Available online on 15.04.2022 at http://jddtonline.info

Journal of Drug Delivery and Therapeutics

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Research Article

Phytochemical Screening, GCMS, FTIR profile of Bioactive Natural Products in the methanolic extracts of *Cuminum cyminum* seeds and oil

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Article Info:

Article History:

Received 17 March 2022
Reviewed 02 April 2022
Accepted 06 April 2022
Published 15 April 2022

Cite this article as:

Ramya S, Loganathan T, Chandran M, Priyanka R, Kavipriya K, Grace Lydial Pushpalatha G, Aruna D, Ramanathan L, Jayakumararaj R, Phytochemical Screening, GCMS, FTIR profile of Bioactive Natural Products in the methanolic extracts of *Cuminum cyminum* seeds and oil, Journal of Drug Delivery and Therapeutics. 2022; 12(2-s):110-118

DOI: http://dx.doi.org/10.22270/jddt.v12i2-s.5280

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Abstract

Seeds of cumin (*Cuminum cyminum* L.) are widely used as a spice for their distinctive aroma. *C. cyminum* have been used in traditional medicine to treat a variety of diseases. Literature presents ample evidence for biomedical activities of cumin which is attributed to its bioactive secondary metabolites - terpenes, phenols, and flavonoids. Besides, health effects of cumin seeds have been experimentally validated through phytochemical analysis depicting the presence of a wide array of bioactive secondary metabolites (BASMs) viz., alkaloid, coumarin, anthraquinone, flavonoid, glycoside, protein, resin, saponin, tannin and steroid. Pharmacological studies indicate that BASMs in seeds of *C. cyminum* exert antimicrobial, insecticidal, anti-inflammatory, analgesic, antioxidant, anticancer, antidiabetic, anti-platelet-aggregation, hypotensive, bronchodilatory, immunological, contraceptive, anti-amyloidogenic, anti-osteoporotic, aldose reductase, α-glucosidase and tyrosinase inhibitory effects. In the present study phytochemical screening, GCMS, FTIR profile of bioactive natural products from *C. cyminum* has been envisaged. Phytochemical screening revealed the presence of alkaloids, anthraquinones, carbohydrates, coumarins, flavonoids, glycosides, proteins, quinones, saponins, steroids, tannins and terpenoids. GC-MS analysis revealed the presence of 21 compounds, of which Cuminaldehyde was prominent. FTIR analysis showed the presence of a strong peak value for 15 compounds and medium peak value for 6 compounds. Many of the compounds in the list could be ADMET bioprospected for biomedical applications as natural drug leads.

Keywords: *Cuminum cyminum*; Cuminaldehyde; Bioactive Natural Products; GCMS; FTIR

INTRODUCTION

Drug development is a complicate, risky, and time-consuming process that can be divided into several stages, including disease-related genomics, target identification/ validation, lead discovery/ optimization, preclinical/ clinical trials[1]. During early stages of drug discovery, activities and specificities of candidate drug lead molecule is assessed at an early stage pharmacokinetics and late stage toxicity[2]. Practically, most of the time, withdrawal of a proven candidate drug lead in the final stage is ascribed to some undesirable efficacy/ safety in absorption, distribution, metabolism, excretion and toxicity (ADMET)[2,3].

Cook et al.[4] comprehensively reviewed the results of AstraZeneca's small-molecule drug projects from 2005 to 2010 based on a longitudinal study and pointed out that unacceptable safety and toxicity were the most important reasons for the failure of more than half of all projects. As with the development of drug discovery, it was realized that it is important to filter and optimize the ADMET properties for drugs at an early stage, which has been accepted and widely used to reduce the attrition rate in drug research and development. A Fail-Early-Fail-Cheap strategy is employed by many of the pharmaceutical companies[5].

Pharmacokinetics and toxicity assessments of preclinical drugs are of significant value in reducing failure rate of new chemical entities in clinical trials[6-8]. In recent years, in vitro and in vivo ADMET prediction methods have been widely used, but it is impractical to perform complex and expensive ADMET experiments on a large number of compounds[9,10]. Thus, *in silico* strategy to predict ADMET properties has become very attractive as a Cost-Saving-High-Throughput alternative to conventional experimental methods[11-17].

Since prehistoric times, humans have used natural products, such as plants, animals, microorganisms, and marine

organisms, in medicines to alleviate and treat diseases[18]. Natural products, which have evolved over millions of years, have a unique chemical diversity, which results in diversity in their biological activities and drug-like properties[19]. Those products have become one of the most important resources for developing new lead compounds and scaffolds[20,21].

World Health Organization (WHO) estimates that 4 billion people, 80 percent of the world population, presently use herbal medicine for some aspect of primary health care. Plant exhibit a wide range of pharmacological activities including antimicrobial, antioxidant, anticancer, hypolipidemic, cardiovascular, central nervous system, respiratory, immunological, anti-inflammatory, analgesic, antipyretic and many other pharmacological effects. In traditional medicine, cumin was used to treat hoarseness, jaundice, dyspepsia and diarrhoea. Seeds were used for stomachic, diuretic, carminative, stimulant, astringent and abortifacient properties[20-23].

