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Original Article

GC-MS Analysis of Bio-Active Compounds in Hydroethanolic Extract of *Caesalpinia sappan*

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ABSTRACT

Background: The presence of phytochemical constituents has been reported from species of the Compositae Caesalpiniaceae. **Objectives:** The present study was designed to determine the bioactive compounds in the heartwood of hydroethanolic extract. **Materials and Methods:** Phytochemical screening of the entire herb of *Caesalpinia sappan* revealed the presence of some bioactive components. Gas Chromatography-Mass Spectrometry (GC-MS) analysis of the heartwood of hydroethanolic extract was performed on GC-MS equipment. **Results:** The phytochemical tests showed the presence of alkaloids, alkaloids, cardiac glycosides, flavonoids, phenols, phlorotannins, reducing sugars, saponins, steroids, tannins, terpenoids, volatile oils, carbohydrates, protein/amino acids in the hydroethanolic extract of *Caesalpinia sappan*. The GC-MS analysis has shown the presence of different phytochemical compounds in the hydroethanolic extract of *Caesalpinia sappan*. A total of 38 compounds were identified. The major components are 9-octadecenoic acid, Oleic Acid, Sarcosine and Dinonanoin. **Conclusion:** From the results, it is evident that *Caesalpinia sappan* contains various photo components and is recommended as a plant of phytopharmaceutical importance.

Keywords: *Caesalpinia sappan* (CS), Heartwood hydroethanolic extraction, Phytochemistry, GC-MS analysis.

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INTRODUCTION

Traditional medicines have been incorporated into conventional healers by humans for centuries due to their pharmacological activity and Research on herbal remedies has produced new drug candidates that are being tested to treat a range of illnesses. Over 80% of respondents of the nation's population rely on conventional medical care for their main healthcare requirements, according to the World Health Organization Group (WHO) in 2008.[1] Living organisms remain essential producers of bioactive substances for the preservation of human health. According to numerous reports, green plants are a source of potent chemotherapeutic agents that are non-phytotoxic, the most structural and readily bio-based.[2] Secondary metabolites from plants have a wide range of intriguing biological activities.

These natural compounds are a major source with a broad range of structural configurations and characteristics.[3] Understanding the active ingredients of plants is beneficial for revealing bioactive molecules, as well as for recognizing new sites of valued phytochemical constituents to produce intricate chemicals and even for understanding the true value of natural remedies.[4] Because many phytoconstituents possess parallel and intertwining mechanisms of action, a novel scientific discipline that also underscores and emphasizes its standardization of natural pharmaceuticals and other goods has emerged. Typically, mass spectrometry is used in conjunction with chromatographic techniques like gas chromatography for the direct measurement of substances found in conventional medicines and plant species. As this methodology has been established to be a useful method for the analysis of non-polar components and volatile essential oils, fatty acids, lipids and alkaloids, GC-MS analysis studies have been used more and more in recent times for the evaluation of plant extracts.[5] Brazil or Sappan wood, also known as *Caesalpinia sappan* (CS), is a plant that belongs to the Leguminosae family. South Asia is where *Caesalpinia sappan* is found and its dried heartwood has long been used as an active component in food and drink.[6] To produce red dye, the plant's heartwood is frequently used. In Thai traditional medicine, the heartwood of the *Caesalpinia sappan* tree has long been used to treat anemia, dermatitis, diarrhea, dysentery and tuberculosis. skin infections, malnutrition, indigestion and dysentery.[7] *Caesalpinia sappan* is used in traditional Chinese remedies that promote increased blood circulation, encourage menstrual flow and possess analgesic and anti-inflammatory properties[8] The highly coveted medicinal plant *Caesalpinia sappan* has been utilized for the

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Alzheimer's disease treatment process,[9] anti-inflammatory,[10] hepatoprotective,[11] analgesic and anti-pyretic activity,[12] anti-bacterial,[13] antioxidative,[14] carcinogenic,[15] anti-viral,[16] Memory Deficits,[17] anti-nociceptive activity,[18] ischemic stroke,[18] anti-allergic,[19] anti-acne,[20] anti-aging.[21] Due to the high cost of psychoactive substances or their negative side effects, researchers are more interested in discovering bioactive substances from natural sources as medicines.

