Instrumental and sensory aroma profile of pomegranate juices from the USA: differences between fresh and commercial juice

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ABSTRACT: Fourteen pomegranate juices (one fresh-squeezed and 13 commercial juices) were studied to determine the aromatic profile of the products. Headspace–solid phase micro-extraction and sensory flavour profile analysis were used to determine the aromatic composition of the juices and were related using partial least squares regression. Up to 83 different aromatic compounds were found in the juices, including terpenes, benzene derivatives, furans, esters, acids, ketones, alcohols and aldehydes. Commercial pomegranate juices did not present a unique sensory or instrumental aromatic profile. The three attributes common to the majority of the juices were an overall sweetness and musty/earthy and grape notes. This study shows the large heterogeneity of the pomegranate juices found on the market, which might be related to the fact that companies are looking for different successful pomegranate juice products using different raw ingredients and processes. Further studies are required to clarify what consumers are expecting in a typical 'pomegranate juice', and which aromatic profile could be successful in improving the acceptance of this healthy product. Copyright © 2010 John Wiley & Sons, Ltd.

Keywords: volatile; Punica granatum L.; SPME; GC–MS; flavour; sensory

Introduction

Pomegranate (Punica granatum L.) is a fruit becoming more popular because of its healthy properties (anti-atherogenic, anti-oxidant, antihypertensive, etc.), which have been widely shown in previous studies.11-14 These healthy properties come from the high anti-oxidant activity of the fruit and are directly related with its phenolic compounds content.5-10

The phenolic content of pomegranate has been reported in fruits from different countries9,10 and in several pomegranate juices,8 demonstrating that anti-oxidant activity of the fruit remains almost intact from fruit to juice. The high anti-oxidant activity of pomegranate juices is mainly caused by the punicalagins and ellagic acid derivatives, compounds located mainly in the rind of the fruit.3 Some methods for extracting the juice, which rub the internal part of the pomegranate rind, may contribute to the extraction of these compounds. Pomegranate juice can be found as 'juice from direct extract', 'juice from concentrate', 'juice concentrate' and 'juice from concentrate with natural flavours'. Product appearance varies from red to brown colour and sometimes with turbidity and some residue present. These variations are conditioned mainly for the different types of processing to elaborate the final juice. The juice can be concentrated to ensure longer storage life and easier transportation, or subjected to a clarification process, reducing the amount of phenolic substances. During concentration, the colour of the juice changes and some volatile compounds are lost.11 During clarification, some sensory properties of the juice will improve (e.g. colour, turbidity, overall appearance and bitterness),12 but the healthy benefits of the juice will be reduced when particles and phenolic substances are removed.

One sensory study found large differences in sensory characteristics among 33 commercial juices; differences mainly found in the aromatic profiles of the products and that could be the result of processing, pomegranate variety or other issues.13 These authors clustered products into five groups of juices, based on overarching sensory properties: dark-fruity; grape; berry; fermented or musty/earthy; and beet attributes.

Although several studies have been conducted on pomegranate juices, none were found that provided information about volatile composition or differences in the instrumental aroma profiles of the juices. Researching these end-products is of great interest, because they are the products which people will consume and which have a direct effect on consumers’ acceptance. Although the aromatic composition of the pomegranate or pomegranate products has not yet been well described, many products can be found in the market labelled 'with pomegranate aroma', such as softeners, hand soap, aromatic candles, flavoured...
water, etc. The extraction method mainly chosen for studying the aroma profile in fruits and derivates is solid phase microextraction (SPME). It is primarily a non-quantitative extraction technique, but the heating of the sample is low and the aroma profile obtained is closer to real than with other extraction techniques, such as simultaneous distillation–extraction or hydrodistillation.\[14\]

The objective of this study was to describe sensory and instrumental aroma characteristics of selected commercial pomegranate juices and to determine their similarity to fresh pomegranate juice. This information will be useful for companies, consumers and researchers to provide a general idea of the aromatic composition of pomegranate products, and not only to improve the aroma of the commercial juices but also to provide ideas in developing fragrances which could be added to cosmetic and other products.

