

GCMS Profiling of Bioactive Phytocompounds in *Irumal Maathirai*: A Traditional Siddha Polyherbo-Mineral Formulation for Cough and Respiratory Ailments

Dr Sathya Priya R¹, Dr G Chenthamarai Selvi²

¹PG Scholar, Department of Nanju Maruthuvam, Government Siddha Medical College and Hospital, Palayamkottai, Tamil Nadu, India.

²Assistant Professor, Department of Nanju Maruthuvam, Government Siddha Medical College and Hospital, Palayamkottai, Tamil Nadu, India.

Corresponding author: Dr Sathya Priya R

DOI: <https://doi.org/10.52403/ijrr.20260566>

ABSTRACT

Irumal Maathirai (IM) is a classical Siddha polyherbal-mineral formulation used for the management of *Irumal* (Cough) and various other respiratory ailments.

Objective: The objective of this study is to characterize the volatile and semi-volatile bioactive compounds present in *Irumal maathirai* by Gas Chromatography and Mass Spectrometry method.

Methods: An ethanolic extract of *Irumal maathirai* was subjected to GC-MS profiling, with compound identification achieved by cross-referencing mass spectra against the NIST library database.

Results: Several distinct peaks were revealed in The Total Ion Chromatogram (TIC). Predominant compounds identified include 10-Octadecenoic acid, methyl ester, Pentadecanoic acid, 13-methyl-, methyl ester, Pyrimidine-5-carboxylic acid, 1,4-dihydro-4-(2-furyl)-1,6-dimethyl-2-methylthio-, ethyl ester, 2-Isopropenyl-4,4,7a-trimethyl-2,4,5,6,7,7a-hexahydrobenzofuran-6-ol.

Conclusion: The identified compounds possess established pharmacological properties, including anti-inflammatory, antimicrobial, bronchodilator and anti-

oxidant effects, which provides a scientific rationale for the traditional therapeutic efficacy of *Irumal Maathirai* in treating various respiratory ailments, supporting its potential as a standardized phytopharmaceutical.

Keywords: *Irumal maathirai*, GC-MS, cough, anti-inflammatory, antimicrobial, bronchodilator, siddha medicine.

INTRODUCTION

Traditional medicine systems have served the world as the primary healthcare backbone for civilizations. Among the various traditional system, Siddha system of medicine is one the oldest traditional treatment modalities originated from the Tamil land of South India.

The Siddha system of medicine relies to the philosophy of "Pancha Bootha" (five elements) theory, which perceives the human body as a microcosm of the universe. It functions on the basis of fundamental principle of maintaining a balance between the three humors: vatham, pitham, kapham. It stands out for its unique use of not just herbs, but also minerals and metals. Within the extensive pharmacopeia, herbo-mineral formulations hold a significant place due to

their perceived potency and therapeutic longevity.

According to the recent report of WHO, respiratory ailments are the 6th leading cause of death. Forum of International Respiratory Societies (FIRS) states that global indoor and outdoor air quality has become worse and exceeds WHO guideline limits. Cough is the most common and predominant symptom encountered in almost all respiratory ailments. However, it can also be a manifestation of various other health conditions. Sometimes, it is self-limiting in nature and sometimes it is the sign of life-threatening serious illness. Chronic cough is more complex and affects approximately 8%-10% of the global population. Nearly 25% of the patients continue to cough (post infectious cough) after the infection has been settle down.

Various treatment modalities have been employed to treat cough. Yet it challenges various global treatment system. One such is Siddha system of medicine which is widely practiced in south India. This system emphasizes various formulation for the treatment of respiratory disorders. One of such classical formulation is Irumal maathirai, a polyherbal-mineral drug indicated for respiratory ailments. The formulation uses various plant and mineral drug including *Glycyrrhiza glabra*, *Aloe barbadensis*, *Piper nigrum* and *Sodium baborate*. The ingredients used in the formulation of Irumal Maathirai have proven anti-inflammatory, anti-microbial, demulcent, anti-oxidant and broncho dilatory effects.

Though the formulation has been used for centuries, its therapeutic efficacy has to be evaluated to meet out the global standards. Phytochemical analysis Irumal maathirai contains various flavonoids, steroids, triterpenoids, phenolic compounds, tannins, and saponins. GCMS profiling of Ethanolic Extract of Irumal Maathirai has been done to isolate the volatile and semi volatile compounds which have therapeutic potential.

