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COMPREHENSIVE ANALYSIS OF THE SIDDHA HERBO-MINERAL FORMULATION SIVA NAMA RASAM USING X-RAY DIFFRACTION AND FOURIER TRANSFORM INFRARED SPECTROSCOPY

Kiruba Annammal Paul Abraham Antonyraj *, Suresh Ramasamy

PG Scholar, Department of Gunapadam (Siddha Pharmacology), National Institute of Siddha, (Affiliated with The Tamil Nadu Dr. M.G. R Medical University), Ministry of Ayush, Chennai, Tamil Nadu, India

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***Corresponding author**
E-mail: kirubaannammal123@gmail.com

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ABSTRACT

The Siddha system of medicine, rooted in ancient Tamil traditions, emphasizes holistic healing by addressing the root causes of diseases. One such traditional herbo-mineral formulation, Siva Nama Rasam (SNR), has been historically used for treating rheumatism, hemorrhoids, and convulsions. Despite its longstanding therapeutic application, SNR lacks scientific validation regarding its chemical composition. This study employs X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR) to characterize SNR and establish its chemical profile. XRD analysis confirms the presence of Lithium Sulfide (Li_2S), Arsenic Sulfide (As_4S_4), and Zinc Sulfide (ZnS), suggesting a highly crystalline structure. FTIR analysis identifies key functional groups, including hydroxyl, amines, carbonyl, and aromatic compounds, which contribute to its potential bioactivity. These findings provide crucial insights into the formulation's physicochemical properties and reinforce its traditional therapeutic claims. By integrating modern analytical techniques with Siddha medicine, this study enhances the credibility, quality control, and potential biomedical applications of SNR. Future research should explore its pharmacological efficacy through *in-vitro* and *in-vivo* studies.

Keywords: Siddha medicine, Siva Nama Rasam, XRD, FTIR, herbo-mineral formulation, chemical characterization, traditional medicine.

INTRODUCTION

The Siddha system of medicine has been practiced since the origins of the Tamil language and stands out for its unique approach compared to other medical systems. Siddha medicine is distinguished by its focus on addressing the root cause of diseases and providing comprehensive remedies that encompass the body, mind, and soul [1]. Siddha medicines are classified into two types, Internal and external. One class of drug that falls under internal medicines is karuppu. In Siddha practice, specific herbal formulations and minerals are used to address multiple health issues, including epilepsy [2]. Siddha practitioners use different approaches to manage conditions such as peptic ulcers, haemorrhoids, and leprosy, often incorporating traditional remedies which addresses the root cause of these ailments. Siddha literature, including ancient texts and manuscripts, provides detailed descriptions of these treatments and their efficacy. The traditional siddha text "Anuboga Vaidya Navaneedham" authored by P. Mohammed Abdullah Sayabu, contains a powerful medicine known as Siva Nama Rasam [3].

SNR, despite its traditional applications, lacks scientific validation in terms of its chemical characterization. Hence, it has been selected for this study. The characterization of a herbo-mineral formulation plays a crucial role in determining its therapeutic potential. In this study, X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR) are employed as analytical techniques to assess the chemical composition of the formulation [4].

XRD is instrumental in examining the structural properties and crystalline nature of the formulation, while FTIR helps identify functional groups and molecular structures within the drug[5]. These techniques contribute to the standardization of traditional formulations by offering precise data on composition, purity, and stability. Such standardization is essential for ensuring batch-to-batch consistency, a persistent challenge in traditional medicine. Furthermore, this characterization not only reinforces the traditional knowledge of Siddha medicine but also enhances the credibility and quality control of SNR, strengthening its potential as an effective treatment for various ailments.

MATERIALS AND METHODS

Choice of the drug

Siva Nama Rasam is a herbo-mineral formulation used for treating "rheumatism, haemorrhoids, and convulsions. It is documented in the Siddha text Anuboga Vaithiya Navaneedham – Part 7, authored by Hakim P. Mohammed Abdullah Sayabu" on pages 76-78.

