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GC–MS Characterization of Volatile Compounds and Anti Inflammatory Activity of the Fruit Rind of *Baccaurea courtallensis*, an Endemic Species of the Western Ghats

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Abstract

Baccaurea courtallensis, an underutilised endemic species of fruit bearing plant in the Western Ghats contains variety of phytochemicals. The objective of the present study was to identify the volatile molecules in the fruit rind and evaluate its anti-inflammatory activity. The dried fruit rind powder and extract made using hexane and ethanol were characterised using Solid Phase Microextraction-Gas chromatography-Mass spectroscopy technique (SPME-GCMS).The experiment identified the presence volatile and semi volatile compounds such as organic acids, fatty acids, furans, and sesquiterpenes. The major compounds detected in hexane extract were ar-curcumene and ar-turmerone while major compound in ethanol extract was acetic acid. In addition to this, dodecanoic acid, tridecanoic acids tetradecanoic acids, 4-tert-butylcyclohexyl acetate, cis-3 hexanal and furfural were also detected. The hexane extract was evaluated for anti-inflammatory effect by bovine serum albumin (BSA) denaturation assay. The extract showed remarkable anti-inflammatory activity (IC_{50} - 121.02 µg/ml). The detected antiinflammatroy activity may be credited to the presence of sesquiterpenes ar-turmerone and Ar-curcumene. The observations suggest that the B. courtallensis fruit rind extract is an encouraging source of phytochemical compounds with biological activites and it has the potential in nutraceutical as well as pharmaceutical industries.

Keywords

Baccaurea courtallensis, Endemic Species, Fruit Rind, GC–MS Characterization, Western Ghats.

INTRODUCTION

Natural products produced by plants are significant sources of pharmaceutical and nutraceutical ingredients due to the presence of versatile structures and wide range of biological activities. Fruits are main source of phytochemicals. Now a days underutilised fruits are in attention owing to the presence of useful phytochemicals which have important biological activities. Furthermore, fruit rinds, which are considered as waste materials, are creating interest as they contain volatile as well as non-volatile secondary metabolites which are having high degree of biological potential like antioxidant, anti-inflammatory and anticancer activities [1, 2].

There is growing trend in the research of phytochemical composition on endemic species of plants in biodiversity spot of Western Ghats [3, 4]. *B. courtallensis* is a fruit bearing tree belonging to Phyllanthacea family. It is mainly grown in the Western Ghats region which is renowned as a world's one of the richest biodiversity spot. The fruit of these plants were consumed by the traditional communities in the nearby areas of Western Ghats for different illnesses [5, 6]. Even though the fruit had shown its nutraceutical and ecological relevance, there is no adequate studies are available on the phytochemical profile as well as bioactivities of *B. courtallensis*. The fruit rinds commonly considered as waste may contain lots of phytocompounds which might be having significant pharmacological activities

Volatile compounds are significant class of natural compounds which add to the aroma and taste of plant products. Many fruits are reservoirs of volatile compounds. Different classes of terpenes, esters, ketones and hydrocarbons are examples of some volatile compounds from plants. Many volatile molecules originated from plants showed anti-inflammatory activity [7]. The reduction of inflammation might involve mechanisms like controlling mediators of inflammation, inhibiting enzymes which generates pro-inflammation, decreasing cytokine production, and lowering oxidative stress. As prolonged inflammation might lead to diabetes, arthritis, heart diseases and cancer, the research for finding out natural compounds with anti-inflammatory activity will be promising in pharmaceutical as well as nutraceutical fields.

Gas Chromatography-Mass spectroscopy (GC-MS) is advanced and most reliable method for the identification of volatile and semi volatile compounds of plant origin. This method involves quick separation using chromatography and spectral characterisation using mass to charge ratio of the compounds. This technique helps to profile the complex phytochemical mixture of plant extracts and correlating these phytochemical compounds with the biological activities [8].

There are little studies available for the biological activities of the phytochemicals from different Baccaurea species [9, 10]. However, no studies are available for the characterisation of volatile compounds and anti-inflammatory activity of fruit rind of *B. courtallensis*. The current research about this particular endemic species might bring a significant impact in the field of natural compounds for pharmaceutical application and also in sustainable promotion of resources from biodiversity region like Western Ghats.

The objective of the current study is to identify the volatile molecules existing in the fruit rinds of *B. courtallensis* using GC- MS and to investigate its anti-inflammatory activity by in vitro assay of the fruit rind and its extracts. The investigation will correlate the identified volatile compounds with anti-inflammatory activity and provide scientific evidence for using this as nutraceutical or pharmaceutical product.

MATERIALS AND METHODS

Collection of Fruits

The fruits were collected from Vannappuram, Idukki with the help of local people. The fruits were cleaned with water after removing the damaged ones, and the seeds were removed from the fruit rinds.

