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GC-MS and FTIR Analysis of Seed Oil Extract of *Cocos nucifera*

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Abstract: The present investigation was carried out to study the GC-MS and FTIR analyses of a seed oil extract of ***Cocos*** *nucifera*. Coconut seed oil has been consumed in tropical countries for thousands of years. According to studies on many indigenous foods, the population consumes a lot of coconut seed oil and is, in general, in good health. Coconut seed oil has a long shelf life and is used in cooking as well as in many daily life industries, including processed foods, baby formulae, medicines, cosmetics, and hair oil. In this study with all these characteristics of good quality, the effects of the oil have been especially reported in cardiovascular diseases, which are due to the presence of unsaturated fatty acids in the oil triglycerides. The GC-MS results revealed the presence of 8 bioactive compounds. The identification of the phytochemical compounds was confirmed based on the retention time, peak area, molecular formula, and molecular weight. Results obtained from infrared spectra indicated functional groups of compounds present in *C. nucifera*.

Keywords: GC-MS, FTIR, Seed oil extract, *Cocos nucifera*

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Introduction

Many years ago, traditional herbal medicine cured the sick and passed it on to the next generation of doctors. The WHO has been working in many countries since 1980 to promote traditional medicine, especially Indian traditional medicine, focusing on plant-based medicines and treatments (Kirtikar *et al*., 1918). Many new diseases have been discovered as a result of our way of life, but the truth is that nature has a cure for all diseases, and medicinal plants contain valuable substances that are still unknown. It is estimated that about 30% of the prescribed drugs contain plant extracts or extracts produced from plants (Nainwal *et al*., 2011). In the medical field, we should spend a little more time and resources on new drugs available from plants. *C. nucifera* is a plant belonging to the family Arecaceae. It is

also known as coconut, coco, and coco-da-bahia (Aragão, 2002). Coconut palm is often considered one of nature's most valuable beautiful plants. Oils, fiber and coconut products are today's consumer products such as soaps, beauty products foods and medicines widely used in products. The coconut palm is one of the most widely used palm trees in the world. Coconuts are used as whole parts including the fibrous, milky flesh, and husk. Several studies on the benefits of coconut and coconut oil have revealed that it can have significant effects on various disorders (Agyemang-Yeboah, 2011). Many advances have been made in current techniques for analytical identification of phytochemical compounds, including GC-MS and FTIR (Hites and Xia, 1995). GC-MS is a compatible, commonly used technique for identification and quantification purposes. FTIR is a very useful tool to detect functional groups present in compounds (Ronald, 1997). In this study GC-MS and FTIR techniques were used to investigate the bioactive compounds in *C. nucifera* seed oil extract.

Materials and Methods

Study area and collection of seed oil extract:

The present study was carried out in PG and Department of Zoology, RD. Govt. Arts College, Sivagangai, Tamil Nadu, India from January, 2022 to May, 2022. The seed oil extract of *C. nucifera* was obtained from the government recognized oil store, Madurai, Tamilnadu, India. Bioactive substances of GC-MS and FTIR were analyzed in Instrumentation Centre, ANJAC College, Sivakasi, Viruthunagar, Tamilnadu, India.

Gas chromatography mass spectroscopy:

The GC-MS analysis of the sample was carried out on Agilent chromatography GC (Model 7820A series) fitted with detector VL-MSD (Model 5977E). The carrier gas Helium was flow at constant 2 ml/min; the GC oven temperature started at 100°C for 1 min then increased at 10°C/min to 270°C held for 30 min. 1.0 µl of the sample was automatically injected into the column (DB-5) with the injector temperature at 270ºC. The injections were performed in split less mode. The compounds were identified based on the comparison of their retention indices (RI), retention time (RT), mass spectra of WILEY, NIST library data of the GC-MS system and literature data.

Fourier Transform Infrared Spectrophotometer:

Fourier Transform Infrared Spectrophotometer is perhaps the most powerful tool for identifying the types of chemical bonds (functional groups) present in compounds. The wavelength of light absorbed is characteristic of the chemical bond as can be seen in the annotated spectrum. By interpreting the infrared absorption spectrum, the chemical bonds in a molecule can be determined. Seed oil extract of *C. nucifera* was used for FTIR analysis. 10 mg of the seed oil extract was encapsulated in 100 mg of KBr pellet, in order to prepare translucent sample discs. The seed oil sample was loaded in FTIR spectroscope (Shimadzu, 8400S), with a scan range from 500 to 4000 cm^{-1} with a resolution of 4 cm^{-1}.

