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Volatile oil composition of *Rosa damascena* Mill. (Rosaceae)

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Abstract

The volatile oil obtained by hydrodistillation of the petals of *Rosa damascena* Mill. (Rosaceae) was analyzed by gas chromatography and gas chromatography/mass spectrometry (GC/MS). The yield of the oil was 0.12 % (v/w). Fifty compounds representing 99.06 % of the oil were characterized. The volatile oil was found rich in sesquiterpenes and aliphatic components, consisting of two monoterpenic esters (0.44 %), nineteen sesquiterpenes (44.05 %), twenty nine aliphatic compounds (54.57 %) including n-octadecanol, n-hexacosane, n-octacosane and n-nonacosane (26.31 %).

Keywords: *Rosa damascena*, Rosaceae, GC-MS, Damask rose, Fragrance.

1. Introduction

Rosa genus, belonging to the Rosaceae family, includes 200 species and more than 18,000 cultivars. One of the most important *Rosa* species is *Rosa damascena* Mill., which is known as "*Gol-e-Mohammadi*" in Persian. This plant is called *Damask rose* because it was originally brought to Europe from Damascus [1]. It is an erect shrub of 12 m in height [2] and primarily cultivated in Turkey, Bulgaria, Iran, India, Morocco, South France, China, South Italy, Libya, South Russia and the Ukraine in the world [3].

R. damascena has attracted considerable attention in horticulture, biochemistry and in pharmacology because of the fragrance of the flowers and the high content of its biologically active substances [4]. Roses are of worldwide economic importance as the centre of a large ornamental shrub and cut flower industry. They also are economically important as a source of essential oils for perfumes and scents [5]. The most important products obtained from oil rose are rose oil, rose water, rose concrete and rose absolute [6]. The rose water were scattered at weddings to ensure a happy marriage and are symbol of love and purity and are also used to aid meditation and prayer [7]. Rose water it mainly used in cosmetics industry in various fairness creams and also for cleansing of face.

Rose oil is mainly used in the perfumery and cosmetics industry as a base component of many of the modern perfumes but it also finds application in the food industry as a flavour additive. The main producers of rose oil are Bulgaria, Turkey, Iran and India. Smaller amounts of rose oil and mainly rose water are produced in the countries of Northern Africa [8]. It is well known for its relaxing effects; traditionally, rose oil is used as a remedy for anxiety, depression and for the treatment of stress related conditions in many parts of the world [9]. Intraperitoneal injection of *R. damascena* essential oil retarded the development of seizure stages in rats [10].

It is reported to possess anticancer [11], anti-aging [12], laxative/purgative [13], hypolipidemic [14,15], antidiabetic [16], antibacterial [17] and antimicrobial activities [18]. In Unani System of Medicine, it is also known as "*Gul-e-Surkh*", widely used as ingredient of various polyherbal formulation *e.g.*"*Safoof-e-Muhazzil*"for the treatment of obesity [19]. The aim of this paper is to identify the chemical composition of the volatile oil of petals of *R. damascena* Mill. by GLC and GC-MS analysis.

2. Material and Methods
2.1. Plant Material and Authentication
The petals of *R. damascena* were purchased from a local market in New Delhi and authenticated by Dr. H. B. Singh, Scientist F and Head, Raw Materials Herbarium and Museum, National Institute of Science Communication and Information Resources (NISCAIR), New Delhi. Voucher specimen of drug was deposited in the Raw Materials Herbarium and Museum, National Institute of Science Communication and Information Resources (NISCAIR), New Delhi, with reference number Ref. NISCAIR/RHMD/consult/-2010-11/1705/05/S.No. 3.

2.2. Isolation of volatile oil
The petals of *R. damascena* (500 g) were hydro-distilled for six hours with Clevenger apparatus. The yield of volatile oil obtained was 0.12 % v/w. The light yellowish coloured volatile oil was collected in the graduated tube. The collected volatile oil was dried over anhydrous sodium sulphate and stored at 4 ^{0}C in the dark.

2.3. GC Analysis
The gas chromatographic analysis of the volatile oil was carried out on Shimadzu 2010 Gas Chromatograph (Japan) equipped with a flame ionization detector (FID) and AB-Innowax 7031428 WCOT fused capillary column (60 m x 0.25 mm x 0.25 µm). The injector and detector (FID) temperatures were maintain at 250 and 270 ºC, respectively. The carrier gas used was nitrogen at a flow rate of 1.21 mL/min with column pressure of 155.1 kPa. The sample (0.2 µl) was injected into the column with a split ratio of 80:1. Component separation was achieved following a linear temperature programmed from 60-230 ºC at a rate of 3 ºC/min and then held at 230 ºC for 9 min, with a total run time of 55.14 min. Percentage of the constituents were calculated by electronic integration of FID peak areas.

