

# Composition of the Essential Oil of *Rosa Damascena* Mill. Cultivated in Romania

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*In the present study we have investigated the chemical composition of the essential oil extracted through hydrodistillation, from fresh petals of Rosa damascena Mill. reared in Romania. The results were compared with those obtained in other specialty studies in order to validate the quality of the essential oil extracted from roses reared in Romania. This volatile oil was analyzed using Gas Chromatography coupled with Mass Spectrometer (GC-MS) and Fourier Transform Infrared Spectroscopy (FTIR). Only a small number of monoterpenes and sesquiterpenes were identified and a large number of aliphatic components. In the examined essential oil, from a total of 85.76% aliphatic components, the aliphatic hydrocarbons represents 76.59% while the oxygenated aliphatic represents only 9.17%. The representative aliphatic hydrocarbons were: heneicosane, nonadecane, tricosane, eicosane and octacosane. The representation of monoterpenes in the obtained essential oil was only of 6.54%. From this total, hydrocarbon monoterpenes accounted 4.43% while oxygenated monoterpenes accounted about 2.11%. The representative hydrocarbon monoterpenes found in the obtained essential oil were (-)- $\beta$ -pinene (1.665%), cis-ocimene (1.024%), sylvestrene (0.549%) and trans-ocimene (0.423%) and the representative oxygenated monoterpenes were nerol (1.039%) and  $\beta$ -Citronellol (0.729%).*

**Keywords:** *Rosa damascena* Mill., essential oil, chemical composition, GC-MS, FTIR

Essential oils are a mixture of numerous compounds characterized by an essence of aromatic plants. Currently, approximately 3000 essential oils are known, 300 of which are commercially important, in particular for the pharmaceutical, food, household and cosmetic industries [1]. Out of these, rose oil is one of the most known and appreciated. *Rosa* genus, belonging to the *Rosaceae* family, includes 200 species and more than 18,000 cultivars [2]. One of the most important *Rosa* species is *Rosa damascena* Mill., which is known as "Gol-e-Mohammadi" in Persian. This plant is called Damascus rose because it was originally brought to Europe from Damascus [2, 3]. Out of about 120 species of roses, mainly four species of rose are used for products based on rose oil: *Rosa damascena* Mill., *Rosa moschata*, *Rosa centifolia* and *Rosa gallica*. But *Rosa damascena* Mill. is traditionally preferred because it has a delicate fragrance and produces a considerable percentage of oil (especially in the industry of perfume and cosmetics) [4].

In traditional systems of medicine, various rose products are used as an astringent, tonic, mild laxative and in treatment of sore throat, enlarged tonsils, heart conditions, eye disease, gall stones, for their cooling effect and as a vehicle for other medicines [4-7]. Essential oil from the rose is reported to have analgesic and antispasmodic

effects [3, 4, 8, 9]. In addition, anti-HIV, anti bacterial and hypnotic activities of rose extract/isolates have been reported [4, 8, 10, 11]. In the recent years, antioxidant, antibacterial and antimicrobial activities of *Rosa damascena* Mill. essential oil have been demonstrated by researchers [2, 3, 8, 12-15].

Rose oil is a volatile oil obtained by hydrodistillation from the fresh flowers of *Rosa damascena* Mill. The main components of rose oil are: (a) oxygenated monoterpenes: citronellol (16–50%), geraniol (15–30%), nerol, linalool (0.7–1.9%), citronellyl acetate, geranyl and neril; (b) sesquiterpenes: farnesol,  $\alpha$ -copaen, cariofilen and cariofilen oxide; (c) non-terpenes:  $\beta$ -phenyl ethyl alcohol (in small amounts because of their high water solubility), phenylethyl acetate, benzyl acetate, myristyl acetate, eugenol (0.3–2.2%), metal ether eugenol, nonyl aldehyde, traces of other aldehydes (propionic, valeric, phenylacetic, salicylic acid, cinnamic etc.) and stearoptene. Under this last denomination are included paraffins with 14-23 carbon atoms in the molecule and which represent 15 to 23% from volatile components. Stearoptenes do not have their own smell but they have fixing properties of other volatile components [16, 17].

*Rosa damascena* Mill. needs moderate temperatures and humid air during flowering to achieve a rich oil content.

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This type of rose is mainly grown in temperate climates, usually at an altitude between 300 and 1800 m [2, 18]. Flowering begins in late May and lasts until the end of June, but in warmer autumns may still have a second flowering wave, but weaker than the first. The fresh damascus rose petals possess a very small quantity of essential oil. One kg of rose oil can be obtained from about 3,000 kg of rose petals [3, 19]. Because of the low oil content and the lack of natural and synthetic substitutes, rose oil is one of the most expensive essential oil in the world markets [4].

The total production of rose oil is approximately 5 metric tons, with Bulgaria and Turkey being the major producers followed by Morocco, Egypt, China, Russia, Iran and India [4]. In Romania the species *Rosa damascena* Mill. is cultivated both as ornamental and therapeutic plant. Also, the Romanian cuisine includes many traditional recipes for sweets and syrups made from rose petals and/or roses extracts. It is well known the fact that 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 [20].

The objectives of this study are the following: (1) the evaluation of chemical composition of essential oil obtained by hydrodistillation from rose petals from the flowers of the species *Rosa damascena* Mill. collected from shrubs reared in Romania (2) comparing of the obtained results with those obtained in other specialty studies [2-4, 18, 21] in order to validate the quality of the essential oil extracted from roses reared in Romania. The obtained volatile oil was analyzed using Gas Chromatography coupled with Mass Spectrometer (GC-MS) and Fourier Transform Infrared Spectroscopy (FTIR).