### Experimental

#### Samples

Fourteen pomegranate juice samples were used for the study, 13 commercial juices and one fresh-squeezed juice (F) prepared from fresh pomegranate arils (Wonderful Cultivar, USA). All the commercial juices were produced in the USA and were available in Manhattan, KS, USA. Two of the samples were ‘juice from direct extract’ (DE), five were ‘juice from concentrate’ (C), one ‘juice concentrate’ (included in the C group) and five were ‘juice from concentrate with natural flavourings added’ (AD) (Table 1). All these products were available in local grocery stores, supermarkets and specialty stores in the area. At least three bottles of each commercial sample were purchased (around 3 litres of each juice).

F juice was prepared by manually extracting the arils from the pomegranate and squeezing them with a kitchen juicer. Three different juices were prepared, one each from three different pomegranates. All nine fruits were purchased during the same week and from the same grocery store. The arils were used whole, without removing the seed or the carpellar membranes, because they would be separated later by the juicer while extracting the juice. No additives or preservatives were added, and no heat treatment was done.

All of the samples were assigned random three-digit codes. The commercial products were stored following the instructions on the packaging and studied before the indicated expiry date. The F juice was studied on the same day it was prepared. For sensory analysis, the concentrates were diluted according to the directions on the packaging.

#### Analysis of Volatile Composition

**Extraction procedure for volatile aroma compounds.** Each sample (2 ml) was hermetically placed in a 10 ml vial with a polypropylene hole cap PTFE/silicone septum. The vials were equilibrated for 10 min at 40°C in the autosampler (Pal System, Model CombiPal, CTC Analytics, Switzerland). After this equilibration time, a DVB/CAR/PDMS fibre (50/30 μm thickness) was exposed to the sample headspace for 30 min at 40°C.\[15\] After sampling, desorption of the analytes from the fibre coating was carried out in the injection port of the gas chromatograph at 250°C for 5 min in splitless mode.

Three replications of each sample juice were done for the instrumental aromatic compounds study. Each replication was from a different bottle of the corresponding commercial sample. Regarding F juice, each replicate was from one of the three prepared juices.

**Chromatographic analyses.** The isolation, identification and semi-quantification of the volatile compounds were performed on a gas chromatograph (Varian GC CP3800; Varian, Walnut Creek, CA, USA) coupled with a Varian mass spectrometer (Saturn 2200) and operated with MS
Workstation software. The GC–MS system was equipped with a VF-5MS column (5% phenyl, 95% dimethylpolysiloxane; Varian; 30 m x 0.25 mm i.d., 1.0 μm film thickness). The starting temperature of the column was 40°C, which was held for 10 min, then increased 8°C/min to 180°C, and finally increased at 10°C/min to 280°C, where was held for 10 minutes. The constant column flow was 1 ml/min, using helium as the carrier gas.

Most of the compounds were identified using two different analytical methods: (a) Kováts indices; (b) mass spectra (authentic chemicals and Wiley spectral library collection).

**Semi-quantification of volatile aroma compounds.** To semi-quantify the volatile compounds, 1,2-dimethoxynbenzene was used as internal standard (final concentration in the sample of 4 mg/kg). The internal standard facilitates the comparison of compounds among samples. Headspace composition is not an accurate representation of the amount of each compound in the sample. All results presented in the discussion were relative to an internal standard; chemical compounds or chemical groups were not compared from a quantitative (or semi-quantitative) point of view. The MS detector was used in scan mode during the study, which is not valid for absolute quantification of volatile compounds.[16]

**Sensory Evaluation with a Trained Panel**

**Panellists.** Five highly trained panellists from the Sensory Analysis Center (Manhattan, KS, USA) participated in this study. Each of the panellists had more than 1000 h of testing experience with a variety of food products. For the current study, the panellists received further orientation on fresh and processed pomegranates.