MATERIALS AND METHODS

Collection of plant material

A plant-based material sappan was purchased from Kerala Ayurvedic Pathimugam, India and Identification and authentication of selected species, (Certificate No.: SS4/No/5-22.) and the plant material was authenticated by Botanist Dr. Nandeesh, Research officer-Sree Siddaganga College, Tumakuru.

Preparation of extract

The heartwood of *Caesalpinia sappan* was shade dried, coarsely powdered under ambient conditions and reduced to a fine powder using an electric grinder to get 40-mesh size powder. The powdered plant material will be subjected to Soxhlet extraction using standard protocol. Thus, the obtained extract was concentrated under reduced pressure at 40°C through a rotator flash evaporator. To create a dry powder of plant extract, the sample extract was freeze-dried. For the characteristics, the lyophilized extract will be kept in airtight amber-colored bottles.[22]

Preliminary phytochemical screening

The hydroethanolic extract was tested for alkaloids, anthraquinone, flavonoids, phenols, steroids, tannins, terpenoids, cardiac glycosides, saponins, phlorotannins, reducing sugars, volatile oils, carbohydrates, protein/amino acids.[23]

GC-MS analysis of bioactive compounds from the sample

Gas chromatography-mass spectrometry was used to identify the bioactive volatile compounds in the ethanolic extract of the sample. The following list of key characteristics summarises some of them.

GC-MS analysis of the sample was carried out using Clarus 680 with non-polar Elite-5MS (5% biphenyl, 95% dimethylpolysiloxane, 30 m×0.25 mm ID×250 µm df) packed into the container and the elements were separated using helium as the carrier gas with a steady flow rate of 2 mL/min. The injector temperature was set at 280°C during the chromatographic run. The 1 µL of extract sample was injected into the instrument the oven temperature was as follows: 100°C (2 min); followed by 200°C at the rate of 10°C min^{-1} and 200°C, where it was held for 3 min and then followed by 300°C at the rate of 25°C min^{-1}; it was held for 10 min. The mass detector conditions were Inlet line temperature of 250°C; ion source temperature of 230°C; and ionization mode electron impact at 70 eV, a scan time of 0.2 sec and scan interval of 0.1 sec. fragments ranging from 40 to 600 Da. The composite spectra were compared to a database of known composite spectra stored in the Gas chromatography-mass National Institute of Standards and Technology (NIST) Library (2014).

Condition Maintained

Mass Condition (EI), Inlet Line Temp=250°C, Source Temp=230°C, Scan: 40 to 600 Da.

Instrumentation Acquisition Parameters Oven: Initial temp 100°C for 2 min, ramp 0°C/min to 200°C, hold 3 min, 25°C/min to 300°C, hold=10 min, Total Run Time=29.00 min, InjA auto=280°C; Volume=1 µL; Split=1:20, Flow Rate=2 mL/min, Carrier Gas=He; Column=Elite-5MS (30.0 m, 0.25 mm ID, 0.25µm).

Identification of phytoconstituents

The National Institute of Standards and Technology (NIST) database, the characteristic peak of the GC-MS was interpreted using a database with more than 62,000 patterns. A comparison was made between the mass spectra of the unknown and known components stored in the NIST library. By connecting the corresponding peak areas to the TIC areas from the GC-MS, quantitative conclusions were reached. The name, molecular formula, molecular weight, retention time, peak area percentage and structure of the test materials were determined.

RESULTS

After the successful cold maceration extraction of the heartwood part of the plant in an investigation, the preliminary phytochemical study revealed that the hydroethanolic extract of CS contains carbohydrates, glycosides, saponins, flavonoids, tannins, triterpenoids, phenolics were present in CS as summarized in (Table 1).

Table 1: Preliminary phytochemical evaluation of hydroethanolic extracts of CS.

Alkaloid	-
Carbohydrates	+
Proteins and Amino Acids	-
Steroids	-
Glycosides	+
Saponins	+
Flavonoids	+
Tannins	+
Triterpenoids	+
Phenolics	+

'+' indicates presence, '-' indicates absence.

Table 2: Compounds identified in the hydroethanolic extract of CS in GC-MS.