Ingredients for Siva Nama Rasam

Table 1: Ingredients of Siva Nama Rasam

Ingredients	Botanical name / Chemical name	Quantity
Purified Gandhagam	Sulphur	50 g
Purified Rasam	Hydrargyrum	50 g
Purified Manosilai	Red orpiment	50 g
Purified Vengaram	Borax	50 g
Purified Karunabi	*Aconitum spicatum*	50 g
Purified Milagu	*Piper nigrum*	50 g

Purification of Raw Drugs

Purification of Gandhagam (Sulphur)

Quantity sufficient of ghee was taken. When ghee is melted, sulfur is added, and the mixture is poured into a vessel containing

milk, where it solidifies. The solidified material is then washed with warm water and allowed to air dry. This process is repeated 30 times [2].

Purification of Rasam (Hydrargyrum)
Mercury (Rasam) underwent purification in a traditional grinder (Kalvam) using brick powder as the initial medium. Following this, it was processed with Turmeric Choornam, grinding each powder for a duration of one hour. The purified mercury was then collected in an earthen vessel. Subsequently, it was subjected to controlled heating along with a specific quantity of *Acalypha indica* herb juice. Finally, the mercury was meticulously washed to ensure thorough purification [2].

Purification of Manosilai (Red orpiment)
Manosilai is grinded well with lemon juice for three hours on Kalvam without interruption and then dried [2].

Purification of Venkaaram (Borax)
A measured quantity of Venkaaram was subjected to frying in an earthen pot [2].

Purification of Karunabi (*Aconitum spicatum*)
For purification, they are soaked in cow's urine for three days and exposed to sunlight daily. After exposure to sunlight cow's urine is replaced by fresh water. After third day, they are dried and preserved [6].

Purification of Milagu (*Piper nigrum*)
For purification, the black pepper seeds were soaked in buttermilk and left undisturbed for one hour and thirty minutes. After which the pepper was strained and thoroughly dried. the pepper was then roasted and preserved [6].

Preparation of Siva Nama Rasam
Rasam (Hydrargyrum) and Gandhagam (Sulphur) were finely ground together until the mixture turned completely black. The remaining three ingredients were individually weighed, ground into a fine powder, and sifted through a cloth before being added to the mixture. The combined mixture was then continuously ground for two hours, followed by the addition of pepper powder, and further ground for an additional 12 hours. The final product was stored in an airtight container [3].

Instrumental Analysis of SNR

XRD Analysis
Powder diffraction data were obtained using an Aeris PANalytical diffractometer (Netherlands) equipped with Ni-filtered copper radiation in Bragg-Brentano geometry. A fine powder sample was prepared as a thin layer on a silicon zero-background holder. The analysis was conducted by measuring the 2θ angle over a range of 10-90 degrees at a scanning speed of 4 degrees per second, utilizing CuKα radiation with a wavelength of λ = 1.5418 Å [7].

FTIR Analysis
The sample was analyzed using a Bruker Alpha-E spectrometer equipped with an ATR (attenuated total reflectance) module. It was carefully positioned on the crystal platform, ensuring proper alignment with the anvil in the up position to achieve optimal contact with the crystal before initiating IR radiation exposure. Spectral measurements were conducted at the specified wavelength, and the corresponding observational peaks/waves were recorded along with their wave numbers for further interpretation. OPUS version 7 software was used for functional group analysis, while signal detection was performed using a DTGS detector. Additionally, baseline correction was applied as needed to refine the results [8].

Table 2: Pattern list of XRD for the analysis of SNR

Visible	Ref. code	Score	Compound Name	Displ. [°2θ]	Scale Fac.	Chem. Formula
*	98-064-2294	65	Lithium Sulfide	0.000	0.951	Li_2S_1
*	98-018-4514	48	Arsenic Sulfide (4/4)	0.000	0.152	As_4S_4
*	98-010-7197	33	Zinc Sulfide	0.000	0.071	Zn_1S_1