**Sample serving.** The juices were shaken and poured into odour-free, disposable 90 ml covered plastic cups (Sweetheart Cup Co. Inc., Owings Mills, MD, USA) for the evaluation. All of the samples were served at room temperature within 30 min before the testing. Each panellist received 60 ml of each product for evaluation. Additional samples were available if needed.

**Sample evaluation procedure.** Twelve 1.5 h sessions were held for the sample evaluations. One or two samples were evaluated each day. All the samples were coded with three-digit random numbers, and the order in which the products were evaluated was randomized. The descriptive attributes used for this study are shown in Table 2 (definitions for each attribute can be found in Koppel and Chambers).[13]

A modified flavour profile method which uses a numerical scale, where 0 represents none and 15 extremely strong, with 0.5 increments, was used.[17,18] The testing room was at 21 ± 1°C and 55 ± 5% RH; the illumination was a combination of natural and non-natural (fluorescent) light.

**Data Analyses**

Partial least squares regression (PLSR) map was conducted using Unscrambler version 9.7 (Camo Software, Oslo, Norway).

**Results and Discussion**

**Sensory Analysis**

Seventeen aroma attributes were found in the 13 commercial samples and the F juice (Table 2). F juice (sample 458) was characterized by having a high fruity aroma with berry, cranberry, fruity dark and floral notes. In addition, some musty/earthy notes and a moderate overall sweetness were detected. DE juices had some differences and were characterized by: fruity, cranberry, grape, musty/earthy and wine-like notes. In general, all these aromatic attributes were present in the AD juices, but not all of
them in the C juices. Cranberry and wine-like notes were absent in all the C juices, and new aromatic notes were detected by the panellists, e.g. fruity dark (samples 197, 488, 555 and 655), candy-like (sample 981), molasses (sample 197), vinegar (samples 225 and 655) and woody (sample 197). Samples 225 and 655 were the only ones with potassium sorbate and potassium benzoate, which might be the origin of the vinegar note.

The AD juices had all the same attributes present that were found in the F and DE juices, including the cranberry and wine-like notes. Because of the added flavourings in the AD samples, new aromatic notes (apple and cherry, sample 846), which were absent in the other juices, were detected by the panellists.

Instrumental Volatile Compounds

Eighty-three aromatic compounds were found in the pomegranate juice samples. Table 3 shows the presence or absence of each of the compounds, according to their chemical families. Alcohols, aldehydes, ketones, esters, furans, benzene derivatives and terpenes were the main aromatic groups but large differences were found, depending on the juice type.

In samples 225 and 655, high amounts of sorbic acid and benzoic acid were found, obviously from the potassium sorbate and potassium benzoate added as preservatives. The presence of these preservatives in high concentrations made it completely impossible to conduct proper instrumental analyses of these juices (40% of the chromatogram time scale was occupied by these two peaks, hiding the presence of other compounds). Therefore, the data presented in Table 4 for these samples is tentative only and the percentages over the total are not shown in Figure 1. Neither of samples 225 and 655 was studied in partial least square regression (PLS2), due to this lack of instrumental data.

As shown in Table 4, the total amounts of volatile compounds were different in the headspace of each sample. Using F juice as the reference, eight of the juices had lower amounts of volatile compounds than this juice and five had higher amounts, but these differences did not seem to be related to the juice type.

Sample 981 was noted for the high amount of total aromatic compounds in its headspace (83.6 mg/kg) when compared with the other samples. This sample was a C juice which could be consumed in the concentrated form or diluted with water as a juice (following the instructions of the label). Despite this high concentration of volatiles, when diluted in its juice form, the sample was characterized by having only four aromatic notes: candy-like, fruity, grape and sweet overall (Table 2). The candy-like attribute was exclusive for this sample, and the sweet overall note was much higher than in any other sample, possibly coming from the high concentration procedure to which the sample was subjected. As can be seen in Figure 1, sample 981 had a significant amount of ketones, represented mainly by β-ionone and a γ-decalactone. β-Ionone is a ketone typical in berries and its descriptors are related with these fruits, being a key odourant in raspberry aroma.[18,20] Regarding the γ-decalactone, it is known that because the aroma of lactones is pleasant, these substances are used for aromatization of food.[21] This may be the case in this sample, because of the higher amounts of the compound compared with the other juices (note that the juice was not indicated as ‘with flavourings added’ on the label of the product, so it was included in the C group during this study). The presence of higher amounts of esters in sample 981 when compared with the others seemed to confirm the presence of some additional flavourings. These compounds were not present in the F or C juices, but only in AD samples. Esters are important aromatic compounds for fruits, synthesized only by intact cells.
### Table 3. Aromatic volatile compounds found in the juice samples

