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SHORT COMMUNICATION

Chemical composition analysis of rose water samples from Iran

Mahmoodreza Moein[1,2], Mohammad M. Zarshenas[3,4], and Shiva Delnavaz[5]

[1]*Medicinal Plants Processing Research Center, Shiraz University of Medical Sciences, Shiraz, Iran,* [2]*Department of Pharmacognosy and* [3]*Department of Traditional Pharmacy, School of Pharmacy, Shiraz University of Medical Sciences, Shiraz, Iran,* [4]*Essence of Parsiyan Wisdom Institute, Traditional Medicine and Medicinal Plant Incubator, Shiraz University of Medical Sciences, Shiraz, Iran, and* [5]*School of Pharmacy, International Branch of Shiraz University of Medical Sciences, Shiraz, Iran*

Abstract

Content: *Rosa damascena* Mill. (Rosaceae) is an important ornamental and medicinal plant and a source of fragrance. Its hydrosol is known in Iran as *golab* (rose water) and has applications in religious ceremonies, food, and pharmaceuticals. Hydrosol is traditionally and industrially produced by distillation. The increase in market demand has led to production of inferior products for hydrosol that contain synthetic essences or essential oils of other plants, or that have been diluted with water. Inferior product often may be distinguished via its color changes and weak odor. However, details need to be determined by chemical analysis.
Objective: The current study evaluated the composition and quality of 10 rose water samples purchased from local markets in Shiraz, capital of Fars province in Iran.
Materials and methods: The essential oils of the samples were extracted and analyzed using gas chromatography-mass spectrometry.
Results: Results revealed that phenethyl alcohol, geraniol, and β-citronellol were the main constituents of most samples. In total, 22 constituents were detected and identified in the samples. Identification was determined for 60.97–96.07% of the essential oil components.
Discussion and conclusion: It was concluded that *Pelargonium* and *Dianthus* essential oils and synthetic essences had been added to some samples. Dibutyl phthalate was also detected in most samples. This substance, which commonly exists as polyethylene terephthalate, may have been released into the samples from their containers.

Keywords

Essential oil, gas chromatography-mass spectrometry, hydrosol, *Rosa damascena*

History

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Introduction

Rosaceae is a family of flowering plants known commonly as roses that encompasses about 3000 species of more than 90 genera (Potter et al., 2007). Among them, the genus *Rosa* includes about 200 species and more than 18 000 cultivars, mostly in the northern hemisphere (Ritz et al., 2005). The Damask rose (*Rosa damascena* Mill.) is a popular variety of Rosaceae that is 1–2 m in height with large colorful flowers (Boskabady et al., 2013). It is an outdoor and indoor ornamental plant cultivated in all parts of the world, including Iran. Besides its role as a fragrance (Dolati et al., 2011), its rose oil has nutritional, pharmacological, and industrial properties (Boskabady et al., 2011; Jabbarzadeh & Khosh-Khui, 2005). The medicinal uses of the Damask rose include those for digestive disorders, chest pain, menstrual bleeding, lung disorders, constipation, tension, and depression (Boskabady et al., 2006, 2013). Several studies on the pharmacological properties of the Damask rose (Boskabady et al., 2011) have reported that rose's essential oil possesses analgesic, anti-inflammatory, hypnotic, antitussive, and antispasmodic properties (Boskabady et al., 2013; Shafei et al., 2010). In addition to the essential oil, hydroalcoholic and aqueous extracts of the Damask rose have shown laxative (Arezoomandan et al., 2011), analgesic (Rakhshandeh et al., 2008) and hypoglycemic effects in animal studies (Gholamhoseinian et al., 2009).

Rose water (hydrosol) is traditionally known as *golab* in Iran and has long been used in religious ceremonies (Haghighi et al., 2008). The product is popular as an additive in the food industry for specialty foods (Nikbakht & Kafi, 2008). The clinical properties of rose water have been reported to provide relief from toothache, aphthous lesions, and gingival and throat inflammation (Norman, 1963). It has been used as a remedy for gastrointestinal complications (Claus et al., 1970), acne (Sharma & Jain, 2013), bacterial infections (Ozkan et al., 2004), and gastric and duodenal spasms (Sharma & Jain, 2013).

The chemical composition of rose water has been studied using different solvents and extraction methods (Agarwal et al., 2005). The main components of hydrosol in ethanol as a solvent are phenethyl alcohol (69.7–81.6%), citronellol (1.8–7.2%), and geraniol (0.9–7%). These components have been also been reported using hydrodistillation (phenethyl alcohol: 30.8%, citronellol: 15.6%, geraniol: 16.8%). Simultaneous distillation–extraction has also been utilized

Correspondence: Mahmoodreza Moein, Department of Pharmacognosy, School of Pharmacy, Shiraz University of Medical Sciences, P.O. Box 71345-1583, Shiraz, Iran. E-mail: mrmoein@sums.ac.ir

to identify the composition of rose water, with phenethyl alcohol (81.27%), citronellol (5.72%), and geraniol (4.43%) reported as the main constituents (Eikani et al., 2005).

