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CHEMICAL COMPOSITION OF THE ESSENTIAL OILS OF *Rosa damascen*a FROM TWO DIFFERENT LOCATIONS IN IRAN

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The rose is widely regarded as the queen of fragrant flowers. The genus "rose" consists of about 150 species of deciduous and semi-evergreen shrubs and climbers, widespread in northern temperate regions. The cultivation of roses dates back to thousands of years. In many cases, the origins and correct names of roses are extremely difficult to elucidate [1]. In the 14th century, *R. damascena* (known as *R. summer*, damask, in the USA) was brought from Persia to Europe by knights returning from the crusades [1]. There are four main species of roses used in essential oil production, namely, *R. damascena* Mill, *R. gallica* L., *R. moshata* Herrm, and *R. centifolia* L. [2]. *R. damascene* Mill. is a vigorous, arching, deciduous shrub with grey-green leaves, divided into five (rarely seven) ovate to elliptic leaflets, up to 6 cm long [1]. Roses have been used since the earliest times in rituals, cosmetics, perfumes, medicines, and aromatherapy [1, 3]. Besides these, a great variety of garden roses also exist, which are bred less for fragrance and more for color and shape [1]. Iranians today use rose water in a variety of foods and sweets such as shole-zard, ghottab, and faloodeh, as well as for medicinal purposes and in religious ceremonies. The essential oils of *R. damascena* are also known for their perfume and are used in cosmetic preparations.

Turkey, the main rose oil producer in the world, uses *R. damascena* Mill. for rose oil production [4]. There are different kinds of traditional and modern devices for the distillation of rose oil [5–7]. Several reports have appeared on the chemical evaluation of rose oils around the world [2, 7–14].

Kovats [15] reported on an intensive study that was carried out on rose oil over a tenyear period in cooperation with scientists at Firmenich, which resulted in the identification of 127 constituents in the oil [16].

Moats and Reynolds [17] published their studies on the extraction of oil from rose petals using the techniques of solvent extraction-(hexane), steam distillation, and high-pressure carbon dioxide and reported that the steam distilled oil was the least favorable [17].

Supercritical carbon dioxide extraction of concretes was carried out by Reverchon et al [18]. Supercritical carbon dioxide extraction is, in principle, a simple process and is widely used to produce extracts for food and pharmaceutical and cosmetic uses. This technique has attracted the attention of many researchers, as reported by Moyler et al [19].

Boelens [20] analyzed Bulgarian rose oil and found that the concentrations are a key issue in thresholds and odor units. Clearly β-damascenone, rose oxides, and citronellol have the greatest impact on the overall olfactive quality of oils. The total number of odor units in hydrodistilled oil is about three times that of the carbon dioxide extract. Perfumers prefer the hydrodistilled oil over the CO_2-extracted oil. Because of this olfactive difference, the market value of CO_2-extracted rose oil is only about one-third the value of hydrodistilled oil.

Kiran [21] reported that the application of higher pressure and temperatures during distillation played an important role in rose oil composition. The odor of rose water distilled under pressure was mixed with the odor of burnt residue. A comparative study of rose oil constituents extracted by dichloromethane from rose water and redistillation of rose water under high and normal pressures was also conducted. The dichloromethane extract of rose water showed higher contents of 2-phenethyl alcohol and lower contents of citronellol, nerol, geraniol, and linalool, as compared with a lower content of 2-phenethyl alcohol and a higher content of citronellol, nerol, geraniol, and linalool in redistilled rose water at higher temperature and atmospheric pressure, respectively [21]. Higher levels of alcohol content were observed in oil extracted and redistilled from rose water than in rose oil distilled directly from the flowers. Ohloff, who reported on the chemistry of natural products, pointed out the impact that various rose oil constituents have as odorants and flavoring materials [16]. Ohloff also discussed the chemistry and sensory properties of these products [16].