Cumin (*Cuminum cyminum* L.) is an annual and herbaceous plant (Family: Apiaceae). It is a multipurpose plant species cultivated in the Middle East, India, China, and several Mediterranean countries, including Tunisia. Its fruit, known as cumin seed, is most widely used for culinary and medicinal purposes[24]. It is generally used as a food additive, popular spice, and flavouring agent in many cuisines. Cumin has also been widely used in traditional medicine to treat a variety of diseases. Pharmacological studies have proven that *C. cyminum* exerts antimicrobial, insecticidal, anti-inflammatory, analgesic, antioxidant, anticancer, antidiabetic, antiplatelet aggregation, hypotensive, bronchodilatory, immunological, contraceptive, anti-amyloidogenic, anti-osteoporotic, aldose reductase, α-glucosidase and tyrosinase inhibitory effects[23]. The medicinal parts were Cumin oil extracted from the ripe fruit and the ripe, dried fruit[25]. Phytochemical analysis of *C. cyminum* revealed that it contains alkaloid, coumarin, anthraquinone, flavonoid, glycoside, protein, resin, saponin, tannin and steroid[23].

Physicochemical characteristics

Moisture content: 8%, PH: 7.3, total ash: 7.5, acid insoluble ash: 18%, alcohol soluble extractive: 6.58%, water soluble extractive: 138% and ether soluble extractive: 11.44 ± 0.20 and 12.36 ± 0.23% in the wet and dry fruits. Crude protein 18.40 ± 0.16 and 19.88 ± 0.20%, crude fibres 21.82 ± 0.13 and 23.57 ± 0.13%, total carbohydrate 55.58 and 60.05% in the wet and dry fruits respectively[23]. Physical properties of the essential oil of cumin seeds: extraction percentage: 2.3-5.7 %, color: colourless or pale yellow, refractive index (20 ºC): 1.47-1.50, density (20 ºC): 0.90-0.94, alcohol solubility (80% v/v): 1:1.3-1:2, aldehyde percentage (Cuminaldehyde): 35-63%, acidity (Cuminic acid): 0.36-1.8, alcohol percentage (Cuminol): 3.5, carbonyl index: 9.32 and steric index: 19.24[23].

Chemical constituents

Phytochemical analysis showed that *C. cyminum* contained: alkaloid, anthraquinone, coumarin, flavonoid, glycoside, protein, resin, saponin, tannin and **steroid**. Nutrient contents of cumin (seeds) were included: calories 7.50, calories from fat 4.00, calories from saturated fat 0.28, protein (g) 0.36, carbohydrates (g) 0.88, dietary fibre (g) 0.22, total fat (g) 0.44, saturated fat (g) 0.04, monounsaturated fat (g) 0.28, polyunsaturated fat (g) 0.06, water (g) 0.16, Ash (g) 0.16, vitamin A (IU) 25.40, vitamin A (RE) 2.54, α-carotenoid (RE) 2.54, beta carotene (µg) 15.24, thiamin – B1 (mg) 0.02, niacin – B3 (mg) 0.10, niacin 0.10, vitamin C 0.16, vitamin E α 0.02, vitamin E (IU) 0.04, vitamin E (mg) 0.02, folate (µg) 0.20, vitamin K (µg) 0.11, calcium (mg) 18.62, copper (mg) 0.02, iron (mg) 1.32, magnesium (mg) 7.32, manganese (mg) 0.06, phosphorus (mg) 9.98, potassium (mg) 35.76, selenium (µg) 0.10, sodium (mg) 3.36, zinc (mg) 0.10, palmitic acid (g) 0.02, oleic (g) 0.28, linoleic acid (g) 0.06 and omega 6 fatty acids (g) 0.06 (79). Organic acids (aspartic, citric, malic, tartaric, propionic, ascorbic, oxalic, maleic and fumaric acids) were isolated from seeds of *Cuminum cyminum*[26]. Cumin fruits contained 2.5 to 4.5% volatile oil and 10% fixed oil (Table 1).

Major compounds in Turkish cumin (*Cuminum cyminum*) seed oil were cuminaldehyde (19.25-27.02%), p-mentha-1,3-dien-7-al (4.29-12.26%), p-mentha-1,4-dien-7-al (24.48-44.91%), γ-terpinene (7.06-14.10%), p-cymene (4.61-12.01%) and β-pinene (2.98-8.90%) . Cuminaldehyde, γ-terpinene, o-cymene, limonene and β-pinene were determined to be the major constituents of Syrian *C. cyminum*. The major compounds in cumin essential oil of Egyptian cultivars were cumin aldehyde (35.25%), tetradecene (12.25%), γ-terpenene (12%), β-ocimene (9.72%), p-mentha-2-en-ol (9%), α-terpinyl acetate (5.32%), α-terpinolene (3%), lmonine (0.5%), myrcene (0.2%), β-pinene (0.9%) and α-pinene (0.19%). Tunisian variety of *C. cyminum* contained cuminlaldehyde (39.48%), gamma-terpinene (15.21%), O-cymene (11.82%), beta-pinene (11.13%), 2-caren-10-al (7.93%), trans-carveol (4.49%) and myrtenal (3.5%) as major components[27]. However, it must be pointed out that in recent times, computational approaches in preclinical studies on drug discovery and development.

