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CHEMICAL VARIABILITY OF ESSENTIAL OIL COMPONENTS OF TWO *Rosa x damascena* GENOTYPES GROWING IN IRAN

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Rose, grown wildly as an ornamental plant, is known to the scientific world as *Rosa damascena* Mill. The genus Rosa includes 200 species and more than 18.000 cultivars [1, 2]. Rose oil is used over the decades for its cooling, astringent, and antiseptic properties. There are four main Rose species used in essential oil production, namely, *R. damascena* Mill., *R. gallica* L., *R. moshata* Herrm., and *R. centifolia* L. [3]. The first species is produced widely in many countries. Turkey and Bulgaria are the greatest producers in the world. This oil is used as rose water, rose cream, rose essence, and in perfumery [4]. Biologic investigations show that rose extract has properties such as antioxidant, antihepatis, antibacterial (i.e., against *Erwinia amylovora*), and antiviral with selective inhibition of protease by virus [5–7]. Water and methanol extracts of *R. damascena* exhibited moderate anti-HIV activity [8]. Different techniques have been used to extract essential oil of this plant, e.g., hydro or steam distillation, solvent extraction, and supercritical fluid extraction [9, 10]. Recently superheated water extraction has been used to extract the volatiles of *R. damascena* using comprehensive two-dimensional gas chromatography with time of flight mass spectrometry [11]. It was found that superheated water extraction gives a slightly higher oil yield than water distillation. The aim of the present work is to determine the essential oil composition of a white sample of *Rosa x damascena*, growing in Central Iran (Kashan area) and carry out a comparative evaluation between this oil and the oil of the other species, pink. To the best of our knowledge, there is no previous report on volatiles of these flowers in the mentioned area.

The flowering aerial parts of two rose species yielded essential oils with intense fragrance. They were subjected to a detailed GC-MS analysis in order to determine possible similarities or differences among them. The oil obtained from the aerial parts of the white sample of *Rosa x damascena* yielded 0.035% v/w with 21 components. The major constituents of the total amount of 99.50% were: citronellol (53.61%), nonadecane (17.57%), geraniol (12.59%), heneicosane (5.46%), and phenyl ethyl acetate (2.95%). The pink species yield was 0.025% v/w with 40 components, representing 99.64% of the total composition. The major components were: citronellol (34.7%), nonadecane (14.5%), heneicosane (10.3%), β-caryophyllene (7.8%), and nerol (5%). Constituents are listed in order of their elution from a DB-5 column in Table 1, showing the variations of the amounts and compositions of essential oils for two specimens of *R. x damascena* from Central Iran (Kashan area). Percentage variations of the main components from the oils of these plants are as below: citronellol (34.7–53.61%), nonadecane (14.5–17.57%), β-caryophyllene (0.18–7.8%), geraniol (0–12.59%), nerol (0–5%), and heneicosane (5–10.3%). The target compounds with the characteristic rose scent of the essential oil of *R. damascena*, such as citronellol, geraniol, nerol, and phenyl alcohol, are found in our samples. The white flower shows a total result of 66.2% for citronellol and geraniol as the monoterpene alcohol contents while the second specimen shows 39.7% for citronellol and nerol. They also contain some components that do not contribute to the fragrance formation, like paraffins (heptadecane, nonadecane, heneicosane, and tricosane). The terpenoide components are classified in Table 1. As can be seen, the major amount of the white flower oil belongs to monoterpene alcohols (67.8%), while the pink sample represents 41.9% for these compounds. The *R. damascena* oil from china has 54.39% of monoterpene alcohols [12], while Turkey samples 1 and 2 have 27.33% and 78.66% [13] and Bulgarian rose oil shows 57.6% [14]. Our plants have no significant amounts of monoterpene hydrocarbons, whereas the pink one shows some sesquiterpenes (10.4%).

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TABLE 1. The Percentage Composition of the Essential Oil of Two *Rosa x damascena* from Kashan Area

