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Influence of maturity age on volatile aroma profile of coconut water from Tall variety

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Abstract

Importance of the work: The Tall coconut variety is commonly used by the coconut-based industry; thus, characteristic profiling of its coconut water is important.

Objectives: To determine the effect of maturity age on the characteristics and volatile aroma compounds of coconut water from the Tall variety.

Materials & Methods: Coconut water samples were collected of maturity aged 6–9 mth from Tall variety palms. The total soluble solids, pH, titratable acidity and color values were determined. Extraction of aroma compounds was performed using solvent extraction and headspace-solid phase microextraction. The extracts were analyzed using gas chromatography-time of flight mass spectrometry.

Results: There were no significant ($p \geq 0.05$) differences among samples for total soluble solids, pH, titratable acidity and color values. In terms of the volatile aroma compounds, all samples contained alcohols, ketones and lactones, as well as several aldehydes, thiols and esters. Potential key volatile aroma compounds detected in the Tall coconut water maturity aged 6–9 mth were acetoin and 1-butanol, which had odor activity values > 1.0. Coconut water from younger maturity ages had a higher presence of alcohols (winey, fruity and sweet aromas) and lactones (coconut-like, creamy and sweet aromas), while the water of more mature coconut fruits contained higher amounts of acetoin (buttery, yogurt-like and creamy aromas) and thiols (sulfury, savory and soup-like aromas).

Main finding: The profiles of volatile aroma compounds could be used to categorize Tall variety coconut water based on its maturity age. Therefore, utilization of coconut water can be determined depending on the desired aroma profile of the final product.

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Introduction

Coconut water is described as having a unique flavor with a sweet and slightly acidic taste (da Fonseca et al., 2009). Young aromatic coconut water from the Dwarf variety has been acknowledged to have superior organoleptic properties due to the presence of aldehydes and esters in the coconut water that make it more preferred by consumers for fresh consumption (Prades et al., 2012a; Burns et al., 2020). However, the industry prefers mature coconut kernel from the Tall variety as the raw material for the production of coconut milk and coconut oil; thus, there is large amount of coconut water from this variety that is ready to be utilized for coconut water-based products (Vani et al., 2020). Coconut water from the Tall variety has potential for development as a functional beverage due to its naturally beneficial chemical composition. For example, it has a potassium content ranging from 220.94 mg/100 mL in a sample aged 5–6 mth to 274.32 mg/100 mL in a sample aged 8–9 mth (Tan et al., 2014).

The composition of coconut water has been reported to depend on the stage of maturity, variety, cultivation practices and plantation region, as well as the soil and environmental conditions (Murasaki-Aliberti et al., 2009; Prades et al., 2012b; Ajibogun and Oboma, 2013; De Marchi et al., 2015). Several studies reported the effect of maturity age on the volatile aroma compounds of coconut water. Jirapong et al. (2015) analyzed coconut water from an aromatic Dwarf variety called 'Nam Hom' and found an increase of 1.4 times in the total volatile organic compounds of the sample when its maturity increased from 6 mth to 8 mth. Luckanatinvong et al. (2018) showed that 'Nam Hom' coconuts should be harvested ideally at age 7 mth to get the desirable pandan aroma from its 2-acetyl-1-pyrroline content. However, there has been lack of published studies exploring how maturity age affects the aroma compounds of coconut water from the Tall variety. The current study addressed this gap by determining if the maturity age affected the volatile aroma compound profile of coconut water from the Tall variety. The information obtained would be useful to the beverage industry, particularly in research and development and in the suitable selection of raw materials based on the intended aroma characteristics of the coconut water-based product.

Materials and Methods

Coconut water

Fresh coconut fruit from coconut trees of the Tall variety (a native species commonly grown in central Thailand) were used as samples. The coconuts were supplied by a coconut farm in Samut Songkhram province, Thailand. Maturity ages of the fruit were 6 mth, 7 mth, 8 mth and 9 mth after the emergence of inflorescence. These coconut fruit samples had meat thicknesses in the range from 0.99 cm to 1.02 cm in the samples aged 6 mth and 9 mth, respectively. Upon arrival in the laboratory, the fruit were immediately dehusked and their shells were cracked to collect the water. All samples were promptly filtered using a food-grade industrial filter bag and stored in clean containers at -18 °C.