## Experimental part

### Materials and methods

The rose petals, from the flowers of the species *Rosa damascena* Mill., were harvested manually, from a specially made rose garden located in Bucharest (Romania), on May 2013, at the early hours of the day and delivered to the laboratory within 20 min after the harvest [22]. All other used reagents were of analytical grade and were purchased from Sigma-Aldrich, Bucharest.

### The essential oil extraction

250 g of fresh petals from flowers of the species *Rosa damascena* Mill. were crushed, transferred in a 2 L round bottom flask and 1.5 L of water were added. The flask was connected to the Clevenger-type apparatus for distillation. The obtained mixture was hydrodistilled for 5 h. The distillate obtained was dried over anhydrous sodium sulphate and stored in air tight amber-colored bottle at 4° C until it was analyzed.

### The analysis of the essential oil

The analysis of the volatile components from the obtained essential oil was carried out on a gas chromatograph coupled with a mass spectrometer Agilent 5975C type. The column used for the separation of the sample components was a DB5-MS capillary column (30 m length × 0.32 mm internal diameter, film thickness 0.25 μm). Hydrogen (99.999% high purity) was used as the carrier gas (inlet pressure 82 737 Pa at a flow rate of 1.6667 × 10<sup>-8</sup> m<sup>3</sup> s<sup>-1</sup> (1 mL min<sup>-1</sup>) (splitting ratio 40:1). Oven temperature was initially 40° C and then was raised progressively to 80° C with a rate of 3° C/min, to 180° C at a rate of 5° C/min and finally was raised to 280° C at a rate of 8° C/min and maintained there for 20 min. For GS-MS analysis, 30 μL of essential oil were introduced in 1 mL of

hexane and then homogenized. The injector temperature was 280° C. The mass spectrometry conditions were as follows: ionization voltage of 70 eV, emission current of 35 mA, scan rate of 2.8 scan/s, mass range of 10–350 amu and ion source temperature of 200° C.

The percentage composition (area percent) of the oils was computed by the normalization method from the GC peak areas, by means of three injections from each sample, without using correction factors. The constituents of the volatile oils were identified by two methods: by comparing their calculated GC retention indices with literature data and by library searching. A mixture of aliphatic hydrocarbons (C8–C24) in hexane was injected as under the above-mentioned temperature programme in order to calculate the retention indices. The generalized equation of Van den Dool and Kratz (1963) was used.

*Kovats retention indices* are calculated using the formula:

$$K = 100 \times \left[ n + \frac{\log t_{Rx} - \log t_{Rn}}{\log t_{Rn+1} - \log t_{Rn}} \right]$$

where:

*x* is the test compound;

*n* is the alkane with *n* carbon atoms into the molecule, whose peak is placed on the left side of the analyzed peak from the chromatogram;

*n+1* is the alkane with *n* carbon atoms into the molecule, whose peak is placed on the right side of the analyzed peak from the chromatogram.

### Fourier Transform Infrared Spectroscopy (FTIR)

The IR fingerprint of the rose essential oils was highlighted using a FTIR spectrophotometer – Thermo SCIENTIFIC Nicolet 6700 Model 912A063, by ATR measurement method. The spectra of the samples are the averages of 32 scans, in the range of 4000 – 800 cm<sup>-1</sup>, with a resolution of 4 cm<sup>-1</sup>.

### Statistical analysis

Analyzing the composition of essential oils from different geographical regions (as a result of the literature studied) and of the one obtained in Romania, it has been observed that the variation of the chemical characteristics analyzed could lead to the identification of types of essential oils. For this we made a classification based on cluster analysis. The IBM SPSS Statistics 20 software was used for the analyses.

## Results and discussions

By the hydrodistillation technique of the rose petals from the flowers of the species *Rosa damascena* Mill., an amount of 0.08% (v/w) essential oil was obtained which was analyzed using Gas Chromatography coupled with Mass Spectrometer (GC-MS). The results are summarized in table 1. A total of forty-two components were identified. As can be seen from figure 1 the volatile oil of *Rosa damascena* Mill. was characterized by a small number of monoterpenes and sesquiterpenes but a large numbers of aliphatic components. In the obtained essential oil, from the total of 85.76% aliphatic components, the aliphatic hydrocarbons dominate and represent 76.59% while the oxygenated aliphatic represents only 9.17%. As shown in figure 2, the representative aliphatic hydrocarbons found in the examined volatile, have been heneicosane, nonadecane, tricosane, eicosane and octosane.

Monoterpenes were only in amount of 6.54% in the essential oil. From this total, hydrocarbon monoterpenes accounted 4.43% while oxygenated monoterpenes accounted about 2.11%. As shown in figure 3, the

