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LC-MS ANALYSIS OF PHYTOCONSTITUENTS IN AQUEOUS EXTRACT OF *Cocos nucifera* Linn. FLOWERS FROM SOUTHERN INDIA

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ABSTRACT

Cocos nucifera Linn. is a tropical tree grown in various parts of the world. The different parts of *Cocos nucifera* are used for food and medicinal purposes. This work aimed to determine and characterize the phytoconstituents in the aqueous extracts of Cocos nucifera flowers. The fresh flowers of *Cocos nucifera* Linn. were collected from southern India. The aqueous extraction of the plant material and the identification and characterization of plant material were performed. 39 compounds were identified and characterized by Liquid-chromatography mass-spectrometry. The major compounds were Nicotiflorin, Myristoyl glycerol, Glucofrangulin B, Valiolone Swainsonine, etc. These bioactive compounds in the *Cocos nucifera* contribute to the pharmacological activities and this can have the promising prospect in drug development.

Keywords: *Cocos* Nucifera, Glucofrangulin B, Myristoyl Glycerol, Nicotiflorin, LC-MS

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INTRODUCTION

Cocos nucifera or coconut palm is a tree usually grown in tropical places. Almost all the parts of the tree, i.e. fruit, oil, leaves, flowers, and roots are used for food as well as medicine. Traditional Ayurvedic medicine widely uses products from cocos nucifera in their formulations. Coconut oil is widely used as cooking media and used for the cosmetic applications. The nutritional status of coconut includes a high amount of saturated fat mainly medium chain saturated fatty acids, a trace amount of monounsaturated and polyunsaturated fat, sodium, carbohydrate, protein, insoluble fiber, sodium, potassium, manganese, iron, copper, selenium etc. Alkaloids, triterpenes, flavonoids, phenols, leucoanthocyanidins, tannins, and steroids were identified in the coconut during the preliminary phytochemical screening.[1,2,3] Coconut is used therapeutically as a home remedy for various illnesses like diabetes, urinary tract infections, viral infections, dandruff, fungal infections, dermatitis, constipation, peptic ulcers, piles, etc.[4,5] The flowers of *Cocos nucifera* are used in ayurvedic formulations like "thenginpookkuladhilehyam" and it is used as a post-delivery tonic in south India.[6,7] There is inadequate scientific evidence to support the therapeutic benefit of *Cocos nucifera* flowers in the treatment of conditions that are claimed by the Indian traditional system of medicine. Pharmacological studies in cocos nucifera flowers across the world revealed activities like anti-inflammatory, anticancer, antidiabetic, antimicrobial, antiepileptic, and antioxidant. In this study, the phytochemical screening was performed in an aqueous extract of cocos nucifera Linn. Using LC-MS method of analysis.[3,4]

EXPERIMENTAL

Plant Collection

The flowers of *Cocos nucifera* were collected from Kannur district, Kerala (India). The collected Cocos nucifera flowers were dried under shade, powdered, and sieved. Authenticated by Dr. Sreeja. P, Taxonomist and Assistant Professor from the Department of Postgraduate Studies and Research in Botany, Taliparamba, India. A voucher specimen was prepared and submitted to the department for future reference.

Preparation of Aqueous Extract of *Cocos nucifera* Flowers

The aqueous extraction of cocos nucifera flowers was done using the Soxhlet extraction method by weighing 25 grams of shade-dried powder in 150 mL of water for 24 hours. After decantation, the supernatant was filtered and evaporated under vacuum using a rotary evaporator.

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Preliminary Phytochemical Screening

Initial qualitative phytochemical investigations were carried out to evaluate the various chemical components found in the aqueous extract of the *Cocos nucifera* flower, including saponins, glycosides, tannins, and alkaloids.

LC-MS Analysis

LC/MS analysis was done using Agilent 6530C Q-TOF LC/MS system with HPLC 1260 Infinity II Prime LC series. The separation was done with a C-18 reverse-phased column (Agilent poroshell 120 EC-C8 µm, 3.0×150 mm) with a mobile phase that consists of Acetonitrile (A) and 0.1 % Ac water (B) in a gradient elution as follows:

Time (min)	A (%)	B (%)
2.00 min	10.00%	90.00%
6.00 min	20.00%	80.00%
10.00 min	30.00%	70.00%
14.00 min	40.00%	60.00%
20.00 min	50.00%	50.00%

ESI ionization technique was employed in negative mode and the general MS parameters were optimized as Nebulizer: 40 psi; source temperature: 325°C; Nitrogen flow: 10L/min; jet stream sheath temperature: 345°C.The total ion chromatogram was extracted using Agilent Mass Hunter software (version 10).

RESULTS AND DISCUSSION

The LC-MS result shows 44 peaks (Fig.-1) in the chromatogram and out of 44 peaks, 39 peaks were identified and characterized by comparing the mass spectra of individual compounds using mass hunter software. The major compounds with molecular structures are given in Table-1. The retention time, molecular mass, and scores of the individual compounds are given in Table-2. The major phytochemicals identified are nicoriflorin, swainsonine, Valiolone, Glucofrangulin B, Caffeyl alcohol, Myristoyl glycerol, Multifidol, and Pseudoprotodioscin[7,8]. The use of cocos nucifera flowers in the treatment of various ailments in traditional systems of medicine was not scientifically evaluated and the identification and characterization of phytoconstituents may boost further studies for predicting the different pharmacological actions.[9,10] Nicotiflorin is a flavonoid, and kaempferol derivative were evaluated for its potent antiglycation and neuroprotective effect. It is also evaluated for its anti-inflammatory and endothelial protective effects. Valiolone is a cyclitol and it is used for the synthesis of antidiabetic drugs, acarbose, and voglibose. Swainsonine identified in cocos nucifera has antitumor activity. Swainsonine reduces the damage to bone marrow cells and it has a protective effect on chemotherapy-induced thrombocytopenia.[11]

