Effect of Beverage Modification with Molecularly Imprinted Polymers (MIPs), Carbon Granules and an Adsorbent Resin on the Organoleptic Properties of Apple, Orange and Cranberry Juice

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Abstract

Aroma and flavour volatile compounds contribute significantly to overall consumer acceptability in many food-related products. Molecularly imprinted polymers (MIPs) have been known to absorb specific volatile odour compounds (VOCs) from alcoholic beverages like red wines but minimal studies have been done to establish how MIPs could modify the overall organoleptic properties (especially the taste) of other beverages. In the present work, apple, orange and cranberry juices were subjected to various treatments with polymers SV7, GV1, CV6, resin Purosorb PAD 600 and activated carbon granules. From, gas chromatography mass spectroscopy (GCMS) analysis a significant decrease in VOCs in all cases was prevalent but was dependent on the contact time (dose and flow rate) between MIPs and the beverage. All samples treated with carbon granules were excluded from further sensory analysis as participants detected a highly unpleasant ashy aftertaste and prominent egg-like odour after informal sensory evaluation. The prominence of these attributes therefore would have hindered this investigation.

Formal sensory analysis of the six selected MIPs and resin treated juices by untrained individuals resulted in differences of each sample based on mainly the colour, aroma and flavour in both apple and cranberry juice. Although, participants ratings were similar, the molecularly imprinted polymers SV7 and GV1 maintained more sensory attributes than the resin Purosorb PAD 600. This is reflected in the hedonic ratings of colour in apple juice with GV1 producing a scoring of 6.4 ± 1.7 verses 4.3 ± 1.9 whilst the aroma intensity values in cranberry juice via treatment with SV7 was rated 5.6 ± 2.3 verses 3.5 ± 2.3. Molecularly imprinted polymer CV6 also performed better than the commercial resin, but, lower contact times are needed in order for participants to have a more holistic sensory experience. Panellists could not discern any significant differences in all six orange juice samples, however, overall trends within the sensory data generated showed that polymer SV7 had a comparatively higher number of beneficial volatiles that were retained. The positive reception that the polymers SV7 and GV1 were able to achieve indicates that there is more scope for modification within the industry utilising these MIPs.

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Abbreviations

MIP, molecularly imprinted polymer; MIPs, molecularly imprinted polymers; GCMS, gas chromatography-mass spectroscopy; SPME, solid phase microextraction; GC, gas chromatography; UV, ultra violet; CAGR, compound growth rate; MAA, methacrylic acid; EGDMA, ethylene glycol dimethacrylate; DVB, divinylbenzene; TRIM, trimethylolpropane trimethacrylate; AIBN, azobisisobutyronitrile; TiO_2, titanium dioxide; SiO_2, silicon dioxide; Fe_3O_4, iron (II, III) oxide; C6, six carbon atoms; H-bond, hydrogen bond; 4VP, 4-vinylphenol; 4VG, 4-vinylguaiacol; 4EP, 4-ethylphenol; 4EG, 4-ethylguaiacol; NIP, non-imprinted polymer; HS-SPME, headspace-solid phase microextraction; GC-MS/MS, gas chromatography tandem mass spectroscopy; MSD, mass selective detector; POF+, positive off-flavour positive; EI^+, electron impact positive ion; RO, reverse osmosis; HCAs, hydroxycinnamic acids; CAR, carboxen; DOP, dioctyl phthalate; BPA, bisphenol A; GA, gallic acid; LDPE, low density polyethylene, PC; polycarbonate; PET, polyethylene terephthalate; FC, from concentrate; NFC, not from concentrate; OAC, odour active compounds; GC-O, gas chromatography-olfactory; OAV, odour activity value; OAVs, odour activity values; VOCs, volatile odour compounds; VOC, volatile odour compound; °Brix, degrees Brix; PTFE, polytetrafluoroethylene; PDMS, poly(dimethylsiloxane); DI, deficit irrigation; PC1, principal component 1; PC2 principal component 2; PCA; principal component analysis; AHC; agglomerative hierarchical clustering.

1. Introduction

Aroma and taste are considered to be the two major factors that influence the flavour of a food or beverage. The subsequent analysis of flavour has attracted the interest of many researchers as volatile flavour compounds in food contribute significantly to overall consumer acceptance. In many ways, differentiating the sensory attributes and perception of a product gives food manufacturers a greater advantage within a given market (Clark, 1998). Juice is attributed as being one of the most popular beverages with orange and apple juice accounting for 29.1% and 27.1%, respectively, of the global demand (Priyadarshini & Priyadarshini, 2018). The complex flavours that various juice products exhibit is due to a wide range of compounds including unsaturated and saturated aldehydes, ketones, alcohols, lactones, terpenoids, organic acids, and esters that indicate the fruity flavours often perceived in the beverage (El Hadi et al., 2013). The overall proportions of volatile constituents are dependent on the type of fruit, cultivar and abiotic and biotic stresses (e.g. orchard management, nutrients in soil, climate and pruning) placed on them during their growth and commercialised practices that manufacturers use to create the final beverage (Pan et al., 2023).

The emergence of molecularly imprinted polymers (MIPs) in the last decade has shown an alternative method of both removing and extracting volatiles that are positive and negative within a product. MIPs are bio-inspired synthetic materials that can selectively reduce or remove organic compounds via a templating strategy (Villa et al., 2021). These polymers are therefore used in a variety of applications from chromatography, solid-phase extraction, and chemical sensors, due to the low cost, easy preparation, chemical stability, predictable specific recognition, and reusability of the polymer (Filipe-Ribeiro et al., 2020). To the best of our knowledge, MIPs have shown to be successful in removing unwanted off-flavours and extracting desirable volatiles for various food-related applications (Anene et al., 2016; Du et al., 2016; Chen & Huang, 2017) but not many published articles have drawn comparisons with the overall effect of MIPs on the sensory profile of beverages. Only two works described in literature have reported significant improvements to the sensory attributes in red wine after the removal of *Dekkera/Brettanomyces* yeasts with MIP treated samples being preferred by panellists compared to that of the non-treated wine (Filipe-Ribeiro et al., 2020; Teixeria et al., 2015). No research has been conducted in relation to how MIPs interact with existing beverages on the market that have desirable characteristics and whether the MIPs would modify the volatile components in a positive way.

In the present work, five absorbent materials, including three MIPs, one resin and carbon granules, were tested to determine their ability to remove volatile compounds from a range of beverages

(apple, orange and cranberry juice) and sensory impact explored. Various treatment protocols were utilised to evaluate the effectiveness of each MIP. Gas chromatography mass spectrometry (GCMS) in conjunction with solid phase microextraction (SPME) was used initially to determine the most significant treatment before sensory analysis was conducted with panellists. This methodology will assess whether the MIP process improves or obstructs the overall organoleptic properties of various fruit beverages currently on the market.

The following research objectives are:

- To determine whether the molecularly imprinted polymers SV7, GV1 and CV6 are more viable for beverage modification compared with other commercial adsorption products currently on the global market.
- To analyse the prospective volatile compounds generated by GCMS and SPME in the original apple, orange and cranberry juice samples compared with the treated ones in order to evaluate the peak area differences.
- From completed statistical analysis, screen selected treated juice samples for formal sensory evaluation to determine consumer acceptability and find any trends within the data.

2. Literature Review

2.1 General Overview of Molecularly Imprinted Polymers (MIPs)

Molecularly imprinted polymers are bio-inspired synthetic materials that are effective in the selective reduction and removal of organic compounds (Villa et al., 2021). As shown in **Figure 1**, the production of MIPs involves the copolymerisation of a functional and monomer and a crosslinker around the template molecule (Bahrani et al., 2021). These crosslinking and functional monomers are essential in providing stability of the bonding sites and polymer network maintaining its strong mechanical properties and porous structure (Villa et al., 2021; Bahrani et al., 2021). Once the MIP structure is formed, the template molecule is removed, leaving behind a highly crosslinked polymer that has a complementary cavity – or rather, the imprinted material (Villa et al., 2021; Sooraj et al., 2021). The cavity itself has a shape, size and spatial arrangement similar to the template molecule utilised during polymerisation, allowing for versatility when the imprinted material rebinds a similar molecule (Bahrani et al., 2021).

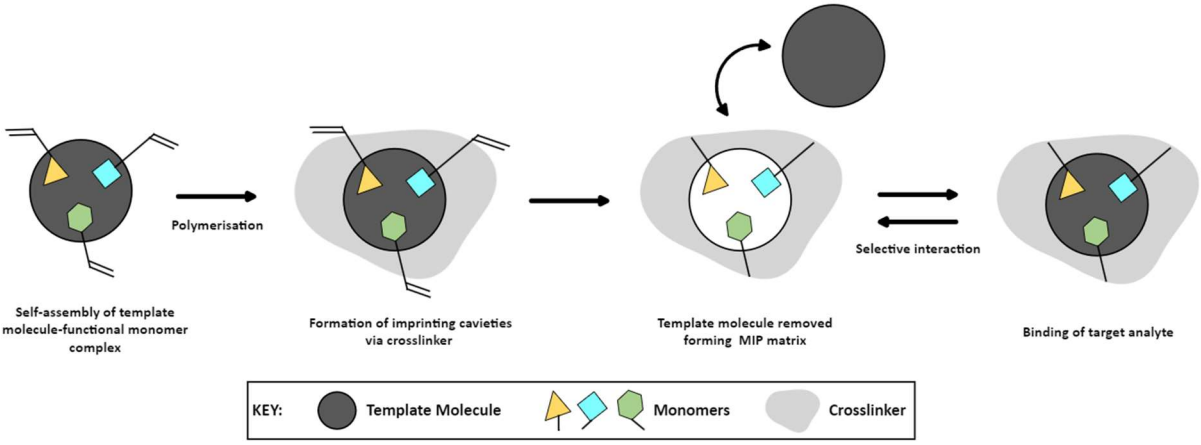


Figure 1. *Schematic for the general manufacture of MIPs adapted from Vasapollo et al. (2011).*[1]

MIPs in general have several advantages whereby they can be synthesised utilising various chemical and biological templates (Sooraj et al., 2021). Due to the high degree of crosslinking, MIPs can have a high chemical, mechanical and thermal resistance – which in turn allows for the polymer to be stable in acidic, alkaline and organic solvent environments depending on the types of monomers utilised (Sooraj et al., 2021). The polymers themselves are easily manufactured, low in cost and can be stored in high or low temperature conditions making them suitable in everyday applications like drug delivery (Filipe-Ribeiro et al., 2020). In addition to this, the structural integrity expressed within the polymers allows for their selectivity and capacity to remain consistent for a long period of time (Sooraj et al.,

2021). The versatility of the manufacturing of the MIPs showcases that there are many iterations possible. Therefore, selecting the appropriate combination of main components (functional monomers, solvents, initiators, etc.), enables the MIP to perform efficiently for the target application.

2.1.1 Template (Target) Molecules

The template (target) molecule is crucial in the development of the molecularly imprinted polymer as it has a large influence on the organisation of the functional groups via the placement of the functional monomers (Vasapollo et al., 2011). This in turn, forms coherent and specific binding sites within the molecule (Sooraj et al., 2021). Essentially, the template molecule must have non-reactive (have chemical inertness) within the chosen polymerisation conditions (Cormack & Elorza, 2004). Which exact functional groups (e.g. thiol groups or hydroquinone moieties) are non-compatible will depend on the application the MIP is needed in as the wrong choice could retard or inhibit the polymerisation kinetics (Sooraj et al., 2021). The use of moderately elevated temperatures (around 60 °C) or UV irradiation must also be taken into consideration as the template molecule will need to remain stable throughout the entire procedure (Bahrani et al., 2021). In addition, solubility of the template (and monomers) should be considered to avoid errors caused by the gradual exit of the template molecule (i.e. choosing wash solvents that will be able to remove the molecule cleanly) are pivotal to the overall performance and application of the imprinted polymer (Bahrani et al., 2021). Therefore, for the various reasons stated above, not all target molecules are compatible for all templating purposes. Commonly, small-sized organic molecules such as sugars, peptides, and nucleotide bases are utilised in molecular imprinting due to their rigid nature which allows for lesser movement and flexibility. Some examples of target molecules used include Bisphenol A, D-Fructose, aspirin, and alanine (Sooraj et al., 2021).

2.1.2 Functional Monomers and Crosslinkers

Functional monomers are essential in providing the high selectivity needed for the polymer. In general, the choice of monomer(s) heavily dictates the functionality of the template molecule with linkage sites (cavities) and interactions providing the foundation for the whole process (Sooraj et al., 2021). Consideration must be taken in terms of monomer reactivity ratios and functionality (e.g., H-bond donor with H-bond acceptor) in order to maximise the polymer matrix's effectiveness and stability (Cormack & Elorza, 2004). Hence, the imprinted polymer matrix must allow for reversibility whereby the functional monomer selected should reversibly bind with the template molecule. The functional monomers themselves can carry basic (vinylpyridine) or acidic (methacrylic acid) groups, or

be hydrophobic in nature (e.g., styrene) – many are able to demonstrate hydrogen bonding (acrylamide). Methacrylic acid (MAA) especially has been widely used in molecular imprinting as this monomer has the ability to act as both a hydrogen bond donor and acceptor (Vasapollo et al., 2011). In most instances, acrylic or vinyl groups as well as noncovalent interactions are utilised more often under free radical polymerisation due to the more successful formation and assembly of the template-monomer complex (Bahrani et al., 2021). A multitude of functional monomers can be commercially manufactured with chemically diverse structures and polarities, with the potential to develop many more by rational design (Cormack & Elorza, 2004). **Figure 2** illustrates some of the more common functional monomers utilised in the non-covalent approach.

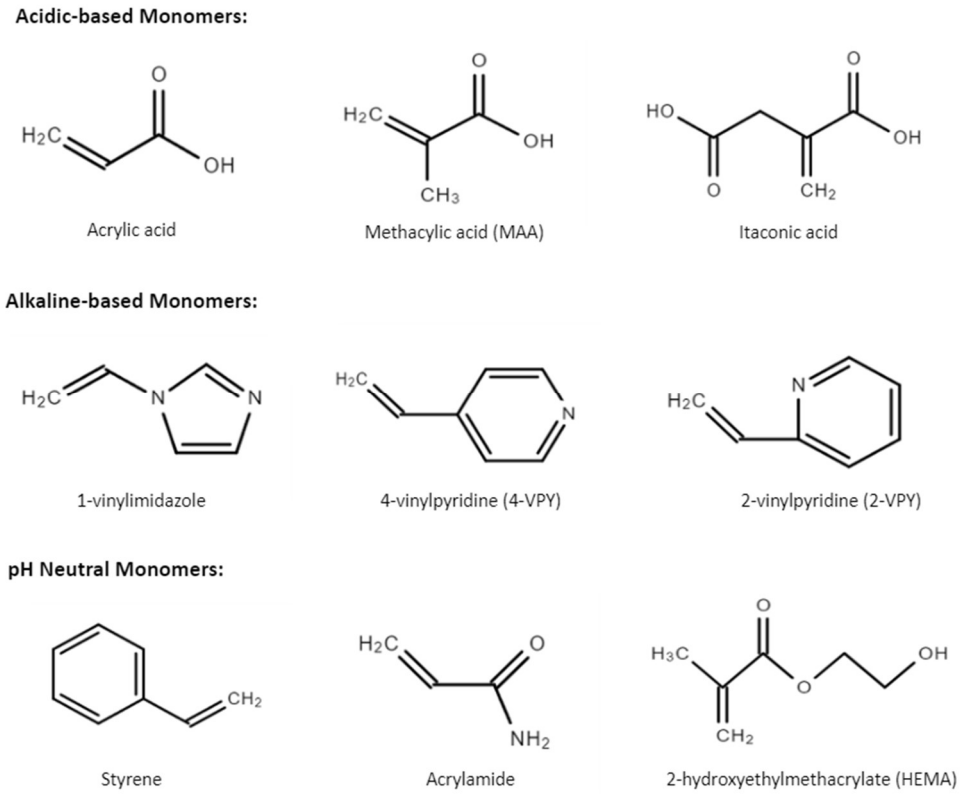


Figure 2. *Common monomers used in the non-covalent approach during molecular imprinting adapted from Vasapollo et al. (2011).*[1]

Another key component in the MIP recipe is the crosslinker which provides the means of a rigid polymer structure around the template molecule which will preserve the MIP's integrity after the template is removed (Sooraj et. al., 2021). Due to their multi-functional capabilities (i.e., having monomers bearing two or more polymerizable vinyl groups and being either soluble or insoluble in nature) these crosslinkers allow for a high amount of non-linear polymer architectures to be produced (Cormack & Elorza, 2004). In general, the crosslinker plays three main roles: it dictates the polymer

morphology, guarantees the stability and shape of the cavities, and provides the mechanical stability of the polymer (Sooraj et al., 2021). **Figure 3** shows some of the most common crosslinkers utilised to manufacture MIPs.

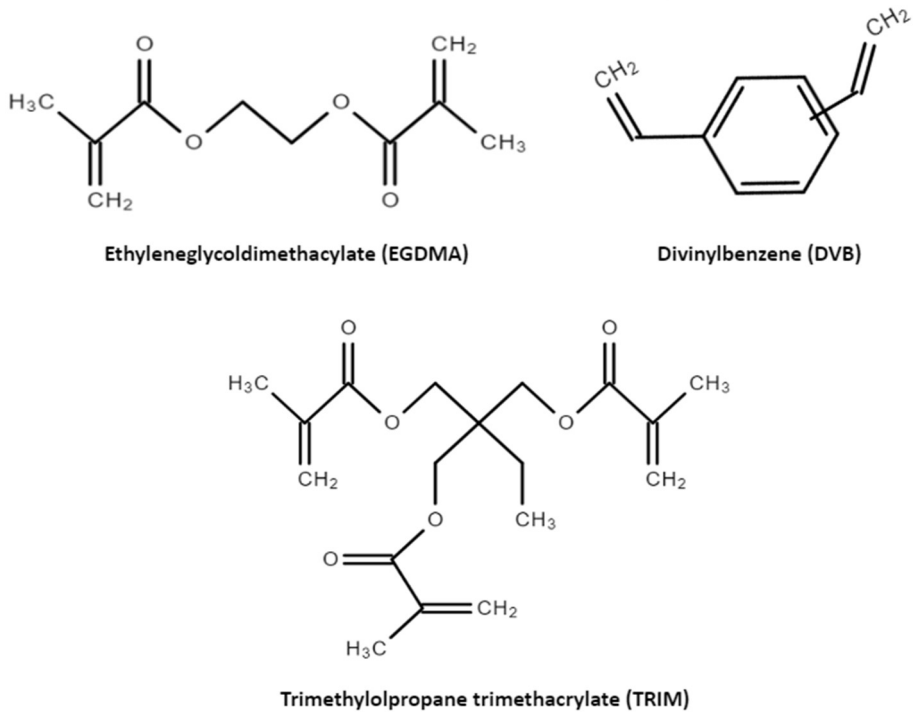


Figure 3. *Skeletal structures of the most common crosslinkers used in molecular imprinting adapted from Vasapollo et al. (2011).*[1]

Highly crosslinked polymers that are non-linear in nature are generally favoured in molecular imprinting as they create permanently porous (microporous) materials with sufficient mechanical stability (Bahrani et al., 2021; Cormack & Elorza, 2004). Too high of a crosslinker ratio will reduce the number of recognition sites whilst too low of a ratio will decrease mechanical stability (Sooraj et al., 2021). Most notably, ethylene glycol dimethacrylate (EGDMA), divinylbenzene (DVB) and trimethylolpropane trimethacrylate (TRIM) are some of the more commonly employed crosslinkers. Yoshimatsu et al. (2007) demonstrated that when trimethylolpropane trimethacrylate (TRIM) acts as the predominant crosslinker during polymerisation the MIP nanoparticles formed were uniform and had a 90% yield compared to 30-40% in DVB. Therefore, depending on the MIP requirements, the crosslinker utilised can vary based on what type of application the imprinting polymer is used for and what functional monomers, solvents and polymerisation techniques are applied.

2.1.3 Types of Monomer-Template Interactions

Good interactions between the template molecule and functional monomer are critical for the MIP to perform correctly. These are obtained by covalent, noncovalent or semi-covalent bonding to form the template-monomer complex. Without these interactions the resulting template molecule would have low affinity to the monomers, fail to create potential recognition sites and would cease to function as intended (Sooraj et al., 2021; Vasapollo et al., 2011). Important characteristics associated with the different types of molecular interactions are presented in **Table 1**.

Table 1. *Brief description of the three main molecular imprinting interactions used in MIP manufacture and their subsequent advantages and disadvantages.*

Type of Interaction	Description of Bond	Advantages	Disadvantages
Covalent	Also known as the preorganised method, in this approach reversible covalent bonds are formed between the template molecule and a functional monomer. After polymerisation, the template is removed (by a chemical reaction). These polymers use reversible covalent bonds such as boronate esters, imines and ketals/acetals groups. In use, the polymer binds the target molecule by forming covalent bonds, and before reuse the bound molecules must be eluted chemically (Sooraj et al. 2021, 2021; Yemiş et al., 2013).	• Stoichiometrically controlled reaction (Bahrani et al., 2021). • Does not require an excess number of functional monomers (Sooraj et al., 2021). • Imprinting cavities are more homogenous and uniform (Yemiş et al., 2013). • Reduction of non-specific interactions between the target molecule and the polymer (Bahrani et al., 2021).	• Has limited template-molecule options (Vasapollo et al., 2011). • Bound molecules are dependent on the number of active sites able to from covalent bonds with the target molecule (Bahrani et al., 2021). • Potential for slow kinetics when the template molecule is removed though this is dependent on the type of MIP manufactured (Sooraj et al., 2021). • Is not suitable for chromatographic or biosensor applications (Sooraj et al., 2021).
Non-covalent	Known as the self-assembly approach, this method is widely used in the preparation of MIPs. The bonds between the template molecule and functional monomer(s) are based on	• An easy method of chemically linking the template molecule and monomer (Sooraj et al., 2021).	• It has no specific stoichiometry as the bonds are known to create heterogenous imprinting cavities (Sooraj et al., 2021).

	hydrogen bonding, ion-pairing, and dipole-dipole interactions (Sooraj et al., 2021; Yemiş et al., 2013).	• Removal of the template is simple (Sooraj et al., 2021). • Numerous functional monomers can be used together (Yemiş et al., 2013). • Stable in hydrophobic environments (Bahrani et al., 2021). • Produces a wide range of affinity constants (Bahrani et al., 2021).	• Easily disrupted in polar environments (Yemiş et al., 2013). • A larger number of functional monomers is required (template-monomer molar ratio of 1:4 or above) in order to push the equilibrium forward (Vasapollo et al., 2011).
Semi-covalent	In this method, the template is covalently bound to afunctional monomer during MIP synthesis, and is then chemically removed (as in covalent method). However, during use, the MIP binds the target via noncovalent interactions like in the non-covalent case. In MIP synthesis, the monomer and template may be directly connected to each other or may be connected via a mediator group (Sooraj et al., 2021).	• High selectivity of imprint cavities from covalent bonding (Sooraj et al., 2021). • Increased speed of template-monomer binding from non-covalent bonding (Bahrani et al., 2021). • There is a wider range of polymerisation conditions (Sooraj et al., 2021). • Only needs a 1:1 or 1:2 template to monomer ratio for processing (Yemiş et al., 2013).	• Template hydrolysis is difficult unless a sacrificial spacer is utilised during MIP manufacture (Yemiş et al., 2013).

Note. Disadvantages for each interaction is dependent on the type of MIP manufactured.

2.1.4 Solvents (Porogen) and Initiators

Solvents are not only responsible for the dissolution of all the components (functional monomers, cross-linkers, template molecules, etc.), but are crucial to the formation of the microporous pores within the polymer structure. The use of thermodynamically good solvents is known to produce polymers with a well-developed pore structure and high specific surface area (Cormack & Elorza, 2004). In fact, the dual nature as both a solvent and pore forming agent gives an overall enhanced MIP interface – ideal for generating long chained polymers that have increased mass transfer, kinetics and permeability (Bahrani et al., 2021). In order to maximise the probability of template-to-functional

monomer complex formation, aprotic solvents such as toluene or chloroform are commonly employed as they stabilise hydrogen bonding via noncovalent interactions (Cormack & Elorza, 2004; Sooraj et al., 2021). However, if hydrophobic forces (covalent interactions) are in play, then protic solvents such as water or methanol are chosen (Vasapollo et al., 2011; Bahrani et al., 2021). The polarity, dielectric constants, and protonation of the solvent used in the reaction greatly impacts the final product formed (Bahrani et al., 2021). Therefore, it is essential that the correct solvent is chosen for the right application.

Initiators are the triggers that activate the reactive agents within the functional monomer to drive the polymerisation process (Bahrani et al., 2021). There are both advantages and disadvantages in selecting one initiator over another based on the technique used in MIP synthesis. In principle, the initial decomposition of the initiator generates free radicals which in turn lead to the polymerisation of the monomers and crosslinkers – the speed and condition in which this happens is contingent on chemical, thermal, photo and electrochemical initiation (Bahrani et al., 2021). For instance, if the template molecule was photochemically or thermally unstable, then an initiator that required photochemical or thermal activation would not be employed (Cormack & Elorza, 2004). Thermal and chemical initiators are generally utilised because they have a more varied temperature range than their counterparts' redox and photochemical initiators which operate at a lower temperature (Bahrani et al., 2021). **Figure 4** illustrates some of the main initiators used in MIP manufacture.

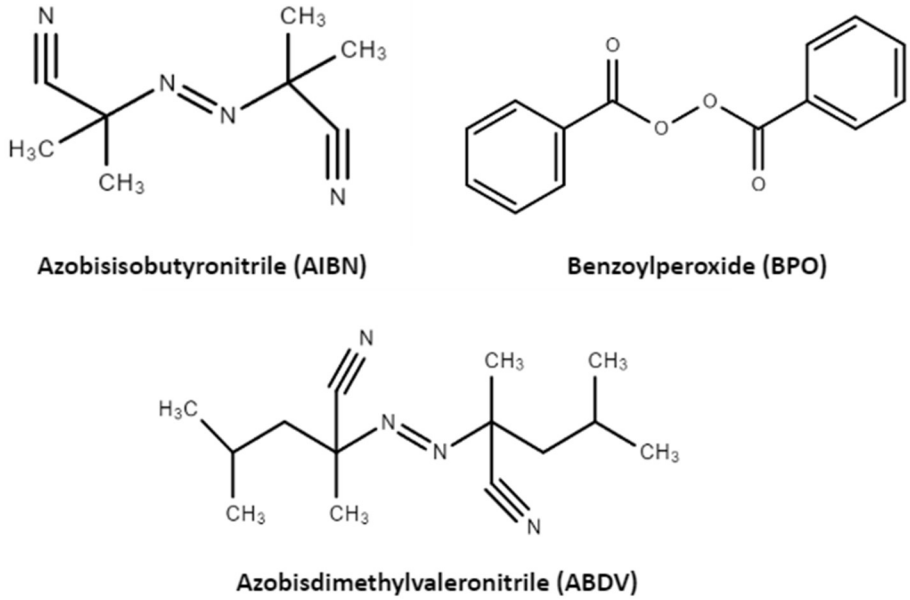


Figure 4. *Structures of the main initiators used in molecular imprinting preparation and synthesis adapted from Winsnuwardhani et al. (2022).*[2]

Due to their diverse chemical structures, many initiators can be used as free radical sources, with peroxide and azo (nitrile) compounds being highly favoured (Vasapollo et al., 2011). Azobisisobutyronitrile (AIBN) for instance, is highly utilised within molecular imprinting as degradation occurs rapidly by either ultraviolet or thermolysis at temperatures between 50 °C – 70 °C (Sooraj et al., 2021; Bahrani et al., 2021). From this degradation, carbon-based free radicals are formed, helping initiate the stable formation of vinyl monomers (Bahrani et al., 2021). It is important to identify the ideal initiator for MIP synthesis. Many factors like the concentration of the initiator (higher concentration increases polymerisation rate and lowers the average molecular weight of the product), temperatures, solubility and production of free radicals can play a part in the final product (Bahrani et al., 2021).

2.1.5 Different Techniques of Molecular Imprinting

When selecting the right approach for molecular imprinting, the end result (the MIP) should be taken into consideration as the different polymerisation techniques influence and control the overall morphology and physicochemical stability after synthesisation (Cormack & Elorza, 2004). As stated before, specific combinations of each variable/component (template molecules, functional monomers, etc.) within MIP synthesis can produce an entirely different MIP depending on what application it is being used for. **Table 2** briefly summaries these procedures and provides the advantages and disadvantages of each.

Table 2. *Brief description of the seven different polymerisation techniques utilised in MIP manufacture and their advantages and disadvantages.*

Type of Polymerisation	Description of Process	Advantages	Disadvantages
Bulk	Template molecules and functional monomers are dissolved in a solvent. Crosslinkers and initiators are then added into the mixture. Nitrogen gas is then flushed in displacing the oxygen. Polymerisation is initiated. Once complete, the bulk polymer is dried, then	• Easiest method of synthesising MIPs (Sooraj et al., 2021). • Has low laboratory requirements – less solvents (Bahrani et al., 2021). • Nice selectivity for the target molecules (Vasapollo et al., 2011).	• High damage to cavities and binding sites due to milling and sieving (Yemiş et al., 2013). • Time consuming with slow binding kinetics with feeble binding (Sooraj et al., 2021). • Low-rate mass transfer and high diffusion barrier (Yemiş et al., 2013).

	mechanically ground to create small particles (Sooraj et al., 2021).		• Requires more template analytes (Bahrani et al., 2021).
Precipitation	Polymeric chains are added and grown in a porogenic solution. Once the particles reach a certain critical mass, they precipitate out due to their low solubility in the solvent. Recovery of the particles is done by using perfluorocarbon which creates small spherical particles that are easy to control (Vasapollo et al., 2011).	• Does not require the use of surfactants (Vasapollo et al., 2011). • Uniform polymer size (Yemiş et al., 2013).	• Extended reaction time (Sooraj et al., 2021). • Large solvent volume and difficulty removing solvent from polymer (Bahrani et al., 2021).
Suspension	Funtional monomers, crosslinker and initiators are dissolved in an solvent. Suspension is formed by mixing the organic phase and the water phase (done by dissolving a surfactant - usually perfluorocarbon within water) since monomers and intiatiors are not soluble. The obtained microspheres are uniform in their size distribution (Yemiş et al., 2013).	• Purification is easier (Yemiş et al., 2013). • Initiator content is low as the polymers utilised are similar to solid resin (Sooraj et al., 2021).	• Weak recognition due to the disruption within the dispersing medium (Bahrani et al., 2021). • Wide range of particle sizes are produced if perfluorocarbon is used (Bahrani et al., 2021).
Emulsion	A process in which functional monomers and template molecules are dispersed by a water- or oil-soluble initiator and stabiliser in an aqueous solution. Emulsifiers are then added into the solution to create a more stable and hydrophilic MIP.	• Uniform particle size distribution (Sooraj et al., 2021). • One of the easiest approaches to create MIP beads (Bahrani et al., 2021).	• Has difficulty removing emulsifier from polymer as it needs more washes (Bahrani et al., 2021). • A low stability of the polymer (Moein et al., 2019).

	Polymerisation then occurs either under the presence of light or heat. Sub-micrometre particles are formed (Bahrani et al., 2021).		
Core-shell	Whereby MIP particles are fixed on the surface of nano-based materials such as TiO_2, chitosan, activated SiO_2, Fe_3O_4, gold nanoparticles, or quantum dot. These materials are used to support the cores for fabrication via surface imprinting. This gives the core part of the MIP added functionality (Sooraj et al., 2021).	• Easier extraction of template molecules (Sooraj et al., 2021). • Larger surface area and smaller particle size (Bahrani et al., 2021). • A higher binding capacity and faster adsorption kinetics (Bahrani et al., 2021).	• Not sensible as chemical sensors due to the incomplete removal of template molecules (Sooraj et al., 2021). • Very slow mass transfer (Sooraj et al., 2021).
Sol-gel	Whereby the cross-linked silica compounds (gels) are formed by creating a colloidal solution (sol) after both hydrolysation and condensation. The chemical reaction itself is irreversible after mixing a metal ion or alkoxide precursor and a water or alcohol solvent (Moein et al., 2019).	• Has higher chemical, mechanical, and thermal stability (Bahrani et al., 2021). • Utilises more eco-friendly solvents like toluene (Bahrani et al., 2021). • Fine powders that are uniform (Moein et al., 2019).	• Long processing time (Moein et al., 2019). • Large capillary stresses (swelling) can occur within the nanoparticles during the drying (Moein et al., 2019). • Known to have very low and non-specific binding capabilities (Moein et al., 2019).
Seed & Iniferter	This method is a derivative of emulsion polymerisation whereby seed-based particles are distributed through a solution. At this stage, swelling of the seed particles occurs. Two-way coagulation and growth then propel the process into a cationic secondary particle	• Can control the kinetic reaction if iniferter is used as an initiator (Ito et al., 2002). • Monodisperse in both shape and size (Bahrani et al., 2021). • Can be used for chromatographic	• Procedure is tedious and prolonged (Bahrani et al., 2021). • Has decreased selectivity (Bahrani et al., 2021). • Aqueous suspension can interfere with polymer synthesis (Ito et al., 2002).

	phase. The iniferter initiator is then used to terminate the growing polymer chains. Thus, allowing for a more controlled nanoparticle size distribution (Ito et al., 2002).	applications (Ito et al., 2002).	

2.2 Various Applications of MIPs in the Removal of Volatiles from Beverages

Molecularly imprinted polymers are known to be used in many applications such as chemical sensors and pharmaceuticals (Filipe-Ribeiro et al., 2020). However, within the beverage industry they have more often than not used to either remove or extract unwanted volatiles from the product or to extract key components such as folic acid. In this section, a number of literature articles have been summarised to determine the overall effect that MIPs have had on various commercial beverages within the global market.

2.2.1 *Dekkera bruxellensis* in Alcoholic Beverages

In the alcohol industry, the contaminating yeasts of the genus *Dekkera/Brettanomyces* (also known as *D. bruxellensis*), under the *Saccharomycetes* class, are responsible for the unwanted volatile phenols 4-vinylphenol (4VP), 4-vinylguaiacol (4VG), 4-ethylphenol (4EP), and 4-ethylguaiacol (4EG) reported in various alcoholic beverages (Lentz, 2018; Pizarro et al. 2009). Derived by the enzymatic decarboxylation of hydroxycinnamic acids (HCAs) to give ferulic and p-coumaric acid, these compounds contribute to the characteristic “Brett” off-flavour (Filipe-Ribeiro et al., 2020). Red wine for instance is highly susceptible to *Dekkera/Brettanomyces* contamination and reproduction due to their lower acidity and frequent storage in wood barrels for aging (Milheiro et al., 2019). If concentrations in red wine (up to 400 µg/L), are detected, then unpleasant aromas such as “leather,” “phenolic,” “horse stable,” and “spice” are often described (Teixeria et al., 2015). As stated previously, not many authors have elaborated on the overall effect of MIP treatment on the sensory profile of different beverages. Only two works described in literature have reported significant improvements to the sensory attributes in red wine when MIPs were incorporated – these articles are summarised below.

Filipe-Ribeiro et al. (2020) investigated the impact on red wine quality, after the removal of volatile phenols, 4-ethylphenol (4EP) and 4-ethylguaiacol (4EG), from an ethylene-based MIP and a non-

imprinted polymer (NIP). Sensory analysis on the colour and aroma of MIP treated wine resulted in a significant decrease of the phenolic attributes, increasing the overall fruity and floral flavours without impacting the colour of the wine. The treated wine exhibited the removal of up to 38 – 63% of wine volatile phenols based on the concentration of volatile phenols present in the alcoholic beverage. Overall, the sensory improvement with the MIP treated wine was significantly higher than the correspondent NIP tested. Authors Teixeria et al. (2015) also showed similar results reporting a significant reduction (40 – 56%) in volatile off-flavours in wine utilising two different MIPs. Treated samples MIP-4EP and MIP-4EG showed no loss of colour and were preferred by panellists with flavour values of 1.5 ± 0.55 and 1.66 ± 0.81, respectively compared to that of 2.83 ± 0.41 for NIP (values depicted here were based on a 1 to 4 scale, being 1 = less intense and 4 = more intense). Both articles concluded that the research conducted could open up good prospects for study possible in industrial applications of MIPs in other beverages affected by off-flavours.

To our knowledge, authors within literature have focused more on how volatile compounds could influence the organoleptic characteristics of alcoholic beverages like cider and beer than ways to extract the phenols associated with the 'Brett' off-flavour through MIPs (Pizzaro et al., 2009; Buron et al., 2012; Lentz, 2018). Within cider and ciders with residual sugars, the yeasts that develop are able to distort the rich flavour and texture of the alcoholic drink (Pizzaro et al., 2009). More specifically, *Dekkera/Brettanomyces* contributes to the degradation of esters that are responsible for the overall fruity aroma and flavour associated with the fermented fruit beverage (Guichard et al., 2017). Pizzaro et al. (2009) studied the impact of volatiles 4EP, 4EG, 4VP and 4EP on five different ciders (A, B, C, D and E) using HS-SPME coupled with GC-MS/MS. The results indicated that ciders B and D expressed a higher concentration of 4EP's (749 ± 11 µg/L and 983 ± 15 µg/L) and 4VP's (1125 ± 10 µg/L and 1241 ± 16 µg/L) than that of the commercial based ciders A, C and E (all with values below 183 µg/L). This was due to both cider samples coming from a press-house rather than being industrially manufactured. In another study done by Buron et al. (2012), eight trained panellists detected 4-EP off-flavours in two commercial based ciders with threshold values of around 1.5 – 2.0 mg/L after orthonasal and retronasal testing.

Beer is known to have a complex array of chemical compounds (upmost of around 1000 – 2000) that give a very distinctive aromas and flavours (Lentz, 2018). Whilst volatile phenols 4-EP, 4-VP, 4-EG and 4-VG do exhibit an undesirable off-flavour within some beer varieties they are still present within the beer in lesser amounts (1 – 5 mg/L) – though there are exceptions to this rule (Lentz, 2018). According to both Callemien & Collin (2009) and Olaniran (2017), a subsequent rise in popularity of specialty beers like Belgian white (made from unmalted wheat) and German Rauch and Weizen (made from

malted wheat) have seen a shift in the acceptance of 4-vinylguaiacol in the beverage. In fact, 4-vinylguaiacol is the main contributor to the distinctive clove-like and peppery-like flavour within these beers often having a threshold of around 20 – 50 mg/L (Callemien & Collin, 2009; Lentz, 2018). By means of brewing "positive off-flavour positive" (POF+) strains of *S. cerevisiae* (a class within *Saccharomycetes*) in the wort after mashing, ferulic acids (roughly 70 – 90%) are able to dominate the mixture ultimately producing 4-vinylguaiacol within the malt and hop of the beer (Lentz, 2008). Therefore, the phenols associated with the hop and malt severely effect the overall flavour, astringency, haze, body and fullness of the alcoholic beverage (Olaniran, 2017). With that being said, majority of the time the compounds produced by *Dekkera/Brettanomyces* yeasts are unwanted within alcoholic beverages. Hence, the removal of said volatile phenols is often critical in improving the sensory characteristics.

2.2.2 Extracted Volatile Compounds from Various Fruit Juices

Within the global market, fruit-based beverages had attributed to a compound annual growth rate (CAGR) of 4% between the years of 2010 – 2014 (Priyadarshini & Priyadarshini, 2018). With expected earnings of around $128,741.1 million by the end of 2017 and a predicted average annual growth rate of 3.7% in future – the overall demand of fruit juices is never likely to decrease in popularity (Priyadarshini & Priyadarshini, 2018). Recent studies within literature have utilised MIPs to extract volatile components from various fruit juices in order to eliminate the instances of components such as patulin – a mycotoxin commonly found in apples derived from fungi such as *Penicillium expansum*, *Aspergillus* and *Byssochlamys nivea* (Khorrami & Taherkhani, 2011). Whilst in other applications, folic acid (vitamin B9) and cinnamic acid are extracted for use within pharmaceutical production and as a food additive (Zengin et al., 2019; Xiang et al., 2017). Employing MIPs to extract said compounds from within fruit-based beverages allows for the optimisation and high recovery rates of these volatile components (Villa et al., 2021). **Table 3** below summaries the analytes extracted from various fruit juices by MIPs and their associated recovery rates of the targeted analyte.

Table 3. *Volatile compounds (analytes) extracted from various fruit beverages utilising molecularly imprinted polymers and their associated recovery rates (%).*

Volatile Compound (Analyte) Extracted	Type of Fruit or Fruit Beverage	Recovery Rates (%)	Type of MIP Used	Reference

Patulin	Cloudy Apple Juice	80	Oxindole-based polymer	Khorrami & Taherkhani (2011)
	Clarified Apple Juice	82 – 98	Silicon dioxide-maleic polymer	Anene et al. (2016)
Folic Acid	Orange Juice	95.5 – 100.5	Polydimethylsiloxane-based polymer	Zengin et al. (2019)
Gallic Acid	Apple Juice	98.5 – 102.3	Multiwalled carbon nanotube-modified with carbon paste electrode	Shojaei et al. (2016)
	Pineapple Juice	98.7 – 103.2		
	Orange Juice	98.1 – 101.8		
Gallic Acid	Grape Juice	95.2	Magnetic mesoporous silica-based MIP	Hu et al. (2015)
	Apple Juice			
	Peach Juice			
	Orange Juice			
Cinnamic Acid	Apple Juice	89.3 – 103.5	Hollow porous-based MIPs	Xiang et al. (2017)
	Orange Juice			
Dioctyl Phthalate	Unspecified Fruit Juice	88.6 – 93.0	Multiwalled carbon nanotube-modified with carboxyl groups	Du et al. (2016)
Bisphenol A	Orange Juice	93.3 – 100.0	Magnetic nanoparticle-based polymer	Wu et al. (2017)
Caffeic Acid Ferulic Acid Hydroferulic Acid Vanillic Acid	Unspecified Fruit Juices	75.3 – 111	Poly (ionic liquid)-based MIP	Chen & Huang (2017)

The elimination of unwanted volatile components such as patulin is crucial in the development of a commercial final apple juice product. In particular, the mycotoxin associated with this analyte can still remain even after processing of the raw apple into juice (Khorrami & Taherkhani, 2011). Within the beverage, the mycotoxin itself is extremely harmful if over 50 ppb (parts per billion) is ingested as it can trigger chronic health risks like epithelial cell degeneration which is why studies done by Khorrami & Taherkhani (2011) and Anene et al. (2016) highlight the importance of eliminating this compound from production. In addition to this, plastic-based components such as dioctyl phthalate (DOP) and bisphenol A (BPA) are also unwanted analytes within food and drink containers that have been studied by authors Du et al. (2016) and Wu et al. (2017) within orange juice and other fruit-based beverages. Both components, respectively, are utilised within the plastic industry to improve flexibility and as a synthesiser within polycarbonate plastics and resins (Wu et al., 2017; Du et al., 2016). On the other side of the spectrum, phenolic acids such as gallic acid (GA) are essential within the drug trimethoprim,

in the food industry and in ink dyes (Shojaei et al., 2016). Because of its versatility and importance in analytical chemistry, GA is beneficial in terms of its antimicrobial, antioxidant and anti-carcinogenic properties (Shojaei et al., 2016). The recovery rates of each analyte are above 75% which indicates a high level of extraction when MIPs are utilised.

2.3 Factors Affecting Organoleptic Properties in Apple, Orange, & Cranberry Juice

Various studies have concluded that the proportions of volatile compounds present in various apple, orange and cranberry cultivars differ depending on preharvest, harvest and postharvest conditions (Espino-Díaz et al., 2016; Massini et al., 2018; Forney 2008; Pan et al., 2023). Various attributes in the given environment can influence the volatile components within the fruit. These abiotic and biotic stresses ultimately interact together to form the basis of the final product's flavour and aroma – whether it be consumed raw or processed. The following sections will discuss the importance of these components on the fruit's volatiles and overall quality in relation to the preharvest, harvest and postharvest factors.

2.3.1 Preharvest Factors of Apple, Orange and Cranberry Fruit

There are many differences in the physiochemical, organoleptic and functional quality of fresh fruits based on the type of cultivar and its corresponding genetic material (Forney, 2008). For instance, Pan et al. (2023) reported that juice made from Chinese sweet oranges gives a higher proportion of terpenes whilst American, Argentinian and Brazilian oranges produce a higher number of aldehydes. Sater et al. (2020) also reported that in a 2016 study, sensory panellists were successfully able to differentiate between four cultivars of *Vaccinium macrocarpon* (a variety of cranberry) based on its aroma compounds. Multiple authors reported that differences in the concentrations of volatiles among apple, orange and cranberry cultivars creates contrasting sensory attributes during maturation (Espino-Díaz et al., 2016; Pan et al., 2023; Sater et al., 2020).

