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Original research

GC-MS analysis of the chemical composition and alcohol content in Rose Water samples of the Isfahan market

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ABSTRACT

Rosa damascena Mill. is an important aromatic plant for the commercial production of rose oil and rose water. Its hydrosol is known in Iran as Golab (rose water) and has applications in religious ceremonies, foods, and pharmaceuticals. The increase in market demand has led to the production of inferior products. The aim of this study was to characterize the chemical composition of 22 rose water samples were purchased from the Isfahan market in October 2022 in aqueous phase and its organic extract and also methanol and ethanol content of these rose water samples by gas chromatography mass spectrometry (GC-MS). The results were used to evaluate the quality of rose water samples and detection of artificial essence use. Methanol and ethanol levels in the tested samples were 5-120 and 20-835 mg/kg. Some samples unusually had no ethanol and methanol. Major constituents of the extracted essence were phenyl ethyl alcohol, β-linalool, eugenol, eugenol methyl ether, geraniol, α-terpineol, citronellol, eugenol methyl ether, terpin hydrate, isopulegol, benzyl alcohol and nerol. These findings show that in order to determine whether rose water samples are real or fake, it is necessary to examine the samples in terms of chemical composition both in the aqueous phase of rose water and in the extracted essential oil as well as in the amount of ethanol and methanol.

Keywords: Rose water; Chemical composition; Methanol; Ethanol; GC-Mass

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1. Introduction

The damask rose *(Rosa damascene Mill.)* has been grown in Iran for centuries for the production of rose water and rose oil, which are currently widely applied in the perfumery, cosmetics and food industry. It is a valuable medicinal plant in traditional and modern medicine. The anti-depressant, antimicrobial, anti-inflammatory, antioxidant, anticancer and anti-diabetic properties, as well as anticonvulsant and hypnotic effects of damask rose, have been confirmed. Rose water known as Golab in Iran, is the primary product of damask rose (Yazdanfar et al., 2022). Rose water is used in religious ceremonies, it is also applied as a flavoring agent in Iranian foods (Boskabady et al., 2011; Mahboubi, 2016).

Iran is one of the most important rose oil and rose water producers in the world. Iran has been mentioned as a country of possible origin of Damask roses (Baser et al., 2003). The quality of rose water depends on the number of its ingredients. For example, phenyl ethyl alcohol is responsible for the nice smell of rose water. The main components of rose water are ethyl alcohol (69.7–81.6%), citronellol (1.8–7.2%), and geraniol (0.9–7%). These components have been also reported using hydro distillation (phenyl ethyl alcohol: 30.8%, citronellol: 15.6%, geraniol: 16.8%). Simultaneous distillation–extraction has also been utilized to describe the composition of rose water, with phenyl ethyl alcohol (81.27%), citronellol (5.72%), and geraniol (4.43%) known as the main constituents (Eikani et al., 2005).

Synthetic essences or essential oils of other aromatic plants are sometimes added to this product to decrease production costs (Loghmani-Khouzani, 2007). Due to the popularity of rose products, especially rose water, the possibility of fraud in the processing of this product has also increased. The purpose of this study was to characterize the chemical composition of 22 rose water samples in aqueous phase and its organic extract and also methanol and ethanol

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content of them. The results were used to evaluate the quality of rose water samples and detecting the use of artificial essential oil and the possibility of fraud.

The presence of alcohols (such as methanol and ethanol), is a matter of great concern. The fermentation of the plant's fibers (i.e., cellulose and pectin) through the manufacturing process, and also the usage of these alcohols as a solvent agent to extract natural ingredients in rose water, lead to their increased residual levels in rose water (Mousavi et al., 2011; Yousefi et al., 2018). Ethanol level in distillates and its toxicity is less than methanol (Mousavi et al., 2011) .

