyde and nonanal. The fruity-sweet odour in juice and other products comes from aliphatic esters such as ethyl 2-methylbutanoate, ethyl 3-methylbutanoate, methyl heptanoate, methyl octanoate, methyl nonanoate. Also, alcohols and aldehydes are frequently identified groups in elderberry chemistry.

In our study, we aimed to determine the volatile compounds in elderberries, which are used as a herbal tea ingredient in Turkey. Hence, the air-dried mature elderberries subjected to microdistillation were analysed by GC and GC-MS systems, simultaneously. The aldehydes were the main groups among the volatiles in elderberries.

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Materials and Methods

Plant Material

Air-dried mature fruits of elderberry were obtained from 'Evçay Company', Yalova, Turkey in 2009.

Isolation of the Volatile compounds

The volatiles were obtained by microdistillation of both dry whole and crushed fruits (50 mg) using an Eppendorf MicroDistiller® with 10 mL distilled water per sample vial. The sample vial was heated to 108°C at a rate of 20°C/min and kept at this temperature for 90 min, then heated to 112°C at a rate of 20°C/min and kept at this temperature for 30 min. The sample was subjected to a final post-run for 2 min under the same conditions. The collecting vial, containing a solution of NaCl (2.5 g) and water (0.5 mL) plus *n*-hexane (350 µL) to trap volatile components, was cooled to –5°C during distillation. After the distillation was completed, the organic layer in the collection vial was separated and analyzed by gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS) systems, simultaneously. The Figure 1 shows the scheme of microdistillation procedure.

GC and GC-MS analyses

The sample was analysed by gas chromatography (GC) with a flame ionization detector (FID) and gas chromatography-mass spectrometry (GC-MS) using an Agilent GC-mass selective detector (MSD) system. The GC-MS analyses were done with an Agilent 5975 GC-MSD system. An Innowax fused silica capillary (FSC) column (60 m × 0.25 mm, 0.25 µm film thickness) was used with helium as the carrier gas (0.8 mL/min). Oven temperature was kept at 60 ºC for 10 min, then programmed to 220 ºC at a rate of 4 ºC/min, then maintained constant at 220 ºC for 10 min, and finally programmed to 240 ºC at a rate of 1 ºC/min. Injector temperature was set at 250 ºC. Split flow was adjusted at 50:1. Mass spectra were recorded at 70 eV with the mass range m/z 35 to 450.

GC analyses were performed using an Agilent 6890N GC system. FID detector temperature was set to 300 ºC and the same operational conditions were applied to a duplicate of the same column used in GC-MS analyses. Simultaneous auto injection was done to obtain equivalent retention times. Relative percentages of the separated compounds were calculated from integration of the peak areas in the GC-FID chromatograms.

Identification of the volatile compounds

The identification of volatile compounds was carried out by comparison of their relative retention times with those of authentic samples or by comparison of their relative retention indices (RRI) to series of n-alkanes. Computer matching against commercial as Wiley GC/MS Library, Adams Library, MassFinder 3 Library (McLafferty, & Stauffer, 1989; Koenig, Joulain, & Hochmuth, 2004) and in-house "Başer Library of Essential Oil Constituents" built up by genuine compounds and components of known oils, as well as MS literature data (Joulain, & König, 1998; ESO, 1999) were used for the identification.

Results and Discussion

34 volatile compounds in elderberries were identified representing 86.1% of the sample. The main compounds were phenylacetaldehyde (32.3%) and benzaldehyde (7.9%). Ethyl linoleate (5.4%), 4-vinyl guaiacol (4.9%), linalool (4.5%), and phenyl ethyl alcohol (4.1%) were also found as other major

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compounds. Table 1. shows the detailed information on the composition of elderberry volatiles. Our results show that the elderberries are rich in aldehydes, ketones, alcohols, esters, terpenes, and fatty acids.

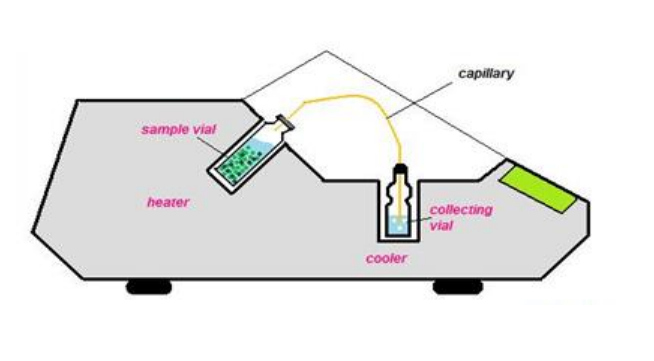
Previous studies indicate that the characteristic aroma of elderberries is due to (*E*)-β-damascenone, dihydroedulan, ethyl-9-decenoate, 2-phenyl ethanol, phenylacetaldehyde and nonanal. The fruity-sweet odour in juice and other products comes from aliphatic esters such as ethyl 2-methylbutanoate, ethyl 3-methylbutanoate, methyl heptanoate, methyl octanoate, methyl nonanoate. At the same time, alcohols such as 2-methyl-1-propanol, 2-methyl-1-butanol and 3-methyl-1-butanol were identified in elderberries. The aldehydes like pentanal, heptanal, octanal contribute the characteristic odor of elderberries. The floral odor of the fruits comes from hotrienol and nonanal. Also, alcohols and aldehydes are frequently identified groups in elderberries (Jensen, et al., 2000; Kaack, et al., 2005; Christensen, et al., 2007; Kaack, 2008).

Table 1. The composition of volatile compounds of elderberries.

RRI	Compound	% of the sample
1000	Decane	2.5
1093	Hexanal	1.4
1136	Isoamyl acetate	1.4
1203	Limonene	1.0
1212	Isoamyl alcohol	<0.1
1244	2-Amylfuran	0.5
1398	2-Nonanone	3.0
1400	Nonanal	1.2
1479	Furfural	<0.1
1541	Benzaldehyde	7.9
1553	Linalool	4.5
1585	5-Methyl furfural	0.5
1590	Bornyl acetate	1.0
1610	Calarene	0.9
1616	Hotrienol	0.6
1663	Phenylacetaldehyde	32.3
1700	Heptadecane	1.1
1800	Octadecane	<0.1
1838	2-Phenyl ethyl acetate	1.6
1838	(*E*)-β-Damascenone	2.5
1853	Ethyl dodecanoate	0.6
1937	Phenyl ethyl alcohol	4.1
2131	Hexahydro farnesyl acetone	1.1
2179	3,4-Dimethyl-5-pentiliden-2-(5H)-furanone	0.5
2218	4-Vinyl guaiacol	4.9
2226	Methyl hexadecanoate	2.0
2239	Carvacrol	<0.1
2262	Ethyl hexadecanoate	1.9
2509	Ethyl linoleate	5.4
2538	Methyl linoleate	<0.1
2583	Methyl linolenate	1.1
2613	Ethyl linolenate	<0.1
2931	Hexadecanoic acid	0.6
	TOTAL	**86.1**

RRI Relative retention indices calculated against *n*-alkanes % calculated from FID data.

Figure 1. The microdistillation.



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