EUROPEAN JOURNAL OF BIOMEDICAL AND PHARMACEUTICAL SCIENCES
http://www.ejbps.com

ISSN 2349-8870
Volume: 12
Issue: 10
Year: 2025

MOLECULAR FINGERPRINTING OF SIDDHA DRUG PARANGIPATTAI CHOORANAM FOR OSTEOARTHRITIS OF KNEE USING FTIR AND GC-MS SPECTRAL ANALYSIS

Kaviya S.*[1], Sakthipriya V.[2], Sathish Kumar P.[3]

[1,2]Third Year PG Research Scholar, Department of Pothu Maruthuvam, Government Siddha Medical College Palayamkottai, Tirunelveli Affliated to The Tamilnadu Dr. MGR. Medical University, Chennai.
[3]Reader, Department of Pothu Maruthuvam, Government Siddha Medical College Palayamkottai, Tirunelveli affliated to The Tamilnadu Dr. MGR. Medical University, Chennai, Tamilnadu India.

***Corresponding Author: Dr. Kaviya S.**
Third year PG Research Scholar, Department of Pothu Maruthuvam, Government Siddha Medical College Palayamkottai, Tirunelveli Affliated to The Tamilnadu Dr. MGR. Medical University, Chennai.
DOI: https://doi.org/10.5281/zenodo.17311287

Article Received on 26/08/2025 **Article Revised on 16/09/2025** **Article Accepted on 07/10/2025**

ABSTRACT
Osteoarthritis of the knee is a prevalent degenerative joint disorder that significantly impairs mobility and quality of life, particularly among aging populations. In this context, Siddha medicine an ancient Indian traditional system offers a promising alternative or complementary approach, emphasizing holistic healing, affordability, and minimal side effects. Rooted in principles such as Pancha Bootham and Mukkutram, Siddha philosophy attributes osteoarthritis primarily to Vali humor imbalance, leading to joint degeneration, followed by Azhal and Iyyam disturbances causing inflammation and restricted movement. Parangipattai (*Smilax china*), a key herb in Siddha formulations, is traditionally used for musculoskeletal, dermatological, and systemic ailments. In the present study, Parangipattai Chooranam (PPC) was subjected to phytochemical characterization using Fourier Transform Infrared Spectroscopy (FTIR) and Gas Chromatography–Mass Spectrometry (GC-MS). FTIR analysis revealed functional groups associated with polyphenols, flavonoids, and terpenoids—compounds known for their anti-inflammatory, antioxidant, and chondroprotective activities. GC-MS identified several fatty acid methyl esters with immunomodulatory and regenerative properties relevant to osteoarthritis therapy. These findings support the ethnopharmacological use of PPC in managing Vatha-related conditions such as knee osteoarthritis. The integration of traditional Siddha knowledge with modern analytical techniques not only reinforces the therapeutic rationale of PPC but also emphasizes the need for further in vitro, in vivo, and clinical studies to ensure its efficacy and safety. This approach bridges traditional wisdom with contemporary science for holistic and evidence-based healthcare.

KEYWORDS: Parangipattai, FTIR, GC-MS, OA KNEE, Siddha.

INTRODUCTION
The World Health Organization (WHO) reports that approximately 70% to 80% of the population in several Asian and African countries rely on traditional systems of medicine as their primary source of health care.[6] In recent decades, there has been a notable resurgence of interest in the AYUSH systems of India—particularly in Siddha medicine, one of the oldest systems of traditional healing. This growing public inclination towards complementary and alternative medical systems is largely attributed to the increasing prevalence of chronic and lifestyle-related disorders, limitations of conventional therapies, and a global shift toward holistic and natural healing approaches. Among the various conditions where Siddha medicine has gained attention, **osteoarthritis of the knee** stands out as a significant focus, due to its high burden on the aging population and limited long-term treatment options in allopathic care. Osteoarthritis of the knee is a degenerative joint disorder characterized by progressive cartilage wear, subchondral bone changes, synovial inflammation, joint space narrowing, stiffness, and chronic pain. It severely affects mobility and quality of life, especially among older adults. While conventional medicine offers non-steroidal anti-inflammatory drugs (NSAIDs), corticosteroids, physical therapy, and eventually joint replacement surgeries, these interventions often come with potential side effects, high costs, and limited disease-modifying capacity. In this context, Siddha medicine is gaining attention as a viable alternative or complementary option, due to its natural origin, minimal side effects, affordability, and holistic treatment approach.

The Siddha system of medicine is built on foundational principles such as *Pancha Bootham* (five elemental forces: earth, water, fire, air, and space), *Mukkutram* (the three vital humors: Vali, Azhal, and Iyyam), and the *96 Thathuvas* (fundamental principles governing physical and mental health). **According to Siddha philosophy, disease arises due to *Amam* which leads to imbalance Mukkutram**, and osteoarthritis is primarily linked to derangement in the Vali humor, leading to joint dryness, degeneration, and pain followed by Pitha humour imbalance were Inflammatory cytokines are released and warmth was present. Iyyam humour was affected which leads to Restricted movement, Swelling.