<table>
<thead>
<tr>
<th>Code*</th>
<th>Compound</th>
<th>KI (Lit.)</th>
<th>KI (Exp.)</th>
<th>Fresh</th>
<th>Direct extract</th>
<th>From concentrate</th>
<th>From concentrate + added flavourings</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>458</td>
<td>943</td>
<td>279</td>
</tr>
<tr>
<td><strong>A1</strong></td>
<td>Ethanethiol</td>
<td>514</td>
<td>**</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>A2</strong></td>
<td>2-Methyl-3-buten-2-ol</td>
<td>582</td>
<td>**</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.12</td>
</tr>
<tr>
<td><strong>A3</strong></td>
<td>1-Pentanol</td>
<td>765</td>
<td>747</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.01</td>
</tr>
<tr>
<td><strong>A4</strong></td>
<td>2,3-Butanediol</td>
<td>800 **</td>
<td>754</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.57</td>
</tr>
<tr>
<td><strong>A5</strong></td>
<td>2-Pentyn-1-ol</td>
<td>772 **</td>
<td>767</td>
<td>–</td>
<td>–</td>
<td>0.01</td>
<td>–</td>
</tr>
<tr>
<td><strong>A6</strong></td>
<td>3-Methyl-2-buten-1-ol</td>
<td>772</td>
<td>781</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.03</td>
</tr>
<tr>
<td><strong>A7</strong></td>
<td>Z-3-Hexen-1-ol</td>
<td>858</td>
<td>861</td>
<td>0.02</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>A8</strong></td>
<td>E-3-Hexen-1-ol</td>
<td>860</td>
<td>859</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>A9</strong></td>
<td>4-Methyl-1-pentanol</td>
<td>875**</td>
<td>851</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.33</td>
</tr>
<tr>
<td><strong>A10</strong></td>
<td>2-Heptanol</td>
<td>911</td>
<td>900</td>
<td>–</td>
<td>–</td>
<td>0.14</td>
<td>0.05</td>
</tr>
<tr>
<td><strong>A11</strong></td>
<td>1-Heptanol</td>
<td>970</td>
<td>971</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>A12</strong></td>
<td>1-Octen-3-ol</td>
<td>979</td>
<td>981</td>
<td>0.01</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>A13</strong></td>
<td>3-Octanol</td>
<td>992</td>
<td>998</td>
<td>0.02</td>
<td>0.03</td>
<td>0.03</td>
<td>–</td>
</tr>
<tr>
<td><strong>A14</strong></td>
<td>3-Ethyl-1-hexanol</td>
<td>1032</td>
<td>1031</td>
<td>–</td>
<td>0.06</td>
<td>0.02</td>
<td>0.07</td>
</tr>
<tr>
<td><strong>B15</strong></td>
<td>Hexanal</td>
<td>802</td>
<td>802</td>
<td>0.13</td>
<td>–</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td><strong>B16</strong></td>
<td>E-2-Hexenal</td>
<td>865</td>
<td>861</td>
<td>–</td>
<td>–</td>
<td>0.04</td>
<td>–</td>
</tr>
<tr>
<td><strong>B17</strong></td>
<td>Heptanal</td>
<td>896</td>
<td>904</td>
<td>0.01</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>B18</strong></td>
<td>Octanal</td>
<td>1001</td>
<td>1007</td>
<td>0.04</td>
<td>0.01</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>B19</strong></td>
<td>Nonanal</td>
<td>1102</td>
<td>1111</td>
<td>0.38</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

