Research Article

Identification of phytoconstituents in ethanolic and aqua-ethanolic extracts of *Solanum indicum* L. through GC-MS

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Abstract

Solanum indicum L. is a commercially important species and ingredient of Dashmoolarishta, an ayurvedic formulation of Indian system of medicine. The present investigation dealt with identification of phytoconstituents in ethanolic and aqua-ethanolic (20:80) root extracts of *S. indicum* using GC-MS analysis. GC-MS analysis of root extracts of *S. indicum* was carried out first-time. GC-MS resulted the presence of Lauric acid, 2-methylbutyl ester (RT- 21.351, 34.54%), Octadecanoic acid (RT- 23.282, 31.76%) and 3, 6-Octadecadiynoic acid methyl ester (RT- 25.107, 10.44%) compounds in ethanolic extract while n-Capric acid isopropyl ester (RT- 21.526, 100%) in aqua-ethanolic extract. The phytochemical compounds identified have been reported to bestow with pharmaceutical and commercial significances.

Keywords: *Solanum indicum*, root, ethanolic and aqua-ethanolic extracts, GC-MS analysis

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Introduction

Solanum indicum L. belonging to family Solanaceae and is commonly known as Birhata or Badi kateri or Indian night shade. It is an erect undershrub of 0.30 to 1.8 m in height (**Figure 1**) and found throughout warmer parts of India, Asia, and Africa upto an elevation of 1.5 m [1]. The national demand of *S. indicum* is 500-1000 MT per annum [2]. All plant parts viz. berries, leaves, roots, seeds and stem of this species have been utilized in traditional system of medicine and are useful in various diseases such as bronchitis, asthma, dry cough, rhinitis, dysuria, leucoderma, sexual disorders, insomnia, cardiac weakness and pruritis [3-6]. The species is among the ten medicinal plants whose roots are principally employed in preparation of Dashmoolarishta, a well-established ayurvedic drug used in the treatment of fatigue, oral sores, and gynecological disorders [7]. The basic dashmool ingredient is utilized in the preparation of more than hundred ayurvedic formulations [8]. In our earlier studies on *S. indicum*, we worked out on evaluation of phenolic, flavonoid contents and antioxidant activity in its leaves, stem and roots [9] and total phenolic and caffeic acid contents in its roots from different agroclimatic regions of Madhya Pradesh state of India [10]. The present study has been focused on GC-MS analysis of ethanolic and aqua-ethanolic root extracts of *S. indicum* for identification of phytocompounds of pharmaceutical and commercial significance.

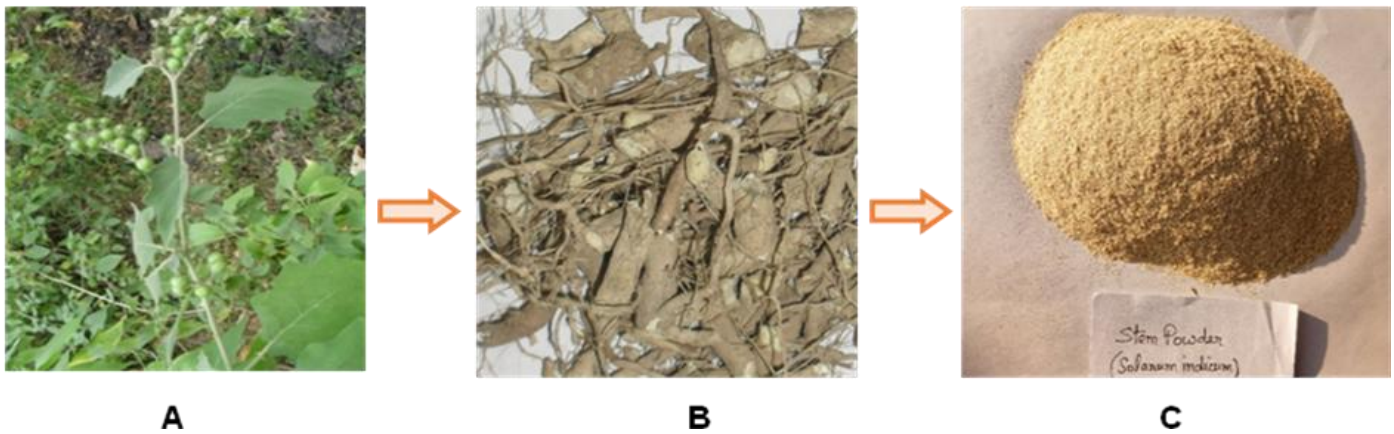

Figure 1 A. *Solanum indicum* plant, B. Roots, C. Root powder

Materials and Methods

Chemicals and reagents

AR grade chemical and solvents and distilled water were utilized in the experiments.