2.4. GC-MS Analysis
The analysis of the volatile constituents were run on a Shimadzu QP-2010 GC-MS system equipped with AB-Innowax 7031428 WCOT column (60 m x 0.25 mm x 0.25 µm) directly coupled to the MS. The carrier gas was helium with a flow rate of 1.21 mL/min. oven temperature was programmed as 50 ºC for 1 min and subsequently held isothermal for 2 min. injector port: 250 ºC, detector: 280 ºC, split ratio 1:50, volume injected: 1 µL of the oil. The recording was performed at 70 eV, scan time 1.5 s; mass range 40-750 amu. Software adopted to handle mass spectra and chromatograph was a Chem station (Figure2).

2.5. Identification
The individual peaks/constituents were identified by gas chromatography by comparison of their retention indices (R.I.) either with those of authentic compounds available in author's laboratory or with those of literature in close agreement to R.I [20-26]. Further identification was made by comparison of fragmentation pattern of mass spectra obtained by GC-MS analysis with those stored in the spectrometer database of NBS 54 K.L, WILEY8 libraries and published literature [27-30]. Retention indices of the components were determined relative to the retention times of a series of n-alkanes relative to C_9-C_{20} on HPS and HP-20M columns.

3. Results and Discussions
Volatile oil of *Rosa damascena* was characterized by very less numbers of monoterpenes (0.44 %) and large numbers of sesquiterpenes (44.05 %) and aliphatic components (54.57 %) with n-hexyl benzoate (2.98 %), trans-2-hexyl-n-octanoate (4.79 %), methyl octadecane (1.90 %), n-octadecanol (4.70 %), n-hexacosane (3.35 %), n-octacosane (2.29 %) and n-nonacosane (26.31 %). Monoterpenes were consists of a monoterpenes ester, 2-isopropyl-5-methylcyclohexyl ester (0.25 %) and citronellyl-n-butyrate (0.19 %) (Table 1; Figure 1).

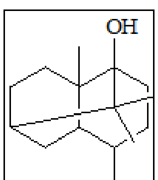
Among nineteen sesquiterpenes (44.05%), all are positively characterized. There are six sesquiterpene hydrocarbons (2.67 %), namely β-patchaulene (0.56 %), α-santalene (0.20 %), β-selinene (0.35 %), α-selinene (0.87 %), and γ-cadinene (0.21 %). There were nine sesquiterpene alcohols (22.16 %) in which prominent sesquiterpene alcohols were t-cadinol (7.75 %), patchaulene alcohol (11.54 %), (2Z,6E) farnesol (0.67 %), viridiflorol (0.47 %), α-cadinol (0.38 %) and β-bisabolol (0.38 %). There are two sesquiterpene oxides (12.37 %), the predominant sesquiterpene oxide was bisabolol oxide (12.18 %) and other caryophyllene oxide (0.19 %). The two sesquiterpene esters (6.85 %) were consists of (2Z,6E)-farnesyl ester (6.53 %) and α-bisabolol acetate (0.32 %)(Table 1; Figure 1).

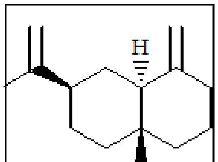
Among twenty nine aliphatic components (54.57 %), there were nineteen aliphatic hydrocarbons (39.61 %), four aliphatic alcohols (5.82 %), four aliphatic esters (8.59 %) and one each aliphatic anhydride (0.18 % and aliphatic carboxylic acid (0.37 %). The aliphatic hydrocarbons were abundantly found in the essential oil among all the aliphatic components. The predominant aliphatic hydrocarbons were n-nonacosane (26.31 %), n-hexacosane (3.35 %), n-octacosane (2.29 %), and methyl octacosane (1.90 %). the predominating aliphatic alcohol was n-octadecanol (4.7 %) with other n-pentadecanol (0.21 %), 2-methyl-2-butanol (0.44 %), and tetradecanol (0.57 %). There were four aliphatic esters (8.59 %) consisting of trans-2-hexanyl-n-octanoate (4.79 %), n-hexyl benzoate (2.98 %), n-octadecanyl acetate (0.78 %) and ethyl acetate (0.44 %). In this report there were no diterpene and aromatic components characterized. Among fifty volatile constituents (99.06 %), fifty five components (98.16 %) were positively characterized and five volatile oil components (0.90) were partially characterized (Table 1; Figure 1).