Siddha treatment protocols aim to restore humoral balance through internal herbal formulations, external therapies like medicated oil massages, fomentation (*Podi kizhi*), yoga, dietary modifications, and rejuvenation therapies (*Kayakalpam*). Several Siddha formulations are traditionally used for the management of osteoarthritis and related musculoskeletal disorders, offering not just symptom relief but also improving joint health, circulation, and tissue regeneration. **Parangipattai** is a well-known medicinal plant widely used in the Siddha system of medicine. Revered for its versatile therapeutic potential, it has been used to manage skin disorders, venereal diseases, urinary tract infections, rheumatic conditions, and venpulli (vitiligo).[3] Its root is rich in phytoconstituents such as flavonoids, saponins, glycosides, β-sitosterol, and resveratrol, which contribute to its broad-spectrum pharmacological actions. Its presence in formulations aimed at detoxification, rejuvenation and immune regulation makes it a cornerstone herb in Siddha therapeutics.

In the present era of evidence-based medicine, there is an increasing emphasis on scientifically validating the efficacy and safety of Siddha drugs to bridge the gap between traditional knowledge and modern medical science. Techniques such as **Gas Chromatography–Mass Spectrometry (GC-MS)** and **Fourier Transform Infrared Spectroscopy (FTIR)** are widely used to analyse the phytochemical constituents and functional groups present in Siddha formulations. The integration of traditional Siddha wisdom with modern scientific methods not only enhances the reliability and credibility of these formulations but also facilitates their wider acceptance in mainstream and global health systems. With rising patient preference for natural therapies and chronic disease management, the scientific exploration and validation of Siddha formulations for conditions such as osteoarthritis of the knee are not just desirable but essential. It paves the way for developing safe, affordable, and effective alternatives that complement conventional treatments and promote a holistic model of health care rooted in both tradition and science.

MATERIALS AND METHODS

Drug Reference: GUNAPADAM PORUTPANBU PART 1 K.S. MURGESHA MUTHALIYAAR.[5]

Drug Ingredients

Table 1: Details of Plant Parangipattai.

Drug Name	Botanical Name	Family	Part used
PARANGIPATTAI	*Smilax china.Linn*	Smilacaceae	Root

Purification

The Drug was brought from Authenticated Raw drug store drug and authenticated in Gunapadam department of Government Siddha Medical college and Hospital, Tirunelveli. After that the drug was dried made into a powder which then purified by Pittaviyal Method (steam cooking in milk) as mentioned in Pathartha guna Sinthamani. A mud pot was taken and it was half filled by milk and half filled by pure water; the mouth of the pot was sealed by a cloth. This chooranam then placed over the cloth and the pot was heated for 3 Hours (1 Saamam). Later drug was dried and powdered then sieved.

Indication: Vatha related disease, Skin disease.

FTIR Analysis

Sample processed using Bruker Alpha-E by ATR module (attenuated total reflectance). Sample positioned on the Crystal platform with perfect alignment of keeping anvil in up position. To ensure that the sample makes good contact angle with the crystal prior to start of the IR radiation exposure. Spectra measurement was achieved with desired wavelength and the corresponding observational peaks/ waves were recorded with wavenumber were subjected to further interpretation. Software used for the analysis is OPUS version 7 for functional group analysis. Signal detection processed through DTGS detector. Baseline correction adjusted as per the requirement.[1]

GC-MS Analysis

Derivatization procedure

For the crude ethanol extracts, a small amount of concentrated sample was taken in a separating funnel and shaken by adding water and ethyl acetate in the ratio of 1:4. The upper layer was collected and concentrated in rotary evaporator to about 1.5 ml. Added 100µl N, O-Bis(trimethylsilyl)trifluoroacetamide and trimethyl chlorosilane (BSTFA+TMCS) and 20µl pyridine and heated at 60°c for 30 minutes. For the layers which are separated from the crude extracts, a small amount of extract was taken and evaporated out totally. To this added acetonitrile and filtered into a conical flask. To the filtrate added 50µl BSTFA+TMCS and heated at 60°c in a water bath for 30 minutes. Filtered using 0.45µ membrane filter to a vial.

GC-MS Procedure

Gas chromatography (GC) analysis was carried out using Agilent 6890N gas chromatography equipped with photon multiplier tube as detector coupled to front injector type 1079. The chromatograph was fitted with HP 5 MS capillary column (30 m ×0.25 mm i.d., film thickness 0.25 _m). The injector temperature was set at 250°C, and the oven temperature was initially at 70 °C hold for 4 mins then programmed to 200°C at the rate of 10°C/min and finally held at 200 °C for 13 min. Helium was used as a carrier gas with the flow rate of 1.5 ml/min. 0.2 micro liter of the sample-SA(diluted with methanol 1:10) were injected in the split less mode. The percentage of composition of the samples were calculated by the GC peak areas. GC–mass spectrometry (GC–MS) analysis of sample was performed using Agilent gas chromatography equipped with JEOL GC MATE-II HR Mass Spectrometer. GC conditions were the same as reported for GC analysis and the same column was used. The mass spectrometer was operated in the electron impact mode at 70 eV. Ion source and transfer line temperature was kept at 250°C. The mass spectra were obtained by centroid scan of the mass range from 50 to 600 amu. The compounds were identified based on the comparison of their retention indices (RI), retention time (RT), mass spectra of WILEY, NIST library data of the GC-MS system and literature data (Adams, 2009).[2]