Retention time (min.)	Name	Formula	Relative concentration (percentage of area, %)	Kovats retention indices, K ( $\times 10^2$ )
3.391	Octane	C <sub>8</sub> H <sub>18</sub>	0.303	0.341
4.784	3-Hexen-1-ol	C <sub>6</sub> H <sub>12</sub> O	0.286	0.398
5.229	1-Hexene	C <sub>6</sub> H <sub>12</sub>	0.438	0.413
9.927	$\beta$ -Pinene	C <sub>10</sub> H <sub>16</sub>	1.665	0.719
10.334	$\alpha$ -Fellandrene	C <sub>10</sub> H <sub>16</sub>	0.109	0.727
10.456	Octanal	C <sub>8</sub> H <sub>16</sub> O	0.106	1.037
10.728	3-Hexen-1-ol, acetate	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	0.097	1.044
10.883	Terpinolen	C <sub>10</sub> H <sub>16</sub>	0.098	1.048
11.414	Sylvestrene	C <sub>10</sub> H <sub>16</sub>	0.549	1.061
12.073	trans-Ocimene	C <sub>10</sub> H <sub>16</sub>	0.423	1.076
12.525	cis-Ocimene	C <sub>10</sub> H <sub>16</sub>	1.024	1.086
14.220	Terpinolen	C <sub>10</sub> H <sub>16</sub>	0.144	1.120
14.946	Linalyl anthranilate	C <sub>17</sub> H <sub>23</sub> NO <sub>2</sub>	1.266	1.134
15.189	Nonanal	C <sub>9</sub> H <sub>18</sub> O	2.485	1.505
15.387	Benzyl Carbinol	C <sub>8</sub> H <sub>10</sub> O	0.127	1.510
16.298	Cyclopropane, trimethyl(2-methyl-1-propenylidene)-	C <sub>10</sub> H <sub>16</sub>	0.245	1.533
16.825	Cyclopropane, trimethyl(2-methyl-1-propenylidene)-	C <sub>10</sub> H <sub>16</sub>	0.122	1.545
18.277	1-Nonene	C <sub>9</sub> H <sub>18</sub>	0.070	1.577
18.796	$\alpha$ -Terpineol	C <sub>10</sub> H <sub>18</sub> O	0.099	1.588
20.335	3-Carene	C <sub>10</sub> H <sub>16</sub>	0.057	1.967
20.430	$\beta$ -Citronellol	C <sub>10</sub> H <sub>20</sub> O	0.729	1.970
20.769	cis-Verbenol	C <sub>10</sub> H <sub>16</sub> O	0.094	1.980
21.325	Nerol	C <sub>10</sub> H <sub>18</sub> O	1.039	1.996
21.813	Neral	C <sub>10</sub> H <sub>16</sub> O	0.146	2.010
25.950	Benzene, 1,3,5-trimethoxy	C <sub>9</sub> H <sub>12</sub> O <sub>3</sub>	0.149	2.584
26.132	Caryophyllene	C <sub>15</sub> H <sub>24</sub>	0.135	2.592
26.937	4-(2,6,6-Trimethyl-cyclohex-1-enyl)-butan-2-ol	C <sub>13</sub> H <sub>24</sub> O	0.080	2.622
27.822	$\alpha$ -Muurolene	C <sub>15</sub> H <sub>24</sub>	0.055	2.655
28.364	$\alpha$ -Muurolene	C <sub>15</sub> H <sub>24</sub>	0.308	2.675
28.696	$\gamma$ -Cadinene	C <sub>15</sub> H <sub>24</sub>	0.094	2.855
28.966	$\delta$ -Cadinene	C <sub>15</sub> H <sub>24</sub>	0.539	2.866
29.292	$\alpha$ -Muurolene	C <sub>15</sub> H <sub>24</sub>	0.111	2.880
29.416	$\alpha$ -Calacorene	C <sub>15</sub> H <sub>20</sub>	0.164	2.885
31.792	$\beta$ -Guaiene	C <sub>15</sub> H <sub>24</sub>	0.162	3.130
32.102	$\beta$ -Guaiene	C <sub>15</sub> H <sub>24</sub>	0.049	3.143
33.209	Nonadecane	C <sub>19</sub> H <sub>40</sub>	0.722	3.190
35.378	Nonadecane	C <sub>19</sub> H <sub>40</sub>	0.109	3.421
36.944	9-Nonadecene	C <sub>19</sub> H <sub>38</sub>	8.470	3.617
36.969	1,2,4-Oxadiazole-3-carboximidamide, N <sup>-</sup> -(1-propionyloxy)-	C <sub>6</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>	4.094	3.618
37.054	9-Nonadecene	C <sub>19</sub> H <sub>38</sub>	0.096	3.622
37.441	Nonadecane	C <sub>19</sub> H <sub>40</sub>	7.033	3.743
37.483	Nonadecane	C <sub>19</sub> H <sub>40</sub>	7.150	3.745
38.654	2-Methyl-7-nonadecene	C <sub>20</sub> H <sub>40</sub>	0.107	3.815
39.107	Eicosane	C <sub>20</sub> H <sub>42</sub>	3.624	-
39.401	Stearaldehyde	C <sub>18</sub> H <sub>36</sub> O	0.165	-
40.165	10-Heneicosene	C <sub>21</sub> H <sub>42</sub>	0.123	-
40.402	10-Heneicosene	C <sub>21</sub> H <sub>42</sub>	0.153	-
40.472	10-Heneicosene	C <sub>21</sub> H <sub>42</sub>	0.077	-
40.578	Heneicosane	C <sub>21</sub> H <sub>44</sub>	6.107	-
40.656	Heneicosane	C <sub>21</sub> H <sub>44</sub>	21.140	-
41.869	Nonadecane	C <sub>19</sub> H <sub>40</sub>	0.527	-
42.173	Stearaldehyde	C <sub>18</sub> H <sub>36</sub> O	0.165	-
42.970	10-Heneicosene	C <sub>21</sub> H <sub>42</sub>	0.433	-
43.098	1-Nitropan	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	6.086	-
43.132	Tricosane	C <sub>23</sub> H <sub>48</sub>	7.977	-
43.386	Oxirane, tetradecyl	C <sub>16</sub> H <sub>32</sub> O	0.031	-
44.193	Nonadecane	C <sub>19</sub> H <sub>40</sub>	0.298	-
44.511	Stearaldehyde	C <sub>18</sub> H <sub>36</sub> O	0.124	-
45.178	10-Heneicosene	C <sub>21</sub> H <sub>42</sub>	0.073	-
45.280	Heneicosane	C <sub>21</sub> H <sub>44</sub>	8.306	-
46.257	Octacosane	C <sub>28</sub> H <sub>58</sub>	0.077	-
47.244	Octacosane	C <sub>28</sub> H <sub>58</sub>	3.175	-

