Study of the chemical compositions of Iranian rose flower essence oil (*Rosa persica*)

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Iranian rose flower or varak (*R. percica* sp.) belongs to the rose flowers species. Being a perennial shrub type it has quite a lot of ramifications which propagate by seed. The purpose of this study is to identify the chemical compositions present in the essence of varak plant (*R. perisca*). For this purpose, this plan was collected from the Ashtian region of Markazi province in (2014) and after drying in ambient temperature the extraction of the essence oil was carried out by implementing steam distillation method. The constituent compositions of the essence oils were separated and identified by the use of gas chromatograph (GC) devices and gas chromatograph connected to mass spectrometry (GC/MS). In the essence of these plants 56 compositions were identified so that the main part of this essence was constituted from hydrocarbon (alkans). Among the identified compositions the active ingredient of heptacosane with (11.6) has the highest percentage and after that stands isobutyl phthalate (11.48), nonacosane (8.88), dibutyl phthalate (6.26), pentacosane (5.96), hexadecanoic acid (3.95), linalool (3.8), ethyl linoleolate (3.73), hexyl hexoate (3.67), octacosane (3.43) are the main constituent compositions of this plant.

Key words: Iranian rose flower (Rosa persica), essence, heptacosane

INTRODUCTION

Varak species by the scientific name of Rosa persica belongs to the Rooideae subgenus and Rosaceae genus. Rose genus consists of many types which are scattered across temperate regions and semi-dry northern hemisphere [1]. Varak genus is a perennial shrub type it has quite a lot of ramifications which propagate by seed. it has wooden shrubs with 30-75 cm height, thorn-like stipules and simple leaves. Yellow petals at the foot with red spots turning to brown and carpel without fluff [2]. phenolyn compositions presence in thorny stems protects this plant against the attacks by the herbivorous insects and micro-organisms and sun ray. Plants belonging to rose genus include many different types of secondary metabolites such as flavonids and tannins [3]. The pharmaceutical significance of antioxidants in preventing cancers and heart blockage diseases and achieving this goal by the consumption of foodstuff containing such compositions for instance acetone extracted from Rosa persica from Iran. teryterpens and cyanic acids have been reported from theses plant [4]

So far, except for a few researches in terms of the constituent components of essence from different species of Rosa in Iran and other countries have not been carried out. Jassbi et al. [6], analyzed the poly phenol antioxidant compositions of Rosa persica in which 5 phenol antioxidants were reported including storing and analytical flavnoids and tannins. Nowak [8] studied fatty acid in different fruits of wild rose species. His findings showed that rose fruits are rich in non-saturated fatty acids especially in species such as *R. rubiginosa, R. rugosa, R. dumalis.* Elisabetsky et al. [5] studied the chemical compositions and antioxidant activities of essence and essential oil of Rosa damascene from the population of Guilan, Iran and concluded that the planted rose flower petals do not taste bitter and thanks to the potential antioxidant activity and appealing flavor can be used as the food flavor flagrant and be used as a preventive factor angst many diseases.

Jassbi et al. [6] carried out a study about the photochemical and horticultural properties of *Rosa canina* which revealed that there is a significant relation between natural habitat and the time of harvesting and the amount of antioxidants, vitamin C and flavonoids.

In this study the constituent compositions of the essence of the *Rosa persica* plant were separated and identified by the use of gas chromatograph (GC) devices and gas chromatograph connected to mass spectrometry (GC/MS). This study was carried out for the first time and in order to detect the constituent compositions of the essence of the plant in natural habitat of Ashtiyan region.

MATERIAL AND METHODOLOGY

Plant collection and essence extraction

Iranian rose flower plant was carried out from the North and East heights of the Ashtiyan town and the Kahrizak valley in June of 2014-2015. In

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order to dry the plants the plant was placed in an air-conditioned room far from sun light and was kept away from any type of light until extracting essence. The drying method is very influential on the active ingredients and if drying is done by the direct sun light the plants would lose their active ingredients [7]. About 100 g of the dried plant was extracted by the use of Clevenger device and the essence was extracted by implementing Hydro distillation method for 4 hours. Essence oils were kept in dark glasses at fridge temperature until device analysis.