RESULTS AND DISCUSSION

FT-IR Analysis

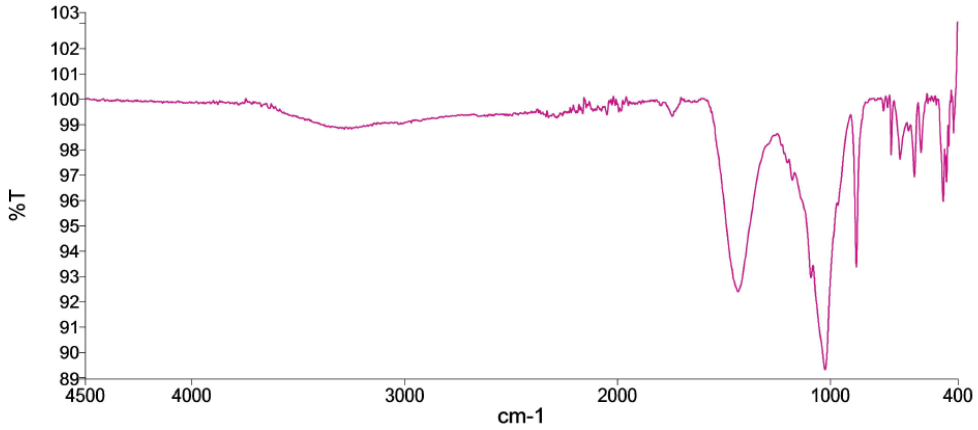

Figure 1: FT-IR spectrum of PPC.

Table 2: FT-IR Peak Table.

S.NO	Peak Position (cm^{-1})	Functional Group / Vibration Type	Possible Phytoconstituents
1.	~3390–3400	O–H stretching (broad)	Alcohols, phenols, flavonoids, tannins
2.	~2920–2850	C–H asymmetric and symmetric stretching (–CH_2/–CH_3 groups)	Aliphatic compounds, fatty acids, terpenes
3.	~1740–1700	C=O stretching (ester, aldehyde, or ketone)	Flavonoid glycosides, triterpenoids, fatty acids esters
4.	~1625–1600	C=C stretching / N–H bending (aromatic rings or amines)	Aromatic compounds, flavonoids, amides
5.	~1410–1380	–CH_3 symmetric bending, COO^- symmetric stretching	Organic acids, polysaccharides
6.	~1260–1200	C–O–C asymmetric stretching / phenolic –OH bending	Esters, ethers, polyphenols
7.	~1080–1020	C–O stretching (alcohols, carbohydrates, ethers)	Polysaccharides, glycosides
8.	~875–700	Aromatic C–H out-of-plane bending	Aromatic rings, phenolic structures
9.	~600–500	Fingerprint region (C–Br, C–I, or metal–oxygen bonds)	Alkaloids, minerals, trace of Phyto-metallic conjugates

The FTIR spectral analysis of Parangipattai Chooranam (PPC) revealed the presence of a broad spectrum of functional groups indicative of diverse phytochemical constituents. Major absorption peaks observed in the range of ~3390–3400 cm^{-1} (O–H stretching) correspond to hydroxyl groups commonly found in phenols,

flavonoids, and tannins. These compounds are well-documented for their potent antioxidant and anti-inflammatory activities, which are highly relevant in the context of osteoarthritis (OA) of the knee, a degenerative joint disease characterized by chronic inflammation, oxidative stress, and progressive cartilage degradation. The spectral region around ~2920–2850 cm^{-1} suggests the presence of aliphatic chains and fatty acid components, potentially contributing to membrane stabilization and anti-inflammatory effects.

Peaks in the region of ~1740–1700 cm^{-1}, attributed to carbonyl (C=O) stretching of esters and ketones, are indicative of flavonoid glycosides, triterpenoids, and fatty acid esters[7], classes of compounds that have demonstrated efficacy in inhibiting inflammatory mediators such as TNF-α, IL-1β, and COX-2, which play a central role in OA pathophysiology.

Furthermore, aromatic C=C stretching and N-H bending observed in the ~1625–1600 cm^{-1} region suggest the presence of aromatic amines and flavonoids, which may exert chondroprotective effects by downregulating matrix metalloproteinases (MMPs) involved in cartilage breakdown.

Functional group vibrations in the ~1410–1380 cm^{-1} region point to symmetric bending and COO^- stretching, confirming the presence of organic acids and polysaccharides that may support extracellular matrix integrity and synovial fluid viscosity. Additional signals in the fingerprint region (~600–500 cm^{-1}) are indicative of metal-oxygen and halogen bonds, suggesting the presence of alkaloids and trace minerals. These elements may contribute to joint tissue repair, mineralization, and modulation of inflammatory pathways at the cellular level.