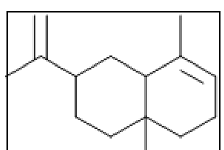
Rosa damascena var. "*trigintipetala*" also known as the oil bearing rose is one of the most important Damask roses industrially cultivated for the production of rose oil and rose water after steam-distillation or rose concrete and rose absolute after solvent extraction [27]. Iranian sample was characterized by high amounts of ecosane (29.88 %), citronellol (25.59 %) and docosane (14.07 %) [28]. Bulgarian rose oil was reported to have citronellol (30.31 %), geraniol (16.96 %), phenyl ethyl alcohol (12.6 %), nerol (8.46 %), hexacosane (3.7 %), nonacosane (2.7 %), ecosane (1.65 %), farnesol (1.36 %) and citronellyl propionate (1.38 %) [29]. Essential oil of its formulation "*Safoof-e-Muhazzil*" reported to contain many constituents *e.g.* eudes-4(14),11-diene (28.61 %), viridiflorollaurate (16.40 %), bisabolene (9.73 %), globulol (9.13 %), thymol (6.14 %), *t*-cadinol (4.15 %), *trans*-cadine-1,4-diene (2.08 %), 2E, 6E-farnesol (1.41), limonene (1.39 %), *δ*-cadinene (1.37 %) and *β*-gurjunene (1.28), which can be compared [30].

Table 1: Volatile oil constituents of *Rosa damascena* Mill.

S. No.	Components	Per cent (%)	Kovats index
1.	Ethyl acetate	0.44	608
2.	2-Methyl-2-butanol	0.34	614
3.	Acetic acid anhydride	0.18	641
4.	2-Isopropyl-5-methyl-cyclohexyl ester	0.25	1281
5.	β-Patchaulene	0.56	1365
6.	α-Santalene	0.20	1420
7.	β-Selinene	0.35	1471
8.	α-Selinene	0.87	1477
9.	γ-Cadinene	0.21	1512
10.	Elemol	0.51	1524
11.	Citronellyl n-butyrate	0.19	1526
12.	n-Hexyl benzoate	2.98	1560
13.	*trans*-2-Hexenyl n-octanoate	4.79	1573
14.	α-Farnesene	0.48	1584
15.	Caryophyllene oxide	0.19	1587
16.	Viridiflorol	0.47	1590
17.	Isospathulenol	0.17	1634
18.	t-Cadinol	7.75	1639
19.	α-Cadinol	0.38	1652
20.	Himachalol	0.29	1656
21.	Bisabolol oxide	12.18	1661
22.	Patchouli alcohol	11.54	1669
23.	β-Bisabolol	0.38	1675
24.	Tetradecanol	0.57	1680
25.	(2Z,6E)-Farnesol	0.67	1722
26.	Methyl heptadecane	0.17	1762
27.	n-Pentadecanol	0.21	1776
28.	n-Heptadecane	0.72	1795
29.	α-Bisabolol acetate	0.32	1798
30.	n-Octadecane	0.18	1802
31.	Methyl pentadecanoate	0.38	1807
32.	(2Z,6E)-Farnesyl acetate	6.53	1824
33.	n-Octadecanyl acetate	0.78	1830
34.	6,10,14-trimethyl-2-pentadecanol	0.32	1846
35.	Methyl octadecane	1.90	1860
36.	Nonadecane	0.32	1895
37.	n-Eicosane	0.63	2000
38.	n-Octadecanol	4.70	2080
39.	n-Docosane	0.19	2195
40.	9-Octadecanoic acid	0.37	2261
41.	n-Tricosane	0.29	2280
42.	n-Tetracosane	0.22	2400
43.	n-Pentacosane	0.33	2500
44.	n-Hexacosane	3.35	2600
45.	Methyl hexacosane	0.40	2640
46.	n-Heptacosane	0.46	2700
47.	n-Octacosane	2.29	2800
48.	2-Methyl octacosane	0.48	2869
49.	3-Methyl octacosane	0.27	2881
50.	n-Nonacosane	26.31	2900
Total		99.06	