Drying of the Fruit Rinds

The fruits were dried using continuous hot air drier at 75^0C temperature for 3 hours to reach the moisture level of less than 15%. The dried material was powdered and taken directly for analysis. It was also taken for solvent extraction

Solvent Extraction

400 ml Hexane was added to 100g fruit rind powder taken in separating funnel. Occasional circulation was given for one hour. The miscella was collected to a round bottom flask. The same process repeated for 4 times. All the washes were collected and filtered using filter paper to remove any undissolved materials. The solvent distilled of from the miscella using a rotary evaporator to get a dry extract. The same procedure was repeated with ethanol also.

GC- MS Characterisation

Sample Preparation

1g sample was added into 20 mL vial sealed with a PTFE-coated silicone septum and analysed by SPME-GC MS. To identify the volatile and semi volatile compounds, retention indices were calculated using a homologous series of n-alkanes as a reference. The mass spectra fragmentation patterns were compared to those in the literature and mass spectra libraries (Flavours and Fragrances of Natural and Synthetic Compounds, 2014; National Institute of Standards and Technology 2014). The chemicals that demonstrated a mass spectral correlation accuracy of more than 90% with library patterns formed the basis of the identification criteria used.

GC, MS & SPME conditions and parameters

The samples were analysed by GC-MS (Agilent 5977A), equipped with GC-7890B and 7693 Auto Sampler, electron impact (EI) mode (electron energy=70eV) with a scan range of 35-450 amu and a scan rate of 3.0 scans/s, and GC-MS solution software. Two capillary columns HP-Innowax (19091N-133, Agilent), 30m length, 250µm inner diameter, 0.25µm thickness were used for separation of the components with flow of 1.6ml/min for Helium. Temperature program of the oven is given table 1.

Table 1: Temperature Program of Oven

Oven temperature	Rate	Hold time(minutes)
50^0C	-	1
50^0C -70^0C	13^0C/minute	0
70^0C -110^0C	25^0C/minute	0.1
110^0C -145^0C	35^0C/minute	4
145^0C -220^0C	8^0C/minute	5
220^0C -250^0C	5^0C/minute	6

The total run time was 35.6 min. Injector temperature for MS is 250^o C. The MS Ion source and MS quad temperature were 230^o C and 150^o C. SPME fibre assembly (50/30 micro meter DVB/CAR/PDMS, Stableflex (Part no:57328-U) and needle size (24 ga) conditioned by inserting them into the GC injector according the supplier's instructions summarized. 1g taken in 20 mL vial sealed with a PTFE-coated silicone septum was analysed by SPME-GC MS. Then the vials were placed in an aluminium thermostated block at 100° C to reach the equilibrium with the headspace. The SPME fibre was subjected to the sample's headspace at 100°C for 10 minutes after the equilibrium time (the extraction time). The next step was to thermally desorb the fibres at the specified temperature for 15 minutes by inserting them directly into the GC's injector port.

Anti-inflammatory activity by BSA Denaturation Assay

Protein denaturation results loose of biological activities of protein molecules. Rheumatoid arthritis, diabetes, and cancer are inflammatory diseases that have been linked to protein denaturation. Hence, substances that can stop proteins from denaturing might potentially aid in the prevention of inflammatory disorders [11]. 100 µl of each sample (5, 10, 50, 100 and 500 µg/ml) is mixed with 45µl (0.4 % w/v) tris buffer saline (pH 6.4) bovine serum albumin and taken as test and distilled water instead of sample with above mixture was considered as control. Afterward, the mixtures were heated at 37°C for 20 min and 70°C for 5 min. After cooling 250 µl of phosphate buffered saline was added. Absorbance was noted at 660 nm.

Percentage of inhibition was calculated using the following formula:

$$\%\, Inhibition \;=\left(\frac{OD\ of\ control - OD\ of sample}{OD\ of\ control}\right) x100$$

Where, O.D is the Optical density

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RESULT AND DISCUSSION

The present study characterised major volatile and semi-volatile phytochemical constituents present in *B. courtallensis* by looking at their retention time and mass fragmentation patterns. Compounds detected are terpenoids, hydrocarbons, and some organic acids. These results shed light on chemical composition of the extract which is not available till now. Figure 1 is a representative chromatogram of GCMS of *B. courtallensis* samples. It was observed that there is clear variation in the composition of volatile chemicals on analysing the fruit rind powder and extracts made using Hexane and ethanol using GC–MS.

Table 2 summarises the major phytochemical molecules present in the fruit rind and extracts made by hexane and ethanol.

