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Chemical Composition of Essential Oil Obtained from a Wild Population of Bulgarian Cardaria draba (L.)

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ABSTRACT: Background: Cardaria draba (L.) is a perennial plant that is used in traditional folk medicine in Asia, Europe, North America, and some regions in Africa. Although there are some studies investigating the pharmacological potential of the herb, scientific data on this plant species are limited. This study aimed to determine for the first time the chemical composition of essential oil (EO) obtained from the flowering aerial parts of Cardaria draba (L.) growing wild in Bulgaria. Methods: For the evaluation of the chemical composition, gas chromatography with mass spectrometry was performed. Results: The main compounds identified in the EO studied belong to different classes, which are not common constituents of essential oils in general. Some of the major compounds were 5-(Methylsulfanyl) pentanentitrile, hentriaconate and phytol. Conclusion: This is the first analysis of EO obtained from Bulgarian Cardaria draba (L.). However, the EO is poor in biologically active compounds and its potential inclusion in herbal pharmaceuticals would be limited.

KEYWORDS: Cardaria draba (L.); folk medicine; herbal extracts

I. INTRODUCTION

Cardaria draba (L.), syn. Lepidium draba, also known as whitetop and hoary cress, is a perennial herbaceous plant belonging to Brassicaceae family that reproduces by seeds and horizontal creeping roots [1–4]. The stem is quite sturdy, straight or spreading, 100 to 800 mm high, covered with colorless fine hairs. The leaves are alternate, simple, mostly serrate, lanceolate to oblong-ovate in shape. While the basal leaves are 40 to 100 mm in length, the leaves at the top of the stem are 20 to 70 mm long. The plant has slightly domed flower clusters in which individual flower stalks grow upward from various points on the branch to approximately the same height [4]. Cardaria draba (L.) grows on native to alkaline soils in a wide range of disturbed habitats, including pastures, croplands, along roadsides, waste and irrigated areas and is indigenous to Southwest and Central Asia, the Mediterranean and Black Sea region of Europe. It also occurs in Algeria and the rest of Africa and is an invasive species in North America, where it was first collected in 1862 [1–6]. In fact, the plant is naturalized or adventive on every continent except Antarctica [5]. Cardaria draba (L.) is thought to have first appeared in England and there is evidence from 1802, 1809 and 1830 to confirm this [7].

Cardaria draba (L.) has a rich history and tradition in folk medicine because of its use for the treatment of many diseases [8,9]. Despite there is limited detail about the consumption of hoary cress, there is an information on the use of the plant as a pot herb [10]. Although the plant can be used fresh or as an ingredient in dishes, there are studies that suggest the use of an infusion of arial parts, taken orally to treat rheumatism, stomach acidification, and to avoid uterine hemorrhages and kidney diseases [8,11]. Decoction of seeds and leaves has been used in pulmonary infections [8].The plant species has biological effects not only on humans but also on other plants. There have been studies showing that extracts of the plant have phytotoxicity on different crops and inhibit the growth of some seeds, such as maize seeds and redroot seeds [6].

Cardaria draba (L.) has been found to contain secondary metabolites such as phenols, saponins, flavonoids, tannins, polyphenolic compounds, polysaccharides, glycosides, alkaloids and some of these secondary metabolites have been proven to have antibacterial, antioxidant, enzyme inhibitory and diuretic effects [1,2,9,12,13].

There are also volatile bioactive compounds that have been shown to possess inhibitory activity against fungi, Gram-negative and Gram-positive bacteria [8]. Moreover, the phenolic compounds are associated with UV protection activity and involvement in processes such as stimulation of nitrogen-fixing nodules, insect attraction, pollination, pigmentation, disease resistance [14]. Nowadays, many pharmaceuticals are based on date of traditional medicine of different

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nations [15]. Currently despite the daily synthesis of new molecules, many novel medicines are expected to have a plant origin [15–17].

The aim of the current study was to investigate the chemical profile of EO obtained from a wild population of Bulgarian Cardaria draba (L.) and to analyze the future perspectives for its potential use.

II. MATERIALS AND METHODS

Plant material

The aerial parts of flowering Cardaria draba (L.) were collected in May 2023 near the city of Plovdiv (42°08'57.4" N 24°49'27.0" E), Bulgaria. A specimen of the species (No: 063362) was deposited in the Herbarium of the Agricultural University Plovdiv (SOA).

Chemicals and Reagents

Purified hexane for GC-MS purchased from Thermo Fisher Scientific GmbH (Bremen, Germany) was used for the dilution of the EO.

