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**Research Article** **Botany**

# SCREENING OF BIOACTIVE COMPOUNDS BY GC-MS, ANTIMICROBIAL ACTIVITY AND *IN SILICO* STUDIES IN *Cynodon dactylon* L. Pers LEAVES

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**ABSTRACT**

In the present study was to investigate the phytochemical screening, histochemical, Fluorescence and antibacterial activity of *Cynodon dactylon* leaves extract. The phytochemical screening *Cynodon dactylon* leaves showed that the presence of saponins, flavonoids, polyphenol, Triterpenoids Steroids, anthroquinone terpenoids and tannin, glycosides whereas Alkaloids, carbohydrate, protein,and phlopatannins were absent in aqueous extract. The methanol extract of *Cynodon dactylon* leaves showed that the presence of, saponins, flavonoids, polyphenol, Triterpenoids terpenoids, Alkaloids, carbohydrate, protein, tannin and glycosides whereas phlopatannins was absent. In the present study twenty compounds were identified from extract of *Cynodon dactylon* leaves by Gas Chromatogram- Mass spectrometry (GC-MS) analysis. The prevailing compounds were Octadecanoic acid, 9-Octadecenoic acid, 1,2-Benzenedicarboxylic acid, 9,12-Octadecadienoyl chloride, 2-Hexadecen-1-Ol and Hexadecanoic acid, methyl ester. The methanolic extract shows antibacterial activity against *Gram-positive (Staphylococcus aureus, Bacillus subtilis) and Gram-negative (Escherichia coli) bacteria.* The methanolic extract shows antifungal activity against *Candida albicans, Aspergillus flavus* and *Aspergillus niger*. *In silico* docking analysis of phytol and oleic acid, angiotensin converting Enzyme (ACE) further proved their anticancer and antidiabetic activity.

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## INTRODUCTION

Plants are widely used as a potent source for isolation of several drugs and formulations in treatment of many diseases. There arises a need to screen medicinal plants for bioactive compounds as a basis for further pharmacological studies (Hassan *et al*, 2007). Medicinal plants form the backbone of traditional medicine in the last few decades with intense pharmacological studies. They are regarded as potential sources of new compounds of therapeutic value and as sources of lead compounds in drug development. Plants are rich sources of secondary metabolites with interesting biological activities. In general, these secondary metabolites are an important source with a variety of structural arrangements and properties (De Fatima *et al*, 2006). Natural products from microbial sources have been the primary source of antibiotics, but with the increasing recognition of herbal medicine as an alternative form of health care, the screening of medicinal plants for active compounds has become very significant (Koduru *et al*, 2006).

The drug-resistant bacteria pathogens have further complicated the treatment of infectious diseases. In recent years, drug resistance to human pathogenic bacteria has been commonly reported from all over the world. However, the situation is alarming in developing as well as developed countries due to indiscriminate use of antibiotics. In the present scenario of emergence of multiple drug resistance to human pathogenic organisms, this has necessitated a search for new antimicrobial substances from natural sources including plants. Plant and plant products play a wide range of antimicrobial properties. Keeping in view, the present study to investigate the phytochemical and antibacterial properties of *Cynodon dactylon*.

## MATERIALS AND METHODS

### Collection of plant materials

The leaves of *Cynodon dactylon* were collected in December 2017 from, Thanjavur district, Tamil Nadu, India. The *Cynodon dactylon* leaves were washed several times with distilled water to remove the traces of impurities from the leaves. Leaves was spread out in a plain paper and shade dried at room temperature for about 10 days and makes a fine powder using grinder mixture. The powder materials were used for further studies.

### Preparation of plant extract:

2 gram of the powder of *C. dactylon* leaves were transferred in to different conical flask (250ml). The conical flask containing 50ml of different solution (methanol and water). The conical flask containing ***C. dactylon leaves*** were shake well for 30 minutes by free hand. After 24 hrs, the extracts were filtered using whatman filter paper No.1 and filtrate used for further analysis.

