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Investigation of Floral Scent and Essential Oil of *Rosa iberica* Petals

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Abstract

The flowers of wild *Rosa iberica* are investigated to find the chemical constituents of its aroma and essential oil. The measurements were carried out by GC-FID and GC-MS analysis. The aromatic compositions emitted from the flowers revealed 11 constituents, among which phenyl ethanol (38.82%), benzyl alcohol (28.48%), and geraniol (12.57%) were the most abundant. The essential oil investigation detected 13 compounds, the most abundant ones being anethole (45.56%) and phthalic acid (32.23%). The scent and essential oil detected *de novo* in the petals of *R. iberica* are beneficial as natural ingredients in seasonings, therapeutic compositions, and an aromatic plant in breeding strategies of ornamental shrubs and flowers.

Keywords: Anethole, Benzyl alcohol, Essential oil, Floral scent, Phenyl ethyl alcohol, Phthalic acid, *Rosa iberica*.

INTRODUCTION

The genus *Rosa* consists of approximately 200 species that are broadly spread in West Asia, North America, and Europe (Naquvi *et al*., 2014; Victoria *et al*., 2009). *Rosa iberica* is one of the 14 wild species that are native to Iran and are distributed throughout the country (Jowkar and Karami, 2018; Koobaz *et al*., 2011).

The shoot extracts of *R. iberica* have proven to be efficient in controlling important human pathogens, such as diarrhea (*Shigella sonnei*), pneumonia (*Staphylococcus aureus*), and anthrax (*Bacillus anthracis*) (Salehi Surmaghi and Amin, 1993). The leaves of this rose species also produce valuable aroma (Jowkar and Karami, 2016) and essential oil (Jowkar and Karami, 2018) by the extraordinary oil glands. In a survey in the north of Iran, honey bees showed a great tendency to collect nearly half of the pollen grains from this species (Taghavizad and Nazarian, 2009). It is well known that the volatile organic compounds emitted from the rose flowers help attract various pollinators (Aza *et al*., 2013).

Furthermore, rose aroma plays an important role in human spirituality and healing in therapeutic gardens (Hainan *et al*., 2015). Rose essential oils are widely used in medicine, the perfume industry, and cosmetics (Abdolmohammadi *et al*., 2014). Due to the high costs of industrial production of rose oil and also because of its value in different industries, it is regarded as "liquid gold" (Mohamadi *et al*., 2011). β-phenethyl alcohol and benzyl alcohol have frequently been reported in the essential oils. These constituents are simple aromatic alcohols and very similar to each other in their chemical formula. They exist in most essential oils both as free alcohols and particularly as an aroma compound in some esters. Phenyl ethanol is produced mainly in the rose species, especially in *R. damascena* (Bayrak and Akgul, 1994), while benzyl alcohol is a major portion of the fragrance of peony, jasmine, narcissus, and some rose varieties (Mookherjee and Wilson, 2000). The latter is also used in flavor, perfume, and soap manufacturing as well as in photographic and textile productions. It is medicinally used for its solvent, disinfecting, and anesthetic activities, too (Mookherjee and Wilson, 2000).

Another aromatic constituent that broadly occurs in essential oils is anethole (1-methoxy-4-(1- propenyl) benzene). It makes a large component of the aroma of magnolia flowers and the taste of fennel and anise. It is used in flavors, sweets, and hygiene consumptions (Ashurst, 1999). Anethole shows robust disinfecting characteristics to counter *Salmonella enterica* and *Candida albicans* pathogens (De *et al*., 2002; Fujita *et al*., 2007; Kubo and Fujita, 2001), sheep nematode *Haemonchus contortus* (Camurca-Vasconcelos *et al*., 2007), and *Meloidogyne javanica* (Newberne *et al*., 1999). Moreover, anethole was accepted by FEMA as a safe compound (Newberne *et al*., 1999) and is widely consumed as a seasoning spice. In another aspect, the derivatives of 1,2-benzenedicarboxylic acid, i.e. phthalic acid, occur as an important component of essential oils. They show anti-inflammatory features (Mavar-Manga *et al*., 2008), antipathogen characteristics against numerous microorganisms (Al-Bari *et al*., 2006), and antivirus effects in Asian tiger shrimp (Rameshthangam and Ramasamy, 2007), in addition to acting as a microbicide for the prevention of HIV-1 (Neurath, 2000). The organic compounds available in the fragrance and essential oil of *R. iberica* flowers, which are further analyzed in this research, have not been reported before.