In Iran, rose water is traditionally and industrially produced by distillation and usually contains 10–50% rose oil (Boskabady et al., 2011). Synthetic essences or essential oils of other aromatic plants are sometimes added to this product to decrease production costs. This practice evidently lowers the quality of the final product, which shows decreased amounts of phenethyl alcohol as the significant compound. In conventional distillation methods of producing rosewater, this compound transfers into the aqueous phase because of its high solubility in water, usually leaving small amounts of phenethyl alcohol remaining in the volatile essence.

The present study analyzed the chemical composition of samples from 10 different brands of rose water purchased from local markets in Iran.

Materials and methods

Sample collection

Ten different brands of rose water were purchased from local market in Shiraz, a city in Fars province of Iran, and were used as samples. The samples were numbered from 1 to 10. Sample 8 was produced by industrial distillation and the rest were produced using traditional distillation methods.

Extraction of essential oils

The essential oils of all samples were extracted using a liquid extractor in two stages for each sample. First, 500 ml of the sample were mixed with 500 ml of petroleum–ether as a solvent. The solvent was heated to 45 °C for 150 min and the essential oils transformed from an aqueous phase to a petroleum–ether phase. The remains of organic phase from the first stage were removed and additional amount (500 ml) of fresh petroleum-ether was entered into the system. As for the first stage, it was heated for 150 min. This stage was carried out to increase the yield of the essential oil in the organic phase.

Essential oil concentration

The essential oil extracted for each sample was concentrated in an IKA RV10 basic rotary evaporator equipped with a Heidolph Rotavac vacuum pump. In this process, 500 ml of petroleum–ether containing the essential oil were heated to 40 °C and vacuumed by rotation of a pump motor at 60 rpm, evaporating the petroleum–ether and leaving the extract. This process produced approximately 50 ml of sample dissolved in a small amount of organic phase (petroleum–ether). The process took 10 min for each sample.

Gas chromatography-mass spectrometry

The concentrated essential oils in each sample were dehydrated and subjected to gas chromatography mass spectrometry (GC/MS) for analysis of the constituents (Agilent Technologies 7890 gas chromatograph coupled with an Agilent Technologies model 5975C mass detector, Palo Alto, CA). The apparatus was equipped with a HP-5MS capillary column [phenyl-methylsiloxane, 30 m × 0.25 mm i.d., Agilent Technologies (60–325/350 °C)]. The oven temperature increased from 60 °C (0 min) to 220 °C in increments of 5 °C/min and held there for 10 min. Helium was selected as the carrier gas and the flow rate was adjusted at a rate of 1 ml/min. The mass spectrometer operated in EI mode at 70 eV. The interface temperature was 280 °C and the mass range was 30–600 *m/z*.

Results and discussion

The data from GC/MS were used to identify the components of the samples. This process compared the resulting Kovats indices (KI) and mass spectra data of the components with those mentioned in the literature (Adams, 1995; Sanseera et al., 2012). Table 1 shows the percentage of the components identified in each sample. In most samples, the major components were phenethyl alcohol, geraniol, and β-citronellol. No geraniol was recorded for five samples; five other samples contained geraniol, with three containing high percentages.

Different percentages of phenethyl alcohol and β-citronellol were found in the samples. Samples of rose essential oil usually contain scant quantities of phenethyl alcohol or none at all. This compound is highly soluble in water and alcoholic and aldehyde monoterpenes are insoluble in water, thus, the proportion of phenethyl alcohol usually increases during the production of rose water (Kurkcuoglu & Baser, 2003).

Table 1 shows the addition of *Pelargonium* essence to some samples. The main components of this essence are geraniol, β-citronellol, and linalool (Verma et al., 2013). As shown in the table, most samples contained these compounds in high percentages. Specifically, Sample 4 contained high amounts of geraniol and β-citronellol, which may have resulted from the addition of *Pelargonium* volatile oil in high amounts.

Table 1 also shows that Sample 1 probably contained *Dianthus* essence; however, there is some controversy about the composition of this sample. It contained a much lower percentage of phenethyl alcohol and much higher percentage of eugenol than the other samples. Other components found in the sample include *trans*-caryophyllene and eugenol-acetate, which were also not detected in other samples. These findings indicate the possibility of the addition of *Dianthus* essential oil to this sample, since about 99% of this oil is eugenol, eugenol-acetate, and caryophyllene (Claus et al., 1970). *Dianthus* essential oil is a colorless to light yellow liquid that darkens and increases in density on contact with air (Claus et al., 1970). Sample 1 was light yellow in color and was the darkest sample. All these findings support the assertion that *Dianthus* essential oil was added to the sample, but there is possibility of a synthetic essence in this sample as well.

There is also more than one possible reason for the percentage of phenethyl alcohol in Sample 8. This sample contained a much higher percentage of phenethyl alcohol than was found in the other samples. It should be noted that Sample 8 was the only sample that was produced industrially. The production process may have separated out most of the lipophilic ingredients from the aqueous phase. Low percentages of geraniol and β-citronellol in this sample support this hypothesis.

