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# Identification of Volatile Compound in Coconut Milk Samples Using GC-MS

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**A B S T R A C T**

The present study was carried out to identity the volatile component in coconut milk samples using direct solvent extraction (Hexane), followed by high-vacuum distillation and gas chromatography-mass spectrometry analysis. The samples were extracted ultrasonically followed by shaking at room temperature and kept overnight at room temperature for cold extraction. Six groups of compounds consisting of alcohols, aldehydes, ketones, acids, esters, lactones, and others were identified. The major volatile compound identified in plain coconut milk were tetracontane, 2-Hexanol and the compounds such as Heptadecane, Ethanone, 1-(3-ethyloxiranyl) were identity in flavoured coconut milk. In commercial coconut milk, Pentane, 3-ethyl-2, 4-dimethyl were found to be higher value than other volatile compound.

## Introduction

Coconut milk, a white opaque liquid, is an emulsion of natural oil in water, extracted from shredded coconut endosperm (*Cocos nucifera* L.) either with or without the addition of water (Simuaug *et al.*, 2004; Tangsuphoom and Coupland, 2005). Coconut milk, the processed and packed milk extracted from fresh matured coconuts is an instant product which can either be used directed or diluted with water to make various preparations such as curries, sweets, desserts, puddings (Anjaya *et al.*, 1996). Coconut milk used as a food ingredient, and also it is an importance substance for health promotion and medicine. Coconut milk may be considered as a substitute for cow milk. It may be used by the people who cannot tolerate cow milk (Rehman *et al.*, 2004). Phospholipids, cephalin and lecithin which have been found in coconut milk (Philippine coconut authority, 2014). Coconut milk is rich in antioxidants, which prevents free radical damage and delay the ageing process. A glass of coconut milk while taking other antioxidants rich foods, such as pecans, raisins and cranberries may boost the immunity while rebuilding the damaged cells in the body (Brown, 2014). It provides fat that is mostly in the form of medium chain fatty acids (MCFA) that is abundant in mother milk

in particular, Lauric acid. It has anti-fungal, antiviral properties (Baldioli *et al.*, 1996).Short term preservation can be easily achieved by pasteurizing the milk at 72 ºC for 20 mins (Seow and Gwee, 1997). Small changes in aroma, either after processing, could be the important determinants of the degree of consumer acceptance of the product. Lin and Wilkens (1970) reported that δ -octalactone, δ -decalactone, and octanol are the major volatile components of coconut meat extracted by distillation. Other compounds identified were 2-heptanol, hexanol, 2-nonanone, 2-octanol, 2-nonanol, octanol, 2-undecanone, ethyl decanoate,2-undecanol, 2-phenylethanol, benzothiazole, α -undecalactone, and dodecanoic acid. Predominant compounds were butanol, hexanol, heptanol, 2-heptanol, octanal, nonanal, 1-octanol,2-nonanol,α-hexalactone,nonanol, octanoic acid, ethyl octanoate, decanal, δ -octalactone, decanol, nonanoic acid,1-undecanol, and δ -decalactone (Jirovetz *et al.*, 2003). Hence, this work focused on determining the volatile compound that occur in pasteurized coconut milk, which ultimately could be related to flavor changes in the product.

## Materials and Methods

### Collection of coconut and extraction of coconut milk

Coconut (West Coast Tall) Variety was purchased from Coconut Research Station, Veppenkulam, Thanjavur district. Spices (Cardamom) were purchased from Thadiyankudisai, Kodaikanal. Coconut milk extracted by grinding process and squeezing out of milk through cleaned muslin cloth likewise cardamom was powdered using mixer grinder and outer layer of husks was removed. The powder of the cardamom was sieved and used as a flavouring agent in flavoured coconut milk. Commercial coconut milk was purchased from department store, used as control.

### Sample preparation

The coconut milk sample was vacuum – filtered through paper (What man filter paper No.1) for homogenization without heat. 10 ml of sample was extracted with 100 ml of HPLC grade hexane in a DURAN laboratory bottle, equipped with a magnetic stirrer, at low speed for 30 min at room temperature. Extractions were carried out 3 times. The hexane fractions containing the volatile compounds were pooled and further purified (nonvolatile removed) by high vacuum distillation at ambient temperature for 2 hr and then at 50º C for 1 hour. Volatiles were condensed in a trap cooled with liquid nitrogen. The resulting aroma extract was evaporated to 5 ml under a gentle steam of $N_2$ gas and then dried over 2 g anhydrous $Na_2SO_4$ to remove water. Extracts were then concentrated to a final volume of 250 µL before analysis.

### Gas Chromatography –Mass Spectrometry analysis

GC-MS was conducted using a 6890 GC/5973 mass selective detector (MSD) system (Aglient Technologies, Palo Alto, Ca., U.S.A). Aroma extracts (1 µL) were injected in hot splitless mode (0.5 min split valve-delay time). Separate were performed on nonpolar (HP-5; 60m length, 0.25 mm i.d and 0.25 µm film thinkness; Quadrex Corp., New haven, Conn., USA.). The GC oven temperature was programmed as follows: initial temperature of 40ºC held for 5 mins, raised at a rate of 2ºC/min to 60º C, raised at a rate of 20º C/min to 90ºC, raised at a rate of 10ºC/min to 200 ºC, and then held at this temperature for 20 min. The carrier gas was helium at a flow rate of 1.7 ml/ min. Injector and MSD transfer line were held at 250 ºC.

