# Profile of Volatile Organic Compounds (VOCs) from Cold-Processed and Heat-Treated Virgin Coconut Oil (VCO) Samples

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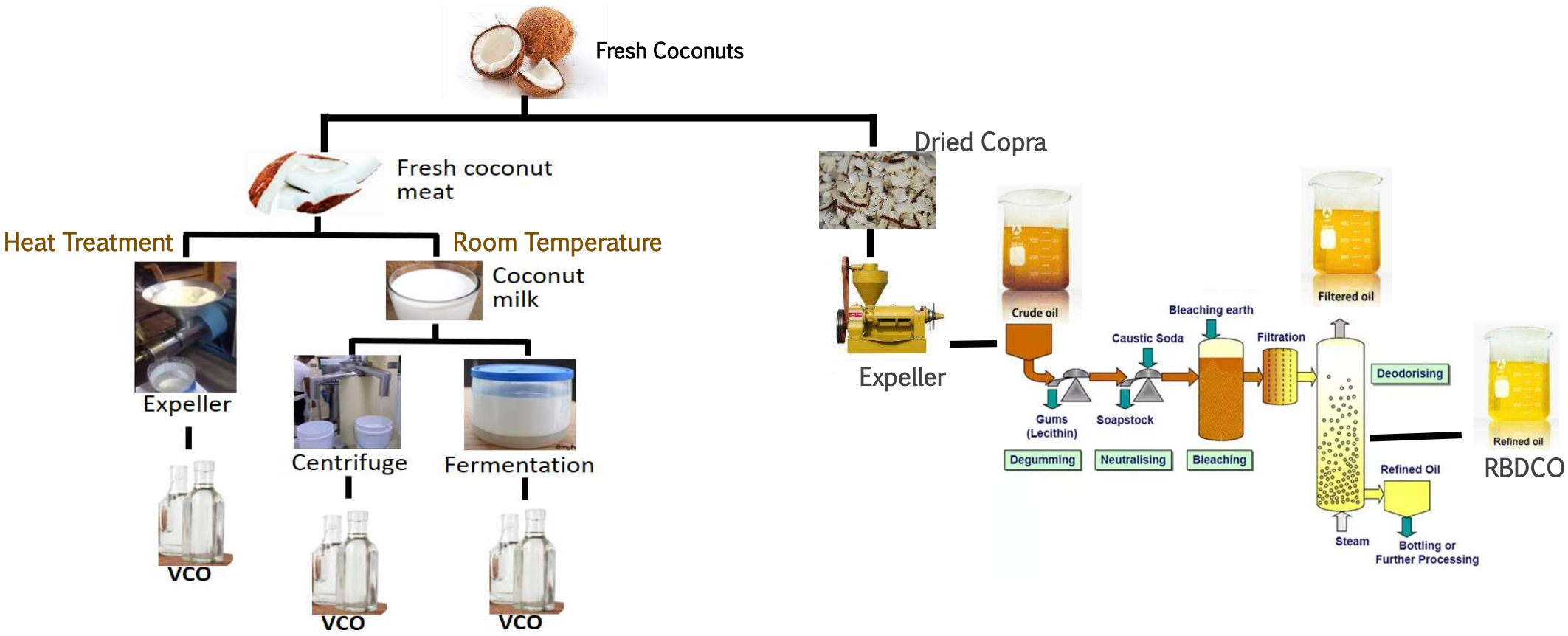
# Production of Virgin Coconut Oil (VCO) and Refined Bleached Deodorized Coconut Oil (RBDCO)



# Volatile Organic Compounds (VOCs) of Coconut Oil

## Source Coconut

ethyl carboxylates

delta-lactones

fatty acids

## Production Process

Maillard reaction

heat

physical separation

moisture

enzymes and microorganisms

oxidation

lipoxygenases (LOX)

