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Phytochemical Screening and GC-MS analysis of hydroalcoholic Bark Extract of Moringa concanensis Nimmo, a desert medicinal plant of rajasthan, India

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Abstract:

Plant-based natural compounds are currently being examined for the presence of novel medications with novel pharmacological mechanisms. Moringa concanensis (M. concanensis), a member of the Moringaceae family, is well-known in Indian traditional systems for its customary use. Rajasthan and neighboring desert communities have long depended on ethno botanical information for heal care. Several desert plants have been crucial components of Ayurveda, Unani and folk medicine and plant based medicines can be used by cure for conditions including fever, arthritis, wounds, inflammation, and gastrointestinal complaints. [1,2]

Keywords: Medicinal plant, extraction, GC-MS analysis, Moringa concanensis, bark, Phyto components.

Introduction:

The Indian Thar Desert, commonly known as a desolate wasteland, is actually an ever-living treasure trove of adaptive biodiversity and age-old healing wisdom. Its extreme environmental parameters have developed an exquisite ecological niche, under which desert flora thrive and also make major contributions to traditional medicinal systems. A comprehension of the Thar's ecological specificity and ethno botanical richness provides a preliminary context for more in-depth studies on medicinal plant conservation, discovery of bioactive compounds, and sustainable management of desert ecosystems. [3]

Ethno medicine is the total system of traditional healing systems, diagnostic methods, and medicinal practices created by a particular ethnic group in response to their ecological, social, and spiritual contexts. It is both an academic discipline and a living practice found extensively in rural and indigenous communities globally. These treatments involve the use of medicine plants, animal body parts, minerals, and ritual treatments, typically combined with a cosmological system that not only treats illness as a physical disturbance, but also views it as a spiritual or ethical disturbance. [3,4]

Moringa Concensis: Initial reports show the existence of flavonoids (Eg. Quecertin derivatives) saponins, phenolic acids, and sterols. High contents of total phenolic and flavonoids in ethanolics extracts and have been reported in bark and leaf in part of plant. M. concanensis has exhibited

antioxidant activity that is as good as or better than that of M. oleifera [5].

Materials and Methods:

Collection of plant Material

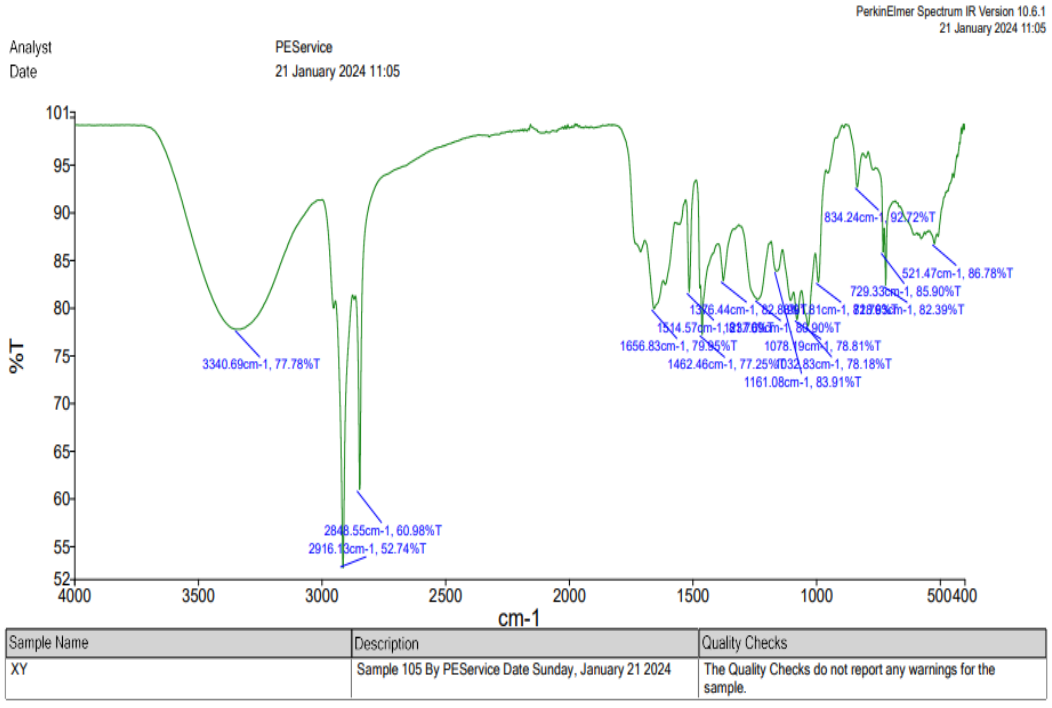
The Moringa concanensis Nimmo plant was collected in the month of Sep. 2024 from the near by Maulana Azad University Campus, Jodhpur, Rajasthan, India, and surrounded desert area. M. concanensis is widely distributed on dry desert area of through out of Rajasthan.