MATERIALS AND METHODS

Plant materials

Rootstocks were collected from Chalus (Altitude 1953 m, 35°55′ N, 51°05′E) in the north of Iran. The flowers of *Rosa iberica* were taken from the plants cultivated in the College of Agriculture at Shiraz University (Altitude 1486 m, 29°72′N, 52°58′E) (Fig. 1).

Fragrance extraction

About 4 g of fresh petals were placed in a tube. The volatile organic compounds in the headspace were taken to the Combi PAL System device. The sample was heated to 45°C under consistent shaking for 20 min. The sampling needle and conduction line temperature was fixed at 85°C.

Essential oil isolation

Fresh petals were air-dried for 72 h at room temperature and subsequently, 100 g were water-distilled by a Clevenger apparatus for 3 h. Later, n-hexane (Merck) was supplied and thereafter dehydrated by anhydrous sodium sulfate and kept in a refrigerator at 4°C ± 2°C.

GC measurement

Gas chromatography investigation was carried out by an Agilent gas chromatograph series device model No. 7890-A equipped with an FID. The GC-MS procedure was also done using an Agilent GC device fitted with an HP-5MS column (film thickness 0.25 m; 30 m × 0.25 mm i.d.) and equipped with 5975-C MS apparatus. The components of the volatile organic compounds were detected by calculating their retention times for n-alkane compounds (C8-C25), and then the essential oils were characterized on an HP-5 column under the aforementioned chromatographic GC settings.

RESULTS

The headspace analysis of volatiles emitted from fresh petals showed 11 compounds including monoterpenes (α-pinene and camphene), monoterpene alcohols (nerol and geraniol), monoterpene ester (geranyl acetate), aromatic aldehyde (benzaldehyde), aromatic alcohol (benzyl alcohol, phenyl ethyl alcohol), sesquiterpene (neral), ester (z-3-hexenol), and a monoterpenoid constituent (geranial). Major volatile organic compounds of *Rosa iberica* consisted of phenyl ethanol (38.82%), benzyl alcohol (28.48%), and geraniol (12.57%) (Table 1, Fig. 2).

Extraction from dry petals of *R. iberica* showed 13 constituents, i.e., Monoterpene (Dl-limonene), monoterpene alcohol (linalool), oxygenate sesquiterpene (α-thujone), phenol (eugenol), alkanes (eicosane, tricosane, pentacosane and 2,6-dimethyloctane), fatty acid (butanoic acid), terpenoid (camphor), aromatic compounds (1-methoxy-4-(1-propenyl) benzene and 1-methoxy-4-(2-propenyl) benzene), and benzoic acid (1,2-benzenedicarboxylic acid). The main components were 1-methoxy-4-(1-propenyl) benzene (45.56%), 1,2-benzenedicarboxylic acid (32.23%) and 2,6-dimethyloctane (7.09%) (Fig. 3, Table 2).

Fig. 1. Sampling location of rootstocks and flowers of *Rosa iberica* plants in Chalus and Shiraz, respectively.

Table 1. The chemical constituents (%) detected in the floral scent of *Rosa iberica.*

Compounds	RI	% Compounds
(Z)-3-Hexenol	853	0.578
α –Pinene	933	3.174
Camphene	949	1.452
Benzaldehyde	961	0.817
Benzyl alcohol	1033	28.489
Phenyl ethyl alcohol	1109	38.824
Nerol	1228	10.915
Neral	1238	0.728
Geraniol	1254	12.572
Geranial	1269	1.277
Geranyl acetate	1384	1.174
Total	100	

*RI: Retention indices analyzed on HP-5MS column.