Measurement of total soluble solids, pH, titratable acidity and color values of coconut water

The total soluble solids was measured using a refractometer (Atago Co. Ltd.; Japan) and the pH of coconut water was determined using a pH meter (Thermo Fisher Scientific; USA). The titratable acidity was measured following the method from Association of Official Analytical Chemists (2000) by titrating the samples with 0.1 N NaOH using phenolphthalein as an indicator. The acidity levels of samples were expressed as grams of malic acid per 100 mL of sample. The Hunter *L*, *a*, and *b* color parameters were measured using an Ultrascan PRO Spectrophotometer (Hunter Associates Laboratory; USA).

Extraction and analysis of volatile aroma compounds in coconut water

Two extraction methods applied: solvent extraction and headspace-solid phase microextraction (HS-SPME). Then, the extracts collected were analyzed using gas chromatography-time of flight mass spectrometry (GC-TOFMS).

Solvent extraction of volatile aroma compounds in coconut water

Solvent extraction was carried out with 2-methyl-3-heptanone (Sigma-Aldrich; USA) as an internal standard and dichloromethane as an extraction solvent (Saemah and Jirapakkul, 2011). Each coconut water sample (250 mL) was spiked with 30 µL of the internal standard (1.45 mg/mL) and extracted twice. Each extraction was performed with 250 mL of the extraction solvent at room temperature for 1 h, while being stirred at low speed. This was followed by a phase separation using a separatory funnel followed by concentration using evaporation with a Vigreux column at 45 °C to reach a volume of 50 mL. Next, the sample was purified with high-vacuum distillation at 10^{-5} Torr at ambient temperature for 2 h and at 50 °C for 1 h. During distillation, the extract was condensed in a trapping tube cooled with liquid N_2. Next, the distilled extract was concentrated under a gentle stream of N_2 gas to a volume of 5 mL. The concentrated extract was passed through a column of glass wool and anhydrous Na_2SO_4 to remove any trace of water and then further concentrated under a gentle stream of N_2 gas to a final volume of 0.5 mL. Lastly, 1 µL of extract was injected using the on-column mode to perform GC-TOFMS.

Headspace-solid phase microextraction of low boiling point volatile aroma compounds in coconut water

Each coconut water sample (5 mL) was placed in a 20 mL vial and added with 5 µL of the internal standard (2-methyl-3-heptanone) at a concentration of 50 ng/mL. Next, the sample was equilibrated at 45 °C for 10 min in a water bath while being stirred at low speed, followed by adsorption of the volatile compounds for 20 min at a similar temperature onto a divinylbenzene/carboxen/polydimethylsiloxane fiber (Supelco; USA) and desorption at the GC inlet port set at 250 °C for 15 min using an SPME inlet liner of 0.75 mm internal diameter (Supelco; USA) with splitless mode (Nasution et al., 2019).

Gas chromatography-time of flight mass spectrometry analysis of volatile aroma compounds in coconut water

For both extraction methods, the analysis of extract was performed using gas chromatography (GC; 7890A; Agilent Technologies; USA) coupled with a Pegasus 4D TOFMS (LECO; USA) using two capillary columns with different stationary phases: polar Stabilwax® (polyethylene glycol) and non-polar Rxi-5 (cross-bond diphenyl dimethyl polysiloxane). Both columns had the following dimensions: 30 m × 0.25 mm internal diameter × 0.25 µm film thickness (Restek; USA). The inlet port, transfer line and mass spectrometry source were set at 250 °C, 250 °C and 200 °C, respectively. The oven temperature commenced at 35 °C for 5 min, raised to 225 °C at 4 °C/min and then held for 10 min. Helium was used as the carrier gas flowing at 1.5 mL/min, while the scanning mass range was set at 30–300 m/z with an acquisition rate of 20 spectra/s and an electron ionization energy of 70 eV (Nasution et al., 2019).

Identification and quantification of volatile aroma compounds in coconut water

The volatile aroma compounds were tentatively identified by comparing their mass spectra with those of the NIST Mass Spectral Library, with confirmation of their retention indices (RIs) performed by comparison with the RIs found in the literature. Alkane series of C6-C30 and C6-C22 were used for the calculation of the RIs of compounds in the polar and non-polar analytical columns, respectively. Several selected compounds were further identified through the injection of standard compounds into a similar GC-TOFMS system.

The calculation of relative concentration of a compound was based on the compound's peak area in the chromatogram compared to that of an internal standard. Among all volatile compounds detected, only those listed in the literature as aroma compounds were reported. The odor activity values (OAVs) of the volatile aroma compounds were calculated as the ratio between the compound's relative concentration and its odor detection threshold in water that was obtained from the literature (Grosch, 2001).