**Ketones**

| **B20** | 3-Hexen-2-one | 760 | – | – | – | – | – | – | – | – | – | – | 0.01 | – | – | – | – |
| **B21** | 4-Methyl-3-penten-2-one | 800 | 799 | – | – | – | – | – | – | – | 0.93 | – | – | – | – | – | – |
| **B22** | 4-Hydroxy-4-methyl-2-pentanone | 840 | 847 | – | – | – | 0.21 | – | – | – | – | – | – | – | – | – | – |
| **B23** | 6-Methyl-5-hepten-2-one | 986 | 987 | 0.01 | – | – | – | – | – | – | – | – | – | – | – | – | – |
| **B24** | 3-Octanone | 990 | 988 | 0.01 | – | – | – | – | – | – | – | – | 0.01 | – | – | – | 0.04 |
| **B25** | α-Sinophorone | 1122 ** | 1142 | – | – | – | – | – | – | – | – | – | – | 0.02 | – | – | – |
| **B26** | β-Damascenone | 1375 ** | 1402 | 0.09 | 0.11 | 0.05 | – | – | – | – | – | – | – | 0.14 | – | 0.15 |
| **B27** | β-Ionone | 1425 | 1501 | – | – | – | – | – | – | – | – | – | – | – | 0.59 | – | – |
| **B28** | γ-Undecalactone | 1547 ** | 1588 | 0.15 | – | 41.7 | 0.02 | 1.82 | – | – | – | – | – | – | – | – | – |

**Acids**

| **B29** | Acetic acid | 602 | ** | – | – | – | 0.06 | 0.10 | 0.10 | 0.02 | 0.29 | – | – | – | – | – | 0.29 |
| **B30** | 2-Methyl butanoic acid | 867 ** | 844 | – | – | – | 0.22 | 0.21 | – | – | – | 0.06 | – | – | – | – |

**Esters**

| **B31** | Ethyl acetate | 610 | ** | – | – | – | – | 1.98 | – | – | – | – | – | – | – | – | – |
| **B32** | Butanoic acid ethyl ester | 798 | 802 | – | – | – | – | – | 0.01 | – | – | – | – | – | 0.08 | – | 0.02 |
| **B33** | Acetic acid butyl ester | 816 | 817 | – | – | 0.01 | – | – | – | – | – | – | – | – | – | – | 0.16 |
| **B34** | 2-Methyl butanoic acid ethyl ester | 849 | 853 | – | – | 0.11 | – | 0.52 | – | – | – | – | 0.26 | 0.27 | 0.05 | 0.11 | – |
| **B35** | 3-Methyl-1-butanol acetate | 878 | 879 | – | – | – | – | 1.65 | – | – | – | – | – | 0.02 | – | – | 0.06 |
| **B36** | Hexanoic acid ethyl ester | 999 | 997 | – | – | – | – | 0.06 | – | – | – | – | – | – | – | – | – |
| **B37** | 3-Hexen-1-ol acetate | 1011 | 1004 | – | – | – | – | – | 0.11 | – | – | – | – | – | 0.20 | – | – |
| **B38** | Acetic acid hexyl ester | 1015 | 1011 | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| **B39** | Z-nerol acetate | 1366 | 1368 | – | – | – | – | – | – | – | – | – | – | – | – | – | – |
| **B40** | Е-nerol acetate | 1381 | 1382 | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – |

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Table 3. Continued.