The amount of methanol and ethanol in rose water samples has been investigated in several articles. (Mousavi et al., 2011; Yousefi et al., 2018). In this article, the content of ethanol and methanol were determined from two points of view. First, high amounts of methanol and ethanol indicate corruption of rose water and due to their toxicity, their amount must be within the permissible limit. The permissible limit of methanol is 150mg/kg and ethanol 2500mg/kg in the Iranian standard (standard.inso.gov.ir, 2022). Second, considering that natural rose water contains various amounts of methanol and ethanol, the samples that do not contain methanol and ethanol are unnatural samples. Therefore, one of the ways to detect fake rose water samples is based on their ethanol and methanol content.

2. Material and Methods

2.1. Sample collection and reagents

A total of 22 bottles of rosewater (22 different brands) were randomly selected and purchased from the local markets and herbalist's shops of Isfahan, Iran, in autumn 2022. The production and expiration date of samples were different. The collected samples were industrially produced rose water. Dichloromethane, ethanol and methanol (all analytical grades) were obtained from Merck (Germany).

2.2. Preparation of rose water extract

The rosewater sample (100 mL) was extracted with 2×50 mL dichloromethane using a separatory funnel. In each step, mixture of rose water and dichloromethane shacked well, then allowed to settle and the organic layer was separated. The organic layer was evaporated under reduced pressure in BUCHI V-855 rotary evaporator at a temperature of 45ºC to get concentrated rose water extract. Finally, 1ml n-hexane was added and mixed well and finally was injected to GC-MS.

2.3. Direct injection of rose water samples to GC-MS

Rose water samples were injected into GC-MS without any preparation to check the hydrophilic compounds in rose water.

2.4. Ethanol and Methanol check

Methanol and ethanol concentrations of each sample were measured by GC-MS, according to the Iranian standard (INSO 22448). At first, the stock solution of ethanol and methanol with a concentration of 1000mg/kg was made in water. Then, working solution of 25, 50, 100, 200, 300mg/kg were made from it. The propanol internal standard solution was made with a concentration of 200mg/kg in water. An equal volume of working standard and internal standard was mixed in the auto sampler vial and injected into the GC-MS. Linear calibration curves for ethanol and methanol were obtained with correlation factors >0.99 (Fig. 1 and Fig. 2). The quantification limit (LOQ) and detection limit (LOD) were calculated based on the standard deviations of the intercept and calibration curve parameters. LOD and LOQ were 16 and 48 mg/kg respectively for ethanol and 9 and 27mg/kg for ethanol.

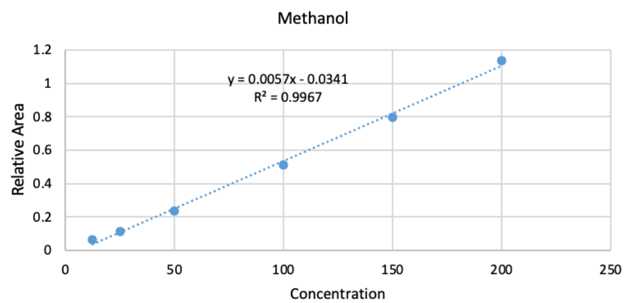

Fig. 1. Calibration curve of methanol

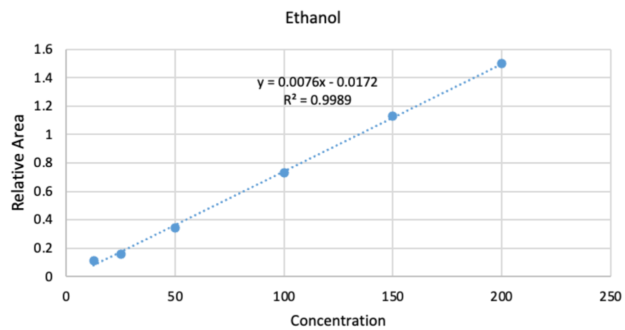

Fig. 2. Calibration curve of ethanol.

An equal volume of the rose water sample was mixed with an equal volume of the internal standard and was injected into the GC-MS. The amount of methanol and ethanol was calculated using standard calibration curve.