MATERIALS AND METHODS

Preparation of the formulation:

The raw drugs used in the formulation of Irumal Maathirai were collected from the authentic herbal drug store in Nagercoil and the drugs were authenticated by the head of the department of Gunapadam, Govt Siddha Medical College, Palayamkottai. The raw drugs were purified and processed and Irumal maathirai was formulated as per classical siddha literature, *Kannusamy Parambarai Vaithiyam*.

Preparation of the extracts for GCMS analysis:

The crude ethanol extracts were prepared by liquid-liquid fractionation method where the metabolites were separated based on their affinity for different solvents. A portion of concentrated ethanolic extract were transferred to a separating funnel. Water and ethyl acetate were added to the extract in the ratio of 1:4 and mixed well by shaking and later allowed to settle. The resulting upper organic phase by organic solvent Ethyl acetate, holding non-polar and semi-polar compound, is transferred carefully. This organic phase is concentrated by removing the excess solvent with the help of rotatory evaporator.

The concentrated compounds were subjected for chemical transformation, silylation, by adding derivatizing agents. A mixture of N, O-Bis(trimethylsilyl)trifluoroacetamide, trimethylchlorosilane (BSTFA + TMCS) and pyridine were added and heated at 60° C for 30 minutes in order to make the molecules more stable and volatile during GCMS procedure.

A small portion of this silylated sample is taken and dried to make it totally free from moisture content. The dried sample is mixed with Acetonitrile and filtered. A mixture of BSTFA and TMCS reagent were added and mixed altogether and heated using boiling water bath at 60° C for about 30 minutes. The solution is filtered through a 0.45 micrometer membrane filter and the obtained clear filter is transferred to chromatography vial.

GC-MS Analysis:

GCMS Analysis was done with Agilent 6890N gas chromatograph with JEOL GC MATE-II HR Mass Spectrometer. A portion of drug sample is dilute with methanol in the ratio of 1:10 and 0.2 micro milliliter is injected into the chromatography column in which helium gas flows at the rate of 1.5ml/min. Under stable thermal conditions (250° C), separation occurs. The separated compounds are allowed to enter the mass spectrometer. A beam of high energy electron (70e V) is bombarded to the compounds and the ionized molecules were scanned across a mass range of 50-600 amu. The data which created a molecular fingerprint is captured

and identified. Based on the retention time (RT) and retention indices (RI), the identified compounds were interpreted with digital database of (NIST) National Institute of Standard and Technology.

RESULTS AND DISCUSSION

GC-MS profiling of the ethanolic extract of Irumal Maathirai identified various bioactive compounds primarily consisting of long-chain aliphatic amines, fatty acid esters, and complex bioactive steroidal derivatives. The obtained chromatogram of the Irumal Maathirai were shown in figure 1 and the identified compounds were tabulated in table 1.