Data analysis

A completely randomized design was used and the experiment was conducted in duplicate. Data collected were reported as mean ± SD values and analyzed using one-way analysis of variance followed by a *post hoc* Duncan's multiple range test. Significant differences were set at $p < 0.05$ and statistical analysis was performed using the SPSS software (version 17; SPSS Inc.; USA).

Results and Discussion

Total soluble solids, pH, titratable acidity and color values of coconut water from Tall variety

Table 1 shows the total soluble solids, pH, titratable acidity and color values of coconut water from the Tall variety. There were no significant effects of maturity age on the *L, a,* and *b* color values, which indicated that the color of the coconut water did not greatly change following maturity. There were no significant differences in pH values among the samples, with values ranging from 5.53 in the sample aged 6 mth to 5.76 in the sample aged 9 mth. Jackson et al. (2004) observed an increase in the pH of their coconut water samples from the Maypan Tall variety during the maturation process from pH 4.6–5.0 at ages 7–10 mth. They reported that the increase in the pH of the coconut water was caused by a reduction in its acid content, which was marked by a reduction in titratable acidity values. Table 1 shows a similar tendency of reduction in titratable acidity, which was also seen in a study by Kannangara et al. (2018) where coconut water from older maturity fruits showed slightly lower titratable acidity than the younger ones.

There were no significant differences found among samples in terms of total soluble solids, although a slightly increasing trend could be observed in samples age from 6 mth to 9 mth. A similar trend was also reported by Tan et al. (2014) who observed changes in characteristics between coconut water aged 5–6 mth and 8–9 mth from the Malayan Tall variety, with total soluble solids values of 5.60 and 6.15, respectively. The titratable acidity levels of the coconut water samples used in the current study were in the range 0.03–0.05 g malic acid per 100 mL sample, which was near the values reported by Soares et al. (2017). The value of titratable acidity is expressed as the amount of malic acid because it is the dominant organic acid found in coconut water (Santoso et al., 1996; Tan et al., 2014).

Volatile aroma compounds identified in coconut water from Tall variety

Table 2 summarizes the volatile aroma compounds identified in the coconut water from the Tall variety that were extracted

Table 1 Total soluble solids, pH, titratable acidity and color values of coconut water from Tall variety

Maturity age	Total soluble solids (°Brix)^{ns}	pH^{ns}	Titratable acidity (g malic acid/100 mL)^{ns}	Color^{ns}		
				L	*a*	*b*
6 months	5.7 ± 0.3	5.59 ± 0.13	0.05 ± 0.01	95.92 ± 3.09	0.12 ± 0.10	1.72 ± 0.07
7 months	5.7 ± 0.3	5.53 ± 0.09	0.05 ± 0.00	94.75 ± 4.09	0.16± 0.13	2.30 ± 0.42
8 months	5.6 ± 0.5	5.62 ± 0.00	0.04 ± 0.00	94.76 ± 3.74	0.13 ± 0.10	2.18 ± 0.14
9 months	5.8 ± 0.3	5.76 ± 0.37	0.03 ± 0.00	94.25 ± 4.69	0.15 ± 0.14	2.19 ± 0.25

^{ns} = non-significant ($p \geq 0.05$)

Table 2 Volatile aroma compounds in coconut water from Tall variety aged 6–9 mth extracted using solvent extraction and headspace-solid phase microextraction (HS-SPME)