2.5. GC-MS analysis and compound identification

Rose water extracts and their alcohol content were analyzed by an Agilent Technologies 7890A Network GC System Chromatograph (Wilmington, USA) with a SQ detector equipped with an Agilent 7693 autosampler (Agilent technologies, USA).

A Stabil wax capillary column (30m x 0.32mmID x 0.25µm film thickness) was used for separation.

The column temperature program for rose water composition check was done from initial temperature 50°C/min and then heated at the rate of 3°C/min to 200ºC and stayed in this temperature for 5 minutes. Carrier gas (helium) flow was 2 mL/min. The injector and detector temperatures were 220°C and 230°C, respectively. 1µl of sample was injected with splitless injection methods. A library search was carried out using the Wiley GC-MS Library. Relative percentage amounts of the separated compounds were calculated from total ion chromatograms by the computerized integrator.

The column temperature program for methanol and ethanol content of rose water was 50°C for 4 min and then heated to 100°C at the rate of 2°C/min and held for 3 min. Then temperature was increased at the rate of 5°C/min to 150°C and held for 5 min. The flow rate was 1 ml/min. The injector and detector temperatures were 220°C and 230°C, respectively. 1µl of sample was injected with 1:100 split mode. The mass scan ranged from 30 to 500 m/z.

3. Results and Discussion

In order to check the compounds in the rose water samples, the extract of rose water with an organic solvent was examined once. Because there was a possibility that some compounds would not enter the organic phase (due to their high hydrophilicity), in order not to lose the study of these compounds, the rose water samples were directly injected into GC-MS without any preparation.

When directly injecting rose water samples, the height of the peaks in the chromatogram is low due to the dilution. To better observe the essence compounds in rose water, the essential oil was extracted using dichloromethane solvent. Dichloromethane is a suitable solvent for extracting rose essence (Agarwal et al., 2005). A sample chromatogram from extract essence of rose water is shown in Fig. 3.

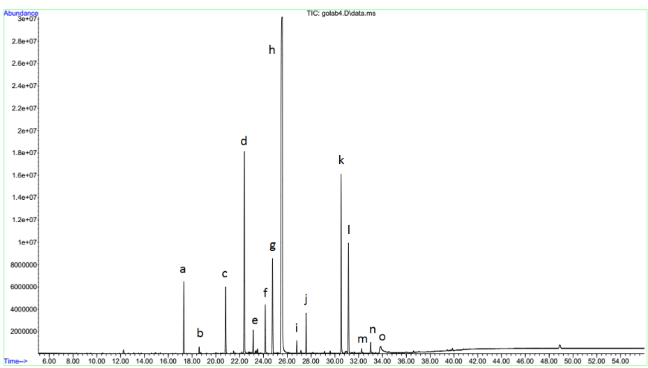

Fig. 3. A sample chromatogram from extract essence of rose water injection (in organic phase) a: linalool, b: β-terpineol, c: α-terpineol, d: β-citronellol, e: cis-geraniol, f: Nerol, g: benzyl alcohol, h: phenyl ethyl alcohol, i: terpin hydrate, j: eugenol methyl ether, k: eugenol, l: hydroxyl citronellol, m: Isopulegol, n: Isopulegol, o: geranic acid.

About thirty-four components were identified in the rose water extracts. The identified components along with their percentage are shown in Table 1. Compounds including linalool, eugenol, geraniol, nerol, α-terpineol, citronellol, eugenol methyl ether, terpin hydrate, isopulegol, hydroxycitronellol, benzyl alcohol and phenyl ethyl alcohol were present in almost all samples.

Decane, dodecane, tridecane and tetradecane were identified in 4 samples (samples 8, 10, 21 and 22). According to studies, the effective ingredients of rose essence are influenced by many factors. The production method of rose water (Moein et al., 2016; Zhao et al., 2016), the genotype of flower used in the process of extracting rose water (Karami et al., 2012), as well as the effect of the freshness of flowers used for extracting rose water (Agarwal et al., 2005; Koksal et al., 2015) on the essence chemical composition have been investigated in several studies.