Isolation of the Essential Oil

A quantity of 100g of air-dried flowering parts of Cardaria draba (L.) was subjected to hydrodistillation for 5 h using a Clevenger-type apparatus to obtain the essential oil. The collected oil was then dried over anhydrous sodium sulfate and stored in dark glass vials at 4 °C until GC-MS analysis.

Chromatographic Conditions

The analysis of the EO was carried out using gas chromatography with mass spectrometry (GC-MS). For the GC-MS analysis, a Bruker Scion 436-GC SQ MS (Bremen, Germany) equipped with a Bruker BR-5ms fused silica capillary column (0.25 µm film thickness and 15 m × 0.25 mm i.d.) was used. The flow rate was fixed to 1 mL/min. The carrier gas used for the analysis was helium. The injection volume was 1 µL and the injector used was split/splitless with a split ratio of 1:20. The oven temperature was set at 40°C for 1 min, increased to 130°C at a rate of 4°C/min, then increased to 240°C at a rate of 5°C/min and finally increased to 300°C at a rate of 15°C/min and held for 2 min. The injector and detector temperatures were set to 250°C and 300°C, respectively. The mass spectra were in full scan mode with a mass range of 50–350 m/z. The separated compounds from the essential oil were identified by MS spectra with spectral data within the Wiley NIST11 Mass Spectral Library (NIST11/2011/EPA/NIH) and the literature data.

III. RESULTS AND DISCUSSION

The essential oil obtained from the aerial parts of the wild Bulgarian Cardaria draba (L.) was pale yellow in color, with a strong odour. The results of GC-MS analyses of the essential oil showed that fifteen constituents, representing 88.24% of the total oil content, were tentatively present. Table 1 and Figure 1 show the chemical composition and the chromatogram of the studied EO.

The volatile compounds identified belong to different classes, some of which are not typical for essential oils. Several of the main classes derived from EO are glucosinolates and their degradation products, fatty acids and carbonyl compounds. Glucosinolates are a group of compounds present in plants or seeds. During autolysis of cells, isothiocyanates and nitriles are formed from glucosinolates by enzymatic degradation [18]. One of the major compounds in the EO was 5-(Methylsulfanyl) pentanenitrile, accounting for 19.24% of the total amount of EO. 5-(Methylsulfanyl) pentanenitrile, also known as erucin nitrile, is a breakdown product of glucosinolate produced by the degradation of glucoerucin [19,20].

Other breakdown products of glucosinolates are isobutyl isothiocyanate and benzyl isothiocyanate, which were present in small amounts in the EO. Isobutyl isothiocyanate originated from the degradation of the isobutyl glucosinolate [20].

Benzyl isothiocyanate is an aromatic compound that is also derived from the degradation of glucosinolates. Although benzyl isothiocyanate could inhibit the growth of Escherichia coli, there have been studies showing that due to the dose it could cause DNA damage and bladder toxicity in rats [21]. Furthermore, the toxic dose is far higher for humans than for rats [21].

Hentriacontane is an alkane hydrocarbon, representing 10.69% of the total oil composition. Earlier studies have suggested that it has various pharmacological effects including antimicrobial, anti-inflammatory and antitumor activities [22].

Compared with previous studies, the major volatile compounds identified in the EO were in different concentrations. The differences in the concentration of compounds in EO are influenced by some factors such as geographical region, soil type, period of collection, growth stage of the plant [23–25].

In our study, we detected the presence of 5-(Methylsulfanyl) pentanenitrile, representing 19.24% of total EO, while another study suggested a content of the same compound 13.8% of total EO [19]. Furthermore, the study indicated that the main constituent in the EO was 4-(Methylsulfanyl) butyl

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isothiocyanate with a content of 28.0%, which is also a glucosinolates degradation product [19].

According to the data, the main volatile compound isolated in EO obtained from Cardaria draba (L.) from some regions in Turkey, is 5-(Methylthio) pentanenitrile, accounting for 41.13% of the EO [26]. Although we have not found the presence of 5-(Methylthio) pentanenitrile, the presence of Benzeneacetaldehyde is almost in the same concentration compared with those in the EO obtained from Turkey Cardaria draba (L.), respectively 2.26% and 2.43% [26].

The investigation of the chemical composition of Cardaria draba (L.) essential oil from West Northern Algeria showed the presence of hexahydrofarnesyl acetone with chemical name 6,10,14-trimethyl-2-pentadecanone as one of the main compounds with concentrations ranging from 11.08% to 20.61% depends on which part of the plant was used to obtain the oil [27]. Despite the fact that in our study the concentration of hexahydrofarnesylaceton was quiet less, representing 1.171% of the total EO, the presence of linalool, phytol, benzaldehyde, nonanal, geranyl acetone and β-ionone was found in both researches in similar concentrations [27].