## Storage

age

hydrolysis

oxidation

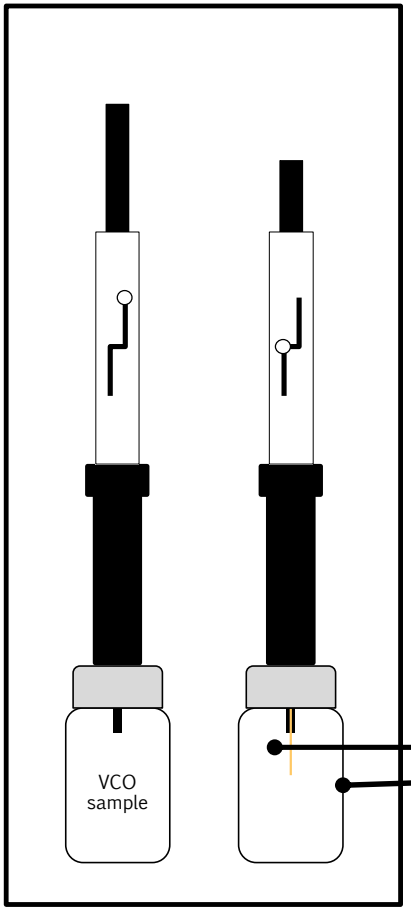
## Deterioration

The VOCs are responsible for the aroma of VCO. The VOCs can come from the coconut meat itself, the process of production, and from degradation processes that occur before, during, and after oil separation.

# Research Objectives

- Identify and quantify the VOCs from VCO samples which were produced using three processes – fermentation, centrifuge, and expeller – as well as refined, bleached and deodorized coconut oil (RBDCO). VCO samples were also collected during on-site observation of each production process.
- Analyze the VOC profiles from various stages of VCO production, as well as old VCO samples,
- Correlate VOC profile to the production process

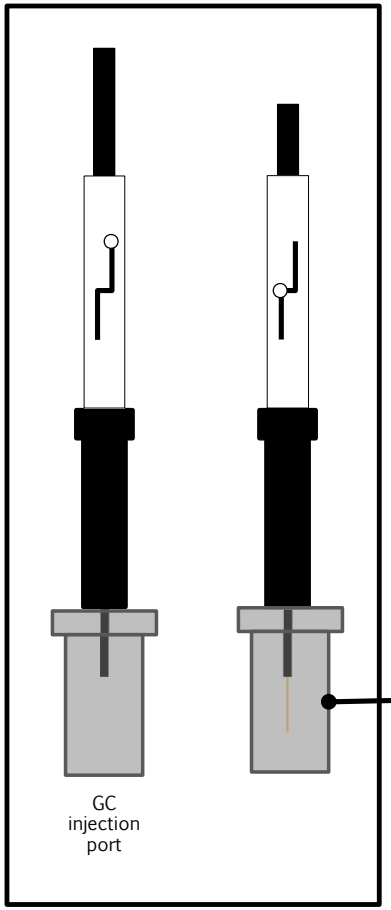
# Methodology




Solid phase microextraction (SPME) was employed to collect the volatile organic compounds present in the headspace of the oil samples.

50/30 µm
DVB/CAR/PDMS
fiber

40°C
20 mins




Collected VOCs were desorbed into the injector port of GCMS that will analyze each compound.