Some samples (samples1, 2 and 8) contain unwanted dibutyl phthalate and diisooctyl phetalate compounds which may have been imported from sample packaging. 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 and may be harmful for human health (Mousavi et al., 2011).

Sample 5 is completely unusual because the only compound in its extracted essential oil is phenyl ethyl alcohol. The manufacturer of this sample may have mixed phenyl ethyl alcohol and water and offered it as rose water or this rose water is made from the residue of rose petals that has been extracted from them before.

Nerol is a character of the freshness of rose water (Baser et al., 2003). Which is not seen in samples 5, 9, 19 and it can be due to the oldness of these samples. The highest amount of nerol is observed in samples 6 (12.5%) and 13 (17.8%).

In order to check the quality of rose water samples and detection of rose water frauds, it is necessary to check the compounds in the aqueous phase of rose water too. For this purpose, the rose water samples were directly injected into the Wax column of GC-MS. A sample chromatogram from direct injection of rose water is shown in Fig. 4.

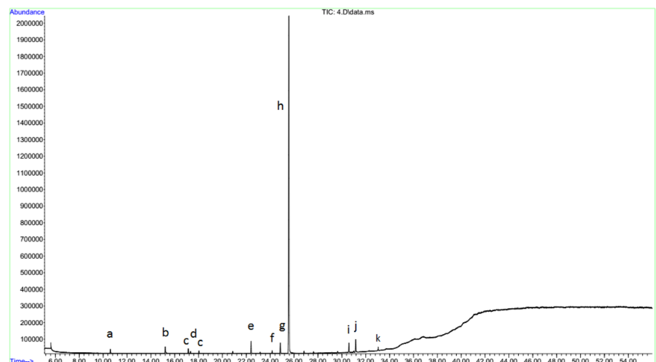

Fig. 4. A sample chromatogram from direct injection of rose water (in aqueous phase) a: 1,3 propan diol, b: acetic acid, c: 2,3 butan diol, d: linalool, e: β-citronellol, f: geraniol, g: L-argenine, h: phenyl ethyl alcohol, i: eugenol, j: hydroxycitronellol, k: 15 crown5.

Since the main composition of rose water in the aqueous phase is phenyl ethyl alcohol, the high percentage of this compound causes the percentage of other substances in the aqueous phase to be negligible. In order to better comparison of the percentage of substances in the aqueous phase, the peak of phenyl ethyl alcohol was removed in the chromatogram and then normalized the peaks. The results are shown in Table 2. Compounds such as 1,3 propanediol, 2,3 butanediol and 15crown5 are observed in the aqueous phase of samples number 2,3,4,9,10,11,12,13,16,17,21 and 22. It seems that these compounds have been used to dissolve the artificial essences added to rose water. Propanediol, butanediol and 15crown 5 are used mainly as a solvent and emulsifier, helping formulations with stability and it indicates the unnaturalness of these rose water samples.

Zarei showed that artificial rosewaters contained mainly polypropylene glycol while in the original samples this alcohol was not observed (Zarei Jelyani et al., 2021).

Table 1. Comparative percentage of the identified compounds in rose water extract of different samples.