Compound	Method of extraction	Retention index[1]	Odor description[2]	Method of identification[3]
Acetaldehyde	HS-SPME	<1000	Nutty, alcoholic (a)	MS, RI
Ethyl acetate	HS-SPME	<1000	Winey (a)	MS, RI, AC
Ethanol	HS-SPME	<1000	Sweet, ethereal (a)	MS, RI
2-Methyl-1-propanol	HS-SPME, solvent extraction	<1100	Sweet, whiskey-like (a)	MS, RI
1-Butanol	HS-SPME, solvent extraction	1148	Winey (a)	MS, RI, AC
3-Methyl-1-butanol	HS-SPME, solvent extraction	1203	Alcoholic (a)	MS, RI, AC
Acetoin	HS-SPME, solvent extraction	1282	Buttery, creamy, yogurt (a)	MS, RI, AC
1-Hexanol	HS-SPME, solvent extraction	1353	Winey, slightly fatty-fruity (a)	MS, RI
Trans-3-hexen-1-ol	Solvent extraction	1366	Green, grass, leafy (a)	MS, RI
2-Ethyl-1-hexanol	HS-SPME, solvent extraction	1488	Sweet, oily, weak rose (a)	MS, RI
Benzaldehyde	Solvent extraction	1516	Almond, bitter (a)	MS, RI, AC
2-(methylthio)-ethanol	Solvent extraction	1524	Sulfury, vegetable-like (a)	MS, RI
1-Octanol	Solvent extraction	1554	Sweet, waxy, orange-rose (a)	MS, RI
Butyrolactone	Solvent extraction	1619	Coconut-like, buttery, creamy, nutty (a)	MS, RI
3-(Methylthio)-1-propanol	Solvent extraction	1711	Meaty, soup-like (a)	MS, RI
δ-Hexalactone	Solvent extraction	1782	Coconut, creamy (a)	MS, RI, AC
4-Methyl-5H-furan-2-one	Solvent extraction	1881	Roast, nutty, sweet, caramel (b)	MS, RI
Phenylethyl alcohol	Solvent extraction	1906	Floral, rose-like (a)	MS, RI, AC
δ-Octalactone	Solvent extraction	1957	Coconut, creamy (a)	MS, RI, AC
Pantolactone	Solvent extraction	2035	Cotton candy (a)	MS, RI
δ-Decalactone	Solvent extraction	2186	Sweet, creamy, milky, peach, nutty (a)	MS, RI, AC

[1] = retention indices from polar column; [2] = odor description from (a) Leffingwell (2004) and (b) Kabir and Lorjaroenphon (2013); [3]; MS = mass spectrometry; RI = matching retention index with literature; AC = injection of authentic compound into similar gas chromatography-time of flight mass spectrometry system

using the solvent extraction and HS-SPME methods. It can be observed that several highly volatile aroma compounds with low boiling points could only be identified using HS-SPME and not using solvent extraction. Therefore, both extraction methods were used to obtain a more complete profile of the volatile aroma compounds in the samples from the low- and high-boiling point volatile compounds. The solvent extraction method was able to extract a large group of volatile compounds, including those with high molecular weights and high boiling points, as well as compounds available at only small concentrations. The low-molecular weight volatile aroma compounds could be detected more conveniently using the HS-SPME method that did not use a solvent; thus, there was no solvent peak that might co-elute and cover the peaks of the highly volatile compounds, such as acetaldehyde, ethyl acetate and ethanol, that tend to appear early in the chromatogram (Augusto et al., 2003).

In all samples of coconut water from the Tall variety used in the current study, the majority of volatile aroma compounds found were alcohols, ketones and lactones (Fig. 1). Jirovetz et al. (2003) identified aldehydes, alcohols and esters as the main aroma compounds in the headspace of mature coconut water from Cameroon. Jirapong et al. (2015) reported alkanes, esters and terpenes as the main volatile organic compounds in the solvent extract of young aromatic coconut water. De Marchi et al. (2015) listed alcohols, aldehydes and ketones as the main volatile compounds in the headspace of young green coconuts from Thailand, with the minor presence of esters, lactones, terpenes, ethers and heterocyclics. Luckanatinvong et al. (2018) identified alcohols, esters, acids and other volatile compounds in the headspace of 'Nam Hom' coconut water. Differences in the type and concentration of volatile compounds found in various studies could be attributed to variation in variety,

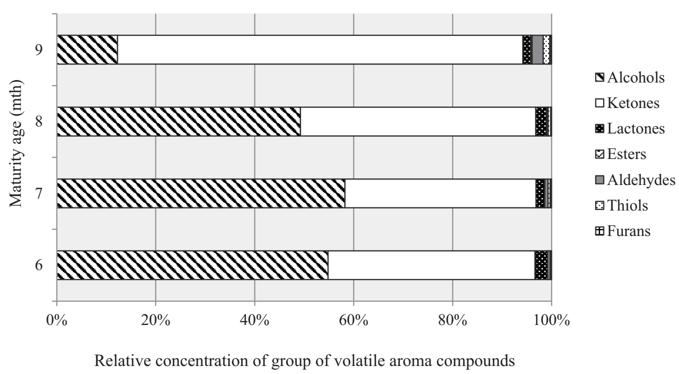

Fig. 1 Relative concentration of groups of volatile aroma compounds in coconut water from Tall variety at different maturity ages

stage of maturity, climatic condition, soil fertility status, sample preparation method, method of extraction and method of analysis (Saittagaroon et al., 1984; Purnomo, 2007; Jirapong et al., 2015).