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<td>943</td>
<td>279</td>
<td>197</td>
</tr>
</tbody>
</table>

**Furans**

A41 Furfural 835 839 – 0.44 1.07 7.54 1.11 0.33 0.52 0.04 0.90 0.61 0.79 0.01 0.37 5.87
A42 2-Furanmethanol 857 858 – – 0.05 – – – – – – – – – – – –
A43 1-(2-Furanyl)-ethanone 911 915 – 0.04 0.03 0.51 0.07 0.03 0.03 – – 0.03 0.11 0.08 0.32
A44 2-Furaldehyde 957 968 – – 2.64 – – – – – – – – – – – –
A45 Furfyl ethyl ketone 1019 1015 – – 0.11 – – – – – – – – – – – –
A46 Furfuryl alcohol 1081 1082 – – – – – – – – – – – – – – – – – –
A47 5-Hydroxymethylfurfural 1241** 1214 – 0.05 – 3.89 – – – – – – 0.75

**Benzene derivatives**

A48 Benzaldehyde 936** 974 – 0.03 2.44 0.12 6.46 0.04 0.10 0.42 0.69 0.22 2.79 0.03 0.34 0.18
A49 Phenol 980 980 – 0.04 – – 0.20 – – – – – – – – – – – –
A50 Benzyl alcohol 1043 1046 – – – – 0.19 – – – – – – – – – –
A51 Eugenol 1348** 1376 – – – – – 0.11 – – 0.03 0.03 0.11 0.32
A52 Methyleugenol 1395 1407 – – – – 0.03 – – – – – – – – – –

**Terpenes**

A53 α-Pinene 939 944 0.03 – – – – – – – – – – – – – – – –
A54 β-Pinene 980 992 0.22 – – – – 1.49 0.03 0.14 – – – – – – – –
A55 3-Carene 1020 1022 – – – – – – 1.49 – – – – – – – –
A56 Eucalyptol 1031 1026 – – – – 0.05 – – – – – – – – – –
A57 4-Carene 1014 1030 – – – – 0.23 – – – – – – – – – –
A58 β-Cymene 1021 1037 – – – – 0.06 – – – – – – – – – –
A59 Z-Ocimene 1041 1039 – – – – – – 0.03 0.23 – – – – – – – –
A60 Limonene 1031 1043 0.34 – – – – – – – – 0.35 – – – – – –
A61 α-Phellandrene 1012** 1046 0.08 – – – – – – – – – – – – – –
A62 E-Ocimene 1052 1051 – – – – – – 0.56 – – – – – – – –
A63 γ-Terpinene 1066 1070 – – – – – – 0.25 – – – – – – – –
A64 Terpinolene 1088 1100 – – – – – – 1.32 0.04 – – – – – – – –
A65 Linalool 1098 1103 – – – – 0.08 – – – – – – – – – –
A66 β-Terpinol 1188** 1167 – – – – 0.61 0.04 – – – – – – – –
A67 4-Terpinol 1179** 1201 0.19 – – – – 0.20 – – – – – – – –
A68 β-Pinen-8-ol 1189 1201 – 0.15 – – – – – – – – – – – –
A69 α-Terpineol 1189 1207 0.32 0.03 0.49 0.37 4.46 0.33 0.09 – – 0.06 0.13 0.02 0.14 0.28
A70 Z-Geraniol 1228 1226 – – – – – – 0.50 – – – – – – – –
A71 Z-Carveol 1230 1234 – 0.12 – – – – – – – – – – – – – –
A72 Thymol 1290** 1245 – – – – – – 0.08 – – – – – – – –
A73 Bergamotene 1435** 1391 0.16 – – – – – – – – – – – – – –
A74 Copaene 1380** 1406 – – – – – – 0.22 – – – – – – – –
A75 2-No-pinene 1436 1430 0.16 – – – – – – – – – – – – – –
A76 α-Farnesene 1487** 1450 1.09 – – – – – – – – – – – – – –
A77 β-Caryophyllene 1418** 1454 0.74 – – – – 2.12 – – – – – – – –
A78 Cedrene ** 1466 0.13 – – – – – – – – – – – – – – – –
A79 Bisabolene 1522 1520 0.31 – – – – – – – – – – – – – –
A80 Valencene 1495** 1523 – – – – – – 0.53 – – – – – – – –
A81 γ-Muurolene 1480** 1538 – – – – – – 0.63 – – – – – – – –
A82 Sesquiphellandrene 1523 1537 0.10 – – – – – – – – – – – – – –
A83 2-Acetylpyrrole 1072 1071 – – – – 0.27 – – – – – – – –