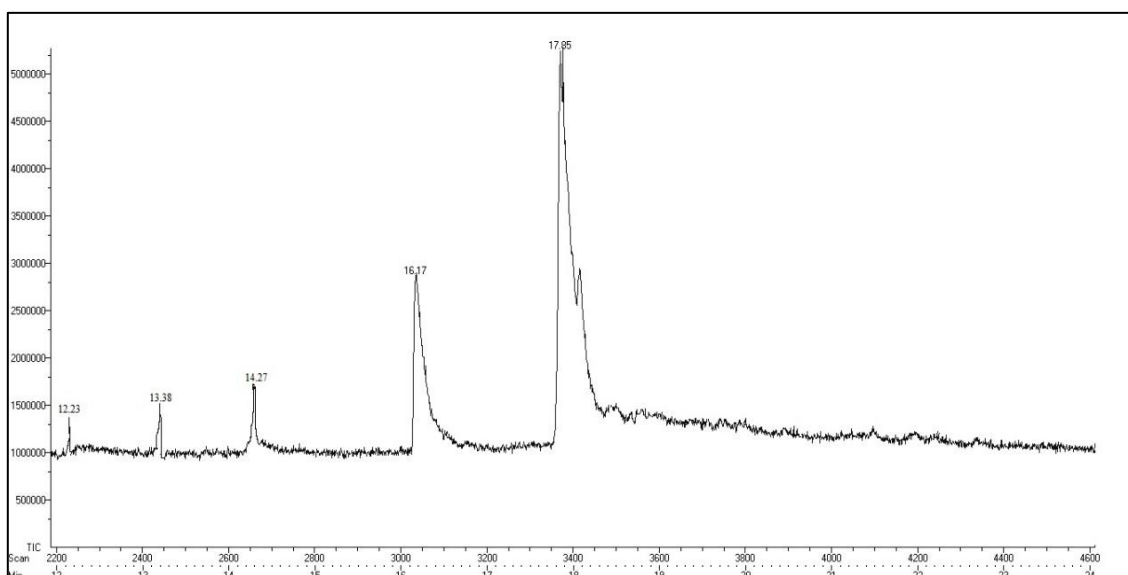


Fig. 1: GC-MS chromatogram of ethanolic extract of irumal maathirai

Significant intense peaks were observed between the retention times (RT) of 12.23 and 17.85 which were tabulated in table in 1. Among the compounds identified, 10-Octadecenoic acid, methyl ester (RT 17.85

mins) is highly abundant followed by Pentadecanoic acid, 13-methyl-, methyl ester (RT 16.17 mins). minor peaks were identified at RT of 12.23, 13.38 and 14.27 minutes.

Table 1: Bioactive compounds identified in ethanolic extract of Irumal Maathirai

S.no.	Retention time (minutes)	Name of the bioactive compounds
1	12.23	2-Isopropenyl-4,4,7a-trimethyl-2,4,5,6,7,7a-hexahydrobenzofuran-6-ol
2	13.38	2,7-Octanedione, 4,4-dimethyl-3-[2-(1-hydroxy-1-methylethyl)-3-methyl-3-butenylidene]-
3	14.27	Pyrimidine-5-carboxylic acid, 1,4-dihydro-4-(2-furyl)-1,6-dimethyl-2-methylthio-, ethyl ester
4	16.17	Pentadecanoic acid, 13-methyl-, methyl ester
5	17.85	10-Octadecenoic acid, methyl ester

[2],[3] 10-Octadecenoic acid, methyl ester, commonly known as methyl oleate, Methyl 10-octadecenoate, is an unsaturated fatty acid methyl ester. It is a potent surfactant and lubricant. [4] Studies confirm that 10-octadecanoic acid hold both antioxidant and antimicrobial property. [5] Docking studies confirms that the compound strongly binds to bacterial proteins and inhibits bacterial growth. [6] Beyond the anti-bacterial property, studies demonstrate that it significantly inhibit the growth of fungal pathogens and posses antifungal action. [7] It scavenges the free radical and provides protection against oxidative damage. Also, it effectively reduces inflammatory markers thereby showing its anti-inflammatory property.

[8][9] Pentadecanoic acid is an essential saturated fatty acid and various research suggests that it activates AMPK and inhibits mTOR pathways, effectively establishing longevity. It effectively lowers pro-inflammatory markers and exhibit anti-inflammatory activity. It also identified to

possess anti-fibrotic and anticancer and anti microbial activity.

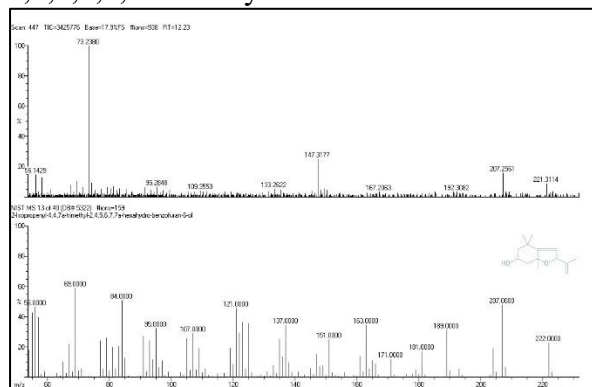
[10] Pyrimidine-5-carboxylic acid, 1,4-dihydro-4-(2-furyl)-1,6-dimethyl-2-methylthio-, ethyl ester is a Dihydropyrimidine derivative.

[11] Dihydropyrimidines play a vital role in synthesis of nucleic acids. Recent research reveal that this compound posses anti-inflammatory, antioxidant, anti-microbial, anti-hypertensive and analgesic activity.