Results

The GC-MS characterization of seed oil extract of *C. nucifera* was identified and presented in Table 1 and Figure 1. Totally, eight major chemical compounds were identified such as Octasiloxane,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl. (0.21%)., 3, Benzodioxole, 5,5' (tetrahyd...., (50.96%)., Pyridine, 1,2,3,6-tetrahydro-1-m.....,(2.04%) 2-Ethylacridine, (5.51%)., Piperonylcyanoacetic acid hydrazide, (14.18%)., 2-Methyl-7-phenylindole (4.72%)., Acetamide, N-(4-fluorophenyl)-2,....(9.80%)., and .gamma.-sitosterol (12.57%) in the seed oil extract of *C. nucifera*. The identification of the phytochemical compounds was confirmed based on the retention time, peak area, molecular formula and molecular weight.

Table 1: GC-MS analysis of seed oil extract of *Cocos nucifera*

S. No.	Retention Time	Area	Compounds	Formula	Molecular weight
1	16.156	0.21	Octasiloxane,1,1,3,3,5,5,7,7,9,9,11,11,13, 13,15,15-hexadecamethyl-	$C_6H_{48}0_7SI_8$	577.20
2	16.403	50.96	1,3-Benzodioxole, 5,5'-(tetrahyd...	$C_{21}H_{22}0_6$	370.4
3	16.745	2.04	Pyridine, 1,2,3,6-tetrahydro-1-m...	$C_9H_{15}NO$	153.22
4	17.210	5.51	2-Ethylacridine	$C_{15}H_{13}N$	207.27
5	17.864	14.18	Piperonylcyanoacetic acid hydrazide	$C_8H_8N_20_3$	180.16
6	18.105	4.72	2-Methyl-7-phenylindole	$C_{15}H_{13}N$	207.27
7	18.440	9.80	Acetamide, N-(4-fluorophenyl)-2,...	$C_{11}H_{14}FNO_2$	211.23
8	20.571	12.57	.gamma.-Sitosterol	$C_{29}H_{50}O$	414.70