MATERIALS AND METHODS

Kingdom - Plantae; **Sub kingdom -** Viridiplantae; **Infra kingdom -** Streptophyta; **Super division** - Embryophyta; **Division** - Tracheophyta; **Sub division -** Spermatophytina; **Class -** Magnoliopsida; **Super order -** Asteranae; **Order -** Apiales; **Family -** Apiaceae; **Genus -** *Cuminum*; **Species -** *Cuminum cyminum*. **Common names** - Jiiraa (Jeera), Zeera (zira, ziira), safed ziiraa (Safed zira), Safed jiiraa (Safaid jeera)

Botanical Description of the plant - *Cuminum cyminum*

Plants – Herbs – usually 10–30(–50) cm tall; **Leaf**: Basal petioles 1–2 cm; sheaths lanceolate, margins white and membranous; blade 3–8 × 2–7 cm; ultimate divisions long-filiform, 15–60 × 0.4–0.7 mm. **Inflorescence**: Umbels many, 2–3 cm across; peduncles 3–10 cm; **Bracts** 2–6 (–8), linear or linear-lanceolate, 10–50 × 0.5–1.2 mm, unequal, entire or apex 2–3-fid, usually longer than the rays, margins membranous; rays (1–)3–6, 3–20 mm, rather stout, very unequal; **Bracteoles** 3–5, similar to bracts, 4–10 × 0.3–0.6 mm, very unequal, sometimes reflexed; umbellules 3–8-flowered; **Flowers**: pedicels 3–6 mm, stout, very unequal. **Calyx:** teeth 0.5–2 mm, longer than the styles. **Petals** ca. 1.4 × 1 mm. Fruit 5–7 × 1.6–2.8 mm; primary ribs short setulose, secondary ribs densely stellate setulose; **Fl**. and **Fr**. Feb–Jun–Sep.

Phytochemical Screening

The cumin seeds were purchased from the local market in Madurai. The methanolic extracts were subjected to chemical tests for the detection of different phytoconstituents using standard procedures[33].

Test for Phenols ($FeCl_3$ Test)

To 1 ml of the extract, 3 ml of distilled water followed by few drops of 10% aqueous Ferric chloride solution was added. Formation of blue or green colour indicates the presence of phenols.

Test for Flavonoids (Shinoda Test)

To 2 ml of the extract, 1 ml of 1% ammonia solution was added. Appearance of yellow colour indicates the presence of flavonoids.

Test for Tannins ($FeCl_3$ Test)

To 1 ml of the extract, 1 ml of 0.008 M Potassium ferricyanide was added and then add 1ml of 0.02 M Ferric chloride containing 0.1 N HCl. Appearance of blue-black colour indicates the presence of Tannins.

Test for Alkaloids (Wagner's Reagent Test)

Approximately, 1 ml of crude extract was mixed with 2 ml of Wagner's reagent. Reddish brown colour precipitate indicates the presence of alkaloids.

Test for Carbohydrates (Fehling's test, Benedict's test)

Fehling's test

Equal volume of Fehling A and Fehling B reagents were mixed together and then add 2ml of crude extract in it and gently boiled. A brick red precipitate appeared at the bottom of the test-tube indicates the presence of reducing sugars.

Benedict's test

1 ml of crude extract was mixed with 2ml of Benedict's reagent and boiled. A reddish brown precipitate was formed which indicates the presence of the carbohydrates.

Test for Proteins (Millon's Test, Ninhydrin Test)

Millon's test

1 ml of crude extract was mixed with 2ml of Millon's reagent; white precipitate appeared which turned red upon gentle heating that confirmed the presence of protein.

Ninhydrin test

1 ml of crude extract was mixed with 2ml of 0.2% solution of Ninhydrin and boiled. A violet colour precipitate was appeared suggesting the presence of amino acids and proteins.

Test for Cardiac glycosides (Keller-Kiliani test)

5 ml of extract was treated with 2 ml of glacial acetic acid containing one drop of ferric chloride solution. This was underlayed with 1 ml of concentrated sulphuric acid. A browning of the interface indicates a deoxy-sugar characteristic of carotenoids. A violet ring may appear below the brown ring, while in the acetic acid layer, a greenish ring may form just gradually throughout thin layer.

Test for Saponins (Foam Test)

2 ml of crude extract was mixed with 5 ml of distilled water in a test tube and it was shaken vigorously. Add some drops of olive oil. The formation of stable foam was taken as an indication for the presence of saponins.

Test for Coumarin (Sodium hydroxide Test)

10 % Sodium hydroxide was added to the extract and chloroform was added. Formation of yellow color shows the presence of Coumarin.

Test for Terpenoids (Salkowski test)

5 ml of extract was mixed with 2 ml of chloroform and 3 ml of concentrated sulphuric acid was carefully added to form a layer. A reddish brown coloration of the inter face was formed which indicates the presence of terpenoids.

Test for Steroids (Salkowski Test)

2 ml of acetic anhydride was added to 0.5 ml of crude extract containing 2 ml of sulphuric acid. The colour changed from violet to blue or green in samples indicates the presence of steroids.

Test for Quinones (Sodium hydroxide Test)

Diluted sodium hydroxide was added to the 1 ml of crude extract. Blue green or red coloration indicates the presence of quinones.