**Table 1**  
THE RETENTION TIME, RELATIVE CONCENTRATION (PERCENTAGE OF AREA) AND KOVATS RETENTION INDICES OF ROSE ESSENTIAL OIL

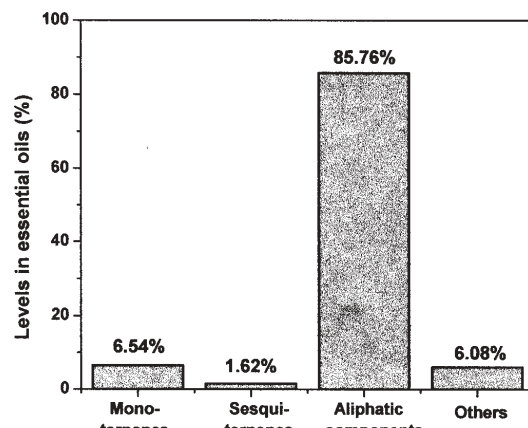


Fig. 1 The levels of monoterpenes and sesquiterpenes versus aliphatic components in the essential oil of *Rosa damascena* Mill.

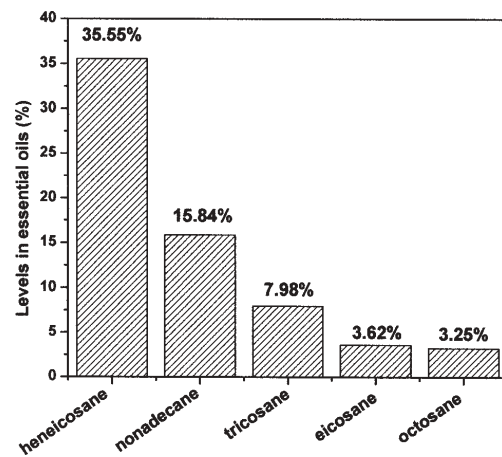


Fig. 2 The levels of representative aliphatic hydrocarbons found in the essential oil of *Rosa damascena* Mill.

representative hydrocarbon monoterpenes found in the essential oil of *Rosa damascena* Mill. are (-)- $\beta$ -pinene (1.665%), cis-ocimene (1.024%), sylvestrene (0.549%) and trans-ocimene (0.423%) and the representative oxygenated monoterpenes are nerol (1.039%) and  $\beta$ -Citronellol (0.729%).

According to some authors [23-25], the fragrance is determined by mixtures of volatiles that can be grouped into the following five major series: hydrocarbons (mostly sesquiterpenes), alcohols (mostly terpenes such as geraniol, nerol, and citronellol), esters (mostly acetates such as hexyl acetate or geranyl acetate), aromatic ethers (3,5-dimethoxytoluene, benzyl methyl ether, and methyl-eugenol), and others such as aldehydes, aliphatic chains, rose oxides, and norisoprenes such as bionone. Among the five rose volatile groups, *R. damascena* and *R. gallica* were in group 2 of alcohol types without orcinol dimethylether, which emit between 35% and 85% alcohol, such as phenylethyl alcohol, citronellol, geraniol, and nerol [26].

According to other authors [27], there are some compounds responsible with fragrance (monoterpenes especially) and fixative effects (some aliphatic hydrocarbons) and therefore responsible for a longer-lasting odour impression (usually tested by

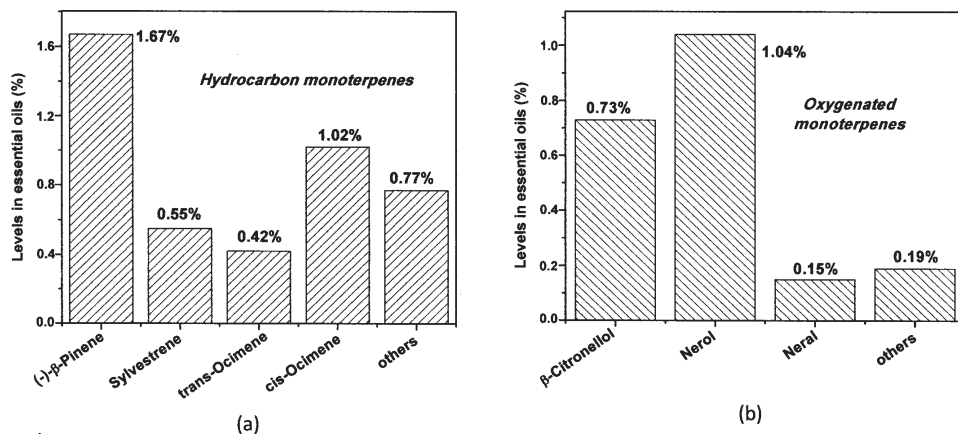


Fig. 3 The levels of representative monoterpenes (a) hydrocarbon and (b) oxygenated in the essential oil of *Rosa damascena* Mill.