### Phytochemical screening

Chemical tests were carried out on the extract using standard procedures to identify the constituents as described by Sofowara (1993), Trease and Evans (1989) and Harborne (1973 and 1984).

### GC-MS Analysis

GC-MS analysis was carried out on Shimadzu 2010 plus comprising a AOC-20i auto sampler and gas chromatograph interfaced to a mass spectrometer instrument employing the following conditions: column RTX 5Ms (Column diameter is 0..32 mm, column length is 30 m, column thickness 0.50 µm), operating in electron impact mode at 70 eV; Helium gas (99.99 %) was used as carrier gas at a constant flow of 1.73 ml /min and an injection volume of 5 µI was employed (split ratio of 10:1), injector temperature 270 ºC; ion source temperature 200 ºC. The oven temperature was programmed from 40 ºC (isothermal for 2 min), with an increase of 8 ºC/min, to 150 ºC, then 8 ºC/min to 250 ºC, ending with a 20 min isothermal at 280 ºC. Mass spectra were taken at 70 eV; a scan interval of 0.5 seconds and fragments from 40 to 450 Da. Total GC running time is 51.25 min. The relative percentage amount of each component was calculated by comparing its average peak area to the total areas. Software adopted to handle mass spectra and chromatograms was a TurboMass Ver 5.2.0 (Srinivasan and Ramarao, 2013).

Interpretation on GC-MS was conducted using the database of National Institute Standard and Technology (NIST) having more than 62,000 patterns. The spectrum of the unknown component was compared with the spectrum of the known components stored in the NIST library. The name, molecular weight and structure of the components of the test materials were ascertained (Dukes, 2013).

### Determination of antimicrobial activity

Antibiogram was done by disc diffusion method (NCCLS, 1993; Awoyinka *et al*., 2007) using plant extracts. Petri plates were prepared by pouring 30 ml of NA /PDA medium for bacteria/fungi. The test organism was inoculated on solidified agar plate with the help of micropipette and spread and allowed to dry for 10 mints. The surfaces of media were inoculated with bacteria/fungi from a broth culture. A sterile cotton swab is dipped into a standardized bacterial/ fungi test suspension and used to evenly inoculate the

entire surface of the Nutrient agar/PDA plate. Briefly, inoculums containing specie of bacteria were spread on Nutrient agar plates for bacteria and fungus strains were spread on potato dextrose agar for. Using sterile forceps, the sterile filter papers (6 mm diameter) containing the crude extracts (50µl) were laid down on the surface of inoculated agar plate. The plates were incubated at 37○C for 24 h for the bacteria and at room temperature (30±1) for 24-48 hr. for yeasts strains. Each sample was tested in triplicate. The antimicrobial potential of test compounds was determined on the basis of mean diameter of zone of inhibition around the disc in millimeters. The zones of inhibition of the tested microorganisms by the samples were measured using a millimeter scale.

***In Silico* Docking Studies**

Protein and ligand structures were obtained from the protein data bank (PDB) database and Pubchem. Automated docking along with a graphical user interface, Auto Dock tools was utilized to generate grids, calculate dock score and evaluate the conformers of activators bound in the active site of protein as targets. A Lamarckian genetic algorithm method, implemented in the program Auto Dock 4.1, was employed. This software used for the estimation of energy during the interaction and identify the best flexible ligand pose with minimum energy. The scoring function is based on the inter-amolecular interaction of ligand and protein during docking. As per genetic algorithm all the torsions were allowed to rotate during docking. The grid map was centred at particular residues of the protein and was generated with Auto Grid. The Lamarckian genetic algorithm and the pseudo-Solis and Wets methods were applied for minimization, using default parameters (Ghose AK, Crippen, 1987; Binkowski et al., 2007; Vidya et al., 2012; Shruthi et al., 2012). Complex structures were modeled using modeling software's Pymol (1.1 version, Delano Scientific LLC, San Carlos, CA, USA), Chimera (1.10.1 version UCSF Resources for biocomputing visualization and informatics, NIH, CA, USA) and Pose view (Trot and Olson, 2010) installed on a desktop equipped with Pentium (R) Dual-E6600 at 3.05 GHz 3.06 GHz processor (2 GB RAM Core CPU) running the Ubuntu 12.01 (LINUX) and Windows XP SP3 operating system.