Coconut water samples from lower maturity ages had higher contents of alcohols (Fig. 1). In a study with five varieties of coconut water aged 8 mth, Prades et al. (2012a) reported that alcohols produced the most varied patterns. Jirovetz et al. (2003) reported nonanol, heptanol and 2-nonanol as the major alcohols found in the headspace of coconut water from ripe coconut fruits in Cameroon, with several of the alcohols playing important roles in producing the fresh, floral and fruity notes of coconut water.

Fig. 1 indicates that the percentage of ketones increased following maturity of the coconut fruit. Prades et al. (2012a) discussed the presence of ketones in coconut water as being responsible for fruity, sweet and creamy or butyric characteristics. They reported the occurrence of higher levels of ketones in coconut water from the Tall and Hybrid varieties as compared to the Dwarf variety at the same stage of maturity (8 mth).

Higher concentrations of lactones were recorded in coconut water from lower maturity ages (Fig. 1). During the maturation process of a coconut fruit, there is an increase in the crude fat and free fatty acid contents of the coconut kernel, especially for shorter-chain saturated fatty acids, such as lauric acid (Assa et al., 2010; Appaiah et al., 2014; Mahayothee et al., 2016). Jackson et al. (2004) reported a slight increase of 1–2% in the fat content of coconut water from the Maypan Tall variety during the initial stage of maturation, prior to the formation of the 'jelly'-like kernel. Jirapong et al. (2015) described a slight increase in short-chain saturated fatty acids and a minor decrease in longer-chain fatty acids in the water of young aromatic Thai coconuts as the fruit increased in maturity from age 6 mth to 7 mth. When the kernel of a coconut fruit starts to thicken, more fat is accumulated in the kernel and less fat is available in the water (Jackson et al., 2004) Therefore, when there are fewer free fatty acids available in coconut water, less lactone formation takes place; consequently, lower amounts of lactones were recorded in coconut water from the more mature coconut fruit.

Relative concentration and odor activity values of volatile aroma compounds in coconut water from Tall variety

Table 3 shows the relative concentrations and odor activity values of the volatile aroma compounds identified in the samples. Among all the alcohols listed, the most abundant ones detected in the samples were ethanol and 1-butanol. There was a decrease in ethanol in the headspace of coconut water when the maturity age increased. This finding could possibly be linked to the presence of acetaldehyde and ethyl acetate. Acetate esters are produced from the carbon of acetaldehyde, while the acetaldehyde might have come from several possible pathways, including enzymatic oxidation of ethanol. Therefore, the decreases in the ethanol and acetaldehyde contents following increasing maturity of the coconut fruit might indicate ethanol was being diverted to acetaldehyde, which was then converted to ethyl acetate. Therefore, the ethyl acetate increased as the coconut fruit matured, as was also observed in apples (Villatoro et al., 2008).

The second-most abundant alcohol identified in the samples was 1-butanol (OAV > 1.0), as shown in Table 3. The odor activity value of a volatile compound represents the ratio of its concentration to its odor detection threshold. Therefore, a compound with an OAV > 1 is expected to make a greater contribution to the aroma of the foodstuff (Grosch, 2001). Having an OAV > 1 indicated the possible important contribution of 1-butanol to the aroma of the coconut water from the Tall variety. In terms of aroma characteristics, 1-butanol, which was also found in coconut milk, was described as providing a fruity odor (Tinchan et al., 2015).

Acetoin, a ketone, was found in the samples used in the current study (Table 3). Though an increasing trend following age could be observed, the average contents of acetoin in the samples were not significantly different. Based on its OAV, acetoin appeared to be the ketone having potential as a key aroma compound in the coconut water throughout maturation. Lasekan and Abbas (2010) and Tinchan et al. (2015) reported acetoin as the most abundant ketone in palm toddy and coconut milk, producing a buttery odor. In addition, acetoin was found in the solvent extract of coconut water from green and yellow coconut varieties (da Fonseca et al., 2009). Acetoin can be biosynthesized from acetaldehyde (Lasekan and Abbas, 2010), which was likely another reason for the declining amount of acetaldehyde in the more mature coconut water (Table 3).