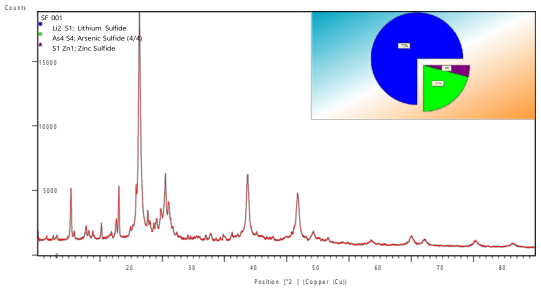

Figure 1: XRD Analysis of SNR

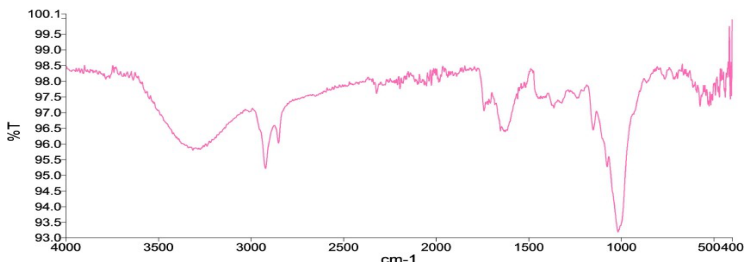

Figure 2: FTIR Analysis of SNR

Table 3: Interpretation of FTIR Peaks obtained for the analysis of SNR

Peak Number	Range (cm-1)	Functional Group
1	3600–3200	O–H Stretching (Hydroxyl group) Indicates alcohols, phenols, or carboxylic acids (broad peak).
2	3400–3250	N–H Stretching (Amines/Amides) Presence suggests primary or secondary amines.
3	3100–3000	C–H Stretching (Aromatic) Indicates aromatic hydrocarbons.
4	2260–2100	C≡C or C≡N Stretching (Triple bond) Possible presence of alkynes or nitriles.
5	1750 – 1650	C=O Stretching (Carbonyl group) Suggests esters, ketones, aldehydes, or carboxylic acids.
6	1000–650	C–H Bending (Out-of-plane bending for aromatics) Suggests aromatic substitution patterns.

RESULTS AND DISCUSSION

XRD Analysis

The XRD results for SNR are presented in Figure 1, with the corresponding diffraction pattern detailed in Table 2.

FTIR Analysis

The FTIR analysis results for SNR are presented in Figure 2, showcasing the peak values, with the corresponding functional groups detailed in Table 3.

X-ray diffraction (XRD) analysis is a non-destructive method used to obtain precise details about a material's crystal structure, chemical composition, and physical characteristics [7]. The X-ray diffraction data indicates a highly crystalline structure with 39 distinct peaks. The most intense peak at 26.32° 2θ (100% relative intensity, d = 3.382 Å) suggests the presence of a dominant phase with well-ordered atomic planes. Peaks at 43.68° 2θ,15.322° 2θ and 23.01° 2θ show significant intensities (29.03%, 22.96 and 22.71%, respectively), indicating secondary phases or additional crystalline planes contributing to the structure. The narrow FWHM (Full Width at Half Maximum) values across the peaks reflect good crystallinity, though minor broadening suggests small crystallites or slight structural disorder in some regions. The varying d-spacing values (1.12–8.81 Å) suggest a mixture of closely packed and more open planes, indicating a complex material with diverse atomic arrangements. These points to a well-defined crystalline structure with multiple phases. The major peaks correspond to Lithium sulfide (Li2S1), Arsenic Sulfide (As4S4) and zinc sulfide (Zn1S1). The strong alignment between the observed data and reference codes indicates that the sample contains both Synthetic lithium-sulfur compound and, Arsenic sulfide and zinc sulfide in well-defined forms, with ZnS possibly being more prevalent. This formulation is a testament to the alchemy of traditional medicine, where precise preparation methods and carefully chosen ingredients create the foundation for synergistic transformations. While the direct formation of Lithium Sulfide (Li_2S), Arsenic Sulfide (As_4S_4), and Zinc Sulfide (ZnS) may not always be spontaneous under normal conditions, traditional processing methods involving controlled heating, maturation, or environmental exposure can promote their formation. The interaction of metals, minerals, and herbal components in such mixtures may facilitate gradual chemical evolution, leading to the development of unique complex salts and sulfur-containing compounds. The sustained-release (SR) lithium is FDA-approved for individuals 12 and older. It is also used off-label for major depressive disorder (adjunct therapy), bipolar disorder without mania, vascular headaches, and neutropenia [9].