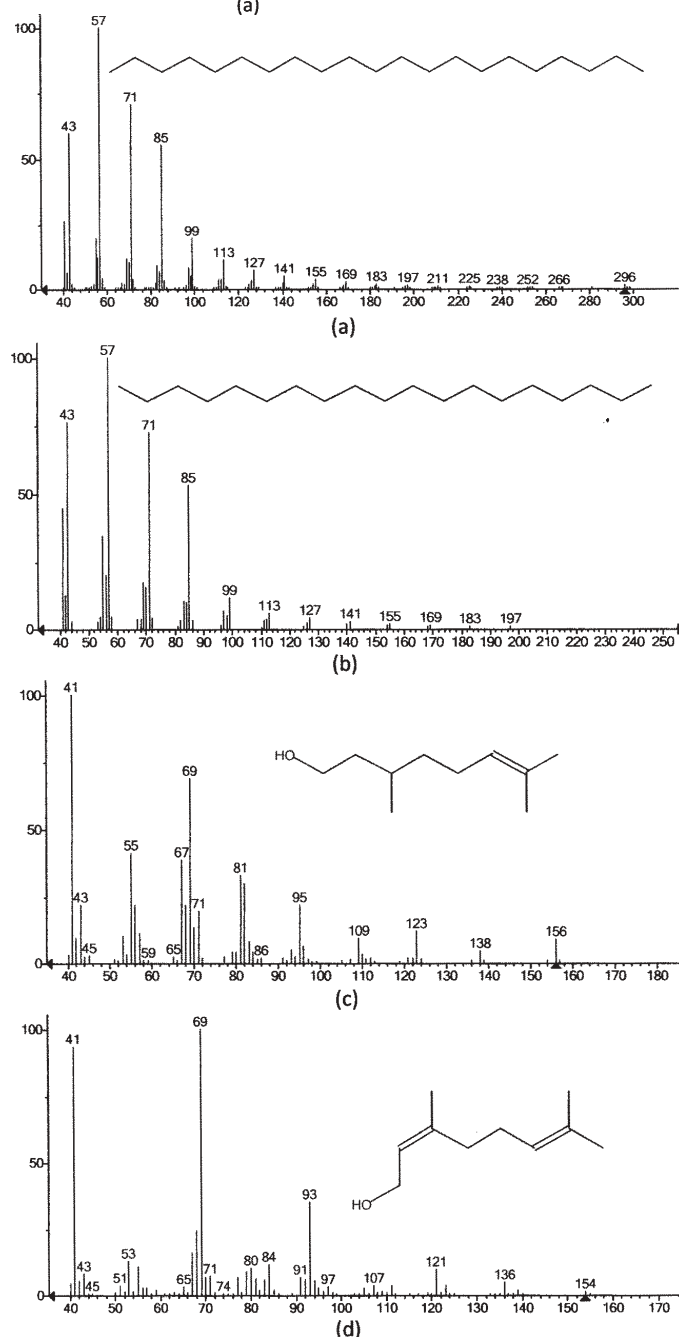


Fig. 4 Mass spectra of (a) heneicosane; (b) nonadecane; (c)  $\beta$ -citronellol; (d) nerol, found in the essential oil of *Rosa damascena* Mill.

olfactory evaluation after application to human skin). From those categories we have found in our essential oil nonadecane (14.2%) and heneicosane (35%) and in small percentages citronellol (0.729%) and nerol (1.039%).

(b)

In figure 4 (a), (b), (c) and (d) are presented the mass spectra of heneicosane, nonadecane, citronellol and nerol, obtained by the technique of Gas Chromatography coupled with Mass Spectrometer.

The above compounds were mentioned by some researchers as being determinants for the basic character of rose oil [23, 28].

In the present work, our results seem to be different from those reported by other authors. The first difference is the obtaining yield of essential oil which was of 0.08% (v/w). This amount is smaller than others reported: Moein et al. have reported 0.16% (v/w), Khouzani et al. 0.10% (v/w) and Verma et al. 0.12% (v/w), respectively [2-4, 18, 21]. The second one, very important also, is related to the composition of the extracted essential oil.

In table 2 are shown, by comparison, the results of five studies regarding the composition of five types of essential oil obtained from species of *Rosa damascena* Mill. reared in five different geographical areas. The results presented in the last column of table 2 are the results of this work.

Moein et al. [3] in his investigation regarding the composition of essential oil of *Rosa damascena* Mill. from South of Iran, from the total of 25 compounds which have been determined, nonadecane (39.73%), heneicosane (32.38%), docosane (7.34%), citronellol (6.14%) and 9-nonadecene (5.69%), were found to be major constituents. Khouzani et al. [2, 18] have found  $\beta$ -citronellol (47.43%), heneicosane (17.45%), disiloxane (17.58%), octadecane (6.13%) and 9-nonadecene (2.63%) as being the major components of essential oil obtained from *Rosa damascena* Mill. from Central Iran. Verma et al [4] have obtained and analyzed essential oil and water of *Rosa damascena* Mill. from India (Uttarakhand). Both oil and water were dominated by the aliphatic hydrocarbons (56.4 and 46.3%, respectively). The representative aliphatic hydrocarbons of the essential oil have been heneicosane (19.7%), nonadecane (13%), tricosane (9.3%), pentacosane (5.3%) and eicosane (2.4%). The Bulgarian rose oil is considered by the perfumers as being of the highest quality. In their study made also on *Rosa damascena* Mill., from Bulgaria this time, Babu et al [21] reported that citronellol (30.31%), geraniol (16.96%), phenyl ethyl alcohol (12.60%), nerol (8.46%), hexa-cosane (3.70%), nonadecane (2.7%) and linalool (2.15%) are the major constituents of essential oil.