GC-MS Analysis

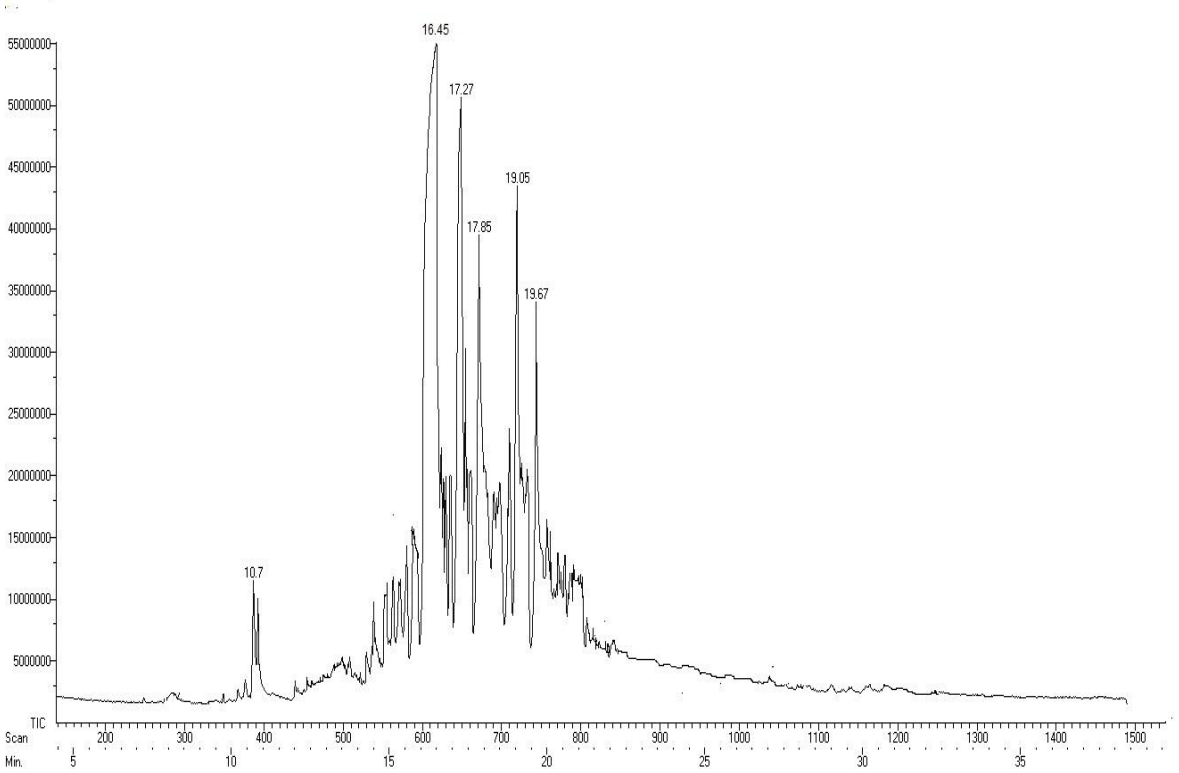

Figure 2: GC profiling of Parangipattai chooranam.

Table 3: Bioactive compounds of Parangipattai chooranam.

S.NO	Retention time	Molecule identified in NIST Library
1.	10.7	2-Propenoic acid, Methyl ester
2.	16.45	Pentadecanoic acid, Methyl ester
3.	17.27	Pentadecanoic acid,13- Methyl, Methyl ester
4.	17.85	2-Butenedoic acid(Z), Monododecyl ester
5.	19.05	Heptadecanoic acid, 15 Methyl, Methyl ester
6.	19.67	Octadecanoic acid, 6-hydroxy, Methyl ester

GC-MS analysis of Parangipattai Chooranam, a classical herbal Siddha formulation, revealed the presence of multiple bioactive constituents, predominantly fatty acid methyl esters, which may contribute to its traditional use in managing osteoarthritis (OA) of the knee.