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TABLE 1. Percentage Composition of the Essential Oil of *R. damascena* Growing in Iran Species

Compound[a]	RI	Ka$_1$	Ka$_2$	Ker$_1$	Ker$_2$	Compound[a]	RI	Ka$_1$	Ka$_2$	Ker$_1$	Ker$_2$
3-Hexen-1-ol	764	-	Tr.	-	Tr.	Thymol	1178	-	-	-	Tr.
Hexanol	782	Tr.	0.1	Tr.	0.2	Geranyl formate	1185	Tr.	-	-	Tr.
Heptanal	809	Tr.	-	Tr.	Tr.	Undecanal	1188	0.1	-	0.1	-
α-Pinene*	855	1.7	0.2	3.1	Tr.	Methyl geranate	1204	-	0.1	-	-
Camphene	867	Tr.	-	Tr.	-	Methyl eugenol	1205	0.7	1.9	0.4	0.1
Heptanol	885	-	Tr.	-	Tr.	Eugenol	1237	0.4	1.5	0.2	1.8
Sabinene*	892	0.1	Tr.	0.3	-	*cis*-2,6-Dimethyl-2,6-octadiene	1249	1.2	0.9	1.7	0.3
6-Methyl-5-hepten-2-one	893	-	-		Tr.	Nerol	1257	0.3	-	-	-
β-Pinene	895	0.4	0.1	0.7	-	Neryl acetate	1258	-	0.1	0.4	-
6-Methyl-5-hepten-2-ol	906	-	-	-	Tr.	*β*-Damascenone	1274	Tr.	Tr.	-	-
β-Myrcene	912	0.6	0.1	1.1	Tr.	Decanoic acid	1275	Tr.	-	-	-
Phellandrene	921	Tr.	-	Tr.	-	Geranyl acetate	1283	1.9	1.3	3.1	0.7
Benzyl alcohol	931	Tr.	0.1	-	Tr.	*α*-Copaene	1285	Tr.	-	-	-
α-Terpinene	933	0.1	-	0.1	-	*β*-Bourbonene	1294	0.3	-	0.3	-
Cymene[b]	936	0.1	0.1	Tr.	Tr.	*β*-Elemene	1302	0.4	0.2	0.6	-
1,8-Cineole	942	0.1	Tr.	Tr.	Tr.	Dodecanal	1307	Tr.	-	Tr.	-
Limonene	945	0.1	Tr.	0.1	0.1	Tetradecane	1316	Tr.	Tr.	Tr.	-
(*Z*)-*β*-Ocimene*	954	Tr.	-	Tr.	-	*β*-Caryophyllene	1319	1.2	0.7	1.2	0.1
(*E*)-*β*-Ocimene*	964	0.1	Tr.	0.1	Tr.	Dihydrobeta-ionone	1324	-	Tr.	-	-
γ-Terpinene	979	0.1	Tr.	0.2	-	*β*-Cubebene	1326	0.1	0.1	0.1	-
Linalool-oxide B	981	-	Tr.	-	Tr.	*α*-Guaiene	1333	1.5	0.9	1.6	0.1
Octanol	983	Tr.	Tr.	-	Tr.	Aromadendrene	1338	Tr.	-	-	-
o-Allyltoluene	994	-	-	-	Tr.	*α*-Humulene	1340	1.3	0.7	1.1	0.1
Dehydro-*p*-cymene	995	-	Tr.	-	-	(*Z*)-*β*-Farnesene	1347	0.1	0.1	0.1	-
α-Terpinolene	1000	0.1	Tr.	0.1	Tr.	2-Butanoic acid, 2-methyl-2-phenylethyl ester	1352	0.1	0.1	0.1	0.1
Nonanal	1005	0.1	-	0.1	-						
Phenyl ethyl alcohol	1011	-	5.8	-	4.9	Benzyl tiglate	1354	-	-	-	0.1
Linalool	1012	0.3	0.7	0.1	0.1	Germacrene D*	1357	3.5	1.6	4.0	-
Perillen	1014	-	-	Tr.	-	*β*-Selinene	1360	0.1	0.1	0.1	-
cis-Rose-oxide	1018	0.2	0.2	0.1	0.3	*β*-Gurjunene	1363	-	Tr.	-	-
Terpin-1-ol	1023	-	Tr.	-	Tr.	2-Tridecanone	1366	-	Tr.	-	-
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	1027	-	-	Tr.	-	*α*-Selinene	1368	0.1	0.1	0.1	-
trans-Rose-oxide	1031	0.1	-	0.1	-	*δ*-Guaiene	1376	1.2	0.7	1.2	0.1
Heptanoic acid	1037	-	-	-	Tr.	*α*-Farnesene	1379	0.3	0.1	0.4	-
Citronellal	1049	Tr.	Tr.	Tr.	Tr.	Pentadecane	1382	1.1	-	1.0	0.1
Nerol oxide	1054	Tr.	0.1	Tr.	0.1	*δ*-Cadinene	1385	0.2	-	0.1	Tr.
Ethyl benzoate	1058	-	0.1	-	-	Elemol	1397	Tr.	Tr.	0.1	Tr.
2-Cyclohexene-1-methanol,2,6,6-trimethyl-	1068	-	0.1	-	Tr.	Sesquirosefurane	1406	Tr.	Tr.	Tr.	-
						Nerolidol	1418	0.2	0.2	0.2	0.2
4-Terpineol	1072	0.1	0.4	Tr.	0.7	Caryophyllene oxide	1428	0.1	Tr.	Tr.	Tr.
Methyl bornyl ether	1075	-	-	Tr.	-	Dodecanoic acid, ethyl ester	1458	0.1	0.1	-	-
cis-Dihydrocarvone	1079	-	Tr.	-	Tr.	Dill apiol	1460	-	-	-	0.1
α-Terpineol	1083	-	-	Tr.	1.8	Hexadecanal	1471	-	-	0.1	-
β-Fenchyl alcohol	1085	-	2.1	-	-	Hexadecane	1462	0.4	0.2	0.3	Tr.
γ-Terpineol	1089	-	0.1	-	-	*γ*-Eudesmol	1484	-	0.1	-	0.1
Decanal	1097	Tr.	-	0.1	-	*t*-Cadinol	1494	0.1	0.1	-	0.1
Dodecane	1113	Tr.	-	Tr.	-	*β*-Eudesmol	1500	0.1	0.1	-	0.1
Citronellol	1139	20.6	30.6	12.6	53.4	Germacrene B	1503	-	0.1	-	0.1
Geraniol	1160	4.8	6.7	3.8	22.7	*α*-Eudesmol	1506	0.2	0.2	-	0.2
Isogeraniol	1161	Tr.	0.1	Tr.	Tr.	6(*E*),8(*E*)-Heptadecadiene	1533	0.1	-	Tr.	-
Citronellyl formate	1167	0.1	0.1	0.1	0.1	(*Z,E*)-Farnesol*	1540	1.8	-	0.1	0.1
Nonanoic acid	1172	-	-	-	0.1	Heptadec-8-ene*	1541	1.1	-	1.0	-