Compound[a]	White, %[b]	Pink, %[b]	RI[c]	Compound[a]	White, %[b]	Pink, %[b]	RI[c]
Myrcene	0.16	-	984	10-epi-γ-Eudesmol	-	0.1	1622
Limonene	0.14	-	1053	Heptadec-8-ene	-	0.2	1670
Linalool	1.38	-	1074	Heptadecane	0.51	1.2	1692
Phenyl alcohol	0.39	3.1	1083	(*Z,E*)-Farnesol	0.24	-	1709
cis-Roseoxide	0.11	0.3	1117	Octadecane	-	0.4	1792
trans-Roseoxide	-	0.1	1128	Phenyl ethyl benzoate	-	0.4	1815
Fenchyl alcohol	-	0.2	1140	1-Nonadecane	-	0.6	1866
α-Terpineol	0.22	-	1182	9-Nonadecene	0.49	-	1874
Dodecane	-	0.2	1196	Nonadecene	-	0.6	1892
Citronellol	53.61	34.7	1214	Nonadecane	17.57	14.5	1901
Nerol	-	5.0	1230	Marrubine	-	2.4	1948
Phenyl ethyl acetate	2.95	0.2	1233	Eicosane	0.31	1.9	1995
Neral	-	0.2	1241	9-Heneicosene	-	0.5	2087
Geraniol	12.59	-	1245	Heneicosane	5.46	10.3	2100
Geranial	0.13	-	1250	Docosane	-	2.5	2191
Methyl geranate	-	0.5	1298	1-Docosanol	-	1.2	2286
Citronellyl acetate	0.25	0.6	1350	Tricosane	1.32	4.3	2299
Lavandulyl acetate	-	0.2	1355	9-Tetracosene	-	0.2	2387
Nerol acetate	1.26	-	1362	Tetracosane	-	1.5	2394
β-Bourbonene	-	0.1	1389	Monoterpenes, %	0.30	-	
Tetradecane	-	0.1	1395	Oxygenated monoterpenes, %			
Methyl eugenol	0.23	0.2	1400	alcohol	67.8	41.9	
β-Caryophyllene	0.18	7.8	1424	aldehyde	0.13	0.2	
α-Humulene	-	1.7	1456	ester	1.51	1.5	
Germacrene D	-	0.4	1481	Sesquiterpenes, %	0.42	10.4	
β-Selinene	-	0.1	1487	Oxygenated sesquiterpenes, %			
(*E,E*)-α-Farnesene	-	0.3	1492	alcohol	0.24	0.1	
Pentadecane	-	0.4	1494	aldehyde	-	-	
Phenyl ethyl tiglate	-	0.1	1550	ester	-	0.1	
Caryophyllene oxide	-	0.2	1577	Total	99.50	99.64	
Hexadecane	-	0.1	1593				

[a]As identified by GC–TOF/MS software; names according to Wiley 7.0 mass spectrs library, and by comparing theirt retention indices.

[b]Percentage of each component is calculated as (peak area of analyte/peak area of analyte/peak area of total ion chromatogram)×100 (in the case of multiple identification, the areas of the peaks that belong to one analyte were combined to find the total area for this particular analyte.

[c]Kovats retention indices (column:DB5).

In Italy, Reverchon et al. [9] obtained citronellol (26.1%), phenylethyl acetate (14.8%), and *n*-nonadecane (10%) from *R. damascena* by steam distillation. We compared a series of data in Table 2, according to the major components of the essential oils of rose flowers from Iran, Turkey, China, India [15], and Bulgaria. As is shown, high percentages in each sample belong to the citronellol and geraniol components. Heneicosane and nonadecane are almost common with various percentages of 2.28–10.3% and 6.44–21%, respectively. Overall, summing up each of the major components in all the samples gives the ranking: citronellol > geraniol > nonadecane > heneicosane > phenyl ethyl alcohol > nonadecene > nerol. The peak of citronellol percentages, as the first major component, belongs to Iranian white sample. Geraniol has the maximum percentage in the second sample of Turkey rose, while it is absent in Iranian pink one. Nonadecane is found in similar percentages in all samples except for Turkish and Bulgarian flowers. A general comparison of the chemical composition of rose oils from the countries mentioned above shows a noticeable difference in the amount of most of the components. Iranian roses are rich in hydrocarbons, whereas these compounds are present in smaller quantities in Turkey roses. By contrast, alcohols are in very high amounts in turkish flowers. The chemical variation of *Rosa damascena* populations from different geographic origins may be due to the environmental influence, but the existence of chemovariations under the same conditions may be determined by genetic factors.

TABLE 2. Essential Oil Comparison of Some *Rosa damascenas* from Different Regions of the World

Compound	Iranian White[a]	Iranian Pink[a]	Chinese Rose [12]	Turkish Rose (1) [13]	Turkish Rose (2) [13]	Bulgarian[c] [14]	Indian [15]
Citronellol	53.61	34.7	30.71	24.47	30.54	33.0	35.14
Nonadecane	17.57	14.5	16.95	6.44	-	9.1	-
Heneicosane	5.46	10.3	7.04	2.28	-	3.0	15.42
Geraniol	12.59		16.11	2.11	36.22	15.8	
Nerol	-	5.0	7.57	0.75	11.19	8.8	21.33
Eicosane	0.31	1.9	4.71[b]		-	-	-
Nonadecene	-	0.6	-	1.8	-	3.2[d]	-
β-Caryophyllene	-	7.8	-	-	-	-	-
Phenylethyl acetate	2.95	-	-	-	-	-	-
Linalool	1.38	-	-	-	1.91	2.7	-
Phenylethyl alcohol	-	-	-	-	1.92	-	-
Phenyl alcohol	0.39	3.1	-	-	-	-	4.32
Benzyl alcohol	-	-	-	-	2.68	-	-

[a]From Kashan area; [b]as 9-eicosane; [c]distilled in 96°C; [d]as *cis*-9-nonadecene derivative.
All numbers are in percent.

The oils of two investigated species are rich in citronellol, and due to this high monoterpene alcohol content, they can be considered in commercial cultivation for perfumery and other applications.

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