Test for Anthraquinones (Borntragers test)

0.5 g of extract was boiled with 10% hydrochloric acid for few minutes in water bath. It was filtered and allowed to cool. Equal volume of $CHCl_3$ was added to the filtrate. Few drops of 10% ammonia was added to the mixture and heated. Formation of rose – pink color indicates of n-hexane, chloroform, ethyl acetate and methanol of the presence of the anthroquinones.

Sample preparation and characterization

For phytochemical screening, 25 g of pulverized seeds were extracted with 125 mL of three solvents namely; methanol, distilled water and methanol/water (1:1) for 72 h. The plant extracts were filtered and concentrated using rotary evaporator under reduced pressure. Preliminary phytochemical analysis was carried out to test for the presence of tannins, saponins, flavonoids, alkaloids, anthocyanins, betacyanins, quinones, glycosides, cardiac glycosides, terpenoids, triterpenoids, phenols, coumarins, steroids and acids in all the three extracts following the standard test methods. Also, 10 g of each powdered plant material was extracted with methanol, distilled water and methanol/distilled water (1:1), respectively, for 72 h. The extracts were filtered and concentrated to 1 mL using BUCHI rotary evaporator under reduced pressure. Then, 1 mL of crude methanolic, water and methanol/ water extracts were taken for FTIR analysis, while 1 mL methanolic extracts were taken in amber GC vials for GC–MS analysis.

GC-MS Analysis

Phyto-components were identified using GCMS detection system as previously with minor modification, whereby portion of the extract was analyzed directly by headspace sampling. GCMS analysis was accomplished using an Agilent 7890A GC system set up with 5975C VL MSD (Agilent Technologies, CA, and USA). Capillary column used was DB5MS (30 m × 0.25 mm, film thickness of 0.25 µm; J&W Scientific, CA, USA). Temperature program was set as follows: initial temperature 50°C held for 1 min, 5°C per min to 100°C, 9°C per min to 200°C held for 7.89 min, and the total run time was 30 min. The flow rate of helium as a carrier gas was 0.811851 mL/min. MS system was performed in electron ionization (EI) mode with Selected Ion Monitoring (SIM). The ion source temperature and quadruple temperature were set at 230°C and 150°C, respectively. The identification of components was based on retention time on the capillary column and matching the GC-MS with the National Institute of Standards and Technology (NIST) library[34].

Fourier Transform Infrared Spectroscopy (FTIR) Analysis

The extracts were analyzed using Agilent Cary 630 FTIR spectrometer equipped with Micro-lab PC software with ATR sampling unit with a resolution of 8 cm^{-1} and scan range of 4000 cm^{-1} to 650 cm^{-1}.

RESULTS

Phytochemical Screening

In the present study, screening for Alkaloids (Wagner's reagent Test) exhibited + result; Anthraquinones (Borntragers Test) showed + result; Carbohydrates (Fehling's test, Benedict's test) indicated ++ result; Coumarins (Sodium hydroxide Test) showed + result; Flavonoids (Shinoda Test) showed ++ result; Glycosides (Keller-Kiliani Test) showed + result; Phenol (FeCl3 Test) showed - result; Proteins (Millon's Test, Ninhydrin Test) indicated ++ result; Quinones (Sodium hydroxide Test) revealed + result; Saponins (Foam Test) showed + result; Steroids (Salkowski Test) presented + result; Tannins FeCl3 Test) showed ++ result; Terpenoids (Salkowski Test) exhibited ++ result (Table 2).

A total of 21 compounds were detected in the GCMS analysis, at RT interval of 4.363 α-Terpinene ($C_{10}H_{16}$) was detected with a MW of 136 in the seeds and oil samples with a percentage peak area of 9.74, 0.0; at RT interval of 4.716 α-Thujene ($C_{10}H_{16}$) was detected with a MW of 136 in seeds and oil samples with a percentage peak area of 0.0, 0.29; while at RT interval of 4.842 α-Pinene ($C_{10}H_{16}$) was detected with a MW of 136 in both the seeds and oil samples with a percentage peak area of 0.12, 0.92; similarly, at RT interval of 5.574 β-Pinene ($C_{10}H_{16}$) was detected with a MW of 136 in the seeds and oil samples with a percentage peak area of 2.1, 0.0; while at RT interval of 5.668 Santolina triene ($C_{10}H_{16}$) was detected with a MW of 136 in both the seeds as well the oil samples with a percentage peak area of -, 11.52; at RT interval of 5.747 α-Myrcene ($C_{10}H_{16}$) was detected with a MW of 136 in the seeds as well as in the oil samples with an average peak area of 0.3, 0.71.

Likewise, at an interval of 6.344 RT ρ-Menthatriene ($C_{10}H_{14}$) was detected with a MW of 134 in the seeds and oil samples with a percentage peak area of 18.77, 24.63; at RT interval of 6.968 Terpinolene ($C_{10}H_{16}$) was detected with a MW of 136 in the seeds and oil samples with a percentage peak area of 15.95, 16.51; at RT interval of 8.614 Limonene ($C_{10}H_{16}$) was detected with a MW of 136 in the seeds and oil samples with a percentage peak area of 0.19, 0.0; at RT interval of 8.752 4-Terpineol ($C_{10}H_{18}O$) was detected with a MW of 154 in the seeds and oil samples with a percentage peak area of -, 0.3; at RT interval of 8.761 1,8-cineole ($C_{10}H_{18}O$) was detected with a MW of 154 in the seeds and oil samples with a percentage peak area of 0.46, 0.14.