250°C
2 mins

# Methodology

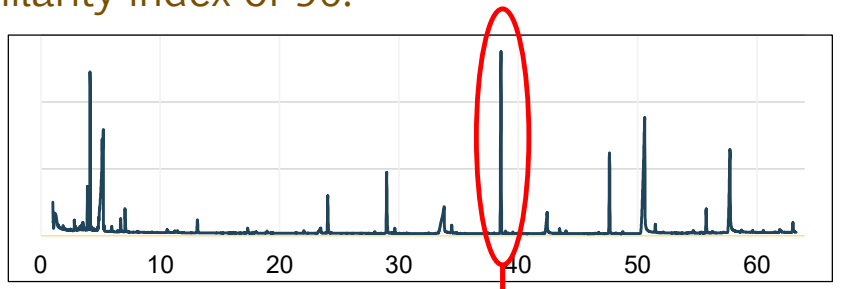
30°C
10 mins

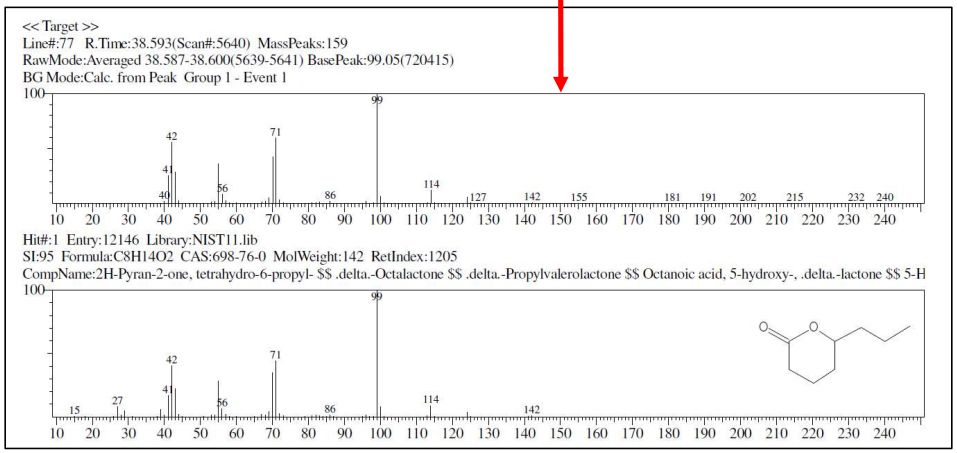
200°C
3°C/min

200°C
EI source
m/z 40 - 240
(quadrupole)

RTX-5MS® column
UHP He @ 1.01 mL/min

Peaks observed from the chromatogram identified by comparing with NIST library with minimum similarity index of 90.