Patchouli alcohol


β-Selinene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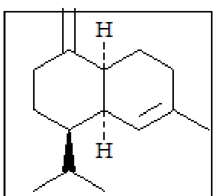
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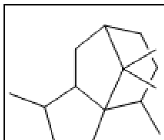
β-Patchaulene


n-Octadecane

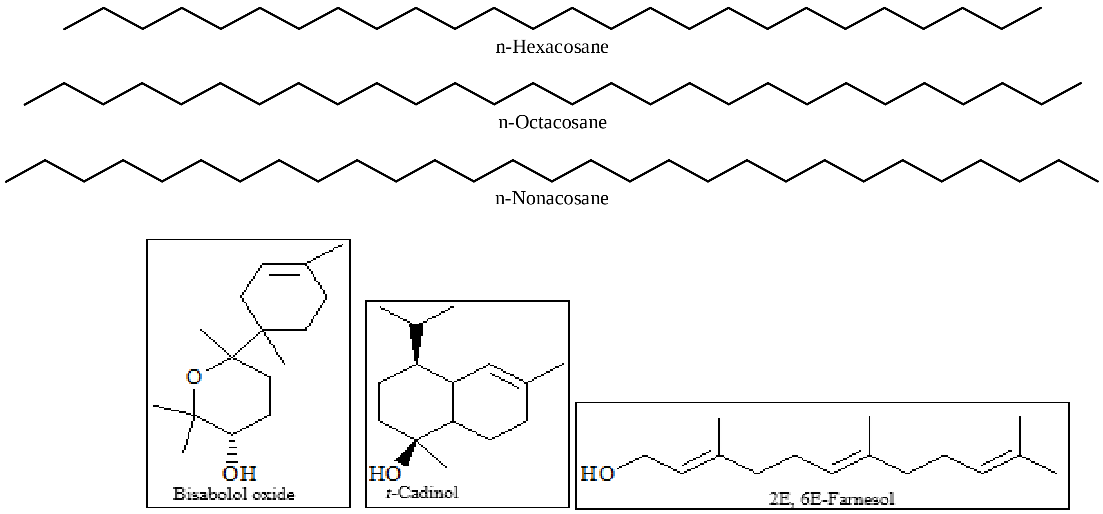

Fig 1: Structures of volatile constituents of *Rosa damascena* oil

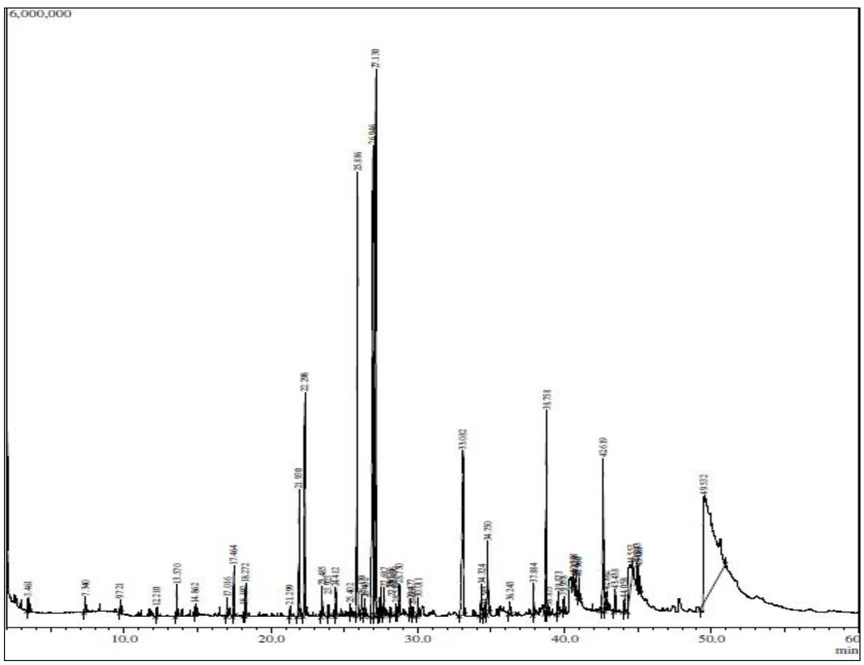

Fig 2: GC-MS spectra of volatile oil of *Rosa damascena*

4. Conclusion

In this report we do not find geraniol, phenyl ethyl alcohol, nerol as reported by earlier researchers [28, 29] while the percentage of hexacosane, octacosane, octadecanol, nonadecane, patchouli alcohol and t-cadinol varies considerably.Variation in the composition of essential oils depends on their genetic variations, geography, time of collection, stages of plant growth and seasonal and environmental factors. Variations in the traded herbal composition occurs on account of geo-climatic conditions of their growth, maturity at the time of collection, species variation at times, substitutability on the basis of perceived efficacy and dubious trade practices [31].

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