**COX-2 enzyme protein structure**

The 3 dimensional structure of the COX-2 enzyme was taken from the Protein Data Bank (PDB) database (www.rcsb.pdb). The RCSB PDB (Research Collaboratory for Structural Bioinformatics, Protein Data Bank) is a repository for the 3D structural data of large biological macromolecules such as proteins and nucleic acids. It provides simple and advanced searches based on annotations related to sequence, structure and function The PDB ID is 6COX which is a complex of COX-2 enzyme with selective inhibitor SC-558 (Amaravani *et al.*, 2012).

**RESULTS AND DISCUSSION**

In the present study was carried out the phytochemical analysis on the *Cynodon dactylon* leaves revealed the presence of medicinally active constituents. The phytochemical characters of the *Cynodon dactylon* leaves investigated and summarized in Table-1 and plate 2 and 3. The phytochemical screening *Cynodon dactylon* leaves showed that the presence of saponins, flavonoids, polyphenol, Triterpenoids Steroids, anthroquinonesm terpenoids and tannin, glycosides whereas Alkaloids, carbohydrate, protein and phlobatannins was absent in aqueous extract. The phytochemical screening *Cynodon dactylon* leaves showed that the presence of, saponins, flavonoids, polyphenol, Triterpenoids terpenoids, Alkaloids, carbohydrate, protein, tannin and glycosides whereas phlobatannins was absent in methanol extract.

Phytochemicals are plant derived chemicals which are beneficial to human health and disease prevention. The term is generally used to refer to those chemicals that may have biological significance, for example antioxidants, but are not established as essential nutrients which when in excess could be detrimental. Scientists estimate that there are thousands of known phytochemicals having the potential to affect diseases such as cancer, stroke and metabolic syndrome and those caused by microorganisms (Anderson et al., 2004).

Hassain et al. (2011) screened phytochemical constituents from methanol leaf extract of *Bombax malabaricum*. Various organic 11 solvent extracts of *Pedalium murex* were subjected to preliminary phytochemical screenings by Thamizh mozhi et al. (2011). Selected 53 traditionally used medicinal plants from western region of India for their qualitative phytochemical screenings, total phenol and flavonoids contents. Pascaline et al. (2011) screened phytochemical constituents of some medicinal plants used by the Nandis of South Nandi District, Kenya.

**Table.1: Qualitative Phytochemical analysis of *Cynodon dactylon* leaves extract**

| S.No | Phytochemicals | Aqueous Extract | Methanol Extract |
|---|---|---|---|
| 1 | Tannin | + | + |
| 2 | Phlobatannins | - | - |
| 3 | Saponnin | ++ | + |
| 4 | Flavonoids | + | ++ |
| 5 | Steroids | + | + |
| 6 | Terpenoids | ++ | ++ |
| 7 | Triterpenoids | + | + |
| 8 | Alkaloids | - | + |
| 9 | Carbohydrate | - | + |
| 10 | Protein | - | + |
| 11 | Anthroquinone | ++ | + |
| 12 | Polyphenol | ++ | + |
| 13 | Glycoside | + | + |

- Absence, + presence and ++ high concentration

**GCMS Analysis**

In the present study twenty chemical constituents have been identified from extract of *Cynodon dactylon* leaves by Gas Chromatogram- Mass spectrometry (GC-MS) analysis. The prevailing compounds were Octadecanoic acid, 9-Octadecenoic acid, 1,2-Benzenedicarboxylic acid, 9,12-Octadecadienoyl chloride, 2-Hexadecen-1-Ol and Hexadecanoic acid, methyl ester. The presence of various bioactive compounds justifies the use of the whole plant for various ailments by traditional practitioners. However isolation of individual phytochemical constituents and subjecting it to biological activity will definitely give fruitful results. (Fig 1, Table 2 and 3).