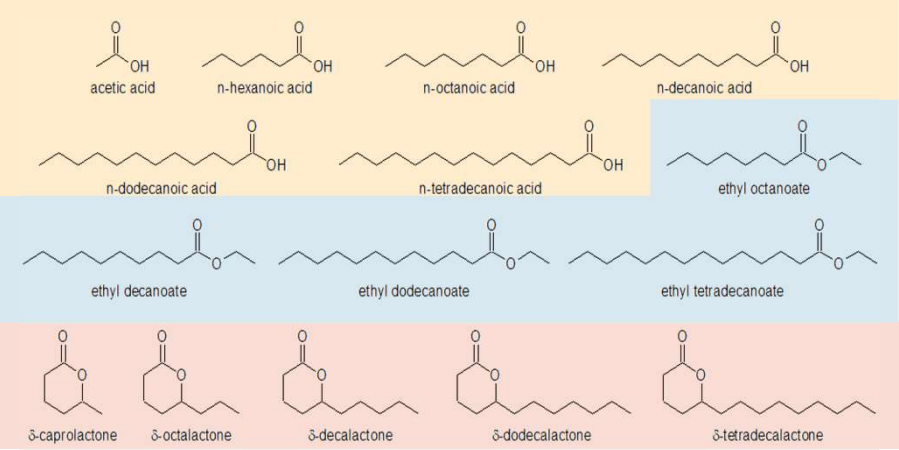



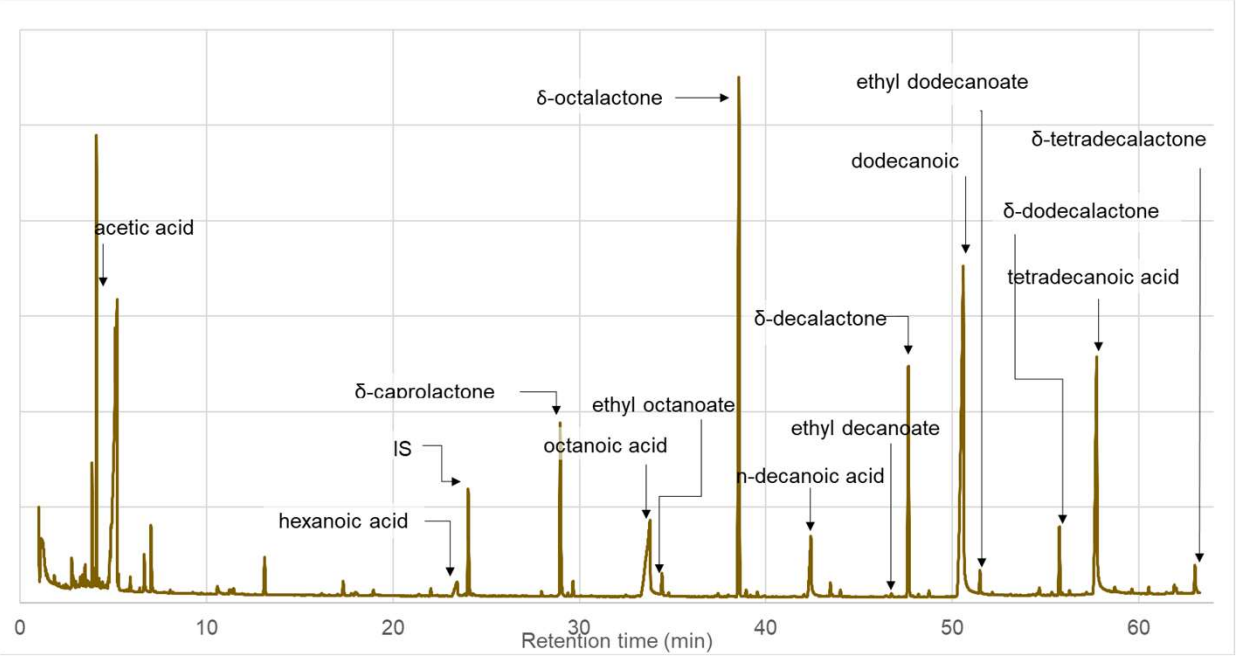
# Results: VCO Samples

| Sample | Exposure time[a] before oil separation | Method of moisture removal from raw VCO | Method of particles removal from raw VCO | Sterilization/ Heat treatment |
|---|---|---|---|---|
| F1-1<br>F1-2 | >24 hrs | Tubular centrifuge | Tubular centrifuge and fine cloth filtration | Hot water for dilution of milk; UV light on oil |
| F2-1<br>F2-2 | <24 hours | Tubular centrifuge and vacuum drying | Tubular centrifuge | Hot water for dilution of milk |
| F3-1<br>F3-2 | <24 hours | Vacuum drying | 0.5 to 1.0-micron bag filtration | None |
| C1-1<br>C1-2 | <24 hours | Disc centrifuge | Paper filter | Hot water to aid in separation |
| C2-1<br>C2-2 | <8 hours | Disc centrifuge | None | None |
| C3-1<br>C3-2 | <8 hours | Settling and vacuum drying | Settling | Blanching of coconut meat |
| E1-1<br>E1-2 | <8 hours | Settling, disc centrifuge, and demoisturizer | Settling and 0.5 to 1.0-micron bag filtration | Oven-drying of ground coconut meat |
| E2-1<br>E2-2 | <8hours | Settling and vacuum drying | Settling, Pressure filter with filter aids | Oven-drying of grated coconut meat |
| E3-1<br>E3-2 | <8hours | Vacuum drying | Filter press | Oven-drying of ground coconut meat |

# Results: Major VOCs of VCO

The major VOCs of VCO can be classified into three subgroups: carboxylic acids, ethyl carboxylates and delta-lactones. These are the same groups that can be found in coconut meat and shreds.