From table 2 it can be seen that five of the seven main components of *Rosa damascena* Mill. essential oil are present in the samples obtained and analyzed in our study, as follows: monoterpene hydrocarbons (4.43%), oxygenated monoterpenes (2.11%), sesquiterpenes hydrocarbons (1.62%), aliphatic hydrocarbons (76.59%), oxygenated aliphatic (9.17%). The results of our study show that the essential oil is dominated by the aliphatic hydrocarbons as in the case of Indian study also. Thus, 9-

Composition of essential oil of <i>Rosa damascena</i> Mill.	South of Iran [23]	Central Iran [26]	India [27]	Bulgaria [28]	Romania (the results of this work)
Monoterpene hydrocarbons (%)	0	0	0.7	1.06	4.43
Oxygenated monoterpenes (%)	6.14	48.58	14.7	63.08	2.11
Sesquiterpenes hydrocarbons (%)	1.74	0	1.4	0	1.62
Oxygenated sesquiterpenes (%)	0	0	0.6	1.36	0
Aliphatic hydrocarbons (%)	92.06	28.13	56.4	8.97	76.59
Oxygenated aliphatic (%)	0	0	0.5	0	9.17
Benzenoid compounds (%)	0	0.26	1.0	12.6	0

**Table 2**  
THE COMPOSITION OF SOME  
ESSENTIAL OILS OBTAINED  
FROM SPECIES OF *ROSA*  
*DAMASCENA* MILL. REARED IN  
DIFFERENT GEOGRAPHICAL  
AREAS AND ROMANIA

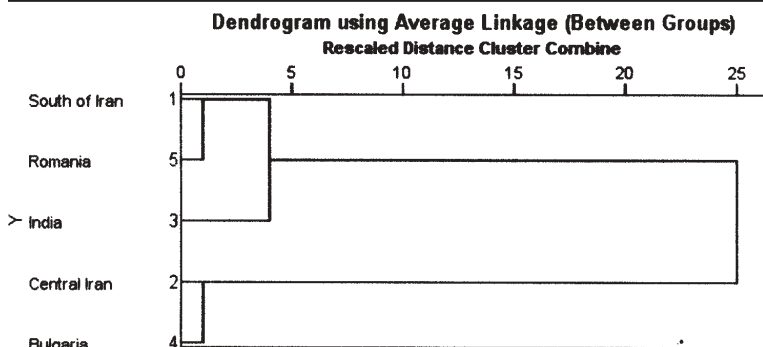


Fig. 5 Dendrogram obtained by the cluster analysis of the percentage composition of essential oils of *Rosa damascena* Mill

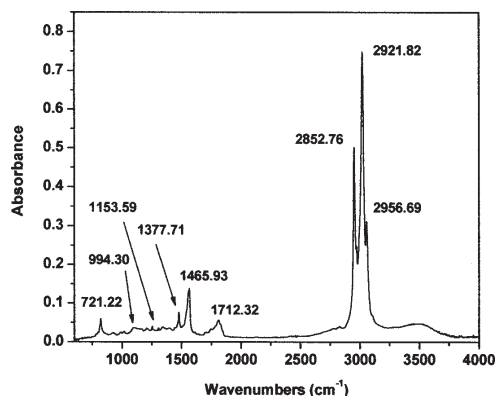


Fig. 6 FTIR spectra of *Rosa damascena* Mill. oil in the range of 4000-600  $\text{cm}^{-1}$

nonadecene (0.1%), nonadecane (15.01%), eicosane (3.62%) and heneicosane (35.55%) are the best represented. Nerol (1.04%),  $\beta$ -citronellol (0.73%) and tricosane (8%) were found in quite good amounts. From all components, only oxygenated monoterpenes are modestly represented. The differences can be attributed to the ecological factors or to some unknown genetic modifications.

Further on, using cluster analysis and based on the similarities of the chemical characteristics of the essential oils analyzed we identified, as seen in the dendrogram presented in figure 5, two types.

The first type consists of the oils from Central Iran and Bulgaria and is characterized by a medium average concentration of oxygenated monoterpenes and a low concentration of aliphatic hydrocarbons. The second type consists of the oils produced in South of Iran, Romania and India. The chemical composition is different, containing a small amount of oxygenated monoterpenes and a high or very high quantity of aliphatic hydrocarbons. Unlike the first type, these also contain a small amount of sesquiterpenes hydrocarbons (less than 2%).