Constituents (%)	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11
Decane	–	–	–	–	–	–	–	20.05	–	14.70	–
Dodecane	–	–	–	–	–	–	–	19.80	–	14.32	–
Tridecane	–	–	–	–	–	–	–	11.38	–	8.66	–
Tetradecane	–	–	–	–	–	–	–	1.30	–	1.21	–
B-Linalool	0.54	2.14	5.00	3.55	–	2.56	10.22	1.38	0.53	2.98	0.49
Hexadecane	–	–	–	–	–	–	–	–	–	0.35	–
Cis-β-Terpineol	–	–	–	0.33	–	–	–	–	0.14	–	–
A-Terpineol	1.33	3.41	4.50	3.49	–	1.44	11.77	1.47	1.50	1.81	0.81
Carvol (carvon)	–	–	–	–	–	–	–	–	–	0.24	–
B-Citronellol	4.80	7.42	8.20	12.00	–	22.20	20.96	3.14	2.75	9.05	1.97
Cis-Geraniol	0.20	0.15	1.00	1.16	–	2.90	1.19	–	–	0.96	0.21
Isogeraniol	–	–	0.39	–	–	1.30	–	–	–	–	–
Nerol	0.76	0.86	2.78	2.75	–	12.50	3.18	0.45	–	4.64	0.72
Benzyl alcohol	–	4.45	3.23	5.10	–	1.78	9.17	1.17	2.76	1.78	4.69
Nonadecane	–	–	0.81	–	–	–	–	–	–	–	–
Phenyl ethyl Alcohol	77.00	63.95	60.63	50.99	91.20	39.50	0.92	32.30	79.70	31.26	75.50
B-Citral or neral	–	–	–	–	–	–	–	–	–	–	–
Eugenol methyl ether	0.67	0.55	0.88	2.10	–	5.70	5.42	0.35	1.10	0.81	0.54
A-Citral	–	–	–	–	–	–	–	–	–	–	–
Terpin hydrate	0.38	1.21	0.90	0.60	–	–	3.46	0.66	0.56	0.28	1.20
Heneicosane	–	–	0.40	–	–	–	–	–	–	–	–
Eugenol	4.50	4.78	6.18	10.20	–	3.90	8.39	1.95	1.90	3.43	4.00
Hydroxycitronellol	3.78	9.02	4.20	5.80	–	3.00	16.83	3.70	9.00	3.09	7.50
Cinnamyl alcohol	–	–	–	–	–	0.82	–	–	–	–	–
Acetic acid phenethyl ester	–	–	–	–	–	–	–	–	–	–	–
Isopulegol	0.33	0.44	0.73	0.57	–	0.55	2.37	–	–	0.41	1.16
Geranic acid	1.11	–	–	1.30	–	1.42	6.00	–	–	0.51	0.46
Dibutyl phthalate	–	1.60	–	–	8.80	–	–	–	–	–	–
Diisooctyl phthalate	4.33	–	–	–	–	–	–	0.82	–	–	–
Terpin hydrate	–	–	–	–	–	–	–	–	–	–	0.20
Benzen acetic acid	–	–	–	–	–	–	–	–	–	–	0.38
Dihydrocarvon	–	–	–	–	–	–	–	–	–	–	–
Phenyl ethanol	–	–	–	–	–	–	–	–	–	–	–
Dihydroeugenol	–	–	–	–	–	–	–	–	–	–	–
Benzoic acid	–	–	–	–	–	–	–	–	–	–	–

Recently, many researches have been done on chemical composition of rose water volatiles and the amount of phenyl ethyl alcohol. A research conducted by Agarwal showed that phenyl ethyl alcohol is the main component of natural rose water but its quantity in rose oil is much less because it is highly polar and water soluble so that most of it remained dissolved in the distillate water (Agarwal et al., 2005). Synthetic essences or essential oils of other aromatic plants are sometimes added to rose water to decrease production costs. This practice evidently lowers the quality of the final product, which shows decreased amounts of phenyl ethyl alcohol as the significant compound (Moein et al., 2014).

In this study, in order to compare rose water samples in terms of the percentage of phenyl ethyl alcohol, all the peaks of the chromatogram were normalized and the percentage of phenyl ethyl alcohol was calculated. The comparison of the percentage of phenyl ethyl alcohol in the aqueous phase of rose water samples is shown in Table 3.