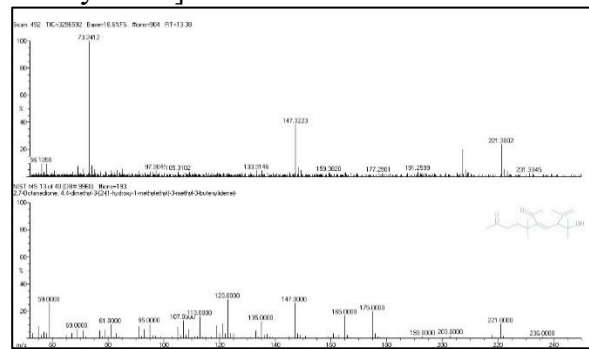
[12] 2-Isopropenyl-4,4,7a-trimethyl-2,4,5,6,7,7a-hexahydro-benzofuran-6-ol is a terpenoid derivative contributing to aromatic and volatile nature of the drug. [13] This volatile terpenoid is known to have decongestant and expectorant qualities. They interact with mucous clearance and act as mild bronchodilator.

2,7-Octanedione, 4,4-dimethyl-3-[2-(1-hydroxy-1-methylethyl)-3-methyl-3-butenylidene]- is a Dione structure with specific aroma and have the property of neutralizing reactive oxidant species.

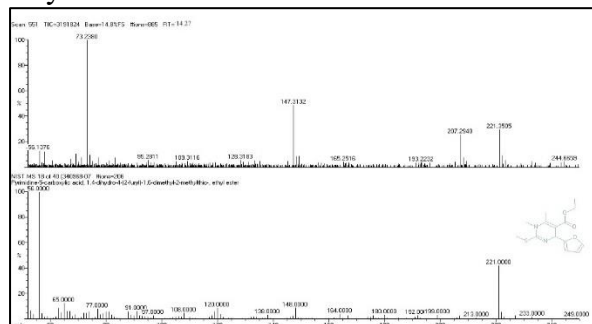
2-Isopropenyl-4,4,7a-trimethyl-2,4,5,6,7,7a-hexahydrobenzofuran-6-ol



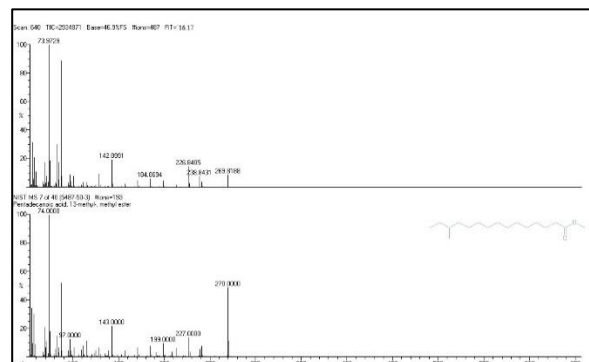
2,7-Octanedione, 4,4-dimethyl-3-[2-(1-hydroxy-1-methylethyl)-3-methyl-3-butenylidene]-



Pyrimidine-5-carboxylic acid, 1,4-dihydro-4-(2-furyl)-1,6-dimethyl-2-methylthio-, ethyl ester



Pentadecanoic acid, 13-methyl-, methyl ester



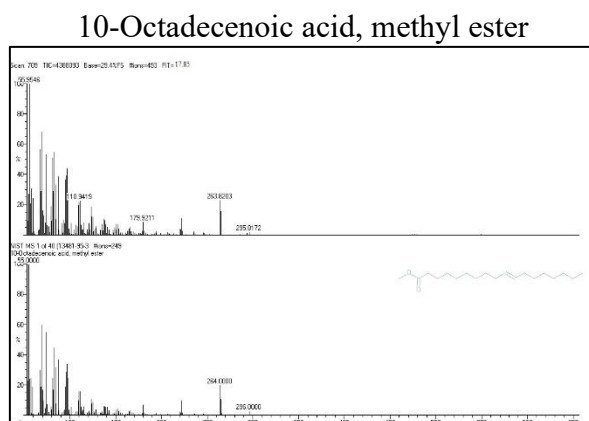


Figure 2. Total Ion Chromatogram (Tic) Of The Compounds Identified (Upper Image) With Matching(Lower Image) From Nist Library Database

CONCLUSION

The identified compound from an ethanolic extract of Irumal maathirai possess anti-inflammatory, anti-microbial, anti-fungal, decongestant, expectorant, bronchodilator and antioxidant properties. The compounds altogether reduce the inflammation in airways and would decrease mucosal accumulation. They also help in bronchial smooth muscle relaxation and facilitate easier breathing. They also help in clearing the invading pathogens. The anti-oxidant property of the identified compounds reduce damage from free radicals and maintain the structural integrity of airways.

Declaration by Authors

Ethical Approval: Approved

Acknowledgement: None

Source of Funding: None

Conflict of Interest: No conflicts of interest declared.