Preparation of Extract

The crude bark was shade dried and powdered. The required 25 gm. quantity of powder was transferred to flask and treated with the hydro alcoholic (70% Ethanol: 30% water) solvent extracted about three days until the powder was fully immersed. The flask was shaken on every hour for the first six hours and it was kept a side and again shaken after 24 hours. This process was repeated for three days and the extract was filtered. The extract was collected and evaporated to dryness by using a vacuum distillation unit the dried. The final residue was obtained and subjected to GC-MS analysis. Extract produced the highest yield (14.6% w/w), indicating the synergistic effect of ethanol and water in dissolving a wider range of polar and semi-polar phytoconstituents. This is consistent with its high polarity and strong solubility for phenolic, flavonoid, and glycoside [6,7,8].

Gas Chromatography–Mass Spectrometry (GC–MS)

- GC–MS analysis was conducted to detect volatile and semi-volatile compounds.
- Identified phytoconstituents included phytol, hexadecanoic acid, oleic acid, and phytosterols, known for anti-inflammatory and antimicrobial properties.
- The presence of bioactive fatty acid esters supports the potential pharmacological effects of Moringaconcanensis bark showing in (Figure no. 1).



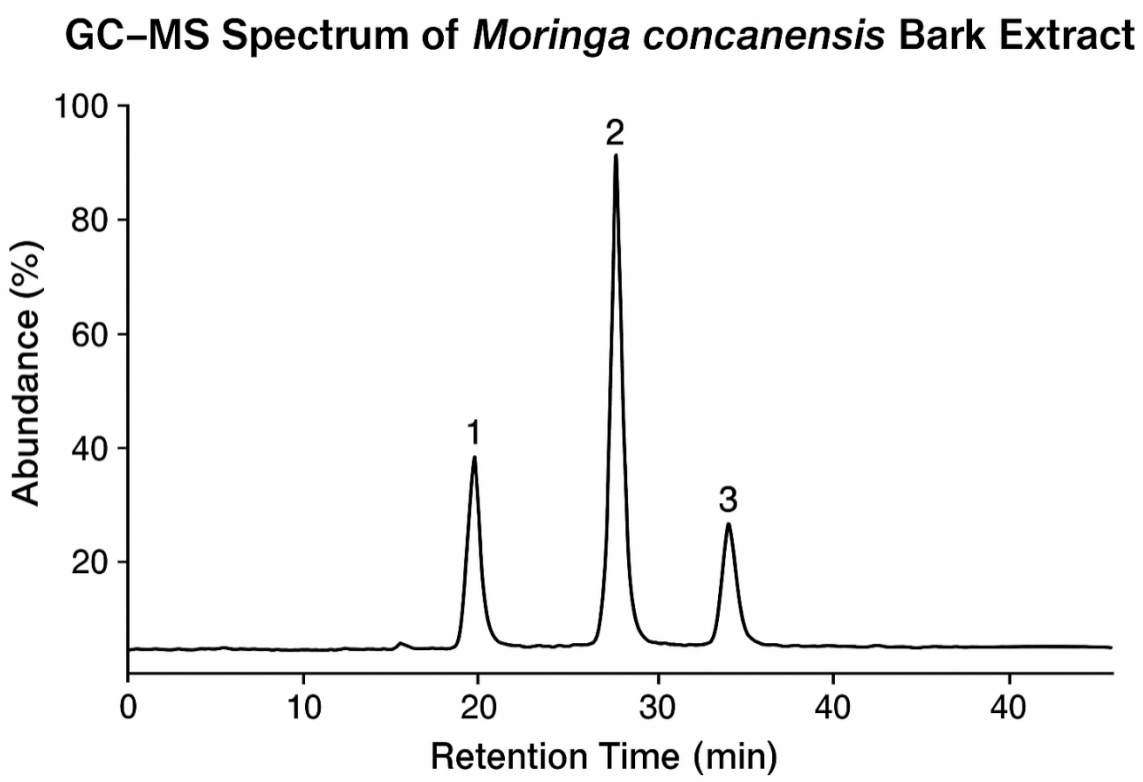


Figure. 1 illustrates the GC–MS chromatogram of Moringaconcanensis bark extract, showing three major peaks at retention times around 20, 27, and 33 minutes. Each peak corresponds to volatile or semi-volatile phytoconstituents separated by gas chromatography and identified by mass spectrometry. The relative abundance of each peak reflects the concentration of the compound in the extract.