Sample 5 unusually did not contain any other compounds other than phenyl ethyl alcohol (as mentioned earlier, this rose water may have been produced from petal waste). In rose water number 1, the percentage of aqueous phase compounds was insignificant and was not integrated so the percentage of phenyl ethyl alcohol in the sample is 100. Among other samples, rose water number 16 and 18 have the highest amount of phenyl ethyl alcohol, and rose water number 7 and 13 have the lowest amount.

Due to the low amount of phenyl ethyl alcohol in the aqueous phase of rose water number 7, as expected, the amount of phenyl ethyl alcohol in its extracted essential oil is negligible too (Table 1). This point indicates the abnormality of this rose water sample.

In the process of producing rose water and other herbal extracts, the plant has picked and used after 48 h of dehydration, and this stress leads to an increase in the concentration of ethanol and methanol in the rose water (Nasouri Gazani et al., 2015). It should be noted that the amount of alcohol in the extract, especially methanol, can never be reduced to zero, thus the presence of methanol determines the authenticity of the plant extract.

The concentrations of the methanol and ethanol of 22 rose water samples were represented in Table 4. The permissible limit of methanol in the national standard of Iran is less than 100 mg/kg, and this level is 2500 mg/kg for ethanol (standard.inso.gov.ir, 2017). Sample number 5 is unusually free of methanol and ethanol, while rose water naturally contains amounts of methanol and ethanol. Samples 4, 9, 11, 21 and 22 contain more than the allowed amount of methanol, which can be due to the aging of rose water in these samples. Other samples contain methanol and ethanol within the permissible limits.

Table 1. Continuation.

Constituents (%)	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22
Decane	–	–	–	–	–	–	–	–	–	12.90	13.66
Dodecane	–	–	–	–	–	–	–	–	–	12.60	13.26
Tridecane	–	–	–	–	–	–	–	–	–	8.20	7.59
Tetradecane	–	–	–	–	–	–	–	–	–	1.15	0.89
β-Linalool	2.40	2.40	5.36	4.22	2.45	5.00	0.50	3.10	1.22	2.93	2.53
Hexadecane	–	–	–	–	–	–	–	–	–	0.30	–
cis-β-Terpineol	–	–	–	–	–	–	–	–	0.47	–	–
α-Terpineol	2.51	2.03	2.20	2.35	2.10	4.87	0.87	1.75	5.59	1.70	2.38
Carvol(Carvon)	–	–	–	–	0.71	1.80	–	–	–	0.24	0.42
β-Citronellol	8.94	24.90	23.10	21.17	12.10	12.20	1.22	24.20	3.53	8.90	6.10
cis-Geraniol	–	4.62	1.22	1.78	0.49	0.74	0.15	15.50	–	4.20	0.53
Isogeraniol	–	–	–	–	–	–	–	3.90	–	–	–
Nerol	1.09	17.80	7.50	9.10	5.27	3.99	0.38	–	0.53	8.70	1.50
Benzyl Alcohol	3.24	0.37	1.10	1.38	3.20	3.45	–	1.30	6.50	2.20	3.20
Nonadecane	–	–	–	–	–	–	–	–	–	–	–
Phenyl ethyl Alcohol	68.23	32.17	41.44	43.00	58.20	44.50	88.40	33.40	48.60	30.40	38.70
β-Citral or neral	-	0.68	–	–	–	–	–	–	–	–	–
Eugenol methyl ether	1.88	6.10	4.90	4.88	1.12	2.50	0.30	6.80	3.00	0.79	0.57
α-Citral	–	0.89	–	–	–	–	–	–	–	–	–
Terpin Hydrate	–	–	0.59	0.62	0.60	1.13	0.70	–	4.26	0.19	0.42
Heneicosane	–	–	–	–	–	–	–	–	–	–	–
Eugenol	4.77	4.10	1.52	2.95	3.60	6.40	2.37	3.20	10.90	1.27	4.70
Hydroxycitronellol	6.90	0.89	8.43	6.98	4.90	6.34	4.40	3.80	14.70	–	3.20
Cinnamyl alcohol	–	1.10	0.77	0.59	–	–	–	1.39	–	–	–
Acetic acid phenethyl ester	–	1.10	0.64	–	–	–	–	–	–	–	–
Isopulegol	–	–	1.19	1.00	1.65	0.89	0.59	0.75	0.70	0.91	0.27
Geranic acid	–	0.62	–	–	–	1.37	–	0.82	–	0.70	–
Dibutyl phthalate	–	–	–	–	–	–	–	–	–	–	–
Diisooctyl phthalate	–	–	–	–	–	–	–	–	–	–	–
Terpin hydrate	–	–	–	–	–	0.28	–	–	–	–	–
Benzen acetic acid	–	–	–	–	1.24	3.10	–	–	–	–	–
Dihydrocarvon	–	–	–	–	0.36	0.54	–	–	–	–	–
Phenyl ethanol	–	–	–	–	0.71	–	–	–	–	–	–
Dihydroeugenol	–	–	–	–	0.92	–	–	–	–	–	–
Benzoic acid	–	–	–	–	0.26	0.76	–	–	–	–	–