Detecting constituent compositions of the essence oils-GC device properties

Gas chromatograph Shimadzu 15A equipped with DB-5 column with 50 m length, internal diameter of 0/25 mm, stationary phase layer thickness of 0/25 micro m and the injection room temperature of 250 c. In heat plan the primary temperature of the column for 3 minutes was kept at 60 c and was increased up to 220 c with the speed of 5 c per minute and was stopped at 220 c for a period of 5 minutes. The detector was FID (Flame Ionization Detector) at 270 c and the carrier gas by the speed of 1ml per minute.

The features of GC/MS device

Agilent 6890 type of gas chromatograph with a column with 30 m length, internal diameter of 25% mm, layer thickness of ./25 micro m of HP-5MS type. The heat plan of the column was arranges as follows: the primary temperature of the oven was 50 c and the interval at this temperature was for a period of 5 m thermal gradient of 3 c at every minute and the rise of temperature up to 240 c by the speed of 15 degrees per minute and rise of the temperature up to 300 c and 3 minutes interval at this temperature. The injection room temperature was 290 c and helium gas was implemented as the carrier gas with the flow speed at. /8 mm per minute. The implemented Mass spectrometry was model Agilent 5973 with ionization voltage of 70 EV and the EI Ionization and the Ionization source temperature 220 c was implemented. The spectrum detection was done by the use of their retention indices and comparing with present indices in reference books and essays and by the use of mass spectrum of standard compositions and utilizing the available data at computer library [8].

RESULTS

The numbers recorded in vertical column of the chromatogram show the rate of frequency of constituent compositions of the essence and the horizontal column display the time of separation and identifying each of the essence constituent

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compositions in the chromatography column (Fig.1).

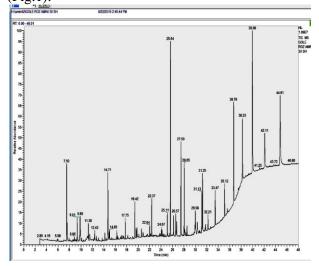


Fig1. Chromatogram of the essence of the Iranian rose flower (Rosa persica)

By considering the output pattern of normal alkanes and the comparison of the obtained mass spectrums from the GC-MS device with standard mass spectrums present in references it became precisely clear that each of the mass spectrums belong to what composition. In order to confirm the identification made by the mass spectrums the Kvats retention indices were implemented whose results are presented at Table 1. As it is evident from among the identified compositions the active ingredient of heptacosane with (11/6) has the highest percentage and after that stands isobutyl phthalate (11/48), nonacosane (8/88), dibutyl phthalate (6/26), pentacosane (5/96), hexadecanoic acid (3/95), linalool (3/8), ethyl linoleolate (3/73), hexyl hexoate (3/67), octacosane (3/43) are the main constituent compositions of this plant.

DISCUSSION

The study and analysis of the chromatogram and the obtained spectrums show the presence of 56 compositions. It was observed that the main part of the essence of the Iranian rose flower (Rosa persica) is composed of hydrocarbon compositions (alkanes). Alkanes are a group of aliphatic hydrocarbons which are totally saturated with The total formula for alkanes is hydrogen. $(C_n H_{2n+2}).$ Among the alkanes the highest percentage belongs to heptacosane. Heptacosane is a hydrocarbon composition as crystals with the formula C₂₇H₅₆ and is indivisible in water. This composition has the melting point of 60 degrees centigrade and the boiling point of 270 centigrade (at a pressure of 15 mm Hg). This composition is divisible in alcohol and it can be found in beeswax. Nonacosane is also a hydrocarbon colorless composition with the formula $C_{29}H_{60}$ with melting point of 63 centigrade. This composition can be found in beeswax and the oil of cabbage leaves. [9] reported the chemical compositions of Rosa damascene essence. Among the detected compositions linalool *seraniol voctadecane v* nonadecane *seranyl* acetone *heptadecane* tricosane *pentacosane heptacosane* are similar to reported chemical compositions by the present study and at the same time the rate of linalool (%3/8)geranyl acetone (%0/24) pentacosane (%5/11) confirms the obtained percentage by the present study. Constituent components of different essences of rose (e.g. *R. persica, R. damascene, R. chinesis, R. rugosa*) are very close to each other and their antioxidant features and properties have been well proved [10]. Reports show that Linanool exists as the main ingredient of several species of aromatic plants that some of these plant species have disease treatment uses in traditional medicine [11] our research also clearly shows the presence of this chemical in chemical composition of the essence of *Rosa persica*.