At an interval of 9.431 (RT) Benzaldehyde ρ-isopropyl ($C_{10}H_{12}O$) was detected with a MW of 148 in the seeds and oil samples with a percentage peak area of 1.27, 0.0; while at RT interval of 9.96 Cuminaldehyde ($C_{10}H_{12}O$) was detected with a MW of 148 in the seeds and oil samples with a percentage peak area of 32.59, 31.65; at RT interval of 10.577 Myrtenal ($C_{10}H_{14}O$) was detected with a MW of 150 in the seeds and oil samples with a percentage peak area of 8.74, 1.78; at RT interval of 10.248 cis-Ocimene ($C_{10}H_{14}O$) was detected with a MW of 150 in the seeds and oil samples with a percentage peak area of 10.26, 4.14; at RT interval of 15.881 α-Terpinen-7-al ($C_{10}H_{14}O$) was detected with a MW of 150 in both the seeds and oil samples with a percentage peak area of 3.98, 4.59;

At and interval of 15.965 (RT) o-Cymen-7-ol was detected with a MW of 150 ($C_{10}H_{14}O$) in the seeds and oil samples with a percentage peak area of 0.0, 1.11; at RT interval of 16.072 γ-Terpinen-7-al was detected with a MW of 150 ($C_{10}H_{14}O$) in the seeds and oil samples with a percentage peak area of 1.95, -0.0; at RT interval of 16.186 Thymol was detected with a MW of 150 ($C_{10}H_{14}O$) in the seeds and oil samples with a percentage peak area of 0.0, 0.35; at RT interval of 16.797 4-Hydroxy-cryptone was detected with a MW of 154 ($C_{10}H_{14}O$) in the seeds and oil samples with a percentage peak area of 1.68, 0.38; at RT interval of 20.047 4-(1-methylethyl)-benzoic acid was detected with a MW of 164 ($C_{10}H_{14}O_2$) in the seeds and oil samples with a percentage peak area of 0.97, 1.43 respectively (Table 3).

FTIR analysis showed the presence of a strong peak value (cm^{-1}) of 700.998 in the reference range of 610-700 with functional group -C=C-H ;C-H bend indicate the presence of Alkynes in the compound; while a peak at 3543.56 with in the reference range of 3500-3700 with O-H (H-bonded), usually broad indicates the presence of Alcohols & Phenols in the compound; similarly, peak at 2873.42 with in the range of 2850-3000 with CH_3, CH_2 & CH bonds shows that alkanes are present in the compound; while a peak at 2856.06 in the range of 2850-3000 with CH_3, CH_2 & CH_2 or 3 bands indicates the presence of alkanes in the compound; however, peak at 2141.56 in the range of 2100-2260 with C-C triple bond indicates alkynes in the compound; a peak at 1716.34 in the range of 1706-1720 with C=O stretching, indicates the presence of a dimer Carboxylic acid in the compound; while peak at 1646.91 in the range of 1640-1690 with a C=N stretching depicts the presence of Imine/ Oxime in the compound; a peak at 1530.24 (range 1500-1550) with N-O stretching depicts the occurrence of a Nitro-compound; while a peak at 1454.06 (range 1400-1500) with C-C Stretch indicates presence of aromatic compound;

At a peak value of 1436.71(cm^{-1}), in the reference range of 1395-1440 a O-H bend was recorded indicating the presence of carboxylic acid in the compound; similarly, at a peak value of 1408.75 within the reference range of 1380-1410 a S=O stretching was recorded indicating the presence of sulfonyl chloride in the compound; while at a peak value of 1070.3 within the reference range of 1030-1070 a S=O was recorded indicating the presence of sulfoxide in the compound; similarly, 897.701; 675-900; a C-H "loop" indicates the presence of aromatic group in the compound; 2991.05; 2850-3000; a N-H stretching shows the presence of alkanes in the compound; while, a medium Peak Value (cm^{-1}) of 2770.24 with in the range of 2695-2830 with C-H (aldehyde C-H) indicates the presence of Aldehydes/ Ketones in the compound.

On the other hand occurrence of a medium peak at 1322.93 within the reference range of 1210-1390 with O-H bending indicates the presence of phenol group in the compound; while occurrence of a medium peak at 1246.75 within the reference range of 1020-1250 with C-N stretching indicates the presence of alkyl aryl ether group in the compound; however a medium peak at 939.163 within the reference range of 910-959 with a O-H bend indicates the presence of carboxylic acids in the compound; while occurrence of a medium peak at 828.882 within the reference range of 550-850 with C-Cl stretch indicates the presence of alkyl halides in the compound; whereas a medium peak at 590.111 within the reference range of 515-690 with a C-Br stretching indicates the presence of Alkyl halides in the compound (Table 4; Fig. 1).