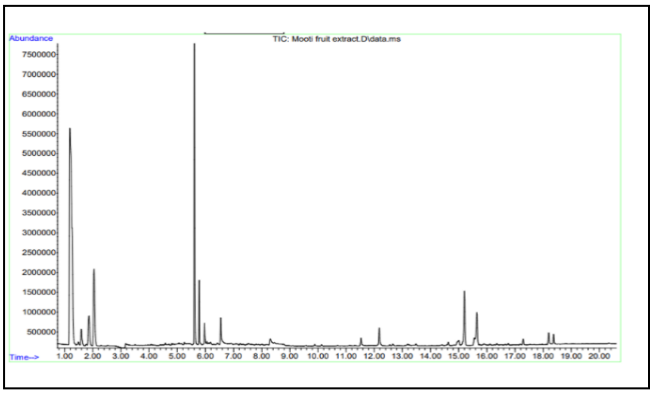

Figure 1: Representative GC-MS Total Ion Chromatogram of *B. courtallensis* sample

Table 2: Area% of Major volatile molecules in Fruit rind, hexane and Ethanol Extracts

			Fruit Rinds		Hexane Extract		Ethanol Extract	
No	Compound Identified	Molecular weight	RT	MS Area %	RT	MS Area %	RT	MS Area %
1	Acetic acid	60.05	5.621	19.732			5.613	52.025
2	Acetylfuran	110.11					6.055	0.463
3	Ar-Curcumene	202.34	8.573	6.361	8.586	18.392		
4	ar-turmerone	216.32	15.536	9.933	15.55	38.494		
5	cis-3-Hexenol	100.16					5.256	0.198
6	Dodecanoic acid	200.32	18.958	18.821				
7	Formic acid	46.03					5.975	2.902
8	Furfural	96.08	5.774	2.769			5.782	6.561
9	Furyl hydroxymethyl ketone	126.11					12.181	3.505
10	Maltol	126.11					11.532	1.738
11	Tetra decanoic acid	228.37	21.986	19.629			20.786	2.980
12	Triacetin	218.21			13.187	7.095		
13	Tridecanoic acid	214.34	21.819	13.356				
14	4-tert-Butylcyclohexyl acetate	198.31			6.491	22.910		
15	5-Hydroxy methylfurfural	126.11	18.358	8.357	18.368	5.953	18.373	1.714

The results showed that the rind powder consists of lipid derived compounds and sesquiterpenes. Medium chain fatty acids like dodecanoic acid (18.8%), tridecanoic acid (13.3%), and tetradecanoic acid (19.6%), and acetic acid (19.7%) were identified in the fruit rind powder. Sesquiterpenes commonly seen in turmeric such as aR-turmerone (9.9%) and ar-curcumene (6.3%) were also identified in the current study. Hexane extract showed ar-turmerone (38.5%) and ar-curcumene (18.4%) as the major compounds. Triacetin (7.1%) and 5-hydroxymethylfurfural (5.9%) were also identified in small percentage. As hexane is a highly nonpolar solvent, extracting volatile compounds would be easier with this solvent system. In contrast, the major compounds identified in ethanol extract showed a different chemical composition in which acetic acid (52.0%) was the major component. Furfural (6.5%) and formic acid (2.9%) were also identified in ethanol extract. As usual ethanol extracted the polar compounds including organic acids. The result showed different chemical profiles for different extracts and for fruit rind powder. The fruit powder contains both fatty acids and sequiterpenes. Hexane extracts contain more sesquiterpenes such as ar-curcumene and ar-turmerone and ethanol extract is composed of organic acids such as acetic acid.

The current study identified some important compounds, such as organic acids, fatty acids, furan derivatives, and sesquiterpenes in the fruit rind. The detected organic acids such as acetic acid, dodecanoic acid, tridecanoic acid and tetradecanoic acid are common plant metabolites found in fruit-derived materials [12]. Volatile compounds like cis-3-hexenol and some furan derivatives may add to the odour and antioxidant properties of the sample [13]. However, the way they were made might also be affected such as by drying or heating it. This is the first study that revealed the presence of sesquiterpenes, ar-turmerone and ar-curcumene in fruit rinds of *B. courtallensis*. This is consistent with the study GC–MS analysis of fruit peel extract of Musa species which also detected ar-turmerone as one of the major volatile constituents. The sesquiterpenes are mainly present in the fruit peels rather than pulp [14].