Collection of plant materials

Roots of *S. indicum* were collected from Chhindwara district of Madhya Pradesh by following the guidelines of good agricultural and collection practices (GACP) for medicinal plants [11].

Processing of plant materials

Plant materials were washed thoroughly in running water to remove soil and other foreign particles. Roots were separated, cut into small pieces and dried in shade for a week. Shade dried material was powdered using pulverizer. The powdered material was utilized for making extracts.

Preparation of extracts

Powdered root sample was subjected to successive extraction with Ethanol and Ethanol: Water (80: 20) (aqua-ethanolic) [12]. A total of 20g of dried powder was extracted in 250 ml of each solvent in successive manner for 12 hrs using soxhlet extraction method. Solvents were evaporated to dryness to yield the respective extracts which were used for GC-MS analysis.

GC-MS analysis

Ethanolic and aqua-ethanolic extracts were subjected to chemical analysis by using GC-MS instrument, Perkin Elmer, USA & Model - Auto system XL with Turbo Mass. Compounds were separated on PE-5MS 30m x 0.250mm x 0.250µm column. Oven temperature was programmed as follows: isothermal temperature of 75^{o}C for min and then increased up to 280^{o}C at the rate of 10^{o}C/min and held for 15min. Injection temperature was 250^{o}C and injection volume was 1µl. EI source temperature was set as 220^{o}C. Helium gas was used as carrier gas at 1 ml/min flow rate. MW range was set at 22 to 620 amu.

Identification of compounds

Interpretation of mass spectrum of GC-MS was conducted using the database of NIST. The spectrum of investigated compounds was compared with spectrum of known compounds stored in NIST. Molecular weight, molecular formula and number of hits were used to identify the name of compounds from NIST.

Results and Discussion

GC–MS was used to carry out the analysis and to identify the phytocompounds. GC–MS analysis resulted the peaks of various compounds in ethanolic root extract, out of which, 03 compounds were identified based on peak area percentage, retention time and structures. In the aqua-ethanolic extract only 01 compound with 100% peak area was detected in GC-MS and was identified. GC-MS chromatograms of ethanolic and aqua-ethanolic extracts of *S. indicum* roots are given as **Figures 2** and **3** respectively. The compounds were identified by comparison of the mass spectra with NIST library. The identified phytocompounds along with their molecular formula, molecular weight, exact mass, retention time (RT) and percentage area are given in **Table 1**. The pharmaceutical as well as commercial importance of the compounds identified in both extracts is given in **Table 2**. Chemical structures of compounds identified by GC-MS in ethanolic and aqua-ethanolic extracts are exhibited in **Figure 4**. Mass spectrum of one of the compounds, Octadecanoic acid is shown as **Figure 5**.