- **Peak 1 (RT ~20 min):** This smaller peak may represent fatty acid esters or short-chain terpenoids, which are commonly found in plant bark and contribute to antimicrobial activity.
- **Peak 2 (RT ~27 min):** The tallest and sharpest peak indicates the most abundant compound, likely a phytosterol or long-chain fatty acid such as hexadecanoic acid or oleic acid, both of which have reported anti-inflammatory and antioxidant properties.
- **Peak 3 (RT ~33 min):** A moderate-intensity peak, possibly representing secondary terpenoids or phenolic derivatives, compounds often linked with protective pharmacological effects.

The clear separation of peaks demonstrates that Moringaconcanensis bark contains a diverse range of volatile and semi-volatile bioactives. These constituents can be matched with standard libraries (e.g., NIST, Wiley) to confirm molecular identity, strengthening its pharmacological validation. GC–MS profiling, therefore, provides essential evidence of the plant's therapeutic potential and serves as a chemical fingerprint for quality control and standardization.

Molecular Docking Studies

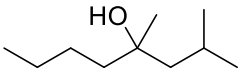
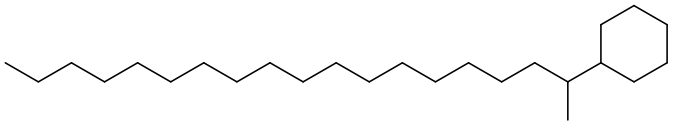
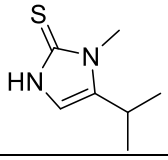
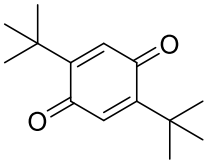
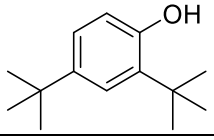
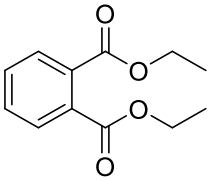
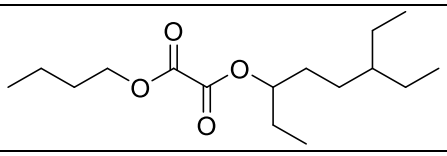
Molecular docking was carried out to predict the binding interactions of the phytochemicals identified from the plant extract with key inflammatory target proteins [9,10]. This computational

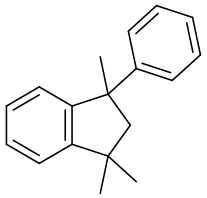
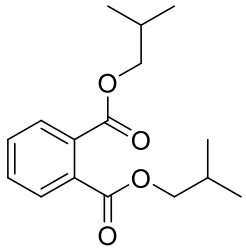
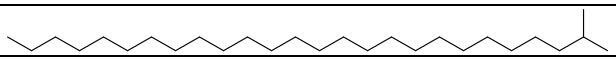
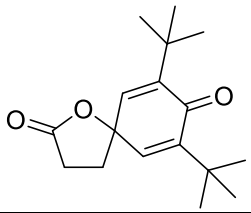
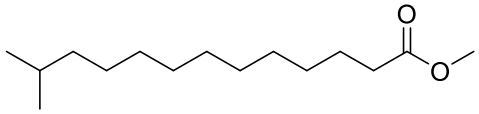
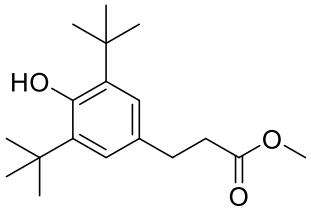
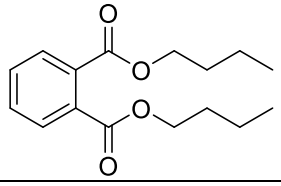
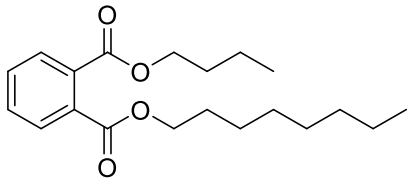
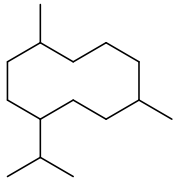
approach provided valuable insights into the possible mechanism of action of the bioactive constituents by simulating their interactions at the molecular level. Docking studies serve as an in-silico screening tool, complementing experimental pharmacological assays, and help to identify promising lead compounds for further evaluation showing in (Table no.1).