A group of lactones (δ-hexalactone, δ-octalactone, δ-decalactone, butyrolactone and pantolactone) was detected in the samples (Table 3). Lactones are responsible for the unique coconut aroma, hence the commonly-used term "coconut-like" to describe their aroma and they are also often stated to give peach-like, creamy-fatty and sweet characteristics (Jirovetz et al., 2003; Lasekan and Abbas, 2010; Santos et al., 2011; Prades et al., 2012a; Tinchan et al., 2015). Similarly, a descriptive sensory analysis performed on coconut milk samples associated lactones with the coconut milk flavor (Wattanapahu et al., 2012). Jirovetz et al. (2003) identified δ-lactones (hexalactone, octalactone, decalactone and dodecalactone) in their sample of coconut water from mature coconut fruit in Cameroon, while Prades et al. (2012a) discovered δ-octalactone, δ-nonalactone and δ-decalactone in their coconut water samples aged 8 mth. Regarding varietal differences, Prades et al. (2012a) reported a higher level of lactones in coconut water from the Tall variety compared to the Dwarf variety, as lipids were deposited in the coconut fruit from the Tall variety at an earlier maturity stage (age 5 mth). Therefore, there was a higher opportunity for the synthesis of fatty acids (which are the source of lactone molecules) through the fatty acid anabolism pathway following cyclization and dehydration of γ- and δ-hydroxy acids (Saittagaroon et al., 1984; Santos et al., 2011; Prades et al., 2012a).

Table 3 shows that δ-octalactone was the most abundant lactone in the samples. This lactone has been identified to be important in providing the characteristic coconut-like aroma in the Tall coconut variety (Santos et al., 2011; Prades et al., 2012a). Saittagaroon et al. (1984) identified δ-octalactone in unroasted and roasted coconut meat samples and Tinchan et al. (2015) also detected it in their samples of canned coconut milk.

Among all the aroma compounds identified, Fig. 2 displays two potential key aroma compounds that had values of OAV > 1, namely acetoin and 1-butanol. It can be observed that there was an increase in the amount of acetoin following maturity. At age 9 mth, acetoin reached a peak of approximately 80% of the total volatile aroma compounds contained in the sample. The high OAV of acetoin in samples from higher maturity ages showed its importance in affecting the aroma of the sample. In coconut water samples aged 9 mth, acetoin was the only volatile aroma compound with an OAV > 1, which gave the unique creamy, buttery and yogurt-like odor characteristics to the sample. The OAV value of 1-butanol dropped to < 1 in the older coconut water (age 9 mth), which indicated its less important role in the aroma of the coconut water in mature coconut fruit. This difference in terms of potential key aroma compounds (with OAV > 1) in coconut water between younger and older coconuts from the Tall variety would be beneficial for selection of the suitable maturity as an ingredient in coconut water-based products. Coconut water at a younger maturity age contains more 1-butanol (Fig. 2); therefore, it would be more suitable for products requiring winey, fruity or tangy notes, such as mixed-fruit beverage products. On the other hand, coconut water with an older maturity age has more acetoin (Fig. 2), which would make it suitable for products needing a creamy or fermented profile, such as yogurt-based products.

Table 3 Relative concentrations and odor activity values of volatile aroma compounds in coconut water from Tall variety