In the initial stages of apple maturation, aldehydes predominate before the alcohol content gradually increases as the apple develops. Finally, esters control the last phase, producing key "fruity" aromatic compounds exhibited within apples and apple-based products (Niu et al., 2019). Similar characteristics are also exhibited in oranges and cranberries in terms of both their ester and aldehyde content the only exception is the fruit's terpene hydrocarbons (e.g., limonene, linalool, and α-pinene) and benzyl compounds (mainly benzyl alcohol and benzoic acid) which do not change significantly during maturation (Perez-Cacho et al., 2008a; Sater et al., 2020). If maturation progresses above optimum

levels, the accumulation of sugars, phenolic and volatile components can occur as a result in the maturation processes decoupling – ultimately changing the fruits' organoleptic profile (Kyriacou & Rouphael, 2018).

In conjunction with changes in maturation and cultivar variation, environmental factors such as weather, geographical location and cultural practices also contribute to the number of aroma volatiles expressed within the final product (Ferguson et al., 1999). Musacchi & Serra (2018) and Pan et al., (2023) stated that the interactions between various cultivars and rootstocks (affects the scion physiology) combined with environmental conditions can impact the overall characteristics of apples and oranges. For instance, a high-radiation environment (increased light accessibility, temperature and humidity) incorporated with optimum soil quality can produce larger and better coloured fruit. However, pronounced exposure to sunlight and high temperatures (greater than 30 – 35 °C) can inhibit the morphological, physiological and metabolic processes of the crop ultimately causing the nutritional and flavour aspects of the fruit to decrease (Kyriacou & Rouphael, 2018).

Whilst cranberries share similar patterns in regard to weather, geographical location and cultural practices they are grown quite differently (Forney, 2008). In order for the fruit to survive in its given environment, cranberries require an adequate fresh water supply and acid peat soil – this is done by the implementation of a bog or marsh (Girard & Sinha, 2012). By allowing for the fresh water supply to flood the cranberry plants they are able to be used continuously every season as the bog protects the berries from frost during spring (Girard & Sinha, 2012). According to Forney (2008), the overall growth, composition and quality of the fruit is an accumulation of various abiotic and biotic stresses including nutrients in soil, water availability and the longevity of the plant.

In addition to this, agronomic factors can also have a substantial impact on apples, oranges and cranberries. The orchard design and its management via pruning plays a crucial role in the overall development of the fruit. For apples high-density planting (HDP) is usually implemented as it provides an excellent canopy-to-root balance without the need to modify and correct by excessive pruning (Musacchi & Serra, 2018). Initial pruning of the flower buds can be controlled based on how many there are on the tree – fruit size is of higher quality if 75% of flower buds are eradicated decreasing irregular crop load (Musacchi & Serra, 2018). Kyriacou & Rouphael (2018) stated that apple fruit trees adapt well to deficit irrigation (DI) as the decrease in vegetation and increase in light exposure ultimately improves the aroma volatiles and total phenol content. Magwaza et al. (2017) had similar findings whereby the ascorbic acid (vitamin C) content of oranges treated in an DI environment increased by 15%. Furthermore, Forney (2003) also emphasized that the general sanitisation (the recycling and management of bog water each season and regular sanding over the bog during winter)

and removal of plant debris (pruning) within bog areas is crucial in the development of the cranberry's growth and vigour. Irrigation management off the plants roots is another important factor that underpins the fruit's overall quality. Because cranberries are partially submerged in water, they rely on a different mode of irrigation management – more specifically water is constantly recycled from its source giving rise to the cranberries distinct flavour attributes without it, carbohydrate stresses can occur (Girard & Sinha, 2012; Hou, 2011).

Not only is the water availability for the root system essential, but the soil nutrition plays a role in the fruits final attributes and yield. For instance, potassium is said to be a crucial element in the manufacture of high-quality citrus fruits as it increases the production of vitamin C, whilst increased nitrogen (dependent on the percentage of acidic peat soil within the cranberry bog) is known to promote essential nutrient uptake during the early stages of the growing session (Magwaza et al., 2017; Hou, 2011). Subsequently, the incorporation of plant growth regulators (such as cytokinins and gibberellic acid) into the roots of orange and apple trees acts as an "carbon partitioner" which stimulates photosynthesis and the flow of nutrients through the phloem – improving tissue growth and the breakdown of sugars for metabolic purposes (Magwaza et al., 2017). Cranberry plants on the other hand utilise fungicides in a different fashion as if added around the time of bloom, they can decrease the chance of any potential infections that would inhibit the cranberries organoleptic abilities (Forney, 2008; Forney, 2003).

One of the final agronomic components that maintains a high fruit quality is pollination. It has been reported by Musacchi & Serra (2018) that most apple cultivars are self-incompatible because of their gametophytic nature whilst others can self-pollinate but only at a rate of around 10%. For most fruits such as oranges, cranberries and apples the flowers themselves are hermaphroditic with honey bees being the most common insect pollinator facilitating and developing the final fruit set (Musacchi & Serra, 2018; Pan et al., 2023; Hou, 2011). The interaction of all these factors therefore, can ultimately determine the final product grown. Hence, careful consideration must be applied at each step to maximise the fruits flavour characteristics and provide consumers with a high-quality end product.

2.3.2 Harvesting Factors of Apple, Orange and Cranberry Fruit

Once the fruit's natural growth and development is complete (i.e., they have reached the optimum level of maturity) they are able to be handled, transported and processed into various commodities for human consumption. Harvest maturity is considered to be a highly influential factor, as if the fruit is picked immaturely the aroma volatiles biosynthesis will be reduced (Pan et al., 2023). Since oranges and cranberries are non-climacteric (does not ripen after harvesting) collection must occur

simultaneously with horticultural or commercial maturity since after postharvest the organoleptic attributes of the fruit remain the same (Kyriacou & Rouphael, 2018). Apples on the other hand are climacteric in nature which means that the fruit is picked before physiological maturity whereby endogenous ethylene synthesis is highly responsive towards the presence of exogenous ethylene resulting in fruit that is able to maintain its physical attributes (Kyriacou & Rouphael, 2018). As reported by Magwaza et al. (2017), vitamin C content within oranges decreases with maturity indicating that an early or mid-harvest is needed for optimum quality. Apples also show similar characteristics as studies done by Dixon & Hewett (2000) indicate that fruit harvested immaturely or late in the season have very low or declining concentrations of volatiles. In terms of cranberries, the primary determining factor is its colour; dark-red cranberries themselves have higher volatile components and lower physiological rates after harvesting (Forney, 2008; Girard & Sinha, 2012). Hence, various maturity indices (e.g., the thiault index responsible for total sugar content) are often employed to monitor and predict the fruit's growth and organoleptic quality for successful application within the given market (Pan et al., 2023; Musacchi & Serra, 2018).

2.3.3 Postharvest Treatment Factors Effecting Apple, Orange and Cranberry Juice

Subsequent postharvest practices such as processing and storage also directly contribute towards the aroma and flavour profile of apple, orange and cranberry juice – more so than any preharvest (I.e. weather, geographical location and cultural practises) and harvest (i.e. maturity) factors presented previously. The following sections will fully analyse the corresponding storage and manufacturing processes that would heavily influence each juices volatile components and subsequently the overall sensory characteristics of the final product.

2.3.3.1 Impact of Storage Conditions on Apple, Orange and Cranberry Juice

Kebede et al., (2019) stated that aroma compounds within apple juice such as hexanal and trans-2-hexenal (associated with the green and grassy aroma) decrease during storage, whilst oxidation and Maillard browning compounds (furfural) increase. Gliszczynska-Swiglo & Tyrakowska (2003) reported a 5 – 21% loss in phenolic acids, 8 – 19% loss in flavonoids and a 6 – 14% decrease in the juices' antioxidant capacity after 11 months of storage at room temperature. Essentially, these polyphenols and volatiles are vulnerable to both enzymatic oxidation (during maceration) and non-enzymatic hydrolysis that occurs during storage (Massini et al., 2018). Various types of reactions have different effects on the quality of both cloudy and clear apple juice during storage. The formation of sediment and a 50% loss of polyphenols is apparent within cloudy apple juice because of the reactions between

pectin and proteins in conjunction with procyanidins (Massini et al., 2018). In regards to clear apple juice, it has been reported that catechins are highly sensitive to polymerisation whilst the majority of polyphenols within the juice remain relatively stable (Massini et al., 2018). Depending on the quality-related (bio)chemical reactions triggered during apple juice processing, the overall flavour of the juice will continue to change during its shelf life (Kebede et al., 2019).

Similar characteristics are exhibited in orange juice, under prolonged storage conditions the overall aroma of orange juice will change significantly depending on the period of time and storage temperature (Pan et al., 2013). It has been reported by Perez-Cacho et al. (2008a) that packaged orange juice that is stored at refrigerated temperatures (4 – 6 °C) for up to 16 weeks has little change in its overall flavour components. However, orange juice that is stored within an ambient environment at higher temperatures (20°C and above) shows a different sensory profile (Pan et al., 2013). Li et al. (2018) investigated that storing orange juice at room temperature and 37°C for 15 days had a significant impact on the beverages' flavour components (e.g., hexanal, decanal and neral). The decline of these desirable compounds caused an increase in terpine-4-ol, 4-ethylguiaicol and p-vinyl guaiacol. Whilst the storage period and temperature are the most important factors that influence orange juice volatiles, there have been other variables that have been investigated. A study by Van Willige et al. (2003) showed that whilst low-density polyethylene (LDPE), polycarbonate (PC), and polyethylene terephthalate (PET) plastic packaging decreased some flavour volatiles, sensory evaluations showed no significant differences between the control and treated samples. In terms of oxygen and light effects, based on research gathered by Perez-Cacho et al. (2008a) there is limited evidence that suggests both factors directly alter the aroma and taste of citrus juices during storage.

On the other side of the spectrum, cranberry juice is sensitive to completely different set of factors. Due to the rapid deterioration of anthocyanin content (the compound responsible for the juice's distinct red colour), cranberry juice has a relatively short shelf-life compared to other fruit juices like apple and orange due to this colour loss (Pappas & Schaich, 2009). Anthocyanins themselves are highly susceptible to oxidation and light degradation during handling and processing (Pappas & Schaich, 2009; Chen et al., 2001). Robards et al. (1999) established that excessive amounts of oxidative polymerisation can be responsible for the formation of sediment within cranberry juice along with ascorbic acid degradation, Milliard browning and loss of the drink's desirable red hue. Pappas & Schaich (2009) further enforced these claims by stating that the type of sugar that is bonded to the anthocyanins influences the juice's stability towards environmental stresses. For instance, anthocyanin arabinosides degrade more easily from exposure to oxygen, light, and variation in vitamin C levels than galactosidases.

2.3.3.2 Impact of Processing on Apple, Orange and Cranberry Juice

Figure 5 (below) showcases a flowchart of the industrial process of cranberry juice. In the current market various juices are processed in two ways – from concentrate (FC) and not from concentrate (NFC). Both methods can also heavily contribute towards the changes in a juice's volatile components and often undergo long storage periods before consumption. The former (FC) utilises pasteurisation and evaporation to remove the majority of the water (but also key aroma volatiles) from the solution. After these steps, the solution can be rehydrated with more water before being packaged and sold commercially. The latter (NFC) is only pasteurised then stored chilled before consumption (Pan et al., 2023). From research conducted by Averbeck & Schieberle (2009), freshly reconstituted juice from concentrate showed similar concentrations of aroma-active compounds to freshly squeezed juice. Hence, juice products are usually developed and manufactured in this manner as the subsequent benefits in the flavour components increases overall palatability.

Cranberry fruit are excellent sources of antioxidants including phenolic compounds, vitamin C, and various minerals such as magnesium (Narwojsz & Borowska, 2010). Around 50 – 65% of the fruit is utilised to manufacture cranberry juices and juice drink products within the United States of America alone (Girard & Sinha, 2012; Pappas & Schaich, 2009). Because fresh cranberries are highly acidic and tart in nature, cranberry juice is generally sweetened with sugar, artificial sweeteners or mixed with other beverages to make it more palatable for consumers (Pappas & Schaich, 2009). The release of these bioactive compounds and antioxidants into the juice is considerably affected by fruit pressing, heated enzymatic maceration, and pasteurisation (Caillet et al., 2011). It is known that any form of heat treatment has a destructive impact on anthocyanin and free radical scavenging properties of cranberry juice (Caillet et al., 2011).

Anthocyanin and ascorbic acid losses were recorded by Narwojsz & Borowska (2010) after various cranberry varieties were subjected to thermal treatment. It was reported that the total anthocyanin loss did not exceed over 40% with phenolic compounds remaining relatively stable. In comparison, strawberry juice resulted in a 41 – 53% and 60 – 70% decrease in anthocyanin and ascorbic acid content, respectively. Both authors concluded that depending on the species of the fruit, the changes in composition would vary during processing and manufacture. It is widely known that fruit pressing or crushing attributes to losses in a juice's flavour characteristics and volatile components (Caillet et al., 2011; Candrawinata et al., 2013; Massini et al., 2018). Although 75% of the antioxidants remain within cranberry juice after pressing, the remaining 25% is lost after the removal of the cranberry pomace (Girard & Sinha, 2012).

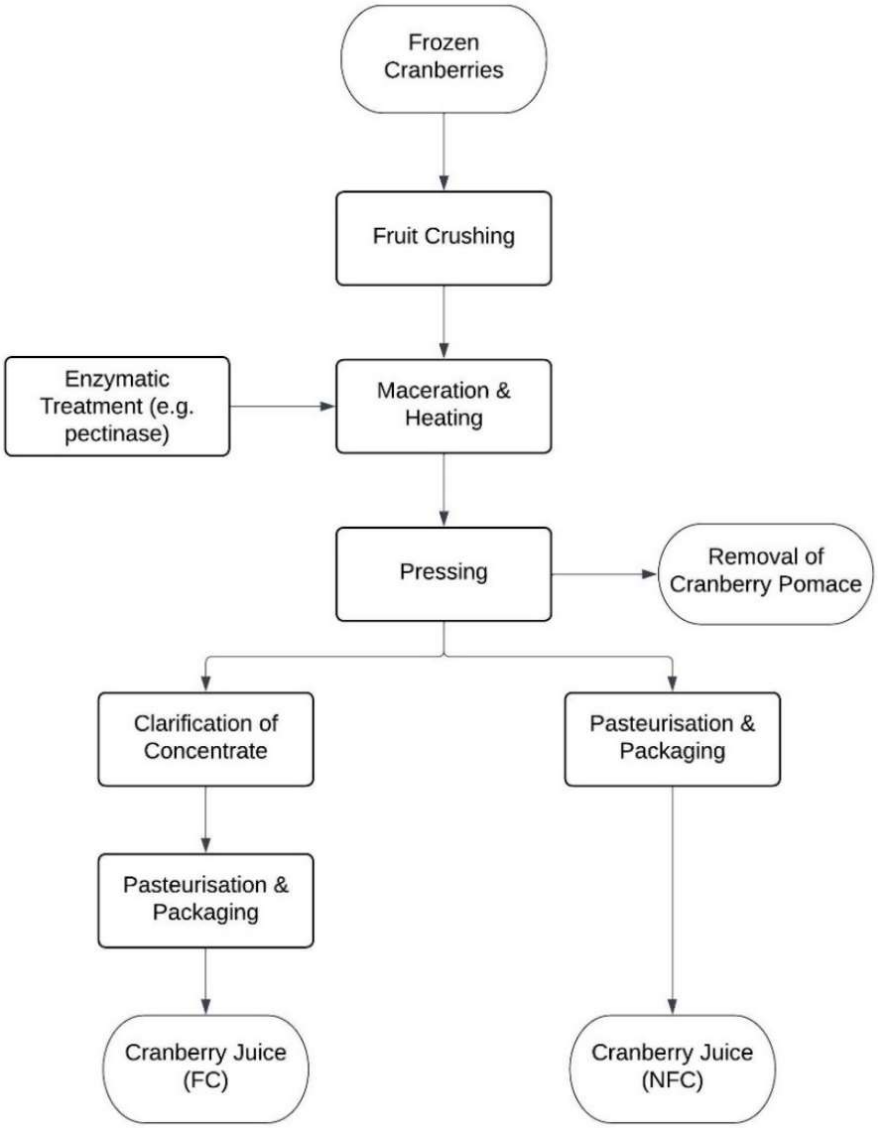


Figure 5. *Flowchart of the production process for cranberry juice from concentrate (FC) and not from concentrate (NFC) adapted from Conidi et al. (2020).*[3]

Heated (enzymatic) maceration is the process in which cranberries are blended with enzymes to digest the fruit into mash (Girard & Sinha, 2012). The addition of highly specific enzymes, such as pectinase, help to partially break down the cell wall of polysaccharides (i.e., pectin and cellulose) causing a decrease in viscosity and improving the overall extractability of various antioxidants and volatile components (Narwojsz & Borowska, 2010; Oszmianski et al., 2009). The main benefit of applying maceration on an industrial scale is that a higher yield of phenolic compounds is often generated within the final product (Girard & Sinha, 2012). Narwojsz & Borowska (2010) discovered that there was a statistically significant ($p < 0.05$) increase in both cranberry juice yield and extractability after fruit maceration. However, it is important to note that the excessive use of enzymes and the heat

treatment of the cranberry mash can result in a slight reduction of antioxidant capacity and undesirable changes in the colour and flavour of the beverage (Caillet et al., 2011). Similar characteristics have been reported in the enzymatic maceration of apples. **Figure 6** (below) showcases the full production process of how apple juice from concentrate and not from concentrate is manufactured. Oszmianski et al. (2009) investigated the effect of various enzymatic treatments on cloudy apple juice, the results demonstrated that a higher polyphenolic content (around 77%), juice yield and cloud-stable juice could be achieved due to enzymatic maceration. However, the procyanidins were significantly lower in the treated juices than the original fruit.

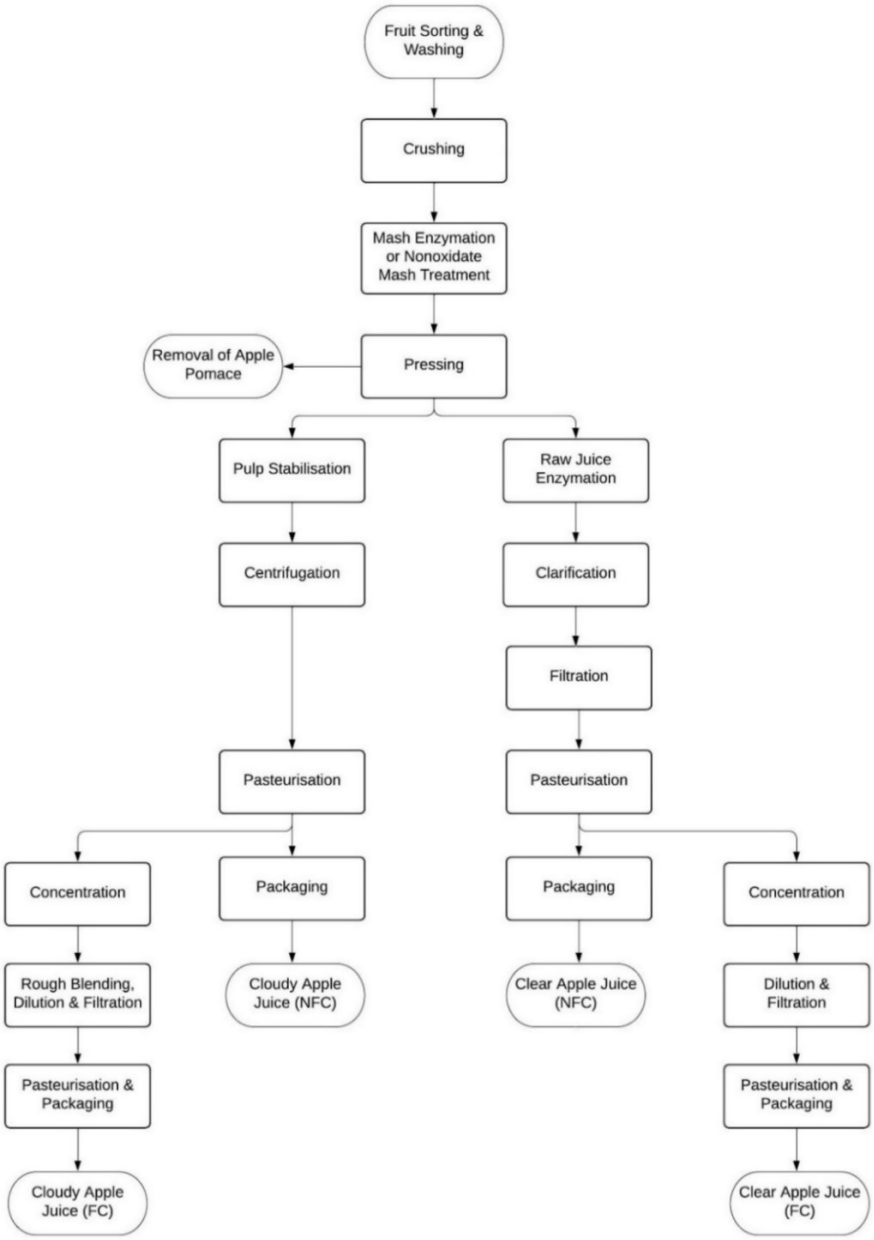


Figure 6. *Flowchart of the process for both clarified and cloudy apple juice from concentrate (FC) and not from concentrate (NFC) adapted from Duan et al. (2023).*[4]

Multiple authors have also concluded that processing increases the likelihood of differences within the apple's polyphenol content (Coelho et al., 2021; Candrawinata et al., 2013; Massini et al., 2018; Oszmianski et al., 2009; Will et al., 2008). It is reported that 58 – 90% of polyphenol compounds are lost during apple juice processing and 15% of aroma volatiles are evaporated at higher temperature processing such as pasteurisation (Will et al., 2008; Coelho et al., 2021). Chen et al. (2013) stated that whilst the process was efficient in controlling bacterial growth, it also resulted in the degradation of various phenolic compounds within most fruit juices. The authors reported that apple juice pasteurised at 94°C had a 48% loss of phenolic compounds compared to juice that was treated at 72°C.

Predominately, the crushing, pressing, clarification and filtration stages create the most variability within both products – more so with clarified apple juice (Candrawinata et al., 2013; Massini et al., 2018). Due to the highly porous and complex nature of the cell wall structure, the adsorption of key flavan-3-ol polyphenols like catechin and proanthocyanin occurs rapidly due to its partial hydrophilic/hydrophobic characteristics (Massini et al., 2018; Oszmianski et al., 2009). More specifically, the majority of the changes during processing occur when the cell walls within the apple are disrupted (broken down chemically) by crushing/pressing or filtration (Candrawinata et al., 2013). The removal of pomace and pulp through pressing and enzymatic treatment also significantly reduces the polyphenol content as they are bound to the cell walls of the apple (Candrawinata et al., 2013; Massini et al., 2018; Oszmianski et al., 2009).

Much like the processing of apple juice, orange juice exhibits similar processing characteristics as shown in **Figure 7** (below). Within orange juice, mono and sesquiterpene hydrocarbons contribute around 74% and 87.4%, respectively in the pulp (cloud), whereas oxygenated compounds (esters, alcohols, and long chained aliphatic aldehydes) are more closely associated with the serum (Brat et al., 2003; Perez-Cacho et al., 2008a). Juice extraction, filtration (through mesh) and centrifugation are three of the four critical stages of where phenolic compounds and flavanones are lost within orange juice production – mainly from the removal of albedo, peel and pulp during manufacture (Gil-Izquierdo et al., 2002). Like filtration, centrifugation is mainly utilised as a means of controlling the total pulp content within the final beverage – based on preferences, consumers can therefore purchase either low or high pulp orange juice (Sentandreu et al., 2011). The process itself makes it easier to separate the pulp from the cloud for pasteurisation at different temperature (to be reincorporated after this phase has occurred) and limits the number of steps required to prepare the juice for evaporation or clarification (Carbonell et al., 2011). According to Perez-Cacho et al. (2008a), a total of around 80% volatile compounds are associated with the pulp and cloud. Hence, if the juice is filtered or centrifugated to remove said pulp, then a vast portion of key aroma compounds are lost.

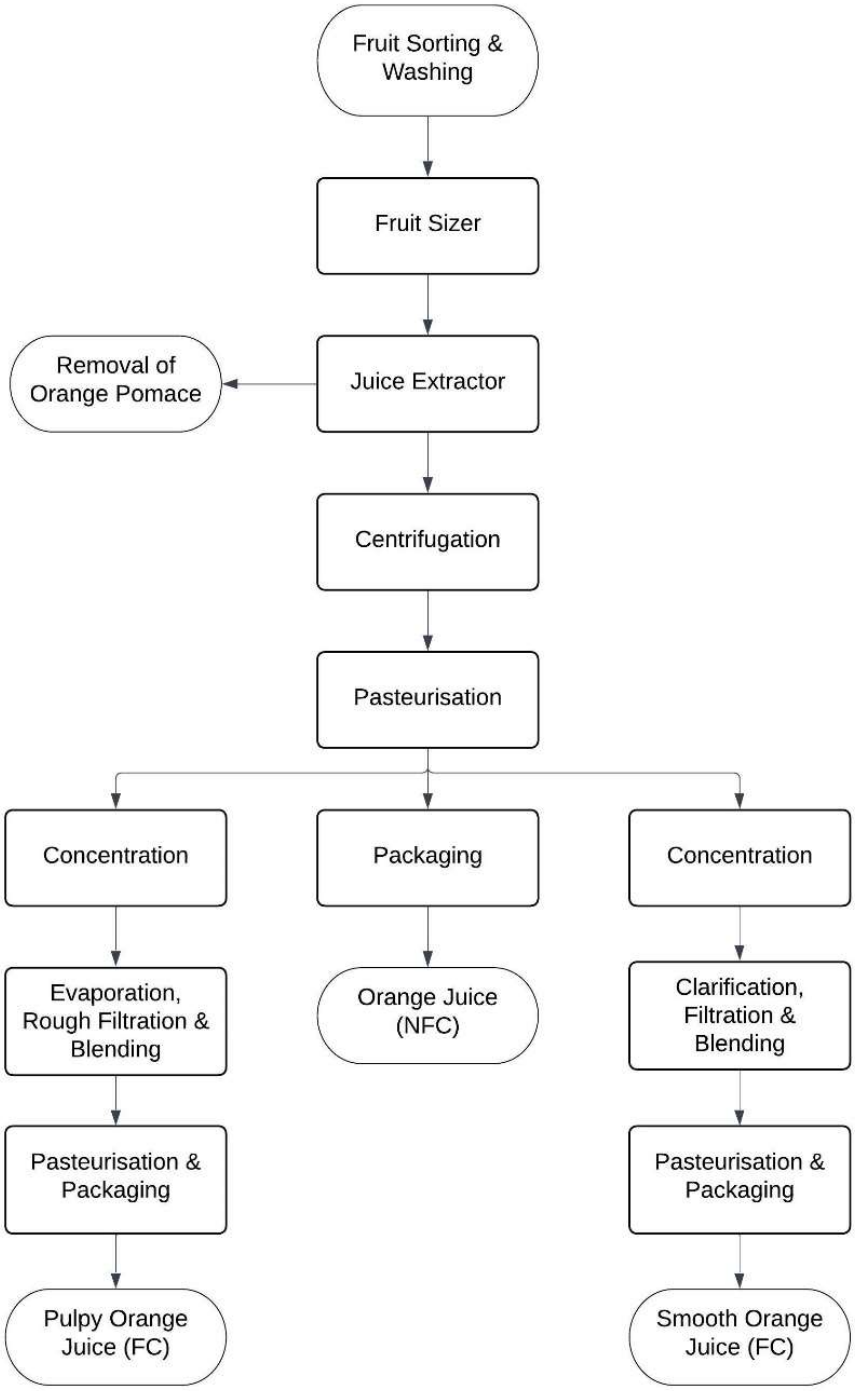


Figure 7. *Flowchart of the process for both pulpy and smooth orange juice from concentrate (FC) and not from concentrate (NFC) adapted from Conidi et al. (2020).*[3]

Many important nutrients (acids, vitamins, minerals and some flavonoids) within orange juice are moderately heat stable under high temperature processing compared to that of apple juice (Sandhu et al., 2012). However, juice aroma and flavour can still be altered due to the loss of crucial volatile components consisting of mainly aldehydes and esters and subsequent development of new precursors (Perez-Cacho et al., 2008a; Pan et al., 2023). Findings from Gil-Izquierdo et al. (2002)

showed that commercially squeezed orange juice treated at both 75 °C and 95 °C for 30 seconds did not distort the overall flavanone content, but in fact, increased vitamin C levels. However, pasteurisation of the pulp within the juice exhibited a 47% antioxidant reduction. When heat is increased, a complex series of chemical reactions takes place within the fruit – namely the degradation of acid-catalysed hydration terpenes to form α-terpineol and the disruption of carbohydrates creating unwanted Maillard-type compounds like furanones or furan aldehydes (Perez-Cacho et al., 2008a).

2.4 Key Aroma-Active Compounds (Volatiles) in Apple, Orange & Cranberry Juice

Volatile compounds (especially aroma-active compounds) are the main sources of aroma and taste perception within apple, orange and cranberry juice. As stated in the previous sections, different volatile components will be present in different concentrations due to numerous abiotic and biotic stresses that the fruit undergoes during its lifecycle. These include, but are not limited to, fluctuations in temperature, type of cultivar (genetic material), orchard management (pruning, irrigation, etc.) and postharvest treatment conditions (thermal processing). It has been reported by Perez-Cacho et al. (2008b) that only 5% of total food volatiles contribute towards perceived aroma. Hence, the implementation of various gas chromatography-mass spectroscopy (GCMS) techniques (e.g., gas chromatography-olfactory) has been widely utilised to characterise and tentatively identify these odour-active compounds (Perez-Cacho et al., 2008a).

In order to precure these threshold values, flavourists usually employ water as a matrix to reconstruct the flavour characteristics of the product as it is odourless in nature (Plotto et al., 2008). However, water cannot mimic the complex metabolic interactions (both volatile and non-volatile) that occur within the food itself (Plotto et al., 2008). As reported by Cliff et al. (2011) it has only been recently that researchers have measured and calculated odour-active compounds (OAC) within varying juice matrixes instead of relying on water as the sole solvent. Due to the wide extent of the volatiles generated and reported within literature for apple, orange and cranberry fruit and fruit-based products (Espino-Díaz et al., 2016; Mastello et al., 2015; Pan et al., 2023; Sater et al., 2020; Gu et al., 2022), a brief overview has been provided with the corresponding sections discussing and outlining the main compounds associated with each juice type and the overall impact that they have on its organoleptic properties (orthonasal and retronasal within varying matrixes).

2.4.1 Volatile Components in Apple Juice

In the last 50 years, researchers have discovered over 300 volatile compounds in the aroma profile of apples (*Malus domestica*) in order to generate a better understanding of the parameters influencing its organoleptic properties – more specifically the aroma-active compounds within the fruit that heavily influences the consumers perception of flavour (Dixon & Hewett, 2000; Espino-Díaz et al., 2016). The most predominant volatile constituents involved in ripe apples and apple juice are esters (78 – 92% of total volatiles) and alcohols (6 – 16% of total volatiles), followed by aldehydes, ketones and ethers (Rita et al., 2011). These constituents – especially alcohols, aldehydes and esters – are essential, even in low amounts, towards the complex flavour characteristics within both apple juice and intact apples (Niu et al., 2019). For instance, as investigated by Dixon & Hewett (2000), ethyl-2-methyl butanoate has a powerful and distinct aroma characteristic of apple whilst trans-2-hexanal contributes to aroma intensity and ethanol enhances the overall aroma quality of the final product manufactured. Each volatile component within apple juice, therefore, coexists positively to form the desired characteristics often perceived within the fruit and fruit-based products such as juice. Relative concentrations of these volatiles depend solely on the enzymatic activity, selectivity and the accessibility of precursors after metabolic reactions (Espino-Díaz et al., 2016).

Table 4 (below) shows the most important compounds associated with apple juice, their flavour descriptions and the water, orthonasal and retronasal threshold values as reported within literature. Due to the limited amount of research reporting the retronasal and orthonasal aspects of apple juice within an apple juice matrix – only three studies conducted by Cliff et al. (2011), Elss et al. (2007), Espino-Díaz et al. (2016) and Mehinagic et al. (2006) tentatively establishes and calculates some threshold values of the most prominent esters, alcohols and aldehydes. Hence, a more comprehensive analysis on the apple volatiles in a water matrix has been provided instead.

Table 4. *Important volatile compounds reported within apple juice, their relative aroma (odour) descriptors, the orthonasal and retronasal detection thresholds (µg/L) within the apple juice matrix and the published odour thresholds of the same compounds in water.*

Number	Chemical Group	Compound	Aroma (Odour) Description[a]	Threshold Value (µg/L)		
				Water	Orthonasal	Retronasal
1	Aldehydes	Acetaldehyde	Green, sweat, pungent	17[b]	-	-
2		Hexanal	Green, grass (cut grass)	11[b]	5[e]	-
3		Trans-2-hexanal	Green, apple	17[b]	-	-
4	Esters	Ethyl acetate	Brandy, pineapple, ethereal-fruity, pleasant	3300[c]	5000 - 13,600[e]	-
5		Butyl acetate	Red apple aroma, banana	66[d]	141[c]	2340[d]
6		Pentyl acetate	Apple, fruity, banana	43[b]	50[f]	160[d]
7		Hexyl acetate	Fruity, solvent-like	2[b]	106[c]	620[d]
8		2-methylbutyl acetate	Apple, fruity	5[d]	650[f]	-
9		Butyl hexanoate	Grass, green apple, fruity	100[d]	700[f]	5490[d]
10		Ethyl hexanoate	Fruity, apple peel	2[c]	2241[c]	-
11		Hexyl hexanoate	Fruity, apple	-	-	520[d]
12		Ethyl propanoate	Fruity, pineapple	10[c]	115[c]	-
13		Ethyl butanoate	Apple, fruity, pineapple	1[d]	46,686[c]	450[d]
14		Hexyl butanoate	Green, apple, fruity	6.4[b]	250[e]	-
15		Methyl 2-methyl butanoate	Apple, fruity, pineapple	17[b]	-	1200 – 1800[g]
16		Ethyl 2-methyl butanoate	Sweet, fruity, strawberry, blackberry, green apple	0.1[d]	8657[c]	600 – 4000[g]
17		Hexyl 2-methyl butanoate	Apple, grape, strawberry, fresh green	6[b]	22[e]	-
18	Alcohols	Ethanol	Slight, sweet, solvent-like	100,000[d]	10,000[e]	-
19		1-Butanol	Sweet, malty, solvent-like, banana	500[d]	-	-
20		1-Hexanol	Herbaceous, green, fruity	500[d]	15[e]	-
21		1-Octanol	Chemical, metal, burnt	110[d]	110[e]	-
22		1-Propanol	Sweet, harsh fusel, banana	400[d]	9[e]	-
23		Trans-2-hexenol	Green fruit, leaf, walnut, caramel	400[d]	-	-

24		2-methyl-1-butanol	Highly diluted, pleasant, malty	300[d]	-	-
25		2-methyl-1-propanol	Sweet, musty, fusel-like	250[d]	5.3, 40[e]	-

Note. Threshold values describe a point at which sensory input can be recognised.

[a,] Aroma (odour) descriptions as reported in literature from Espino-Díaz et al. (2016), Coelho et al. (2021) and Dixon & Hewett (2000).

[b, c, d] Odour threshold values in water reported from Coelho et al. (2021), Niu et al. (2019) and Cliff et al. (2011) respectively.

[e, f] Orthonasal threshold values in an apple juice matrix reported from both Espino-Díaz et al. (2016) and Mehinagic et al. (2006) respectively, unless specified by other superscript lettering.

[g,] Retronasal threshold values in an apple juice matrix reported from Elss et al. (2007), unless specified by other superscript lettering

2.4.1.1 Aldehydes within Apple Juice

The two main aroma-active aldehydes within apple juice have been reported as being hexanal and trans-2-hexanal by multiple authors (Coelho et al., 2021; Kebede et al., 2020; Mehinagic et al., 2006; Dixon & Hewett, 2000). Distinctively imparting a green, grassy and apple-like aroma in intact apples and apple juice, both these compounds are known to be strong indicators of potential change in the product's green-apple profile (Kebede et al., 2020). It has been suggested by authors Espino-Díaz et al. (2016) and Mehinagic et al. (2006) that these hexanal compounds are present at high levels in apple juice due to the disruption of tissue cells from commercial processing (i.e., crushing/pressing). As stated previously, various apple varieties have different concentrations of volatiles due to the abiotic and biotic stresses (e.g., the climate, soil type, orchard management and processing) in their given environment.

Fructuoso & Cortada (2010) reported that the concentrations of hexanal within 'Golden Delicious' apples were four to five times less than 'Cox's Orange Pippin' and 'Jonathan' varieties as well as 100 times less for the compound trans-2-hexanal. Meanwhile, Rita et al. (2011) investigated the main volatile compounds within Lithuanian Auksis-based apple juice – reporting that 2-hexenal and hexanal contributed 50.1% and 10.5% respectively towards the juice's aroma. Acetaldehyde on the other hand has been known to appear in varieties that undergo an absence of oxygen during storage (Espino-Díaz et al., 2016). Often imparting a pungent and green-like flavour due to fatty acid synthesisation causing browning of apple tissue, the volatile itself has been reported not to contribute much towards the overall organoleptic properties of apple juice (Espino-Díaz et al., 2016; Dixon & Hewett, 2000).

2.4.1.2 Esters within Apple Juice

There is no single compound responsible for an apple's organoleptic profile as most odorants are present in all varieties but in varying proportions (Dixon & Hewett, 2000). Esters, however, are the most predominant component with several studies attributing them to be the most potent aroma volatiles within apples and apple-based products like apple juice (Mehinagic et al., 2006; Coelho et al., 2021; El Hadi et al., 2013; Niu et al., 2019). In fact, ester compounds respectively account for 81%, 85%, 90%, 93% and 98% in 'Mondial Gala,' 'Granny Smith,' 'Fuji,' 'Golden Delicious' and 'Pink Lady' cultivars (Fructuoso & Cortada, 2010). Acetates, propionates, butanoates and hexanoates are crucial ester compounds that contribute the best organoleptic attributes in many apple varieties (Fructuoso & Cortada, 2010). For instance, butyl acetate, hexyl acetate and 2-methyl butyl acetate, butyl

hexanoate and hexyl hexanoate have been reported by Mehinagic et al. (2006), Coelho et al. (2021) and Fructuosa & Cortada (2010) as volatiles that are the most abundant in various apple cultivars.

Characterised by their fruity and apple-like attributes, these compounds are known to positively enhance the overall aroma within apples and apple juice. Interestingly, within the 'Red Delicious' variety it has been stated that volatiles ethyl butanoate, ethyl 2-methyl butanoate, hexyl acetate and ethyl hexanoate are the most potent odorants contributing to the aroma and subsequently its intensity (Niu et al., 2019; Coelho et al., 2021). Within literature these compounds have also been very prevalent in many apple varieties like 'Pink Lady,' 'Elstar,' 'Fuji' and 'Cox Orange' (El Hadi et al., 2013; Elss et al., 2007; Espino-Díaz et al., 2016; Fructuoso & Cortada, 2010). Other compounds such as hexyl 2-methylbutanoate, hexyl butanoate, methyl 2-methylbutanoate and ethyl propanoate have also been described as being crucial volatiles boosting flavour perception and intensity within apples and apple-based products by imparting fruity (pineapple/apple after tastes) and green profiles (Coelho et al., 2021; El Hadi et al., 2013; Elss et al., 2007). Finally, both pentyl and ethyl acetate are known to produce positive fruity and apple aromas – especially ethyl acetate as it is one of the most abundant volatile esters often perceived by consumers (Niu et al., 2019; Fructuoso & Cortada, 2010).

2.4.1.3 Alcohols within Apple Juice

Alcohols are the second most important group after esters because of their high concentrations within apple juice and contribute heavily towards apple flavour (Cliff et al., 2011). The most abundant alcohol reported within literature is 1-butanol – mainly located within the apple peel – its sweet, malty-like aroma is highly desirable because of its characteristic apple flavour (Mehinagic et al., 2006; Rita et al., 2011; Fructuoso & Cortada, 2010). Other short-chain alcohols that have reported to be crucial aroma-active compounds are 1-hexanol, 1-octanol, trans-2-hexenol and 1-propanol which give apple juice its herbaceous, fruity and sweet sensation within the apple juice and are known to enhance the apples aroma intensity (Espino-Díaz et al., 2016; López et al., 1997; Coelho et al., 2021; Mehinagic et al., 2006). Volatiles 2-methyl-1-butanol and 2-methyl-1-propanol have been heavily associated with the apple juice's overall quality although they are not considered genuine constituents of apple fruit (Espino-Díaz et al., 2016; Rita et al., 2011). These compounds are formed from the decarboxylation of amino acids leucine and isoleucine after apple juice production (Rita et al., 2011). Furthermore, from the reduction of acetaldehyde under anaerobic conditions, ethanol is another volatile compound that is utilised to assess the quality of the apple juice (Coelho et al., 2021; Espino-Díaz et al., 2016). These components, however, are described as being undesirable within apple juice at high concentrations as they produce a pungent and solvent-like flavour (Coelho et al., 2021). Ethanol especially, is known

to be able to stimulate or inhibit the fruit's metabolism altering various biochemical pathways within the juice by either enhancing ester and alcohol formation or by decreasing non-ethyl esters and aldehydes (Dixon & Hewett, 2000).

2.4.2 Volatile Components in Orange Juice

Over 200 volatile compounds have been detected within orange juice, and like apple juice, only a small portion of them are aroma-active (Perez-Cacho & Rouseff, 2008b). The majority of volatiles within orange juice consist of aldehydes (mainly acetaldehyde, hexanal, octanal and decanal) and esters (especially ethyl butanoate) but it has been reported that a small portion of alcohols (linalool and α-terpineol being major constituents), ketones (mainly nootkatone) and terpenes (such as myrcene, limonene and α-pinene) exhibit odour activity within the juice (Mastello et al., 2015). According to Brat et al. (2003) and Sandhu et al. (2012), around 70 - 80% of hydrocarbons (monoterpene and sesquiterpene) reside within the pulp whilst 80 - 90% of oxygenated volatiles (esters, alcohols, and aliphatic aldehydes) are based within the serum or orange peel portion of the orange. Many of these aroma-active compounds have varying degrees to which they contribute to the sensory characteristics of orange juice – some more dominant than others. For instance, ethyl butanoate is commonly known as a key indicator for desirable attributes within orange-based products, imparting a pineapple-like flavour, whilst β-pinene (one of the more aroma-active terpene hydrocarbons) creates a more positive aroma intensity to orange juice (Perez-Cacho & Rouseff, 2008b).

Table 5 (below) shows the most important compounds associated with orange juice, their flavour descriptions and the water, orthonasal and retronasal threshold values as reported within literature. Unlike orthonasal and retronasal values reported and calculated in apple juice (see **Table 4** above), more research has been conducted within a deodorised orange juice matrix by Plotto et al. (2004) and Plotto et al. (2008) on the most prominent esters, alcohols, aldehydes, ketones and terpene hydrocarbons that impact the juices overall organoleptic perception. A comprehensive analysis has therefore been provided on how each volatile interacts within various matrixes (i.e., water and orange juice). Interestingly, the findings from both articles indicates that each volatile within orange juice has more of an aroma impact than its corresponding taste. Ultimately suggesting that odour is a more prevalent factor in the orange juices sensory characteristics rather than its retronasal counterpart.