DISCUSSION

Ethnobotanical studies and phytochemical screening remains the mainstay in the hunt of bioactive secondary metabolites from natural sources. But computational approaches in preclinical studies on drug discovery and development play a major role[35-46]. Therefore, simultaneous progress in both the fields has become the rule of the day. In a study, Romeilah *et al.*[47], isolated 20 compounds from the *C. cyminum* (seeds) oil

including: α-pinene 2.14, sabinene 1.01, β-pinene 4.89, β-myrcene 1.45, α-terpinene 0.84, p-cymene 1.77, limonene 0.24, α-terpinene 1.07, α-terpinolene 0.08, Camphor 0.12, Terpinen-4-ol 0.04, α-terpineol 2.47, geraniol 0.07, geranyl acetate 4.11, β-caryophyllene 3.44, α-phellandrene 1.09, cuminaldehyde 60.01, thymol 2.04, β-farnesene 3.01 and caryophyllene oxide 6.12.

However, Gachkar *et al.*[48], isolated 32 compounds from *C. cyminum* oil including: isobutyl isobutyrate 0.8, *a*-thujene 0.3, *a*-pinene 29.1, sabinene 0.6 , myrcene 0.2 , *d*-3-carene 0.2, *p*-cymene 0.3, limonene 21.5, 1,8-cineole 17.9, (*E*)-ocimene 0.1, *g* -terpinene 0.6, terpinolene 0.3, linalool 10.4, *a*-campholenal 0.03, *trans*-pinocarveole 0.07 , *d*-terpineole 0.09, terpinene-4-ol 0.5, *a*-terpineole 3.17, *trans*-carveole 0.4, *cis*-carveole 0.07, geraniol 1.1, linalyl acetate 4.8, methyl geranate 0.2, *a*-terpinyl acetate 1.3, neryl acetate 0.09, methyl eugenol 1.6, *b*-caryophyllene 0.2, *a*-humulene 0.2, spathulenol 0.07, caryophylleneb epoxide 0.1, humulene epoxide II 0.08 and acetocyclohexane dione-2 0.4.

Chaudhary *et al.*,[49] identified as much as 49 components in the essential oil constituents of the *C. cyminum* fruit that represented 99.78% of total detected constituents. The essential oil was characterized by the presence of monoterpene (79.61%), sesquiterpene (2.66%), aromatic (16.55%) and aliphatic compounds (0.66%). Among 34 monoterpenes detected, there were 14 hydrocarbons (41.28%), 12 alcohols (5.76%), 06 keto compounds (31.92%), 01 aldehyde (0.54%) and 02 esters (0.11%).

However, predominant monoterpene hydrocarbon was γ-terpinene (23.22%) followed by α-phellandrene (12.01%), α-pinene (1.78%) and α-terpinene (1.24%). Among 12 monoterpenic alcohols, p-menth-2-en-7-ol (3.48%) was the major alcoholic constituent and trans-dihydrocarvone (31.11%) was the prominent monoterpenic ketone in the essential oil[50]. Sesquiterpenes identified in the oil were teresantalol (2.62%) and karvaknol (0.04%)[49]. Aromatic compounds detected were p-cymene (15.87%), 8a-methyl octahydro-2 (1H)- naphthalenone, 2-isopropyl-5-methyl phenol, p-cymen-7-ol, o-cymen-5-ol, p-cymen-3-ol, 6-allyl-4,5-dimethoxy-1,3-benzodioxole and 2,a,8,8-tetramethyl decahydrocyclopropanal [d] naphthalene. The aliphatic compounds included 1- (1, 2, 3-trimethyl-2- cyclopenten-1-yl) ethanone, 3-isopropyl phenol, 2-methyl-4-isopropyliden-cyclopentan-1-al, 1-methyl-4-iso propyl-3-cyclohexen-1-ol, 2-isopropenyl-5-methyl-hex-4-enal, 4-isopropyl cyclohex-1,3-dien-1-yl) methanol, 4-isopropyl-1-cyclohexen-1-carbaldehyde, hexadecylene oxide and (3,4-dimethyl-2-oxo-cyclopenten-1-yl) acetic acid.

Similarly, that analysis of the methanolic extract of the fruits of *C. cyminum* led to the isolation of five terpenic and steroidal constituents, they were characterized as 1,4,5,8-tetrahydroxynaphthyl geranilan-10'-al 1'-oate, lanost-5,20 (22)-dien-3α-olyl *n*docosanoate, labdan-6α,16,20-triol-16-(10',11'- dihydroxy anthraquinone-2'-oate), stigmast-5-en- 3β-O-D-arabinopyranosyl-2'-benzoate and lanost-5,24-dien-3β-ol 3β-O-D- arabinopyronosyl-2'- *n*octadec- 9'', 12''-dienoate. The characteristic odour of cumin was attributed to the presence of sminaldehyde, 1, 3-p-menthadien-7al, 1-4-p-menthadien-7-al. 14 free amino acids were also isolated from the seeds. While, flavonoid glycosides isolated from the plant were included apigenin-7-glucoside, luteolin-7-glucoside, luteolin-7-glcuronosyl glucoside, luteolin and apigenin. Total polypheols in cumin were 4.98± 0.31. (mg GAE/g DW). Phenols (salicylic acid, gallic acid, cinnamic acid, hydroquinone, resorcinol, P-hydroxybenzoic acid, rutin, coumarine, quercetin) were isolated from seeds of *C. cyminum*[51].