Volatile aroma compound	Odor detection threshold (μg/L)[1]	Relative concentration (μg/L)				Odor activity value			
		Age 6 mth	Age 7 mth	Age 8 mth	Age 9 mth	Age 6 mth	Age 7 mth	Age 8 mth	Age 9 mth
Acetaldehyde	15 (a)	8.4 ± 7.1^{a}	9.0 ± 3.9^{a}	4.5 ± 3.0^{a}	6.8 ± 4.9^{a}	< 1	< 1	< 1	< 1
Ethyl acetate	5 (a)	0.4 ± 0.3^{a}	1.7 ± 1.6^{a}	1.7 ± 1.6^{a}	3.3 ± 0.5^{a}	< 1	< 1	< 1	< 1
Ethanol	100000 (a)	204.7 ± 101.3^{a}	172.3 ± 15.3^{a}	131.3 ± 47.7^{a}	105.0 ± 11.0^{a}	< 1	< 1	< 1	< 1
2-Methyl-1-propanol	7000 (a)	112.8 ± 50.4^{a}	87.2 ± 56.3^{a}	63.7 ± 22.7^{a}	19.9 ± 5.0^{a}	< 1	< 1	< 1	< 1
1-Butanol	500 (a)	689.6 ± 321.4^{ab}	783.1 ± 27.5^{ab}	991.4 ± 451.6^{a}	136.9 ± 56.6^{b}	1.4	1.6	2.0	< 1
3-Methyl-1-butanol	250 (a)	29.0 ± 2.6^{a}	15.2 ± 4.4^{a}	18.0 ± 15.0^{a}	5.1 ± 1.0^{a}	< 1	< 1	< 1	< 1
Acetoin	800 (a)	810.3 ± 288.2^{a}	718.2 ± 216.5^{a}	1188.0 ± 790.5^{a}	1042.0 ± 859.9^{a}	1.0	< 1	1.5	1.3
1-Hexanol	2500 (a)	13.6 ± 5.0^{a}	10.4 ± 4.3^{a}	7.5 ± 3.3^{a}	6.4 ± 5.4^{a}	< 1	< 1	< 1	< 1
Trans-3-hexen-1-ol	110 (b)	3.0 ± 0.5^{a}	4.5 ± 2.0^{a}	4.8 ± 2.4^{a}	4.7 ± 0.6^{a}	< 1	< 1	< 1	< 1
2-Ethyl-1-hexanol	270000 (a)	3.3 ± 0.5^{ab}	4.7 ± 0.3^{a}	2.9 ± 0.6^{b}	3.2 ± 0.7^{ab}	< 1	< 1	< 1	< 1
Benzaldehyde	350 (a)	1.2 ± 0.2^{a}	2.5 ± 2.4^{a}	1.3 ± 0.7^{a}	21.4 ± 18.2^{a}	< 1	< 1	< 1	< 1
2-(Methylthio)-ethanol	120 (c)	1.3 ± 0.4^{c}	2.7 ± 0.9^{bc}	4.4 ± 0.7^{b}	8.4 ± 1.5^{a}	< 1	< 1	< 1	< 1
1-Octanol	110 (a)	5.2 ± 4.5^{a}	5.7 ± 5.5^{a}	9.1 ± 7.0^{a}	10.9 ± 8.6^{a}	< 1	< 1	< 1	< 1
Butyrolactone	1000 (d)	2.2 ± 0.9^{a}	4.9 ± 1.8^{a}	3.3 ± 2.3^{a}	6.1 ± 1.7^{a}	< 1	< 1	< 1	< 1
3-(Methylthio)-1-propanol	250 (e)	2.1 ± 0.9^{b}	6.0 ± 0.1^{ab}	9.0 ± 4.2^{a}	8.8 ± 0.9^{a}	< 1	< 1	< 1	< 1
δ-Hexalactone	n.a.	17.8 ± 10.8^{a}	12.6 ± 2.1^{a}	24.9 ± 19.2^{a}	3.3 ± 0.0^{a}	n.a.	n.a.	n.a.	n.a.
4-Methyl-5H-furan-2-one	n.a.	2.2 ± 1.3^{a}	4.9 ± 1.8^{a}	3.9 ± 0.1^{a}	4.5 ± 0.8^{a}	n.a.	n.a.	n.a.	n.a.
Phenylethyl alcohol	750 (a)	0.8 ± 0.5^{a}	0.9 ± 0.2^{a}	1.6 ± 0.9^{a}	0.9 ± 0.7^{a}	< 1	< 1	< 1	< 1
δ-Octalactone	400 (a)	23.7 ± 16.7^{a}	10.3 ± 0.8^{a}	21.4 ± 9.1^{a}	8.7 ± 2.5^{a}	< 1	< 1	< 1	< 1
Pantolactone	n.a.	4.2 ± 4.0^{a}	3.4 ± 3.0^{a}	4.5 ± 2.1^{a}	1.1 ± 1.0^{a}	n.a.	n.a.	n.a.	n.a.
δ-Decalactone	100 (a)	1.6 ± 1.0^{a}	0.6 ± 0.2^{a}	0.6 ± 0.5^{a}	1.4 ± 1.3^{a}	< 1	< 1	< 1	< 1

[1] = odor detection thresholds from (a) Leffingwell & Associates (2008), (b) Boonbumrung et al. (2001), (c) Hansen et al. (1992), (d) Buttery and Ling (1998) and (e) Fritsch and Schieberle (2005);
Mean±SD in each row superscripted with different lowercase letters are significantly ($p < 0.05$) different; n.a. = not available
Each concentration value was calculated primarily from solvent extraction, except for those detected only using headspace-solid phase microextraction.