Table 5. *Important volatile compounds reported within orange juice, their relative aroma (odour) descriptors, the orthonasal and retronasal detection thresholds (µg/L) within the orange juice matrix and the published odour thresholds of the same compounds in water.*

Number	Chemical Group	Compound	Aroma (Odour) Description[a]	Threshold Value (µg/L)		
				Water[b]	Orthonasal[c]	Retronasal[d]
1	Aldehydes	Acetaldehyde	Solvent-like (alcohol), fruity, fresh, floral	25	187	152
2		Hexanal	Green, grassy (cut grass)	10.5	151	88
3		Octanal	Green, citrus-like (lemon), fruity, soapy	8	233	97
4		Nonanal	Melon, citrus-like, floral	5	312	165
5		Decanal	Green, citrus-like (lemon)	5	204	97
6		(Z)-dec-4-enal	Citrus-like	0.004	-	-
7		(Z)-hex-3-enal	Green, leaf-like, grassy	0.25	26.9	12.1
8		(E)-non-2-enal	Green, floral, metallic	0.08	1.52	0.055
9		(E, E)-2,4-nonadienal	Fatty	0.1	-	-
10		(E, E)-2,4-decadienal	Fatty	0.2	1.71	1.13
11		Citral (a and b)	Green, fruity, citrus-like, lemon	41.4[c]	1230	714
12	Esters	Methyl butanoate	Fruity, strawberry	28	116	120
13		Ethyl butanoate	Fruity, pineapple, orange, sweet	1	1.71	1
14		Ethyl acetate	Fruity, solvent-like, sweet, tangerine/orange	5	6037	3554
15		Ethyl hexanoate	Fruity (apple, almond), orange	5	3.5	2.30
16		Ethyl propanoate	Sweet, fruity, grapefruit	0.1	256	146
17		Ethyl octanoate	Spicy, floral, fruity	15	-	-
18		Ethyl 2-methyl butanoate	Fruity, sweet, apple	0.006	0.080	0.055
19		Ethyl 2-methyl propanoate	Fruity, sweet, apple	0.1	-	-
20	Alcohols	Hexanol	Grass, floral, resin-like	200	-	-
21		(Z)-3-hexen-1-ol	Fatty, grassy, leaves	70	348	243
22		Terpinen-4-ol	Woody, stale, floral	3.7	-	-
23		1-octanol	Herbal, green, grapefruit	130	-	-

24		Linalool	Floral, sweet, fruity, lemon	6	113	105
25		Geraniol	Citrus-like, green, minty, rose, floral	2.3	-	-
26		α-terpineol	Mint, green, fruity, citrus	28	25,900	9060
27	Terpenes	α-pinene	Pine, woody, citrus peel, chemical	5	1650	2010
28		β-pinene	Citrus, wood, terpene-like, pungent	140	37,200	36,100
29		*d*-limonene	Minty, citrus-like (lemon), fruity, anise	200	13,700	13,330
30		γ-terpinene	Green, chemical, woody	0.2	3260	2140
31		β-myrcene	Mossy, musty, medicine, balsamic	14	773	500
32		Valencene	Lemon, floral	10.5	4756	3749
33	Ketones	β-ionone	Violet-like (lilac), rose, floral	0.007	-	-
34		Carvone	Minty	8.2	-	-
35		1-octen-3-one	Mushroom, metallic	1	-	-
36		Nootkatone	Pungent, aromatic, musty	501	2240	1300

Note. Threshold values describe a point at which sensory input can be recognised.

[a,] Aroma (odour) descriptions as reported in literature from Mastello et al. (2015), Rega et al. (2003) and Perez-Cacho & Rouseff (2008b).

[b,] Odour threshold values in water reported in Pan et al. (2023), unless specified by other superscript lettering.

[c, d,] Orthonasal and retronasal threshold values in an orange juice matrix reported from both Plotto et al. (2004) and Plotto et al. (2008), respectively

2.4.2.1 Aldehydes within Orange Juice

Within orange juice there are four different kinds of odour-active aldehydes; saturated aliphatic, terpene, unsaturated, and phenolic. These are produced via fatty acid pathways (Perez-Cacho & Rouseff, 2008b). Being primarily been found within the peel, both saturated and terpene aldehydes produce a fruity (citrus-like) aroma whilst unsaturated aldehydes are responsible for the green/fatty/metallic odours (Perez-Cacho & Rouseff, 2008b). Within these subsets, acetaldehyde is one of the most dominant compounds found in freshly squeezed orange juice imparting a fresh, solvent-like aroma and pungent flavour (Pan et al., 2023). Many authors attribute this compound as being an important indicator for maturity, as acetaldehyde is known to improve orange juice's organoleptic properties and overall perception (Perez-Cacho & Rouseff, 2008a; Pan et al., 2023). However, due to its high volatility (as it is mainly located within aqueous essence), thermal processing and filling from concentrate is known to decrease its concentration in the beverage (Averbeck & Schieberle, 2009). Straight-chain aldehydes octanal, nonanal and decanal (responsible for green and citrus-like notes) are also known for their ability to enhance the aroma and flavour of orange juice. These compounds are largely prevalent within the beverage as commercial juice pressing is able to extract more of them from the peel due to its high pressure (Pan et al., 2023).

Hexanal, whilst highly regarded as a key aroma-active compound in many fruits such as raspberries and pomegranates, is considered not essential within orange juice, only contributing a slight "green" aroma (Perez-Cacho & Rouseff, 2008b). Compounds such as (Z)-hex-3-enal are derived from the degradation of both linoleic and linolenic acid via the formation and lipoxygenase-catalysation of fatty acid hydroperoxides during processing (El Hadi et al., 2013; Averbeck & Schieberle, 2009). A number of volatile degradation products are created depending on the location of the double bonds (due to fatty acid moiety) as well as the synthesis and degradation of hydroperoxide (Perez-Cacho & Rouseff, 2008b). **Figure 8** (below) showcases some of these degradation products with linolenic acid and the potential pathways in order to form these compounds. Interestingly, Perez-Cacho & Rouseff (2008b) stated that (E, Z)-isomeric odorants have varying sensory characteristics with (E)-isomers often being associated with off-odours and (Z)-isomers being more palatable. Monoterpene aldehyde citral (derived from orange peel oil) is not only responsible for the formation of derivatives geranial (citral a) and neral (citral b); but is also considered important in orange juice flavour, especially when present above the threshold level in water (Mastello et al., 2015).

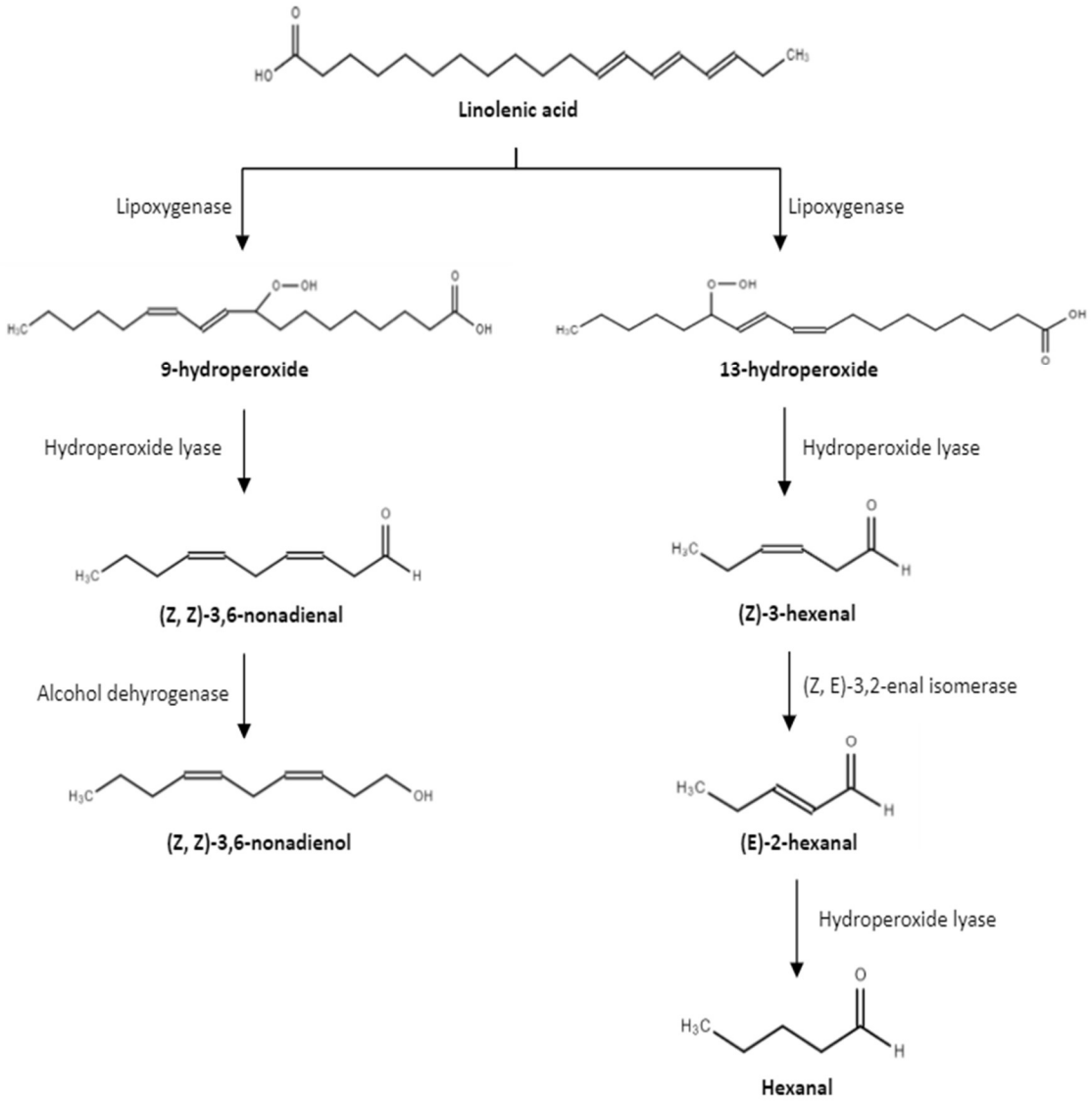


Figure 8. *Degradation of some linolenic acid derived molecules adapted from El Hadi et al. (2013).*[5]

2.4.2.2 Esters within Orange Juice

Esters are the most critical component as they are responsible for the pleasant characteristic fragrances associated with the fruits. Ethyl butanoate has been cited by multiple authors as one of the most potent odorants within orange juice often imparting a sweet fruity-orange note (Perez-Cacho & Rouseff, 2008a; Plotto et al., 2004; Rega et al., 2003; Pan et al., 2023). In fact, the ester itself is reported to exceed all others in abundance within orange juice and is utilised as an artificial flavour in the food industry (Mastello et al., 2015; Pan et al., 2023). A study done by Plotto et al. (2008) on the threshold values within deodorised orange juice showcased that ethyl butanoate had the highest recorded retronasal and orthonasal odour activity value (OAV).

Averbeck & Schieberle (2009) also corroborated this with their own research findings where ethyl butanoate had the highest flavour dilution factor of 2,084. Other important esters within orange juice include ethyl-2-methylbutanoate, ethyl-2-methylpropanoate and ethyl hexanoate as they are known to be present above their sensory threshold values within water (Perez-Cacho & Rouseff, 2008b; Plotto et al., 2008). Aroma-active esters ethyl acetate, ethyl propionate, ethyl hexanoate and ethyl octanoate are not as critical to the juice's profile because they possess low to mid odour activity – often indirectly or minorly influencing the juices organoleptic quality (Perez-Cacho & Rouseff, 2008b). Ethyl hexanoate especially can create musty, rancid and rotten-like off-flavours if levels are above its threshold detection value (Pan et al., 2023). Esters are synthesised from alcohols by acyl-CoA's. Two different pathways exist to form these compounds – the fatty acid pathway and amino acid biosynthetic pathway (El Hadi et al., 2013; Perez-Cacho & Rouseff, 2008b). The former is responsible for the manufacture of branched-chained esters whilst the latter produces straight-chained esters (Pan et al., 2023). Both pathways are known to produce a diverse set of esters – for instance Pan et al. (2023) discovered that C6-alcohols (having six carbon atoms) can be transformed into hexyl, (2, E)-hexenyl, and (3, Z)-hexenyl after esterification. Once industrialised processing occurs (i.e., heated maceration or pasteurisation), the overall concentration of these components decreases as hydrolase enzymes destabilises the bonds in the ester compounds (Perez-Cacho & Rouseff, 2008b).

2.4.2.3 Terpene Hydrocarbons within Orange Juice

Terpene hydrocarbons quantitatively and qualitatively are the main constituents in orange juice, located mainly within the peel and pulp. These compounds account for 95% of the volatile fraction and are formed by both isopentenyl diphosphate and dimethylallyl diphosphate via two different pathways (Perez-Cacho & Rouseff, 2008a; El Hadi et al., 2013; Pan et al., 2023). However, their overall contribution to the juice's sensory profile is limited because of their high orthonasal threshold values – meaning that they are mid-level volatiles (Pan et al., 2023). Out of the six aroma-active compounds listed in **Table 5** (above), d-limonene was revealed by multiple authors as a major component contributing around 45 – 90% of total terpenoids within processed orange juice (Saini et al., 2022; Cabral et al., 2010; Mustafa, 2015; Plotto et al., 2004). Research conducted by Cabral et al. (2010) found that within the peel oil of Citrus aurantium (a variety of bitter orange), 77.9% of d-limonene was extracted after cold-pressing whilst Rega et al. (2003) reported a value of 93% in fresh orange juice after SPME analysis. In spite of its high percentage, not much is known about how limonene contributes to the juice's overall sensory profile. Bi et al. (2020) theorised that d-limonene enhances other volatiles within the matrix via headspace partitioning. The compound valencene (a

sesquiterpene with a lemon and floral like aroma) has also been noted to heavily contribute towards flavour and aroma within the fruit although it is present in much lower quantities than limonene (Cabral et al., 2010).

In addition to this, orange β-myrcene has been noted by multiple authors to be the second most abundant aroma-active terpene within orange juice imparting a mossy and balsamic-like aroma (Averbeck & Schieberle, 2009; Plotto et al., 2004; Cabral et al., 2010). Although only contributing around 7.43% within the peel oil and having a low orthonasal threshold value, the odour that it produces dominates even more than that of d-limonene (Mustafa, 2015; Perez-Cacho & Rouseff, 2008a). However, if present above its threshold value, it can negatively impact the processed orange juice as it is known to cause pungent and bitter notes within the product (Baldwin et al., 2012). Finally, volatiles γ-terpinene, α-pinene and β-pinene are also common terpene hydrocarbons detected in GC analysis. El Hadi et al. (2013) found that γ-terpinene and α-pinene had a profound effect on Japanese summer oranges (*Citrus natsudaidai*), even though both terpenoids were present in smaller amounts. β-pinene (a bicyclic terpene) on the other hand contributes approximately 3.40% within orange juice and is solely dependent on how much peel oil is in the final product (Cabral et al., 2010; Perez-Cacho & Rouseff, 2008b). Although these compounds are less abundant, they are still known as key background volatiles that contribute positively towards the juice's overall sensory profile – especially its aroma (Perez-Cacho & Rouseff, 2008b).

2.4.2.4 Alcohols and Ketones within Orange Juice

Linalool has been established by most researchers as the most potent alcohol within orange juice and has been noted as a mid-level odorant (Plotto et al., 2008; Perez Cacho & Rouseff, 2008a; Rega et al., 2003; Saini et al., 2022). Mainly residing within the peel oil (between values of 0.89 – 2.92%), linalool is known to possess a distinctive sweet floral-like aroma (Mustafa, 2015; Cabral et al., 2010). Subsequently, the volatile compounds α-terpineol (green odour), terpinen-4-ol (woody and stale notes) and geraniol (green and minty odour) are formed after the acidic degradation (at a pH of 3.8) of linalool by oxidative hydration-dehydration reactions (Bi et al., 2020; Perez Cacho & Rouseff, 2008a). It has been reported by Perez-Cacho & Rouseff (2008b), that both α-terpineol and 4-terpinenol are strong indicators of aged and temperature abused juice, often imparting stale and metallic off-flavours. Geraniol is said to be an off-flavour with its concentration increasing in canned (RFC) reconstituted from concentrate (Perez-Cacho & Rouseff, 2008a). However, gas-chromatography olfactory (GC-O) analysis showed that these compounds are rarely aroma-active. Hexanol, (Z)-3-hexen-1-ol and 1-octanol on the other hand are reduced by the alcohol dehydrogenase from their

aldehyde counterparts hexanal, (Z)-3-hexan-1-al and 1-octanal (Pan et al., 2023). These alcohols, especially 1-octanol, are considered to be critical volatiles in fresh orange juice odour conveying fruity/floral and herbal profiles (Rega et al., 2003). However, their concentration solely depends on the type of cultivar utilised during manufacturing and processing.

Arguably the most potent ketone odorant within orange juice is 1-octen-3-one. Formed by the decomposition of lipids, the odour and flavour are often described as "mushroom and metallic" (Pan et al., 2023). The odour threshold value in water is reported as being between 0.005 – 1 µg/L (Perez Cacho & Rouseff, 2008b). As reported by Plotto et al. (2008), nootkatone is known as a sign of extreme oxidation within orange juice even though it is mainly found in grapefruit juice. In fact, both nootkatone and carvone were both present after thermal concentration whilst other key aroma volatiles decreased during evaporation (Averbeck & Schieberle, 2009). The orthonasal threshold value of around 2240 µg/L indicates that nootkatone is of key importance – with El Hadi et al. (2013) stating that the ketone had one of the highest odour activity values within citrus fruit juices.

However, because of its low concentration (approximately 0.1 mg/L) the volatile is highly unlikely to have a huge impact on the juices organoleptic profile and only acts as a background component in orange juice (Plotto et al., 2008; Mahattanatawee et al., 2005). Carvone on the other hand, is formed by the degradation of limonene's unsaturated sites via oxidation, the ketone itself is known to reduce the overall quality of the juice and possesses a strong minty off-flavour (Perez-Cacho & Rouseff, 2008a; El Hadi et al., 2013). Finally, studies conducted by Mahattanatawee et al. (2005) found that β-ionone contributed 22% of the total GC-O floral component in fresh orange juice. Considering that it has an extremely low odour threshold in water and orange juice, it still manages to create a potent sweet violet-like aroma (Perez Cacho & Rouseff, 2008a).

2.4.3 Volatile Components in Cranberry Juice

Due to their high tannin content and sour nature (pH < 3.0), fresh cranberries are mainly processed and manufactured into processed goods to make them more palatable for consumers. Cranberry juice in itself has added sugars since fresh cranberries only contain a sugar content of around 4% (Zhang et al., 2019a). According to Zhu et al. (2016), the fruit's unique and distinct aroma is derived from hundreds of volatile compounds coexisting during its maturity and ripening stages. However, it is important to note that not all compounds in cranberry juice are aroma-active in nature. More specifically, cranberry juice alone is reported to possess multiple alcohols, esters (less so than apple and orange fruits), aldehydes, acids and terpene hydrocarbons (Zhang et al. 2019b).

Like orange and apple, the number of volatiles within the cranberry fruit is solely dependent on the specific cultivar utilised and the resulting environmental and physiological triggers during its growth. For instance, the compound α-terpineol in European (*Vaccinium oxycoccos,* L.) and American (*Vaccinium macrocarpon,* Ait.) cultivars is representative of 13% and 9.7% of total volatiles, respectively (Gu et al., 2022). Among these volatile constituents, benzyl compounds such as benzyl alcohol, benzaldehyde and benzoic acid are significant contributors towards cranberry juice's organoleptic properties with each imparting sweet, green and honey notes and heavily influencing the aroma and overall quality of the product (Gu et al., 2022; Sater et al., 2020; Zhu et al., 2016).

Table 6 (below) shows the most important compounds associated with cranberry juice, their flavour descriptions and the water threshold values as reported in literature. Due to the limited data available on the retronasal (taste) and orthonasal (aroma) aspects of a cranberry juice matrix, this has not been included. Within the corresponding body paragraphs discussing each main volatile compound some of the OAVs and respective concentrations have been provided as a substitute. However, a comprehensive analysis has been provided on the water values within a cranberry juice matrix. These threshold values are based on the research derived from authors Zhang et al. (2019b), Zhu et al. (2016) and Zhang et al. (2019a).

Table 6. *Important volatile compounds reported within cranberry juice, their relative aroma (odour) descriptions and the water detection thresholds (ug/L).*

Number	Chemical Group	Compound	Aroma (Odour) Description[a]	Water Threshold Value (µg/L)
1	Aldehydes	Hexenal	Green, grassy (cut grass)	9[c]
2		(E)-2-hexenal	Green, grassy	8.2[c]
3		Benzaldehyde	Chemical, green, almond-like	320[c]
4		Octanal	Pungent, fruit-like	1[c]
5		Pentanal	Fruity, berry, nutty	12[b], 22[c]
6		(E)-2-heptenal	Fruity, musty, cheesy	13[c]
7		(E)-2-octenal	Citrus (orange), fatty	3[c]
8		(E)-2-nonenal	Fatty (greasy), green, grassy	0.4[c]
9	Esters	Ethyl 2-methylbutyrate	Fragrant, fruit, sweet	0.1[c]
10		Ethyl butyrate	Fruity	0.1[b]
11		Ethyl benzoate	Floral, fruity, musty, herb	100[b]
12		Ethyl hexanoate	Fruity, floral	0.3[b], 5[c]
13		Ethyl butanoate	Fruity, sweet, pineapple	1[c]
14		Ethyl acetate	Floral, fragrant	5[b]
15		Hexyl acetate	Fruity, solvent-like	115[c]
16	Terpenes	Linalool	Floral, fragrant, lemon-like	10[c]
17		Citronellol	Fresh, floral, rose-like	-
18		α-terpineol	Fresh (green-like), minty, lilac	28[b, c]
19		Eucalyptol	Orchid, mint	-
20	Ketones	β-ionone	Violet-like (lilac), rose, floral	7[c]
21	Acids	Benzoic acid	Fruity, cheesy, acidic	85,000[d]
22		2-methylbutyric acid	Fruity, cheesy, acidic	10[d]
23	Alcohols	Benzyl alcohol	Vanilla, sweet, fruity	1.2[b], 100[c]
24		4-penten-2-ol	Fruity	-

25		Octanol	Chemical, metal, burnt	110[c]
26		Nonanol	Glycyrrhiza (liquorice), mellow-like	1000[c]
27		Hexanol	Grass, floral, resin-like	500[c]

Note. Threshold values describe a point at which sensory input can be recognised by individuals.

[a,] Aroma (odour) descriptions as reported in literature from Zhang et al. (2019a), Zhang et al. (2019b) and Zhu et al. (2016).

[b, c, d] Odour threshold values in water reported in Zhang et al. (2019b), Zhu et al. (2016) and Zhang et al. (2019a) respectively.

2.4.3.1 Aldehydes within Cranberry Juice

There is a general consensus between multiple authors that aldehydes are the most abundant volatile compounds in cranberries and cranberry-based products like juice (Sater et al., 2020; Ruse et al., 2012; Zhang et al., 2019a; Gu et al., 2022). According to previous investigations, the most aroma-active aldehydes within cranberry juice are benzaldehyde, (E)-2-hexenal, (*E*)-2-octenal, (*E*)-2-nonenal, octanal, hexanal and pentanal (Cosme et al., 2022; Gu et al. 2022). All these components are heavily responsible for the cranberry's aroma potency and have often been described as the green (grassy/leafy), fatty, and fruity flavours within cranberry juice. These compounds are produced by enzyme-catalysed degradation of unsaturated fatty acids (Zhu et al., 2016; Zhang et al., 2019a). Studies conducted by Zhu et al. (2016) on four different types of American cranberries ('Early Black,' 'Howes,' 'Searles,' and 'McFarlin') have shown hexanal, (E)-2-hexenal, pentanal, (E)-2-octenal and (E)-2-nonenal as having high odour activity values (OAVs). Benzaldehyde especially is known to be an extremely important volatile compound as it is present at high amounts within various cranberry cultivars such as 'Steven,' 'Bergman' and 'Pilgrim' (Ruse et al. 2012). Although most aldehydes contribute positively towards the organoleptic properties of the juice and fruit, they can also be perceived as unpleasant paint-like and rancid off-flavours when present at higher levels due to their low threshold values (Zhu et al., 2016).

2.4.3.2 Esters within Cranberry Juice

Ethyl 2-methylbutyrate has been reported by Gu et al. (2022) and Zhu et al. (2016) to be a significant contributor to the cranberry aroma possessing OAVs between 10–33. According to Cosme et al. (2022), ethyl 2-methylbutyrate is predominantly known to greatly enhance the overall aroma and flavour of cranberry juice. Ethyl acetate is highly prevalent in the cranberry juice, at concentrations around 156–526 ug/L (Zhang et al., 2019a). Despite other acetate compounds (e.g., hexyl acetate) contributing fruity and floral aspects to cranberry products, ethyl acetate can impart negative vinegar or nail polish remover scents at higher concentrations of around 120–160 mg/L (Zhang et al., 2019a). Furthermore, ethyl benzoate has also been established as a prominent volatile by numerous authors (Ruse et al., 2012; Zhang et al., 2019a; Pappas & Schaich, 2009; Zhang et al., 2019b). Its overall perception within cranberries and cranberry juice is that of floral, fruity, musty, and herbal profiles (Zhu et al., 2016). Subsequently, with ethyl benzoate having a OAV less than 1 indicates that whilst it does not contribute much towards cranberry's sensory profile, it still impacts the aroma quality within the product positively by acting as a background 'enhancer' for other volatile components (Gu et al., 2022; Zhang et al. 2019a). Volatiles ethyl hexanoate and ethyl butanoate have previously been

reported within apple and orange juices. These are quite common within a number of different fruits, and are known for their characteristic fruity, sweet and pineapple-like odours. Within cranberries and cranberry juices, these volatiles impact both the aroma and flavour, though they are present at lower amounts with aroma intensities between 1.2–2.4 and 3.7–5.7 respectively (Zhu et al., 2016).

2.4.3.3 Terpene Hydrocarbons within Cranberry Juice

Within cranberry juice, monoterpenes account for 60% of the total volatile concentration (Gu et al., 2022). Among them, α-terpineol exhibits the highest concentration within the aroma profile of the fruit – contributing the floral and sweet notes within various cranberry products (Ruse et al., 2012; Zhu et al., 2016; Zhang et al., 2019a). Investigations done by Zhang et al. (2019b) on cranberry wines showed that the volatile compound had a OAV between 8-17, while Zhang et al. (2019a) found its concentration to be around 185-233 µg/L. Because of its extremely high potency, α-terpineol is able to significantly influence the intensity of the juice's aroma, and is known as a key aroma compound characteristic of the fruit itself (Zhu et al., 2016). Linalool is another volatile that is considered to be a critical volatile, though it is present at lower concentrations (around 3.65-18.1 µg/L), the compound is still highly significant towards the cranberry juice's aroma imparting floral, lilac and lavender notes (Pappas & Schaich, 2009; Zhang et al., 2019a).

In addition to this, the presence of both monoterpenes' eucalyptol and citronellol (responsible for floral, rose-like aromas) have been determined by multiple authors as being crucial compounds within cranberries and cranberry juices (Gu et al., 2022; Crouteau & Fagerson, 1968; Zhang et al., 2019a). Eucalyptol and citronellol are known in juice made from American cranberries to contribute 12% and 9% respectively towards the total volatile content of the beverage (Crouteau & Fagerson, 1968). Eucalyptol especially, although detected at a lower threshold level than other volatile compounds (0.29-0.60 µg/L), possesses a distinctive minty aroma and flavour and is derived from the acid-catalysed cyclization of α-terpineol (Zhang et al., 2019a).

2.4.3.4 Ketones, Acids and Alcohols within Cranberry Juice

Only one major ketone has been recently identified within literature that influences the cranberry juice's sensory profile – β-ionone (Cosme et al., 2022; Gu et al., 2022). Imparting a floral aroma and exhibiting high odour activity values (approximately 73), this compound has been stated to positively impact the overall aroma (Zhu et al., 2016). In terms of acidic components within the juice, benzoic acid has been established as the dominant force behind the acidic, fruity and cheesy odours present

in cranberries and cranberry-based products. Though benzoic acid is present at higher threshold values (155-288 mg/L), its lower OAV (around 2.1) suggests that it does not contribute much towards the total aroma profile (Zhang et al., 2019a). In fact, within fresh cranberry juice it has been reported by Pappas & Schaich (2009) that benzoic acid only accounted for 41mg/L (in free form) and 0.47% in the total volatile fraction. Although, benzoic acid is considered as a background constituent, it is able to enhance the overall fruity aroma within the beverage when present in moderate amounts (Zhang et al., 2019a). Furthermore, multiple authors Cosme et al. (2022), Gu et al. (2022) and Zhu et al. (2016) have also commented on the role 2-methylbutyric acid plays within cranberry juice. Like benzoic acid, 2-methybutyric acid contributes significantly towards the overall aroma of the beverage with OAV between 18-37 – this volatile is commonly perceived as having an acidic aroma and fruity flavour (Zhu et al., 2016).

In terms of alcohols, benzyl alcohol has been described as a major component within cranberry juice and is attributed to the fruity and sweet profiles (Zhang et al., 2019b; Sater et al., 2020; Ruse et al., 2012). In fact, benzyl alcohol accounted for 29.2% and 21.6% within European and American cranberry varieties, respectively and accounted for 23.1% of total volatile concentration (Gu et al., 2022). Zhang et al. (2019b) also determined that benzyl alcohol is a major volatile, finding concentrations between 753 to 2604 µg/L in fermented cranberry-based wines. In addition to this, Ruse et al. (2012) remarked that benzyl alcohol had an extremely positive impact on both the flavour characteristics but also on its potential antioxidative properties. The compound's prevalence within the fruit is solely dependent on the pH of the final product.

Subsequently, octanol and nonanol have also been discovered to impart 'mellow' notes but are found in lesser amounts within cranberries and cranberry based products (Zhu et al., 2016). However, hexanol has been reported to have an aroma intensity between 4.7-6.8% in various cranberry varieties/cultivars and is classed as a key sensory compound. All are responsible for the enhancement of other volatile components and are more background flavours that are known for their green and grassy characteristics (Zhu et al., 2016). Finally, 4-penten-2-ol has been reported to impart a fruity aroma though present in lower amounts in cranberry juices due to the fluctuation in temperature during processing which impacts its stability (Ruse et al., 2012). However, the volatile is still considered to contribute towards the aroma intensity (Gu et al., 2022).

2.5 Summary of Literature

Molecularly imprinted polymers (MIPs) are bio-inspired synthetic materials which can be used for the reduction and removal of organic compounds via a template strategy. MIPs can be produced with many different variations, which means that there are many iterations possible that can tailor a MIP with specific properties depending on the type of application needed within the food industry. For instance, the removal of patulin (a mycotoxin from spoiled apples) from cloudy and clarified apple juice was done using two different MIPs - an oxindole MAA and an SiO_2 maleic based polymer respectively (Khorrami & Taherkhani, 2011; Anene et al., 2016). The effect that MIPs and their components have on the sensory aspects have only been studied in wines by two authors Filipe-Ribeiro et al. (2020) and Teixeria et al. (2015). Hence, the need to further investigate how MIPs influence the overall organoleptic properties of other beverages is crucial in understanding if they can improve the final food product manufactured.

In saying this, there are multiple factors that could contribute towards the flavour profiles of apple, orange and cranberry juices. For instance, high temperature processing is known to decrease aroma-active volatile compounds by 15% in apple juice and 47% and 40% of antioxidants within orange and cranberry juices, respectively (Coelho et al. 2021; Gil-Izquierdo et al., 2002; Narwojsz & Borowska, 2010). In addition to this, various cultivars will have different proportions of constituents based on the abiotic and biotic stresses (e.g., orchard management, climate and pruning) placed on them during the growing season and during harvesting. These factors all have an impact on the flavours and aromas produced during the fruit's preharvest, harvest and post-harvest cycles which adds another layer of complexity towards how consumers perceive the different juice products.

There are many different volatiles listed in apple, orange and cranberry juice that contribute towards the final product's organoleptic perception – with some components being more prominent than others. For instance, in apple juice, ethyl-2-methyl butanoate (an ester) gives off a distinct fruity apple aroma whilst ethanol (an alcohol) contributes to the overall aroma quality (Dixon & Hewett, 2000). Multiple authors have utilised various gas chromatography mass spectroscopy techniques to determine and calculate the presence of these volatile constituents (Rega et al., 2003; Perez-Cacho et al., 2008a; Mastello et al., 2015; Niu et al., 2019; Bi et al., 2020). The results from the total ion chromatographs have given researchers a better indication of what volatiles are being produced and their abundance levels within the various samples tested. With the knowledge now known from literature, the characterisation of the main volatiles within apple, orange and cranberry juice is important in order to establish how they have been affected by the MIPs during different treatments.

3. Materials and Methods

3.1 Preparation of Column and Absorbent Materials

Five different beverage treatment materials were acquired from three different commercial manufacturers. Three food-safe MIPs, called SV7, GV1, and CV6 (Amaea, Hamilton, New Zealand), a commercial beverage treatment resin Purosorb PAD 600 (Purolite Corporation, Huzhou, China) and activated carbon (Z Filter Carbon Universal, Still Spirits, Auckland, New Zealand). 10 g (dry weight) of each material was measured into three empty 12 g solid load cartridges/columns (Hawach Scientific, Xi'an, China). Before and after the materials were added, each column had two stainless-steel mesh frits placed on the top and bottom to secure the material. The mesh frits were cut to fit the cartridges diameter of 22 mm in order to prevent the polymers from escaping treatment. See **Appendix 1** for weights recorded within each column. The filled column is then inverted (distributor cap end down) and placed onto a clamp stand as shown in **Figure 9**. It is important to note that all activated carbon columns needed to be refilled after each treatment as carbon is a one-use material and is typically not cleaned and reused commercially. The other four materials are designed to be cleaned (eluted) and reused many times.

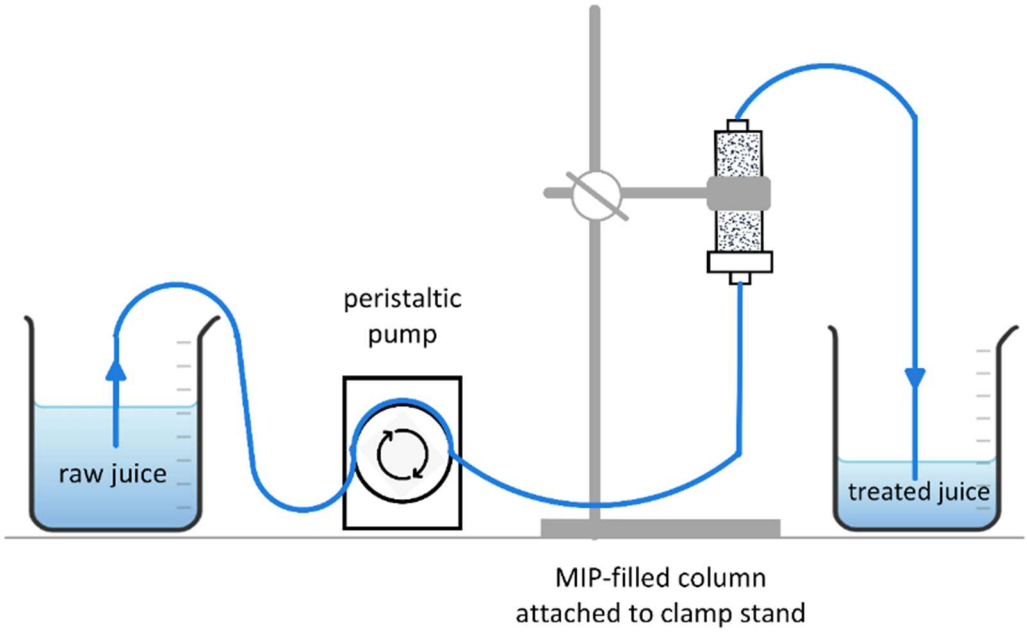


Figure 9. *Diagram showing the experimental apparatus set up and components.*

Tygon S3 E-3603 flexible tubing (Saint-Gobain Performance Plastics, Auckland, New Zealand) was attached to both ends of the peristaltic pump and column fitted to the column with luer lock fittings.

At both ends of the cartridge, the flexible tubing is secured with a cable tie to prevent the beverage from leaking during processing. The actual feed rate of the peristaltic pump was calculated and adjusted according to the pump's instruction manual before conditioning of the absorbent materials took place. The dry beads were first conditioned with several volumes of reverse osmosis (RO) water at 100 mL min^{-1} to remove any residual fine particles that may have been present. The pump rate was then slowed down to 15 mL min^{-1} for 20 minutes to allow all the pores to absorb liquid. Another 200 mL of RO water was then pumped through quickly to flush out any leftover compounds within the column. Finally, air was pumped through at 300 – 500 mL min^{-1} to expel as much liquid as possible from the cartridge.

3.2 Treatment of Juice Samples with Absorbent Materials

The pre-conditioned column was connected to the pump and receiving vessels with appropriate tubing (as shown in **Figure 9**) before treatment began. Three beverages were purchased from a local supermarket (Palmerston North, New Zealand) – these included apple juice (°Brix 12.8 with pH 3.57), orange juice (°Brix 11.1 with pH 3.76), and cranberry juice (°Brix 11.0 with pH 2.47). The juice was packaged in plastic bottles and kept at room temperature (approximately 20 °C) for analysis. To prevent blockage within the column, the orange juice was filtered with a fine mesh material to remove the sediment/pulp. It is also important to note that cleaning of the column and pumping system occurs after each run to remove any residual juice/sugars from the MIP beads (see **Section 3.2.1**). Following treatment, each column was stored in the refrigerator at 4 °C to ensure no microbial growth occurs within the MIP beads and resin.

Table 7. *Experimental design for the various treatment agents and beverages.*

Juice	Absorbent Material	Column number	Flow rate (mL/min)	Volume of beverage passed (L)	Dose rate (g/L)	Treatment time (min)
Apple Orange Cranberry	**Amaea SV7 Amaea GV1 Amaea CV6 Purosorb PAD 600 Activated Carbon Granules**	Column 1	15	0.5	20	33
				1	10	67
				2	5	133
		Column 2	35	0.5	20	14
				1	10	29
				2	5	57
		Column 3	60	0.5	20	8
				1	10	17
				2	5	33

As detailed in **Table 7**, three sets of columns were run for each beverage at three different flow rates. Samples were taken from the bulk passed beverage after a volume equivalent to 20, 10 and 5 g of MIP per litre of beverage had been passed. This meant that in total, nine different treatment rates were samples for each beverage. 250 mL from each treatment was taken and stored in a PTFE (polytetrafluoroethylene) bottle at -20 °C for future sensory analysis. Additionally, at every treatment rate described, 20 mL of the treated beverage was filtered using a 0.45 µm nylon filter (with a 25 mm diameter) attached to a 12 mL sterile luer lock syringe (Interlab, Wellington, New Zealand) and stored at -20 °C in glass vials for gas chromatography analysis. The remainder of the treated beverage was utilised for Brix (AlphaTech Systems Ltd, Auckland, New Zealand) and pH (Thermo Fisher Scientific, Massachusetts, United States) testing to see if there were any changes after being processed with the different MIPs, resin and carbon. Calibration with pH 4.0 and 7.0 solutions were performed before testing the juice samples. See **Appendix 1** for °Brix (degree Brix) and pH values of all juice samples.

3.2.1 Cleaning of Pump System

To clean the columns after use, 200 mL of RO water was pumped through at 100 mL min^{-1} to remove any residual juice/sugars left behind. Then, 200 mL of 96.4% food-grade ethanol (Southern Grain Spirits, Christchurch, New Zealand) was pumped through at 15 mL min^{-1} The elution with ethanol will strip the small phenols/colour and other bound compounds from the column, preparing it for reuse. Air was then pumped through the column at 300 – 500 mL min^{-1} to expel as much ethanol as possible – inverting the column for maximum efficiency until all sample is passed. Another 400 mL of RO water at 100 mL min^{-1} is passed to remove any residual ethanol left within the MIP beads, resin and cartridge. Finally, air was pumped through the column again at 300 – 500 mL min^{-1} to expel all of the RO water leftover within the system. Cleaning of the system was done after each treatment to restore the resins' ability to treat the next beverage (for SV7, GV1, CV6 and Purosorb PAD 600) and to ensure no contamination of the treated beverages. For all carbon treatments, however, no ethanol is needed until the final pass (to clean the system) as the activated carbon within the column was replaced each time.

3.3 Solid-Phase Microextraction (SPME)

From literature, it was recommended to use DVB/CAR/PDMS as it detects a broader range of aroma active volatiles within the sample (Zambonin et al., 2004; Rega et al., 2003; Teixeria et al., 2015). The methodology for SPME analysis was loosely based on research conducted by Zambonin et al (2004). A Stableflex 50/30µm thick DVB/CAR/PDMS fibre (Supelco, Darmstadt, Germany) was utilised to extract

volatiles from the headspace of treated and untreated apple, orange and cranberry juice samples. The fibre was conditioned in splitless/split mode within the GC injector port for 4 hours at 270 °C. Before each extraction took place, the fibre was held at room temperature for 2 minutes to equilibrate. 5 mL aliquots of juice sample (defrosted at 4 °C) was transferred into 20 mL glass vials. The vials were then sealed with PTFE/Silicone-lined (Grandado, Hong Kong) aluminium crimp caps (Agilent Technologies, California, United States). For headspace extraction, the 20 mL vials were then placed in a 50 °C incubator with the DVB/CAR/PDMS fibre for 30 minutes before SPME analysis. All injections were performed manually with an 8-minute GC injection time for each sample. SPME analysis was done in triplicate.

3.4 Gas Chromatography and Mass Spectroscopy (GCMS) Analysis

GCMS analysis was performed by an Agilent 7890A gas chromatograph and interfaced, by a GC transfer line, to a 5975C MSD (Mass Selective Detector) with a triple-axis detector (Agilent Technologies, California, United States). The GC chromatographic column consisted of a fused silica HP-5ms capillary column with a length of 30 m, inner diameter of 0.20 mm and 0.25 µm film thickness (Agilent Technologies, California, United States). The capillary column was connected to the split/splitless injector that had an inner diameter of 0.75 mm. The carrier gas used was helium which was operated at a flowrate of 1.3 mL min^{-1}. The methodology for chromatographic and mass spectroscopy analysis was loosely based on conditions set by Zambonin et al (2004). The oven temperature program was from: 50 °C (2 min) to 190 °C at 30°C/min; from 190 °C (3 min) to 200 °C at 2 °C/min; from 200 °C (4 min) to 250 °C at 15 °C/min and then held at 250 °C (1 min). A column head pressure of 15 psi and an injector temperature of 270 °C was used. The injector is operated in splitless/split mode with an 8 min sampling time. The GC transfer line is maintained at 270 °C. The mass spectrometer was operated at the electron impact positive ion (EI^+) mode with a source temperature of 230 °C. The electron energy was 70 eV and the filament current is 200 µA.

3.4.1 Identification and Quantification of Volatile Compounds

Compound identification was made by comparison of mass spectra matches within the Agilent MSD Productivity ChemStation software database library. Among the 200 (approximately) volatile compounds identified from the three different juices; 8, 13 and 9 key compounds were selected for apple, orange and cranberry juice respectively on the basis of their abundance in the headspace, their impact on the flavour and aroma profile, and/or their chemical class. For quantification, the total sum normalisation (as a percentage amount) was obtained by integrating the peak areas of all key

compounds in the treated samples and then divided by the peak area for that analyte in the control juice. Relative uncertainties were calculated from triplicate values.

3.5 Sensory Evaluation

Before formal sensory analysis, informal testing was conducted for every sample with three people (laboratory personnel) to give an initial indication of the specific flavour/aroma characteristics of each sample. Participants were asked to comment and describe any significant flavour or aroma attributes that they perceived within the various apple, orange and cranberry juice samples. See **Appendix 2** for these testing results. For the subsequent formal sensory evaluation, a non-trained sensory panel consisting of around 34–35 consumers (professors, laboratory personnel and local residents) evaluated six selected apple, orange and cranberry juice samples individually. The selection of 34–35 consumers was based on availability during the COVID-19 outbreak, subsequent time constraints during juice processing resulting in a low volume of samples, and low costs placed on this dissertation. Although it can be acknowledged that significant differences between samples would be difficult to distinguish, authors Stone et al. (2012) and Moskowitz et al. (2008) have stated that using a small sample size (between 25–75 untrained persons) can show trends and provide direction from the sensory data generated.

The consumers were asked to rate the samples on a 9-point hedonic scale, with 1 = dislike extremely and 9 = like extremely. Intensity scales were also employed to rate the perceived intensities of specific attributes of the samples, from 0 to 10, being 0 = low and 10 = high. Refer to **Appendix 3** for all sensory questionnaires utilised for the six-selected apple, orange and cranberry juice samples. The 9-point hedonic and 10-point intensity scales of this nature were utilised in accordance with literature from Stone et al. (2012), Lawless & Heymann (2010) and Moskowitz et al. (2008) as they have been used to reliably show consumer liking and perceived intensity rating for untrained individuals. Participants were required to evaluate the six apple, orange and cranberry juice samples one at a time. A constant volume of 7 mL of each juice was served in 10 mL plastic portion cups at 4 °C to participants in individual sensory booths. Participants were separated and asked to remain silent during the entire evaluation to remove any possible inferences and bias from others. Panellists were also asked to cleanse their palates with water and wafer crackers before evaluating each sample. Data was collected electronically using the RedJade sensory software (California, United States of America). The results gathered were analysed to determine whether treatment with MIPs, an absorbent resin or carbon granules had an effect on the sensory properties of the samples. Ethical approval was granted by

Massey University's Human Ethics Committee (MUHEC) with the corresponding application code 4000026008.

3.6 Statistical Analysis

The averages of the concentration of each compound obtained from the GCMS-SPME (**Appendix 4**) were used for multivariate analysis. Agglomerative hierarchal clustering (AHC) using Euclidean distance and ward linkage was used to explore the grouping of the samples into clusters based on the concentrations of the compounds. In addition to this, principal component analysis (PCA) was used to visualise the relationships among the different compounds and samples. Treatments were labelled 1 to 46 for each juice for easier identification as shown in **Table 8**. Both the AHC and PCA were performed with the relative recovery of the 8 (apple), 13 (orange) and 9 (cranberry) aroma compounds detected in each juice. The results from the multivariate analysis were used to screen all 46 treatments to find the final six for formal sensory evaluation. A one-way ANOVA with Tukey's HSD post hoc test was carried out on the sensory data obtained for the six-juice samples for apple, orange and cranberry. Statistical significance was established at $p < 0.05$. The average value for each attribute from the sensory evaluation used in PCA to corroborate the relationship between the different sensory attributes (aroma, flavour, etc.) and six selected apple, orange and cranberry juice samples. Data was analysed using XLSTAT software (Addinsoft, France) and RedJade.

