

## Essential Oil Composition of *Rosa damascena* Mill Cultivated in Central Iran

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The essential oil of *Rosa damascena* Mill cultivated in central Iran (Kashan region) from the petals and whole flower (petals and retals), were extracted using a Clevenger apparatus in aqueous and acidic (10% v/v) solutions. Depending on the conditions of the steam distillation, eighteen major components of the essential oil extracts were identified by GC-MS in a 0.4-1% yield. The volatile components obtained from the retals were compared with the volatile oil from whole flowers (retals and petals) in aqueous and acidic solutions. The major differences were, first, some of the effective component in the retals, like  $\beta$ -citronellol, which is responsible for the higher quality of the rose oil obtained in a better yield, and, secondly, some of the toxic components, like 2-octanamine (0.47% in E sample), which can reduce the quality of the rose oil and which are completely removed in the acidic solution. According to the GC-MS results,  $\beta$ -citronellol (14.5-47.5%), nonadecane (10.5-40.5%), geraniol (5.5-18%) and heneicosane (7-14%), were the major components of the oil.

### INTRODUCTION

The fragrance of the rose flower captured by extraction is one of the most valuable flavours and fragrances produced. The most common aroma concentrates of rose are rose oil and rose water, derived from steam distillation. *Rosa damascena* Mill (which is known as Gole Mohammadi in Persian) belongs to the family of Rosaceae, many species and variety of which are cultivated throughout the world as an ornamental plant. *Rosa damascena* needs moderate temperatures and humid air during flowering to achieve a rich oil content. This type of rose is mainly grown in temperate climates, usually at an altitude between 300-1800 m. *Rosa damascena* is well known as medicinal herbal. In addition to its perfume, in traditional medicine, several pharmacological effects of this plant, such as a therapeutic effect on premenstrual breast

tenderness and reduction of inflammation, especially of the neck, were reported [1]. Also rose oil is famous, not only for its wide application in perfumery and cosmetics, but also, along with its aroma properties, it is a valuable natural drug agent possessing bacteriostatic, antihistological, gall curative, antispasmodic and relaxing etc. [1]. Avicenna showed that rose oil has uses in aroma-therapy for treatment of cardiac diseases [2].

There are different kinds of traditional and modern devices for the extraction of volatile oil from *Rosa damascene* [3-7]. A number of reports have appeared on the chemical evaluation of rose oil [8,9] and exhaustive reviews have been published by placeCity-Lawrence [10,11]. Rose oil can be contaminated with aliphatic amines. Some common toxicological properties for aliphatic amines have been reported in [12].

The objective of the present study is focused on the evaluation of neutral and acidic media on the steam-distillation of *Rosa damascene* and also a comparative study of the components in whole flowers and petals. To the best of the authors knowledge, no such studies have been reported in the literature on Iranian essential rose oil.

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## EXPERIMENTAL/PLANT MATERIAL

The petals and whole flowers (petals and sepals) of *Rosa damascena* were collected during its flowering period, which begins in May to mid-June, depending on the amount of sunshine and the altitude of the growing region in Kashan (central region of Iran). The flowers are picked in the early morning, when starting to bloom. They are taken to the distillatory apparatus as quickly as possible and utilized for distillation.

## ISOLATION OF VOLATILES

In the first analysis, the petals of the Vidorj regions (200 g) were placed on the cleverger apparatus [13] and the volatile fraction was isolated by steam-distillation for 4 h, according to the method recommended in the European pharmacopoeia [14]. The essential oil (0.5 mL) was collected from the rose water using a separator funnel. Secondly, equally in two sets of cleverger apparatus, the sepals and petals (200 g) of the flowers from the Vidorj and Dorrin regions were extracted, using steam-distillation in distilled water and 0.8 and 0.2 mL of essential oil was collected, respectively. The third experiment was carried out on 200 g of sepals and petals of the Khonb and Ghemsar regions with 10% v/v sulfuric acid in water. 0.4 mL and 0.6 mL of essential oil was obtained, respectively. The oils which were light yellow in color were dried over anhydrous calcium chloride and stored in vials at a low temperature (2°C) until analysis.

## GC AND GC-MS ANALYSES

The extracted oil was analyzed by GC and GC-MS. GC analysis was carried out on a Hewlett-Packard-6890 gas chromatograph equipped with a Free-Induction Decay (FID) detector and an HP-5MS fused silica column (30 m × 0.25 mm i.d., film thickness, 0.25 μm). Oven temperature was held at 60°C for 3 min and then programmed to 220°C at a rate of 6°C/min. The injector and detector (FID) temperatures were 290°C and the carrier gas was helium with a flow of 1 mL/min. The volume injected was 0.1 × 1 of the oil and the split ratio was 1:20.