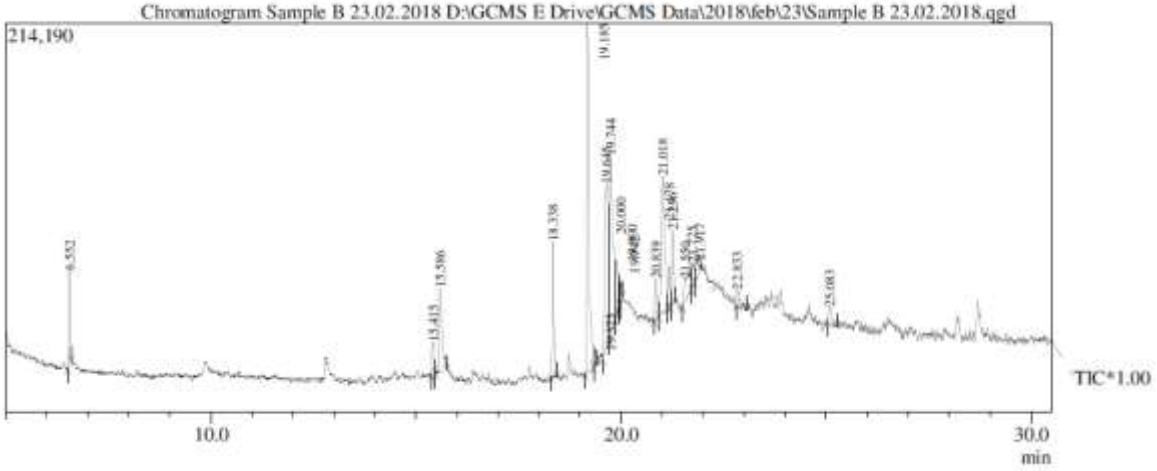



**Fig 1: Chromatogram obtained from the GC-MS with the *Cynodon dactylon* leaves extract**

**Table 2: Components identified in ethanolic extract of *Cynodon dactylon* leaves (GC- MS study)**

Peak Report TIC

| Peak# | R.Time | I.Time | F.Time | Area% | Height% | A/H | Mark | Name |
|---|---|---|---|---|---|---|---|---|
| 1 | 6.552 | 6.508 | 6.600 | 2.86 | 6.08 | 2.09 | | UNDECANE |
| 2 | 15.415 | 15.367 | 15.467 | 1.77 | 2.12 | 3.71 | | HEXADECANE, 1-CHLORO- |
| 3 | 15.586 | 15.467 | 15.750 | 6.37 | 5.43 | 5.21 | V | Phthalic acid, di-(1-hexen-5-yl) ester |
| 4 | 18.338 | 18.292 | 18.425 | 5.29 | 8.72 | 2.69 | | 2-Pentadecanone, 6,10,14-trimethyl- |
| 5 | 19.185 | 19.125 | 19.333 | 18.48 | 22.62 | 3.63 | | OCTADECANOIC ACID, METHYL ESTER |
| 6 | 19.375 | 19.333 | 19.400 | 0.86 | 0.96 | 3.98 | V | Pentanoic acid, 2-[(phenylmethoxy)imino]-, tr |
| 7 | 19.645 | 19.550 | 19.700 | 15.09 | 10.59 | 6.34 | | 9-OCTADECENOIC ACID (Z)- |
| 8 | 19.744 | 19.700 | 19.858 | 15.67 | 11.58 | 6.02 | V | 1,2-BENZENEDICARBOXYLIC ACID, DIE |
| 9 | 19.900 | 19.858 | 19.933 | 3.19 | 3.38 | 4.20 | V | 2,4,4-Trimethyl-1-pentanol |
| 10 | 19.942 | 19.933 | 19.967 | 0.83 | 2.29 | 1.62 | V | 2-Propynoic acid, methyl ester |
| 11 | 20.000 | 19.967 | 20.042 | 0.90 | 1.30 | 3.08 | V | L(+)-GLUTAMINIC ACID HYDROCHLOR |
| 12 | 20.839 | 20.792 | 20.917 | 2.27 | 2.57 | 3.93 | | Dichloroacetic acid, nonyl ester |
| 13 | 21.018 | 20.917 | 21.133 | 11.68 | 8.84 | 5.87 | V | 9,12-Octadecadienoyl chloride, (Z,Z)- |
| 14 | 21.178 | 21.133 | 21.208 | 1.86 | 2.64 | 3.14 | V | 2-HEXADECEN-1-OL, 3,7,11,15-TETRAME |
| 15 | 21.256 | 21.208 | 21.325 | 3.44 | 4.83 | 3.17 | V | HEXADECANOIC ACID, METHYL ESTER |
| 16 | 21.550 | 21.500 | 21.708 | 3.75 | 1.55 | 10.72 | | 2-HEPTADEC-5"-EN-1"-YLOXY TETRAH |
| 17 | 21.725 | 21.708 | 21.792 | 1.46 | 1.65 | 3.93 | V | ANTHRACENE, 9-(ETHYL-2,2-D2)- |