Sl. No.	Name of the Compound	MF	MW	Peak Area (%)
1	9,12-Octadecadienal, dimethyl acetate	$C_{20}H_{38}O_2$	310.2	6.75
2	2-(4-Chloro-phenoxy)-nicotinic acid	$C_{12}H_8ClNO_3$	249	4.90
3	Pyridate	$C_{19}H_{23}ClN_2O_2S$	378.1	4.52
4	1-(4-Methoxyphenyl) imidazoline-2-thione	$C_{10}H_{10}N_2OS$	206.05	4.34
5	Pyridine	$C_{12}H_{15}NO_2$	205.1	3.50
6	6-Methoxy-4-methylquinoline-2-thiol	$C_{11}H_{11}NOS$	205	2.96
7	1-[1-(3-Chlorophenyl)-1,2,3-triazol-4-yl] cyclohexan-1-amine	$C_{14}H_{17}ClN_4$	276.1	2.50
8	Pyrazol-5(4H)-one, 3-(4-nitrophenyl)	$C_9H_7N_3O_3$	205	2.30
9	Trimethylsilyl (5-benzyl-3,6-dioxopiperazin-2-yl) acetate	$C_{16}H_{22}N_2O_4Si$	334.1	2.30
10	Dimethyl(bis[(4,8,8-trimethyldecahydro-1,4-methanoazulen-9-yl) methoxy]) silane	$C_{32}H_{56}O_2Si$	500.40	1.94
11	9-Octadecenoic acid	$C_{21}H_{42}O_2Si$	354.2	57.6
12	Hexadecylamine	$C_{22}H_{49}NSi$	355.3	17.6
13	11-Octadecenoic acid	$C_{21}H_{42}O_2Si$	354.2	5.07
14	13-Octadecenoic acid	$C_{21}H_{42}O_2Si$	354.2	4.68
15	N-(2-Hydroxyethyl)-4-(oxo(phenyl)acetyl) benzamide tms.	$C_{20}H_{23}NO_4Si$	369.1	4.68
16	Oleic Acid	$C_{21}H_{42}O_2Si$	354.2	2.59
17	Sarcosine	$C_{26}H_{49}NO_3$	423.3	2.59
18	Dinonanoin monocaprylin	$C_{29}H_{54}O_6$	0.47	2.59
19	Isopentedrone	$C_{12}H_{17}NO$	191	33.5
20	7,8-Diazabicyclo[4.2.2]deca-2,4,7-trien-7-oxide	$C_8H_{10}N_2O$	150	3.67
21	2H-[1,2,4]Triazole-3-sulfonic acid benzyl-methyl-amide	$C_{10}H_{12}N_4O_2S$	252	3.53
22	2-Aminohydratropic acid	$C_9H_{11}NO_2$	165	3.12
23	1-Propanol, 3-(ethylthio	$C_5H_{12}OS$	120	2.88
24	2-[3-(4-Methoxyphenyl)-1,2,4-oxadiazol-5-yl] aniline	$C_{15}H_{13}N_3O_2$	267	2.57
25	Benzenemethanamine, N,α-dimethyl	$C_9H_{13}N$	135	2.34
26	3-Amino-1-chloro-4-phenyl-2-butanone	$C_{10}H_{12}ClNO$	197	2.26
27	N-(2-Phenylpropan-2-yl) acetamide	$C_{11}H_{15}NO$	177	2.08
28	Propane, 1-[(1-methylethyl) thio]	$C_6H_{14}S$	118	1.84
29	Benzamidine	$C_7H_8N_2$	120	12.2
30	Hydrazine carboxamide, 2-(phenyl methylene)	$C_8H_9N_3O$	163	6.64
31	3-Pyridinecarbonitrile, 1,4-dihydro-1-methyl	$C_7H_8N_2$	120	16.3
32	2-Aminohydratropic acid	$C_9H_{11}NO_2$	165	5.41
33	: p-Toluic acid, 2-phenylethyl ester	$C_{16}H_{16}O_2$	240	4.78
34	Hydrazinecarboxamide, 2-(phenylmethylene)	$C_8H_9N_3O$	163	6.64
35	1,2-Naphthalenediol, 1,2,3,4-tetrahydro	$C_{10}H_{12}O_2$	164	1.60
36	Pyridine, 5-ethenyl-2-methyl	C_8H_9N	119	3.88
37	m-Toluic acid, 2-phenylethyl este	$C_{16}H_{16}O_2$	240	3.58
38	o-Toluic acid, 2-phenylethyl ester	$C_{16}H_{16}O_2$	240	2.18