Table-1 the identified constituents of the essence of the Iranian rose flower (Rosa persica)

| No | Composition | Percentage | RI | No | Composition | Percentage | RI |
|----|------------------------------------|------------|--------|----|---------------------------------|------------|--------|
| 1 | Linalool | 3.8 | 1098.7 | 29 | Tetradecanal | 1.87 | 1709.4 |
| 2 | Nonanal | 1.27 | 1102.7 | 30 | Octyloctanoate | 0.16 | 1776.7 |
| 3 | Menthone | 0.17 | 1155 | 31 | Tetradecanoic acid, ethyl ester | 0.42 | 1793.6 |
| 4 | Menthol | 1.51 | 1175.2 | 32 | Octadecane | 0.3 | 1798 |
| 5 | Butyl caproate | 0.19 | 1190.9 | 33 | Hexahydrofarnesyl acetone | 1.16 | 1844.8 |
| 6 | Terpineol <alpha-></alpha-> | 1.2 | 1194.2 | 34 | Isobutyl phthalate | 11.48 | 1870.9 |
| 7 | Ethyl octanoate | 1.28 | 1197.5 | 35 | Nonadecane | 1.03 | 1898 |
| 8 | d-Carvone | 0.61 | 1243.1 | 36 | Butyl cyclohexyl phthalate | 1.29 | 1917.6 |
| 9 | Hexanoic acid, 3-methylbutyl ester | 0.21 | 1247.9 | 37 | Hexadecanoic acid, methyl ester | 0.71 | 1925.9 |
| 10 | Hexanoic acid, 2-methylbutyl ester | 0.74 | 1250.6 | 38 | Dibutyl phthalate | 6.26 | 1965.8 |
| 11 | Geraniol | 0.81 | 1258.1 | 39 | Hexadecanoic acid, ethyl ester | 3.95 | 1994.3 |
| 12 | Prenylhexanoate | 0.43 | 1292.9 | 40 | Hexadecyl acetate | 0.14 | 2009.2 |
| 13 | Undecanal | 0.19 | 1303.9 | 41 | Octadecanal | 0.48 | 2020.7 |
| 14 | 2,4-Decadienal, (E,E)- | 0.2 | 1316.1 | 42 | Heneicosane | 1.14 | 2098.9 |
| 15 | Undecenal<2E-> | 0.39 | 1361 | 43 | Methyl linolenate | 0.47 | 2102.2 |
| 16 | Hexyl hexoate | 3.67 | 1382.3 | 44 | Phytol | 0.88 | 2118.2 |
| 17 | Ethyl decanoate | 0.47 | 1391.7 | 45 | Ethyl linoleate | 2.12 | 2162.4 |
| 18 | Tetradecane | 0.37 | 1394.9 | 46 | Ethyl linoleolate | 3.73 | 2169.1 |
| 19 | Octanoic acid, isopentyl ester | 0.4 | 1445.3 | 47 | Ethyl octadecanoate | 0.16 | 2193.4 |
| 20 | Geranyl acetone | 0.16 | 1450.2 | 48 | Docosane | 0.32 | 2197.8 |
| 21 | Heptylhexanoate | 0.16 | 1479.6 | 49 | Eicosanal | 0.73 | 2223.4 |
| 22 | Tridecanal | 1.04 | 1506 | 50 | Tricosane | 1.93 | 2297.1 |
| 23 | Hexyl octanoate | 1.87 | 1577.7 | 51 | Tetracosane | 1.87 | 2397.6 |
| 24 | Lauric acid, ethyl ester | 0.4 | 1590.1 | 52 | n alkane | 5.96 | |
| 25 | Hexadecane | 0.44 | 1594.4 | 53 | n alkane | 4.32 | |
| 26 | Tridecanal | 0.12 | 1607.6 | 54 | n alkane | 11.6 | |
| 27 | Benzophenone | 0.53 | 1629.5 | 55 | n alkane | 3.43 | |
| 28 | Heptadecane | 0.55 | 1693.8 | 56 | n alkane | 8.88 | |

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