| 18 | 21.917 | 21.792 | 21.942 | 1.72 | 0.75 | 10.15 | V | 6-Heptenyl acetate |
| 19 | 22.833 | 22.808 | 23.075 | 1.22 | 1.05 | 5.17 | | SILICONE POLYMER |
| 20 | 25.083 | 25.042 | 25.267 | 1.31 | 1.06 | 5.49 | | SILICATE ANION TETRAMER |
| | | | | 100.00 | 100.00 | | | |

**Table 3: Biological Activity of phyto-components identified in the ethanolic extracts of the *Cynodon dactylon* leaves by GC-MS**

| S.No. | Name of the compound | Biological activity** |
|---|---|---|
| 1. | Octadecanoic acid | Antioxidant, **anti-inflammatory**, nemaicide, pesticde, Anti-androgenic flavor, hemalytic, 5- Alpha reductase inhibitor |
| 2. | 9-Octadecenoic acid | Antihypertensive, Increase HDL and decrease LDL Cholesterol |
| 3. | 1,2-Benzenedicarboxylic acid | Antimicrobial activity |
| 4. | 9,12-Octadecadienoyl chloride | Antimicrobial activity |
| 5. | Hexadecanoic acid, methyl ester | Anti oxidant, hypocholesterolemic, nematicide, pesticide, lubricant, anti androgenic, flavour, hemolytic-5-α reductase inhibitor. |

****Source: Dr.Duke's phytochemical and ethnobotanical databases [Online database.**

Karpagasundari and Kulothungan, (2014) screened the bioactive components of *Physalisminima* leaves have been evaluated using GC-MS. GC-MS analysis of extract of *Physalisminima* leaves revealed the existence of heneicosanoic acid (25.22), bicyclo [4.1.0] hepta-2,

4-dien (27.41) octadecanoic acid (CAS), stearic acid (31.19) and octadeca-9, 12-dienoic acid (32.02).

Similarly the work was done by GC-MS analysis of bioactive components of *Hugonia mystax L*. (Linaceae). Thirteen compounds were identified. 1,2-benzene dicarboxylic acid, diisooctyl ester (48.75 %) was found to be major component followed by n- hexadecanoic acid (13.52 %), phytol (9.25 %), squalene (6.41 %), vitamin E (4.09 %), dianhydromannitol (3.56 %), 9,12–octadecadienoic acid (Z,Z)–(3.20%) and 3,7,11,15 – tetramethyl -2-hexadecen -1-ol (2.85 %) .