Table 1. Percentages of the identified compounds in the ten rose water samples.

Number	Compound	Reference KI	Calculated KI	1	2	3	4	5	6	7	8	9	10
1	Linalool	1098	1100	8.99	1.53	–	4.07	1.95	0.51	1.38	1.93	0.65	–
2	Phenethyl alcohol	1110	1114	12.02	20.83	47.78	33.42	39.53	33.79	37.7	73.31	26.8	34.94
3	beta-Citronellol	1228	1228	5.9	3.36	5.3	10.26	8.56	5.57	8.15	8.37	6.54	2.66
4	Geraniol	1255	1255	11.67	3.95	2.34	24.01	12.59	–	–	–	–	–
5	*m*-Thymol	1290	1290	1.26	1.3	–	1.17	–	–	–	–	–	–
6	Eugenol	1356	1359	17.75	2.51	3.61	3.05	2.26		2.88	3.63	–	–
7	Methyleugenol	1401	1405	–	–	1.04	0.67	–	1.27	1.09	1.51	–	–
8	Curzerene	1496	1499	–	5.4	3.93	2	2.66	7.33	3.04	1.17	4.58	11.04
9	Myristicin	1520	1524	–	2.22	–	–	1	1.76	1.26	–	–	–
10	Dibutyl phthalate	1965	1965	–	18.78	11.38	6.84	8.84	10.09	18.01	3.98	9.88	13.88
11	Nonane	900	900	0.31	–	–	–	–	–	–	–	–	–
12	Alpha-pinene	939	935	0.71	–	–	–	–	–	–	–	–	–
13	*m*-Cymene	1022	1026	1.15	–	–	–	–	–	–	–	–	–
14	Benzyl alcohol	1032	1033	–	–	–	–	0.46	–	–	0.85	–	–
15	gamma-Terpinene	1062	1060	0.47	–	–	–	–	–	–	–	–	–
16	alpha-Terpineol	1189	1193	–	–	–	2.23	–	–	–	1.32	1.49	–
17	Carvacrol	1298	1301	3.63	–	–	–	–	–	–	–	–	–
18	*trans*-Caryophyllene	1419	1425	3.44	–	–	–	–	–	–	–	–	–
19	Eugenol acetate	1524	1529	0.71	–	–	–	–	–	–	–	–	–
20	Heptadecane	1700	1710	–	1.08	–	–	–	–	–	–	–	–
21	Nonadecane	1900	1899	2.35	–	–	–	–	–	–	–	–	–
22	Docosane	2200	2199	0.4	–	–	–	–	–	–	–	–	–
	Citronellol + geraniol			17.57	7.31	7.64	34.27	21.15	5.57	8.15	8.37	6.54	2.66
	Oxygenated monoterpinoids			31.45	10.35	7.64	41.74	23.1	13.46	9.53	11.62	8.68	2.66
	Non oxygenated monoterpinoids			2.33	–	–	–	–	–	–	–	–	–
	Oxygenated Sesquiterpinoids			3.44	5.4	3.93	2	2.66	7.33	3.04	1.17	4.58	11.04
	Non oxygenated Sesquiterpinoids			–	–	–	–	–	–	–	–	–	–
	Known compounds			70.36	61.17	75.38	87.72	77.85	60.97	73.51	96.07	49.9	62.52

Table 1 shows Sample 2 contained the largest amount of dibutyl phthalate, followed by Samples 7, 10, 3, and 6 in decreasing order. Samples 8, 4, 5, and 9 contain the lowest amount of this compound in decreasing order; Sample 1 contained no dibutyl phthalate. Dibutyl phthalate is a component of polyethylene terephthalate (PET) containers. In low-quality PET containers, this compound may be released into the liquid contained in the bottle. This substance is toxic to the kidneys, liver, and central nervous system and may damage these organs under repeated or prolonged exposure (Franz, 2002; Montuori et al., 2008). The existence of dibutyl phthalate in the samples most likely results from storage of these products in large PET containers following production or from distribution of the products in plastic bottles. The low percentage of this substance in the Sample 8 confirms this assumption, since this sample was the only one packed in a glass bottle.

Conclusion

This research studied the chemical composition of 10 rose water samples. The essential oils were extracted and identified using GC/MS. In most samples, phenethyl alcohol, geraniol and β-citronellol were the main constituents. Geraniol was found in large amounts in half of the samples. The percentages of the main compounds differed strongly between the industrially produced sample and the other samples.

The results also revealed a high probability for the addition of *Pelargonium* essence to some samples. The main compounds of this essential oil (geraniol, beta-citronellol, and linalool) were detected in these samples. *Dianthus* essence or synthetic essence was also apparently added to one sample. This was inferred based on the different compositions and colors of this sample with respect to the other samples.

Dibutyl phthalate was found in most samples. This compound, which is generally released from PET containers, may be harmful for human health. Results of this study indicate that increased monitoring should be considered to ensure the safety and quality of nutritional and ethnopharmacological rose water.

Declaration of interest

The authors report no declarations of interest.

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