* Code used to simplify Figures 2 and 3.
** Tentatively identified: only mass spectral data. Values are the mean of three replications.
during the β-oxidation of fatty acids or from amino acid metabolism. Generally, when the fruits are homogenized, the esters are rapidly hydrolysed by the hydrolase enzymes present, and the fruit aroma flattens. AD samples had esters in their volatile profile. These could be the compounds responsible for the apple, beet, cherry, floral and fruity notes.

Sample 846 (belonging to the AD group) had the highest fruity aromatic note, highlighted by the presence of more alcohols than the other juices. The main components in this sample were Z- and E-3-hexen-1-ol, present in the F juice and in other fruits such as berries. The high concentration of these alcohols in some samples compared with the other samples indicated that this might be one of the compounds in the added flavourings of AD samples.

Benzenederivatives were present in all the juices except the F juice. These compounds come from the degradation of lignin and phenolic acids and their aromatic notes are variable, depending on the compound being formed, usually either vanilla, woody, smoky or spicy. Benzaldehyde was the main compound from this family, being present in all the commercial juices (DE, C and AD). Almond, cherry and sweet are the descriptors for this compound, which is normally found in almonds and other nuts and is common in ‘artificial’ cherry flavours. Although this compound was absent in the F sample, the small amount of benzaldehyde in some commercial juices, and its presence in the C juices, indicated that this might not be an added flavouring or that small amounts of this compound might be enough to produce a heightened fruit flavour in the juices (its odour threshold in water is only 0.35 mg/l).

The two aromatic groups which seemed to represent a huge difference between commercial and F juice were terpenes and furans. Terpenes seemed to be the predominant group in the F juice, which had no furans. Commercial juices had furans, and terpenes were never the main group. Some terpenes with hydroxy groups are naturally present in fruit juice, at least in part as glycosides. These terpene glycosides hydrolyse, either enzymatically (β-glucosidase) or because of the low pH of the juices. The latter process is strongly accelerated by heat treatments, changing the terpene profile in the juices.

Furan compounds, which were present in the commercial samples and not in the F sample, are commonly associated with heated products and have been related previously with Maillard reactions and caramel-like aromas, coming from the toasting process in some nuts, such as almonds. The processing in the commercial juices implicates some pasteurization (e.g. samples 328 and 403) or other heating methodology to preserve the juice, so furan compound development is expected (mainly furfural). The presence of the molasses attribute in the sensory analysis of sample 197 (C) might be due to the presence of these compounds in its volatile composition. This attribute was not found in sample 403 (AD), which also was characterized by large amounts of furans and furfural, but the presence of added flavourings with low odour thresholds in the sample could hide this aromatic note in favour of the fruity or cranberry notes that highlighted in the juice.

### Relationship between Sensory and Instrumental Aromas

When taking into account the first two dimensions of the PLSR biplot (PLS1 and PLS2), 48% variation in the instrumental data explained only 37% of variation in the sensory data (Figure 2). Despite the low variation explained, different groups could
be differentiated in this figure, C juices on the one hand and F, DE and AD juices on the other hand. The presence of some compounds originated during the concentration stage of these samples might hide and/or modify some aromatic attributes expected in the pomegranate juices. In addition, some aromatic compounds could have been lost during the concentration step. Fruit juice concentrates are elaborated using evaporation, freezing or a process involving high-pressure filtration. Concentration by evaporation is the preferred industrial process, but this process leads to losses in aromatic compounds if it is not combined with an appropriate aroma recovery step. One example of this on C juice could be sample 982, in which the candy-like or overall sweet attribute was so intense that it hid the fruity and cranberry notes that the terpenes present in the sample should provide to the juice.