**Anti-bacterial activity of *Cynodon dactylon* leaves extract**

Nowadays there exist more than 250 types of infections caused by bacteria. Among these microorganisms, we find the *Bacillus subtilis Escherichia coli* and *Staphylococcus* that are known to be one of the main elements of human physiological flora. Methanolic extract of *Cynodon dactylon* were screened against bacteria. The antibacterial activity was determined by measuring the diameter of zone of inhibition recorded. The ethanolic extract shows significant activity against *Escherichia coli, Bacillus subtilis* and *Staphylococcus aureus* (plate 4). The results of the *Cynodon dactylon* extract was correlated with the standard drug and show that the methanolic extract shows good activity against all bacterial strains.

**Anti-fungal activity of *Cynodon dactylon* leaves extract**

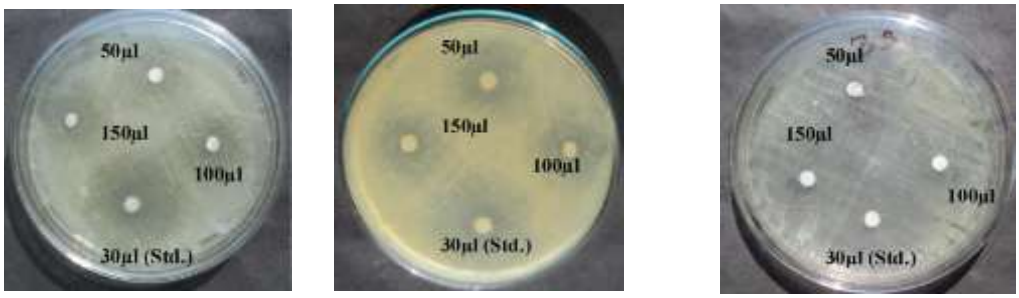
Fungi are ubiquitous in the environment, and infection due to fungal pathogens has become more common. The aim of this work was to evaluate in vitro the potential antifungal activity of medicinal *Cynodon dactylon* leaves extract against *Candida albicans, Aspergillus flavus* and *Aspergillus niger*. The methanolic extract of *Cynodon dactylon* were screened against fungi. The antifungal activity was determined by measuring the diameter of zone of inhibition recorded. The ethanolic extract shows significant activity against *Candida albicans, Aspergillus flavus* and *Aspergillus niger* (plate 4). The results of the *Cynodon dactylon* extract was correlated with the standard drug and show that the methanolic extract shows good activity against all fungal strains.

**Table 4: Antimicrobial activities of *Cynodon dactylon* leaves**

| **Bacteria** | | | | |
|---|---|---|---|---|
| **Microorganisms** | **50µl** | **100µl** | **150µl** | **Standard** |
| *Escherichia coli* (mm) | 13.50±0.94 | 16.75±1.17 | 19.00±1.33 | 14.25±0.99 |
| *Staphylococcus aureus* (mm) | 11.50±0.80 | 11.50±0.80 | 12.75±0.89 | 11.00±0.77 |
| *Bacillus subtilis* (mm) | 6.75±0.47 | 7.25±0.50 | 7.00±0.49 | 9.00±0.63 |
| **Fungus** | | | | |
| *Candida albicans* (mm) | 10.25±0.71 | 13.25±0.85 | 14.25±0.99 | 10.00±0.70 |
| *Aspergillus flavus* (mm) | 8.25±0.57 | 9.25±0.64 | 9.75±0.68 | 10.25±0.71 |
| *Aspergillus niger* (mm) | 14.75±1.03 | 13.25±0.92 | 10.50±0.71 | 7.50±0.52 |