Table 8. *Identification of the various absorbent treatments on apple, orange and cranberry juice samples for agglomerative hierarchal clustering (AHC) and principal component analysis (PCA).*

Identification Number	Description of Absorbent Material Treatment
1	Control (untreated juice)
2	20g/L SV7 (Column 1)
3	10g/L SV7 (Column 1)
4	5g/L SV7 (Column 1)
5	20g/L SV7 (Column 2)
6	10g/L SV7 (Column 2)
7	5g/L SV7 (Column 2)
8	20g/L SV7 (Column 3)
9	10g/L SV7 (Column 3)
10	5g/L SV7 (Column 3)
11	20g/L GV1 (Column 1)
12	10g/L GV1 (Column 1)
13	5g/L GV1 (Column 1)
14	20g/L GV1 (Column 2)
15	10g/L GV1 (Column 2)

16	5g/L GV1 (Column 2)
17	20g/L GV1 (Column 3)
18	10g/L GV1 (Column 3)
19	5g/L GV1 (Column 3)
20	20g/L CV6 (Column 1)
21	10g/L CV6 (Column 1)
22	5g/L CV6 (Column 1)
23	20g/L CV6 (Column 2)
24	10g/L CV6 (Column 2)
25	5g/L CV6 (Column 2)
26	20g/L CV6 (Column 3)
27	10g/L CV6 (Column 3)
28	5g/L CV6 (Column 3)
29	20g/L Purosorb PAD 600 (Column 1)
30	10g/L Purosorb PAD 600 (Column 1)
31	5g/L Purosorb PAD 600 (Column 1)
32	20g/L Purosorb PAD 600 (Column 2)
33	10g/L Purosorb PAD 600 (Column 2)
34	5g/L Purosorb PAD 600 (Column 2)
35	20g/L Purosorb PAD 600 (Column 3)
36	10g/L Purosorb PAD 600 (Column 3)
37	5g/L Purosorb PAD 600 (Column 3)
38	20g/L Carbon (Column 1)
39	10g/L Carbon (Column 1)
40	5g/L Carbon (Column 1)
41	20g/L Carbon (Column 2)
42	10g/L Carbon (Column 2)
43	5g/L Carbon (Column 2)
44	20g/L Carbon (Column 3)
45	10g/L Carbon (Column 3)
46	5g/L Carbon (Column 3)

Note. Columns 1, 2 and 3 (also known as COL. 1, 2 and 3) denotes the type of flowrate utilised during treatment of the three different juices (apple, orange and cranberry).

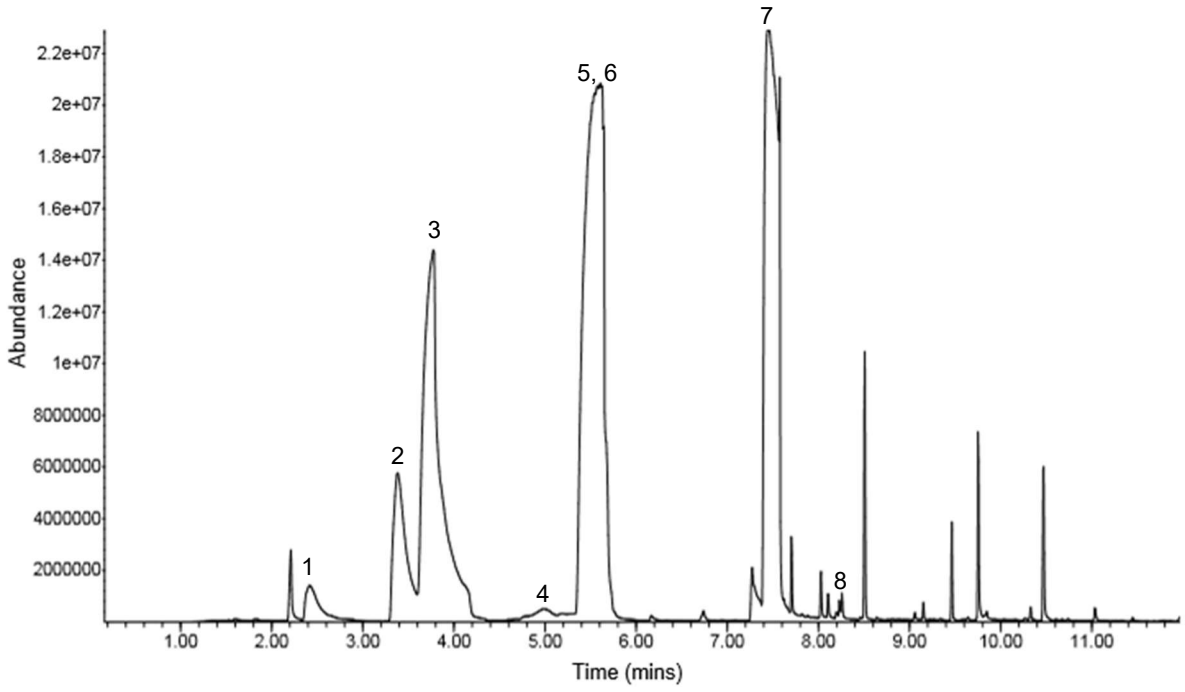
4. Results and Discussion

4.1 Analysis of GCMS and SPME Apple, Orange & Cranberry Samples

A selected chromatograph of the compounds generated via GCMS analysis have been provided to showcase the volatiles detected within each juice. All other treated samples showed the same volatiles as the control but with varying abundances. Relative peak areas for each apple, orange and cranberry volatile can be found in **Appendix 4**. Principal component analysis (PCA) was constructed to give further insight into the relationship between the various MIP and resin treated samples and volatile compounds. In addition to this, agglomerative hierarchical clustering (AHC) was used to provide groups based on distances between samples. **Appendix 5** showcases the results by class for each juice sample treated with the MIPs and commercial resin. These tables corroborate the information presented in the dendrograms but give a simplistic view of which samples are alike for each juice.

4.1.1 Identification of Key Volatiles in Apple Juice Chromatograph

Compounds hexanal, butyl acetate and hexyl acetate have often been described in the literature as being significant aroma-active volatiles within apple juice as they often provide essential grassy, red apple and fruity notes to the beverage (Coelho et al., 2021; Cliff et al., 2011). Hence, it is of no surprise to find these compounds within the generated chromatogram as presented in **Figure 10**.



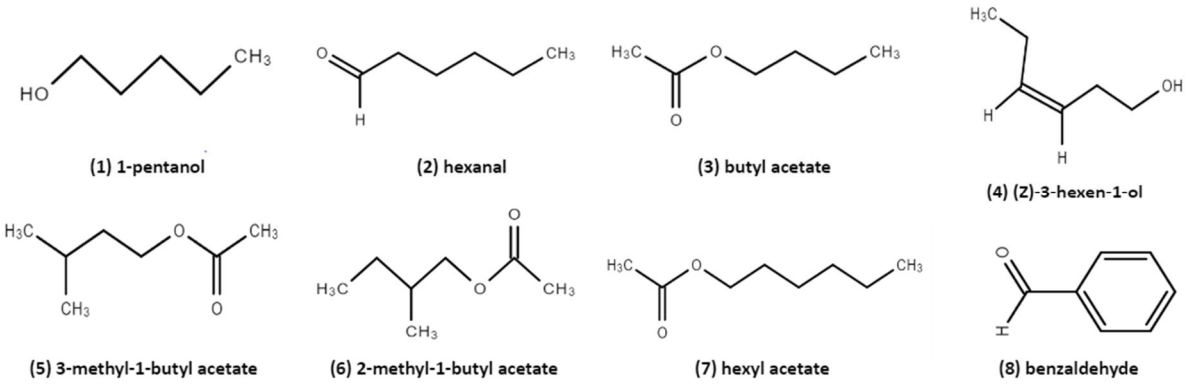


Figure 10. *Chromatogram of untreated apple juice (control) by GCMS-SPME and corresponding skeletal diagrams of the main compounds 1 to 8 detected.*

The detection of alcohols 1-pentanol (fusel-like) and (Z)-3-hexen-1-ol (grassy) within all the apple juice samples indicates their importance within the apple juices complexity. (Z)-3-hexen-1-ol, a derivative of the aldehyde (Z)-3-hexan-1-al, is formed by oxidation with alcohol dehydrogenase upon mechanical damage. This compound heavily influences the juice's aroma (Pan et al., 2023). The volatile 1-pentanol on the other hand has been reported by both Kebede et al. (2019) and Espino-Díaz et al. (2016) as a potential marker for volatile flavour change within apple juice during its shelf life and as a trigger for the formation of pentyl esters. Furthermore, the prevalence of esters 3-methyl-1-butyl acetate and 2-methyl-1-butyl acetate (fruity and banana-like) is believed to not only enhance the juices overall aroma, but acts as an indicator of volatile changes during maturation (Mehinagic et al., 2016). Interestingly, benzaldehyde was also detected within apple juice which provides a caramel and almond-like flavour. Its presence within the juice can be potentially due to Strecker degradation (the conversion of an α-amino acid into an aldehyde via an imine intermediate) interacting with the beverage's sugars (Coelho et al., 2021).

4.1.1.1 Distribution of Apple Juice Volatiles via Principal Component Analysis

The principal component analysis (PCA) on the associated effect each MIP treatment (coloured dots) had on the apple juice volatiles (red dots) is shown in **Figure 11**. Results showed that the two main principal components (PC1 and PC2) accounted for 78.23% of the total variability in the forty-six apple juice samples, with PC1 accounting for 58.81% and PC2 19.42% respectively.

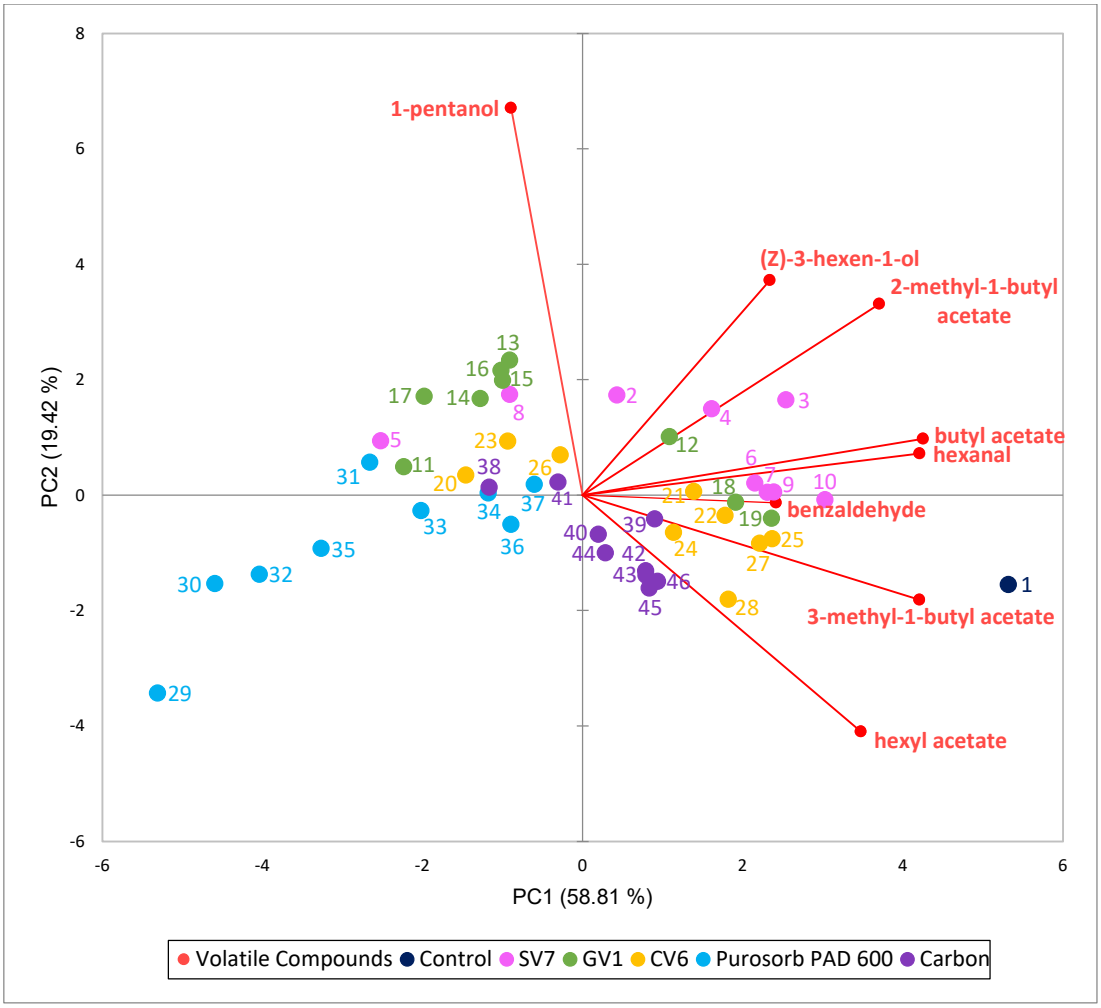


Figure 11. *Principal component analysis (PCA) of volatile compounds (red) in apple juice and the corresponding absorbent material treatments. PC1 representing the first principal component and PC2 for the second principal component.*

As expected, the control (1) sample was positively loaded on PC1 and correlated with most of the volatiles as it is the original (control) product with a high concentration of the key volatile compounds. Among the samples, polymers SV7 (2, 3, 4, 6, 7, 9, 10), CV6 (21, 22, 24–28) and carbon (39, 40, 42–46) have had a more positive association with all volatiles (hexyl acetate, hexanal, butyl acetate, etc.) apart from the alcohol 1-pentanol. These volatile components are shown to heavily dominate PC1, therefore have significant influence on the sensory properties of the apple juice. Since these treatments have retained most of the aroma-active compounds, it can be concluded that they still contain the desirable fruity and sweet characteristics, though at lower levels. The opposite can be said for polymer Purosorb PAD 600 (29–37) and GV1 (11, 13–17), whereby the samples are negatively associated with all available apple volatiles apart from 1-pentanol insinuating that the MIP heavily stripped out essential ester, aldehyde and alcohol components from the beverage potentially impacting the apple juice's sensory prospects. A possible reason for this could be the overall specificity and manufacture of the

polymers which were able to bind and absorb more volatile components from the beverage. Interestingly, apple juice samples treated by both polymers also experienced an increase in 1-pentanol. Kebede et al. (2020) deduced that the alcohol 1-pentanol increases immediately after apple juice processing. The findings concluded that 1-pentanol was a crucial shelf-life indicator for volatile aroma changes triggered by either juice pasteurisation or oxidative reactions during continued storage. With this being said, it is plausible that the high levels of 1-pentanol within Purosorb PAD 600 and GV1 samples could be due to the decrease in other key apple volatiles or that both polymers were the catalyst for chemical reactions during treatment.

4.1.1.2 Agglomerative Hierarchical Clustering Analysis of Apple Juice Samples

In terms of apple juice, the dendrogram shows five well-defined clusters as shown in **Figure 12** below. The first cluster (labelled B) is clearly discernible and is composed mainly of SV7 and some GV1 polymers. It can be deduced that these samples have higher levels of apple VOCs. Two other clusters (A) and (C) share similar characteristics to (B) as they are located on the same clade though at a shorter distance (less than 5 between the main clusters). A group of samples (C) has been established as having similar levels of volatile components with the majority of CV6 and carbon-treated samples being almost identical. This is in agreement with the PCA results in which apple juice treated with SV7, CV6 and carbon samples were positioned at some distance from the others on the biplot. Cluster (A) stands alone so it can be deduced that this sample is substantially different from the distribution of the remaining clusters due to its higher volatile capacity.

The fourth (D) and fifth (E) clusters convey GV1 and Purosorb PAD 600 as polymers that exhibited the least number of apple VOCs due to the distance being greater than 50. This is collaborated by GCMS values in **Table 23**, **Appendix 4** whereby the various samples eight volatile compounds had decreased from the original apple juice sample (1). For instance, compound hexanal for sample 11 (GV1) had a peak area of 34.8% whilst sample 29 (Purosorb PAD 600) had a value of 3.6% compared to that of the control (114.8%). It can be assumed that clusters (B) and (E) are well separated due to the variation of volatile components after treatment whereby polymer SV7 had a less intense process than Purosorb PAD 600 regardless of the dose and flow rates. Hence, the dendrograms ability to produce clear groupings within the samples after analysing their associated characteristics is compelling. Yu et al. (2018) analysed juice volatiles from 13 different citrus fruits (e.g. mandarins, blood and sour oranges) and found the procedure to be quite useful for determining sub-groups within the different citrus varieties.

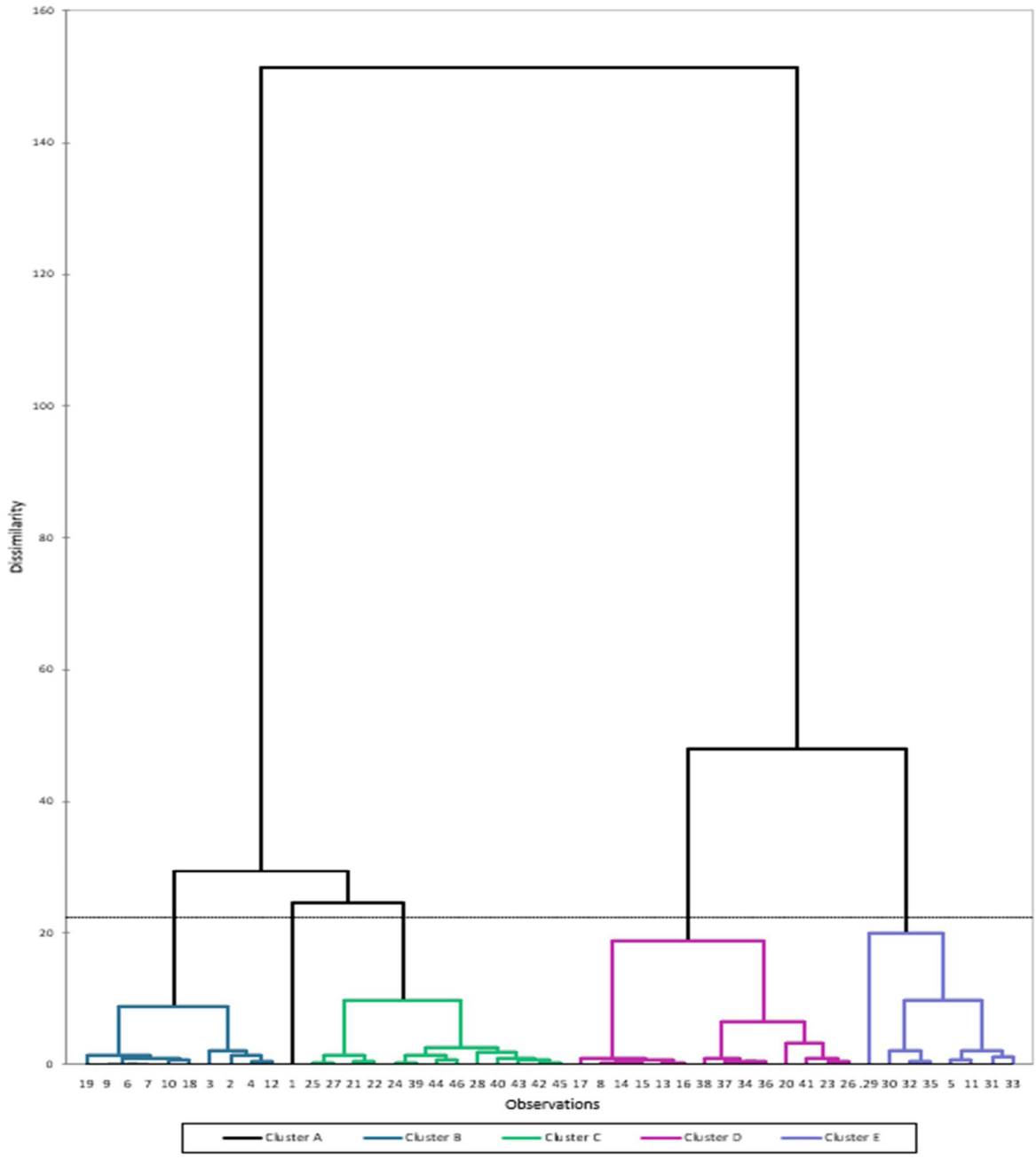


Figure 12. *Dendrogram of hierarchical cluster analysis of treated apple juice with different molecularly imprinted polymers verses control sample.*

4.1.2 Identification of Key Volatiles in Orange Juice Chromatograph

Authors such as Plotto et al. (2004) and Plotto et al. (2008) have already established volatile compounds α-pinene, β-pinene, limonene, 1-octanol, linalool, benzaldehyde and decanal as key organoleptic compounds within orange juice. These compounds were all found in the present work, as shown in the example chromatogram below (**Figure 13**).

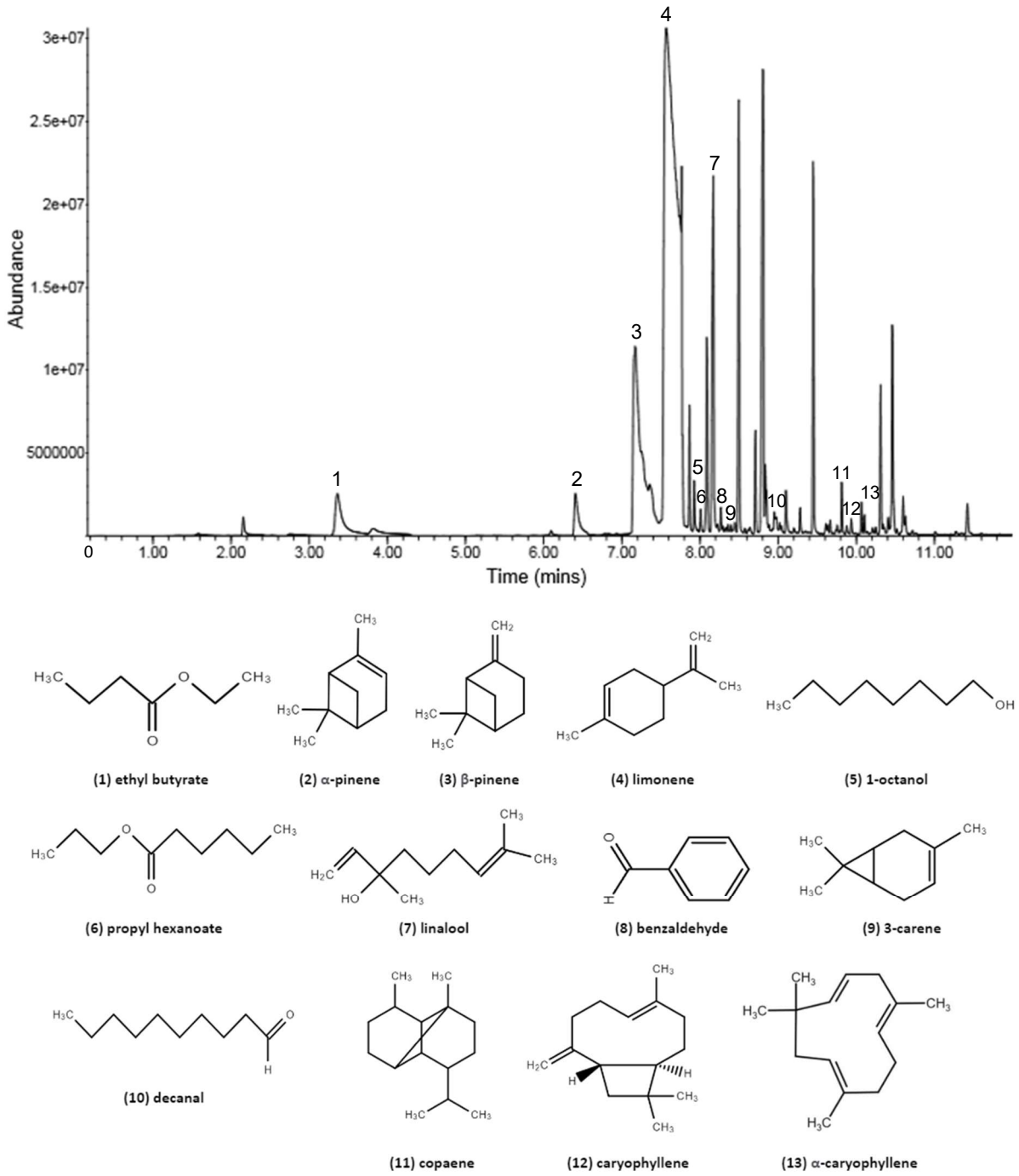


Figure 13. *Chromatogram of untreated orange juice (control) by GCMS-SPME and corresponding skeletal diagrams of the main compounds 1 to 13 detected.*

Ethyl butyrate, although naturally found in citrus fruits has been noted by Pan et al. (2023) to be a food additive as its fragrance is reminiscent of freshly squeezed orange. Copaene on the other hand has been recognised for its distinctive aroma, often imparting a spicy, earthy and dill-like odour. Copaene has been described as one of the principal aroma-active volatiles by Sádecká et al. (2014) as its overall intensity remains unchanged during a 4-month storage period. On the other hand, caryophyllene and α-caryophyllene give the orange juice its characteristic spicy, woody and clove-like

fragrance whilst 3-carene exhibits a turpentine-like and sweet odour (Sádecká et al., 2014; Li et al., 2018). As reported by Vavoura et al. (2022), caryophyllene, α-caryophyllene and 3-carene have been known to enhance the orange flavour in the beverage. To our knowledge, no authors have reported the presence of propyl hexanoate in oranges and orange juice during GCMS analysis. If they have then its significance or the impact it has on the beverage's aroma or flavour characteristics has not been described. However, Oteiza et al. (2014) found that propyl hexanoate (formed during ripening or processing) imparted floral, fruity and sweet notes within apple juice. Considering the nature of hexanoate esters as providers of fruity-based aromas, it can therefore be assumed that propyl hexanoate presents similar characteristics in orange juice.

4.1.2.1 Distribution of Orange Juice Volatiles via Principal Component Analysis

Figure 14 (below) showed that PC1 and PC2 explained 63.24% and 16.10% of the variation in the orange juice data respectively. Similar, to apple juice the PCA biplot, the 13 volatile compounds were positively loaded on PC1, symbolising their overall importance to the beverage's organoleptic properties. It can be noted that the projections for all active variables are significantly lower than both apple and cranberry biplots. This is most likely due to the filtration of the orange juice whereby the pulp/cloud portion was removed as it interfered with MIP treatment. Since the pulp and cloud in of itself contains 80% of all volatile compounds, its removal would cause them to be less prominent within the solution (Perez-Cacho et al., 2008a).

Unlike the apple juice biplot, less samples remained within the lower and upper right quadrants after various MIP treatments. All SV7 treated samples (2–10) maintained the highest proportion of volatile components suggesting that the polymer did not impact the aroma of orange juice as significantly as other MIP treatments. Similar characteristics were exhibited with Purosorb PAD 600 whereby the active observations (namely samples 29–37) had a negative correlation with all orange aroma-active volatiles. As stated previously, the overall formulation of the polymer plays a significant role in how many volatile components are absorbed into its porous structure (Filipe-Ribeiro et al., 2020; Sooraj et al., 2021). In fact, the Purosorb PAD 600's principal applications have been identified as hydrophobic organic species separation, juice debittering and polyphenol extraction by the manufacturers. In this case, the poly(divinylbenzene)-based polymer was able to extract more hydrophobic organic compounds such as linalool, 1-octanol and decanal from the beverage which is reflected in the biplot above.

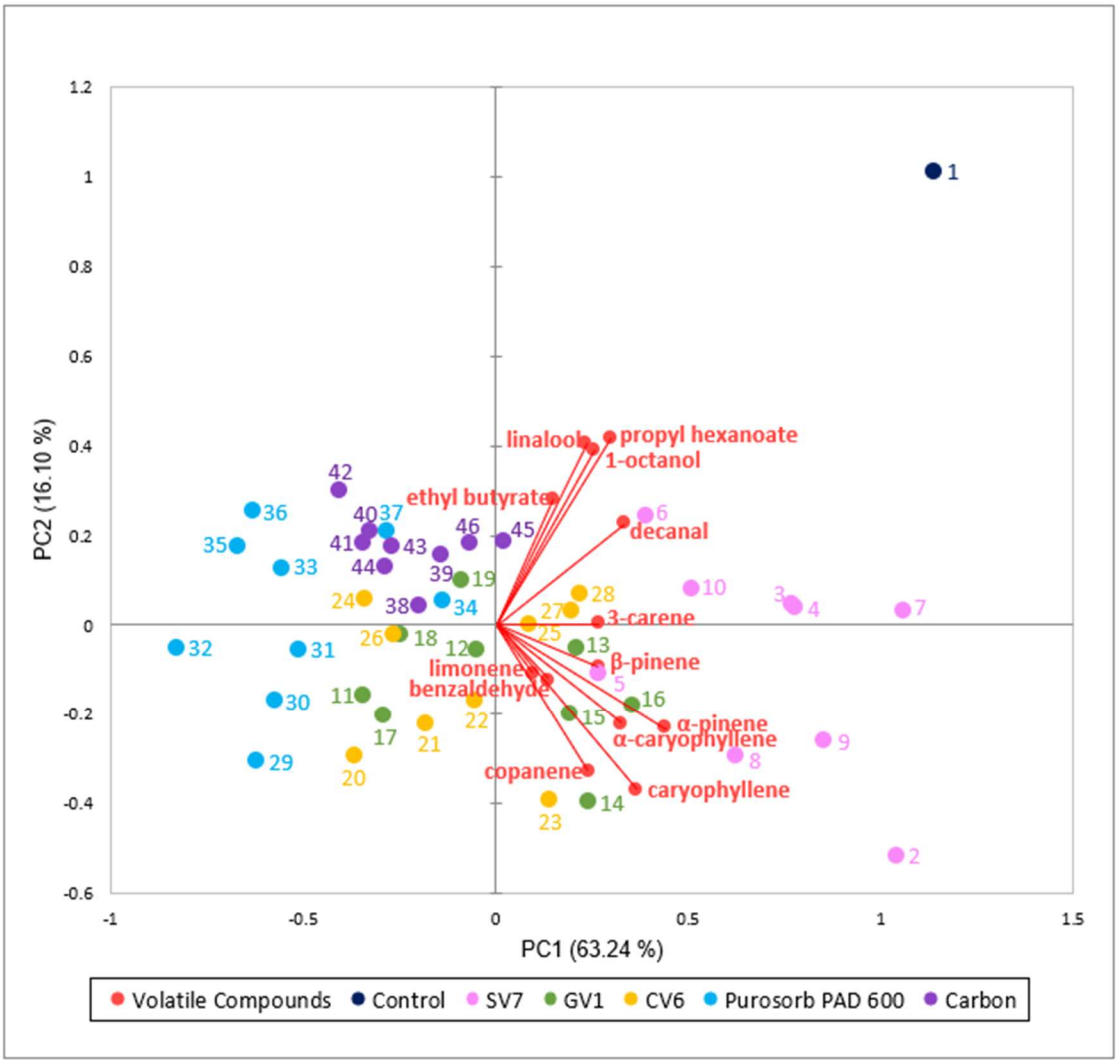


Figure 14. *Principal component analysis (PCA) of volatile compounds (red) in orange juice and the corresponding absorbent material treatments. PC1 representing the first principal component and PC2 for the second principal component.*

Interestingly, the carbon-treated samples (38–46) had a highly negative association – with major decreases in volatile compounds such as limonene, β-pinene and benzaldehyde. This is completely different from the apple juice PCA, whereby all carbon-treated samples had a positive impact on the aroma and flavour. It is unclear as to why this phenomenon has occurred in orange juice, whilst both apple and cranberry juice had a positive correlation with the carbon treatment. Activated carbon is known to successfully reduce the presence of patulin from apple juice whilst significantly improving the colour and clearness of the beverage (Kadakal et al., 2002). In addition to this, Kadakal et al. (2004) also discovered an improvement in the colour and clearness of the juice but several water-soluble vitamins such as ascorbic acid and thiamine were reduced. In saying this, studies done by Pandiarajan et al. (2018) and Ramutshatsha-Makhwedzha et al. (2022) have found that activated carbon derived from orange peels have the ability to adsorb certain dyes (e.g. methylene and methyl orange) and

herbicides. In fact, Pandiarajan et al. (2018) stated that because the fruit peel contains high levels of lignin, cellulose, carboxyl and pectin substances the likelihood of absorbent-adsorbate interactions increases enhancing their overall binding capacity. Hence, it is plausible that some of these components were present within the juice after commercial pressing ultimately interacting with the carbon granules and decreasing the active volatiles within the beverage.

Samples treated with polymers CV6 and GV1, operated similarly, both having positive and negative correlations with the orange juice volatiles. Most notably, GV1 samples 13–16, 23 and CV6 samples 25, 27 and 28 all maintained a decent level of aroma-active volatiles. Generally, higher dose rates and lower flow rates seemed to have impacted the samples more (this is notable in all treated juice samples). For instance, juice treated at a flow rate or dose rate of 15 mL/min and 20g/L respectively, tended to have a decrease in the number of components. This is most likely due to the beverage having more exposure to the MIP beads during this specific treatment. It can be deduced that both polymers have components had to have been manufactured in a similar manner where either the template (target molecule), functional monomer or crosslinker was the cause of their performance.

4.1.2.2 Agglomerative Hierarchical Clustering of Orange Juice Samples

The orange juice dendrogram (**Figure 15** below) shows a completely different trend to apple juice whereby clusters (A), (D) and (E) are grouped together due to their slight similarity to one another. As expected cluster (A) is at a greater distance (> 20) compared with other samples due to it being the original (control) product. SV7 polymers (cluster E) retained the highest amount of VOC's in orange juice (distance of 7) whilst carbon (cluster D) follows closely behind at a Euclidean distance of 3. It is interesting to compare the dendrogram (below) with the PCA biplot (**Figure 14**) as whilst both distinguish key differences, AHC visualises the chemical similarities between samples more holistically than PCA simply due to its analytical use of PC1 and PC2. Patras et al. (2011) had similar findings when classifying the antioxidant and anthocyanin levels of 14 common vegetables and fruits in vitro. The authors discovered that PCA and AHC visualisations differed in green peppers and carrots whilst all others (e.g. red peppers, cranberries) showed consistent patterns and trends. In our results, carbon-treated samples exhibited a negative correlation to SV7-based juice samples in the biplot whilst the dendrogram (below) indicates that carbon samples shared some similarities with SV7 and the control. When comparing the peak area values from **Table 24** (located in **Appendix 4**) the carbon samples only had a slight difference from SV7 samples indicating in some compounds they are closer in nature than the PCA biplot shows. For instance, carbon-treated sample 39 for the volatile limonene had a peak area of 98.2% compared to that of 90.9% for the SV7 sample (3).

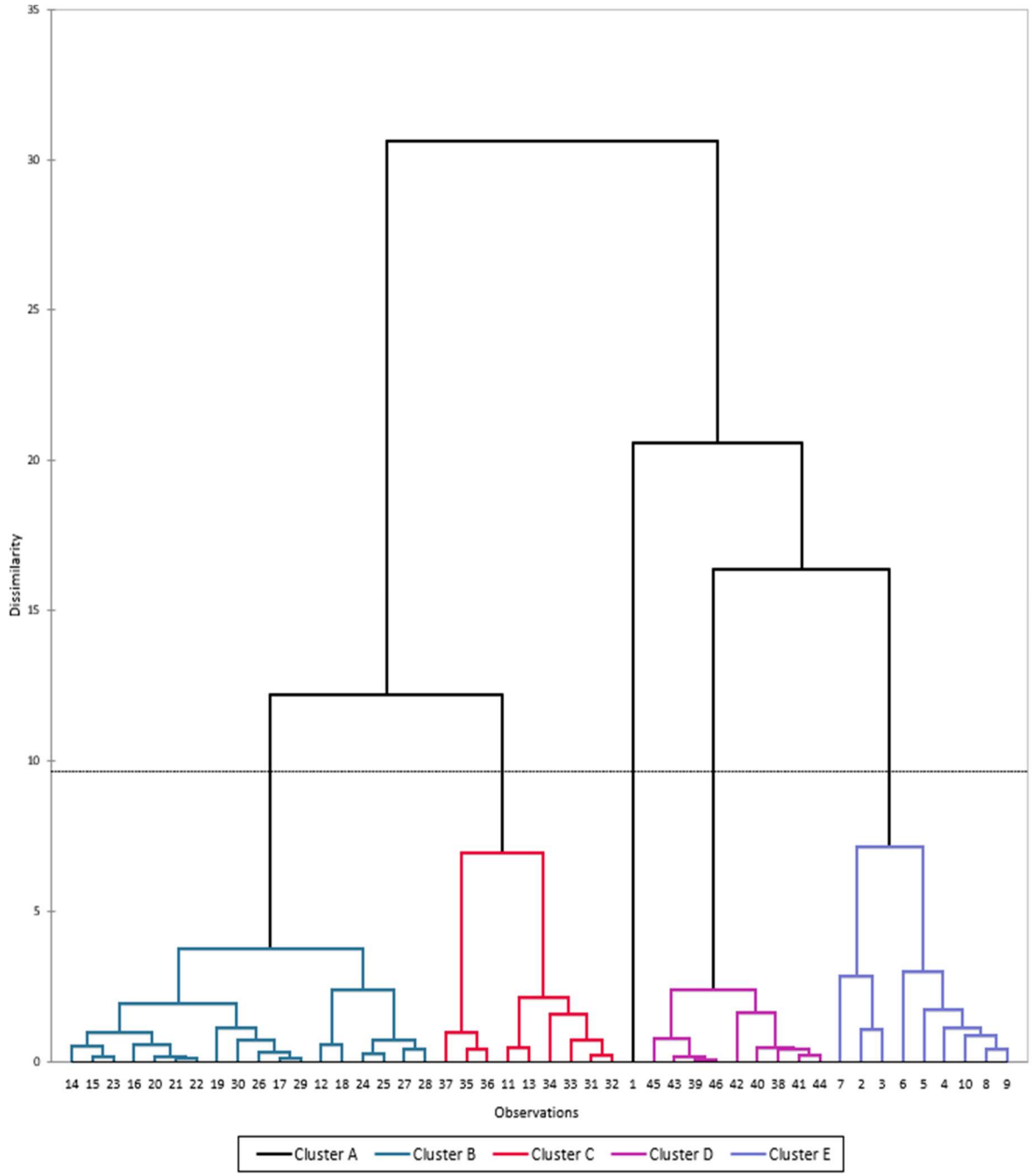


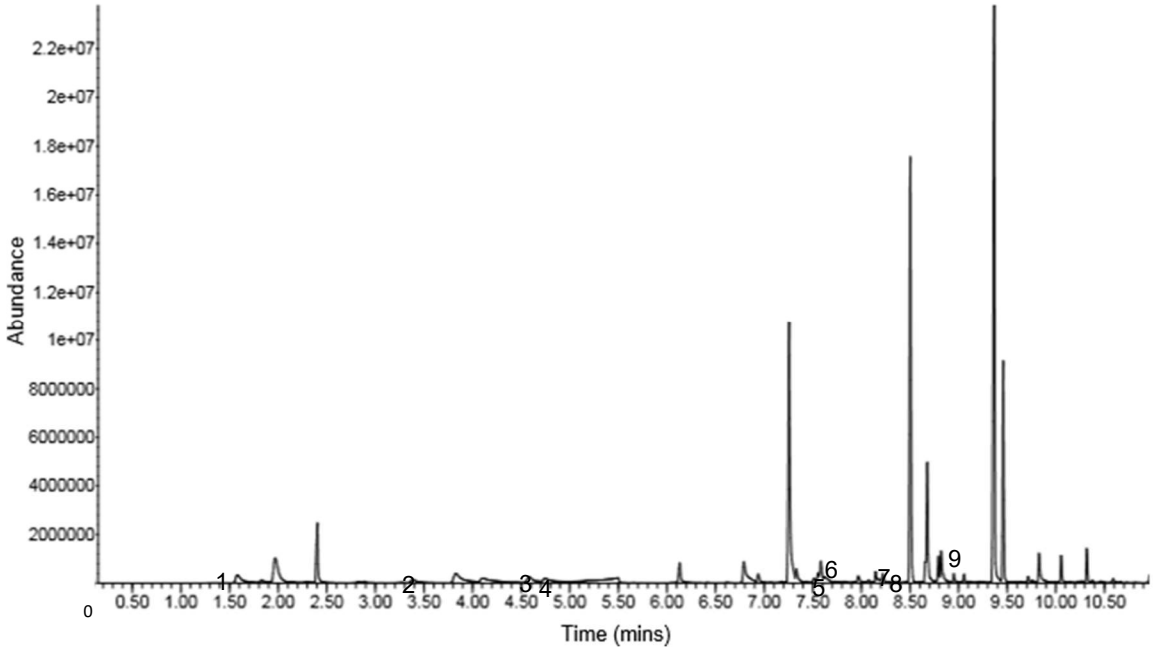
Figure 15. *Dendrogram of hierarchical cluster analysis of treated orange juice with different molecularly imprinted polymers verses the control sample.*

Whilst clusters (A) and (E) maintained relatively high amounts of the 13 orange-based volatiles, cluster (C) treated by Purosorb PAD 600 contained the least. The polymer itself has consistently removed most of the volatile components from all juice types tested. Whilst it is effective in its treatment, the potential of the MIP to reduce key organoleptic profiles within orange juice during sensory may be severe based on the results above. Hu et al. (2015) found their magnetic mesoporous silica

microspheres (MMS) MIPs had larger surface areas to accommodate more recognition sites, excellent selectivity and faster kinetic binding properties that effectively removed folic acid from multiple fruits juices. In addition to this, Zengin et al. (2019) PDMS (poly-dimethylsiloxane)-based MIPs also shared similar properties in its application to remove gallic acid within orange juice. Hence, it can be deduced that depending on the application the MIP is used for, it can perform at its highest capacity. In the case of Purosorb PAD 600 samples, GCMS analysis (**Table 24**, **Appendix 4**) showed that the polymer itself reduced the majority of key peak areas compared with the control sample (1) – especially, at higher contact times. The mixture of polymers GV1 and CV6 in Cluster (B) shows that the treatment wasn't as harsh as Purosorb PAD 600 as exhibited by its < 5 distance. These factors are also reiterated in the PCA biplot (**Figure 14**) with CV6 and GV1 performing almost identically to one another. A potential reason as to why samples 11 to 28 presented in this manner could be because the polymers utilised were manufactured similarity to remove certain orange juice components (e.g. vitamin C and other antioxidants) more so than apple and cranberry.

4.1.3 Identification of Key Volatiles in Cranberry Juice Chromatograph

Compounds ethyl acetate, ethyl butyrate, ethyl-2-methylbutyrate, eucalyptol, linalool, benzaldehyde and benzoic acid listed in **Figure 16** (below) have been identified as aroma-active volatiles that heavily contribute towards the cranberry juice's organoleptic characteristics by authors Zhang et al. (2019a), Zhang et al. (2019a) and Zhu et al. (2016). These volatiles are known to contribute and provide key floral, fruity and fragrant odours to the beverage.