Table 2. Compounds identified in direct injection of different rose water samples into the GC-MS.

Constituents (%)	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11
1,3 Propan diol	–	–	5.17	5.67	–	–	–	–	9.80	–	6.40
15 Crown5	–	–	–	3.10	–	–	–	–	–	3.70	–
2,3 Butan diol	–	6.04	–	10.29	–	–	–	–	–	–	–
6,7 Dihydro7hydroxy linalool	–	–	–	–	–	5.10	–	–	–	–	–
Acetic acid	–	9.10	6.50	11.00	–	–	2.60	30.14	17.10	–	5.20
Bezene acetic acid	–	–	–	–	–	–	84.40	–	–	–	–
Butiric acid	–	19.30	–	–	–	–	–	–	–	–	–
cis-Geraniol	–	–	16.40	3.6	–	5.60	–	–	–	9.20	–
Eugenol	–	7.20	17.68	13.22	–	3.18	–	–	9.51	5.00	9.20
Eugenol methyl ether	–	–	–	–	–	4.10	–	–	–	–	–
Geranyl vinyl ether	–	–	–	–	–	4.90	–	–	–	–	4.20
Hydroxycitronellol	–	30.40	5.87	17.70	–	34.20	3.70	–	36.71	17.50	42.60
L-Argenine	–	12.40	13.39	14.89	–	3.78	4.70	10.40	11.90	9.80	8.70
Butyrate	–	–	–	–	–	–	1.20	–	–	–	–
Nerol	–	–	8.00	–	–	–	–	–	–	–	–
Terpin hydrate	–	6.50	–	–	–	–	–	9.10	4.34	3.30	11.20
Terpineol	–	–	–	–	–	3.84	–	–	2.88	5.42	4.30
β-Citronellol	–	8.40	22.89	16.00	–	27.70	2.70	13.62	7.66	36.80	4.60
β-Linalool	–	–	3.98	2.87	–	7.42	–	36.60	–	8.97	–

Table 2. Continuation.