TABLE 1. (continued)

Compound[a]	RI	Ka$_1$	Ka$_2$	Ker$_1$	Ker$_2$
(*E,E*)-Farnesol*	1556	-	-	2.5	0.5
Heptadecane	1559	6.0	-	4.4	0.4
Benzyl benzoate	1565	0.2	-	-	0.1
(*E,E*)-Farnesal*	1567	-	-	0.1	-
Heptadecadiene	1569	Tr.	-	-	-
(3*E*)-Octadecene*	1614	0.2	-	0.2	Tr.
Hexadecanal	1645	0.2	-	-	-
(16*E*)-Octadecenal	1647	-	-	0.3	-
Phenethyl benzoate	1648	-	-	-	0.1
Benzoic acid, 2-phenyl ester	1650	0.2	-	-	-
Octadecane	1653	0.6	0.4	0.5	0.1
Octanoic acid, 2-phenylethyl ester	1664	Tr.	-	-	-
Farnecyl acetate	1671	0.1	Tr.	0.1	-
Hexahydrofarnesyl acetone	1688	Tr.	-	Tr.	-
1,13-Tetradecadiene	1719	0.2	0.1	0.1	-
Benzene acetic acid, 2-phenyl ethyl ester	1720	-	-	-	Tr.
1-Nonadecene	1732	12.9	6.0	8.6	-
(5*Z*)-Nonadecene	1737	0.1	0.1	-	1.0
Nonadecane	1752	2.7	17.9	22.8	3.4
Hexadecanoic acid	1778	-	-	-	0.1
(5*E*)-Eicosene	1800	0.1	0.2	-	Tr.
(3*E*)-Eicosene	1803	0.5	-	-	-
Hexadecanoic acid, ethyl ester	1808	0.1	-	-	-
(9*E*)-Eicosene	1813	0.1	-	0.4	-
Eicosane	1823	3.1	1.4	2.4	0.3
10-Heneicosane	1870	-	-	0.4	0.1
9-Heneicosane	1872	-	0.2	-	-
9-Nonadecene	1873	0.6	-	-	-
1-Octadecene	1889	0.5	-	-	-
9-Heneicosene	1889	-	-	0.3	-
Heneicosane	1895	13.5	4.8	9.6	1.5
Geranyl isovalerate	1911	0.1	-	Tr.	-
Linoleic acid, ethyl ester	1918	0.1	Tr.	-	-
Ethyl linolenate	1920	-	Tr.	-	-
1-Dococene	1952	0.1	-	Tr.	-
Docosane	1960	0.4	0.1	0.3	0.1
1-Tricocene	2016	0.5	-	-	-
9-Tricosene	2016	-	0.1	0.3	0.1
2,6,10,14-Tetramethylhexadecane	2025	-	-	-	0.3
Tricosane	2027	2.6	0.6	2.0	-
Geranyl propionate	2039	0.1	-	-	-
Tetracosane**	2087	0.1	Tr.	0.1	Tr.
Pentacosane	2148	0.7	0.1	0.6	0.1
Hexacosane	2210	0.1	0.2	Tr.	0.4
Heptacosane	2260	0.6	0.1	0.5	0.1
Octacosane	2322	Tr.	-	-	-
Nonacosane	2397	0.1	Tr.	0.1	-