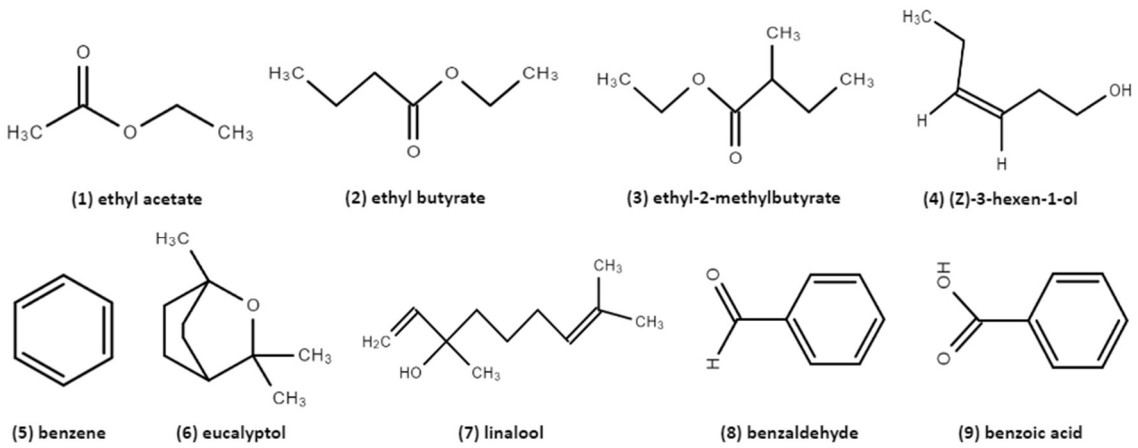


Figure 16. *A chromatogram of untreated cranberry juice (control) by GCMS-SPME and corresponding skeletal diagrams of the main compounds 1 to 9 detected.*

In terms of its presence in cranberry juice, (Z)-3-hexen-1-ol is not as prevalent as other grassy and green-like VOC's (e.g. hexanal, benzaldehyde and (E)-2-hexenal) that contribute more towards the beverage's aroma and flavour (Zhu et al., 2016). It is quite common for majority of fruits (e.g., tomatoes, green kiwifruit, apples) to contain (Z)-3-hexen-1-ol as it contributes leafy and green profiles via the degradation of unsaturated fatty acids whereby the double bond adopts a Z-configuration (Zhu et al. 2016). The compound is often released upon mechanical damage bought about by juice pressing (Zhang et al., 2019a). Hence, the detection of (Z)-3-hexen-1-ol in this case, suggests that the compound is more of a background volatile in cranberry juice. On the other hand, aromatic phenylalanine derivatives such as benzoic acid, benzyl alcohol and benzaldehyde are all derived from the volatile benzene via oxidation (Sater et al., 2020). Given benzene's importance in contributing a sweet and honey-like aroma and for its overall conversion into other vital components, it has been considered by Zhu et al. (2016) and Sater et al. (2020) as being one of the most important VOCs in cranberry-based products such as juice.

4.1.3.1 Distribution of Cranberry Juice Volatiles via Principal Component Analysis

Results from **Figure 17** show that PC1 and PC2 explained 54.44% and 13.59% (68.03% total) of the variation in the data respectively. All volatiles were positively loaded on PC1. Unlike the apple and orange juice PCA analysis, treated cranberry juice samples (active observations) were highly clustered together in the centre of the biplot and not as diverse suggesting that the polymers did not affect the compounds as strongly. Consistently, Purosorb PAD 600 (30 – 37) has had a negative connotation with all active variables throughout its use. Hence, it is of no surprise that the polymer was able to significantly decrease the volatiles from cranberry juice. Majority of the CV6, SV7, GV1 and carbon

polymers were especially similar in their organoleptic properties – with only slight differences in volatile content as indicated in the biplot below and GCMS-SPME data from **Table 25** in **Appendix 4**.

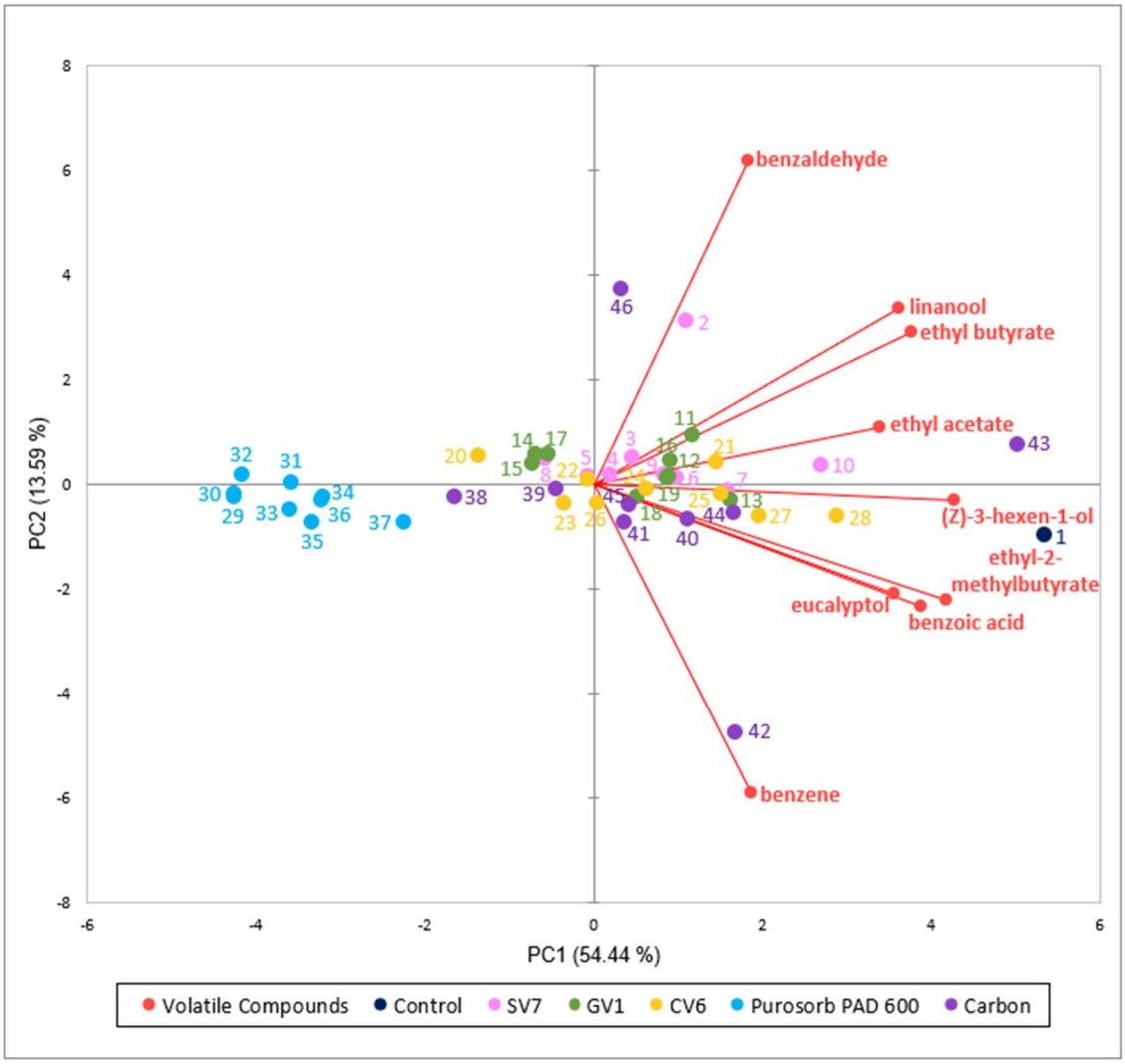


Figure 17. *Principal component analysis (PCA) of volatile compounds (red) in cranberry juice and the corresponding absorbent material treatments. PC1 representing the first principal component and PC2 for the second principal component.*

The outliers 1 (control), 2, 10, 28, 42, 43, and 46 have been distinguished as samples that contain the highest amounts of the 9 identified active variables. The fact that cranberry juice retained more of its volatile components compared to other juices signifies that either the molecularly imprinted polymers weren't manufactured with the right capabilities to effectively remove the aroma-active compounds or the polymers removed other aspects such as tannins and polyphenolic compounds which provide the bitterness and astringency typically exhibited in cranberry-based products. The results obtained in this study contribute to a gap in research of how different molecularly imprinted polymers impact the organoleptic profile of cranberry juices especially as not much is available within literature than

its counterpart's orange and apple juice. According to the current results for all juice types, samples treated with different polymers, dose rates and flow rates were very well distinguished, revealing that the overall impact that these factors have on their organoleptic profile is profound.

4.1.3.2 Agglomerative Hierarchical Clustering of Cranberry Juice Samples

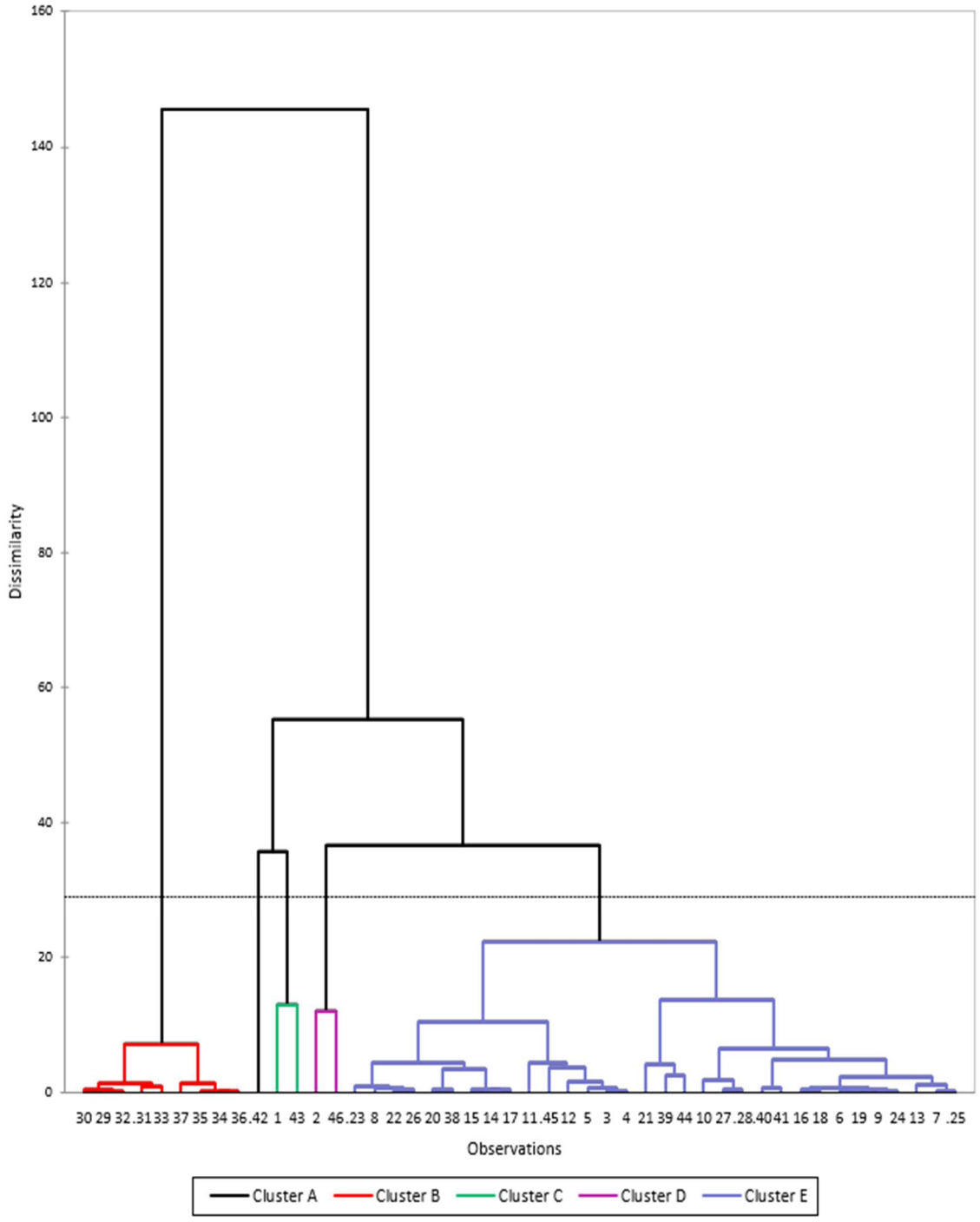


Figure 18. *Dendrogram of hierarchical cluster analysis of treated cranberry juice with different molecularly imprinted polymers verses the control sample.*

From **Figure 18** (above), Cluster (E) contains the majority of the treated samples with a total of 32 (**Table 28**, **Appendix 5**) showing a high number of similarities. Predominantly, this cluster is composed of cranberry samples treated with polymers SV7, GV1, CV6 and carbon. This phenomenon was also present within the PCA biplot (**Figure 17**) whereby the samples were highly compacted together. It can be assumed that these MIPs weren't meant for volatile extraction within cranberry juice which led to its lower performance. In addition to this, Cluster (D) on the other hand grouped samples 2 and 46 together based on similarities in their GCMS peak areas. For instance, the volatile linalool had peak area values of 130% and 124% respectively. Evidence found by Sater et al. (2020) stated that cranberry compounds present in minuscule amounts were still able to heavily influence the qualitative experience of berry aroma and flavour. Therefore, it can be deduced that cranberry juice itself is more robust in nature to physical and chemical changes.

Interestingly, sample 42 (cluster A) which was treated with carbon granules was determined to be significantly different from all other distributions. When looking at the volatile peak areas from **Table 25** (**Appendix 4**), sample 42 displays a high amount of benzene (327.4 %) which could explain its dissimilarity from the others. Similarly, sample 43 (carbon-treated) has been established as being almost identical to the control (1) when in fact the peak areas have an average difference of around 32. Compounds linalool (182.5%), ethyl acetate (136.8%), and ethyl butyrate (141.5%) within sample 43 could have accounted for the similarities to the control. The discrepancies between samples may be due to calculation of peak areas during GCMS analysis which could have offset future data analysis. As expected, the only polymer that exhibited any distinct difference would be Purosorb PAD 600 (cluster B) given that its Euclidean distance is greater than 140. As stated in previous sections, the manufacturing of the polymer would most likely have allowed for more volatile components to be absorbed.

4.2 Sensory Analysis of Apple, Orange and Cranberry Juice

This section will outline and give understanding of the connection between the sensory aspects of the MIP-treated juice samples and its consumer acceptability. Although more consumers ($n \geq 100$) are needed in consumer studies (Kemp et al., 2009) to increase the power of statistical analysis, the low number of participants used in this study due to circumstances beyond the control of the researcher, the number of participants used in this study can still provide overall trends in the sensory data generated as reported by authors Stone et al. (2012) and Moskowitz et al. (2008). So that the objective can pursued, a 9-point hedonic and 10-point intensity scales were employed in order for panellists to rate their level of liking and how strongly they perceived attributes of the six different apple, orange

and cranberry samples. Lawless & Heymann (2010) stated that the implementation of both these scales would not only provide direction for product optimisation but allow for better visualisation of consumer liking of the product with regards to its overall liking. In addition to this as stated by Moskowitz et al. (2008) panellists are able to utilise both hedonic and intensity scales to accurately determine a multitude of sensory attributes on a product either individually (one at a time) or all at once in an evaluation session. The six samples were chosen on the basis of PCA and AHC analysis and informal testing results (located in **Appendix 2**). Predominantly, samples treated with SV7, CV6, GV1 and Purosorb PAD 600 were utilised to better understand their overall effect on the beverages. All carbon-treated samples were excluded from sensory analysis based upon the fact that from informal testing results, the samples were found to have a distinct egg-like smell and unpleasant ashy carbon aftertaste and were thus not well received by the panellists. The juice samples will be discussed individually from one another to determine whether polymers were viable within that beverage as it is expected that the polymers would interact with the various juice's compounds differently.

4.2.1 Analysis of Acceptability for MIP Treated Apple Juice Samples

As indicated in **Table 9**, hedonic ratings for sweetness, tartness, apple flavour and overall liking remained relatively consistent to one another with only slight differences throughout the six different MIP formulations. Ratings for the colour showed significant differences in consumer opinion for all six treated apple juice samples with both sample 1 (6.5 ± 1.9) and sample 3 (6.4 ± 1.7) retaining the characteristic golden hue of the apple juice more than the others. These results suggest that participants tended to like sample 1 (control) and sample 3 (10g/L GV1 COL.1) out of the six evaluated solely based on its colour. On the other side of the spectrum, the lowest mean scored values for apple aroma were samples 2 and 4 with participants rating them from "Dislike slightly" to "Dislike moderately," indicating that the corresponding polymers of SV7 and Purosorb PAD 600 reduced the majority of the crucial aroma-active aldehydes and esters from these samples. As stated by Rita et al. (2011), Niu et al. (2019) and Espino-Díaz et al. (2016) these two compound groups are the dominant chemical groups within intact apples and apple-based products with esters making up about 78 – 92% of total volatiles. Hence, the reduction of identified aldehyde volatiles hexanal, (Z)-3-hexen-1-ol and esters butyl acetate, hexyl acetate, 3-methyl-butyl acetate, and 2-methyl-butyl acetate within samples 2 and 4 would removal crucial 'fruity,' 'green' and 'grassy' fragrances inhibiting the overall sensory experience.

Subsequently, the colour of samples 2, 4, and 6 had lower average hedonic scores of 5.0, 4.3, and 4.8 respectively, suggesting that participants "Neither liked nor disliked" or "Slightly disliked" their colour,

which is most likely due to the pale-yellow hue (almost transparent-like) that the treated samples exhibited. Interestingly, findings from Filipe-Ribeiro et al. (2020) also found a slight reduction (19%) in the colour composition and intensity of red wines – but not enough for participants to voice concern, with values remaining at 3.6 on a scale of 5. It is widely known that during the production of clarified apple juice, significant losses occur in the juice's flavour characteristics, phenolic content and volatile composition (Caillet et al., 2011; Massini et al., 2018). Hence, a potential reason as to why the MIPs heavily impacted the appearance (colour) in this study could be that the overall formulation of the commercial apple juice utilised was not able to fully withstand the treatment process.

Table 9. *Mean scores for **liking** of sensory attributes of the six apple juice samples collected during consumer testing and their corresponding standard error using a 9-point hedonic scale (n = 34).*

Sample No.	Colour	Apple Aroma	Sweetness	Apple Flavour	Tartness	Overall Liking
1	6.5 ± 1.9^{A}	6.8 ± 1.8^{A}	6.8 ± 2.0^{A}	6.6 ± 1.9^{A}	5.6 ± 1.7^{A}	6.2 ± 1.8^{A}
2	5.0 ± 1.6^{BC}	5.9 ± 1.5^{AB}	6.3 ± 1.8^{A}	6.3 ± 1.7^{A}	6.0 ± 1.5^{A}	6.1 ± 1.8^{A}
3	6.4 ± 1.7^{A}	6.5 ± 1.5^{A}	6.7 ± 1.8^{A}	6.5 ± 1.5^{A}	6.1 ± 1.6^{A}	6.4 ± 1.7^{A}
4	4.3 ± 1.9^{C}	5.0 ± 1.7^{B}	5.6 ± 1.8^{A}	5.5 ± 1.7^{A}	5.2 ± 1.5^{A}	5.3 ± 1.9^{A}
5	6.1 ± 1.3^{AB}	6.6 ± 1.7^{A}	6.6 ± 1.8^{A}	6.6 ± 1.4^{A}	5.8 ± 1.6^{A}	6.1 ± 1.8^{A}
6	4.8 ± 1.4^{C}	6.3 ± 1.6^{A}	6.8 ± 1.8^{A}	6.6 ± 1.4^{A}	5.8 ± 1.7^{A}	6.2 ± 1.5^{A}

Note. Statistical differences were tested using ANOVA and Tukey's honesty significant difference (HSD) post hoc test. Different letters in each column indicate statistically significant difference among the samples at $p < 0.05$. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.1, (3) 10g/L GV1 COL.1, (4) 20g/L Purosorb PAD 600 COL.1, (5) 10g/L CV6 COL.2 and (6) 20g/L CV6 COL.2.

Table 10. *Mean scores of sensory attribute **intensities** of the six apple juice samples collected during consumer testing and their corresponding standard error using a 10-point line scale (n = 34).*

Sample No.	Apple Aroma Intensity	Sweetness Intensity	Apple Flavour Intensity	Tartness Intensity
1	6.9 ± 1.8^{A}	5.6 ± 1.9^{A}	6.5 ± 1.4^{A}	4.7 ± 2.4^{A}
2	4.8 ± 2.5^{BC}	5.9 ± 2.1^{A}	5.5 ± 2.0^{AB}	4.1 ± 1.8^{A}
3	6.1 ± 2.2^{AB}	6.0 ± 1.8^{A}	6.4 ± 1.8^{A}	4.9 ± 2.1^{A}
4	3.6 ± 2.3^{C}	5.3 ± 2.0^{A}	4.8 ± 2.1^{B}	4.3 ± 2.2^{A}
5	6.2 ± 2.2^{AB}	6.0 ± 1.8^{A}	6.5 ± 1.9^{A}	4.5 ± 2.2^{A}
6	5.4 ± 2.1^{AB}	5.8 ± 1.8^{A}	6.2 ± 1.7^{A}	4.6 ± 2.0^{A}

Note. Statistical differences were tested using ANOVA and Tukey's honesty significant difference (HSD) post hoc test. Different letters in each column indicate statistically significant difference among the samples at $p < 0.05$. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.1, (3) 10g/L GV1 COL.1, (4) 20g/L Purosorb PAD 600 COL.1, (5) 10g/L CV6 COL.2 and (6) 20g/L CV6 COL.2.

The difference in acceptability for each sample resulted from both the apple aroma and appearance (colour) more than anything else, which in turn may be influenced by the chemical changes from external factors such as the MIPs. Hence, a common trend that was shown in these results was that

panellists liked a golden colour and strong fruity aroma to their apple juice than a pale-yellow product that had no aroma. This is also corroborated in **Table 10** (above) whereby participants rated the intensity of certain attributes from 0 (low) to 10 (high). A closer examination of both the apple aroma and flavour intensities for samples 2 and 4 showcases a difference from all other samples with values of 4.8 and 3.6 for apple aroma and 5.5 and 4.8 for apple flavour respectively. These ratings reiterate the fact that these MIPs would not be as suitable for commercial use for apple juice as they drastically change the total composition of the final product unless much lower contact times are taken into consideration. These results also corroborate the findings of Moskowitz et al. (2008) whereby untrained participants are able to rate the sensory attributes in a comprehensive manner without the need of extensive training in both the intensity of the stimulus and its overall likeability. Furthermore, Stone et al. (2012) also stated that intensity scales of this nature are approximately equal in reliability with other standard scales for untrained individuals.

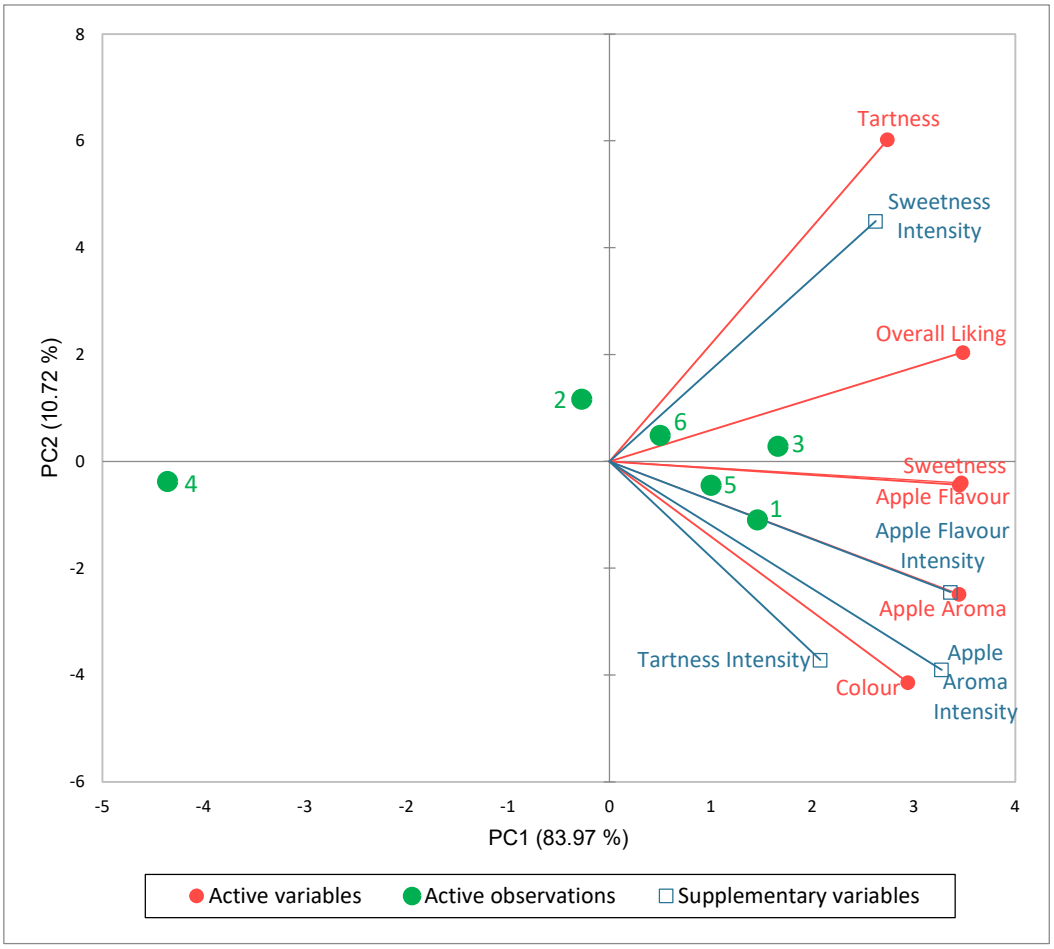


Figure 19. *Principal component analysis (PCA) biplot of the six selected apple juice samples. Supplementary variables are the intensity which were overlaid on the hedonic variables. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.1, (3) 10g/L GV1 COL.1, (4) 20g/L Purosorb PAD 600 COL.1, (5) 10g/L CV6 COL.2 and (6) 20g/L CV6 COL.2.*

For a better visual understanding of all hedonic and intensity attributes in relation to the six different MIP samples a PCA biplot was generated and is shown in **Figure 19** above. Results showed that the two main principal components (PC1 and PC2) accounted for 94.69% of the total variability in the six apple juice samples, with PC1 accounting for 83.97% and PC2 10.72% respectively. The liking for the fruit's apple aroma, apple flavour, colour, sweetness as well as overall liking were attributed to PC1, whilst the tartness and tartness intensity vectors contributed largely to the discrimination on PC2. Upon further investigation, the majority of the samples (1, 3, 5 and 6) were all positively associated with all hedonic and intensity attributes. The overall liking was, in turn, more positively associated with the intensity of sweetness and tartness perception in the upper right quadrant along the PC1 axis. This is in agreement with previous PCA and AHC analysis done on the relationship between the eight apple volatiles and the treated samples whereby GV1 and CV6 retained some of the highest amounts of each compound. A comparison of the different treatments (20g/L verses 10g/L) for CV6 shows that the corresponding dose rates affected the sensory attributes, with sample 5 having a higher proportion of colour, apple aroma, apple flavour and sweetness than sample 6. Hence, it can be concluded that the volume or amount of product that is passed through the MIPs can alter the sensory profile by a decent amount but does not alter the juice significantly to which the esters present are completely removed.

Curiously, sample 2 which was treated with the SV7 polymer performed slightly lower in comparison to previous PCA and AHC findings where it was shown to retain the most aroma-active volatiles. It can be concluded that the panellists simply did not like the colour of sample 2 as indicated in their ratings in **Table 9** and from comments from some participants (**Table 29** in **Appendix 6**) attributing the lack of apple aroma and its unappealing pale colour (appearance) to its low rating. As stated by Moskowitz et al. (2008) descriptive commentary in connotation with participants overall liking ratings provides valuable information on sensory characteristics as well as research guidance. In addition to this, most of the participants agreed that sample 4 (treated with polymer Purosorb PAD 600) had the least amount of apple aroma, apple flavour and colour with several comments stating its pale colour, nondescript odour and weak flavour for its poor performance. From **Figure 19**, sample 4 was also negatively correlated with all corresponding hedonic and intensity sensory attributes as it was on the opposite side of these variables on the PCA biplot. These results confirm the findings from GCMS, PCA and AHC analysis whereby Purosorb PAD 600 removed the majority of the VOCs from apple juice only leaving behind "diluted sugar water." This phenomenon may have been due to the addition of other additives to make up for the loss of natural sugars after juice pressing and pasteurisation (Caillet et al., 2011). Ultimately, its overall utilisation in juice applications could use some improvement whereby

less contact time (i.e. a higher flow rate or lower dose rate) is needed in order to maintain a more holistic sensory experience.

4.2.2 Analysis of Acceptability for MIP Treated Orange Juice Samples

As indicated in **Table 11** and **Table 12**, all of the hedonic and intensity ratings remained within a range of 5.1 to 6.3 with ANOVA showing no significant differences ($p > 0.05$). These results indicate panellists did not perceive any significant differences between the six orange juice samples evaluated with most of the hedonic scores ranging from "Neither like nor dislike" and "Like slightly" suggesting that participants were neutral about the liking of samples. With the scores being so close together on the intensity and hedonic scales it can be deduced that the samples were either similar in terms of acceptability and intensity or the sample size was too low to show any significant differences between the six orange juice products. A potential reason as to why participants had difficulty in relation to the six orange juice samples could be due to the filtration of the orange juice prior to MIP treatment as small bits off pulp restricted the flow of the beverage during processing which would have left behind a more artificial tasting product. More specifically, Perez-Cacho et al. (2008a) reported that 80% of volatile content remains within both the serum and pulp portion. Hence, the removal of the sediment would have had impacted the organoleptic properties of the orange juice even before treatment with the MIPs creating a sample that was not representative of the original product used.

Table 11. *Mean scores for **liking** of sensory attributes of the six orange juice samples collected during consumer testing and their corresponding standard error using a 9-point hedonic scale (n = 35).*

Sample No.	Colour	Orange Aroma	Sweetness	Orange Flavour	Sourness	Overall Liking
1	6.1 ± 1.6^{A}	6.0 ± 1.7^{A}	5.7 ± 1.7^{A}	6.2 ± 1.7^{A}	6.2 ± 1.6^{A}	6.2 ± 1.7^{A}
2	6.1 ± 1.7^{A}	6.1 ± 1.5^{A}	5.9 ± 1.4^{A}	6.3 ± 1.5^{A}	6.1 ± 1.3^{A}	6.1 ± 1.5^{A}
3	5.6 ± 1.7^{A}	5.7 ± 1.7^{A}	5.7 ± 1.5^{A}	5.8 ± 1.6^{A}	6.0 ± 1.3^{A}	5.9 ± 1.4^{A}
4	6.3 ± 1.4^{A}	6.3 ± 1.3^{A}	5.8 ± 1.7^{A}	6.1 ± 1.6^{A}	6.2 ± 1.6^{A}	6.2 ± 1.7^{A}
5	5.3 ± 1.6^{A}	6.0 ± 1.6^{A}	6.0 ± 1.6^{A}	6.2 ± 1.4^{A}	5.9 ± 1.3^{A}	5.9 ± 1.6^{A}
6	5.9 ± 1.7^{A}	5.9 ± 1.4^{A}	5.5 ± 1.6^{A}	6.2 ± 1.5^{A}	5.8 ± 1.3^{A}	5.8 ± 1.6^{A}

Note. Statistical differences were tested using ANOVA and Tukey's honesty significant difference (HSD) post hoc test. Different letters in each column indicate statistically significant difference among the samples at $p < 0.05$. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.1, (3) 10g/L GV1 COL.1, (4) 20g/L SV7 COL.2, (5) 20g/L GV1 COL.2 and (6) 10g/L Purosorb PAD 600 COL.1.

Table 12. *Mean scores of sensory attribute **intensities** of the six orange juice samples collected during consumer testing and their corresponding standard error using a 10-point line scale (n = 35).*

Sample No.	Orange Aroma Intensity	Sweetness Intensity	Orange Flavour Intensity	Sourness Intensity
1	5.4 ± 2.4^{A}	5.1 ± 2.0^{A}	6.0 ± 1.8^{A}	5.3 ± 2.2^{A}

2	5.9 ± 2.1^{A}	5.5 ± 1.8^{A}	6.2 ± 1.6^{A}	5.5 ± 2.2^{A}
3	5.4 ± 2.0^{A}	5.7 ± 1.6^{A}	5.7 ± 1.7^{A}	5.4 ± 1.9^{A}
4	5.7 ± 2.0^{A}	5.7 ± 2.0^{A}	5.7 ± 2.1^{A}	4.6 ± 2.1^{A}
5	5.3 ± 1.9^{A}	5.7 ± 2.2^{A}	6.0 ± 1.3^{A}	5.5 ± 2.1^{A}
6	5.3 ± 2.0^{A}	5.8 ± 1.8^{A}	5.8 ± 1.6^{A}	5.2 ± 2.0^{A}

Note. Statistical differences were tested using ANOVA and Tukey's honesty significant difference (HSD) post hoc test. Different letters in each column indicate statistically significant difference among the samples at $p < 0.05$. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.1, (3) 10g/L GV1 COL.1, (4) 20g/L SV7 COL.2, (5) 20g/L GV1 COL.2 and (6) 10g/L Purosorb PAD 600 COL.1.

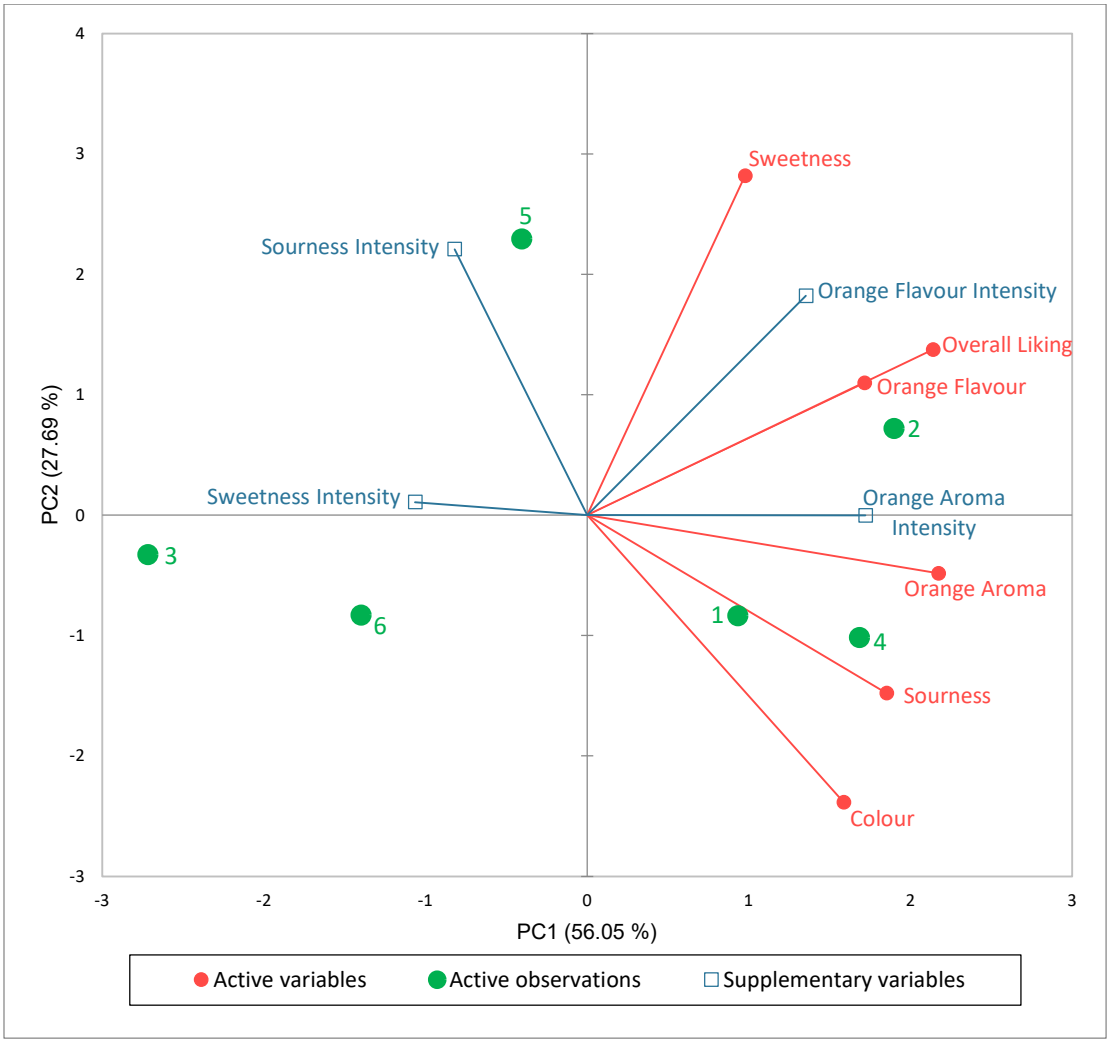


Figure 20. *Principal component analysis (PCA) biplot of the six selected orange juice samples. Supplementary variables are the intensity which were overlaid on the hedonic variables. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.1, (3) 10g/L GV1 COL.1, (4) 20g/L SV7 COL.2, (5) 20g/L GV1 COL.2 and (6) 10g/L Purosorb PAD 600 COL.1.*

Although hedonic and intensity results were similar there is still an underlying pattern to be obtained from the orange juice data generated. As reported by Moskowitz et al. (2008) and Stone et al. (2012) a small sample size number is adequate for preliminary project phases whilst giving general direction and insight for future analysis. As established in **Figure 20** (above), PC1 and PC2 explained 56.05% and

27.69% (83.74% total) of the variability in the data respectively. The biplot shows that sweetness, orange flavour, and orange flavour intensity contributed significantly to the variation in the PC1 (in the upper right quadrant) and were positively related to overall liking. In contrast, orange aroma, orange aroma intensity, sourness and the colour were all positively loaded on PC1 in the lower right quadrant and were negatively correlated with the intenseness of both sourness and sweetness.

From the PCA it can be revealed that samples 2 and 4 had comparatively high scores of all positive attributes than 3, 5 and 6. On this basis, it provides an indication that most consumers are more likely to reject orange juice samples that were too sweet and too sour. Sample (6) treated with Purosorb PAD 600 was located diagonally in relation to sweetness, orange flavour intensity and overall liking, indicating that the sample was low in these attributes. Thus, it was impacted negatively overall with a lower association to these key attributes and liking. Previous PCA and AHC analysis on the 13 aroma-active volatiles via GCMS also confirmed that the polymer was able to decrease the total VOCs content within orange juice by a significant amount. Given its high sorption rate and exceptional binding properties its overall performance in separating these compounds was much more formidable than any of the other MIPs utilised during testing. Compellingly, sample 5 processed by polymer GV1 was also negatively associated with all other attributes having a comparatively high sourness intensity. As expected, both SV7 samples (2 and 4) had a comparatively higher appearance (colour), orange flavour, orange aroma and sweetness even surpassing the control (1). As documented in GCMS analysis, out of all the MIPs utilised, SV7 retained the most volatiles within the orange juice samples. Hence, solely based on its performance the SV7 polymer is the more viable option.

4.2.3 Analysis of Acceptability for MIP Treated Cranberry Juice Samples

From **Table 13**, in all six cranberry samples evaluated, the hedonic ratings for colour, sweetness, tartness, bitterness, cranberry flavour, astringency and overall liking shared similar values of around 5.2 to 6.7. Overall, the ratings were predominantly between 5 and 7 suggesting that consumer liking ranged from “Neither like nor dislike,” to “Like moderately”. The only significant difference detected was with the cranberry aroma. Given sample 4 is rated far lower compared to all others suggests the polymer Purosorb PAD 600 removed key aroma-active cranberry volatiles as shown in previous GCMS data which is reflected in the hedonic sensory results. Sample 6 treated with GV1 on the other hand, only had a slight difference of 0.9 from the control (1) demonstrating that participants could still detect the aroma, though it may have been less prominent.

Table 13. *Mean scores for **liking** of sensory attributes of the six cranberry juice samples collected during consumer testing and their corresponding standard error using a 9-point hedonic scale (n = 34).*

Sample No.	Colour	Cranberry Aroma	Sweet-ness	Tartness	Bitterness	Cranberry Flavour	Astringency	Overall Liking
1	6.1 ± 1.8^{A}	6.6 ± 1.6^{A}	5.3 ± 2.0^{A}	5.5 ± 1.5^{A}	5.7 ± 1.5^{A}	6.3 ± 1.4^{A}	5.2 ± 1.4^{A}	6.0 ± 1.7^{A}
2	6.2 ± 1.5^{A}	6.3 ± 1.3^{A}	5.9 ± 1.8^{A}	6.2 ± 1.7^{A}	5.9 ± 1.4^{A}	6.7 ± 1.1^{A}	5.6 ± 1.4^{A}	6.2 ± 1.6^{A}
3	5.9 ± 1.7^{A}	6.2 ± 1.4^{A}	5.3 ± 1.8^{A}	5.7 ± 1.7^{A}	5.5 ± 1.4^{A}	6.3 ± 1.5^{A}	5.3 ± 1.6^{A}	5.3 ± 2.0^{A}
4	5.5 ± 1.7^{A}	4.9 ± 1.7^{B}	5.5 ± 1.6^{A}	5.5 ± 1.5^{A}	5.4 ± 1.5^{A}	5.7 ± 1.6^{A}	5.4 ± 1.6^{A}	5.3 ± 1.6^{A}
5	6.1 ± 1.8^{A}	6.2 ± 1.5^{A}	5.6 ± 1.6^{A}	5.2 ± 1.5^{A}	5.4 ± 1.3^{A}	6.0 ± 1.6^{A}	5.0 ± 1.5^{A}	5.4 ± 1.5^{A}
6	6.1 ± 1.6^{A}	5.7 ± 1.4^{AB}	5.8 ± 1.3^{A}	5.9 ± 1.4^{A}	5.7 ± 1.4^{A}	6.5 ± 1.1^{A}	5.6 ± 1.5^{A}	5.9 ± 1.6^{A}

Note. Statistical differences were tested using ANOVA and Tukey's honesty significant difference (HSD) post hoc test. Different letters in each column indicate statistically significant difference among the samples at $p < 0.05$. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.2, (3) 10g/L GV1 COL.2, (4) 10g/L Purosorb PAD 600 COL.1, (5) 20g/L CV6 COL.3 and (6) 20g/L GV1 COL.2.

Table 14. *Mean scores of sensory attribute **intensities** of the six cranberry juice samples collected during consumer testing and their corresponding standard error using a 10-point line scale (n = 34).*

Sample No.	Cranberry Aroma Intensity	Sweetness Intensity	Tartness Intensity	Bitterness Intensity	Cranberry Flavour Intensity	Astringency Intensity
1	6.6 ± 2.1^{A}	6.1 ± 2.4^{A}	6.1 ± 2.5^{A}	4.2 ± 2.4^{A}	6.7 ± 1.5^{A}	4.3 ± 2.7^{A}
2	5.6 ± 2.3^{AB}	6.3 ± 2.3^{A}	5.5 ± 2.0^{A}	3.6 ± 2.5^{A}	6.1 ± 1.9^{AB}	5.1 ± 2.9^{A}
3	4.9 ± 2.2^{BC}	6.0 ± 2.4^{A}	6.0 ± 2.2^{A}	4.1 ± 2.0^{A}	5.6 ± 2.3^{AB}	5.1 ± 2.4^{A}
4	3.5 ± 2.3^{C}	6.1 ± 2.2^{A}	5.3 ± 2.2^{A}	3.5 ± 2.3^{A}	5.0 ± 2.3^{B}	5.3 ± 2.4^{A}
5	5.8 ± 2.2^{AB}	6.2 ± 2.5^{A}	5.4 ± 2.9^{A}	3.9 ± 2.3^{A}	5.5 ± 1.9^{AB}	4.8 ± 2.7^{A}
6	4.5 ± 2.3^{BC}	5.7 ± 2.1^{A}	5.2 ± 2.1^{A}	3.1 ± 2.0^{A}	5.8 ± 1.7^{AB}	4.9 ± 2.4^{A}

Note. Statistical differences were tested using ANOVA and Tukey's honesty significant difference (HSD) post hoc test. Different letters in each column indicate statistically significant difference among the samples at $p < 0.05$. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.2, (3) 10g/L GV1 COL.2, (4) 10g/L Purosorb PAD 600 COL.1, (5) 20g/L CV6 COL.3 and (6) 20g/L GV1 COL.2.

On closer inspection, significant differences ($p < 0.05$) were observed in both the aroma and flavour intensities of the samples as shown in **Table 14**. Several participants indicated that sample 4 had a lack of aroma with one comment stating it smelt like playdough (**Table 31** in **Appendix 6**). This is corroborated by the lower rating of 3.5 ± 2.3 on the intensity scale. Subsequently, the overall flavour in this sample was rated at a 5.0 ± 2.3 with participants indicating that the astringent, sour and sweet attributes were masking and overpowering its potency. Removal of key aroma and flavour compounds (e.g. benzene, benzenic acid and (Z)-3-hexen-1-ol) could have played a significant role in its low ratings with the balance of flavours being out of alignment (Caillet et al., 2011; Gu et al., 2022). As stated by Reed et al. (2006), tannins, which are responsible for the astringency and bitter notes would have increased due to the elimination of these key aldehydes, alcohols and esters. It is known that additional sugars are present within cranberry juice and cranberry-based products to combat the overall tartness the fruit produces which is potential reason as to why panellists could still taste a higher amount of sweetness in not only sample 4 but all others treated (Blumberg et al., 2013). Sample 3, 5 and 6 were similar in cranberry intensity but overall, the polymer did not extract as much VOCs

from the juice and was able to maintain the flavour profiles more. Ratings for sample 2 (SV7) showed only a small difference between the control (1) demonstrating that this treatment performed relatively better than polymers GV1, CV6 and Purosorb PAD 600.