Constituents (%)	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22
1,2,3 Trimethoxy propan	–	11.50	–	–	–	–	–	–	–	–	–
1,3 Propan diol	13.30	20.60	–	–	4.00	4.37	–	–	–	6.74	8.70
15 Crown5	–	–	–	–	–	–	–	–	–	–	–
2,3 Butan diol	–	–	–	–	6.12	10.95	–	–	–	–	–
6,7 Dihydro7hydroxy linalool	–	–	–	–	–	–	–	–	–	–	–
Acetic acid	15.70	–	–	11.60	12.83	9.39	–	–	76.58	–	–
Benzyl alcohol	–	–	–	–	8.40	–	–	–	–	13.40	16.52
Bezene acetic acid	–	–	–	–	–	–	–	–	–	–	–
Butiric acid	–	–	–	–	–	–	–	–	–	–	–
cis-Geraniol	–	7.50	17.70	–	–	–	–	5.12	–	9.00	3.80
Citronellol epoxide	–	–	–	69.50	–	–	–	–	–	–	–
Dipropylene glycol	–	15.50	–	–	–	–	–	–	–	–	–
Eugenol	8.70	–	–	–	–	5.16	11.40	1.91	3.47	–	8.26
Eugenol methyl ether	–	2.00	5.50	–	–	–	–	4.20	–	–	–
Geranyl vinyl ether	–	–	–	–	–	–	–	–	–	–	–
Hydroxycitronellol	32.60	7.60	18.00	18.70	47.16	40.11	22.10	44.74	11.71	5.50	20.00
Isopulegol	–	1.80	–	–	2.00	9.67	–	5.44	–	–	–
L-Argenine	15.10	–	–	–	–	6.23	–	1.84	3.91	–	–
Linalyl butyrate	–	–	5.60	–	–	–	–	–	–	–	–
Nerol	–	1.00	–	–	–	–	–	–	–	22.56	–
Oxym methoxy phenyl	–	–	–	–	–	–	43.00	–	–	–	–
Terpin	–	–	–	–	3.00	2.84	–	–	–	–	–
Terpin hydrate	–	1.00	–	–	11.67	9.83	7.00	6.60	2.13	–	5.24
Terpineol	–	1.90	–	–	–	3.54	8.00	2.95	–	5.47	6.00
β-Citronellol	14.20	21.00	53.00	–	2.10	4.87	–	24.57	2.17	24.63	26.10
β-Linalool	–	3.70	–	–	–	–	8.10	3.13	–	9.53	5.90

Table 3. The percentage of phenylethyl alcohol in the aqueous phase of rose water samples.

Sample	%Phenylethyl Alcohol	Sample	%Phenylethyl Alcohol
1	100.00	**12**	82.70
2	87.00	**13**	41.10
3	82.50	**14**	73.20
4	82.70	**15**	72.80
5	100.00	**16**	86.30
6	69.30	**17**	77.00
7	10.70	**18**	86.10
8	84.00	**19**	58.70
9	78.70	**20**	55.90
10	82.00	**21**	84.00
11	74.00	**22**	83.80

Table 4. The amount of methanol and ethanol in rose water samples.

Sample	Methanol (ppm)	Ethanol (ppm)	Sample	Methanol (ppm)	Ethanol (ppm)
1	23.44	36.93	**12**	55.63	477.71
2	49.28	131.89	**13**	5.85	27.09
3	80.75	530.75	**14**	29.15	170.63
4	111.02	777.99	**15**	24.82	162.63
5	–	–	**16**	51.23	321.21
6	28.19	81.34	**17**	97.29	459.97
7	14.66	20.43	**18**	33.52	151.59
8	39.93	–	**19**	32.46	151.88
9	119.01	834.86	**20**	41.31	45.85
10	50.75	218.86	**21**	120.13	384.78
11	107.86	743.15	**22**	115.44	684.14

4. Conclusion

In this study, 22 samples of rose water present in Isfahan market were studied in terms of chemical composition and the amount of ethanol and methanol. Artificial rose water contained 1, 3 propanediol, 2, 3 butanediol and 15crown 5 and sometimes methanol and ethanol was not observed in these samples. The presence of ethanol and methanol confirms an original rose water sample, while diol compounds and 15crown5 confirms an artificial one. Moreover, when diol compounds and 15crown 5 are present with ethanol and methanol alcohols, it indicates that the original and artificial samples were mixed. For the accurate selection of rose water, the presence of all identified compounds is essential. Rose water samples that contain low amounts of main ingredients of rose water essence are most likely prepared from flower waste after several times of rose water production.

Due to the toxicity and carcinogenicity of synthetic essential oils for edible purposes, considering that rose water is also used in baking and cooking in Iran, it is necessary to continuously control this substance in terms of its naturalness by food organizations.

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Conflict of interest

The authors declare that there is no conflict of interest.

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