GC/MS analysis was performed on a HP-6890 mass selective detector coupled with a HP-6890 gas chromatograph, equipped with a cross-linked 5% pH ME siloxane HP-5MS capillary column (30 m × 0.25 mm i.d., film thickness, 0.25 μm) and operating under the same conditions as described above. The MS operating parameters were as follows: Ionization potential, 70 eV; ionization current, 2A; ion source temperature, 200°C; resolution, 1000.

## IDENTIFICATION OF COMPONENTS

The components of the oil were identified by GC retention indices relative to *n*-alkanes and computer matched with a Wiley 275 Library, as well as by comparison with the fragmentation pattern of the mass spectra with those of authentic samples or with data published in the literature [15-17]. The percentage compositions of the samples were computed from the GC peak areas.

## RESULTS AND DISCUSSION

In this study, more than 95 macro- and micro-components were found in the essential oil of *Rosa damascena* from the Kashan regions. The oil yield (1% v/w) from the flavor of *Rosa damascena* was determined by a gravimetric method and calculated in percentage, with respect to the starting mass of the plant material. Eighteen compounds were identified, representing more than 95% of the total oil (Table 1).

The major constituents are listed in order of their elution from a HP-5Ms column. The constituent of the oil was β-citronellol (15-47.5%), nonadecan (24-40.5%), geraniol (0-18%) and hencosane (7-14.5%).

The advantage of using sulfuric acid was in the removal of trace aliphatic amines, which were present in some cases and the disadvantage was in removing geraniol, linalool, geraniol acetate, *cis* fransol and nerol. Also, the percentage of β-citronellol was reduced to half in this solution.

Bulgarian rose oil was reported, which was as follows: β-citronellol (30.31%), geraniol (16.96%), phenyl ethyl alcohol (12.60%), nerol (8.46%), hexacosane (3.70%), nonadecane (2.7%), linalool (2.15%), β-Ionone (1.00%), ecosane (1.65%), docacosane (1.27%), farnesol (1.36%), neryal acetate (1.41%), citronellyl propionate (1.38%), geraniol (1.35%), α-pinene (0.60%), myrceen (0.46%), *cis* rose oxide (0.55%), decanal (0.51%), terpine-4-ol (0.55%), β-caryophyllene+citronellyl act (0.81%), *iso* borneol (0.57%), heptadecane (0.92%) [18].

The comparison of the results with the literature showed significant differences for oils, which can be attributed to ecological factors, genetic differences or the development stages of the plant parts analyzed.

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**Table 1.** The percentage composition of the essential oil of *Rosa damascena* identified with GC/MS

No	Compound	A%	B%	C%	D%	E%	RI/S	RI/R
1	$\beta$ -Citronellol	47.43	32.49	23.55	26.05	14.88	1212	1228
2	Nonadecane	-	23.99	39.70	40.68	10.39	1921	1900
3	Geraniol	-	18.12	5.65	-	-	1232	1255
4	Phenyl Ethyl Alcohol	0.26	0.39	-	0.22	0.41	1075	1110
5	Henicosane	17.45	9.64	-	13.89	7.3	2114	2100
6	9-Nonadecen	2.63	4.89	4.26	4.95	3.34	1860	1893
7	Eicosane	0.66	1.29	1.87	1.71	20.5	2007	2000
8	Linalool	-	0.29	-	-	-	1095	1100
9	Citronellyl acetate	-	0.13	-	-	-	1326	1354
10	Methyl eugenol	-	0.55	0.87	2.55	1.78	1364	1401
11	Cis-farnesol	-	1.57	-	-	-	1686	1697
12	Heptadecane	1.10	1.37	1.59	-	1.55	1703	1700
13	Pentadecane	0.16	0.13	1.32	2.65	0.96		
14	Docosane	-	-	19.50	0.44	7.03	2202	2200
15	Nerol	1.15	-	-	-	-	1212	1228
16	Disiloxane	17.58	-	-	-	-		
17	Octadecane	6.13	-	-	-	-	1799	1800
18	Pentacosane	-	-	-	-	2.42	2505	2500
	Total	94.55	94.98	98.31	93.14	94.55		

A: Petals of Vidorj regions extracted in distilled water;

B: Whole flower (petals and sepals) of Vidoj regions extracted in distilled water;

C: Whole flower (petals and sepals) of Dorrin regions extracted in distilled water;

D: Whole flower (petals and sepals) of Ghamsar regions extracted in 10% sulfuric acid;

E: Whole flower (petals and sepals) of Khonab regions extracted in 10% sulfuric acid;

GC-MS: The RI of the component was according to an authentic standard;

%: Relative percentage obtained from peak area;

RI: Retention index, S: Sample and R: Ref. [14].

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