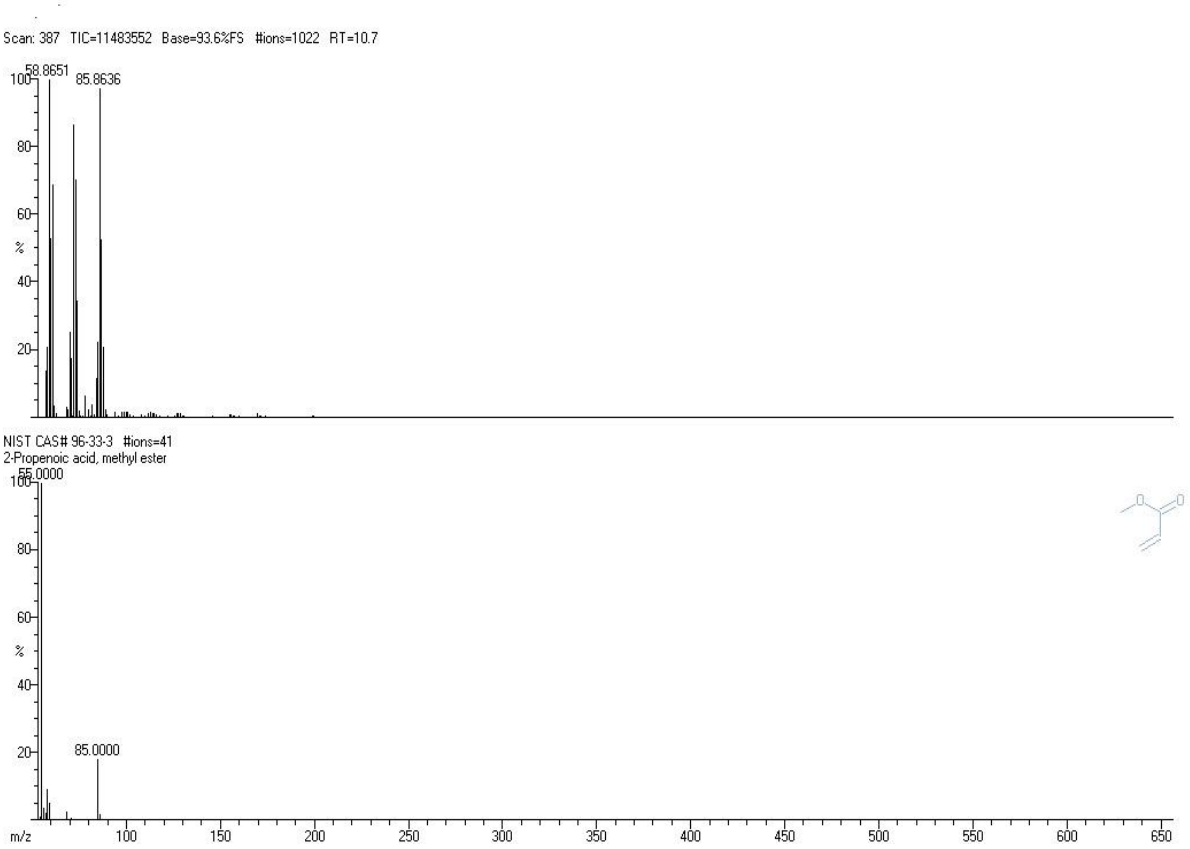

Figure 3: Methyl 2-propenoate.

From the fig 3, the compound Methyl 2-propenoate (RT: 10.7 min) may enhance the percutaneous absorption of co-existing bio actives in herbal preparations. Its presence could potentially facilitate the bioavailability of therapeutic constituents across joint tissues.

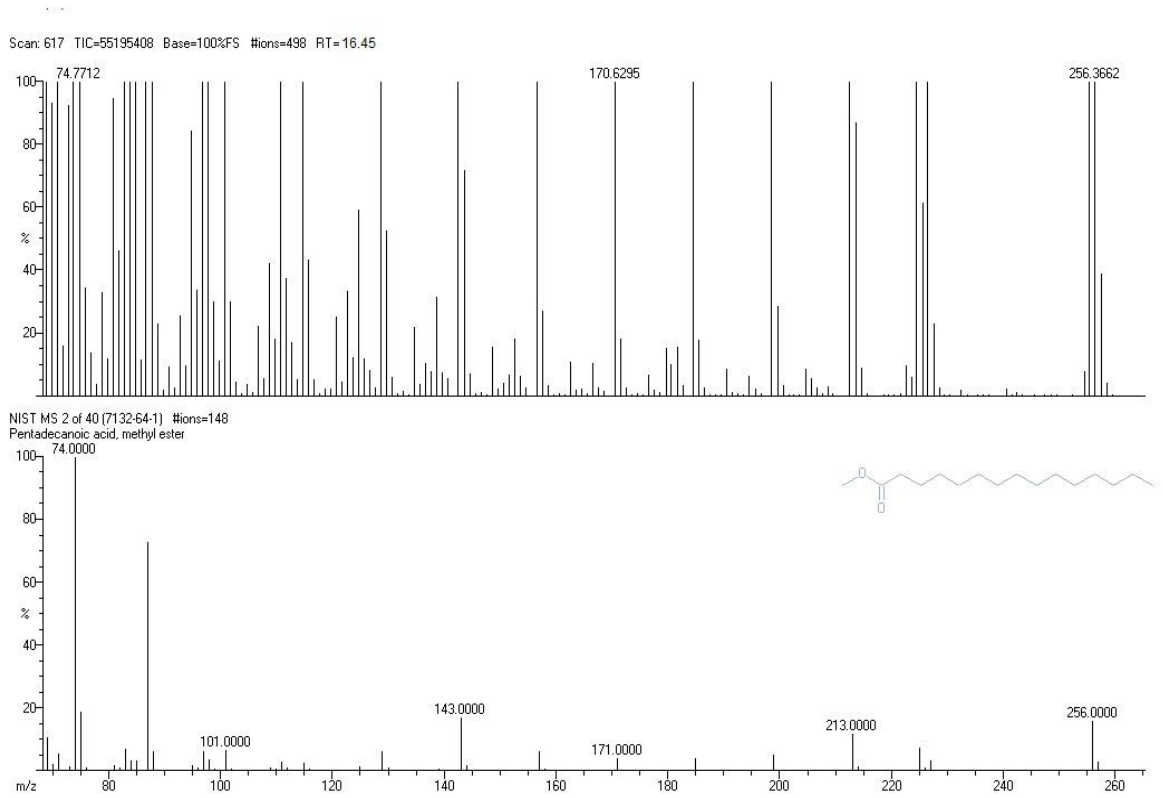

Figure 4: Pentadecanoic acid, methyl ester.