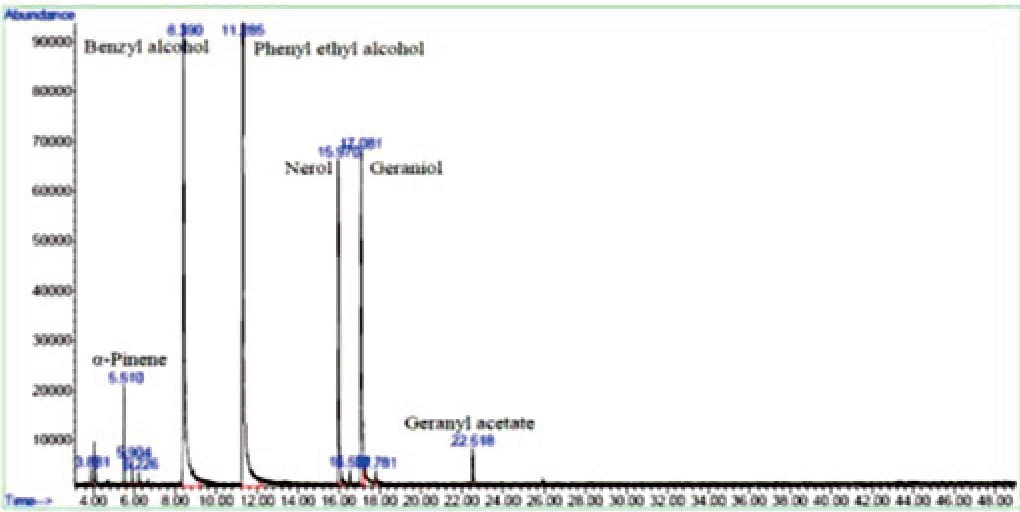

Fig. 2. GC-MS spectra of volatile organic compounds of *Rosa iberica* petals.

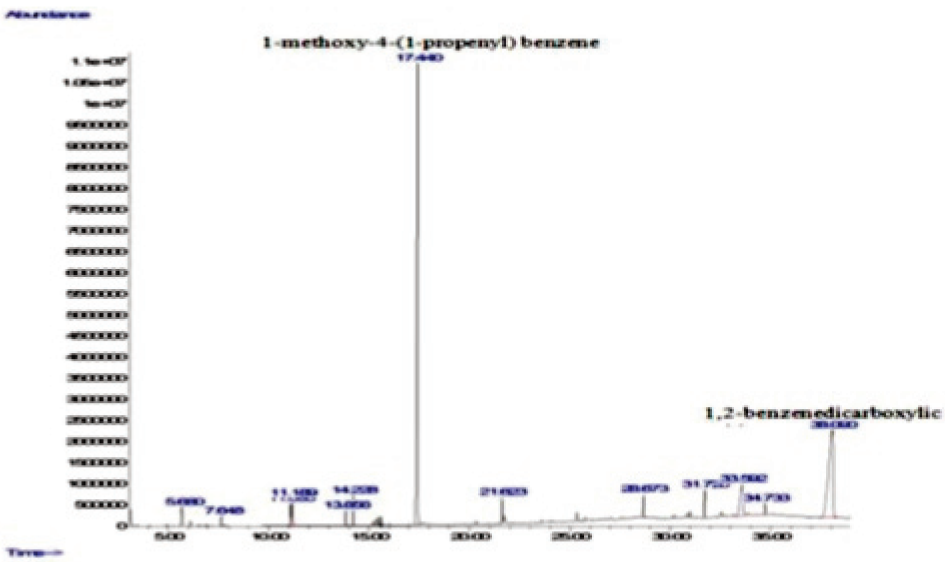

Fig. 3. GC-MS spectra of the essential oils of *Rosa iberica* petals.

Table 2. Chemical compounds (%) extracted from the essential oils of *Rosa iberica* petals.

Compounds	RI	% Compounds
Butanoic acid	808	0.939
α.Thujone	928	2.35
2,6-Dimethyloctane	938	7.09
Dl-Limonene	1022	1.49
Linalool	1099	1.53
Camphor	1141	1.284
Benzene, 1-methoxy-4-(1-propenyl)	1155	45.46
Benzene, 1-methoxy-4-(2-propenyl)	1202	1.79
Eugenol	1355	1.51
Eicosane	2000	1.48
Tricosane	2300	0.89
1,2-Benzendicarboxylic acid	2499	32.23
Pentacosane	2500	1.92
Total	99.95	

*RI: Retention indices analyzed on HP-5MS column.