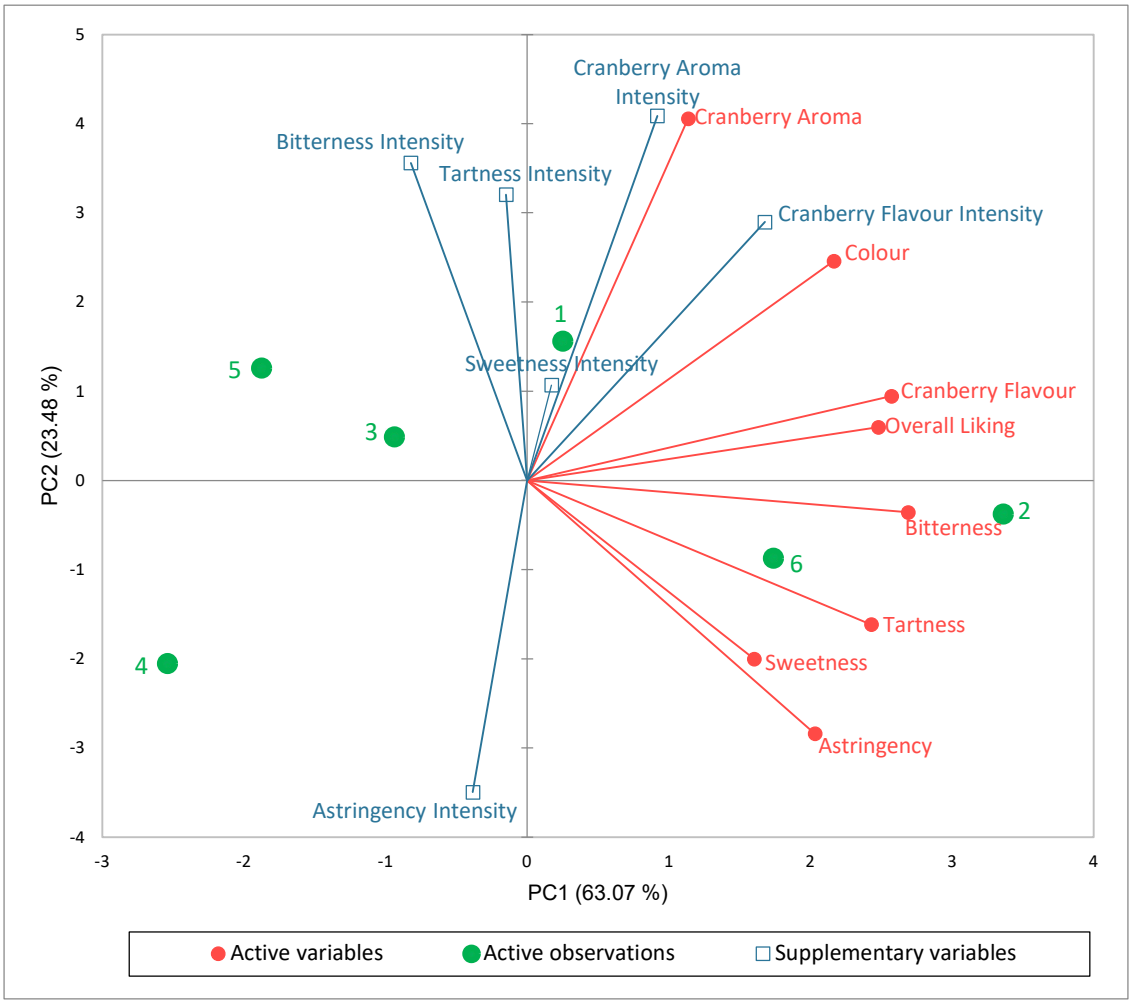


Figure 21. *Principal component (PCA) biplot of the six selected cranberry juice samples. Supplementary variables are the intensity which were overlaid on the hedonic values. Sample numbers correlate as follows (1) control, (2) 10g/L SV7 COL.2, (3) 10g/L GV1 COL.2, (4) 10g/L Purosorb PAD 600 COL.1, (5) 20g/L CV6 COL.3 and (6) 20g/L GV1 COL.2.*

The cranberry juice biplot (**Figure 21**) accounted for 86.55% of the total variability within the data with PC1 and PC2 being 63.07% and 23.48% respectively. Given its ability to remove majority of critical volatile components from the beverage, sample 4 treated with Purosorb PAD 600 was negatively associated with liking for colour, cranberry aroma, cranberry flavour and overall liking. However, it was rated high in astringency intensity. As indicated from panellists' commentary in **Table 31** (**Appendix 6**), the relationship between sample 4 and the intensity of the astringency (located in the lower left quadrant) directly correlates with participants' dislike of the sample because of its dry and ashy aftertaste. Authors Zhu et al. (2016) and Reed et al. (2006) stated that cranberry juice often

displays a dry aftertaste due to the tannins within the fruit. Descriptive commentary of this nature, is known to be crucial in the understanding of participants overall liking of the product providing relevant information on sensory characteristics (Moskowitz et al., 2008). Samples 3 (10g/L GV1 COL.2) and 5 (20g/L CV6 COL.3) were associated with both the intensity of bitterness and tartness. When looking at the corresponding GCMS values and PCA analysis on the interaction between these compounds it can be shown that CV6 and GV1 were similar in their performance. It can be concluded that participants liked sample 2 to any of the MIP treated samples solely based on its cranberry flavour, colour, tartness, bitterness, sweetness, astringency and overall liking. Hence, it can be concluded the sample treated by SV7 was able to maintain more volatile components which in turn made the sensory experience more positive.

5. Conclusions

The following study was to determine whether MIPs were viable to modify the organoleptic properties of existing fruit-based beverages on the current market. The acceptability and organoleptic attributes of apple, orange and cranberry juice were assessed via participants during sensory evaluation. In general, the results indicated that the polymer SV7 was the most liked treatment in orange and cranberry juice whilst polymer GV1 was more liked within apple juice. These MIPs were able to maintain the overall organoleptic properties (i.e. flavour, aroma and colour) typically reserved in the original product, though at slightly lower levels. The polymer CV6 performed adequately however lower contact times is needed in order for consumers to have a more holistic sensory experience. This is due to participants detecting bitter and astringent-notes within cranberry and drastic colour and aroma changes in apple juice. Among the six samples for apple, orange and cranberry juices, Purosorb PAD 600 (resin) far exceeded in its performance to remove volatile components with panellists labelling the sample as being diluted with a general lack of colour, flavour and aroma. Even though the hedonic and intensity ratings between all the samples were quite small – especially for orange juice, participants were still able to detect and describe slight differences within the MIP treated samples and the commercial resin showing an overall trend in the sensory data generated.

Even though this work has certain limitations including a small sample size (34 – 35 individuals), varying consumer perceptions and demographics for each juice type, the results have still provided insight into the modification of juices for potential commercialisation within industry. Additionally, the experimental techniques developed in this research could be utilised in future comparisons by others contributing to the effects that these polymers have on different beverages sensory characteristics. Further studies could investigate the impact of MIP processing on the colour changes as although participants described this phenomenon occurring no other experimental procedure was utilised to verify how much the colour had changed – particularly in apple juice samples. Other pertinent studies that could be done is to test more juices (e.g. pomegranate or feijoa) on the global market which could even expand into alcoholic beverages such as cider and beer. The deterioration of the carbonation of cider and beer after MIP treatment, however, will need to be taken into consideration by potentially reintroducing carbon dioxide back into the product. The relationship between polyphenolic compounds (e.g. quercitrin and catechins) with the MIPs could also provide further understanding of how they would affect a beverages sensory profile. Finally, a broader range of contact and exposure times of the MIP when the beverage is processed would help pinpoint exact parameters for manufactures to work with. Specifically tailoring this would broaden the consumers preferences more and increase their overall acceptability of the product.

6. References

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7. Endnotes

[1] Adapted from "Molecularly Imprinted Polymers: Present and Future Prospective," by G. Vasapollo, R. D. Sole, L. Mergola, M. R. Lazzoi, A. Scardino, S. Scorrano and G. Mele, 2011, *International Journal of Molecular Sciences, 12*(9), p. 5908-5945. Copyright 2011 by Creative Commons Attribution. Adapted with permission. https://creativecommons.org/licenses/by/3.0/

[2] Adapted from "Molecularly-Imprinted SERS: A Potential Method for Bioanalysis," by H. A. Wisnuwardhani, S. Ibrahim, R. R. Mukti and S. Damayanti, 2022, *Scientia Pharmaceutica, 90*(3), p. 54. Copyright 2022 by Creative Commons Attribution. Adapted with permission. https://creativecommons.org/licenses/by/4.0/

[3] Adapted from "Membrane-based Operations in the Fruit Juice Processing Industry: A review," by C. Conidi, R. Castro-Muñoz and A. Cassano, 2020, *Beverages, 6*(1), p. 18. Copyright 2020 by Creative Commons Attribution. Adapted with permission. https://creativecommons.org/licenses/by/4.0/

[4] Adapted from "Implementation of the HACCP System for Apple Juice Concentrate Based on Patulin Prevention and Control," by S. Duan, F. Liu, Q. Qin, Q. Jia, X. Cao, Z. Hua, Y. Fan and C. Wang, 2023, *Foods, 12*(4), p. 786. Copyright 2023 by Creative Commons Attribution. Adapted with permission. https://creativecommons.org/licenses/by/4.0/

[5] Adapted from "Advances in Fruit Aroma Volatile Research," by M. A. M. El Hadi, F. J. Zhang, F. F. Wu, C. H. Zhou and J. Tao, 2013, *Molecules, 18*(7), p. 8200-8229. Copyright 2013 by Creative Commons Attribution. Adapted with permission. https://creativecommons.org/licenses/by/3.0/

8. Appendices

8.1 Appendix 1 – Supplementary Data on Column Weights, Brix and pH Values.

The sections below present the raw data from the experiments, including the MIPs, resin and carbon weights (grams) utilised for each juice treatment for all apple, orange and cranberry samples. The °Brix (degrees Brix) values and pH values have also been provided for each juice. It is important to note that the carbon treatments are the only components that were refilled after every juice treatment due to the fact they do not have the same specificity as molecularly imprinted polymers SV7, GV1, CV6 and resin Purosorb PAD 600.

8.1.1 – MIP, Resin & Carbon Weights within Each Column Used for Juice Treatment

Table 15. *MIP weights in grams used for dose rate treatments of 20 g/L, 10 g/L and 5 g/L for each column with apple, orange and cranberry juice*.

Type of MIP	Column Number	Type of Juice	Weight (g)
SV7	1	Apple	10.0735
	2		10.0718
	3		10.0734
	1	Orange	10.0724
	2		10.0718
	3		10.0721
	1	Cranberry	10.0834
	2		10.0748
	3		10.0712
GV1	1	Apple	10.0572
	2		10.0512
	3		10.0571
	1	Orange	10.0563
	2		10.0524
	3		10.0459
	1	Cranberry	10.0573
	2		10.0570
	3		10.0568
CV6	1	Apple	10.0545
	2		10.0091
	3		10.0501
	1	Orange	10.0012
	2		10.0342
	3		10.0011

	1	Cranberry	10.0438
	2		10.0440
	3		10.0432
Purosorb PAD 600	1	Apple	10.0801
	2		10.0445
	3		10.0815
	1	Orange	10.0691
	2		10.0554
	3		10.0562
	1	Cranberry	10.0832
	2		10.0828
	3		10.0830

Note. Column numbers are associated with the type of treatment utilised. Column 1 was used for treatments at a flowrate of 15 mL/min, column 2 was used for treatments at 35 mL/min and column 3 at a flowrate of 60 mL/min .

Table 16. *Carbon weights in grams for each column used for treatment (20 g/L, 10 g/L and 5 g/L) of apple, orange and cranberry juice.*

Type of MIP	Column Number	Type of Juice	Dose Rate (g/L)	Weight (g)
Carbon	1	Apple	20	10.0115
			10	10.0221
			5	10.0103
	2		20	10.0073
			10	10.0071
			5	10.0040
	3		20	10.0200
			10	10.0059
			5	10.0145
	1	Orange	20	10.0161
			10	10.0523
			5	10.0594
	2		20	10.0267
			10	10.0465
			5	10.0505
	3		20	10.0226
			10	10.0173
			5	10.0432
	1	Cranberry	20	10.0042
			10	10.0242
			5	10.0576
	2		20	10.0216
			10	10.0217
			5	10.0175

	3		20	10.0438
			10	10.0160
			5	10.0235

Note. Columns that were filled with carbon had to be refilled after each treatment as the carbon cannot be regenerated.

8.1.2 – Brix and pH Measurements for Juice Samples

Table 17. *°Brix and pH readings recorded in triplicate for apple juice control, each molecularly imprinted polymer (SV7, GV1, CV6), Purosorb PAD 600, and carbon-treated samples.*

Sample Name	°Brix	pH
Control	12.8	3.57
	12.8	3.57
	12.8	3.57
20g/L SV7 Column 1	12.4	3.55
	12.5	3.56
	12.5	3.56
10g/L SV7 Column 1	10.1	3.56
	10.3	3.57
	10.9	3.56
5g/L SV7 Column 1	12.7	3.57
	12.8	3.57
	12.7	3.57
20g/L SV7 Column 2	12.7	3.57
	12.3	3.57
	12.3	3.57
10g/L SV7 Column 2	12.8	3.55
	12.4	3.54
	12.5	3.55
5g/L SV7 Column 2	12.6	3.57
	12.7	3.57
	12.6	3.56
20g/L SV7 Column 3	12.8	3.60
	12.7	3.60
	12.8	3.59
10g/L SV7 Column 3	11.9	3.53
	11.9	3.54
	11.9	3.53
5g/L SV7 Column 3	10.0	3.57
	10.1	3.57
	10.1	3.57
20g/L GV1 Column 1	11.9	3.60

	12.0	3.59
	11.9	3.60
10g/L GV1 Column 1	12.4	3.60
	11.9	3.58
	12.1	3.60
5g/L GV1 Column 1	10.9	3.58
	10.1	3.58
	10.8	3.59
20g/L GV1 Column 2	10.0	3.58
	10.2	3.58
	10.0	3.59
10g/L GV1 Column 2	10.0	3.58
	10.2	3.58
	10.5	3,58
5g/L GV1 Column 2	10.1	3.52
	10.7	3.53
	10.2	3.52
20g/L GV1 Column 3	10.8	3.59
	10.4	3.60
	10.4	3.59
10g/L GV1 Column 3	10.0	3.53
	10.0	3.53
	10.2	3.52
5g/L GV1 Column 3	10.0	3.55
	10.2	3.55
	10.5	3.55
20g/L CV6 Column 1	10.1	3.49
	9.5	3.50
	10.3	3.50
10g/L CV6 Column 1	10.6	3.54
	10.3	3.54
	10.3	3.54
5g/L CV6 Column 1	10.4	3.59
	10.3	3.59
	10.5	3.58
20g/L CV6 Column 2	10.1	3.51
	10.3	3.50
	10.0	3.50
10g/L CV6 Column 2	10.8	3.51
	10.7	3.51
	10.2	3.50
5g/L CV6 Column 2	11.0	3.57
	9.8	3.56

	10.9	3.58
20g/L CV6 Column 3	10.0	3.55
	10.2	3.55
	10.0	3.55
10g/L CV6 Column 3	10.4	3.59
	10.3	3.59
	9.9	3.59
5g/L CV6 Column 3	9.8	3.55
	10.7	3.55
	10.0	3.55
20g/L Purosorb PAD 600 Column 1	8.0	3.54
	7.4	3.54
	7.8	3.54
10g/L Purosorb PAD 600 Column 1	9.9	3.63
	9.5	3.63
	9.7	3.64
5g/L Purosorb PAD 600 Column 1	8.0	3.55
	7.9	3.55
	7.8	3.55
20g/L Purosorb PAD 600 Column 2	9.5	3.59
	10.0	3.59
	9.8	3.60
10g/L Purosorb PAD 600 Column 2	9.3	3.57
	9.7	3.58
	9.6	3.58
5g/L Purosorb PAD 600 Column 2	11.1	3.63
	11.2	3.62
	11.1	3.63
20g/L Purosorb PAD 600 Column 3	10.8	3.53
	10.8	3.53
	10.8	3.54
10g/L Purosorb PAD 600 Column 3	11.1	3.61
	10.8	3.60
	11.0	3.61
5 g/L Purosorb PAD 600 Column 3	11.0	3.62
	11.1	3.62
	11.1	3.62
20 g/L Carbon Column 1	9.1	3.66
	9.5	3.67
	9.5	3.66
10 g/L Carbon Column 1	9.6	3.61
	9.5	3.61
	9.5	3.62

5 g/L Carbon Column 1	10.9	3.54
	11.0	3.55
	11.2	3.55
20 g/L Carbon Column 2	9.2	3.65
	9.6	3.65
	9.7	3.65
10 g/L Carbon Column 2	10.8	3.65
	10.8	3.65
	10.7	3.65
5 g/L Carbon Column 2	10.9	3.57
	11.1	3.57
	11.2	3.57
20 g/L Carbon Column 3	9.1	3.61
	9.3	3.61
	9.6	3.61
10 g/L Carbon Column 3	10.7	3.55
	10.7	3.55
	10.9	3.56
5 g/L Carbon Column 3	9.9	3.55
	10.1	3.55
	10.6	3.55

Table 18. *°Brix and pH readings recorded in triplicate for orange control, each molecularly imprinted polymer (SV7, GV1, CV6), Purosorb PAD 600), and carbon-treated samples.*

Sample Name	°Brix	pH
Control	11.1	3.76
	11.0	3.76
	11.1	3.76
20g/L SV7 Column 1	9.4	3.76
	9.4	3.76
	9.6	3.76
10g/L SV7 Column 1	9.4	3.78
	9.6	3.79
	9.5	3.79
5g/L SV7 Column 1	9.0	3.80
	8.9	3.81
	9.1	3.80
20g/L SV7 Column 2	9.1	3.87
	9.2	3.88
	8.9	3.87
10g/L SV7 Column 2	8.4	3.86
	8.3	3.86

	8.5	3.86
5g/L SV7 Column 2	8.4	3.80
	7.7	3.80
	8.3	3.80
20g/L SV7 Column 3	8.2	3.83
	8.4	3.83
	8.6	3.83
10g/L SV7 Column 3	7.8	3.82
	8.2	3.82
	8.4	3.81
5g/L SV7 Column 3	7.8	3.83
	7.8	3.83
	8.0	3.83
20g/L GV1 Column 1	8.8	3.84
	8.5	3.84
	8.5	3.83
10g/L GV1 Column 1	9.1	3.80
	9.2	3.80
	9.1	3.80
5g/L GV1 Column 1	8.4	3.82
	8.3	3.82
	8.6	3.82
20g/L GV1 Column 2	9.0	3.81
	8.9	3.81
	9.0	3.80
10g/L GV1 Column 2	8.3	3.79
	8.3	3.79
	8.3	3.79
5g/L GV1 Column 2	8.5	3.81
	8.6	3.81
	8.6	3.81
20g/L GV1 Column 3	9.0	3.86
	9.0	3.86
	9.1	3.85
10g/L GV1 Column 3	7.8	3.85
	8.0	3.85
	7.7	3.85
5g/L GV1 Column 3	7.8	3.87
	7.7	3.88
	7.4	3.88
20g/L CV6 Column 1	8.1	3.88
	8.3	3.88
	8.5	3.87

10g/L CV6 Column 1	8.4	3.87
	8.6	3.87
	8.8	3.87
5g/L CV6 Column 1	7.1	3.85
	7.1	3.85
	7.4	3.85
20g/L CV6 Column 2	7.9	3.80
	7.8	3.80
	7.7	3.80
10g/L CV6 Column 2	7.5	3.86
	7.5	3.86
	7.7	3.86
5g/L CV6 Column 2	7.4	3.83
	7.9	3.83
	7.2	3.83
20g/L CV6 Column 3	7.3	3.88
	7.1	3.89
	6.9	3.88
10g/L CV6 Column 3	7.1	3.87
	6.9	3.87
	7.1	3.86
5g/L CV6 Column 3	8.3	3.90
	8.4	3.89
	8.3	3.90
20g/L Purosorb PAD 600 Column 1	7.4	3.90
	7.4	3.89
	7.5	3.90
10g/L Purosorb PAD 600 Column 1	7.4	3.89
	7.8	3.89
	7.9	3.90
5g/L Purosorb PAD 600 Column 1	9.6	3.80
	9.6	3.80
	9.8	3.80
20g/L Purosorb PAD 600 Column 2	7.2	3.82
	7.8	3.82
	8.1	3.82
10g/L Purosorb PAD 600 Column 2	7.6	3.82
	7.3	3.82
	7.1	3.82
5g/L Purosorb PAD 600 Column 2	8.1	3.79
	8.1	3.79
	8.4	3.80
	8.2	3.85

20g/L Purosorb PAD 600 Column 3	8.2	3.85
	8.1	3.85
10g/L Purosorb PAD 600 Column 3	9.1	3.84
	9.2	3.84
	9.3	3.84
5 g/L Purosorb PAD 600 Column 3	9.9	3.85
	9.9	3.85
	10.0	3.84
20 g/L Carbon Column 1	9.3	3.88
	9.3	3.88
	9.3	3.88
10 g/L Carbon Column 1	7.8	3.85
	7.8	3.85
	7.1	3.85
5 g/L Carbon Column 1	8.9	3.80
	8.9	3.80
	9.2	3.80
20 g/L Carbon Column 2	9.7	3.87
	9.8	3.86
	9.8	3.87
10 g/L Carbon Column 2	7.6	3.85
	7.3	3.85
	7.3	3.85
5 g/L Carbon Column 2	8.3	3.83
	7.8	3.83
	8.4	3.82
20 g/L Carbon Column 3	10.0	3.86
	10.1	3.86
	10.0	3.86
10 g/L Carbon Column 3	9.2	3.85
	9.2	3.85
	9.1	3.85
5 g/L Carbon Column 3	8.1	3.81
	8.4	3.81
	8.5	3.81

Table 19. *°Brix and pH readings recorded in triplicate for cranberry juice control, each molecularly imprinted polymer (SV7, GV1, CV6) and Purosorb PAD 600 and carbon-treated samples.*

Sample Name	°Brix	pH
Control	11.0	2.47
	11.0	2.46
	11.0	2.46
20g/L SV7 Column 1	9.7	2.49

	9.7	2.49
	10.3	2.48
10g/L SV7 Column 1	10.3	2.47
	10.1	2.47
	10.5	2.47
5g/L SV7 Column 1	10.4	2.46
	10.5	2.46
	10.5	2.46
20g/L SV7 Column 2	10.4	2.51
	10.2	2.49
	10.5	2.49
10g/L SV7 Column 2	10.0	2.53
	10.1	2.52
	10.2	2.52
5g/L SV7 Column 2	11.3	2.56
	11.0	2.56
	11.0	2.56
20g/L SV7 Column 3	12.4	2.55
	12.4	2.55
	12.6	2.55
10g/L SV7 Column 3	12.6	2.53
	12.7	2.52
	12.8	2.53
5g/L SV7 Column 3	12.6	2.52
	12.5	2.52
	12.7	2.52
20g/L GV1 Column 1	11.9	2.52
	12.0	2.52
	12.1	2.52
10g/L GV1 Column 1	11.9	2.51
	12.1	2.51
	12.3	2.51
5g/L GV1 Column 1	11.3	2.52
	11.8	2.52
	12.2	2.52
20g/L GV1 Column 2	11.7	2.55
	11.7	2.55
	11.7	2.55
10g/L GV1 Column 2	12.5	2.53
	12.5	2.53
	12.5	2.53
5g/L GV1 Column 2	12.0	2.53
	12.5	2.53

	12.2	2.53
20g/L GV1 Column 3	12.6	2.53
	12.8	2.53
	12.5	2.53
10g/L GV1 Column 3	12.5	2.53
	13.1	2.53
	13.1	2.52
5g/L GV1 Column 3	11.9	2.54
	11.9	2.54
	12.2	2.54
20g/L CV6 Column 1	10.4	2.55
	10.2	2.55
	10.4	2.55
10g/L CV6 Column 1	11.0	2.54
	11.7	2.54
	11.8	2.54
5g/L CV6 Column 1	11.8	2.54
	11.9	2.54
	12.0	2.54
20g/L CV6 Column 2	11.8	2.55
	12.0	2.55
	12.0	2.55
10g/L CV6 Column 2	12.7	2.54
	13.1	2.54
	12.7	2.54
5g/L CV6 Column 2	12.8	2.52
	12.5	2.52
	12.4	2.52
20g/L CV6 Column 3	12.3	2.53
	12.0	2.53
	12.0	2.53
10g/L CV6 Column 3	12.7	2.52
	12.7	2.52
	12.8	2.52
5g/L CV6 Column 3	12.0	2.52
	12.2	2.52
	12.5	2.52
20g/L Purosorb PAD 600 Column 1	11.1	2.53
	11.3	2.53
	11.4	2.53
10g/L Purosorb PAD 600 Column 1	11.6	2.54
	11.8	2.54
	11.7	2.54

5g/L Purosorb PAD 600 Column 1	11.9	2.50
	12.1	2.51
	12.1	2.51
20g/L Purosorb PAD 600 Column 2	11.8	2.54
	11.9	2.55
	11.9	2.55
10g/L Purosorb PAD 600 Column 2	12.0	2.56
	11.9	2.56
	12.0	2.55
5g/L Purosorb PAD 600 Column 2	12.3	2.52
	12.7	2.52
	12.8	2.52
20g/L Purosorb PAD 600 Column 3	12.3	2.54
	12.6	2.54
	12.6	2.54
10g/L Purosorb PAD 600 Column 3	12.0	2.54
	12.0	2.54
	12.2	2.54
5 g/L Purosorb PAD 600 Column 3	13.2	2.56
	13.4	2.55
	13.6	2.55
20 g/L Carbon Column 1	10.3	2.56
	10.2	2.57
	10.3	2.57
10 g/L Carbon Column 1	11.2	2.69
	11.2	2.69
	11.2	2.69
5 g/L Carbon Column 1	12.8	2.68
	13.0	2.68
	12.9	2.68
20 g/L Carbon Column 2	10.4	2.70
	10.4	2.70
	10.6	2.70
10 g/L Carbon Column 2	12.6	2.67
	12.9	2.67
	12.6	2.67
5 g/L Carbon Column 2	10.6	2.63
	10.6	2.63
	10.8	2.63
20 g/L Carbon Column 3	10.4	2.68
	10.9	2.68
	10.9	2.68
10 g/L Carbon Column 3	12.2	2.67

	12.2	2.67
	12.2	2.67
5 g/L Carbon Column 3	11.1	2.60
	11.4	2.60
	11.4	2.61

8.2 Appendix 2 – Informal Sensory Evaluation Results

Three participants were asked to record and describe the overall attributes they detected after tasting each treated and untreated juice. This testing was utilised to give a general indication of what the treated samples organoleptic attributes were like before formal sensory analysis took place, and guided the choice of samples to advance to formal testing.

Table 20. *Preliminary testing commentary from three different laboratory personnel on both the treated and untreated (control) apple juices samples.*

Sample Tasted	Participants (1 – 3) Comments
Control	***1:*** A bit too sugary. Less tart/sour. Not much apple flavour but the apple aroma is very good.
	2: Sweet and sour. Rich apple flavour and aroma. Like this sample.
	3: Very sweet. Apple aroma and flavour is strong and powerful. Too sweet for my tastes.
20 g/L SV7 Column 1	***1:*** Diluted water.
	2: Watery. Subtle sweetness. Prevalent apple flavour.
	3: Diluted.
10 g/L SV7 Column 1	***1:*** Fruity and sweet with a slight tartness.
	2: Sour and sweet – heavily balanced. Nice apple flavour.
	3: Fresh apple. Tastes sweet.
5 g/L SV7 Column 1	***1:*** Sweet, apple flavour. Very fruity aroma.
	2: Sweet and sour. Again, a nice balance in this sample.
	3: Light. Watery.
20 g/L SV7 Column 2	***1:*** Very fresh. Sweet but slightly diluted. There was a slight bitter note.
	2: Bland tasting, a bit sweet. Like a tiny bit of sugar has been added to water.
	3: Sweeter. Fresh apple taste and aroma. No aftertaste.
10 g/L SV7 Column 2	***1***: Diluted slightly, still sweet and had a prominent apple taste.
	2: Sweet but watery.
	3: Ripe apple taste. Sweet.
5 g/L SV7 Column 2	***1:*** Diluted water.
	2: Sour and watery.
	3: Diluted taste.
20 g/L SV7 Column 3	***1:*** A lot of sweetness. Slightly tart.
	2: Apple flavour is there, but the sample is a bit bland.
	3: Too sweet. Did not enjoy this sample.
10 g/L SV7 Column 3	***1:*** Sweet, but not as much as the previous sample.
	2: Sweet, a bit of apple flavour. Sample is a bit bland.
	3: Clear apple taste. Not bad.
5 g/L SV7 Column 3	***1:*** Sweet and also tart. A bit sour but not overpowering.

	2: Bland. No flavour whatsoever.
	3: Sweet. Slightly unpleasant to my taste buds.
20 g/L GV1 Column 1	***1:*** Watery.
	2: Watery and sour.
	3: Sweet and sour. Balanced flavours. Like this sample.
10 g/L GV1 Column 1	***1:*** Watery with a bitter aftertaste.
	2: Sweet and watery.
	3: Watery.
5 g/L GV1 Column 1	***1:*** Watery and sour. With a tangy aftertaste.
	2: Watery. Sour aftertaste.
	3: Apple flavour and aroma too light.
20 g/L GV1 Column 2	***1:*** Watery.
	2: Watery and sweet.
	3: Watery.
10 g/L GV1 Column 2	***1:*** Watery.
	2: Watery and sweet.
	3: Watery. Very diluted.
5 g/L GV1 Column 2	***1:*** Apple flavour prevalent. More sour than sweet.
	2: Sweet and sour. Very good apple flavour and aroma.
	3: Very sweet.
20 g/L GV1 Column 3	***1:*** Watery and sour.
	2: Watery and slightly sweet.
	3: Watery.
10 g/L GV1 Column 3	***1:*** Fruity. A balance of sweet and sourness.
	2: Sweet but there is not a lot of apple flavour or aroma to the sample.
	3: Like this apple juice taste. Good balance of sweetness, sourness and apple flavour, and apple aroma.
5 g/L GV1 Column 3	***1:*** Watery and slightly sweet. Like sugar water.
	2: Watery though its slightly sweet and sour.
	3: Similar as the previous sample. However, sourness is prevalent more in this sample. Like this sample.
20 g/L CV6 Column 1	***1:*** Diluted and watery. Hint of sweetness.
	2: Sweet. There is a strong apple flavour. Though it tastes flat.
	3: Watery.
10 g/L CV6 Column 1	***1:*** Kind of sweet, slightly diluted.
	2: Sweet with a bland flavour.
	3: Like this sample. Not too sweet, though a little bit sour.
5 g/L CV6 Column 1	***1:*** Watery and bitter.
	2: Watery apple-like flavour. It's a bit diluted.
	3: Watery.
20 g/L CV6 Column 2	***1:*** Watery but sour and also bitter.
	2: Sourness is there. A bit watery with a slight apple flavour and aroma.
	3: Light taste. Sweeter.

10 g/L CV6 Column 2	***1:*** Slightly watery with a sour taste.
	2: A bit sweet. Apple flavour is slightly prevalent.
	3: Fresh taste. Good.
5 g/L CV6 Column 2	***1:*** Watery. Slight apple flavour and aroma but not much.
	2: Watery and sour.
	3: Watery.
20 g/L CV6 Column 3	***1:*** Watery and sour.
	2: Apple flavour/aroma is only there slightly (probably diluted). Sour.
	3: Watery. Sour.
10 g/L CV6 Column 3	***1:*** Watery but slightly sweet.
	2: Watery and sour.
	3: Sweeter. Fresh apple juice taste.
5 g/L CV6 Column 3	***1:*** Similar as the previous sample.
	2: Watery and sour.
	3: Light juice taste. Balanced.
20 g/L Purosorb PAD 600 Column 1	***1:*** Sour (but not overpowering), very watery and diluted.
	2: Sweet though its diluted.
	3: Watery.
10 g/L Purosorb PAD 600 Column 1	***1:*** Watery though there is slight sourness, sweetness and tartness.
	2: Sweet and sour. A bit of apple flavour and aroma detected.
	3: Sweet though the sample is sourer.
5 g/L Purosorb PAD 600 Column 1	***1:*** Watery and sour.
	2: A bit watery. Sourness and apple flavour comes through a lot.
	3: Fresh apple taste.
20 g/L Purosorb PAD 600 Column 2	***1:*** Same as previous sample.
	2: Watery and a little bit sour. Sample isn't that great. Tastes like really bad acid water that's kind of bland.
	3: Watery. Don't like this sample.
10 g/L Purosorb PAD 600 Column 2	***1:*** Watery but slightly sweet.
	2: Watery and sweet.
	3: Too sweet. Can't taste much apple.
5 g/L Purosorb PAD 600 Column 2	***1:*** Sweet and sour (more sweetness detected though)
	2: Very sweet and sour. Though a bit diluted still tastes nice.
	3: Taste is good. Sweet.
20 g/L Purosorb PAD 600 Column 3	***1:*** Same as previous sample.
	2: High apple flavour and aroma present. Sweet and sour is balanced.
	3: Sweeter. Ok taste.
10 g/L Purosorb PAD 600 Column 3	***1:*** Sourness more prominent. Sample also has a hint of sweetness.
	2: Sweet and sour. A bit watery.
	3: Very sweet. Don't like it at all.
5 g/L Purosorb PAD 600 Column 3	***1:*** Similar attributes detected to previous apple juice sample.
	2: Bland flavour – just flat flavours all around.
	3: Sour more than sweet. Good, like this sample a lot.

20 g/L Carbon Column 1	***1:*** Sweet. No carbon aftertaste in this sample.
	2: Sweet but the aftertaste is not pleasant at all.
	3: A little bit watery with slight sweetness. Unpleasant aftertaste.
10 g/L Carbon Column 1	***1:*** Heavy carbon aftertaste.
	2: Strong carbon taste and smell. Could not decern any other attributes in the sample because of this.
	3: Fresh apple taste comes through. But there was a strong carbon taste and smell to the sample.
5 g/L Carbon Column 1	***1:*** Carbon aftertaste but there is a slight sweetness.
	2: Sweet and sour. Carbon taste still there.
	3: Very sweet. Carbon aftertaste.
20 g/L Carbon Column 2	***1:*** A lot more sweetness detected in this sample. Carbon aftertaste.
	2: Sweet but had a strong carbon smell and ashy aftertaste.
	3: Too sweet. Strange aftertaste still there.
10 g/L Carbon Column 2	***1:*** No carbon aftertaste detected in this sample. Has a nice sweet and sour balance to it.
	2: Sweet.
	3: Sweet. Can't taste the apple flavour.
5 g/L Carbon Column 2	***1:*** Slightly sweet, but sourness dominates more. No carbon aftertaste.
	2: Watery and slightly sweet. Disappointing sample.
	3: Diluted. Not a good sample. No aftertaste.
20 g/L Carbon Column 3	***1:*** No carbon aftertaste. Sour in nature.
	2: Sour and a bit watery.
	3: Sour. No aftertaste. Not very impressive.
10 g/L Carbon Column 3	***1:*** Sweet but had a carbon/ashy aftertaste.
	2: Watery had a strange carbon aftertaste.
	3: Strange aftertaste is back in this sample. Hint of sweetness kind of well-balanced. An ok sample.
5 g/L Carbon Column 3	***1:*** Sour but had a carbon/ashy aftertaste.
	2: Similar to the previous sample.
	3: Sourness detected a bit. Watery. Aftertaste is still there – almost metal-like.

Note. Numbers (1 to 3) represent each person's commentary on the various samples.

Table 21. *Preliminary testing commentary from three different laboratory personnel on both the treated and untreated (control) orange juice samples.*

Sample Tasted	Participants (1 – 3) Comments
Control	***1:*** Watery and diluted – orange flavour (the taste itself is very synthetic). Had a sour aftertaste and was bitter on the tongue.
	2: Sour and diluted. A bit of orange flavour (but synthetic). Not the best one. Disliked this sample.

	3: Sour and very diluted. Did not taste like actual orange, more like orange flavouring. Strong tangy and bitter aftertaste.
20 g/L SV7 Column 1	***1:*** Diluted watery sample.
	2: Sour but has some orangey flavour present.
	3: Watery orange juice.
10 g/L SV7 Column 1	***1:*** Sourer/tart – barely any sweetness.
	2: Strong orange flavour juice (more like an additive), sweeter.
	3: Sweeter than the previous sample. Strong synthetic orange flavour.
5 g/L SV7 Column 1	***1:*** Still slightly sour – has a very prominent orange flavour and aftertaste (almost artificial like). Sweeter than previous sample.
	2: Taste similar to previous sample, but less sour.
	3: Less sour. Similar to previous sample.
20 g/L SV7 Column 2	***1:*** Balanced flavours of sweet and sour. Slightly tangier.
	2: Very sweet and no aftertaste, less sour.
	3: Very sweet. Less sour.
10 g/L SV7 Column 2	***1***: Diluted and watery sample.
	2: Sweet and sour aftertaste, prominent orangey flavour.
	3: Slightly diluted compared to previous sample. Though orange flavour and sweetness still present.
5 g/L SV7 Column 2	***1:*** Diluted and watery sample.
	2: Yuck aftertaste. Very diluted and not acceptable.
	3: Diluted. Not a good sample.
20 g/L SV7 Column 3	***1:*** More mouthfeel with a sharp and sour aftertaste.
	2: Sour and just about right sweetness.
	3: Balanced sourness and sweetness.
10 g/L SV7 Column 3	***1:*** Watery, diluted and sour.
	2: Sweet and sour, a bit of orange flavour.
	3: Not much orange flavour detected. More sourness.
5 g/L SV7 Column 3	***1:*** Watery diluted and sour.
	2: A bit diluted but sweet, less sour.
	3: Diluted still but still has sweet and sour notes.
20 g/L GV1 Column 1	***1:*** Orange flavouring – not that sour.
	2: Sweet but diluted.
	3: Watery orange juice.
10 g/L GV1 Column 1	***1:*** More prominent orange flavour and aroma. Very sour. There was a hint of sweetness detected but the sourness was very overpowering.
	2: Sour aftertaste with a strong orange flavour.
	3: Sourer than usual. Orange flavour was detected in both the taste and the aroma.
5 g/L GV1 Column 1	***1:*** Sample tasted similar to the previous one.
	2: Sweet, diluted.
	3: Diluted orange juice.

20 g/L GV1 Column 2	***1:*** Tangy aftertaste. Not much sweetness. The sharpness of sour component overpowered all other attributes.
	2: Sweet and sour. Detectable orange flavour. Particularly like this one.
	3: Sweeter. Bitter aftertaste.
10 g/L GV1 Column 2	***1:*** Similar characteristics to the previous sample. Less sour.
	2: Strong sourness also sweet (very strong flavour).
	3: Sweet juice. Less bitterness afterwards.
5 g/L GV1 Column 2	***1:*** Diluted and watery.
	2: Diluted, no taste (no sweet/sour attributes)
	3: Watery orange juice.
20 g/L GV1 Column 3	***1:*** Sour with the orange flavour being very prominent.
	2: Sweet, orange flavour present.
	3: Sweet. Strong orange taste. Less bitter.
10 g/L GV1 Column 3	***1:*** Sweet and less sour tasting.
	2: Similar to the previous sample.
	3: Sweeter than previous sample. Strong taste. Less bitter.
5 g/L GV1 Column 3	***1:*** Diluted and sour.
	2: Sweet. Strong orange flavour. No sour aftertaste.
	3: Sweet. A slight bitter aftertaste but not as overpowering as the other samples tasted.
20 g/L CV6 Column 1	***1:*** No flavour. Diluted and doesn't taste like anything.
	2: Bland taste.
	3: Watery sample and very diluted.
10 g/L CV6 Column 1	***1:*** Very flavourful – the overall sweetness and sourness is enhanced.
	2: Strong sour, sweet flavour.
	3: Stronger orange taste, sweeter.
5 g/L CV6 Column 1	***1:*** Diluted and watery.
	2: Diluted (more pronounced sweetness than sour)
	3: Diluted sample.
20 g/L CV6 Column 2	***1:*** No flavour whatsoever. Tasted like water but had a bitter aftertaste.
	2: Sour but diluted.
	3: More diluted sample. Barely can taste any of the orange flavour.
10 g/L CV6 Column 2	***1:*** Similar attributes to the previous sample tasted.
	2: Sweet but diluted.
	3: Watery
5 g/L CV6 Column 2	***1:*** Slightly diluted. Had a prominent sour taste afterwards.
	2: Sweet and sour. Like this sample a lot.
	3: Sweeter. Compared to previous sample. More like orange juice.
20 g/L CV6 Column 3	***1:*** Orange flavour (balanced). Slightly sweet and less sour.
	2: Strong flavours (mixture of sour and sweet)
	3: Sweet juice, no bitterness whatsoever.
10 g/L CV6 Column 3	***1:*** Absolutely nothing. Just plain water with a weird tangy and bitter aftertaste.

	2: Sour more than sweet but a bit watery.
	3: Milder flavour.
5 g/L CV6 Column 3	***1:*** More sour but still watery and diluted.
	2: Sweeter with a prominent orange flavour but diluted still.
	3: Watery.
20 g/L Purosorb PAD 600 Column 1	***1:*** Diluted. No flavour, basically water with citric acid powder.
	2: Sour and orangey flavour but heavily diluted.
	3: Like water. Very light taste.
10 g/L Purosorb PAD 600 Column 1	***1:*** Diluted but with a slight sourness and sweetness.
	2: Similar characteristics as the previous sample.
	3: Slightly sweeter.
5 g/L Purosorb PAD 600 Column 1	***1:*** Diluted again. But, less sour than previous sample.
	2: Diluted and slightly sweet.
	3: Sweet.
20 g/L Purosorb PAD 600 Column 2	***1:*** Tasted like water, had no flavour at all. Bitter aftertaste.
	2: Diluted. Tastes like bitter water. Absolutely disgusting. Don't like this sample at all.
	3: Like water with a hint of sourness.
10 g/L Purosorb PAD 600 Column 2	***1:*** Water but with a slight sour tang.
	2: Sour and orange favour prevalent. Slightly sweet.
	3: Similar to the previous sample. But has slightly more body to it.
5 g/L Purosorb PAD 600 Column 2	***1:*** Water but a sour taste to it. Slight sweetness. Overall balanced.
	2: Not too sour and orangey. Like this sample a lot.
	3: Sweeter.
20 g/L Purosorb PAD 600 Column 3	***1:*** Sourness is still there and well as the sample being diluted.
	2: Sweet and orangey.
	3: Watery.
10 g/L Purosorb PAD 600 Column 3	***1:*** Same flavours as the previous sample.
	2: Sweet like the previous sample but more diluted.
	3: Very light tasting but bitter.
5 g/L Purosorb PAD 600 Column 3	***1:*** Diluted still but with a subtle sweetness and sourness. Not as bad as other samples tasted previously. Orange flavour is prevalent.
	2: Sweet, subtle sourness, and powerful orangey flavour. Not so much of an aftertaste.
	3: Watery. Slightly sour.
20 g/L Carbon Column 1	***1:*** Sour and watery. Bad chalky aftertaste which isn't ideal.
	2: Sweet. Though had a very ashy carbon-like aftertaste that wasn't really acceptable. Wouldn't drink this if it was available for sale.
	3: Watery. Strange aftertaste detected.
10 g/L Carbon Column 1	***1:*** Predominately sour. Increases afterwards. Slight orange flavour. Ashy/chalky aftertaste is still there.
	2: Sour and sweet with same carbon aftertaste.
	3: Bitter aftertaste. Slightly stronger orangey flavour in this sample.

5 g/L Carbon Column 1	***1:*** Diluted, watery and sour. Carbon aftertaste prevalent still.
	2: Diluted and sour with carbon aftertaste.
	3: Watery.
20 g/L Carbon Column 2	***1:*** Watery. Nothing more to taste.
	2: Way more diluted than the previous samples. Carbon aftertaste present still.
	3: Watery.
10 g/L Carbon Column 2	***1:*** Similar to the previous sample. Carbon aftertaste still present.
	2: No flavour whatsoever. Like water. Ashy aftertaste.
	3: Just like water.
5 g/L Carbon Column 2	***1:*** Slight sour notes within the beverage.
	2: Sour and sweet. Carbon-like aftertaste.
	3: Sweeter.
20 g/L Carbon Column 3	***1:*** Orange flavour is present in a small amount. Sour but not overbearing. Ashy carbon taste is still there.
	2: Very bland tasting. Not much of a carbon aftertaste in this sample.
	3: Sweeter.
10 g/L Carbon Column 3	***1:*** Diluted flavours and aroma. Tastes like water with ash in it.
	2: Sour and a bit diluted in terms of sweetness. Not bad overall.
	3: Less sweet.
5 g/L Carbon Column 3	***1:*** Similar to previous sample. Slightly less of a carbon aftertaste.
	2: Sour and sweet. Ashy aftertaste still there a bit but not as prevalent.
	3: Watery.

Note. Numbers (1 to 3) represent each person's commentary on the various samples.