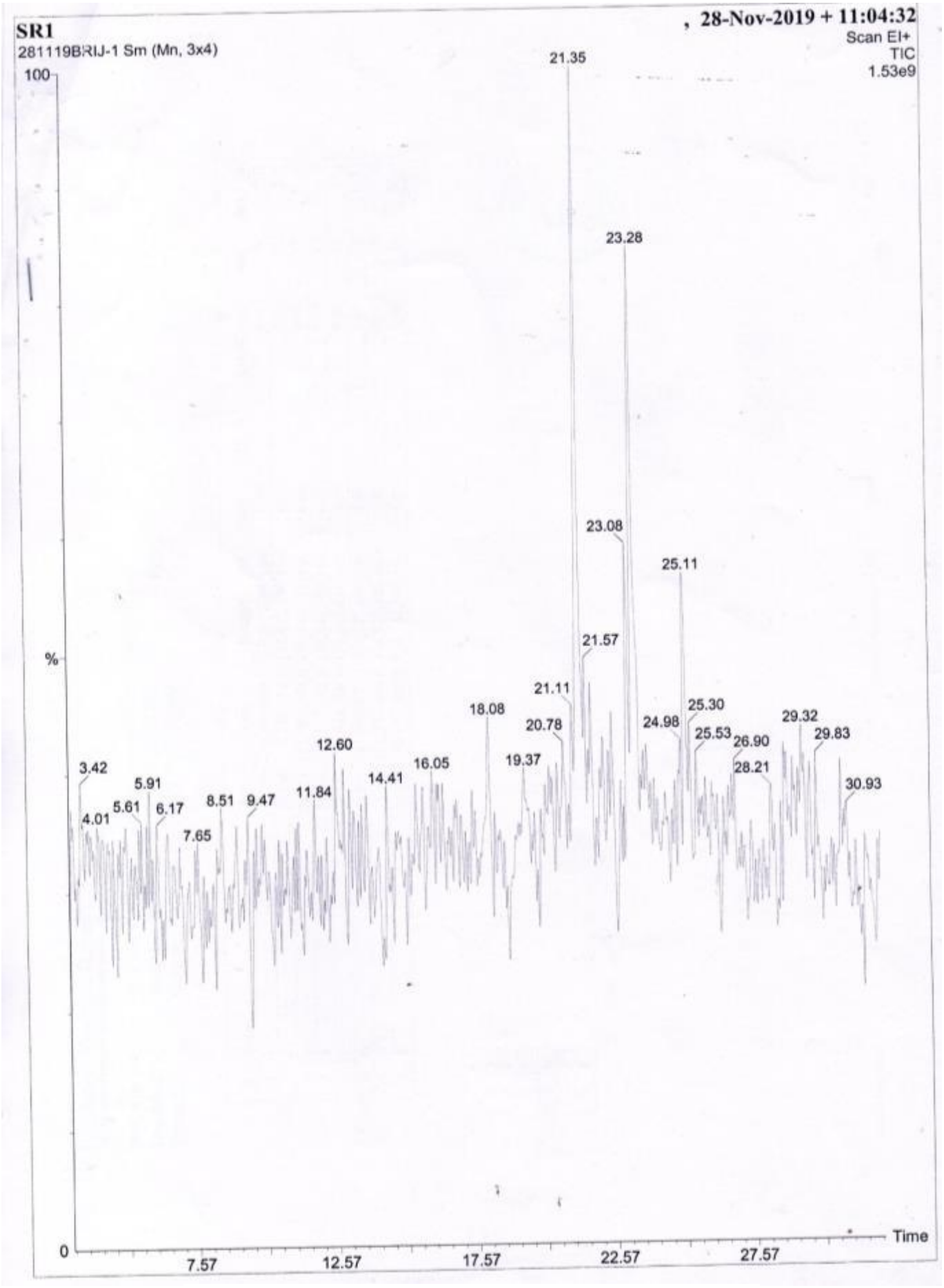

Figure 2 GC-MS chromatogram of ethanolic extract of *S. indicum* root

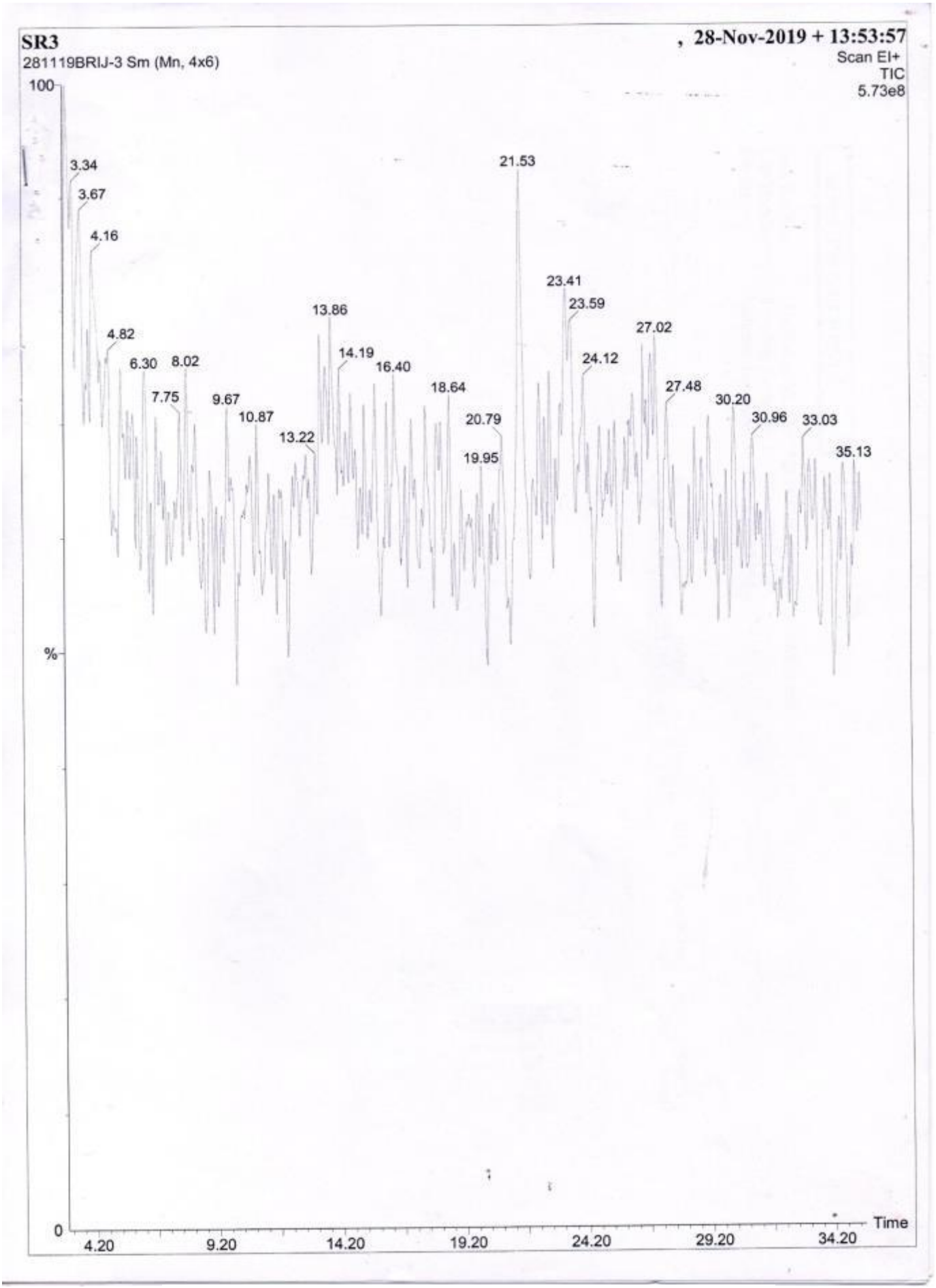

Figure 3 GC-MS chromatogram of aqua-ethanolic extract of *S. indicum* root

Table 1 Phytocompounds identified in ethanolic and aqua- ethanolic (20:80) extracts by GC-MS

Extracts	Name of phytocompounds	Molecular Formula	Molecular Weight	Exact Mass	RT (min)	Area %
Ethanolic	Lauric acid, 2-methylbutyl ester or 2-methyl-1-butyl laurate	$C_{17}H_{34}O_2$	270	270.45	21.351	31.54
	Octadecanoic acid	$C_{18}H_{36}O_2$	284	284.48	23.282	31.76
	3,6-Octadecadiynoic acid methyl ester	$C_{19}H_{30}O_2$	290	290.40	25.107	10.44
Aqua- ethanolic (20:80)	n-Capric acid isopropyl ester or Isopropyl decanoate	$C_{13}H_{26}O_2$	214	214.34	21.526	100

Table 2 Bioactivity/ importance of phytocomponents identified in ethanolic and aqua- ethanolic (20:80) extracts by GC-MS