Tr.: less than 0.05%.

[a] Method of identification: RI, MS; *RI, MS, CoI; **V.

[b] Correct isomer not determined.

Ka$_1$ = first oil rose of Kashan; Ka$_2$ = second oil rose of Kashan; Ker$_1$ = first oil rose of Kerman; Ker$_2$ = second oil rose of Kerman.

A comparative study of volatile components of *R. damascena* has been carried out, using various techniques, namely direct thermal desorption (DTD), superheated water extraction (SWE), and water distillation (WD) [22]. It was found that SWE gave a slightly higher oil yield than WD. The phenyl ethyl alcohol content, which is highly desirable in rose oil, was significantly higher using the DTD (36.52%) and SWE (38.14%) techniques than with the WD (1.92%) technique. WD gave a higher content of citronellol (30.54%) and geraniol (36.22%) when compared with the SWE and DTD techniques. DTD volatiles showed a greater total number of different components than either the SWE or WD methods. It was hence concluded that the DTD is a promising method for qualitative analysis of volatiles of *R. damascena* [22].

According to the results of the other researchers, namely Moates [17], Moyler [19], Boelens [20], Kiran [21], and Ozel [22], the hydrodistillation method is suitable and economical for factory oil production.

The objective of the present study is focused on the evaluation of hydrodistillation method and the chemical composition of rose oil distilled from different species. This simple, rapid, and economical method was applied to the identification and determination of *R. damascena* Mill. from two species which are mostly cultivated in Iran. To the best of our knowledge, no such studies have been reported in the literature until now.

The damask rose (*Rosa damascena* Mill.) is cultivated at different locations in Iran. The flowers are picked early in the morning before sunrise during the months of May and June and used for distillation.

A direct-fired field distillation unit containing a distillation tank (capacity: 3000 L) and a condensation column and receiver, all made of stainless steel and which can process 300–500 kg fresh rose flowers/batch, was installed at an altitude of 2600 m. Fresh rose flowers (340 kg) were charged into the distillation unit along with 200 L fresh water. The unit was heated by water steam. The system was kept open to atmospheric pressure until the temperature rose to 70°C, and consequently the air present in the unit was replaced by the vapor. After complete removal of air from the unit, the air vent was closed and the whole unit was operated as a closed system under pressure to distill the oil. The pressure, temperature, and rate of distillation were controlled manually. The vapors produced in the still were condensed in a condensation column and collected in a receiver equipped with cold water circulation. The process was completed after the collection of 500 L of distilled rose water. The oil collected (first oil, crude oil, or direct oil) in the receiver was separated from the rose water and dried over anhydrous Na_2SO_4. The oil samples were analyzed by GC/MS and GC/FID. The oil compositions of distilled rose are shown in Table 1.

Rose water collected in the receiver was redistilled in a redistillation tank in 3000 L stills to yield more rose oil (this oil is known as second oil, cooked oil, or indirect oil). The redistilled rose oil was dried over anhydrous Na_2SO_4. The second oil samples were also analyzed by GC/MS and GC/FID. The oil compositions of redistilled rose water are shown in Table 1.

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