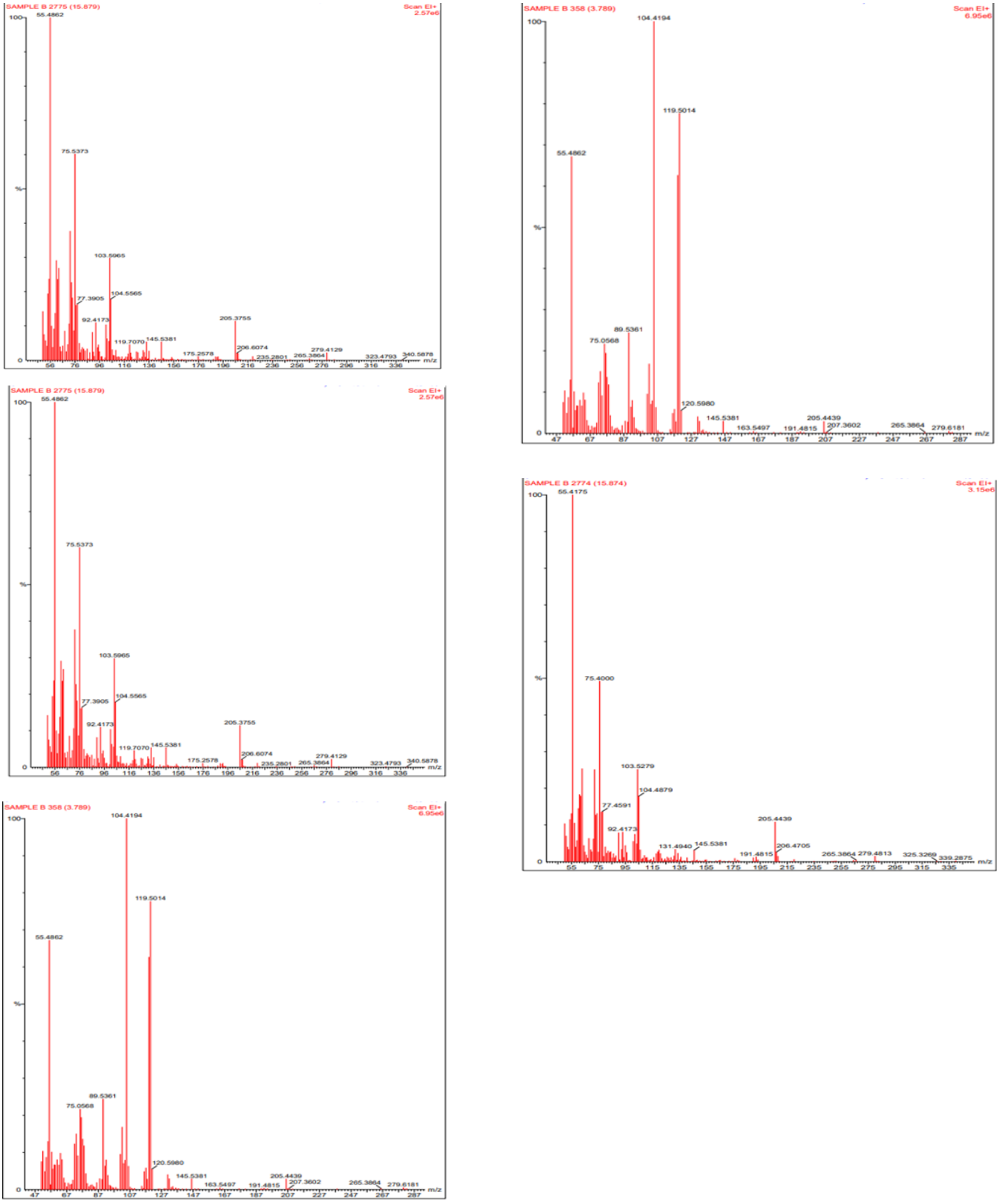

Figure 1: Chromatogram of hydro-ethanolic extract of CS.