The result of the study can be considered positive in the following sense: even if the extraction yield is smaller, the

**Table 3**  
THE INFRARED CHARACTERISTIC BANDS OBSERVED IN  
*ROSA DAMASCENA* MILL. OIL

Band position ( $\text{cm}^{-1}$ )	Class of Compounds
2956.69	$-\text{CH}_3$ asymmetric and symmetric stretching vibrations
2921.8 and 2852.7	$-\text{CH}_2-$ , symmetric and symmetric stretching vibrations
1712.32	C=O stretch in non-conjugated ketones, carbonyls
1465.93	C-H asymmetric and symmetric bend
1377.71	C-H asymmetric and symmetric bend;
	OH bend (phenol or tertiary alcohol)
1153.59	C-O stretch (tertiary alcohol);
	C-O-C stretch (alkyl-substituted ether),
994.30	$-\text{CH}_2-$ (methylene - cyclohexane ring vibrations),
	C-H in-plane bend (aromatic)
721.22	$(-\text{CH}_2-)_n$ rocking ( $n \geq 3$ ); skeletal C—C vibrations

quantities of major constituents are superior to those under discussion for comparison. The amount of nonadecane (15.01%) is superior to the Indian (13%) and Bulgarian (2.7%) amounts, the amount of eicosane (3.62%) is superior to the Indian (2.4%), Central Iranian (0.66%) and Bulgarian (1.65%) amounts. The amount of heneicosane (35.55%) is superior to South Iranian (32.38%), Central Iranian (17.45%) and Indian (19.7%) amounts.

Depending on the destination, the presence in a large amount or the absence of one of the components may be advantages for the quality of products which are based on essential oil (fragrance, cream, drug, oil for aromatherapy etc.).

#### Fourier Transform Infrared Spectroscopy (FTIR)

Fourier transform infrared spectroscopy is one of the most widely employed techniques for functional groups identification. Figure 6 and table 3 showed the infrared spectrum and the characteristic bands observed in *Rosa damascena* Mill. oil in the range of 4000-800  $\text{cm}^{-1}$ . The characteristic bands of the saturated aliphatic  $\text{sp}^3$  C-H bonds are observed in the range of 2956-2852  $\text{cm}^{-1}$  which are assigned to  $\nu_{\text{as}}(\text{CH}_3)$ ,  $\nu_{\text{as}}(\text{CH}_2)$ , and  $\nu_{\text{s}}(\text{CH}_2)$  respectively (the bands situated at 2921.8  $\text{cm}^{-1}$  and 2852.7  $\text{cm}^{-1}$  correspond to methylene C-H asymmetric and symmetric stretching vibrations respectively, and the band

situated at 2956.69 cm<sup>-1</sup> is due to methyl C-H asymmetric and symmetric stretching vibrations). Any band structures observed between 3150 and 3000 cm<sup>-1</sup> are almost exclusively an indication of the unsaturation (C = C - H) and/or a presence of aromatic rings but their absence in the obtained IR spectrum is indicative of the absence of aromatic compounds [29]. The absorption located at 1712 cm<sup>-1</sup> corresponds to the C=O stretch in non-conjugated ketones, carbonyls and in ester groups [30]. In addition, the band observed between 1465-1377 cm<sup>-1</sup> can be attributed to C-H groups or OH bend (phenol or tertiary alcohol). On the other hand, the strong methylene/methyl band which appeared at 1435-1436 cm<sup>-1</sup>, the weak methyl band which appeared at 1375-1376 cm<sup>-1</sup> and the CH<sub>2</sub> rocking vibration band which appeared at 758-759 cm<sup>-1</sup> are indications for a long-chain linear aliphatic structure [29, 31]. The bands located in the range of 1153-950 cm<sup>-1</sup> can be attributed to -CH<sub>2</sub>- (methylene - cyclohexane ring vibrations), C-H in-plane bend (aromatic), C-O stretch (primary or tertiary alcohol) or C-O-C stretch (alkyl-substituted ether). The band observed at and 721 cm<sup>-1</sup> can be attributed to aromatic C-H bending, methylene (CH<sub>2</sub>)<sub>n</sub> rocking (n≥3) or skeletal C-C vibrations.

### Conclusions

The composition of essential oil obtained by hydrodistillation from fresh petals of *Rosa damascena* Mill. cultivated in Romania was determined using Gas Chromatography coupled with Mass Spectrometer (GC-MS). The essential oil is characterized by a small number of monoterpenes and sesquiterpenes but a large number of aliphatic components. From the total of 85.76% aliphatic components, the aliphatic hydrocarbons represents 76.59% while the oxygenated aliphatic represents only 9.17%.

For functional groups identification the Fourier Transform Infrared Spectroscopy (FTIR) technique was used. The presence of the saturated aliphatic was outlined by the bands located at 2921.8 cm<sup>-1</sup>, 2852.7 cm<sup>-1</sup> and 2956.69 cm<sup>-1</sup> respectively. The band located at 1712 cm<sup>-1</sup> usually marks the presence of ketones, carbonyls and ester groups. The phenols or tertiary alcohols have been found between 1465-1377 cm<sup>-1</sup> while the primary alcohols and the alkyl-substituted ether were found between 1153-950 cm<sup>-1</sup>. The band located at 721 cm<sup>-1</sup> reveals the presence of aromatic compounds.

The obtained results were compared with those published by authors from South and Central Iran, India and Bulgaria, countries very well known for *Rosa damascena* Mill. cultivation. We can say that the Romanian essential oil is dominated by the aliphatic hydrocarbons as in the case of the Indian essential oil. 9-nonadecene (8.56%), nonadecane (15.01%), eicosane (3.62%) and heneicosane (35.55%) are the best represented. Nerol (1.04%), β-citronellol (0.73%) and tricosane (8%) were found in quite good amounts. From all components, only oxygenated monoterpenes are modestly represented.