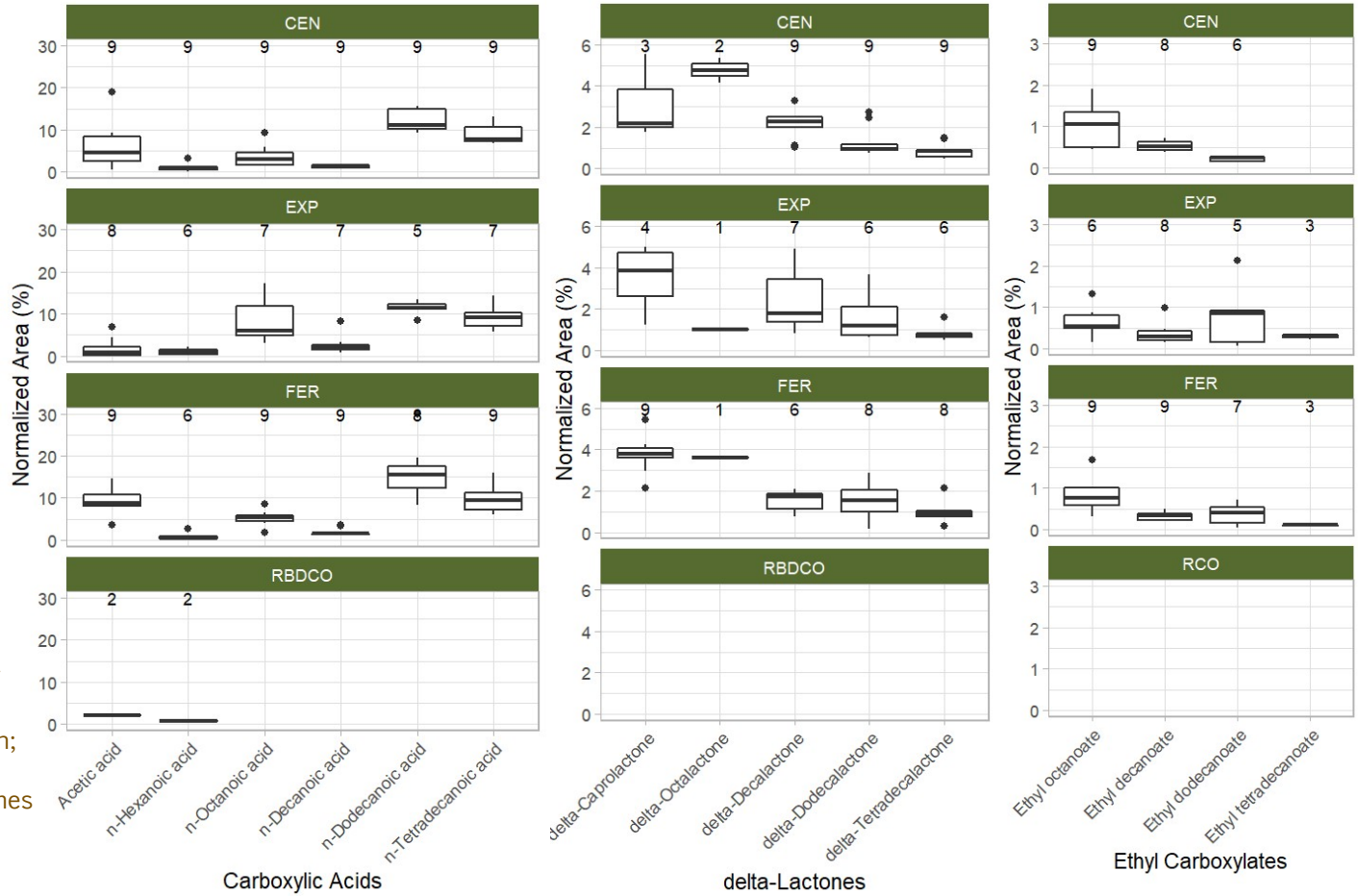


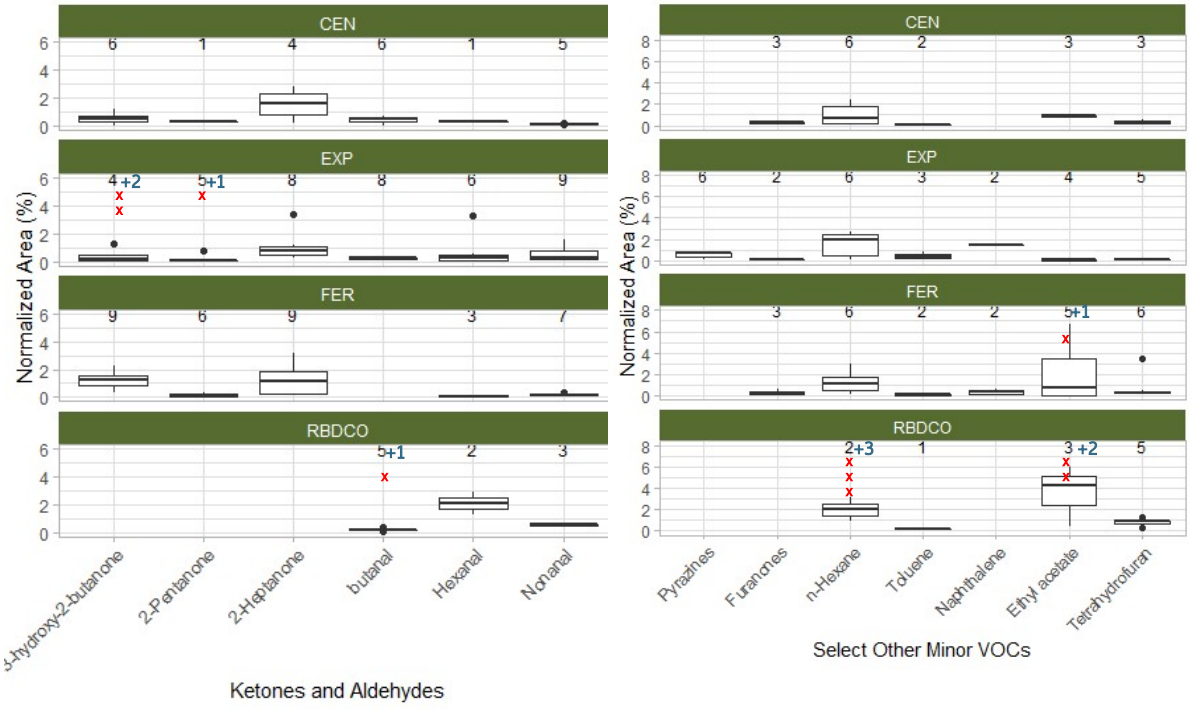
# Results: Major VOCs

- Thirteen compounds were frequently observed (>50%) across all samples analyzed.
- The major VOCs except acetic acid and n-hexanoic acid were not found in the RBDCO samples.
- There is wide variability in the normalized areas per VOC, especially in expeller samples.

Range of relative amounts (based on normalized areas of the components in the GC-MS TIC) of the of the major VOCs in VCO from different processes (CEN, centrifugation; EXP, expeller; FER, fermentation) and of RBDCO. The numbers on top of every box represent the number of