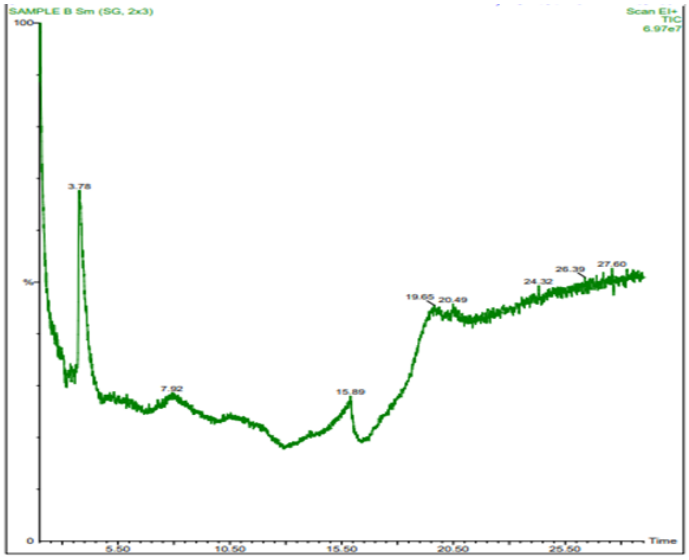

Figure 2: Mass Chromatogram of CS hydroethanolic extract.

DISCUSSION

Gas chromatography mass is one of the most effective methods for determining the constituents of organic material, including long-chain and branched-chain hydrocarbons, alcohols, acids and esters. CS-ethanolic extract underwent GC-MS analysis, which identified 438 compounds (phytochemical constituents) that may be responsible for the plant's medicinal properties (Figures 1 and 2). Based on the molecular formula and molecular weight, peak area, it was confirmed that the phytochemical compounds were what they claimed to be. The compounds identified (Table 2), It is discovered that, 9-Octadecenoic acid (57.6%), Isopentedrone (33.5%) and Hexadecylamine (17.6%) is found as the major compound and the other thirty-five minor compounds such as 9,12-Octadecadienal (6.75%), 2-(4-Chloro-phenoxy)-nicotinic acid (4.90%), Fenpyrate (4.52%), 1-(4-Methoxyphenyl) imidazoline-2-thione (4.34%), Pyridine (3.50%), 6-Methoxy-4-methylquinoline-2-thiol(2.96%),1-[1-(3-Chlorophenyl)-1,2,3-triazol-4-yl] cyclohexan-1-amine (2.50%), Pyrazol-5(4H)-one, 3-(4-nitrophenyl) (2.30%), Trimethylsilyl (5-benzyl-3,6-dioxopiperazin-2-yl) acetate (2.30%),Dimethyl(bis[(4,8,8-trimethyldecahydro-1,4-methanoazulen-9-yl) methoxy]) silane (1.94%), 11-Octadecenoic acid (5.07%), 13-Octadecenoic acid (4.68%), N-(2-Hydroxyethyl)-4-(oxo(phenyl)acetyl) benzamide tms (4.68%), Oleic Acid (2.59%), Sarcosine (1.93%), Dinonanoin (0.47%).7,8-Diazabicyclo[4.2.2]deca-2,4,7-trien-7-oxide (3.67%), 2H-[1,2,4]Triazole-3-sulfonic acid benzyl-methyl-amide (3.53%),2-Aminohydratropic acid (3.12%), 1-Propanol, 3-(ethylthio) (2.88%),2-[3-(4-Methoxyphenyl)-1,2,4-oxadiazol-5-yl]aniline (2.54%), Benzenemethanamine, N,α-dimethyl (2.34%), 3-Amino-1-chloro-4-phenyl-2-butanone (2.16%), N-(2-Phenylpropan-2, yl)acetamide (2.08%), Propane, 1-[(1-methyl ethyl)thio] (1.84%), Benzamidine (12.2%), Hydrazine carboxamide (6.64%),3-Pyridinecarbonitrile (6.13%), 2-Amino-2-phenylpropanoic acid (5.41%), p-Toluic acid (4.78%), Hydrazine carboxamide (6.64%), 1,2-Naphthalenediol (4.60%), 5-Vinyl-2-picoline (3.88%), m-Toluic acid (3.58%), o-Toluic acid (2.88%). The present study helps to predict the formula and structure of 38 biomolecules. Further investigation may lead to isolation of bio-active compounds and their structural elucidation and screening of pharmacological activity will be helpful for further drug development.

CONCLUSION

The Gas chromatography-mass method is a simple and quick quantitative method to determine bioactive substances, requiring only a few grams of plant parts. The investigation is important since certain of the biomolecules have biological activity. 38 distinct chemical compounds that have various pharmacological properties can be discovered in the hydroethanolic extract of *Caesalpinia sappan*. So, every active ingredient can be extracted separately, used in clinical trials to evaluate effectiveness and transformed from a crude drug into a novel one.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ABBREVIATIONS

CS: *Caesalpinia sappan*; **GC-MS:** Gas chromatography-mass spectroscopy; **MF:** Molecular formula; **MW:** Molecular Weight; **WHO:** World Health Organization Group; **NIST:** National Institute of Standards and Technology.