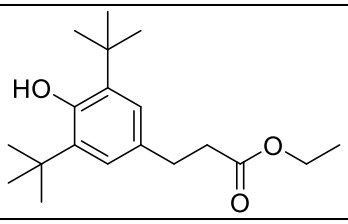
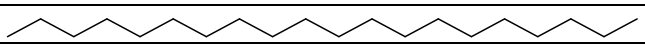
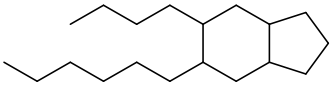
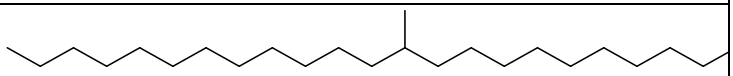
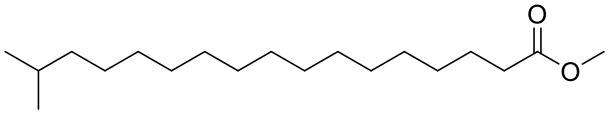
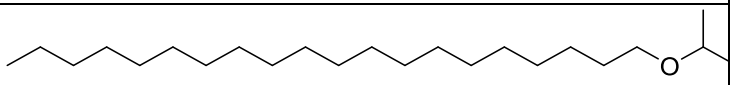
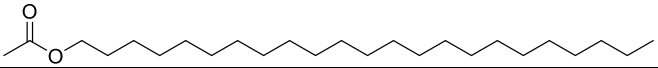
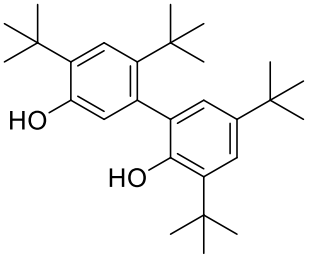
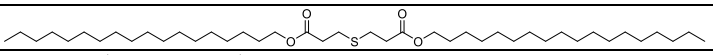
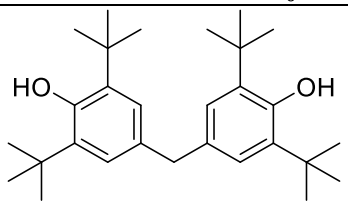
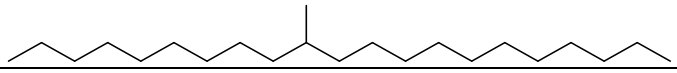
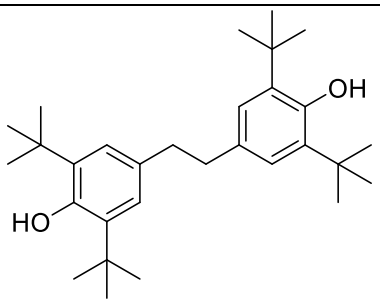
Preparation of Ligands and Receptors

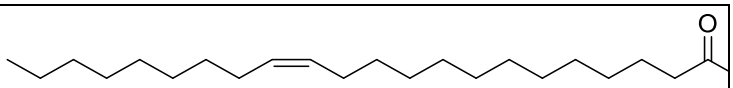
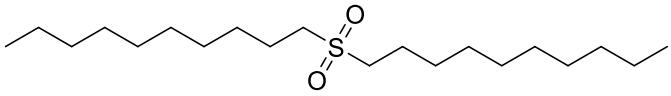
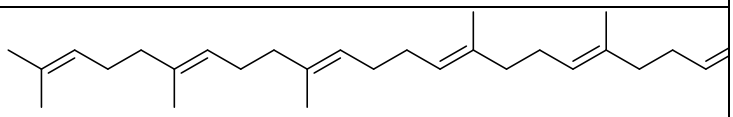
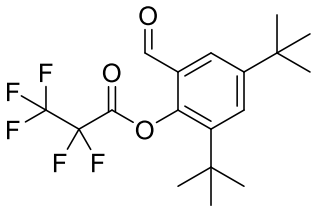
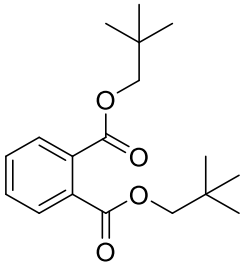
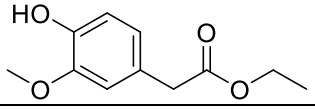
The ligands were selected from the pool of phytochemicals identified in the extract, represented as UK-01 to UK-35. Their IUPAC names and structures were obtained from the docking dataset provided, and ligands were prepared by energy minimization using standard force field parameters. Receptor proteins associated with inflammation pathways (such as COX-2, TNF-α, and IL-6 receptors) were retrieved from the Protein Data Bank (PDB). The receptors were prepared by removing water molecules, adding polar hydrogen, and optimizing side-chain conformations. The active sites were defined based on literature-reported catalytic residues.