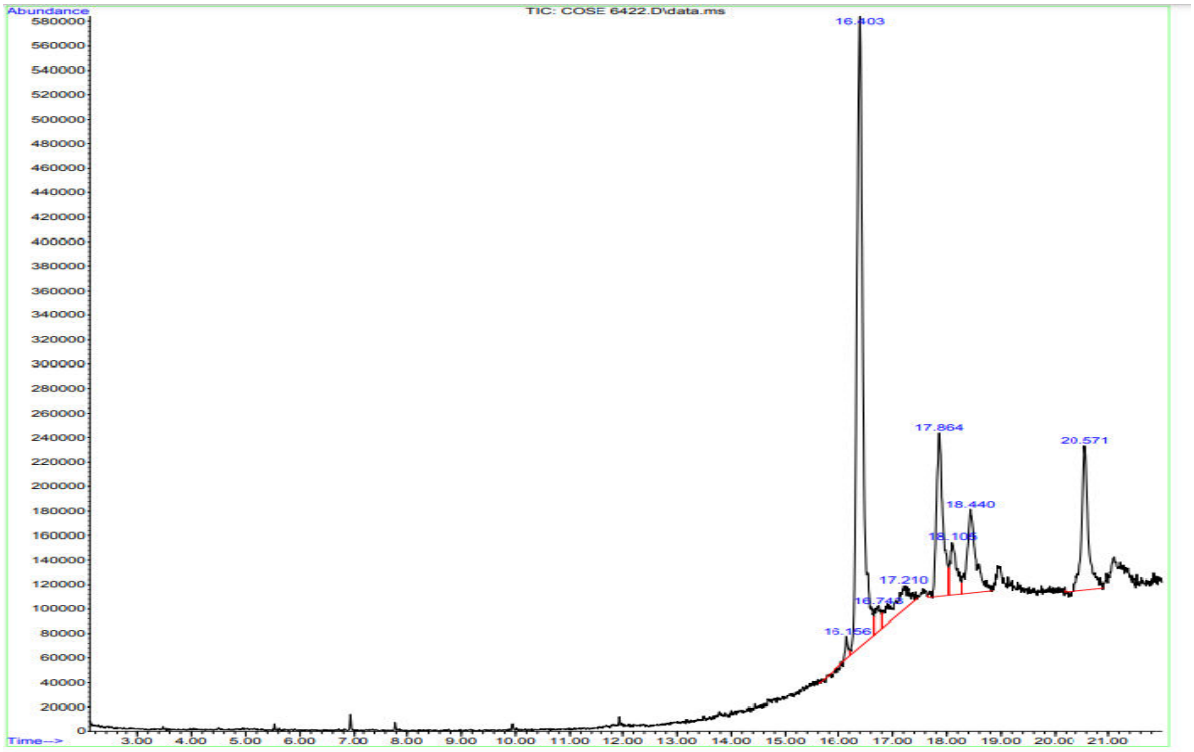

Fig. 1: GC-MS analysis of seed oil extract of *Cocos nucifera*.

Table 2: Functional groups of the components of seed oil extract of *Cocos nucifera* by FTIR

Sl. No.	Absorption (cm^{-1})	Functional Groups	Compounds	Intensity
1	722.29	C=C bending	Alkene	Strong
2	1109.96	C-O Stretching	Secondary alcohol	Strong
3	1155.28	C-O Stretching	Tertiary alcohol	Strong
4	1236.29	C-O Stretching	Alkyl aryl ether	Strong
5	1746.42	C=O Stretching	Esters	Strong
6	2731.02	C-H Stretching	Aldehyde	Medium
7	2852.52	N-H Stretching	Amine salt	Strong, broad
8	2959.56	O-H Stretching	Carboxylic acids	Strong, broad
9	3649.07	O-H Stretching	Alcohols	Medium, Sharp