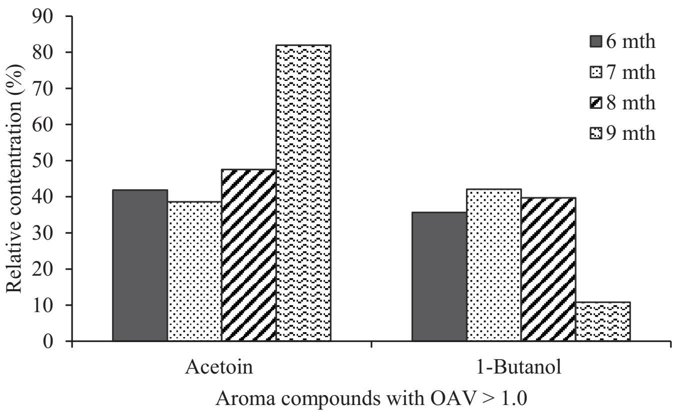

Fig. 2 Relative concentration of potential key volatile aroma compounds with odor activity value (OAV) > 1.0 in coconut water from Tall variety at different maturity ages

In addition to the alcohols, ketones and lactones, there were also other groups of volatile aroma compounds detected in the coconut water samples, such as esters, aldehydes and thiols (Fig. 1). An aromatic ester (ethyl acetate) was detected in the headspace of coconut water samples (Table 2). Esters have been reported to provide fruity and sweet odors (Saittagaroon et al., 1984). Prades et al. (2012a) identified several esters in five varieties of coconut water from coconut fruits aged 8 mth, although they appeared in low amounts and had no specific aroma characteristics. Ethyl acetate (the ester detected in the current study) was also found in virgin coconut oil, where it was mapped to a nutty aroma (Santos et al., 2011).

Regarding the aldehydes (Fig. 1), benzaldehyde was identified in the samples using solvent extraction, while acetaldehyde was identified in the headspace of samples (Table 2). Acetaldehyde was also identified in the headspace of coconut water aged 8 mth from five varieties by Prades et al. (2012a), who stated that the aldehydes were associated with green, fresh and almond aroma characteristics. Prades et al. (2012a) also reported that coconut water from the Tall variety contained the lowest level of aldehydes of the five studied varieties. Several low-molecular weight aldehydes might come from the autoxidation of fatty acids or from the action of lipoxygenase on polyunsaturated fatty acids (Prades et al., 2012a). Jirapong et al. (2015) reported several polyunsaturated fatty acids in coconut water, while Meethaworn and Siripanich (2017) detected lipoxygenase activity in coconut water. Therefore, the availability of free fatty acids as the precursors, and lipoxygenase as the enzyme, could contribute to the presence of aldehydes in coconut water.

The few thiols, or sulfur-containing compounds, that were identified in the samples were 2-(methylthio)-ethanol and 3-(methylthio)-1-propanol (Table 2). There were increasing amounts of thiols observed with increasing maturity age of the samples (Table 3). Thiols, such as methionol (3-methylthio-1-propanol), have been reported to provide soup-like, meaty, boiled potato-like, vegetable-like and savory characteristics in food (Seow et al., 2010; McGorrin, 2011). Thiols were abundant in the essential oil of coconut water from the yellow coconut variety in Brazil (da Fonseca et al., 2009). Its increasing amount in the samples following maturity explains the higher savory and sulfury aroma found in the water of more mature coconut fruit. The formation of thiols requires sugars and sulfur-containing compounds such as methionine, which both have been reported to be available in coconut water from the Tall variety (Santoso et al., 1996; Seow et al., 2010; Tan et al., 2014).

Conclusion

Maturity age did not have significant effects on the total soluble solids, pH, titratable acidity and color values of coconut water from the Tall variety. Alcohols, ketones and lactones were the major volatile aroma compounds in the samples. Among these compounds, acetoin and 1-butanol were potential key aroma compounds with values of OAV > 1.0. Coconut water from lower maturity (aged 6–7 mth) of the Tall variety contained more alcohols and lactones that contributed winey, fruity, sweet, coconut-like and creamy odor characteristics. The coconut water from the Tall variety with higher maturity ages (aged 8–9 mth) had more acetoin and thiols that contributed buttery, yogurt-like, sulfury and soup-like aromas. These findings should help to categorize coconut water from the Tall variety based on the aroma profiles of its compounds at different maturity stages. Therefore, utilization of selected maturity of coconut water from the Tall variety can be carried out accordingly to suit the desired aroma properties of the intended product.

Conflict of Interest

The authors declare that there are no conflicts of interest.

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