SUMMARY

The current study sought to identify potential bioactive molecules present in the hydroethanolic extract of *Caslapinea sappan*. The presence of different molecules was identified by GCMS. Out of 39 bioactive molecules. We have analyzed (9-octadecenoic acid (57.6%), Isopentedrone (33.5%) and Hexadecyl amine (17.6%) was found in the highest concentration. Identified is a potential therapeutic agent for the treatment of neuroprotective and anti-inflammatory agents.

REFERENCES

1. Bao H, Zhang LL, Liu QY, Feng L, Ye Y, Lu JJ, *et al*. Lin LG. Cytotoxic and Pro-Apoptotic Effects of Cassane Diterpenoids from the Seeds of *Caesalpinia sappan* in Cancer Cells. Molecules. 2016;18: 21(6):791. doi: 10.3390/molecules21060791, PMID: 27322234.
2. Atanasov AG, Zotchev SB, Dirsch VM; International Natural Product Sciences Taskforce; Supuran CT. Natural products in drug discovery: advances and opportunities. Nat Rev Drug Discov. 2021;20(3):200-16. doi: 10.1038/s41573-020-00114-z, PMID: 3351048.

3. Bonura A, Giacomarra M, Montana G. The Keap1 signaling in the regulation of HSP90 pathway. Cell Stress Chaperones. 2022;27(3):197-204. doi: 10.1007/s12192-022-01253-5, PMID: 35362892.
4. de Oliveira-Júnior RG, Ferraz CAA, de Oliveira AP, Araújo CS, Oliveira LFDS, *et al.* Phytochemical and pharmacological aspects of *Cnidoscolus Pohl* species: A systematic review. Phytomedicine. 2018;15;50:137-47. doi: 10.1016/j.phymed.2017.08.017, PMID: 30466972.
5. Chen SY, Gao Y, Sun JY, Meng XL, Yang D, Fan LH, *et al.* Traditional Chinese Medicine: Role in Reducing β-Amyloid, Apoptosis, Autophagy, Neuroinflammation, Oxidative Stress and Mitochondrial Dysfunction of Alzheimer's Disease. Front Pharmacol. 2020;22:11:497. doi: 10.3389/fphar.2020.00497, PMID: 32390843.
6. Pattananandecha T, Apichai S, Julsrigival J, Ogata F, Kawasaki N, Saenjum C. Antibacterial Activity against Foodborne Pathogens and Inhibitory Effect on Anti-Inflammatory Mediators' Production of Brazilin-Enriched Extract from *Caesalpinia sappan* Linn. Plants (Basel). 2022;27: 11(13):1698. doi: 10.3390/plants11131698, PMID: 35807650.
7. Murillo-Villicaña M, Noriega-Cisneros R, Peña-Montes DJ, Huerta-Cervantes M, Aguilera-Méndez A, Cortés-Rojo C, *et al.* A. Antilipidemic and Hepatoprotective Effects of Ethanol Extract of *Justicia spicigera* in Streptozotocin Diabetic Rats. Nutrients. 2022;6:14(9): 1946. doi: 10.3390/nu14091946, PMID: 3556591.
8. Kim HY, Lee HJ, Zuo G, Hwang SH, Park JS, Hong JS, *et al.* Antinociceptive activity of the *Caesalpinia eriostachys* Benth. ethanolic extract, fractions and isolated compounds in mice. Food Sci Nutr. 2022;7: 10(7):2381-9. doi: 10.1002/fsn3.2846, PMID: 35844922.
9. Anil PP, Shams R, Dash KK, Kalsi R. A Comprehensive Review on Bioactive Compounds Found in *Caesalpinia sappan*. Molecules. 2023;25: 28(17):6247. doi: 10.3390/molecules28176247, PMID: 37687076.
10. Rangel-Huerta OD, Pastor-Villaescusa B, Aguilera CM, Gil A. A Systematic Review of the Efficacy of Bioactive Compounds in Cardiovascular Disease: Phenolic Compounds. Nutrients. 2015;29: 7(7):5177-216. doi: 10.3390/nu7075177, PMID: 26132993.