Free radical scavenging and antioxidant activity of silver nanoparticles synthesized from *Cuminum cyminum* (Cumin) seed extract could be used as an effective antioxidant[52]. However, *C. cyminum* roots, stems and leaves, and flowers were investigated for their total phenolic, flavonoids, and tannins contents. In all *C. cyminum* organs, total phenolic content ranged from 11.8 to 19.2 mg of gallic acid equivalents per gram of dry weight (mg of GAE/g of DW). Among the polyphenols studied, 13 were identified in roots, 17 in stem and leaves, and 15 in flowers. The major phenolic compound in the roots was quercetin (26%), whereas in the stems and leaves, p-coumaric, rosmarinic, trans-2-dihydrocinnamic acids and resorcinol were predominant. In the flowers, vanillic acid was the main compound (51%)[53]. A total of 19 phenolic compounds were successfully identified during the ripening of cumin seeds. Rosmarinic acid was the major phenolic acid for the unripe seeds, while, half ripe and full ripe seeds were dominated by p-coumaric acid.

CONCLUSION

Phytochemical screening of bioactive natural products from *Cuminum cyminum*, GCMS analysis revealed the presence of 21 compounds, FTIR profile with the manifestation of strong and medium peak corresponding to the presence different functional groups in the compounds detected. The unique range of natural products in GCMS/ FTIR profile *C. cyminum* if ADMET prospected could be exploited for a wide range of biomedical applications.

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Table 1: Nutritional value per 100 g of *Cuminum cyminum*

Energy	**1,567 kJ (375 kcal)**
CHEMICAL CONSTITUENT	**QUANTITY**
Carbohydrates	44.24 g
Sugars	2.25 g
Dietary fibre	10.5 g
Fat	22.27 g
Saturated	1.535 g
Monounsaturated	14.04 g
Polyunsaturated	3.279 g
Protein	17.81 g
VITAMINS	**QUANTITY % (DV)**
Vitamin A equiv.	8% (64 µg)
beta-Carotene	7% (762 µg)
Vitamin A	1270 IU
Thiamine (B1)	55% (0.628 mg)
Riboflavin (B2)	27% (0.327 mg)
Niacin (B3)	31% (4.579 mg)
Vitamin B6	33% (0.435 mg)
Folate (B9)	3% (10 µg)
Vitamin B12	0% (0 µg)
Choline	5% (24.7 mg)
Vitamin C	9% (7.7 mg)
Vitamin D	0% (0 µg)
Vitamin D	0% (0 IU)
Vitamin E	22% (3.33 mg)
Vitamin K	5% (5.4 µg_)
MINERALS	**QUANTITY %DV†**
Calcium	93% (931 mg)
Iron	510% (66.36 mg)
Magnesium	262% (931 mg)
Manganese	159% (3.333 mg)
Phosphorus	71% (499 mg)
Potassium	38% (1788 mg)
Sodium	11% (168 mg)
Zinc	51% (4.8 mg)
OTHER CONSTITUENTS	**QUANTITY**
Water	8.06 g

Table 2 Phytochemical analysis of phytocompounds from *Cuminum cyminum*

PHYTOCONSTITUENTS	TEST	PRESENT/ ABSENT
Alkaloids	Wagner's reagent Test	**+**
Anthraquinones	Borntragers Test	**+**
Carbohydrates	Fehling's test, Benedict's test	**++**
Coumarins	Sodium hydroxide Test	**+**
Flavonoids	Shinoda Test	**++**
Glycosides	Keller-Kiliani Test	**+**
Phenol	$FeCl_3$ Test	**-**
Proteins	Millon's Test, Ninhydrin Test	**++**
Quinones	Sodium hydroxide Test	**+**
Saponins	Foam Test	**+**
Steroids	Salkowski Test	**+**
Tannins	$FeCl_3$ Test	**++**
Terpenoids	Salkowski Test	**++**

+++ = Abundantly present; ++ = moderately present; + = slightly present; - = absent

Table 3: GCMS analysis of phytocompounds from fruits of *Cuminum cyminum*

SNO	COMPOUND NAME	RT	MW	MF	% AREA	
					SEEDS	OIL
1.	α-Terpinene	4.363	136	$C_{10}H_{16}$	9.74	-
2.	α-Thujene	4.716	136	$C_{10}H_{16}$	-	0.29
3.	α-Pinene	4.842	136	$C_{10}H_{16}$	0.12	0.92
4.	β-Pinene	5.574	136	$C_{10}H_{16}$	2.1	-
5.	Santolina triene	5.668	136	$C_{10}H_{16}$	-	11.52
6.	α-Myrcene	5.747	136	$C_{10}H_{16}$	0.3	0.71
7.	ρ-Menthatriene	6.344	134	$C_{10}H_{14}$	18.77	24.63
8.	Terpinolene	6.968	136	$C_{10}H_{16}$	15.95	16.51
9.	Limonene	8.614	136	$C_{10}H_{16}$	0.19	-
10.	4-Terpineol	8.752	154	$C_{10}H_{18}O$	-	0.3
11.	1,8-cineole	8.761	154	$C_{10}H_{18}O$	0.46	0.14
12.	Benzaldehyde ρ-isopropyl	9.431	148	$C_{10}H_{12}O$	1.27	-
13.	**Cuminaldehyde**	**9.96**	**148**	**$C_{10}H_{12}O$**	**32.59**	**31.65**
14.	Myrtenal	10.577	150	$C_{10}H_{14}O$	8.74	1.78
15.	cis-Ocimene	10.248	150	$C_{10}H_{14}O$	10.26	4.14
16.	α-Terpinen-7-al	15.881	150	$C_{10}H_{14}O$	3.98	4.59
17.	o-Cymen-7-ol	15.965	150	$C_{10}H_{14}O$	--	1.11
18.	γ-Terpinen-7-al	16.072	150	$C_{10}H_{14}O$	1.95	--
19.	Thymol	16.186	150	$C_{10}H_{14}O$	--	0.35
20.	4-Hydroxy-cryptone	16.797	154	$C_{10}H_{14}O$	1.68	0.38
21.	4-(1-methylethyl)-benzoic acid	20.047	164	$C_{10}H_{14}O_2$	0.97	1.43