S. No.	Name of compound	Nature of compound	Biological Activity/ Importance
1.	Lauric acid, 2-methylbutyl ester or 2-methyl-1-butyl laurate	Saturated fatty acid ester	It comes under the category of flavoring agents. Mixture of 2-methyl-1-butyl laurate and 3-methyl-1-butyl laurate used in cosmetic, dermatological, or pharmaceutical compositions [13].
2.	Octadecanoic acid	Saturated fatty acid	5-α-reductase inhibitor, hypocholesterolemic, suppository, cosmetic, lubricant, surfactant & softening agent, perfumery, propecic, flavor [14-16].
3.	3,6-Octadecadiynoic acid methyl ester	Unsaturated fatty acid ester	Anti-asthma, pesticides, Neurons protective, anti-inflammatory, and hepato-protective property [17].
4.	n-Capric acid isopropyl ester or Isopropyl decanoate	Saturated fatty acid ester	It is a food additive and flavoring agent. It is added to food for human consumption. Recommendation for use of isopropyl decanoate in fragrance concentrate is up to 5.0% [18].

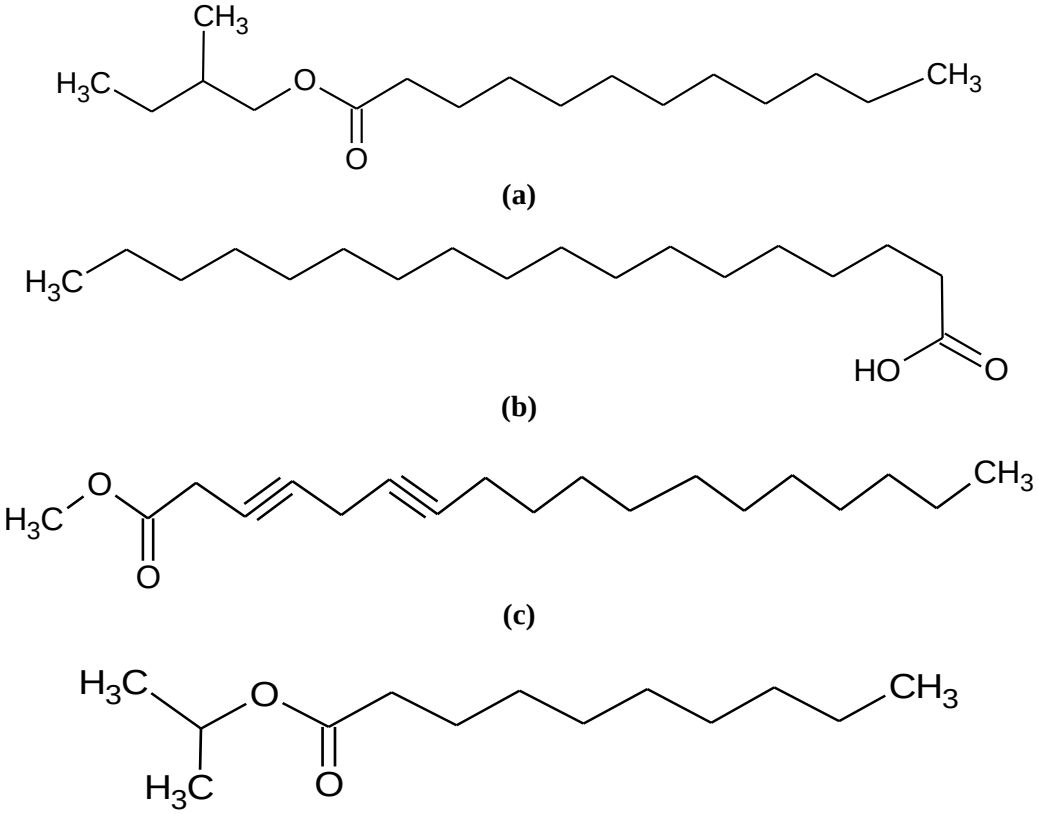

Figure 4 Chemical structures of phytocompounds identified by GC-MS (i) ethanolic extract (a) Lauric acid, 2-methylbutyl ester (b) Octadecanoic acid (c) 3, 6-Octadecadiynoic acid methyl ester (ii) Aqua-ethanolic extract (d) n-Capric acid isopropyl ester