Phytol is a diterpene alcohol that accounts for 5.609% of the total EO. It has diverse biological effects such as antioxidant, anti-inflammatory, cytotoxic, antimicrobial, metabolism-modulating and immunomodulatory activities [28]. There are studies showing that phytol has cytotoxic activity against some tumor cells, and its cytotoxicity depends on the dose used [29].

Table 1. Volatile constituents of the EO obtained from Cardaria draba L., distributed in Bulgaria, expressed as a percentage of total EO.

No	Compound	Formula	Class of compound	% of total EO
1	Isobutyl isothiocyanate	C_5H_9NS	GDP	1.202
2	Benzaldehyde	C_7H_6O	CC	0.887
3	Benzeneacetaldehyde	C_8H_8O	CC	2.460
4	Linalool	$C_{10}H_{18}O$	OM	0.738
5	Nonanal	$C_9H_{18}O$	CC	1.511
6	5-(Methylsulfanyl) pentanenitrile	$C_6H_{11}NS$	GDP	19.243
7	Benzyl Isothiocyanate	C_8H_7NS	GDP	0.764
8	Dihydrodehydro-beta-ionone	$C_{13}H_{20}O$	O	0.305
9	Not identified			41.968
10	Geranyl acetone	$C_{13}H_{22}O$	CC	0.243
11	Hexahydrofarnesyl acetone	$C_{18}H_{36}O$	S	1.171
12	Beta-Ionone	$C_{13}H_{20}O$	CC	1.307
13	n-Hexadecanoic acid	$C_{16}H_{32}O$	FA	0.144
14	Phytol	$C_{16}H_{32}O$	DA	5.609
15	Hentriacontane	$C_{31}H_{64}$	AH	10.690
GDP – glucosinolate degradation products				

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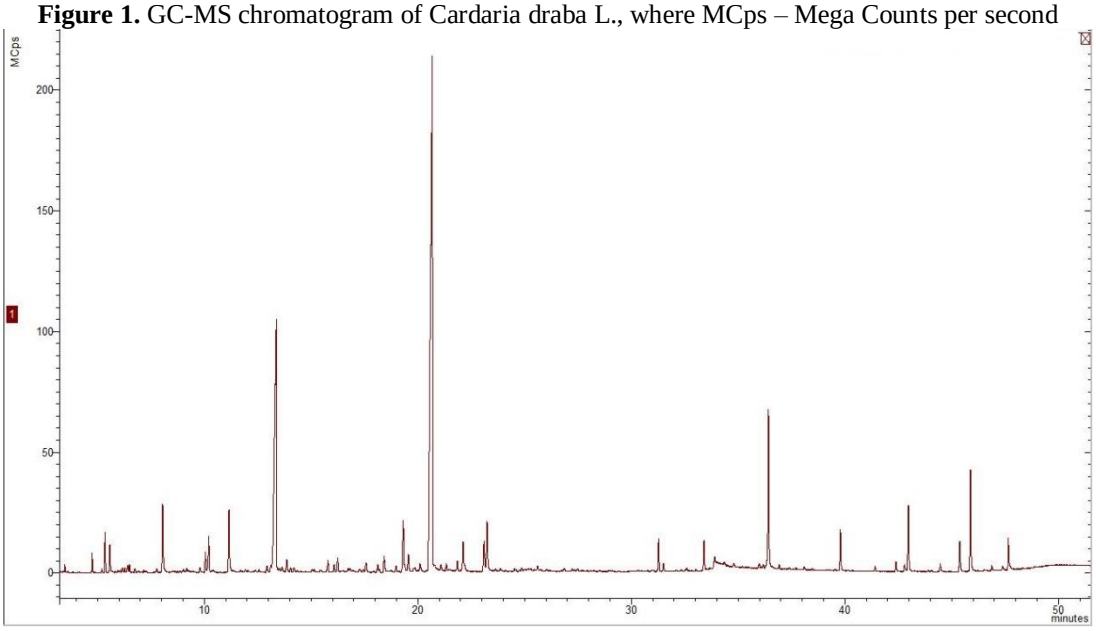
CC – carbonylic compounds
OM - oxygenated monoterpenes
S - sesquiterpenes
FA – fatty acids
AH – alkane hydrocarbons
DA – diterpene alcohols

Figure 1. GC-MS chromatogram of Cardaria draba L., where MCps – Mega Counts per second



IV. CONCLUSION

The chemical profile of the essential oil of Cardaria draba (L.), growing wild in Bulgaria, was investigated for the first time by gas chromatography – mass spectroscopy method. The conducted GC-MS analysis indicated the presence of fifteen volatile constituents, representing 88.24% of the total EO. However, the EO is poor in biologically active compounds and its potential inclusion in herbal medicinal products would be limited.

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