MSD conditions were as follows: electron – impact ionization voltage was 70 electron volts, scan range was 30 to 300 *m/z* at a rate of 2.74 scan/s.

## Results and Discussion

In the present study, the volatile compounds presented in coconut milk samples were analyzed by GC-MS analysis. The results revealed that there are ten compounds were identified in plain coconut milk. It contain the bioactive compounds such as tetracontane, it has strong antimicrobial activity, which can destroy food borne pathogens prevent from many disease and 2 hexonal was used in fruit and vegetable processing and preservation (Fig. 1 and Table 1).

Volatile compound such as Heptadecane, Pentane, 3-ethyl-2,4-dimethyl, Ethanone, 1-(3-ethyloxiranyl), Tetrahydrofuran, 2,2-dimethyl were identified in flavoured coconut milk. Heptadecane is a major component of *Spirulina platensis*, which contains high levels of proteins, amino acids, vitamins, beta carotene.It has been shown that the strong antioxidative effects of have therapeutic benefits in renal disease and inhibit the proliferation of human liver cancer cells (Fig. 2 and Table 2).

In commercial coconut milk, Pentane, 3-ethyl-2,4-dimethyl, 3-Hexen-2-one, Etrahydrofuran, 2,2-dimethyl, 1-Heptacosanol, 2-Pentanone, 3-ethyl-3-methyl were identified (Fig. 3 and Table 3).