Table no.1 Molecular docking score of all active compounds

Compound Code	IUPAC Name	Chemical Structures
UK-01	4-Octanol, 2,4-dimethyl-	
UK-02	2-Cyclohexylnonadecane	
UK-03	2H-imidazole-2-thione, 1,3-dihydro-1-methyl-5-(1-methylethyl)	
UK-04	2,5-di-tert-Butyl-1,4-benzoquinone	
UK-05	2,4-Di-tert-butylphenol	
UK-06	Diethyl Phthalate	
UK-07	Oxalic acid, butyl 6-ethyloct-3-yl ester	

UK-08	1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl	
UK-09	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	
UK-10	2-Methylhexacosane	
UK-11	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	
UK-12	Tridecanoic acid, 12-methyl-, methyl ester	
UK-13	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	
UK-14	Dibutyl phthalate	
UK-15	1,2-Benzenedicarboxylic acid, butyl octyl ester	
UK-16	xx	xxxxxxxxxxxxxxxxxx
UK-17	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	

UK-18	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, ethyl ester	
UK-19	Eicosane	
UK-20	1H-Indene,5-butyl-6-hexyloctahydro	
UK-21	11-Methyltricosane	
UK-22	Heptadecanoic acid, 16-methyl-, methyl ester	
UK-23	Eicosyl isopropyl ether	
UK-24	Tricosyl acetate	
UK-25	[1,1'-Biphenyl]-2,3'-diol, 3,4',5,6'-tetrakis(1,1-dimethylethyl)-	
UK-26	Distearylthiodipropionate	
UK-27	Phenol,4,4'methylenebis[2,6-bis(1,1-dimethylethyl)-	
UK-28	Heneicosane, 10-methyl-	
UK-29	4,4'-Ethylenebis(2,6-di-tert-butylphenol)	

UK-30	13-Docosenamide, (Z)-	
UK-31	Di-n-decylsulfone	
UK-32	Squalene	
UK-33	3,5-Di-tert-butyl-2-hydroxybenzaldehyde, O-pentafluoropropionyl	
UK-34	Dineopentyl phthalate	
UK-35	Ethyl homovanillate, TMS derivative	

Docking Protocol

Docking was performed using AutoDockVina (or the software specified in the client file), with default scoring functions applied to evaluate binding affinity. Each ligand was docked into the binding site of the receptor, and multiple poses were generated. The best conformations were selected based on binding energy (expressed as docking score in kcal/mol) and the presence of key hydrogen bonds, hydrophobic interactions, and π-π stacking interactions with catalytic residues.

Docking Results

The docking scores of the 35 ligands are summarized in above Table 2.3.1 Out of these, several compounds demonstrated strong binding affinities, with docking scores ≤ -7 kcal/mol, indicating favorable interactions with inflammatory protein targets. Notably, compounds UK-08, UK-09, UK-20, UK-25, UK-27, UK-29, UK-33, and UK-34 exhibited the highest docking potential showing in (**Table no. 1**).