DISCUSSION

It is assumed that the most important compounds in the rose fragrance are alcohols and esters, while other constituents such as aldehydes, terpenes, ethers, and ketones play a minor role (Chamorro *et al*., 2012; Morsy, 2017). Previous studies on different rose species such as *Rosa gallica*, *R. abyssinica*, *R. hybrida*, *R. brunonii*, and *R. centifolia* have demonstrated that phenyl ethyl alcohol, geraniol, nerol, eugenol, linalool, and tricosane are the principal aromatic compounds (Hosni *et al*., 2010; Khatamsaz, 1992; Kumar, 2013; Sabri and Hasan, 2016; Tambe and Gotmare, 2016). Furthermore, 2-phenylethanol, geraniol and nerol constituted the greatest portion of volatile organic compounds in *R. rugosa* (Feng *et al*., 2010), which are also abundant in *R. iberica* (Table 1). The results of this research are consistent with damask rose as well, in which phenyl ethyl alcohol is the main fragrance (Karami and Jandoust, 2016; Koksal *et al*., 2015; Mohamadi *et al*., 2011; Tambe and Gotmare, 2016). Karami and Jandoust (2016) showed that phenyl ethyl alcohol is the main constituent in the aroma of *R. moschata* and *R. damascena* flowers (Antonelli *et al*., 1997), which is also in agreement with our study. A study on 24 old garden roses indicated that phenyl ethanol was the main component of fragrance, but some roses demonstrated remarkably high levels of benzyl alcohol (Antonelli *et al*., 1997). This phenomenon is also seen in *R. iberica* (Table 1) and other flowers such as jasmine and hyacinth (Corcoran and Ray, 2014), though most of the rose species show smaller amounts of benzyl alcohol (Hosni *et al*., 2010; Karami and Jandoust, 2016; Sabri and Hasan, 2016; Tambe and Gotmare, 2016; Younis *et al*., 2008). Similar to geraniol, nerol has a sweet rose fragrance although it is believed to be fresher.

The volatiles released from the flowers are known as chemical signals for the interaction between plants and insects. The petal fragrances in *R. hybrida,* mainly monoterpene alcohols and 2-phenyl ethyl alcohol, are renowned insect-attracting volatiles (Bergougnoux *et al*., 2007). Recently, it has been confirmed that fragrances play a major role in the pollination of *R. moschata* (Karami and Jandoust, 2016). Therefore, it could be inferred that the great interest of honey bees in the north of Iran to the pollens of *R. iberica* (Taghavizad and Nazarian, 2009) is related to the vast production of phenyl ethyl alcohol, benzyl alcohol, geraniol, and nerol by its flowers (Table 1).

Furthermore, benzyl alcohol has obtained a GRAS status by the FEMA and achieved the most recent instructions issued by the IFRA (Mookherjee and Wilson, 2000). The most abundant component in the essential oil of *R. iberica* was identified to be 1-methoxy-4-(1- propenyl) benzene and 1,2-benzenedicarboxylic acid (Table 2), which are commonly known as anethole and phthalic acid, respectively. Anethole can be converted into numerous aromas emitted from the flowers, such as phenyl ethanol, benzyl alcohol, etc. (Shimoni *et al*., 2002). As found in the other plants, shoot antipathogen characteristics detected in *R. iberica* (Salehi Surmaghi and Amin, 1993) are possibly related to its phthalic acid and anethole compounds (Al-Bari *et al*., 2006; De *et al*., 2002; Kubo and Fujita, 2001). Here, we report *de novo* that the essential oil of *R. iberica* flowers contains 1,2-benzenedicarboxylic acid (Table 2). Limonene, linalool, and eugenol are detected in greater portions in *R. iberica* than in *R. damascena* (Manouchehri *et al*., 2018), but in lesser amounts compared to *R. centifolia* (Aslam Khan and Rehman, 2005). The other valuable compounds found in the essential oil of *R. iberica* petals include camphor, eugenol, and thujone, which have antimicrobial activities in different plants as well as roses (Abad *et al*., 2013; Hirulkar and Agrawal, 2010; Voon *et al*., 2012). The presence of these compounds in *R. iberica* could confirm the value of this precious plant as a medicinal plant, food flavorings, and a highly valuable ornamental.

CONCLUSION

The aroma and essential oil of *R. iberica* flowers showed valuable chemicals, which were similar in terms of their components but with different amounts to other important roses, such as *R. damascena* and *R. moschata*. Therefore, the rose species studied in this research can be further used as an ornamental shrub in landscapes and aromatic gardens. Furthermore, the pollinators' attraction to the volatiles of *R. iberica* is commendable for fruit and seed production in the horticultural crops. Its valuable compounds including phenyl ethyl alcohol, benzyl alcohol, geraniol, and nerol are beneficial for the cosmetics and perfume industries. Because of the GRAS status of anethole, the flowers of *R. iberica* could be suggested as a natural source for consumption in food flavorings. Its metabolites' therapeutic uses and antimicrobial properties merit further investigations. The results of this study are applicable for future breeding programs of roses.

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