Although there was a low variation explained, some general tendencies seemed to appear in the PLS study (Figure 2): six of the seven furan compounds (A41–A47) seemed to be related to the woody, molasses and fruity-dark notes. These attributes are typical of processed foods. On the other side of the graph, terpenes (A53–A82) and esters (A31–A40) were associated with candy-like and sweet overall notes.

A second PLS regression was done to determine the differences among the F, DE and AD juices. The results for the first two dimensions of the PLSR biplot are shown in Figure 3. Once the concentrate juices were eliminated from the PLS study, 48% of variation in the instrumental data for the first two dimensions of the PLSR biplot (PLS1 and PLS2) explained 61% of the variation in the sensory data, and 33% of variation in the instrumental data in the second two dimensions of the PLSR biplot (PLS3 and PLS4) explained 27% of the variation in the sensory data (a total of 81% of variation in the instrumental data explained 88% of the variation in the sensory results).

While juice from fresh squeezed arils was characterized by having high fruity-dark, floral, fruity and sweet overall notes, commercial juices had more cranberry, wine-like and grape notes. Fresh-squeezed juice was characterized by the presence of aldehydes (A15, 17–19) and terpenes (A54, 56, 61, 65, 68, 75–79 and 82), while the commercial juices had a combination of compounds which included mainly alcohols (A1–14) and some esters and furans (A32–37, and A41, 44 and 47, respectively). No experiments were done to test the relationship between the identified compounds and the sensory attributes, but these tentative results seemed to show that aldehydes and terpenes contributed to the fruity, sweet overall and fruity dark notes of the F juice. Also, the combination of alcohols, esters and terpenes seemed to contribute to the grape and wine-like notes in the AD juices. With the aim of confirming these statistical results, a real quantification of the compounds may be done. Once the compounds have been quantified, sensory analysis would determine the corre-

**Figure 2.** PLS regression map showing the relationship between instrumental data correlated with sensory data in all the juices studied. Fresh-squeezed, F juice; direct extract, DE juices; from concentrate, C juices; Conc + aroma, AD juices. Sensory parameters were characterized as indicated in Table 2; instrumental data, aromas (A1–A83, codes indicated in Table 3).
sponding descriptors associated with each one of the compounds or groups of compounds (using a non-aromatic juice, with the same characteristics as the pomegranate juice, as a base to spike the compounds).

**Conclusions**

Up to 83 aromatic compounds were found in the 14 pomegranate juices. All juices had different instrumental and sensory aromatic profiles. The main differences in chemical composition between fresh-squeezed and commercial juices were the percentages of terpenes and furans. Fresh-squeezed juice was mainly characterized by the presence of terpenes and aldehydes, while furans were important contributors in the commercial juice aromas. Different processing methodologies to manufacture the juice can change the aromatic profile of the fresh juice, particularly in juices from concentrate, as shown in the PLS study. Seventeen different sensory attributes were found in these pomegranate juices, including fruity, floral or musty notes. Each one of the samples was characterized by the presence of only some of the attributes (three to nine different aromatic notes, depending of the sample). Juice from fresh-squeezed arils was characterized by having more, floral, fruity and sweet OV notes, compared with commercial juices from direct extract and with added flavourings, which had more cranberry, wine-like and grape notes. Juices from concentrate were highlighted by fruity dark notes and the presence (in some samples) of other notes typical in processed foods (e.g. molasses, candy-like). Methodologies to improve pomegranate juice extraction or preservation, or even artificial aromas of pomegranate, should be developed with the aim of creating higher quality products which can increase the consumption of pomegranate juice and allow consumers to take advantage of its health-promoting properties.

**References**


**Figure 3.** PLS regression map showing the relationship between instrumental data correlated with sensory data in fresh squeezed juice, juices from direct extract and juices from concentrate with added flavourings. Fresh-squeezed, F juice; direct extract, DE juices; Conc + aroma, AD juices. Sensory parameters were characterized as indicated in Table 2; instrumental data, aromas (A1–A83, codes indicated in Table 3)