times the particular VOC was detected. (The total number of samples per category are 9 for CEN, EXP and FER, and 5 for RBDCO)



# Results: Minor VOCs

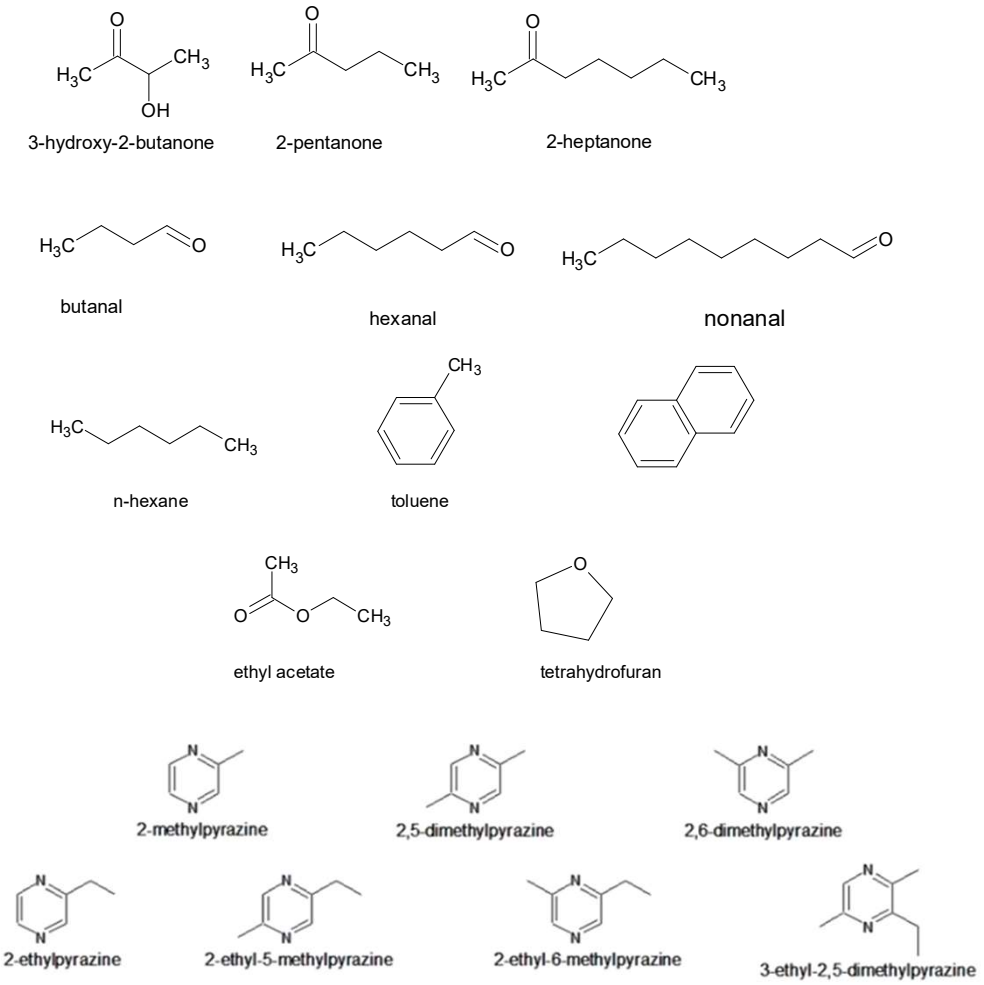



Range of relative amounts (based on normalized areas of the components in the GC-MS TIC) of the of select minor VOCs in VCO from different processes (CEN, centrifugation; EXP, expeller; FER, fermentation) and of RBDCO. The numbers on top of every box represent the number of times the particular VOC was detected. The total number of samples per category are 9 for CEN, EXP and FER, and 5 for RBDCO. The x mark is a datapoint beyond the scale of the graph