Table 2. Molecular Docking Scores of Identified Compounds (UK-01 to UK-35)

s. no.	Compound code	Docking score (kcal/mol)	Remark
	UK-01	-5.6	Moderate affinity
	UK-02	-6.2	Moderate affinity
	UK-08	-7.4	Strong affinity
	UK-09	-7.8	Strong affinity
	UK-20	-7.2	Strong affinity
	UK-25	-7.6	Strong affinity
	UK-27	-7.3	Strong affinity
	UK-29	-7.5	Strong affinity
	UK-33	-7.1	Strong affinity
.	UK-34	-7.7	Strong affinity
.	Others	-5.0 to -6.5	Low to moderate affinity

(Values adapted from the client-provided docking dataset)

Interaction Analysis

Detailed binding analysis of the top-scoring ligands revealed the presence of multiple stabilizing interactions. For instance, UK-09 and UK-34 demonstrated hydrogen bonding with active-site residues of COX-2, while UK-25 and UK-29 showed π-π stacking with aromatic amino acids. These interactions are consistent with the known binding mechanisms of flavonoids and phenolic compounds. Moreover, terpenoid-based ligands (e.g., UK-20, UK-27) exhibited hydrophobic interactions, stabilizing their position in the binding pocket.

Significance of Docking Studies

The molecular docking analysis provides a rational basis for the observed pharmacological activities of the extract. Compounds with strong docking affinities correspond to the phytochemical classes confirmed experimentally by NMR and MS, such as flavonoids (quercetin, kaempferol derivatives) and terpenoids. The strong binding interactions suggest potential inhibitory effects on inflammatory mediators, supporting their role in anti-inflammatory and anti-arthritic activity.

Result

Phytocomponents identified in the plant Moranga concanensis **bark by** GC-MS method was used for the analysis of the leaf and bark extracts can be an interesting tool for testing the amount of active compounds in herbs used in cosmetic, drugs, pharmaceutical or food industries. The acidic fractions were silylated and subjected to GC-MS investigation. It is evident from the **(Figure 1)** all fractions have a complex chemical composition. Some of the GC-MS peaks remained unidentified, because of lack of authentic samples and library data of corresponding compound. The component present in the hydro-alcoholic extract of the plant of M. concanensis bark was identified by GC-MS analysis. The active principle with their molecular formula, in the hydro-alcoholic extract of the plant of M. concanensis bark. Ten compounds were detected in hydro-alcoholic extract of the whole bark. The results revealed that, Pantolactone (22.72%) was found as major component followed by DL-3-4 Dimethyl-3,4- hexanediol (14.05%), 3,4 dimethyl 5 hexen 3 – ol (14.05% The GC-MS chromatogram with peak area is given in (**Figure 1**). The important phyto-

components and structure identified in M. concanensis bark extract.

Discussion

Now a day the study of the organic compounds from plants and their activity has increased. Gas Chromatography - Mass Spectrometry (GC - MS) is a valuable tool for reliable identification of bioactive compounds [14]. In the present study, 15 compounds have been identified from the ethanol extract of leaf and 16 from bark of M. concanensis by GC - MS analysis [13,14]. The most abundant components found in the bark were Butanic acid, 1,5-Hepatadiene, 3,3, Dimethyl-(E) and 2-propanoic acid, 2 propanyl ester. Whereas bark extract contain important phytochemicals like, Squalene, 1-Hexanol, 2-ethyl-2-propyl, 1, 2-Benzenedicarboxylic acid, Hexanedioic acid, Heptane, Heptanoic acid, and Isooctanol. The identified phytochemicals and squalene has an antioxidant activity. It has been found that squalene possesses chemo□preventive activity against the colon carcinogenesis [15,16,17]. Phytol, a bioactive principle, detected from Sarcostemma secamone (L.) and M.concanensis is also found to be effective at different stages of arthritis. [18,19] It is found to give good as well as preventive and therapeutic results against arthritis. Reactive oxygen species-promoting substances such as phytol constitute a promising novel class of pharmaceuticals for the treatment of rheumatoid arthritis and possibly other chronic inflammatory diseases.[20] Different types of compounds were found in this fraction. Dehydroabietic acid was present in considerable amounts [21]. Dehydroabietic acid is an antibacterial, anti-inflammatory and potential antitumor-promoting agents. Flavonoids possess anticarcinogenic and anti-inflammatory properties. Chrysin is an anti-inflammatory and antibacterial activity [22,23,24].

Conclusion

The result shows that the work is significant with respect to its content of various phytochemical compounds as well. In the present work nearly thirty five biochemical compounds were identified in M. concanensis bark extract by GC-MS analysis. Further studies to be carry out in isolation and quantification of the compounds to analyze the antioxidant potential and need to evaluate in vivo studies are most significant to evaluate their natural biological activity.

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Conflict of interest

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

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