REFERENCES

1. National institute of standards and technology, NIST standard reference database 69: NIST chemistry webbook.
2. <https://cymitquimica.com/cas/17257-43-1/>
3. National Center for Biotechnology Information (2026). PubChem Compound Summary for CID 25642, Methyl 10-octadecenoate. Retrieved April 28, 2026 from <https://pubchem.ncbi.nlm.nih.gov/compound/Methyl-10-octadecenoate>.
4. Ali, J., Ikram, M., Zahoor, M. *et al.* Role of phytochemicals present in *Azadirachta indica* leaves extracts in controlling toxigenic fungi and inhibition of aflatoxins biosynthesis. *Discov Food* **6**, 104 (2026). <https://doi.org/10.1007/s44187-026-00845-9>
5. Almuhayawi, M. S., Alruhaili, M. H., Gattan, H. S., Alharbi, M. T., Nagshabandi, M. K., Hagagy, N., Almuhayawi, S. M., Al Jaouni, S. K., Selim, S., Mostafa, E. M., & Elnosary, M. E. (2024). *In vitro* and *in silico* biopotentials of phytochemical compositions and antistaphylococcal and antipseudomonal activities of volatile compounds of *Argania spinosa* (L.) seed oil. *Frontiers in bioengineering and biotechnology*, *12*, 1348344. <https://doi.org/10.3389/fbioe.2024.1348344>
6. Krishnappa, S., Karthik, Y., Pratap, G. K., Shantaram, M., Umarajashekhar, A., Soumya, J., Bhatt, B., Sayed, S. M., Alhelaify, S. S., Aharthy, O. M., & Mushtaq, M. (2024). Exploration of bioactive compounds from *Olea dioica* in Western Ghats of Karnataka using GC-MS. *Biotech*, *14*(3), 63. <https://doi.org/10.1007/s13205-023-03888-2>
7. Alqahtani, F. Y., Aleanizy, F. S., Mahmoud, A. Z., Farshori, N. N., Alfaraj, R., Al-Sheddi, E. S., & Alsarra, I. A. (2019). Chemical composition and antimicrobial, antioxidant, and anti-inflammatory activities of *Lepidium sativum* seed oil. *Saudi journal of biological sciences*, *26*(5), 1089–1092. <https://doi.org/10.1016/j.sjbs.2018.05.007>
8. National Center for Biotechnology Information (2026). PubChem Compound Summary for CID 13849, Pentadecanoic Acid. Retrieved April 28, 2026 from <https://pubchem.ncbi.nlm.nih.gov/compound/Pentadecanoic-Acid>.

9. Venn-Watson, S., & Schork, N. J. (2023). Pentadecanoic Acid (C15:0), an Essential Fatty Acid, Shares Clinically Relevant Cell-Based Activities with Leading Longevity-Enhancing Compounds. *Nutrients*, 15(21), 4607. <https://doi.org/10.3390/nu15214607>
10. National Center for Biotechnology Information (2026). PubChem Compound Summary for CID 332931, 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-methyl-2-oxo-4-(2-thienyl)-, ethyl ester. Retrieved April 28, 2026 from <https://pubchem.ncbi.nlm.nih.gov/compound/332931>.
11. Kaur, R., Chaudhary, S., Kumar, K., Gupta, M. K., & Rawal, R. K. (2017). Recent synthetic and medicinal perspectives of dihydropyrimidinones: A review. *European journal of medicinal chemistry*, 132, 108–134. <https://doi.org/10.1016/j.ejmech.2017.03.025>
12. National Center for Biotechnology Information (2026). PubChem Compound Summary for CID 536443, 2-Isopropenyl-4,4,7a-trimethyl-2,4,5,6,7,7a-hexahydro-benzofuran-6-ol. Retrieved April 28, 2026 from <https://pubchem.ncbi.nlm.nih.gov/compound/536443>.
13. Baser, K. H. C., & Buchbauer, G. (2015). *Handbook of Essential Oils: Science, Technology, and Applications*. CRC Press.

How to cite this article: Sathya Priya R, G Chenthamarai Selvi. GCMS Profiling of bioactive phytochemicals in *Irumal Maathirai*: a traditional siddha polyherbo-mineral formulation for cough and respiratory ailments. *International Journal of Research and Review*. 2026; 13(5): 687-692. DOI: <https://doi.org/10.52403/ijrr.20260566>