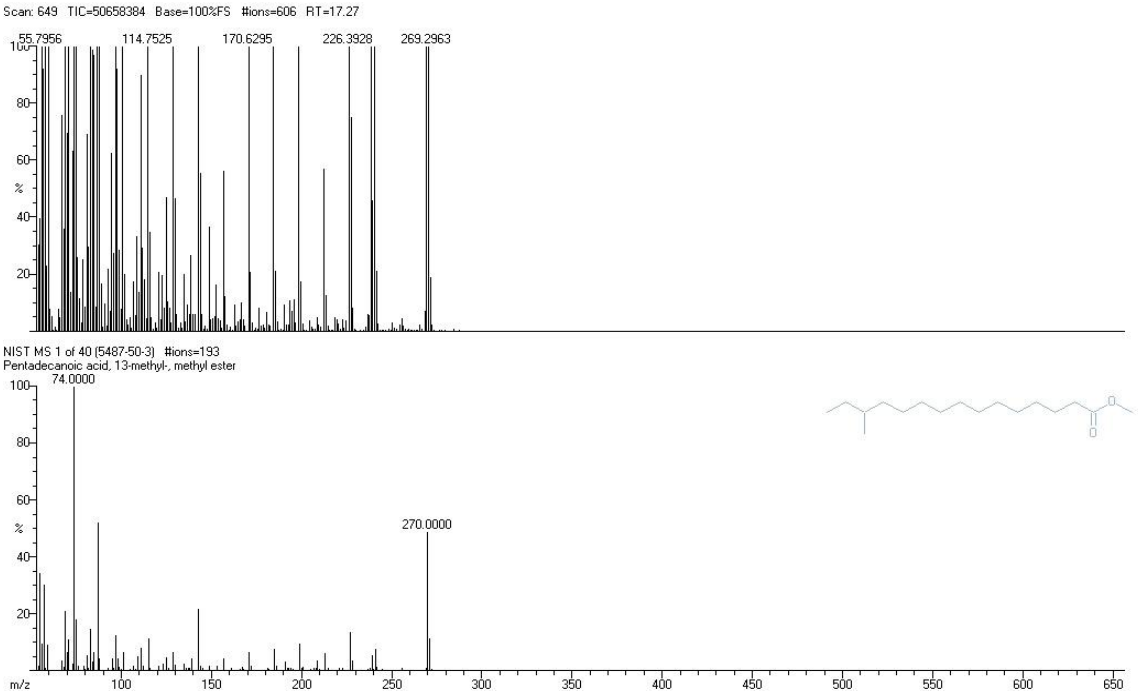

Figure 5: 13-methylpentadecanoic acid, methyl ester.

Pentadecanoic acid, methyl ester (RT: 16.45 min) and 13-methylpentadecanoic acid, methyl ester (RT: 17.27 min) are saturated and branched-chain fatty acid derivatives, respectively, which have demonstrated notable anti-inflammatory and antioxidant properties in experimental models.[4] These properties are crucial in osteoarthritis management, where inflammatory cytokines such as IL-1β and TNF-α play a major role in cartilage destruction and synovitis.

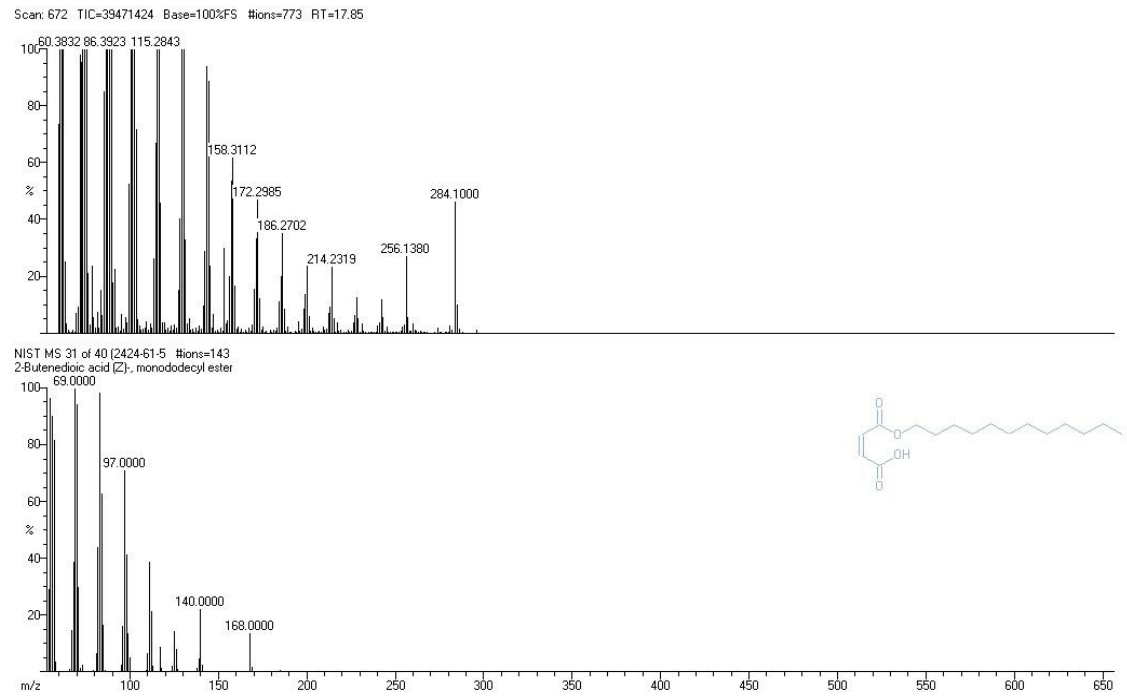

Figure 6: (Z)-2-Butenedioic acid, monododecyl ester.