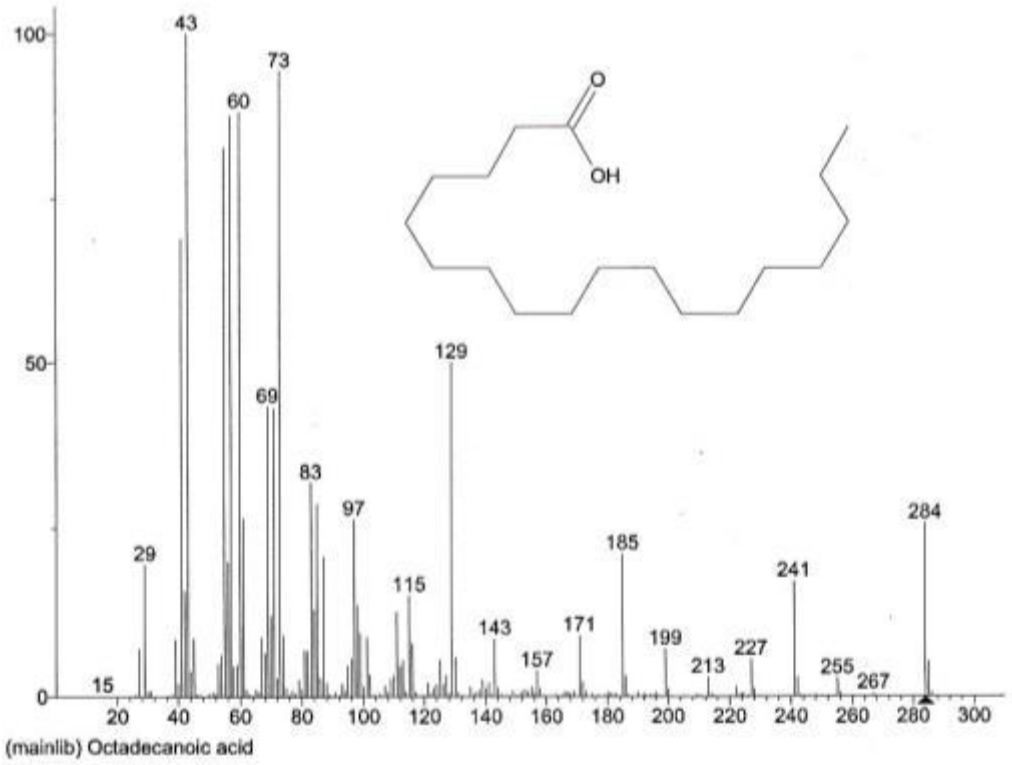

Figure 5 Mass spectrum of Octadecanoic acid identified by GC-MS in ethanolic extract

In the ethanolic extract, the main compounds were lauric acid, 2-methylbutyl ester, a saturated fatty acid ester (a, 31.54 %), Octadecanoic acid, a saturated fatty acid (b, 31.76 %) and 3,6-Octadecadiynoic acid methyl ester, an unsaturated fatty acid eater (c, 10.44 %) were the main compounds. In aqua-ethanolic extract, only one compound with 100% abundance namely n-Capric acid isopropyl ester, a saturated fatty acid ester (d) was detected. Table 2 showed the commercial significance of the identified compounds. In the literature, the mixture of 2-methyl-1-butyl laurate and 3-methyl-1-butyl laurate is reported to be utilized in cosmetic, dermatological, or pharmaceutical compositions [13]. Octadecanoic acid shows 5-α-reductase inhibitor activity, hypo cholesterolemic property and used in suppository, cosmetic, lubricant, surfactant and softening agent, perfumery, propecic, flavor [14-16]. 3,6-Octadecadiynoic acid methyl ester is reported to contain anti-asthma, pesticides, neurons protective, anti-inflammatory, and hepato-protective properties [17]. n-Capric acid isopropyl ester is being used as a food additive and flavoring agent. It is added to food for human consumption [18]. On comparison of both extracts, it can be noticed that ethanolic extract is rich in phytocompounds than aqua-ethanolic.

Conclusion

Since time immemorial, the medicinal plants have been utilized as a remedy to cure several ailments of mankind. These plants have also been the sources for wide range of commercially importance phytocompounds of therapeutic potential. GC-MS analysis investigated the important compounds in both the extracts of *S. indicum* root. The identification of these phytocompounds is adding more significance to this plant. Further studies may be carried out on isolation and characterization of more phytocompounds along with their biological activities.

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