These results can be considered positive for the following reason: even if the extraction yield is smaller, the quantities of major constituents are superior to those under discussion for comparison. The amount of nonadecane (15.01%) is superior to the Indian (13%) and Bulgarian (2.7%) amounts, the amount of eicosane (3.62%) is superior to the Indian (2.4%), Central Iranian (0.66%) and Bulgarian (1.65%) amounts. The amount of heneicosane (35.55%) is superior to South Iranian (32.38%), Central Iranian (17.45%) and Indian (19.7%) amounts. Depending on the destination, the presence in a large amount or the absence of one of the components may be advantages for the quality of

products which are based on essential oil (fragrance, cream, drug, oil for aromatherapy etc.). The differences between the fifth kinds of essential oils under discussion can be attributed to the ecological factors or to some unknown genetic modifications.

In a previous paper was studied the chemical composition of the essential oil *Artemisia absinthium* [32].

### References

1. SHAABAN H.A.E., EL-GHORAB A.H., SHIBAMOTO T, J Essent. Oil Res., **24**, No. 2, 2012, p. 203.
2. PERUMAL K., MOORTHY T. A. S., SAVITHA J. S., Asian J. Biol. Sci., **3**, No. 2, 2012, p. 330.
3. MOEIN M, KARAMI F, TAVALLALI H., GHASEMI Y, IJPS Winter, **6**, No.1, 2010, p. 59.
4. VERMA R.S., PADALIA R.C., CHAUHAN A., Arch. Biol. Sci., **63**, No. 4, 2011, p. 1111.
5. HUNT S. R, Pharm. J. **189**, 1962, p.589.
6. KAUL V. K., Damask rose-cultivation and processing in supplement to cultivation and utilization of aromatic plants, Edits, S.S. Handa and M. K. Kaul, Regional Research Laboratory, Jammu, 1998.
7. SCHWEISHEIMER W, Perfums Cosmet. Savons, **4**, 1961, p. 62.
8. BASIM E., BASIM H., Fitoterapia, **74**, No.4, 2003, p. 394.
9. LIBSTER M., Delmar's Integrative Herb Guide for Nurses, Cengage Learning, Albany, 2002.
10. MAHMOOD, N., PIACENT, S.K., PIZZA, C., BRUKE, A., KHAN, A., A. HAY, Biochem. Biophysic. Res. Communic. **229**, 1996, p. 73.
11. RAKHSHANDEH, H., SHAKERI, M.T., GHASEMZADEH M.R., Iranian J. Pharm. Res. **6**, No. 3 2007, p. 193.
12. ACHUTHAN CR, BABU BH, PADIKKALA J., Pharm Biol., **41**, No. 5, 2003, p. 357.
13. OZKAN G, SAGDIC O, BAYDAR NG, BAYDAR H., Food Sc Technol Int, **10**, no. 4, 2004, p. 277.
14. BUCKLE, J., Clinical Aromatherapy. Essential Oils in Practice, Second Edition Paperback, New York, Churchill Livingstone, 2003.
15. MIRALI N., AZIZ R., NABULSIL, Int. J. Med. Arom. Plants, **2**, No. 1, 2012, p. 41.
16. ELIU-CEAU<sup>a</sup>ESCU V, RADOIA<sup>a</sup> G., CADARIU T., Odorante si aromatizante: chimie, tehnologie, aplicatii, Editura Tehnică, București, 1988.
17. KUMAR R., SHARMA S., SOOD S., AGNIHOTRI V.K., SINGH V., SINGH B., J. Essent Oil Res., **26**, No. 3, 2014, p. 147.
18. LOGHMANI-KHOZANI H., SABZI FINI O., SAFARI J., Scientica Iranica, **14**, No. 4, 2007, p. 316.
19. BASER K.H.C., Perf. Flav. **17**, No. 3, 1992, p. 45.
20. NAQUVI K.J., ANSARI S. H., ALI M., NAJMI A. K., Journal of Pharmacognosy and Phytochemistry, **2**, No. 5, 2014, p.177.
21. BABU K.G.D., KAUL K.V., Flavour Fragr. J., **20**, No. 2, 2005, p. 222.
22. British Pharmacopoeia 1993, British Pharmacopoeia Commission, Publisher Stationery Office Books, 1994, 2 editions.
23. CHINOUL, Assessment report on Rosa gallica L., Rosa centifolia L., Rosa damascena Mill., flos, European Medicines Agency, Committee on Herbal Medicinal Products (HMPC), 2013.
24. ANTONELLI A.; FABBRI, C; GIORGIONI, ME; BAZZOCCHI, R. J. Agric. Food Chem., **45**, No. 11, 1997, p. 4435
25. DEBENER, TH.; LINDE, M., Critical Reviews In Plant Sciences, **28**, No.4, 2009, p. 267
26. FLAMENT I.; DEBONNEVILLE, C; FURRER A., ACS SYMPOSIUM SERIES, **525**, 1993, p. 269
27. L. JIROVETZ, G. BUCHBAUER, A. STOYANOVA, A. BALINOVA, Z. GUANGJIUN, M. XIHAN, Flavour Frag. J., **20**, No.1, 2005, p. 7.
28. C. MESAROS, M. CULEA, A. IORDACHE, O. COZAR, Bulletin UASVM Agriculture, **66**, No.1, 2009, p.111
29. MADIVOLI E.S., GITU L., GUMBA E., Chemistry and Materials Research, **2**, No. 4, 2012, p.13.
30. IKBAL S., AL-SHEIBANY, National Journal of Chemistry, **19**, 2005, p. 366.
31. VANKAR P.S., SHUKLA D., Appl. Nanosci., **2**, No. 2, 2012, p.163.
32. BERECHET, M.D., STELESCU, M.D., MANAILA, E., CRACIUN, D., Rev. Chim. (Bucharest), **66**, no. 11, 2015, p. 1814

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