Table 22. *Preliminary testing commentary from three different laboratory personnel on both the treated and untreated (control) cranberry juice samples.*

Sample Tasted	Participants (1 – 3) Comments
Control	***1:*** Very sweet. Sour notes present after the initial hit of sweetness. Astringency detected in the aftertaste.
	2: Very strong flavour – too much for my liking. Very sweet and sour. Also has a strong astringent aftertaste.
	3: Very sweet. Not that enjoyable. Has a strong cranberry flavour but bitter aftertaste.
20 g/L SV7 Column 1	***1:*** Very mild sour taste. Slightly sweet. Astringency is gone.
	2: Higher sugar content more than sourness.
	3: Watery.
10 g/L SV7 Column 1	***1:*** Very sour, not as sweet as the previous sample. No astringency.
	2: Sour and sweet. Well balanced.
	3: Sweeter.
5 g/L SV7 Column 1	***1:*** Sour aftertaste. No astringency in sample. Subdued sweetness.
	2: Diluted sourness and sweetness.

	3: Sweet and sour but watery.
20 g/L SV7 Column 2	***1:*** Sour aftertaste. No astringency present.
	2: Similar to the previous sample.
	3: Watery.
10 g/L SV7 Column 2	***1***: Sour and less astringent. Very bitter aftertaste.
	2: Very sour with some sweetness.
	3: Very diluted. Not good at all.
5 g/L SV7 Column 2	***1:*** Similar characteristics to the previous sample.
	2: Diluted with a slight sweetness and very sour still.
	3: Sweeter and a bit sour also has a fresh taste.
20 g/L SV7 Column 3	***1:*** Watery and heavily diluted.
	2: Watery.
	3: Diluted.
10 g/L SV7 Column 3	***1:*** Slight cranberry flavour detected. Less sour than previous samples.
	2: More sweet cranberry flavour than sour.
	3: Sweeter. Has prominent cranberry taste and aroma.
5 g/L SV7 Column 3	***1:*** Sour, has a slight cranberry taste. Not as sweet but the astringency has come back in this sample.
	2: More sourness than sweetness.
	3: Sweet and sour.
20 g/L GV1 Column 1	***1:*** Watery and diluted.
	2: Diluted.
	3: Diluted.
10 g/L GV1 Column 1	***1:*** Slight sweetness but sourness overpowers it. Less astringent.
	2: Very sweet.
	3: Slightly sweet.
5 g/L GV1 Column 1	***1:*** More sour than sweet. Less astringent.
	2: Sweet and sour. Balanced,
	3: Sweet with a fresh cranberry taste.
20 g/L GV1 Column 2	***1:*** Increase of sweetness. Not as sour.
	2: Sweet and a bit sour.
	3: Sweeter. Balanced flavours in this sample. Very nice.
10 g/L GV1 Column 2	***1:*** Slight sweetness and sourness (balanced). Sour notes not present in the aftertaste.
	2: Diluted but sweet still.
	3: Slightly sweet. Like this sample a lot. Not as sour (its subtle).
5 g/L GV1 Column 2	***1:*** Sweet, less sour. No aftertaste or astringency detected.
	2: Sour, less sweet than usual.
	3: Sweeter, not too bad.
20 g/L GV1 Column 3	***1:*** Watery and diluted.
	2: Diluted and watery. Did not like this sample.
	3: Watery but sour.
10 g/L GV1 Column 3	***1:*** Diluted and sour. Less sweetness.

	2: Diluted and sour.
	3: Sweeter. Ok taste. But it is rather diluted and watery.
5 g/L GV1 Column 3	***1:*** Same as previous sample.
	2: Diluted but sweet.
	3: Slightly diluted. A bit of sweetness there.
20 g/L CV6 Column 1	***1:*** Sweet, not sour at all. No astringency.
	2: Sweet and bland.
	3: Fresh taste. Sweet.
10 g/L CV6 Column 1	***1:*** Diluted and sour. Not that much sweetness to the sample.
	2: Sweet and bland.
	3: Diluted and watery.
5 g/L CV6 Column 1	***1:*** Diluted and watery.
	2: Watery and sweet. Disliked this sample. Just tasted like sugar water.
	3: Watery and sour. Not sweet at all.
20 g/L CV6 Column 2	***1:*** Diluted and watery but still has a slightly sour taste.
	2: Sweet and sour.
	3: Watery and not that sweet.
10 g/L CV6 Column 2	***1:*** Extremely sour. Has a chalky and astringent aftertaste.
	2: Sour and sweet. There was a nice cranberry flavour to sample. Astringency was prominent within the aftertaste.
	3: Slightly sweet.
5 g/L CV6 Column 2	***1:*** Diluted but slightly sour and sweet.
	2: Sweet. Strong cranberry flavour and aroma.
	3: Sweeter and fresh.
20 g/L CV6 Column 3	***1:*** Watery with a hint of sourness. Hint of cranberry flavour and aroma.
	2: Watery but with some sweetness and sourness. Strong cranberry flavour and aroma detected.
	3: Very nice. Has a fresh berry taste to it. Like this sample a lot.
10 g/L CV6 Column 3	***1:*** Diluted and watery. But the sweetness and sourness are mildly balanced in this sample.
	2: Watery and sour. Absolutely no sweetness perceived.
	3: Less sweet and diluted.
5 g/L CV6 Column 3	***1:*** Very sour, not a lot of sweetness to it. Astringency is heavily there.
	2: Sour and sweet.
	3: Slightly sweet Ok taste. Though aftertaste is bitter.
20 g/L Purosorb PAD 600 Column 1	***1:*** Extremely sour and diluted/watery.
	2: Watery and very bland.
	3: Watery.
10 g/L Purosorb PAD 600 Column 1	***1:*** Very sour and slightly sweet.
	2: Watery and very sour.
	3: Sweeter. Ok, but the sample isn't that impressive.
5 g/L Purosorb PAD 600 Column 1	***1:*** Diluted and sour.
	2: Watery and bland. Not enjoyable at all.

	3: Very light taste. Hint of sweetness and sourness.
20 g/L Purosorb PAD 600 Column 2	***1:*** Diluted but sour.
	2: Seriously diluted and didn't taste like much.
	3: Just like water.
10 g/L Purosorb PAD 600 Column 2	***1:*** No sweetness whatsoever in this sample. Extremely sour. Very overpowering.
	2: Balanced sweetness and sourness. Good sample.
	3: Sweet. But the sugary taste is very unpleasant.
5 g/L Purosorb PAD 600 Column 2	***1:*** Sweet and sour. Rather balanced but the sourness carries on into the aftertaste.
	2: Same as previous sample tasted.
	3: Way too sweet for my liking.
2 0g/L Purosorb PAD 600 Column 3	***1:*** Watery and bitter.
	2: No flavour. Very, very bland and watery. Did not enjoy this sample.
	3: Light tasty but sour.
10 g/L Purosorb PAD 600 Column 3	***1:*** Watery and bitter.
	2: Bland and very unenjoyable. Bitter aftertaste that was unpleasant.
	3: Watery.
5 g/L Purosorb PAD 600 Column 3	***1:*** Watery and bitter.
	2: Similar attributes as the previous sample tasted.
	3: Sour and watery.
20 g/L Carbon Column 1	***1:*** Heavy carbon aftertaste. Very diluted and watery with ashy flavour.
	2: Sour. Carbon aftertaste.
	3: Watery.
10 g/L Carbon Column 1	***1:*** Sourness is prominent. Carbon aftertaste is still there.
	2: Sour and sweet. A bit of a bitter aftertaste.
	3: Very interesting taste. Like it a lot.
5 g/L Carbon Column 1	***1:*** No carbon aftertaste. Diluted and watery.
	2: Sweet and sour but it's diluted a bit.
	3: Very sweet. Almost sickening sweet.
20 g/L Carbon Column 2	***1:*** Watery with carbon aftertaste.
	2: Watery.
	3: Watery.
10 g/L Carbon Column 2	***1:*** Watery with a carbon aftertaste.
	2: Bland with little flavour.
	3: Watery. Sour and slightly sweet. Carbon aftertaste prominent.
5 g/L Carbon Column 2	***1:*** Slightly bitter aftertaste as well as metallic tang. Watery.
	2: Watery but sour. Disliked this sample.
	3: Watery. Sour and not sweet.
20 g/L Carbon Column 3	***1:*** Sweet and sour but it was diluted.
	2: Sweet with a strong cranberry flavour. Although it had a strong carbon smell and aftertaste.
	3: Very sweet. Don't like this sample.

10 g/L Carbon Column 3	***1:*** Sour tasting. Carbon aftertaste was there again.
	2: Sour and a bit bitter.
	3: Sweet. Has some caramel after taste for some reason.
5 g/L Carbon Column 3	***1:*** Same as the previous sample tasted.
	2: Sour. Very bitter aftertaste and the carbon smell is off-putting.
	3: Sweet and sour (well balanced). Very nice sample.

Note. Numbers (1 to 3) represent each person's commentary on the various samples.

8.3 Appendix 3 – Formal Sensory Evaluation Questionnaires

The following appendixes and figures below outline and detail the questionnaires utilised during formal sensory evaluation of the six selected apple, orange and cranberry juice samples. Participants were asked a multitude of questions based upon the different fruit juices characteristics. For instance, cranberry juice is known to be astringent and bitter whilst apple juice is known for its tartness and sweetness. RedJade's software provided the necessary sample codes by means of a block design. Participants were also asked to comment and provide opinions on each sample tasted after going through all attribute-based (i.e. sweetness and bitterness) questions.

8.3.1 – Formal Sensory Questionnaire for Apple Juice Samples

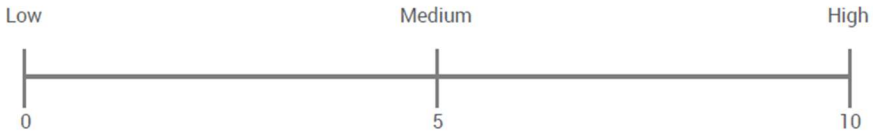
1 Please select the phrase that best describes how much you like or dislike the **COLOUR** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

2 Please select the phrase that best describes how much you like or dislike the **APPLE AROMA** (fruity aroma) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

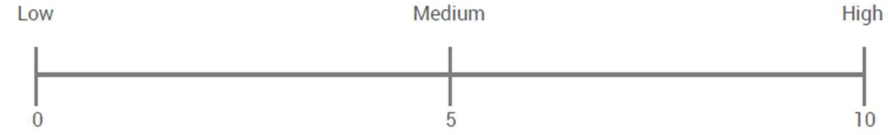
3 Please rate the **INTENSITY** of the **APPLE AROMA** (fruity aroma) in Sample {{sample_code}}.



4 Please select the phrase that best describes how much you like or dislike the **SWEETNESS** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

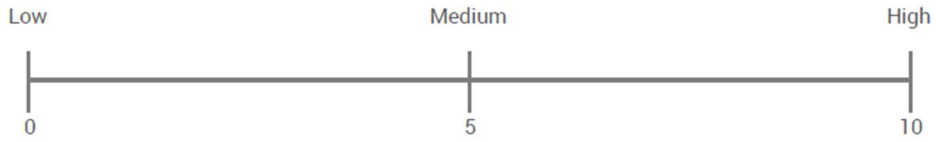
5 Please rate the **INTENSITY** of the **SWEETNESS** in Sample {{sample_code}}.



6 Please select the phrase that best describes how much you like or dislike the **APPLE FLAVOUR** (fruity flavour) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

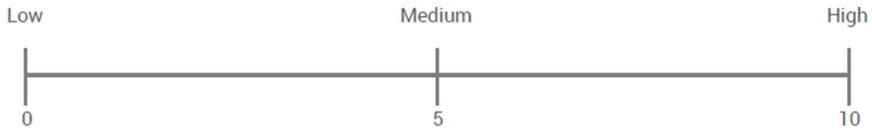
7 Please rate the **INTENSITY** of the **APPLE FLAVOUR** (fruity flavour) in Sample {{sample_code}}.



8 Please select the phrase that best describes how much you like or dislike the **TARTNESS** (defined as a sharp sour taste) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

9 Please rate the **INTENSITY** of the **TARTNESS** (defined as a sharp sour taste) in Sample {{sample_code}}.



10 Please select the phrase that best describes your **OVERALL OPINION** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

11 Please rate the **INTENSITY** of the **AFTERTASTE** in Sample {{sample_code}}.

Much Too Weak	Slightly Too Weak	Just About Right	Slightly Too Strong	Much Too Strong
○	○	○	○	○

ℙ NOTE: Only answer this question if on question #1 of questionnaire page your answer was one of the following: "Slightly Too Strong" "Much Too Strong"

12 From the previous question, please describe (in as much detail as possible) the aftertaste you detected.

13 Do you have any additional comments about Sample {{sample_code}}? If not, then please write no.

Figure 22. *Questionnaire for the six selected apple juice samples during formal sensory evaluation.*

8.3.2 – Formal Sensory Questionnaire for Orange Juice Samples

1 Please select the phrase that best describes how much you like or dislike the **COLOUR** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

2 Please select the phrase that best describes how much you like or dislike the **ORANGE AROMA** (citrus aroma) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

3 Please rate the **INTENSITY** of the **ORANGE AROMA** (citric aroma) in Sample {{sample_code}}.

Low	Medium	High
0	5	10

4 Please select the phrase that best describes how much you like or dislike the **SWEETNESS** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

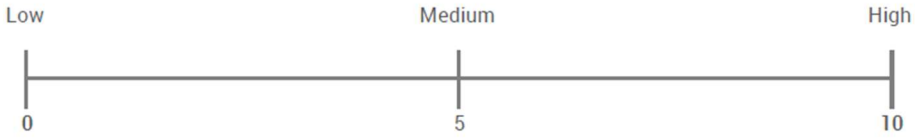
5 Please rate the **INTENSITY** of the **SWEETNESS** in Sample {{sample_code}}.

Low	Medium	High
0	5	10

6 Please select the phrase that best describes how much you like or dislike the **ORANGE FLAVOUR** (fruity flavour) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

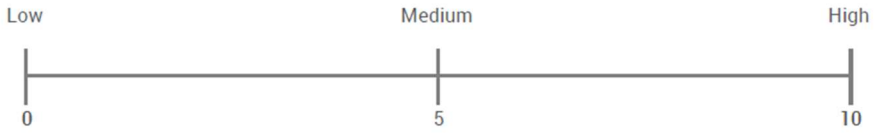
7 Please rate the **INTENSITY** of the **ORANGE FLAVOUR** (fruity flavour) in Sample {{sample_code}}.



8 Please select the phrase that best describes how much you like or dislike the **SOURNESS** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

9 Please rate the **INTENSITY** of the **SOURNESS** in Sample {{sample_code}}.



10 Please select the phrase that best describes your **OVERALL OPINION** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

11 Please rate the **INTENSITY** of the **AFTERTASTE** in Sample {{sample_code}}.

Much Too Weak	Slightly Too Weak	Just About Right	Slightly Too Strong	Much Too Strong
○	○	○	○	○

NOTE: Only answer this question if on question #1 of questionnaire page your answer was one of the following: "Slightly Too Strong" "Much Too Strong"

12 From the previous question, please describe (in as much detail as possible) the aftertaste you detected.

13 Do you have any additional comments about Sample {{sample_code}}? If not, then please write no.

Figure 23. *Questionnaire for the six selected orange juice samples during formal sensory evaluation.*

8.3.3 – Formal Sensory Questionnaire for Cranberry Juice Samples

1 Please select the phrase that best describes how much you like or dislike the **COLOUR** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

2 Please select the phrase that best describes how much you like or dislike the **CRANBERRY AROMA** (fruity aroma) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

3 Please rate the **INTENSITY** of the **CRANBERRY AROMA** (fruity aroma) in Sample {{sample_code}}.

Low — Medium — High

0 — 5 — 10

4 Please select the phrase that best describes how much you like or dislike the **SWEETNESS** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

5 Please rate the **INTENSITY** of the **SWEETNESS** in Sample {{sample_code}}.

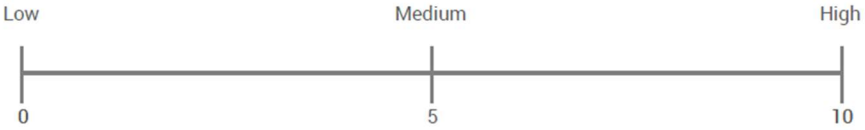
Low — Medium — High

0 — 5 — 10

6 Please select the phrase that best describes how much you like or dislike the **TARTNESS** (defined as a sharp sour taste) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

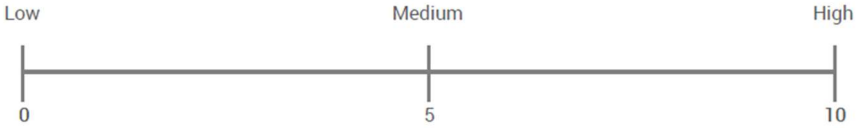
7 Please rate the **INTENSITY** of the **TARTNESS** (defined as a sharp sour taste) in Sample {{sample_code}}.



8 Please select the phrase that best describes how much you like or dislike the **BITTERNESS** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

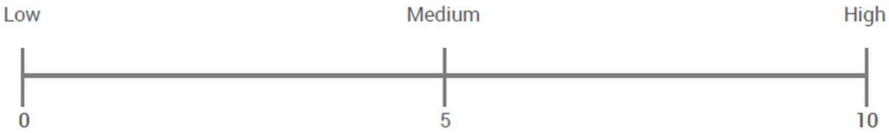
9 Please rate the **INTENSITY** of the **BITTERNESS** in Sample {{sample_code}}.



10 Please select the phrase that best describes how much you like or dislike the **CRANBERRY FLAVOUR** (fruity flavour) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

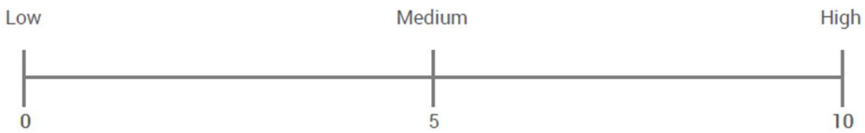
11 Please rate the **INTENSITY** of the **CRANBERRY FLAVOUR** (fruity flavour) in Sample {{sample_code}}.



12 Please select the phrase that best describes how much you like or dislike the **ASTRINGENCY** (defined as the tightness or dry sensation in the mouth) of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

13 Please rate the **INTENSITY** of the **ASTRINGENCY** (defined as the tightness or dry sensation in the mouth) in Sample {{sample_code}}.



14 Please select the phrase that best describes your **OVERALL OPINION** of Sample {{sample_code}}.

Dislike Extremely	Dislike Very Much	Dislike Moderately	Dislike Slightly	Neither Like Nor Dislike	Like Slightly	Like Moderately	Like Very Much	Like Extremely
○	○	○	○	○	○	○	○	○

15 Please rate the **INTENSITY** of the **AFTERTASTE** in Sample {{sample_code}}.

Much Too Weak	Slightly Too Weak	Just About Right	Slightly Too Strong	Much Too Strong
○	○	○	○	○

NOTE: Only answer this question if on question #1 of questionnaire page your answer was one of the following: "Slightly Too Strong" "Much Too Strong"

16 From the previous question, please describe (in as much detail as possible) the aftertaste you detected.

17 Do you have any additional comments about Sample {{sample_code}}? If not, then please write no.

Figure 24. *Questionnaire for the six selected cranberry juice samples during formal sensory evaluation.*

8.4 Appendix 4 – Data of Identified Compounds by Total Peak Area

Total sum normalisation expresses the total peak area (given as a percentage) of certain target compounds generated by GCMS analysis. Area value was integrated manually and calculated by the computer software program. Total sum normalisation generally exhibits greater validity when chromatographs closely resemble each other. In the case of this dissertation, all chromatographs (not shown) were fairly similar in their characteristics and retention times but had varying peak area abundances. Hence, this method was utilised to determine the relative concentrations of each analyte (volatile compound) after GCMS-SPME analysis. The calculated data of which can be found in the following tables below.

Table 23. *Normalisation of identified GCMS compounds by the average of triplicate total peak areas and their relative uncertainties (%) for apple juice.*

No.	Sample Name	Compound's Total Peak Area and Uncertainty (%)							
		1-pentanal	Hexanal	Butyl acetate	(Z)-3-hexen-1-ol	3-methyl-1-butyl acetate	2-methyl-1-butyl acetate	Hexyl acetate	Benzaldehyde
1	Control Apple	105.8 ± 3.7	114.8 ± 6.1	108.9 ± 4.9	109.8 ± 4.3	107.9 ± 4.0	84.5 ± 8.9	106.9 ± 3.9	100.1 ± 5.3
2	20g/L SV7 (COL.1)	202.7 ± 5.1	78.2 ± 9.2	70.4 ± 5.7	93.6 ± 7.3	37.1 ± 7.6	98.2 ± 6.3	19.7 ± 8.3	45.1 ± 7.6
3	10g/L SV7 (COL.1)	168.7 ± 6.9	103.5 ± 8.2	89.3 ± 6.0	127.6 ± 5.6	68.4 ± 7.5	109.8 ± 7.3	32.4 ± 8.3	49.8 ± 6.3
4	5g/L SV7 (COL.1)	182.9 ± 4.7	96.9 ± 8.2	83.8 ± 5.3	113.4 ± 7.6	61.5 ± 4.0	91.5 ± 8.8	24.4 ± 5.0	50.3 ± 5.7
5	20g/L SV7 (COL.2)	195.9 ± 8.3	32.3 ± 9.2	31.9 ± 5.9	85.4 ± 6.0	12.8 ± 5.5	52.6 ± 8.4	5.7 ± 4.5	45.1 ± 2.7
6	10g/L SV7 (COL.2)	125.5 ± 6.5	97.8 ± 6.4	90.3 ± 5.1	104.4 ± 5.2	77.9 ± 4.8	91.5 ± 7.9	41.6 ± 6.9	41.3 ± 5.8
7	5g/L SV7 (COL.2)	122.5 ± 6.6	96.9 ± 7.2	89.1 ± 6.1	104.7 ± 4.7	80.8 ± 5.7	91.6 ± 6.9	46.7 ± 4.3	44.1 ± 6.9
8	20g/L SV7 (COL.3)	204.9 ± 4.8	51.4 ± 6.2	50.3 ± 3.9	106.5 ± 6.2	24.7 ± 4.3	81.6 ± 4.3	12.7 ± 6.3	42.8 ± 7.1
9	10g/L SV7 (COL.3)	118.4 ± 3.8	100.5 ± 6.9	92.0 ± 5.9	106.4 ± 7.6	81.7 ± 6.1	92.9 ± 5.1	47.1 ± 6.2	38.7 ± 3.7
10	5g/L SV7 (COL.3)	119.6 ± 5.5	102.2 ± 6.5	94.6 ± 6.2	111.5 ± 5.1	90.1 ± 4.9	93.1 ± 9.1	55.6 ± 4.0	52.5 ± 8.0
11	20g/L GV1 (COL.1)	173.0 ± 4.5	34.8 ± 7.8	37.8 ± 9.5	65.2 ± 8.2	16.3 ± 7.9	64.5 ± 8.5	8.8 ± 6.4	42.8 ± 4.4
12	10g/L GV1 (COL.1)	173.5 ± 6.4	87.0 ± 7.3	78.0 ± 6.1	103.0 ± 7.8	64.5 ± 5.1	84.7 ± 9.5	26.2 ± 4.8	42.3 ± 4.4
13	5g/L GV1 (COL.1)	232.5 ± 5.8	52.9 ± 8.5	52.9 ± 5.7	123.6 ± 9.6	24.7 ± 8.8	77.4 ± 5.3	10.7 ± 9.7	38.9 ± 4.0
14	20g/L GV1 (COL.2)	207.8 ± 6.5	46.4 ± 6.7	46.3 ± 4.0	107.4 ± 8.2	22.5 ± 5.2	73.2 ± 7.1	11.3 ± 7.1	42.6 ± 8.4
15	10g/L GV1 (COL.2)	218.6 ± 5.3	50.2 ± 8.6	50.3 ± 6.4	116.6 ± 7.6	24.7 ± 6.7	74.8 ± 8.6	10.8 ± 8.1	43.9 ± 8.3
16	5g/L GV1 (COL.2)	218.7 ± 4.2	49.0 ± 6.9	45.2 ± 4.6	136.8 ± 6.1	23.5 ± 4.9	69.9 ± 7.2	12.0 ± 5.6	43.9 ± 7.0
17	20g/L GV1 (COL.3)	222.7 ± 4.7	41.1 ± 5.6	35.8 ± 4.2	111.5 ± 7.6	17.0 ± 6.1	58.9 ± 5.6	9.2 ± 4.2	39.4 ± 6.5
18	10g/L GV1 (COL.3)	121.1 ± 4.9	93.0 ± 10.2	84.8 ± 6.7	105.7 ± 4.6	75.5 ± 10.0	77.0 ± 7.3	43.1 ± 10.9	52.4 ± 5.5
19	5g/L GV1 (COL.3)	113.4 ± 7.9	101.6 ± 6.2	90.0 ± 4.5	122.1 ± 5.3	88.4 ± 3.6	69.8 ± 7.3	56.5 ± 4.1	38.5 ± 6.7
20	20g/L CV6 (COL.1)	109.7 ± 5.4	32.0 ± 8.1	32.5 ± 6.2	130.1 ± 5.2	15.6 ± 8.7	48.5 ± 5.6	6.0 ± 7.9	75.9 ± 4.4
21	10g/L CV6 (COL.1)	96.2 ± 4.4	76.6 ± 6.6	64.0 ± 7.9	129.5 ± 8.5	57.8 ± 10.3	73.2 ± 7.5	29.8 ± 5.3	77.3 ± 3.6
22	5g/L CV6 (COL.1)	72.1 ± 4.2	79.9 ± 6.0	69.5 ± 4.3	131.4 ± 4.9	67.1 ± 5.2	76.3 ± 7.8	37.7 ± 5.1	68.2 ± 7.9
23	20g/L CV6 (COL.2)	131.3 ± 6.6	44.9 ± 6.6	40.6 ± 4.7	148.6 ± 4.2	25.2 ± 8.3	57.1 ± 5.6	12.1 ± 4.4	54.4 ± 5.5
24	10g/L CV6 (COL.2)	71.2 ± 6.2	68.3 ± 6.0	65.0 ± 4.7	122.6 ± 3.9	65.3 ± 5.0	71.5 ± 8.2	40.3 ± 3.7	55.4 ± 6.9

25	5g/L CV6 (COL.2)	64.3 ± 4.7	81.7 ± 6.7	72.9 ± 5.7	128.2 ± 6.3	72.6 ± 4.8	80.9 ± 9.1	53.5 ± 5.0	72.7 ± 9.7
26	20g/L CV6 (COL.3)	105.5 ± 9.9	46.8 ± 6.7	44.4 ± 5.0	152.1 ± 6.8	30.0 ± 6.8	66.9 ± 3.6	17.2 ± 5.1	62.5 ± 3.8
27	10g/L CV6 (COL.3)	72.4 ± 9.4	78.3 ± 7.7	72.1 ± 4.1	121.1 ± 5.6	74.7 ± 5.2	81.2 ± 7.5	56.7 ± 5.7	66.9 ± 4.9
28	5g/L CV6 (COL.3)	14.3 ± 8.3	75.3 ± 7.9	67.4 ± 5.0	109.9 ± 7.4	72.4 ± 4.6	79.3 ± 9.2	58.0 ± 4.9	54.8 ± 3.4
29	20g/L Puro (COL.1)	66.7 ± 8.5	3.6 ± 1.8	2.2 ± 0.8	9.3 ± 1.8	3.2 ± 0.4	-	38.2 ± 5.4	1.3 ± 0.2
30	10g/L Puro (COL.1)	116.7 ± 5.5	14.9 ± 6.5	4.6 ± 1.1	32.3 ± 7.9	2.7 ± 0.2	11.3 ± 5.4	1.4 ± 0.4	47.0 ± 8.3
31	5g/L Puro (COL.1)	151.9 ± 8.0	26.1 ± 7.3	29.5 ± 5.5	112.5 ± 8.1	11.5 ± 2.5	39.3 ± 5.2	3.4 ± 0.6	44.7 ± 7.3
32	20g/L Puro (COL.2)	89.9 ± 9.6	13.1 ± 7.2	8.1 ± 1.4	57.3 ± 7.8	6.0 ± 0.7	25.2 ± 6.2	5.0 ± 0.8	40.0 ± 5.0
33	10g/L Puro (COL.2)	115.4 ± 5.5	44.4 ± 8.1	26.9 ± 9.0	87.5 ± 5.4	20.1 ± 8.2	51.9 ± 7.6	13.0 ± 6.3	46.0 ± 9.7
34	5g/L Puro (COL.2)	96.2 ± 8.9	57.1 ± 6.8	41.0 ± 5.6	113.4 ± 7.8	24.7 ± 5.4	58.1 ± 4.8	12.6 ± 6.8	42.0 ± 5.2
35	20g/L Puro (COL.3)	85.5 ± 6.2	54.4 ± 6.7	41.3 ± 4.8	98.5 ± 5.2	32.4 ± 6.7	64.6 ± 4.5	24.4 ± 4.9	42.0 ± 3.7
36	10g/L Puro (COL.3)	85.5 ± 7.6	54.4 ± 6.6	41.3 ± 5.2	98.5 ± 6.8	32.4 ± 6.6	64.6 ± 6.1	24.4 ± 6.3	42.0 ± 6.1
37	5g/L Puro (COL.3)	127.1 ± 5.8	59.1 ± 6.9	47.0 ± 8.6	108.5 ± 10.1	36.6 ± 8.0	66.1 ± 4.7	25.6 ± 6.1	41.1 ± 8.4
38	20g/L Carbon (COL.1)	101.4 ± 9.0	37.9 ± 5.8	37.8 ± 4.8	123.1 ± 3.6	29.1 ± 5.9	61.3 ± 6.4	15.2 ± 4.1	49.7 ± 5.8
39	10g/L Carbon (COL.1)	92.1 ± 7.5	69.1 ± 6.1	60.2 ± 4.3	115.8 ± 5.5	64.7 ± 5.1	75.5 ± 6.3	40.1 ± 4.7	48.0 ± 5.5
40	5g/L Carbon (COL.1)	76.3 ± 8.7	59.1 ± 8.5	56.3 ± 5.2	99.7 ± 6.4	56.9 ± 9.4	76.5 ± 5.9	33.4 ± 10.1	40.3 ± 5.5
41	20g/L Carbon (COL.2)	81.5 ± 6.3	46.1 ± 6.9	44.5 ± 4.9	158.3 ± 5.8	37.2 ± 5.5	62.7 ± 6.3	24.5 ± 6.5	46.6 ± 3.6
42	10g/L Carbon (COL.2)	59.5 ± 4.2	63.7 ± 6.3	57.5 ± 4.1	97.6 ± 4.7	64.5 ± 5.1	75.7 ± 5.7	50.1 ± 5.6	45.9 ± 4.8
43	5g/L Carbon (COL.2)	50.5 ± 7.7	67.7 ± 7.2	61.0 ± 5.0	106.0 ± 7.3	67.5 ± 4.9	71.1 ± 4.5	51.2 ± 4.7	34.3 ± 6.4
44	20g/L Carbon (COL.3)	84.0 ± 4.1	52.5 ± 7.4	52.7 ± 4.9	107.0 ± 7.4	58.6 ± 4.2	63.5 ± 8.1	46.2 ± 4.2	51.9 ± 2.9
45	10g/L Carbon (COL.3)	58.7 ± 10.0	64.1 ± 7.4	57.8 ± 5.5	94.3 ± 5.9	65.5 ± 4.5	70.0 ± 9.2	57.4 ± 4.2	47.7 ± 6.7
46	5g/L Carbon (COL.3)	70.9 ± 8.3	60.3 ± 5.8	57.8 ± 4.2	103.5 ± 6.2	66.9 ± 4.5	59.7 ± 4.4	55.7 ± 4.8	64.8 ± 4.4

Note. (-) means compound was not detected within gas chromatography-mass spectroscopy (GCMS) analysis. Puro means the resin Purosorb PAD 600.

Table 24. *Normalisation of identified GCMS compounds by the average of triplicate total peak areas and their relative uncertainties (%) for orange juice.*

No.	Sample Name	Compound's Total Peak Area and Uncertainty (%)												
		Ethyl butyrate	α-pinene	β-pinene	Limonene	1-octanol	Propyl hexanoate	Linalool	Benzaldehyde	3-carene	Decanal	Copaene	Caryophyllene	α-caryophyllene
1	Control Orange	79.6 ± 2.3	72.8 ± 2.5	77.7 ± 3.9	92.7 ± 2.3	110.5 ± 5.1	122.9 ± 6.1	117.5 ± 2.7	63.1 ± 7.6	93.5 ± 7.9	124.9 ± 7.9	72.4 ± 3.1	100.6 ± 3.2	93.0 ± 5.7
2	20g/L SV7 (COL.1)	35.2 ± 5.8	134.8 ± 3.2	89.4 ± 4.4	101.4 ± 2.9	49.8 ± 4.0	56.8 ± 9.5	59.5 ± 5.3	55.8 ± 3.6	78.5 ± 9.2	73.6 ± 9.8	114.2 ± 6.6	156.6 ± 8.4	111.1 ± 10.0
3	10g/L SV7 (COL.1)	53.1 ± 5.5	106.9 ± 4.2	81.7 ± 4.0	90.9 ± 9.7	72.6 ± 7.2	55.9 ± 6.0	76.3 ± 6.9	63.5 ± 9.7	69.7 ± 9.2	85.6 ± 8.8	88.3 ± 6.2	128.9 ± 1.2	79.7 ± 9.7
4	5g/L SV7 (COL.1)	44.3 ± 4.7	113.8 ± 3.8	81.8 ± 4.1	97.3 ± 4.8	59.2 ± 8.6	51.9 ± 7.6	64.0 ± 3.3	56.4 ± 7.3	64.1 ± 8.5	126.5 ± 5.9	84.7 ± 4.3	112.7 ± 2.7	85.4 ± 4.3
5	20g/L SV7 (COL.2)	28.5 ± 3.6	103.0 ± 8.7	73.2 ± 3.9	95.6 ± 3.3	27.5 ± 3.7	56.5 ± 3.5	38.4 ± 5.2	59.1 ± 8.8	51.4 ± 2.5	96.0 ± 6.8	79.1 ± 4.7	88.7 ± 5.4	68.2 ± 4.5
6	10g/L SV7 (COL.2)	61.3 ± 2.6	106.6 ± 2.8	60.1 ± 4.3	86.4 ± 2.4	52.3 ± 6.0	50.9 ± 2.8	61.1 ± 4.6	57.9 ± 1.7	73.4 ± 4.4	96.1 ± 6.6	58.6 ± 6.3	84.0 ± 3.8	70.7 ± 2.9
7	5g/L SV7 (COL.2)	42.8 ± 3.8	126.0 ± 4.2	85.0 ± 9.4	105.5 ± 6.0	63.0 ± 4.7	102.5 ± 8.1	78.6 ± 3.1	60.6 ± 7.4	74.8 ± 8.4	73.3 ± 8.8	74.3 ± 4.2	139.8 ± 8.0	110.6 ± 8.0
8	20g/L SV7 (COL.3)	36.5 ± 4.9	124.7 ± 5.8	72.5 ± 6.1	98.6 ± 5.3	37.0 ± 5.6	29.7 ± 4.8	54.5 ± 2.8	57.7 ± 5.8	70.4 ± 6.4	106.4 ± 8.8	92.0 ± 8.1	110.7 ± 7.2	89.3 ± 5.7
9	10g/L SV7 (COL.3)	42.1 ± 4.2	120.1 ± 5.6	82.2 ± 6.3	106.7 ± 3.8	48.1 ± 5.3	46.3 ± 9.8	65.6 ± 4.1	62.2 ± 3.1	75.7 ± 5.1	98.9 ± 6.5	98.5 ± 6.9	134.2 ± 8.3	90.9 ± 7.9
10	5g/L SV7 (COL.3)	49.3 ± 5.2	97.1 ± 5.4	72.8 ± 4.8	103.9 ± 3.1	53.3 ± 8.9	47.0 ± 8.9	72.9 ± 4.8	52.9 ± 5.8	65.7 ± 6.1	95.1 ± 7.2	84.0 ± 6.3	101.5 ± 8.1	75.6 ± 5.3
11	20g/L GV1 (COL.1)	28.2 ± 6.1	40.0 ± 5.0	54.5 ± 7.3	92.3 ± 4.6	21.1 ± 8.7	20.5 ± 4.4	38.2 ± 4.0	69.6 ± 8.0	45.2 ± 2.9	58.7 ± 6.5	58.6 ± 3.3	86.7 ± 7.9	74.5 ± 7.3
12	10g/L GV1 (COL.1)	33.1 ± 8.1	81.9 ± 9.1	60.9 ± 8.9	94.3 ± 5.6	30.2 ± 6.0	33.8 ± 7.3	42.2 ± 4.5	61.0 ± 3.3	56.6 ± 8.0	76.2 ± 6.2	66.9 ± 8.7	80.3 ± 5.6	57.2 ± 3.6

13	5g/L GV1 (COL.1)	38.8 ± 5.4	68.2 ± 8.4	65.8 ± 7.2	101.4 ± 4.7	48.1 ± 8.6	37.4 ± 8.1	59.1 ± 4.4	77.6 ± 5.3	63.0 ± 7.9	71.2 ± 8.6	76.9 ± 6.8	99.2 ± 3.7	80.6 ± 2.9
14	20g/L GV1 (COL.2)	28.7 ± 3.8	78.4 ± 5.4	69.5 ± 4.4	106.3 ± 3.1	31.3 ± 8.6	33.2 ± 7.5	45.8 ± 8.2	51.1 ± 9.8	60.1 ± 4.4	61.5 ± 5.0	95.7 ± 5.3	119.7 ± 2.1	90.0 ± 4.2
15	10g/L GV1 (COL.2)	31.2 ± 4.2	79.4 ± 3.2	74.2 ± 5.0	107.8 ± 2.7	35.4 ± 6.3	39.4 ± 7.8	46.9 ± 3.6	55.6 ± 5.9	57.2 ± 3.0	74.1 ± 8.7	84.7 ± 5.0	106.5 ± 6.1	69.1 ± 7.1
16	5g/L GV1 (COL.2)	36.9 ± 5.2	94.1 ± 5.5	81.3 ± 6.2	111.3 ± 3.4	45.3 ± 7.9	44.6 ± 5.5	59.6 ± 6.3	53.4 ± 5.1	60.7 ± 3.7	59.7 ± 5.8	88.8 ± 6.8	109.5 ± 3.3	74.2 ± 5.7
17	20g/L GV1 (COL.3)	25.3 ± 4.1	60.8 ± 5.6	60.2 ± 6.3	98.2 ± 2.9	21.2 ± 5.8	22.8 ± 6.5	33.9 ± 4.2	51.0 ± 3.0	49.5 ± 5.9	58.1 ± 10.0	69.3 ± 4.8	83.0 ± 3.3	61.0 ± 6.8
18	10g/L GV1 (COL.3)	34.6 ± 4.3	80.3 ± 4.6	59.2 ± 7.3	93.1 ± 5.0	30.0 ± 9.1	25.1 ± 6.0	45.0 ± 7.3	56.3 ± 6.6	49.6 ± 4.6	57.1 ± 8.1	56.2 ± 6.1	68.6 ± 5.3	53.5 ± 9.2
19	5g/L GV1 (COL.3)	43.8 ± 4.4	68.9 ± 5.2	62.9 ± 6.5	96.7 ± 3.3	47.7 ± 4.1	36.0 ± 2.5	55.9 ± 5.7	62.0 ± 4.1	50.3 ± 3.2	56.7 ± 9.1	65.0 ± 6.0	77.1 ± 2.2	59.8 ± 4.2
20	20g/L CV6 (COL.1)	24.0 ± 3.0	75.2 ± 8.7	56.6 ± 5.2	92.2 ± 3.0	17.0 ± 4.5	15.7 ± 7.2	28.6 ± 5.5	47.7 ± 7.0	40.5 ± 5.5	50.8 ± 8.3	73.4 ± 7.7	80.5 ± 5.3	52.4 ± 8.9
21	10g/L CV6 (COL.1)	28.6 ± 7.0	76.6 ± 4.0	60.7 ± 3.7	96.5 ± 2.9	28.1 ± 6.4	22.5 ± 7.8	37.5 ± 4.3	44.1 ± 6.6	45.7 ± 7.2	57.1 ± 8.2	78.5 ± 4.9	86.5 ± 4.5	60.3 ± 5.3
22	5g/L CV6 (COL.1)	30.6 ± 4.7	77.5 ± 8.9	65.2 ± 4.3	99.9 ± 2.9	34.5 ± 8.5	28.9 ± 9.3	47.4 ± 7.4	50.9 ± 4.0	50.0 ± 3.6	58.0 ± 6.5	81.9 ± 3.3	92.3 ± 1.5	58.6 ± 7.7
23	20g/L CV6 (COL.2)	21.0 ± 5.9	83.3 ± 2.6	69.1 ± 4.0	105.1 ± 5.1	26.4 ± 5.6	26.1 ± 3.2	38.6 ± 6.1	48.7 ± 4.5	50.1 ± 4.7	77.7 ± 5.4	90.5 ± 6.8	111.8 ± 4.9	76.7 ± 4.4
24	10g/L CV6 (COL.2)	32.2 ± 4.5	58.5 ± 6.3	53.2 ± 5.9	85.6 ± 6.3	34.8 ± 7.4	23.3 ± 6.1	46.7 ± 7.3	50.0 ± 2.5	47.3 ± 5.8	62.4 ± 9.3	57.8 ± 8.6	71.5 ± 9.5	53.2 ± 6.0
25	5g/L CV6 (COL.2)	35.1 ± 5.4	77.9 ± 7.4	64.5 ± 4.3	99.0 ± 3.1	41.8 ± 5.7	33.5 ± 3.0	56.8 ± 6.0	51.7 ± 4.8	56.5 ± 3.8	78.7 ± 6.7	71.4 ± 3.9	91.0 ± 5.6	64.8 ± 9.2
26	20g/L CV6 (COL.3)	31.9 ± 4.4	53.8 ± 8.1	59.0 ± 3.8	94.5 ± 4.3	31.8 ± 8.2	28.8 ± 4.8	46.0 ± 5.3	51.4 ± 5.8	51.1 ± 3.9	58.6 ± 6.6	67.0 ± 5.8	80.8 ± 4.1	56.8 ± 5.8
27	10g/L CV6 (COL.3)	36.7 ± 3.4	68.0 ± 5.3	71.2 ± 4.3	105.3 ± 2.7	44.4 ± 9.1	41.0 ± 4.1	61.5 ± 3.9	47.7 ± 3.3	59.5 ± 5.8	86.2 ± 5.5	81.1 ± 5.6	99.5 ± 4.1	66.5 ± 5.2

28	5g/L CV6 (COL.3)	34.8 ± 3.3	72.0 ± 5.5	76.0 ± 4.4	107.4 ± 3.4	46.0 ± 5.5	41.0 ± 3.5	61.9 ± 4.7	61.4 ± 6.5	59.4 ± 4.1	94.3 ± 7.9	77.0 ± 3.5	93.9 ± 3.3	59.1 ± 4.1
29	20g/L Puro (COL.1)	9.4 ± 3.0	50.6 ± 6.1	52.9 ± 5.4	90.2 ± 2.9	14.4 ± 4.8	12.8 ± 5.2	17.2 ± 4.8	42.6 ± 3.2	38.7 ± 4.8	43.9 ± 9.0	61.8 ± 4.6	79.6 ± 3.9	51.4 ± 9.0
30	10g/L Puro (COL.1)	16.8 ± 3.3	57.6 ± 4.1	36.0 ± 8.8	84.0 ± 5.8	24.4 ± 7.3	16.1 ± 6.2	29.3 ± 3.9	44.5 ± 8.8	40.1 ± 4.0	42.4 ± 9.0	58.5 ± 10.0	76.1 ± 9.9	55.2 ± 9.9
31	5g/L Puro (COL.1)	32.7 ± 4.8	33.8 ± 4.7	37.1 ± 4.0	84.6 ± 3.3	28.3 ± 7.6	28.0 ± 4.6	31.6 ± 6.9	54.4 ± 0.8	39.2 ± 6.4	48.0 ± 8.8	57.7 ± 8.6	91.8 ± 2.7	56.8 ± 6.1
32	20g/L Puro (COL.2)	22.7 ± 4.4	26.9 ± 7.4	27.9 ± 8.3	82.3 ± 3.6	21.3 ± 3.6	16.7 ± 9.5	23.1 ± 5.2	43.8 ± 4.7	36.8 ± 5.6	39.4 ± 8.8	48.3 ± 5.9	75.0 ± 1.2	44.9 ± 9.7
33	10g/L Puro (COL.2)	36.2 ± 3.1	30.0 ± 3.3	39.0 ± 5.3	86.1 ± 3.1	31.7 ± 5.3	29.7 ± 8.9	35.3 ± 4.0	44.0 ± 7.5	41.3 ± 2.9	59.6 ± 6.9	49.6 ± 5.7	79.1 ± 4.7	49.0 ± 3.9
34	5g/L Puro (COL.2)	35.0 ± 5.8	49.4 ± 6.7	61.5 ± 5.3	99.3 ± 3.8	47.8 ± 8.2	40.5 ± 8.4	56.5 ± 6.5	59.7 ± 3.3	51.1 ± 6.1	47.2 ± 6.1	66.5 ± 8.2	92.8 ± 9.4	61.5 ± 8.9
35	20g/L Puro (COL.3)	29.0 ± 3.6	43.3 ± 7.0	31.0 ± 6.5	80.5 ± 5.0	37.9 ± 3.8	29.4 ± 7.8	40.4 ± 9.6	38.2 ± 9.2	31.9 ± 7.2	44.8 ± 8.4	50.5 ± 6.8	64.7 ± 2.5	39.3 ± 9.8
36	10g/L Puro (COL.3)	35.7 ± 4.5	42.4 ± 5.8	30.3 ± 5.5	84.4 ± 3.1	37.1 ± 5.7	38.9 ± 4.3	44.9 ± 5.9	33.3 ± 6.2	34.9 ± 5.1	43.3 ± 7.7	49.2 ± 5.0	65.2 ± 5.2	39.0 ± 5.9
37	5g/L Puro (COL.3)	37.6 ± 3.5	53.5 ± 8.5	54.3 ± 3.9	94.7 ± 3.3	43.6 ± 4.7	47.1 ± 7.0	52.7 ± 5.4	33.7 ± 6.8	40.2 ± 8.5	56.6 ± 7.2	61.4 ± 8.3	81.2 ± 5.3	44.9 ± 4.7
38	20g/L Carbon (COL.1)	25.2 ± 3.6	73.2 ± 4.3	61.4 ± 4.2	97.9 ± 2.4	35.8 ± 8.4	26.8 ± 7.3	54.6 ± 4.5	31.1 ± 4.0	38.3 ± 7.2	75.3 ± 7.4	66.8 ± 7.2	75.8 ± 4.7	51.1 ± 7.9
39	10g/L Carbon (COL.1)	30.6 ± 4.8	75.0 ± 4.4	65.1 ± 7.6	98.2 ± 4.4	37.3 ± 5.9	32.6 ± 6.5	53.8 ± 5.7	26.7 ± 5.3	41.0 ± 3.8	90.5 ± 7.7	64.0 ± 5.3	73.6 ± 1.8	43.3 ± 8.2
40	5g/L Carbon (COL.1)	32.0 ± 6.5	71.9 ± 4.8	54.0 ± 8.0	89.6 ± 7.5	40.6 ± 6.8	34.8 ± 4.7	56.3 ± 8.1	24.1 ± 6.5	38.6 ± 8.1	61.3 ± 9.7	57.9 ± 8.1	63.3 ± 1.8	44.1 ± 6.6

41	20g/L Carbon (COL.2)	31.0 ± 4.2	62.5 ± 6.6	54.8 ± 6.4	92.2 ± 4.0	38.9 ± 7.6	33.3 ± 5.6	58.8 ± 2.6	31.8 ± 2.1	39.1 ± 3.3	57.2 ± 5.8	55.8 ± 2.8	70.2 ± 3.7	45.1 ± 7.2
42	10g/L Carbon (COL.2)	39.7 ± 3.3	70.5 ± 5.1	51.0 ± 7.2	84.3 ± 3.9	38.6 ± 4.9	41.8 ± 6.7	55.4 ± 5.7	36.2 ± 4.3	35.6 ± 6.2	53.0 ± 5.3	45.2 ± 8.8	57.6 ± 7.5	39.3 ± 7.8
43	5g/L Carbon (COL.2)	30.5 ± 5.4	64.6 ± 3.3	57.4 ± 5.0	93.1 ± 2.6	38.5 ± 4.6	32.1 ± 6.2	50.5 ± 4.0	26.8 ± 6.0	37.6 ± 9.3	80.6 ± 5.2	57.8 ± 5.3	71.7 ± 2.9	47.0 ± 4.7
44	20g/L Carbon (COL.3)	25.4 ± 4.1	66.7 ± 4.1	60.3 ± 4.0	96.6 ± 3.0	40.3 ± 9.5	35.6 ± 7.0	51.9 ± 5.6	32.5 ± 3.2	37.4 ± 7.4	64.2 ± 4.9	61.2 ± 5.5	70.7 ± 3.9	45.0 ± 6.6
45	10g/L Carbon (COL.3)	35.3 ± 5.3	97.8 ± 3.4	68.6 ± 7.4	97.2 ± 4.8	42.6 ± 6.6	42.8 ± 2.5	55.1 ± 7.1	29.2 ± 7.8	42.2 ± 5.0	90.0 ± 6.3	59.9 ± 8.1	72.9 ± 6.9	45.8 ± 9.7
46	5g/L Carbon (COL.3)	28.8 ± 3.8	79.9 ± 7.2	65.4 ± 5.9	101.0 ± 3.2	41.8 ± 7.7	39.0 ± 5.3	56.4 ± 7.6	29.9 ± 6.5	37.4 ± 5.6	93.1 ± 7.4	63.5 ± 3.7	74.8 ± 2.3	46.7 ± 5.9

Note. (-) means compound was not detected within gas chromatography-mass spectroscopy (GCMS) analysis. Puro means the resin Purosorb PAD 600.