The compound (Z)-2-Butenedioic acid, monododecyl ester (RT: 17.85 min), from above fig.6, states that it was an ester derivative of fumaric acid, which may possess lipid-regulating and anti-inflammatory activities and support its potential to modulate joint inflammation. On note it improve lipid metabolism within inflamed synovial fluid.

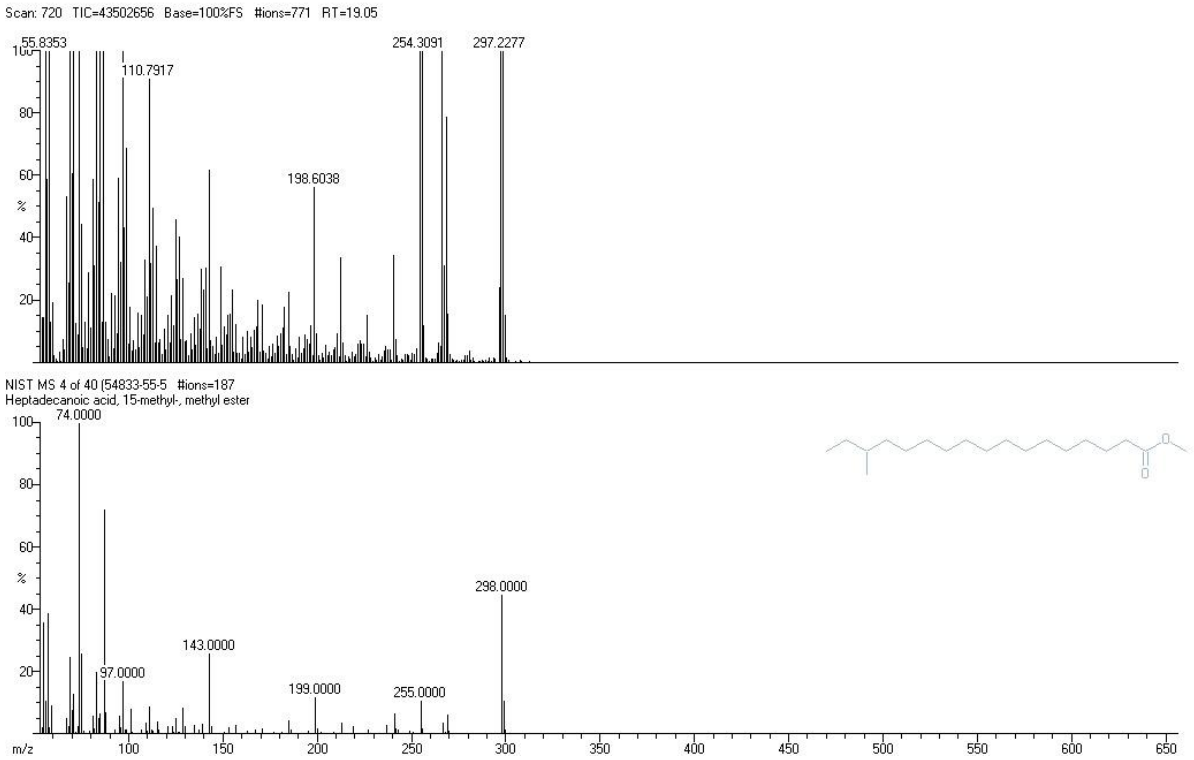

Figure 7: 15-methyl-heptadecanoic acid, methyl ester.

15-methyl-heptadecanoic acid, methyl ester (RT: 19.05 min), another branched-chain fatty acid methyl ester, has been associated with immunomodulatory effects. Its role in downregulating inflammatory markers and maintaining joint homeostasis may help alleviate OA symptoms, particularly in chronic conditions.