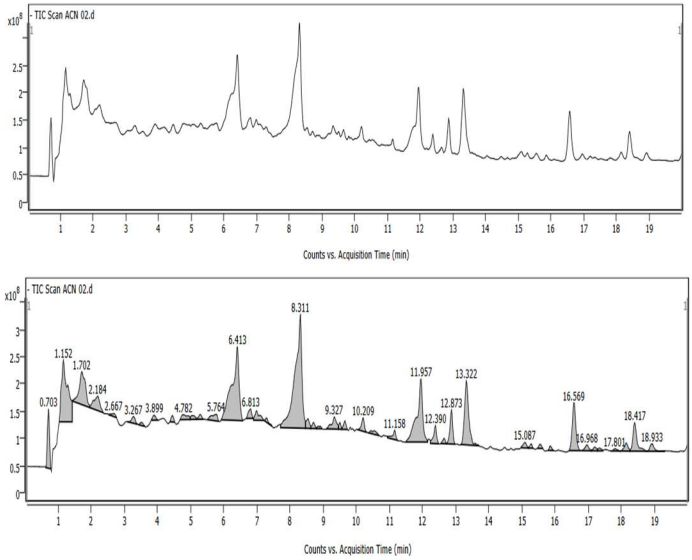
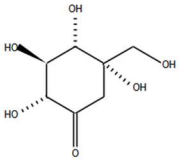
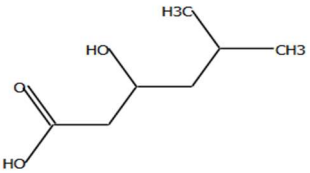
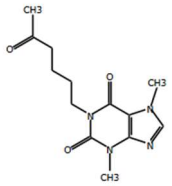
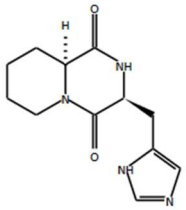
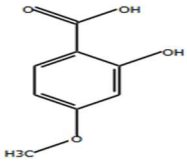
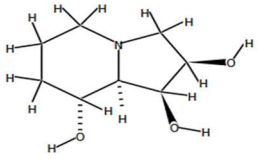
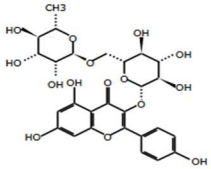
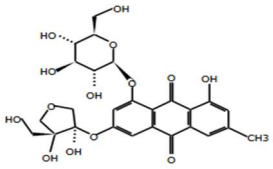
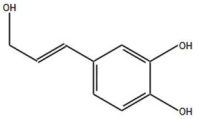
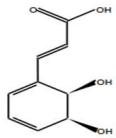
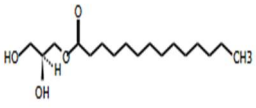
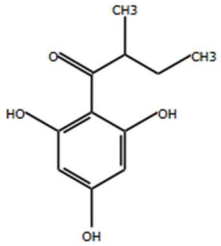


Fig.-1: LC-MS Chromatogram of Aqueous Extract of *cocos nucifera* Linn. Flowers

Glucograngulin B is an anthraquinone glycoside and has antioxidant, antitumor, and antifungal activity.[12] Thus, the results of the LC-MS ANALYSIS of cocos nucifera flower aqueous extract indicating the presence of phytoconstituents helps to gain insight into the various medicinal properties that are claimed by the traditional Indian system of medicine[13, 14].

Table-1: Molecular Structures of Identified Compounds

Valiolone		3-Hydroxyisoheptanoic acid	
Pentoxifylline		Histidylproline diketopiperazine	
4-Methoxy salicylate		Swainsonine	
Nicotiflorin		Glucofrangulin B	
Caffeyl alcohol		cis-3-(3-Carboxyethenyl)-3,5-cyclohexadiene-1,2-diol	
Myristoyl glycerol		Multifidol	

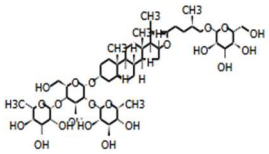
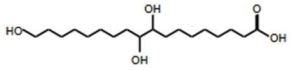
Pseudoprotodioscin		Phloionolic acid	

Table-2: LC-MS Results of Identified Compounds

Compound	Retention time	Molecular weight	Score
Valiolone	0.703	192.060	96.66
Pentoxifylline	2.184	278.137	95.27
4-Methoxy salicylate	3.267	168.042	97.30
Nicotiflorin	3.899	594.160	96.09
Caffeyl alcohol	5.281	166.060	97.02
Myristoyl glycerol	9.327	302.246	97.33
Pseudoprotodioscin	18.41	1030.53	95.22
Histidylproline diketopiperazine	2.667	248.127	96.46
Swainsonine	3.500	173.106	96.10
Glucofrangulin B	5.764	564.149	96.87
cis-3-(3-Carboxyethenyl)-3,5-cyclohexadiene-1,2-diol	8.311	182.05	97.18
Multifidol	13.322	210.090	96.45
Phloionolic acid	12.873	332.257	95.96

CONCLUSION

It is concluded that the LC-MS analysis data in the study may boost the further study of *Cocos nucifera* on the scientific authentication of traditional knowledge for the treatment of various ailments.

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CONFLICT OF INTERESTS

There is no conflict of interest for the writers with the content.

AUTHOR CONTRIBUTIONS

All the authors contributed significantly to this manuscript, participated in reviewing/editing, and approved the final draft for publication. The research profile of the authors can be verified from their ORCID IDs, given below:

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