**Fig.1** Chromatogram obtained from GC-MS with plain coconut milk

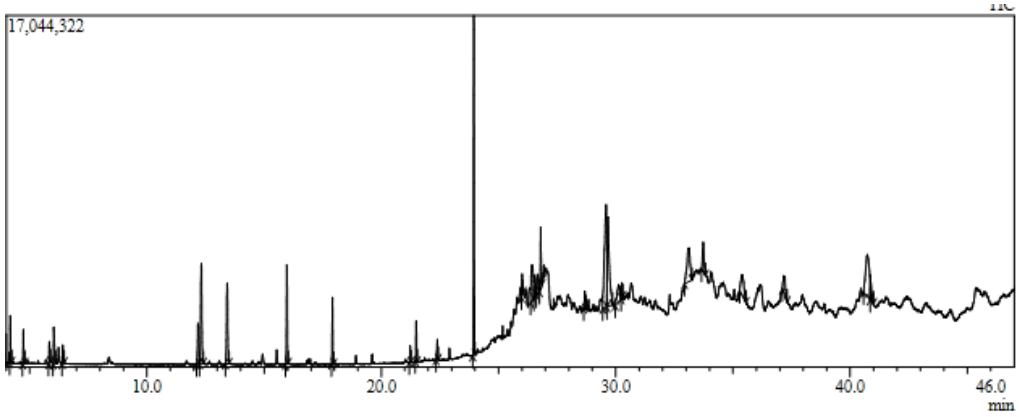


**Fig.2** Chromatogram obtained from GC-MS with flavoured coconut milk

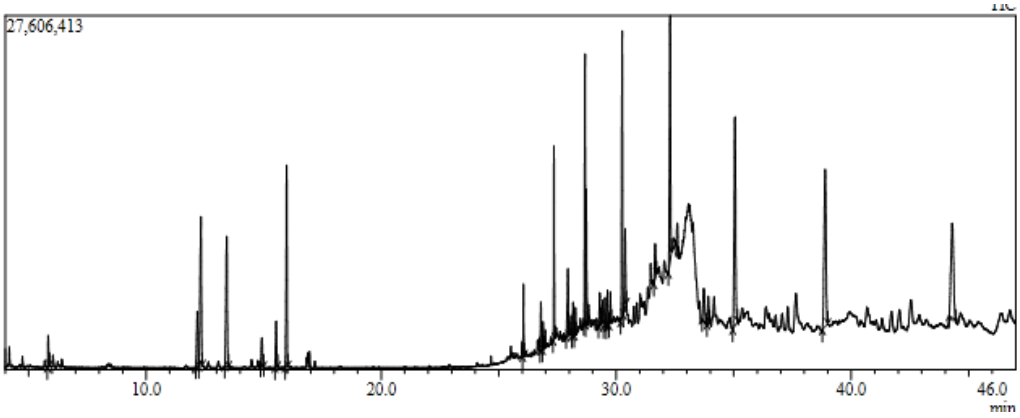

**Fig.3** Chromatogram obtained from GC-MS with commercial coconut milk

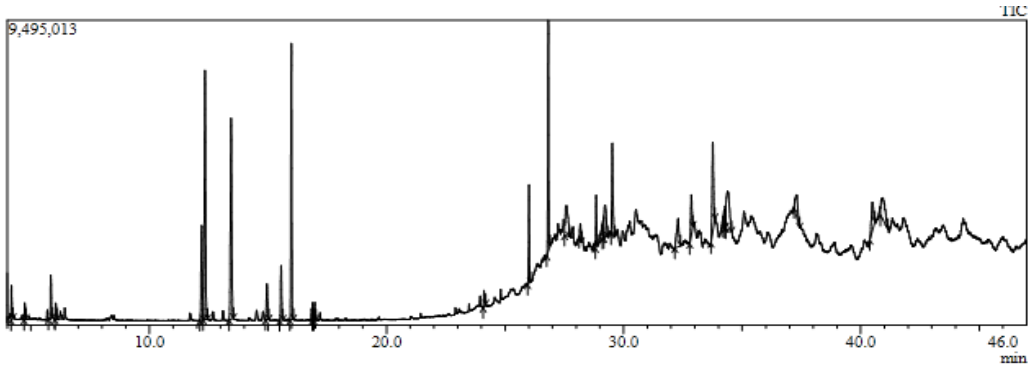


**Table.1** Volatiles compound identified in plain coconut milk by GC-MS analysis

| Retention time (min) | Name of the compound | Peak area (%) |
|---|---|---|
| 4.174 | 2-Pentanol, 2-methyl- | 1.52 |
| 4.731 | 3-Pentanol, 3-methyl- | 1.23 |
| 5.840 | 2-Hexanone | 0.85 |
| 6.031 | Cyclopentanol, 1-methyl- | 1.64 |
| 6.412 | 2-Hexanol | 6.412 |
| 12.185 | Tetrahydrofuran, 2,2-dimethyl- | 2.58 |
| 17.915 | Eucalyptol | 2.21 |
| 21.488 | alpha.-Terpineo | 1.26 |
| 22.391 | Geraniol | 0.87 |
| 26.005 | 2H-Pyran-2-one, tetrahydro-6-pentyl- | 0.70 |
| 28.680 | Heptadecan | 0.77 |
| 29.660 | Tetracontane | 10.18 |
| 30.115 | 1-Hexacosano | 2.56 |
| 33.124 | Pentatriacontane- | 5.61 |

**Table.2** Volatiles compound identified in flavoured coconut milk by GC-MS analysis

| Retention time (min) | Name of the compound | Peak area (%) |
|---|---|---|
| 26.793 | Dodecanoic acid | 1.33 |
| 26.885 | Heneicosane | 0.66 |
| 27.351 | Heptadecane | 3.58 |
| 27.942 | Pentadecane, 2,6,10-trimethyl | 2.08 |
| 28.163 | Pentadecane, 8-hexyl- | 1.07 |
| 28.266 | Heptadecane, 2-methyl | 0.63 |
| 28.669 | Heptadecane | 6.38 |
| 29.298 | Eicosane | 1.05 |
| 5.831 | 2-Hexanone | 0.80 |
| 12.176 | Tetrahydrofuran, 2,2-dimethyl | 2.25 |
| 12.328 | Pentane, 3-ethyl-2,4-dimethyl | 6.31 |
| 13.427 | Ethanone, 1-(3-ethyloxiranyl)- | 5.67 |
| 14.923 | Hexane, 2-nitro- | 1.06 |
| 15.529 | 2-Pentanone, 3-ethyl-3-methyl- | 1.41 |

**Table.3** Volatiles compound identified in commercial coconut milk by GC-MS analysis

| Retention time (min) | Name of the compound | Peak area (%) |
|---|---|---|
| 4.182 | 2-Pentanol, 2-methyl- | 0.99 |
| 4.744 | 3-Pentanol, 3-methyl- | 0.50 |
| 5.842 | 2-Hexanone | 1.50 |
| 6.051 | Cyclopentanol, 1-methyl- | 0.59 |
| 12.205 | etrahydrofuran, 2,2-dimethyl | 5.18 |
| 12.347 | Pentane, 3-ethyl-2,4-dimethyl | 13.52 |
| 14.958 | Hexane, 2-nitro- | 1.94 |
| 15.554 | 2-Pentanone, 3-ethyl-3-methyl- | 2.26 |
| 15.988 | 3-Hexen-2-one | 10.10 |
| 16.889 | 1-Nonen-4-ol | 0.49 |
| 24.111 | n-Decanoic acid | 0.57 |
| 27.589 | 1-Heptacosanol | 3.51 |
| 28.840 | delta.-Dodecalactone | 1.74 |
| 32.296 | 2-Methylhexacosane - | 2.70 |

Plants contains variety of phytochemical components, many of them are biologically active compounds and known to have pharmacological activities (Gu *et al.*, 2014). The bioactive secondary metabolites have been shown to reduce the risk and progression of diseases such as cancer, cardiovascular disease, neurodegenerative diseases, etc by scavenging free radicals through various biological mechanism (Ansari and Khodagholi, 2013).

The results of GC-MS indicated that coconut milk samples contained numerous bioactive components belongs to various classes such as polyphenols, alkaloids, flavonoids, steroids that will provide health benefits. Coconut milk rich in antioxidants, which prevents free radical damage. It can help reverse previous damage and delay ageing process. Coconut can be effectively processed into coconut milk beverages as a substitute for cow milk beverages with improved nutritional value for health concerned consumers.

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