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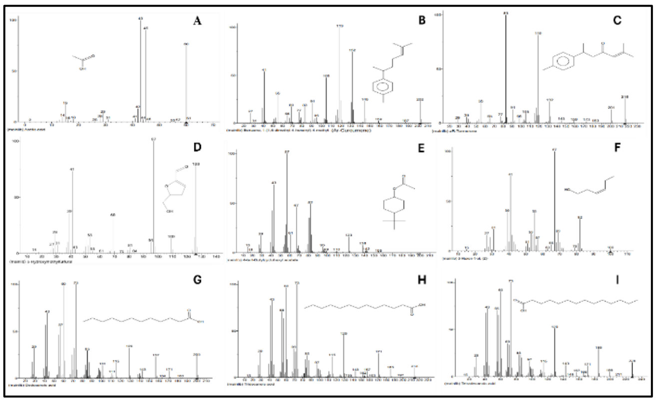

Figure 2: Mass Fragments of Major compounds of Hexane Extract of *B. courtallensis* (A) Acetic acid; (B) Ar-Curcumene; (C) ar-turmerone; (D) 5-Hydroxymethyl furfural; (E) 4-tert - Butylcyclohexyl acetate; (F) Cis 3-Hexen-1-ol (G) Dodecanoic acid; (H) Tridecanoic acid; (I) Tetra decanoic acid

Anti Inflammatory Activity Using BSA Denaturation Assay

Bovin Serum Albumin (BSA) denaturation assay was used to assess the anti-inflammatory potential of BCE extract. This is a well-known in vitro method for estimating the anti-inflammatory activity by measuring protein stabilization. This assay assesses the capability of for the inhibition of heat-induced protein denaturation, and indicating its capacity to reduce inflammatory reactions [15].

The fruit rind extract showed that protein denaturation was inhibited in the BSA assay in a way that depended on the concentration. The percentage of inhibition went up continuously from 3.78% to 66.53% when the concentration went up from 5 to 500 µg/mL. This shows that the substance protects proteins from being denatured by heat. Near to 100 µg/mL, there was a moderate inhibition, which is close to the half-maximal response. The IC_{50} value of 121.02 µg/mL reveals that the extract has anti-inflammatory power.

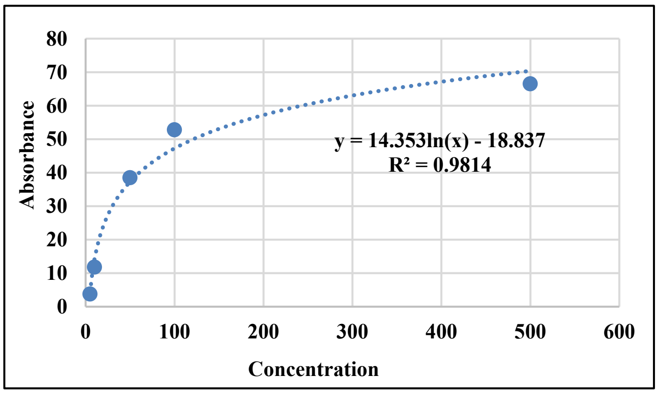

Figure 3: Graphical representation of BSA Denaturation study of the *B. courtallensis* fruit rind extract (IC_{50} = 121.02 µg/ml)

The IC_{50} value of 121.02 µg/ml is significant as the test is conducted in the crude extract. The anti-inflammatory activity of the extract can be interrelated to the presence of volatile compounds in the category of sesquiterpenes such as ar-turmerone and ar-curcumene. These molecules are widely recognised as antioxidant and anti-inflammatory agents [16-18]. Ar-turmerone is main pharmacologically active volatile component usually found in *Curcuma longa* is known for the suppression of inflammatory mediators such as TNF-α, IL-1β, IL-6, nitric oxide, cyclooxygenase through the inhibition of NF-κB and MAPK signalling pathways [19]. Ar-curcumene, a different sesquiterpene found in the fruit rind extract, also connected with anti-inflammatory and antioxidant effects. Experiments have illustrated that ar-curcumene inhibits oxidative stress, scavenges free radicals, and also diminishes inflammation [20]. Ar-curcumene may thus interact with ar-turmerone synergistically to enhance the protein stabilisation and anti-inflammatory effects observed in the present study.

CONCLUSION

The current study efficiently identified the volatile and semi volatile phytochemical compounds identified in the fruit rind of *B. courtallensis* using SPME-GC-MS technique. The anti-inflammatory potential of the hexane extract was demonstrated through BSA denaturation assay. The inferences confirmed distinctive phytochemical profiles in the fruit rind powder and solvent extracts, with the hexane extract revealing a high concentration of sesquiterpenes, including ar-turmerone and ar-curcumene, whereas the ethanol extract was rich in organic acids, particularly acetic acid. The hexane extract displayed a robust concentration-dependent result on protein denaturation, with an IC_{50} value of 121.02 µg/ml. This means that it has reasonable anti-inflammatory activity even when it is not purified. The biological activity observed may be linked with the occurrence of sesquiterpenes and other volatile compounds recognised for antioxidant and anti-inflammatory effects.

This study is a first time scientific report on the volatile composition and anti-inflammatory properties of *B. courtallensis* fruit rind, thus contributing important intuitions for future pharmacological and nutraceutical studies. Additional research concentrating on purification, isolation of active components, and in vivo studies is recommended to completely evaluate its therapeutic potential and possible industrial uses.

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