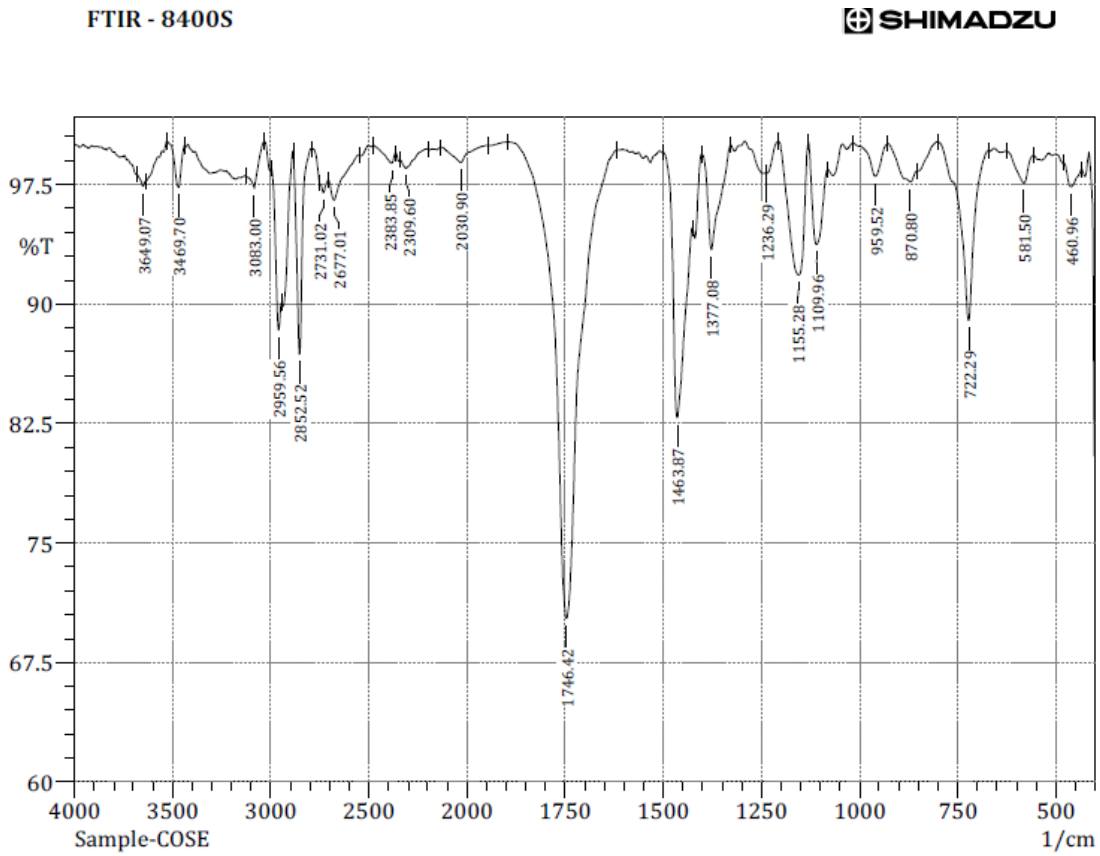

Fig. 2: FT-IR spectrum of seed oil extract of *Cocos nucifera.*

FTIR analysis of seed oil extract of *C. nucifera* was carried out and presented in Figure 2. The compounds indicated show the band at 3649.29, 2959.56, 2852.52, 2731.02, 1746.42, 1236.29, 1155.28, 1109.96 and 722.29 cm^{-1}. The broad band at 3649.29 cm^{-1} OH stretching in alcohol groups. The presence of peaks at 2959.56 cm^{-1} and 2852.52 cm^{-1} corresponding to the O-H stretch carboxylic acids and N-H stretch of amine salts. The band at 2731.02 cm^{-1} to assign the C-H stretch aldehyde. The peak at 1746.42 cm^{-1},1236.29 cm^{-1} and 1155.28 cm^{-1} in C=O stretch esters, C-O stretch alkyl aryl ether, and tertiary alcohol. The peaks at 1109.96 cm^{-1}, and 722.29cm^{-1} were observed to the C-O stretching secondary alcohol, C=C bend alkene, respectively (Fig. 2).

Discussion

The essential seed oil extract interferes with the basic metabolic, biochemical, physiological, and behavioural functions of arthritis, observes essential rapid action against inhalation or neurotoxic action, and there is evidence of interference (Enan, 2005). According to Khan *et al.* (2021), octasiloxane, 1, 1, 3, 3, 5, 5, 7, 7,9, 9, 11, 11, 13, 13, 15, 15-hexadecamethyl (Kumaradevan et al., 2015) and 2-ethylacridine (Husseinnihashemi et al., 2015) have antimicrobial and antioxidant activities. Also, 2-methyl-7-phenylindole was identified in an ethanolic root extract of *Plumbago zeylanica,* and the extract exhibited antimicrobial activity (Ajayi *et al*., 2011).

El-Sawi and Mohamed (2002) previously reported that 21 compounds were identified in the herb and seed oils, accounting for 90.2% and 95.6% of the total amounts, respectively. GC-MS analysis of the seed oil extract of *C. nucifera* revealed compounds toxic to pests and parasites.

FTIR is a recently well-accepted method for the identification of bioactive compounds because it offers simple product sampling and high-speed analysis. FTIR spectroscopy enables molecular imaging of complex plant samples, allowing identification and characterization of molecular components of biological tissues (Christian, 2014). FTIR spectroscopy has proven to be reliable and sensitive method for the detection of biomolecular composition. Similar results were observed by Chandran (2014), Chandran (2021) and Ramya *et al*. (2022).

Conclusion

Essential seed oils of plants containing volatile compounds is known to exhibit larvicidal, insecticidal, and anti-arthritic properties. These plant seed oils may be a useful source of compounds used in the control of arthropods of agricultural, medical and veterinary importance. The fatty acids of coconut oil provide a high percentage of repellent against mosquitoes, insects, ticks, mites, sandflies and stinging flies. These compounds of coconut seed oil extract give longer protection against insects feeding blood than any other known natural repellent. It has antibacterial, anti-inflammatory, antiviral and antifungal effect and also provides extra moisture to the skin. Plant seed oils may serve as a suitable alternative to synthetic antagonists in the future as they are relatively eco-friendly, safe, inexpensive and readily available in many parts of the world.

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