- Pyrazines were observed only from from expeller samples
- Ketones, in particular 3-hydroxy-2,3-butanone (acetoin) and 2-heptanone were detected at significant amounts in expeller samples; these key ketones were not found in RBDCOs
- Various aldehydes were detected in VCOs and RBDCOs
- There is a wide variability in the normalized area of ethyl acetate in Expeller VCO and RBDCO.

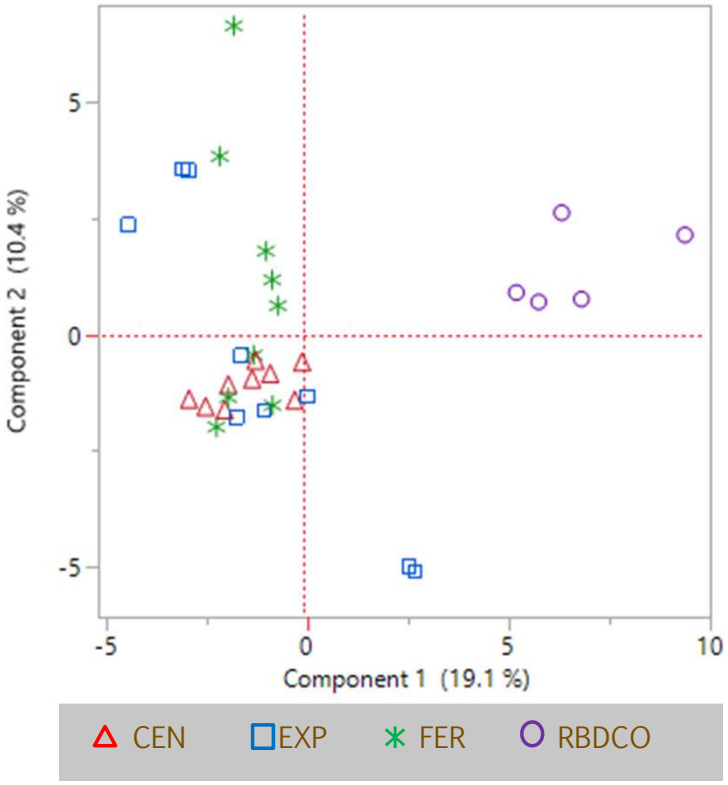
# Results: Minor VOCs

- Minor VOCs detected in fermentation and centrifuge samples are benzoic acid, butanoic acid and pentadecanoic acid.
- Other ketones detected include 2-pentadecanone and 2-undecanone
- Hydrocarbons like alkanes and alkenes were observed especially in RBDCO samples; the 13-yr. old RBDCO sample had the greatest number of these compounds

