

Concentrate apple juice industry: aroma and pomace valuation as food ingredients

Elisabete Coelho ^{1,*}, Mariana Pinto ¹, Rita Bastos ¹, Marco Cruz ¹, Cláudia Nunes ^{1,2}, Sílvia M. Rocha ¹ and Manuel A. Coimbra ¹

¹ LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.; ecoelho@ua.pt, a39045@ua.pt, ritabastos@ua.pt, mcruz@ua.pt, smrocha@ua.pt, mac@ua.pt

² CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, 3810-193, Portugal; claudianunes@ua.pt

* Correspondence: ecoelho@ua.pt; Tel.: +351 234 370706 (E.C.)

Supplementary Material:

Table S1. GC peak area of apple hydrodistillate obtained from the wet apple pomace and apple aroma resultant from the industrial juice processing, analysed by HS-SPME/GC-MS, and divided in positive and negative aroma and chemical families, according to the heatmap of **Figure 4**.

<i>Compound</i>	<i>Chromatographic peak area (10⁻⁷)</i>			
	<i>Apple pomace hydrodistillate (n=3)</i>	<i>Standard Deviation</i>	<i>Apple aroma (n=3)</i>	<i>Standard Deviation</i>
Positive aroma				
Alcohols				
Butanol	0.3	0.1	10.0	1.8
1-Hexanol	13.2	4.5	176.1	12.1
<i>Trans</i> -2-hexenol	0.0	0.0	25.6	1.0
6-methyl-5-hepten-2-ol	0.2	0.4	0.0	0.0
Aldehydes				
Acetaldehyde	0.1	0.2	1.6	0.2
Hexanal	4.5	4.0	41.6	3.8
Heptanal	0.4	0.6	0.0	0.0
<i>Trans</i> -2-hexenal	0.9	0.9	82.7	4.6
Octanal	0.3	0.5	0.0	0.0
<i>Trans</i> -2-heptenal	2.4	1.7	0.0	0.0
Nonanal	2.1	2.8	0.0	0.0
Benzaldehyde	41.0	15.8	2.2	0.4
Esters				
Methyl Acetate	1.7	1.1	0.0	0.0
Ethyl Acetate	5.5	3.2	32.3	2.9
Ethyl propionate	0.0	0.0	3.4	0.5
Propyl acetate	0.0	0.0	3.2	0.5
Methyl butanoate	0.0	0.0	1.3	0.0
Ethyl butanoate	0.1	0.1	36.3	2.6
Ethyl-2-methyl-butanoate	0.1	0.1	47.2	5.1
Butyl Acetate	0.3	0.1	127.0	10.1
Isoamyl Acetate	0.3	0.1	0.0	0.0
2-Methylbutyl acetate	0.0	0.0	88.4	7.4
Butyl propionate	0.0	0.0	5.2	1.3
Pentyl acetate	0.0	0.0	5.1	0.8
Methyl Hexanoate	0.1	0.2	0.0	0.0
Butyl 2-methylbutanoate	0.5	0.3	13.0	0.9
Ethyl Hexanoate	0.6	0.2	11.2	1.1
Hexyl Acetate	3.8	1.0	177.6	8.0
<i>Trans</i> -2-hexenyl acetate	0.0	0.0	10.3	0.5
Butyl Hexanoate	1.2	0.9	25.6	1.0
Hexyl butanoate	1.6	1.4	25.6	1.0
Hexyl (Iso)butanoate	3.1	1.4	0.0	0.0
Hexyl 2-methylbutanoate	2.6	2.3	12.3	1.4

Ethyl octanoate	0.3	0.4	0.0	0.0
Hexyl 2-butenate	1.4	1.2	0.0	0.0
Hexyl hexanoate	2.6	0.7	0.0	0.0
Ethyl Benzoate	0.4	0.4	0.0	0.0
Hexyl octanoate	0.0	0.0	0.0	0.0
Ethylphenylacetate	0.3	0.3	0.0	0.0
Methyl (E,Z)-2,4-decadienoate	0.5	0.5	0.0	0.0
2-Phenylethyl acetate	0.4	0.3	0.0	0.0
Ethyl (E,Z)-2,4-decadienoate	0.9	0.7	0.0	0.0
Ethyl benzoate	0.0	0.0	0.1	0.0
Butyl benzoate	0.7	0.6	0.0	0.0
Benzyl acetate	0.0	0.0	0.2	0.0
2-Phenylethyl acetate	0.0	0.0	0.1	0.0
Butyl Phenylacetate	0.2	0.2	0.0	0.0
Hexyl benzoate	0.3	0.2	0.0	0.0
Ketone				
6-Methyl-5-hepten-2-one	19.3	10.2	0.0	0.0
Phenols				
Estragole	15.2	1.9	6.2	0.3
<i>Trans</i> -anetole	0.5	0.8	0.3	0.1
Methyl Eugenol	0.8	0.7	0.0	0.0
Norisoprenoids				
β -Ionone	0.6	0.5	0.0	0.0
(E,Z)-Pseudoionone	1.2	0.1	0.0	0.0
(E,E)-Pseudoionone	0.4	0.6	0.0	0.0
Geranyl acetone	2.1	1.3	0.2	0.4
Linalool	0.7	1.3	0.0	0.0
Geranial	1.3	1.1	0.0	0.0
α -Bergamotene	0.2	0.4	0.0	0.0
(E,E)- α -Farnesene	10.8	16.4	0.0	0.0
<i>E</i> -Geraniol	0.4	0.7	0.0	0.0
(<i>E</i>)-Nerolidol	0.7	0.1	0.0	0.0
Farnesol isomer 1	0.2	0.2	0.0	0.0
(<i>E,E</i>)-Farnesal	0.1	0.1	0.0	0.0
(<i>E</i>)-Farnesene	0.1	0.1	0.0	0.0
Farnesol isomer 2	6.9	8.0	0.0	0.0
Negative aroma				
Acids				
Acetic acid	0.1	0.1	0.0	0.0
Octanoic acid	0.8	0.7	0.0	0.0
Nonanoic acid	0.4	0.3	0.3	0.3
Decanoic acid	0.5	0.4	0.0	0.0
Alcohols				
Ethanol	1.5	0.8	7.4	0.7
Isoamyl Alcohol	0.3	0.4	0.0	0.0
2-Metilbutanol	0.0	0.0	7.0	0.5
Pentanol	0.1	0.1	0.0	0.0
1-Octen-3-ol	0.3	0.3	0.0	0.0

1-Octanol	3.6	1.0	1.8	0.3
nonanol	0.0	0.0	0.4	0.1
1-Decanol	0.5	0.4	0.0	0.0
Aldehydes				
(<i>E,E</i>)-2,4-Heptadienal	0.9	0.9	0.0	0.0
2-Nonenal	1.8	1.6	0.0	0.0
<i>E</i> -2-Decenal	2.5	0.7	0.0	0.0
(<i>E,E</i>)-2,4-nonadienal	0.4	0.7	0.0	0.0
(<i>E,Z</i>)-2,4-Decadienal	11.7	1.2	0.0	0.0
2,3-Dimethylbenzaldehyde	0.3	0.5	0.0	0.0
(<i>E,E</i>)-2,4-Decadienal	14.4	3.7	0.0	0.0
Ketones				
3-Octanone	0.0	0.0	0.0	0.0
1-Octen-3-one	0.2	0.3	0.0	0.0