In pharmaceutical applications, arsenic sulfide has shown promise as an anticancer agent, particularly in the treatment of acute promyelocytic leukemia (APL), where it induces apoptosis and cell cycle arrest in malignant cells [10]. Arsenic sulfide has been widely utilized in traditional medicine systems such as Siddha, Ayurveda, and Traditional Chinese Medicine (TCM) for treating skin disorders, inflammatory conditions, and certain malignancies [11]. Zinc sulfide (ZnS) is added to topical formulations in dermatology due to its antimicrobial effects and is also used in sunscreens for UV protection. Studies are investigating ZnS nanoparticles for their potential in photodynamic therapy (PDT) for cancer treatment and as antimicrobial agents in wound dressings and medical devices to help prevent infections [12]. The FT-IR spectrum analysis reveals the presence of alcohols, indicating the existence of hydroxyl (-OH) groups. These groups are commonly linked to water solubility and can engage in hydrogen bonding, which may contribute to enhanced biological activity. Likewise, the detection of carboxylic acids suggests an acidic nature of the compound. Additionally, the presence of amines indicates nitrogen-containing groups, which may contribute to its basic properties [13]. Amines are essential in biological systems, frequently serving as ligands in enzyme reactions or as key elements in drug development due to their capability to bind with biological targets[14]. The identification of aromatic compounds and unsaturated hydrocarbons in the spectrum indicates the presence of delocalized electrons, which can improve the stability and reactivity of the compound. Aromatic compounds are well known for their antioxidant properties, aiding in the neutralization of free radicals and minimizing oxidative stress in biological systems. Additionally, the presence of saturated hydrocarbons, such as alkanes or lipid components, suggests a potential role in energy storage or as a structural component of biological membranes[15]. The detection of carbonyl groups (C=O), commonly found in ketones, aldehydes, or esters, adds to the chemical complexity of the sample. These carbonyl-containing compounds are known for their diverse reactivity, making them essential in organic synthesis and contributing to distinct biological activities [16]. For instance, esters are commonly used in pharmaceuticals and fragrances, highlighting their importance in both medicinal chemistry and sensory applications [17]. In summary, the presence of these functional groups highlights a complex chemical composition, where both aliphatic and aromatic structures are present. The intricate nature of SNR suggests its potential for various biological activities, including antioxidant, antimicrobial, anti-epileptic, and anti-inflammatory effects. These properties align with its traditional use in treating conditions like Kaakkai vali (Epilepsy), Magotharam (Ascites), Kunmam (Peptic ulcer) and Vali Noigal (Joint diseases). X-ray diffraction and FT-IR analysis reveal a complex material comprising crystalline structure of Lithium sulfide (Li_2S_1), Arsenic Sulfide (As_4S_4) and zinc sulfide (Zn1S1), alongside various functional groups[18]. These include hydroxyl, carboxylic acids, amines, aromatic compounds, unsaturated and saturated hydrocarbons, and carbonyl groups. This diverse chemical composition suggests

potential biological activities, such as antioxidant, antimicrobial, and anti-inflammatory effects.

CONCLUSION

This study marks a groundbreaking attempt to scientifically authenticate SNR through the use of advanced analytical techniques such as XRD and FTIR. These methodologies generate a distinctive chemical profile of the formulation, establishing a reference point for future *in-vitro* and *in-vivo* investigations. Additionally, further standardization can be implemented to assess quality parameters, ensuring consistency in future research. The innovative aspect of this work lies in its effort to integrate traditional wisdom with modern scientific principles, thereby laying a strong foundation for the global recognition of Siddha medicine.

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ABBREVIATIONS

SNR: Siva Nama Rasam;
XRD: X-Ray Diffraction;
FTIR: Fourier Transform Infrared Spectroscopy;
ATR: Attenuated Total Reflectance;
FWHM: Full Width at Half Maximum.

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