Table 4: IR spectral frequencies of functional groups in methanolic fruit extract of *C. cyminum*

Peak Value (cm^{-1})	Reference Ranges	Functional group (Bonds)	Peak Intensity	Nature of the Compound
3543.56	3500-3700	O-H (H-bonded), usually broad	Strong	Alcohols & Phenols
2991.05	2850-3000	N-H stretching	Strong	Alkanes
2873.42	2850-3000	CH_3, CH_2 & CH	Strong	Alkanes
2856.06	2850-3000	CH_3, CH_2 & CH_2 or $_3$ bands	Strong	Alkanes
2770.24	2695-2830	C-H (aldehyde C-H)	Medium	Aldehydes/ Ketones
2141.56	2100-2260	C-Ctriple bond	Strong	alkynes
1716.34	1706-1720	C=O stretching, dimer	Strong	Carboxylic acid
1646.91	1640-1690	C=N, Stretching	Strong	Imine/Oxime
1530.24	1500-1550	N-O Stretching	Strong	Nitro-compound
1454.06	1400-1500	C-C Stretch	Strong	Aromatic
1436.71	1395-1440	O-H bend	Strong	Carboxylic acid
1408.75	1380-1410	S=O stretching	Strong	Sulfonyl chloride
1322.93	1210-1390	O-H bending	Medium	Phenol
1246.75	1020-1250	C-N Stretching	Medium	Alkyl aryl ether
1070.3	1030-1070	S=O	Strong	Sulfoxide
939.163	910-959	O-H bend	Medium	Carboxylic acids
897.701	675-900	C-H "loop"	Strong	Aromatics
828.882	550-850	C-Cl Stretch	Medium	Alkyl halides
700.998	610-700	-C=C-H ;C-H bend	Strong	Alkynes
590.111	515-690	C-Br stretching	Medium	Alkyl halides

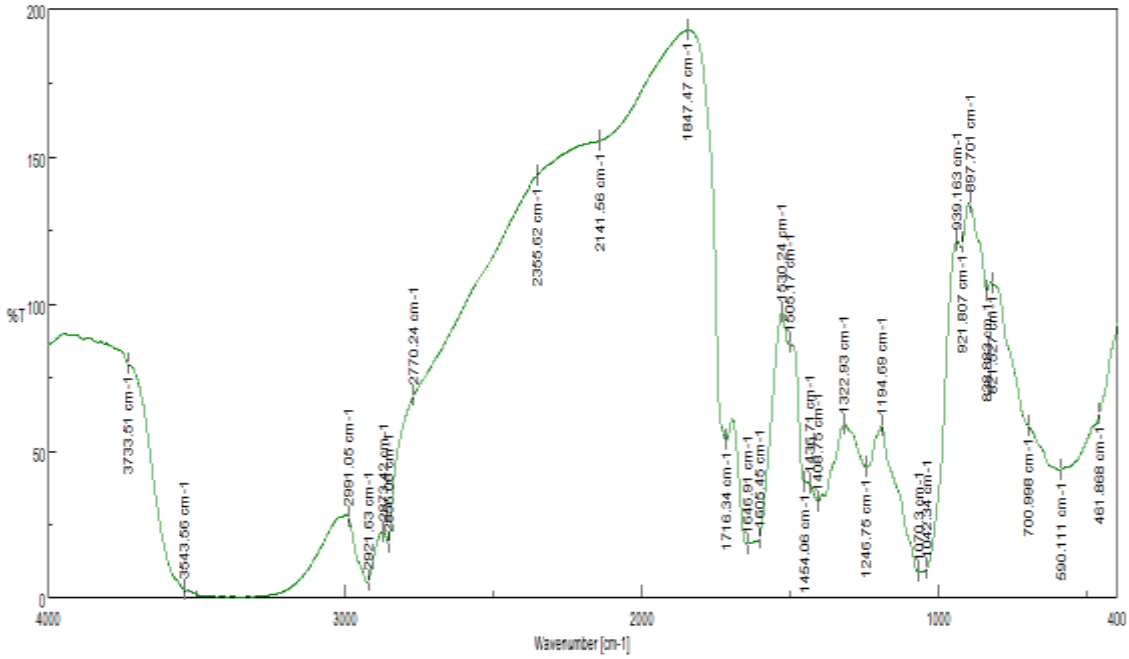

Figure 1: FTIR spectrum of methanolic fruit extract of *C. cyminum*