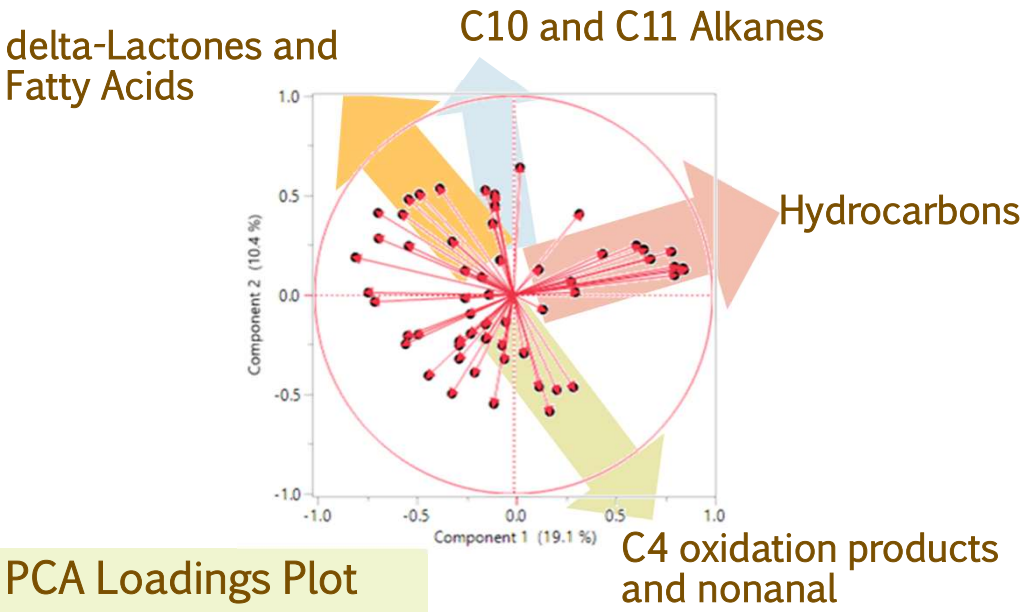


# Results: Principal Component Analysis (PCA)

## PCA Scores Plot




## PCA Loadings Plot

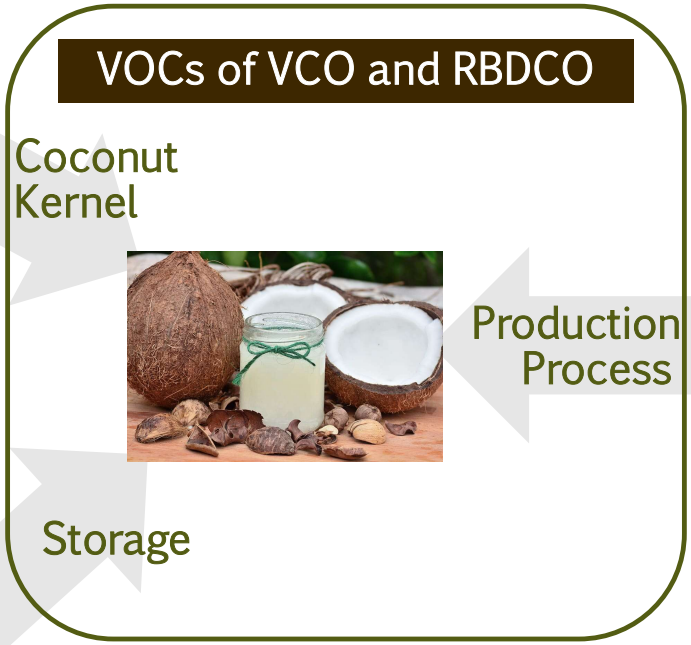



- RBDCO are separated from VCO samples and this is due to the hydrocarbons.
- VCOs prepared by centrifugation are more clustered together than VCOs from produced through other processes.
- VCO from expeller method displayed the highest variability

# Results: Discussion

- The major VOCs of VCO, except acetic acid comes, from the coconut kernel. These substance are extracted by the oil during production
- These are removed during the refinement, deodorization and bleaching process. Thus, these are no longer found in RBDCOs.

- VOCs are also produced during storage.
- Hydrocarbons can be produced during the storage. This can be triggered by microbiological factors.
- Diffusion can decrease VOCs while exposure to physico-chemical factors lead to increase in VOCs




- The VCO process can affect the relative amounts of the major VOCs that will transfer from the kernel to the oil.
- The process also affects the type of minor VOCs in the VCO products.
- Pyrazines found only in expeller samples can be produced if there is heat involved.
- Acetic acid and a variety of other short chain compounds can be produced by microbial/enzymatic action depending on the time and exposure to moisture.
- Exposure to other physico-chemical factors (light, air, presence of iron) during production leads to hydrolysis, oxidation and other processes.

# Conclusion

- Fourteen major VOCs were detected in the headspace of VCO: acetic acid; the fatty acids and the corresponding delta-lactones of C6, C8, C10, C12, and C14, and the ethyl carboxylates of C8, C10, and C12.
- Fourteen minor VOCs were likewise detected. These can be grouped into five types: carboxylic acids (formic acid, butanoic acid, benzoic acid, and pentadecanoic acid), ketones (acetoin, 2-heptanone), alcohol (ethanol), aldehydes (acetaldehyde, hexanal, benzaldehyde), esters (ethyl acetate, methyl tetradecanoate), and hydrocarbons (n-hexane and toluene).
- Five pyrazines were detected in expeller VCO.
- Various hydrocarbons from C5 to C14 were noted to be higher in old RBDCO and VCO samples.

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DEPARTMENT OF SCIENCE AND TECHNOLOGY

VCOP VIRGIN COCONUT OIL PHILIPPINES

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