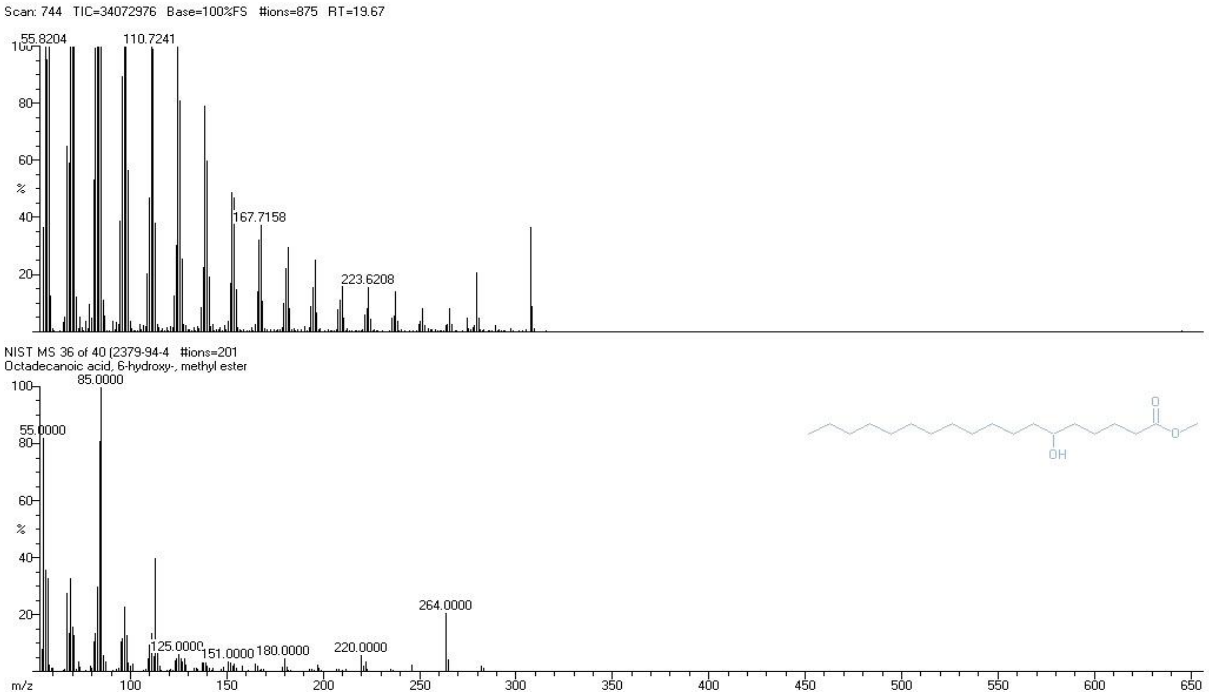

Figure 8: 6-hydroxy-octadecanoic acid, methyl ester.

Furthermore, 6-hydroxy-octadecanoic acid, methyl ester (RT: 19.67 min), a hydroxylated fatty acid, is known for its wound-healing, antioxidant, and chondroprotective actions. It may contribute to cartilage regeneration, synovial membrane repair, and lubrication of joint tissues—an essential aspect of OA therapy.

CONCLUSION

The comprehensive phytochemical evaluation of Parangipattai Chooranam (PPC) through FTIR and GC-MS analyses reveals the presence of a diverse array of bioactive constituents that may underlie its traditional therapeutic efficacy in osteoarthritis of the knee. FTIR spectral data confirmed the presence of key functional groups associated with polyphenols, flavonoids, organic acids, and terpenoids—compounds well-documented for their antioxidant, anti-inflammatory, and chondroprotective activities. These functional groups are particularly relevant in the context of osteoarthritis, which involves chronic inflammation, oxidative stress, and progressive cartilage degeneration. Complementarily, the GC-MS analysis identified several fatty acid methyl esters and related derivatives, including pentadecanoic acid methyl ester, 13-methylpentadecanoic acid methyl ester, and 6-hydroxy-octadecanoic acid methyl ester. These compounds are known to possess anti-inflammatory, immunomodulatory, and regenerative properties, which align with the pharmacological requirements of osteoarthritis management. Collectively, the results substantiate the ethnopharmacological relevance of PPC and provide a scientific rationale for its traditional use in Siddha medicine for musculoskeletal disorders classified under Vatha conditions. The presence of multi-targeted bioactive compounds supports its potential role as a complementary therapeutic agent in the management of knee osteoarthritis. However, further studies, including in vitro, in vivo, and clinical investigations, are warranted to elucidate the pharmacodynamic mechanisms, optimize dosage regimens, and ensure safety and efficacy in human populations.

Declaration by Authors

ACKNOWLEDGEMENT: NONE.

Source of Funding: None.

Conflict of Interest: The authors declare no conflict of interest.

REFERENCES

1. https://people.chem.ucsb.edu/neuman/robert/orgchembyneuman.book/15%20EstersAmidesRelated/15Separates/15Text.pdf
2. https://sciencesolutions.wiley.com/solutions/technique/gc-ms/wiley-registry-nist-mass-spectral-library/
3. Qadir A, Aqil M, Ali A, Ahmad FJ, Ahmad S, Arif M, Khan N. GC-MS analysis of the methanolic extracts of *Smilax china* and *Salix alba* and their antioxidant activity. Turk J Chem., Apr. 1, 2020; 44(2): 352-363. doi: 10.3906/kim-1907-5. PMID: 33488162; PMCID: PMC7671229.
4. Singh D, Mehghini P, Rodriguez-Palacios A, Di Martino L, Cominelli F, Basson AR. Anti-Inflammatory Effect of Dietary Pentadecanoic Fatty Acid Supplementation on Inflammatory Bowel Disease in SAMP1/YitFc Mice. Nutrients, Sep. 8, 2024; 16(17): 3031. doi: 10.3390/nu16173031. PMID: 39275347; PMCID: PMC11397537.
5. Vaithiyarathinam K.S Murugesa Muthaliyar, GunapadamMooligai, published by Director of Indian medicine and Homeopathy, chennai., 106.
6. WHO guidelines for assessing quality of herbal medicines with reference to contaminants and residues, World Health Organization, Geneva, 2007.
7. Gaddam, Susmila & Kotakadi, Venkata Subbaiah & Allagadda, Rajasekar & Vasavi, Thirumalanadhuni & Siva Gayathri, Velakanti & Samanchi, Srilakshmi & Thangellamudi, Devaraju & Masarapu, Hema & P, Uma & Ch, Appa & Zereffa, Enyew. Bioinspired multifunctional silver nanoparticles by Smilax Chenensis and their enhanced biomedical and catalytic applications. Scientific Reports., 2024; 14. 10.1038/s41598-024-77071-9.