Table 25. *Normalisation of identified GCMS compounds by the average of triplicate total peak areas and their relative uncertainties (%) for cranberry juice.*

No.	Sample Name	Compound's Total Peak Area and Uncertainty (%)								
		Ethyl acetate	Ethyl butyrate	Ethyl-2-methyl butyrate	(Z)-3-hexen-1-ol	Benzene	Eucalyptol	Linalool	Benz-aldehyde	Benzoic acid
1	Control Cranberry	89.5 ± 4.9	107.2 ± 5.3	101.8 ± 6.7	104.7 ± 9.0	107.7 ± 8.2	99.5 ± 6.0	95.0 ± 4.6	86.2 ± 9.4	108.5 ± 3.4
2	20g/L SV7 (COL.1)	69.3 ± 7.3	175.8 ± 1.5	35.4 ± 2.5	70.0 ± 1.9	48.7 ± 9.1	-	130.6 ± 2.9	87.9 ±6.8	21.7 ± 8.4
3	10g/L SV7 (COL.1)	60.5 ± 7.8	69.1 ± 3.6	40.6 ± 3.9	70.9 ± 5.2	22.9 ± 5.2	95.5 ± 5.2	52.6 ± 9.6	80.5 ± 8.8	36.4 ± 5.1
4	5g/L SV7 (COL.1)	60.7 ± 8.5	65.0 ± 6.9	37.6 ± 5.1	70.4 ± 2.8	21.8 ± 6.2	101.9 ± 5.2	40.8 ± 7.5	74.5 ± 6.5	34.7 ± 2.1
5	20g/L SV7 (COL.2)	52.5 ± 9.7	69.7 ± 1.6	42.0 ± 5.7	54.4 ± 5.5	36.5 ± 6.5	88.9 ± 9.7	48.2 ± 3.5	75.2 ± 9.2	37.1 ± 6.3
6	10g/L SV7 (COL.2)	69.9 ± 8.1	71.5 ± 5.9	56.9 ± 6.0	70.3 ± 5.9	39.1 ± 6.3	79.1 ± 6.7	55.2 ± 7.5	77.0 ± 6.8	48.8 ± 2.7
7	5g/L SV7 (COL.2)	75.7 ± 9.4	72.3 ± 1.9	69.7 ± 4.6	74.5 ± 6.6	48.8 ± 6.5	77.0 ± 7.2	60.3 ± 8.6	77.0 ± 5.9	55.9 ± 6.7
8	20g/L SV7 (COL.3)	56.0 ± 6.1	59.4 ± 5.5	44.5 ± 9.1	54.7 ± 3.3	24.0 ± 6.6	56.3 ± 5.5	45.8 ± 8.9	76.4 ± 8.3	36.6 ± 2.4
9	10g/L SV7 (COL.3)	67.6 ± 3.9	62.3 ± 1.9	52.2 ± 8.7	80.7 ± 9.9	53.8 ± 4.3	67.6 ± 5.5	49.9 ± 3.2	83.6 ± 8.7	46.3 ± 2.4
10	5g/L SV7 (COL.3)	82.7 ± 6.9	96.0 ± 7.0	79.2 ± 2.3	98.2 ± 2.3	67.3 ± 7.1	82.2 ± 5.9	77.5 ± 8.7	85.4 ± 9.6	42.2 ± 1.7
11	20g/L GV1 (COL.1)	53.7 ± 4.5	150.3 ± 1.9	42.0 ± 3.4	63.3 ± 2.9	39.3 ± 5.2	90.8 ± 6.2	60.4 ± 6.6	77.5 ± 9.3	37.8 ± 4.7
12	10g/L GV1 (COL.1)	72.6 ± 7.4	90.9 ± 9.0	49.4 ± 8.9	72.0 ± 4.9	39.8 ± 5.1	101.4 ± 5.2	57.9 ± 3.4	67.2 ± 8.3	25.6 ± 2.8
13	5g/L GV1 (COL.1)	67.4 ± 4.2	75.0 ± 1.0	64.4 ± 4.2	81.5 ± 7.0	49.8 ± 7.0	110.2 ± 5.9	49.0 ± 7.5	78.3 ± 9.1	44.5 ± 2.7
14	20g/L GV1 (COL.2)	68.2 ± 1.5	48.7 ± 6.7	31.5 ± 9.5	62.8 ± 1.7	46.5 ± 3.9	66.2 ± 6.3	37.8 ± 6.9	84.1 ± 7.1	21.0 ± 5.6
15	10g/L GV1 (COL.2)	76.2 ± 2.5	41.1 ± 8.8	38.9 ± 6.2	68.4 ± 2.6	31.5 ± 6.7	61.5 ± 6.4	31.9 ± 7.9	76.5 ± 7.5	18.3 ± 6.2
16	5g/L GV1 (COL.2)	70.5 ± 4.4	67.4 ± 4.4	53.9 ± 7.8	90.3 ± 4.8	31.2 ± 8.6	75.9 ± 9.1	52.1 ± 3.4	79.8 ± 8.6	34.2 ± 3.1
17	20g/L GV1 (COL.3)	59.5 ± 2.9	51.2 ± 2.3	40.5 ± 5.7	68.3 ± 3.5	35.4 ± 6.5	58.8 ± 7.4	34.7 ± 6.6	84.8 ± 6.9	28.5 ± 9.0
18	10g/L GV1 (COL.3)	59.7 ± 2.1	63.1 ± 3.4	58.1 ± 4.6	82.8 ± 2.9	35.7 ± 7.5	76.1 ± 9.1	47.1 ± 7.2	67.9 ± 9.7	36.3 ± 3.5
19	5g/L GV1 (COL.3)	69.2 ± 6.6	71.8 ± 2.7	59.7 ± 2.8	79.0 ± 3.0	36.1 ± 7.4	74.2 ± 5.2	51.6 ± 8.0	75.1 ± 9.6	40.2 ± 4.0
20	20g/L CV6 (COL.1)	44.3 ± 4.8	49.9 ± 8.3	30.6 ± 2.8	53.4 ± 6.5	26.5 ± 9.5	67.7 ± 8.0	45.1 ± 6.6	75.6 ± 9.8	16.4 ± 9.0
21	10g/L CV6 (COL.1)	131.5 ± 7.4	60.0 ± 7.8	47.5 ± 6.6	73.7 ± 1.7	35.8 ± 9.0	83.2 ± 5.1	55.8 ± 3.6	73.8 ± 8.8	38.3 ± 1.2
22	5g/L CV6 (COL.1)	52.1 ± 2.1	53.5 ± 1.6	50.9 ± 7.6	69.0 ± 3.0	36.0 ± 9.0	61.5 ± 5.7	43.0 ± 6.7	78.0 ± 9.1	43.3 ± 9.9

23	20g/L CV6 (COL.2)	39.3 ± 4.2	58.8 ± 2.3	52.2 ± 7.2	69.6 ± 3.3	38.1 ± 8.0	72.0 ± 7.1	47.0 ± 8.5	64.3 ± 6.7	32.0 ± 2.2
24	10g/L CV6 (COL.2)	57.7 ± 3.9	65.9 ± 0.7	56.4 ± 3.4	77.7 ± 6.8	58.5 ± 5.9	73.0 ± 7.4	49.4 ± 8.0	78.2 ± 6.9	39.1 ± 2.8
25	5g/L CV6 (COL.2)	67.3 ± 5.0	68.8 ± 8.1	72.2 ± 6.8	74.5 ± 8.3	50.7 ± 4.3	88.3 ± 7.3	62.0 ± 9.9	77.8 ± 7.2	48.5 ± 3.1
26	20g/L CV6 (COL.3)	43.1 ± 2.8	59.6 ± 0.5	54.9 ± 6.7	64.0 ± 7.6	48.8 ± 4.8	68.6 ± 4.9	50.0 ± 4.1	71.4 ± 8.7	46.6 ± 1.9
27	10g/L CV6 (COL.3)	59.5 ± 5.0	77.1 ± 2.7	81.1 ± 2.5	92.6 ± 8.6	45.5 ± 9.1	81.1 ± 8.2	60.1 ± 7.3	69.1 ± 9.6	59.0 ± 1.7
28	5g/L CV6 (COL.3)	69.3 ± 2.2	90.9 ± 0.7	87.9 ± 7.1	97.0 ± 7.3	65.5 ± 6.6	86.6 ± 6.4	74.5 ± 9.5	72.0 ± 7.8	63.8 ± 1.5
29	20g/L Puro (COL.1)	22.7 ± 3.4	8.7 ± 3.0	8.0 ± 5.3	12.4 ± 3.4	22.5 ± 5.9	31.1 ± 4.4	17.8 ± 8.6	58.6 ± 6.9	16.7 ± 2.0
30	10g/L Puro (COL.1)	30.1 ± 5.7	13.4 ± 0.4	9.3 ± 5.3	20.1 ± 2.8	25.8 ± 7.3	18.2 ± 7.6	12.8 ± 5.8	54.0 ± 8.8	13.3 ± 2.0
31	5g/L Puro (COL.1)	42.4 ± 4.8	18.8 ± 1.8	14.4 ± 7.5	33.8 ± 3.0	15.2 ± 7.8	20.1 ± 6.5	14.6 ± 8.0	57.4 ± 9.6	15.4 ± 4.9
32	20g/L Puro (COL.2)	27.5 ± 3.5	12.0 ± 2.6	9.2 ± 2.5	15.5 ± 5.0	12.9 ± 4.1	22.0 ± 7.9	17.0 ± 5.3	62.5 ± 8.6	17.8 ± 5.3
33	10g/L Puro (COL.2)	35.2 ± 2.8	15.4 ± 7.7	13.8 ± 8.3	25.2 ± 5.0	10.1 ± 8.1	20.9 ± 4.5	15.3 ± 8.9	48.7 ± 9.1	34.7 ± 1.5
34	5g/L Puro (COL.2)	58.5 ± 1.9	22.8 ± 3.1	16.1 ± 9.2	39.8 ± 6.0	19.2 ± 4.8	29.3 ± 9.7	22.2 ± 8.9	46.2 ± 5.2	8.2 ± 1.2
35	20g/L Puro (COL.3)	53.8 ± 2.5	19.3 ± 6.8	19.7 ± 3.0	38.1 ± 5.7	20.3 ± 5.2	26.5 ± 6.6	18.7 ± 5.4	37.5 ± 8.3	13.7 ± 2.1
36	10g/L Puro (COL.3)	56.1 ± 3.3	20.6 ± 1.4	22.3 ± 8.5	34.7 ± 5.6	19.4 ± 5.9	26.8 ± 7.2	18.1 ± 3.9	48.9 ± 9.5	12.3 ± 7.8
37	5g/L Puro (COL.3)	49.2 ± 2.8	32.1 ± 3.3	34.2 ± 4.0	57.8 ± 7.1	22.0 ± 4.5	39.3 ± 7.5	29.1 ± 7.6	41.3 ± 9.2	16.8 ± 4.4
38	20g/L Carbon (COL.1)	38.7 ± 7.1	38.0 ± 7.0	34.5 ± 5.5	48.1 ± 2.0	33.6 ± 4.1	69.6 ± 8.3	45.2 ± 3.4	61.5 ± 7.5	19.5 ± 3.1
39	10g/L Carbon (COL.1)	86.7 ± 4.5	44.3 ± 0.7	30.8 ± 4.9	56.3 ± 6.0	26.8 ± 3.9	64.5 ± 6.7	69.8 ± 3.5	50.9 ± 7.9	33.2 ± 3.7
40	5g/L Carbon (COL.1)	54.8 ± 4.7	74.7 ± 6.0	65.2 ± 8.9	90.3 ± 4.1	34.5 ± 5.2	89.4 ± 7.3	74.2 ± 3.7	50.4 ± 8.9	36.5 ± 2.2
41	20g/L Carbon (COL.2)	52.7 ± 6.6	61.3 ± 2.2	55.3 ± 3.1	72.2 ± 3.7	41.2 ± 8.1	76.8 ± 7.1	65.1 ± 6.4	53.4 ± 8.7	43.7 ± 1.3
42	10g/L Carbon (COL.2)	76.8 ± 9.1	55.0 ± 6.9	58.0 ± 5.5	65.1 ± 4.0	327.4 ± 4.8	80.3 ± 7.3	55.4 ± 7.9	44.2 ± 9.9	51.6 ± 1.2
43	5g/L Carbon (COL.2)	136.8 ± 6.8	141.5 ± 4.8	82.9 ± 3.7	82.1 ± 3.4	47.6 ± 6.5	87.5 ± 6.4	182.5 ± 8.9	52.4 ± 9.8	67.3 ± 4.4
44	20g/L Carbon (COL.3)	96.8 ± 5.4	75.0 ± 5.1	57.4 ± 5.2	74.7 ± 3.6	42.8 ± 4.5	77.8 ± 5.4	83.4 ± 5.4	49.9 ± 8.3	56.0 ± 2.7
45	10g/L Carbon (COL.3)	58.9 ± 4.0	78.2 ± 1.8	21.0 ± 6.9	65.0 ± 4.8	44.5 ± 5.5	85.9 ± 5.5	54.8 ± 5.7	61.6 ± 6.5	65.0 ± 2.8
46	5g/L Carbon (COL.3)	81.4 ± 6.4	57.0 ± 1.7	12.8 ± 9.6	53.0 ± 7.2	29.8 ± 7.2	44.3 ± 4.4	124.2 ± 8.8	131.6 ± 7.8	29.0 ± 1.3

Note. (-) means compound was not detected within gas chromatography-mass spectroscopy (GCMS) analysis. Puro means the resin Purosorb PAD 600.

8.5 Appendix 5 – Agglomerative Hierarchical Clustering Supplementary Data

Agglomerative hierarchical clustering (AHC) analysis only provides groups based on the distances between samples – samples in the same cluster are closer to each other than those in a different cluster and visualised as dendrograms. The difference between cluster analysis and PCA is that the former merges pairs of samples based on their similarities via distance whilst the latter reveals any patterns associated with large data sets. Observation analysis acquired from AHC leads to a new form of categorisation between samples that have been treated and untreated. The tables below showcase a simplified version of the dendrograms discussed in the main body of the dissertation. The maximum, average and minimum distances from the centroid represent how far away samples are from the original (control) apple, orange and cranberry juice samples.

Table 26. *Agglomerative hierarchical clustering of processed apple juice samples grouped by class.*

Class	One	Two	Three	Four	Five
Objects	1	10	8	14	13
Sum of weights	1	10	8	14	13
Within-class variance	1	0.188	0.433	0.427	0.105
Min. distance	0.000	0.217	0.366	0.351	0.127
Avg. distance	0.000	0.384	0.577	0.615	0.294
Max. distance	0.000	0.766	1.037	0.815	0.561
Samples[a]	Control (1)	20g/L SV7 COL.1 (2) 10g/L SV7 COL.1 (3) 5g/L SV7 COL.1 (4) 10g/L SV7 COL.2 (6) 5g/L SV7 COL.2 (7) 10g/L SV7 COL.3 (9) 5g/L SV7 COL.3 (10) 10g/L GV1 COL.1 (12) 10g/L GV1 COL.3 (18) 5g/L GV1 COL.3 (19)	20g/L SV7 COL.2 (5) 20g/L GV1 COL.1 (11) 20g/L Puro COL.1 (29) 10g/L Puro COL.1 (30) 5g/L Puro COL.1 (31) 20g/L Puro COL.2 (32) 10g/L Puro COL.2 (33) 20g/L Puro COL.3 (35)	20g/L SV7 COL.3 (8) 5g/L GV1 COL.1 (13) 20g/L GV1 COL.2 (14) 10g/L GV1 COL.2 (15) 5g/L GV1 COL.2 (16) 20g/L GV1 COL.3 (17) 20g/L CV6 COL.1 (20) 20g/L CV6 COL.2 (23) 20g/L CV6 COL.3 (26) 5g/L Puro COL.2 (34) 10g/L Puro COL.3 (36) 5g/L Puro COL.3 (37) 20g/L Carbon COL.1 (38) 20g/L Carbon COL.2 (41)	10g/L CV6 COL.1 (21) 5g/L CV6 COL.1 (22) 10g/L CV6 COL.2 (24) 5g/L CV6 COL.2 (25) 10g/L CV6 COL.3 (27) 5g/L CV6 COL.3 (28) 10g/L Carbon COL.1 (39) 5g/L Carbon COL.1 (40) 10g/L Carbon COL.2 (42) 5g/L Carbon COL.2 (43) 20g/L Carbon COL.3 (44) 10g/L Carbon COL.3 (45) 5g/L Carbon COL.3 (46)

Note. Minimum (min.), average (avg.) and maximum (max.) show the distances from the centroid respectively. Objects show how many samples are within that particular class or cluster.

[a] Sample name and its corresponding identifying number in brackets.

Table 27. *Agglomerative hierarchical clustering of processed orange juice samples grouped by class.*

Class	One	Two	Three	Four	Five
Objects	1	9	9	18	9
Sum of weights	1	9	9	18	9
Within-class variance	0.000	0.251	0.172	0.144	0.057
Min. distance	0.000	0.273	0.223	0.135	0.134
Avg. distance	0.000	0.450	0.369	0.348	0.214
Max. distance	0.000	0.672	0.679	0.581	0.344
Samples[a]	Control (1)	20g/L SV7 COL.1 (2) 10g/L SV7 COL.1 (3) 5g/L SV7 COL.1 (4) 20g/L SV7 COL.2 (5) 10g/L SV7 COL.2 (6) 5g/L SV7 COL.2 (7) 20g/L SV7 COL.3 (8) 10g/L SV7 COL.3 (9) 5g/L SV7 COL.3 (10)	20g/L GV1 COL.1 (11) 5g/L GV1 COL.1 (13) 5g/L Puro COL.1 (31) 20g/L Puro COL.2 (32) 10g/L Puro COL.2 (33) 5g/L Puro COL.2 (34) 20g/L Puro COL.3 (35) 10g/L Puro COL.3 (36) 5g/L Puro COL.3 (37)	10g/L GV1 COL.1 (12) 20g/L GV1 COL.2 (14) 10g/L GV1 COL.2 (15) 5g/L GV1 COL.2 (16) 20g/L GV1 COL.3 (17) 10g/L GV1 COL.3 (18) 5g/L GV1 COL.3 (19) 20g/L CV6 COL.1 (20) 10g/L CV6 COL.1 (21) 5g/L CV6 COL.1 (22) 20g/L CV6 COL.2 (23) 10g/L CV6 COL.2 (24) 5g/L CV6 COL.2 (25) 20g/L CV6 COL.3 (26) 10g/L CV6 COL.3 (27) 5g/L CV6 COL.3 (28) 20g/L Puro COL.1 (29) 10g/L Puro COL.1 (30)	20g/L Carbon COL.1 (38) 10g/L Carbon COL.1 (39) 5g/L Carbon COL.1 (40) 20g/L Carbon COL.2 (41) 10g/L Carbon COL.2 (42) 5g/L Carbon COL.2 (43) 20g/L Carbon COL.3 (44) 10g/L Carbon COL.3 (45) 5g/L Carbon COL.3 (46)

Note. Minimum (min.), average (avg.) and maximum (max.) show the distances from the centroid respectively. Objects show how many samples are within that particular class or cluster.

[a] Sample name and its corresponding identifying number in brackets.

Table 28. *Agglomerative hierarchical clustering of processed cranberry juice samples grouped by class.*

Class	One	Two	Three	Four	Five
Objects	2	2	32	9	1
Sum of weights	2	2	32	9	1
Within-class variance	0.926	0.968	0.184	0.071	0.000
Min. distance[a]	0.680	0.696	0.134	0.110	0.000
Avg. distance[b]	0.680	0.696	0.389	0.238	0.000
Max. distance[c]	0.680	0.696	0.853	0.410	0.000
Samples[d]	Control (1) 5g/L Carbon COL.2 (43)	20g/L SV7 COL.1 (2) 5g/L Carbon COL.3 (46)	10g/L SV7 COL.1 (3) 5g/L SV7 COL.1 (4) 20g/L SV7 COL.2 (5) 10g/L SV7 COL.2 (6) 5g/L SV7 COL.2 (7) 20g/L SV7 COL.3 (8) 10g/L SV7 COL.3 (9) 5g/L SV7 COL.3 (10) 20g/L GV1 COL.1 (11) 10g/L GV1 COL.1 (12) 5g/L GV1 COL.1 (13) 20g/L GV1 COL.2 (14) 10g/L GV1 COL.2 (15) 5g/L GV1 COL.2 (16) 20g/L GV1 COL.3 (17) 10g/L GV1 COL.3 (18) 5g/L GV1 COL.3 (19) 20g/L CV6 COL.1 (20) 10g/L CV6 COL.1 (21) 5g/L CV6 COL.1 (22) 20g/L CV6 COL.2 (23) 10g/L CV6 COL.2 (24) 5g/L CV6 COL.2 (25)	20g/L Puro COL.1 (29) 10g/L Puro COL.1 (30) 5g/L Puro COL.1 (31) 20g/L Puro COL.2 (32) 10g/L Puro COL.2 (33) 5g/L Puro COL.2 (34) 20g/L Puro COL.3 (35) 10g/L Puro COL.3 (36) 5g/L Puro COL.3 (37)	10g/L Carbon COL.2 (42)

			20g/L CV6 COL.3 (26) 10g/L CV6 COL.3 (27) 5g/L CV6 COL.3 (28) 20g/L Carbon COL.1 (38) 10g/L Carbon COL.1 (39) 5g/L Carbon COL.1 (40) 20g/L Carbon COL.2 (41) 20g/L Carbon COL.3 (44) 10g/L Carbon COL.3 (45)		

Note. Minimum (min.), average (avg.) and maximum (max.) show the distances from the centroid respectively. Objects show how many samples are within that particular class or cluster.

[a] Sample name and its corresponding identifying number in brackets.

8.6 Appendix 6 – Participant Commentary from Formal Sensory Evaluation of Juices

After each of the six-selected apple, orange and cranberry juice samples were tasted, participants were asked to comment on the overall organoleptic characteristics (i.e. what attributes stood out to them the most) and if they detected any unpleasant aftertastes. The following tables below represent the individuals' opinions and preferences of each juice.

Table 29. *Summary of participant's commentary on the six selected apple juice samples.*

Participant Code	Sample Identifier	Sample Name	Comments
1001	1	Control	The sweetness of the sample was a bit too much.
	2	10g/L SV7 (COL.1)	Very watered down. Could not taste a thing apart from the tartness. Also, could not smell anything. Colour of the sample was very pale.
	3	10g/L GV1 (COL.1)	Sample was very balanced. Probably my most preferred one. The sweetness wasn't so overpowering so that you could actually taste the apple flavour and tartness
	4	20g/L Puro (COL.1)	Balanced sweet and sour but more on sour side.
	5	10g/L CV6 (COL.2)	Water and diluted but could smell apple. Tartness was alright.
	6	20g/L CV6 (COL.2)	Overall flavour is much better. Slight sweetness and sourness. Not too sweet. Aroma is lacking though.
1002	1	Control	The taste lingers in the mouth after drinking
	4	20g/L Puro (COL.1)	Sour taste
	6	20g/L CV6 (COL.2)	The taste is too strong to my likeness
	2	10g/L SV7 (COL.1)	Like the original taste of the juice in the sample
1003	4	20g/L Puro (COL.1)	Quite a strong and intense aftertaste
	1	Control	I liked this one a lot
1005	2	10g/L SV7 (COL.1)	It was intense sweetness but was mixed with tart and a bit if sourness as well
	3	10g/L GV1 (COL.1)	The tartness and sweetness were too strong in the aftertaste
	4	20g/L Puro (COL.1)	It was bit more tart than the previous sample
	6	20g/L CV6 (COL.2)	It has an astringent and mouth drying aftertaste
	1	Control	The apple flavour wasn't natural and it had artificial sweeteners I think
	5	10g/L CV6 (COL.2)	The apple flavour had a bit of fermented or aged taste which I didn't like
1006	4	20g/L Puro (COL.1)	Slightly too weak overall in terms of apple sweet and tart
1007	1	Control	Sweet
	2	10g/L SV7 (COL.1)	Astringency detected in aftertaste
	3	10g/L GV1 (COL.1)	Very tart
	5	10g/L CV6 (COL.2)	Sweet

	6	20g/L CV6 (COL.2)	Astringent aftertaste
1008	4	20g/L Puro (COL.1)	Taste like apple cider vinegar or some fermented juice
1009	5	10g/L CV6 (COL.2)	Too sweet and not enough apple flavour. There's a bit not bland aftertaste but acceptable
	2	10g/L SV7 (COL.1)	The tartness and apple flavour are quite strong but there's also good level of sweetness.
	3	10g/L GV1 (COL.1)	I like the sourness in this sample not too strong but can still taste it
	4	20g/L Puro (COL.1)	The tartness is slightly higher than sweetness but overall, it's a good sample
	6	20g/L CV6 (COL.2)	This sample taste just about right and there's a good balance between sweetness and sourness
1010	2	10g/L SV7 (COL.1)	The colour was not the most appealing but flavour ratios were good. Apple fruity flavour and sweetness sits quite strongly in the mouth afterwards
	3	10g/L GV1 (COL.1)	Almost off bitter aftertaste and dryness that sits. The strength of the above stated outweighs the nice notes.
	1	Control	Nice after taste flavour with no bad notes sitting in the mouth. Notes meaning the flavour, taste, texture, feel.
	4	20g/L Puro (COL.1)	After taste was tarty and sweet, which mellowed out quite fast
	5	10g/L CV6 (COL.2)	Not much after taste but nice after taste.
	6	20g/L CV6 (COL.2)	Very sweet initially
1011	1	Control	No
	3	10g/L GV1 (COL.1)	Too sweet
1012	1	Control	I like that it has darker colour, tastes and smells good.
	2	10g/L SV7 (COL.1)	Taste good again. Just the colour is pale
	3	10g/L GV1 (COL.1)	Good taste. The colour is my liking here
	4	20g/L Puro (COL.1)	Taste very good. The only comment would be the colour is too pale
	5	10g/L CV6 (COL.2)	Pretty good
	6	20g/L CV6 (COL.2)	Taste good. Just the colour not my liking here
1015	2	10g/L SV7 (COL.1)	Tastes diluted
	6	20g/L CV6 (COL.2)	Tastes a bit watery
1016	4	20g/L Puro (COL.1)	No apple taste left
	5	10g/L CV6 (COL.2)	A little bit too sweet
	6	20g/L CV6 (COL.2)	A bit sweet
1018	2	10g/L SV7 (COL.1)	Nice flavour
	4	20g/L Puro (COL.1)	Lacks aroma, sweetness and flavour
1019	1	Control	Super sour initially
	4	20g/L Puro (COL.1)	Not fruity enough, too pale in colour
1020	3	10g/L GV1 (COL.1)	Sweet lingering aftertaste, slightly sticky
	4	20g/L Puro (COL.1)	Sweet aftertaste.
	6	20g/L CV6 (COL.2)	Sweet aftertaste
1022	1	Control	Aftertaste of old/slightly off apples

	4	20g/L Puro (COL.1)	Aftertaste reminds me of cheap apple juice
1023	1	Control	Very sweet aftertaste
	3	10g/L GV1 (COL.1)	Too sweet of an aftertaste
	5	10g/L CV6 (COL.2)	Too sweet and slightly unnaturally sour.
1025	1	Control	A bit too sweet
	6	20g/L CV6 (COL.2)	This one is too sweet for me
	2	10g/L SV7 (COL.1)	This one is my favourite
	3	10g/L GV1 (COL.1)	Didn't like the colour or sweetness
	4	20g/L Puro (COL.1)	This one seemed lighter, didn't cling to the mouth
1028	2	10g/L SV7 (COL.1)	Low apple flavour but good sweetness level. Slight lingering tartness afterwards.
	6	20g/L CV6 (COL.2)	Slight tartness lingered after tasting sample. However, it was not very strong
	3	10g/L GV1 (COL.1)	The apple aroma seemed slightly different to other samples
	4	20g/L Puro (COL.1)	The pale colour made me think it would be weak but it had a strong sweet flavour
	5	10g/L CV6 (COL.2)	Strong sweetness and tartness which over powered the apple flavour
1029	3	10g/L GV1 (COL.1)	Sweetness and tartness not balanced
	5	10g/L CV6 (COL.2)	Too sweet
1030	1	Control	Too sweet
	4	20g/L Puro (COL.1)	Weak, non-descript, no flavour and too pale
	5	10g/L CV6 (COL.2)	Too sweet
1032	6	20g/L CV6 (COL.2)	Strong sweet lingering aftertaste
1033	5	10g/L CV6 (COL.2)	Fairly good
1034	1	Control	Strong dislike, tastes like chemicals
	2	10g/L SV7 (COL.1)	Aftertaste was too intense
	3	10g/L GV1 (COL.1)	Apple tastes off
	4	20g/L Puro (COL.1)	Weird smell, quite chemically

Note. Comments provided are only from participants that felt inclined to write about a particular sample. The annotation 'Puro' is the shorted form of resin Purosorb PAD 600. The control is the original apple juice sample (untreated).

Table 30. *Summary of participant's commentary on the six selected orange juice samples.*

Participant Code	Sample Identifier	Sample Name	Comments
1001	1	Control	Tastes the best of all, would buy a bottle
	2	10g/L SV7 (COL.1)	Tastes great
	3	10g/L GV1 (COL.1)	Flavour does not linger at all, vanishes way too quickly
	4	20g/L SV7 (COL.2)	Another very weak tasting sample, does not taste very orangey, tastes watered down
	5	20g/L GV1 (COL.2)	Orange tastes a little bit off, like an orange that's a few weeks past it's best before date
	6	10g/L Puro (COL.1)	Good aftertaste, but no bitterness or flavour. Tastes like a weak version of cool change orange drink

1002	1	Control	Like a very over ripe orange
	4	20g/L SV7 (COL.2)	Aroma and colour of sample wasn't too bad but the overall flavour was seriously diluted and tasted like water with citric acid in it. A tangy bitter aftertaste.
	5	20g/L GV1 (COL.2)	Has too much of an artificial orange flavour to it
	2	10g/L SV7 (COL.1)	Could taste a sweetness there but more sour which I liked. Aroma was strong and the colour payoff was good.
	3	10g/L GV1 (COL.1)	Well balanced orange juice. Like the initial sweet taste that turns into sour after it sits in the mouth for a bit
	6	10g/L Puro (COL.1)	Diluted sour water with hint of orange flavour coming though
1003	3	10g/L GV1 (COL.1)	More distinct sweet aftertaste
	1	Control	I have a preference for less sweet tastes based on past diabetic experiences.
1004	1	Control	The sourness remains in the mouth
1005	4	20g/L SV7 (COL.2)	The best
1006	6	10g/L Puro (COL.1)	Didn't taste like just orange. Almost pineapple juice taste
1008	5	20g/L GV1 (COL.2)	This sample taste sweet and doesn't have much sourness
1010	1	Control	Really disliked the aroma
	2	10g/L SV7 (COL.1)	Tasted waterier than 831.
	4	20g/L SV7 (COL.2)	Couldn't really taste the orange flavour
1012	1	Control	Not very like orange juice. Some other fruits taste
	2	10g/L SV7 (COL.1)	It's good
	3	10g/L GV1 (COL.1)	It's good
	4	20g/L SV7 (COL.2)	Less orange flavour, mild in sweet and sour as well
	5	20g/L GV1 (COL.2)	It's good
	6	10g/L Puro (COL.1)	Similar to market orange juice
1013	1	Control	Unusual smell. The colour is good because I like my orange juice more orange then yellow.
	2	10g/L SV7 (COL.1)	Unusual taste
	3	10g/L GV1 (COL.1)	Not sweet enough.
	4	20g/L SV7 (COL.2)	Unusual smell in mouth
	5	20g/L GV1 (COL.2)	Not sweet enough for me
	6	10g/L Puro (COL.1)	Not sweet enough again. The smell is not like fresh orange juice that I like.
1018	3	10g/L GV1 (COL.1)	The astringency is too strong for my liking
	4	20g/L SV7 (COL.2)	Slight bitter and astringency
	6	10g/L Puro (COL.1)	Has slight astringent aftertaste
1020	6	10g/L Puro (COL.1)	Sample has hints of brown colour
1021	2	10g/L SV7 (COL.1)	Too sour
1022	6	10g/L Puro (COL.1)	Leaves a slightly unpleasant feel in the mouth after
	1	Control	Colour was a bit too weak for orange juice, almost watery looking
	3	10g/L GV1 (COL.1)	Good colour

	4	20g/L SV7 (COL.2)	An almost dirty sour taste is leftover with none of the sweetness in the aftertaste
	5	20g/L GV1 (COL.2)	Slightly watery looking colour
1023	1	Control	Aftertaste was long lasting but not in a bad way.
	3	10g/L GV1 (COL.1)	Very tasty, great mouthfeel. Perfect sweetness for me
	4	20g/L SV7 (COL.2)	Tastes like store bought orange juice
	5	20g/L GV1 (COL.2)	It's hard to describe but I mentally know sweet things are bad for me, but like them so I got conflicted answering whether I liked it. My tongue objectively liked it but my brain was like 'I am going to have a huge insulin spike'.
1025	6	10g/L Puro (COL.1)	Too acid for the fruit flavour
1026	4	20g/L SV7 (COL.2)	Just a bit strong
	5	20g/L GV1 (COL.2)	Tanginess stays longer than ideal
1027	1	Control	Sticks in the mouth a bit long
	4	20g/L SV7 (COL.2)	My favourite
1029	1	Filtered Orange	Subtle
	5	20g/L GV1 (COL.2)	Tame
1030	1	Control	A bit bitter
1031	5	20g/L GV1 (COL.2)	Taste a bit diluted
1032	1	Control	Slightly artificial taste
1034	3	10g/L GV1 (COL.1)	Taste diluted
1035	1	Control	Bitter

Note. Comments provided are only from participants that felt inclined to write about a particular sample. Puro is the shorted form of resin Purosorb PAD 600. The control is the original orange juice sample (untreated). 831 is the code for the control sample.

Table 31. *Summary of participant's commentary on the six selected cranberry juice samples.*

Participant Code	Sample Identifier	Sample Name	Comments
1001	3	10g/L GV1 (COL.2)	Bitter, dry, tight aftertaste
	4	10g/L Puro (COL.1)	Dry and tight
1002	2	10g/L SV7 (COL.2)	Good balance of sweet and tart. No bitterness at all and the astringency wasn't that bad
1003	1	Control	The aftertaste lasted quite some time in a negative way. I disliked this one a lot
	2	10g/L SV7 (COL.2)	Quite a strong aftertaste that lasted some time
1004	1	Control	Sour and taste like medicine
1005	3	10g/L GV1 (COL.2)	Very sour
1006	4	10g/L Puro (COL.1)	Sour
	5	20g/L CV6 (COL.3)	Bitter
	6	20g/L GV1 (COL.2)	Strong astringency
	1	Control	Good flavour and willing to buy
1007	3	10g/L GV1 (COL.2)	Bitter aftertaste, metallic. Aroma is more apple aroma than cranberry
	4	10g/L Puro (COL.1)	Astringent, bitter
	6	20g/L GV1 (COL.2)	Aroma is more apple aroma than cranberry

1008	3	10g/L GV1 (COL.2)	Strong astringent and bitter aftertaste for me. Not enough sweet and sourness for me and weak cranberry flavour
	4	10g/L Puro (COL.1)	Slight bitter aftertaste
	6	20g/L GV1 (COL.2)	Astringent aftertaste is too strong
	1	Control	It has tolerable bitter aftertaste
1009	2	10g/L SV7 (COL.2)	There is a bit tangy taste at the end but the overall flavour was good
	3	10g/L GV1 (COL.2)	A bit astringent aftertaste but a good balance of sweetness and tartness
1010	1	Control	Sweet and tart
	3	10g/L GV1 (COL.2)	Tart mouthfeel
	5	20g/L CV6 (COL.3)	Higher astringent
	6	20g/L GV1 (COL.2)	Too sweet
1011	5	20g/L CV6 (COL.3)	Not too bitter for me
	1	Control	Too bitter at the end
	2	10g/L SV7 (COL.2)	This one too bitter
	3	10g/L GV1 (COL.2)	Not too bitter which is great
	4	10g/L Puro (COL.1)	Too bitter
	6	20g/L GV1 (COL.2)	Very bitter at the end
1014	3	10g/L GV1 (COL.2)	The first sip felt too strong and stayed in the mouth for a while
	5	20g/L CV6 (COL.3)	The taste stays in the throat
1015	1	Control	A little bit astringent but not in a bad way could be better carbonated. The previous sample 294 is better than 812
	3	10g/L GV1 (COL.2)	Lingering dry sensation in the mouth. Most artificially cranberry flavoured out of the bunch
	4	10g/L Puro (COL.1)	Strong in taste astringency and tartness are strong and slight cranberry lacking in aroma. Smells like play dough quite unpleasant
	2	10g/L SV7 (COL.2)	Hard on the throat but most cranberry tasting of the bunch
	5	20g/L CV6 (COL.3)	Second in rank for tasting a bit too artificial-like.
1018	4	10g/L Puro (COL.1)	The sweetness is still there. Looked and tasted like lolly water
	5	20g/L CV6 (COL.3)	Ongoing sweetness
	6	20g/L GV1 (COL.2)	Don’t like the colour
1019	3	10g/L GV1 (COL.2)	A bit sweet, and dry sensation leaves a long time
	5	20g/L CV6 (COL.3)	Fruit flavour and dry sensation are a bit strong
	4	10g/L Puro (COL.1)	Sour taste covers cranberry flavour
1020	2	10g/L SV7 (COL.2)	Astringent
	3	10g/L GV1 (COL.2)	Apple aroma instead of cranberry. Astringent, bitter
	4	10g/L Puro (COL.1)	Astringent
	6	20g/L GV1 (COL.2)	Astringent
	5	20g/L CV6 (COL.3)	The aroma of this sample is more apple than cranberry
1021	1	Control	Chemical test
	3	10g/L GV1 (COL.2)	Strong chemical taste

	4	10g/L Puro (COL.1)	Too sweet
	5	20g/L CV6 (COL.3)	Chemical taste
1024	3	10g/L GV1 (COL.2)	Bitterness and tightness sit in the mouth after
	5	20g/L CV6 (COL.3)	The dryness in the mouth and bitterness sits for a while
	1	Control	Good colour, flavours worked well together with none outweighing the other. Nice flavour overall
	4	10g/L Puro (COL.1)	Aftertaste is pleasant but not very flavourful
1025	3	10g/L GV1 (COL.2)	Tart aftertaste
1026	2	10g/L SV7 (COL.2)	Not a big fan of sweet juice
	3	10g/L GV1 (COL.2)	Same comment
	4	10g/L Puro (COL.1)	Too sweet - can't tell any difference between samples. All seem to be too sweet
	5	20g/L CV6 (COL.3)	Same comment as other samples
	6	20g/L GV1 (COL.2)	Too sweet like other samples
1029	3	10g/L GV1 (COL.2)	Slightly tangy aftertaste. Too intense, couldn't do more than a few sips
	1	Control	Good aftertaste
	2	10g/L SV7 (COL.2)	Tasted quite intense
	4	10g/L Puro (COL.1)	Looks too light, but tastes great
	5	20g/L CV6 (COL.3)	Weak after taste, too sweet
	6	20g/L GV1 (COL.2)	Tastes good, hard to discriminate between bitterness and tartness
1030	6	20g/L GV1 (COL.2)	Good
1031	5	20g/L CV6 (COL.3)	Weird filmy feeling afterwards
1032	5	20g/L CV6 (COL.3)	Bitter, not too sweet.
1034	1	Control	Bitter aftertaste

Note. Comments provided are only from participants that felt inclined to write about a particular sample. The annotation 'Puro' is the shorted form of resin Purosorb PAD 600. The control is the original cranberry juice sample (untreated). Codes 294 and 812 are samples 20 g/L GV1 (COL.2) and the control respectively.