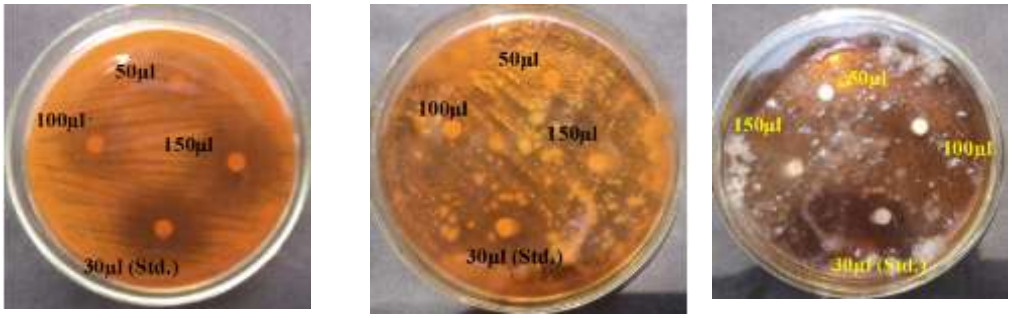
Values were expressed as Mean ± SD.
Bacterial standard - Chloramphenicol
Fungal standard - Fluconazole

**Plate 4: Anti-bacterial activity of *Cynodon dactylon* leaves extract**




***Escherichia coli*** ***Staylococcus aureus*** ***Bacillus subtilis***

**Plate 4: Anti-fungal activity of *Cynodon dactylon* leaves extract**




***Candida albicans*** ***Aspergillus flavus*** ***Aspergillus niger***

Siva Sakthi *et al* . (2011) evaluated the antibacterial potentiality of ethanol and ethyl acetate solvent extracts of mature leaves of *Datura metel* against nine pathogenic bacterial isolates *viz*., *Staphylococcus aureus, Bacillus subtilis, Bacillus cereus, Escherichia coli, Salmonella typhi, Shigella flexneri, Klebsiella pneumoniae, Vibrio cholerae* and *Pseudomonas aeruginosa*. The turbidity of the bacterial inoculums was compared with 0.5 Mc Farland standards and the antibacterial potential of *Datura metel* ethanol extract was tested by using Agar well diffusion method. The ethanol extract of *Datura metel* (100 mg/ml) showed maximum zone of inhibition (26 mm) against *Pseudomonas aeruginosa, Escherichia coli* and *Bacillus subtilis*. *Staphylococcus aureus* showed less zone of inhibition (8 mm). The ethyl acetate extract of *Datura metel* (100 mg/ml) showed maximum zone of inhibition (19 mm) against *Escherichia coli*. There was no zone of inhibition against *Pseudomonas aeruginosa*.

Gupta *et al.* (2010) investigated antibacterial activity of five ethanolic and aqueous plant extracts against *S. aureus, Pseudomonas aeruginosa* and *Bacillus subtilis* and their results showed that the ethanolic extracts of four plants (*Achyranthes aspera, Cynodon dactylon, Lantana camara* and *Tagetes patula*) were effective against all tested microorganisms with MIC's ranged from 25 to 125 mg/ml.

***In silico* studies**

Inflammation is the response of an organism to invasion by a foreign body such as bacteria, parasites and viruses. Studies on inflammation have become one major focus of global scientific research. Cyclooxygenases (COX) are the key enzymes in the synthesis of prostaglandins, the main mediators of inflammation, pain, and increased body temperature (hyperpyrexia). The body produces two main isoforms of COX proteins, that is, cyclooxygenases1 (COX-1) and cyclooxygenases-2 (COX-2). The COX-1 is responsible for formation of important biological mediators such as prostanoids, including prostaglandins, prostacyclin, and thromboxane, and involved in pain causing, blood clotting, and protecting the stomach (Watson et al., 2000), whereas COX-2 is involved in the pain by inflammation and plays a major role in prostaglandin biosynthesis in inflammatory cells and central nervous system (Chhajed et al., 2010).

COX-2 inhibition is desirable for anti-inflammatory responses as it is expressed during inflammation by proinflammatory molecules, This COX-2 is believed to be the target enzyme for the anti-inflammatory activity of anti-inflammatory drugs. As selective COX-2 inhibitors are preferred drugs and since natural products have been proven to be the richest source of medicinal entities with chemical diversity, this would be better option in search of lead in drug discovery (Rosen et al., 2009).

Identification and screening of bioactive molecules and their binding sites in the protein are challenging for drug development. Therefore, we planned to find out the binding ability of Octadecanoic acid with COX 2 using computational biology tools. The docked ligand molecules were selected based on docking energy and good interaction with the active site residues and the results are shown in Table 5 and 6. Hydrogen bond was indicated by dashed lines in green between atoms involved and rest of the interactions were hydrophobic.

The activation energy (-9.25671 Kcal/mol) was found with Octadecanoic acid (Figure 3 and 4). From the *in silico* docking results, it is quite evident that plant-derived compounds have the great

potential against anti-inflammatory activity of inflammatory mediator protein COX 2.

*In silico* molecular docking in one of the most powerful techniques to discover novel ligand for proteins of known structure and thus play key role in structure based drug. Investigators often use docking computer programs to find the binding affinity for molecules that fit a binding site on the protein. Hence in this present work we have carried out *in silico* molecules docking to analyze the binding properties of the mediator called COX-2 with 3 different compounds reported from *Cynodon dactylon leaves* . The wet analysis carried out by us showed very good result with regard to anti-inflammatory property of this plant extract. So the present study may act as supportive evidence that substantiate property of this plant extract., Octadecanoic acid has potential inhibiting ability was identified from this *Cynodon dactylon leaves* with COX-2.

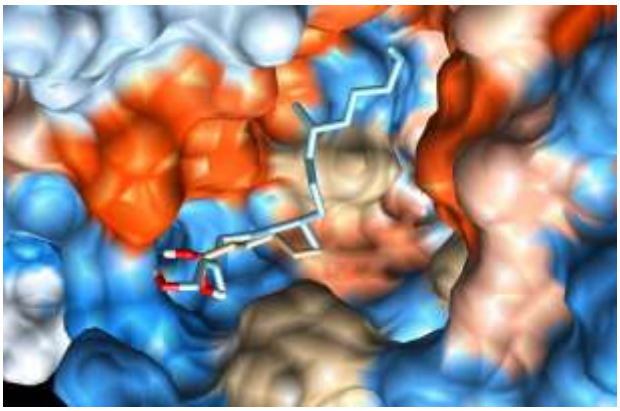
**Table 5: Cyclooxygenase-2 Enzyme binding site**

| S. No. | Ligands | Amino acids in the binding pocket |
|---|---|---|
| 1. | Octadecanoic acid | Arg 208, Glu276 |

**Table 6. Docking results of Octadecanoic acid compounds against Cyclooxygenase-2 Enzyme**

| Sl.No. | Ligands | Moleccular formula | Molecular Weight [g/mol] | Hydrogen donor | Hydrogen acceptor | Docking Energy Level (*kcal/mol*) |
|---|---|---|---|---|---|---|
| 1. | Octadecanoic acid | $C_{18}H_{36}O_2$ | 410 | 01 | 02 | -9.256 |

**Fig 3 Electrostatic surface of COX- 2 alongside of the amino acids motif with Octadecanoic acid**



## CONCLUSION

Overall, it can be concluded from the present study that *Cynodon dactylon* leaves contains rich source of phytochemicals. This study is the first scientific report that provides convincing phytochemicals and antibacterial activity evidence for the relevance of *Cynodon dactylon* leaves thus providing scientific validity to its traditional consumption by the local populace of south India. *Cynodon dactylon* leaves extract had a good potential for therapeutic use against infectious diseases caused by bacterial and fungal pathogens.

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