11. Lee JH, Ahn NH, Choi SB, Kwon Y, Yang SH. Natural Products Targeting Amyloid Beta in Alzheimer's Disease. Int J Mol Sci. 2021;26: 22(5):2341. doi: 10.3390/ijms22052341, PMID: 33652858.
12. Li J, Zhao T, Qiao H, Li Y, Xia M, Wang X, *et al.* Research progress of natural products for the treatment of ischemic stroke. J Integr Neurosci. 2022;28: 21(1):14. doi: 10.31083/j.jin2101014, PMID: 35164450.
13. Ansong JA, Asante E, Johnson R, Boakye-Gyasi ME, Kuntworbe N, Owusu FWA, *et al.* Formulation and Evaluation of Herbal-Based Antiacne Gel Preparations. Biomed Res Int. 2023;18:2023:7838299. doi: 10.1155/2023/7838299, PMID: 38146392.
14. Nathan VK, Rani ME. Natural dye from *Caesalpinia sappan* L. heartwood for eco-friendly coloring of recycled paper-based packing material and its *in silico* toxicity analysis. Environ Sci Pollut Res Int. 2021;28(22):28713-19. doi: 10.1007/s11356-020-11827-4, PMID: 33543441.
15. Pattananandecha T, Apichai S, Julsrigival J, Ogata F, Kawasaki N, Saenjum C. Antibacterial Activity against Foodborne Pathogens and Inhibitory Effect on Anti-Inflammatory Mediators' Production of Brazilin-Enriched Extract from *Caesalpinia sappan* Linn. Plants (Basel). 2022;27: 11(13):1698. doi: 10.3390/plants11131698, PMID: 35807650.
16. Vij T, Anil PP, Shams R, Dash KK, Kalsi R, Pandey VK, *et al.* A Comprehensive Review on Bioactive Compounds Found in *Caesalpinia sappan*. Molecules. 2023;25: 28(17):6247. doi: 10.3390/molecules28176247, PMID: 37687076.
17. Saini R, Dhiman NK. Natural Anti-inflammatory and Anti-allergy Agents: Herbs and Botanical Ingredients. Anti inflamm Antiallergy Agents Med Chem. 2022;21(2):90-114. doi: 10.2174/1871523021666220411111743, PMID: 35410623.
18. Wu SQ, Otero M, Unger FM, Goldring MB, Phrutivorapongkul A, Chiari C, *et al.* Anti-inflammatory activity of an ethanolic *Caesalpinia sappan* extract in human chondrocytes and macrophages. J Ethnopharmacol. 2011;18: 138(2):364-72. doi: 10.1016/j.jep.2011.09.011, PMID: 21963554.
19. Nasim N, Sandeep IS, Mohanty S. Plant-derived natural products for drug discovery: current approaches and prospects. Nucleus (Calcutta). 2022;65(3):399-11. doi: 10.1007/s13237-022-00405-3, PMID: 36276225.
20. Ghosh P, Das C, Biswas S, Nag SK, Dutta A, Biswas. *et al.* Phytochemical composition analysis and evaluation of *in vitro* medicinal properties and cytotoxicity of five wild weeds: A comparative study. F Res. 2020;2:9:493. doi: 10.12688/f1000research.22966.1, PMID: 32676186.
21. Syamsunarno MRA, Safitri R, Kamisah Y. Protective Effects of *Caesalpinia sappan* Linn. and Its Bioactive Compounds on Cardiovascular Organs. Front Pharmacol. 2021;5:12:725-45. doi: 10.3389/fphar.2021.725745, PMID: 34603037.
22. Wan YJ, Xu L, Song WT, Liu YQ, Wang LC, Zhao MB, *et al.* The Ethanolic Extract of *Caesalpinia sappan* Heartwood Inhibits Cerebral Ischemia/Reperfusion Injury in a Rat Model Through a Multi-Targeted Pharmacological Mechanism. Front Pharmacol. 2019;5:10:29. doi: 10.3389/fphar.2019.00029, PMID: 308047.
23. Li Y, Dong M, Wu Z, Huang Y, Qian H, Huang C. Activity Screening of the Herb *Caesalpinia sappan* and an Analysis of Its Antitumor Effects. Evid Based Complement Alternat Med. 2021;25:2021: 9939345. doi: 10.1155/2021/9939345, PMID: 34257693.

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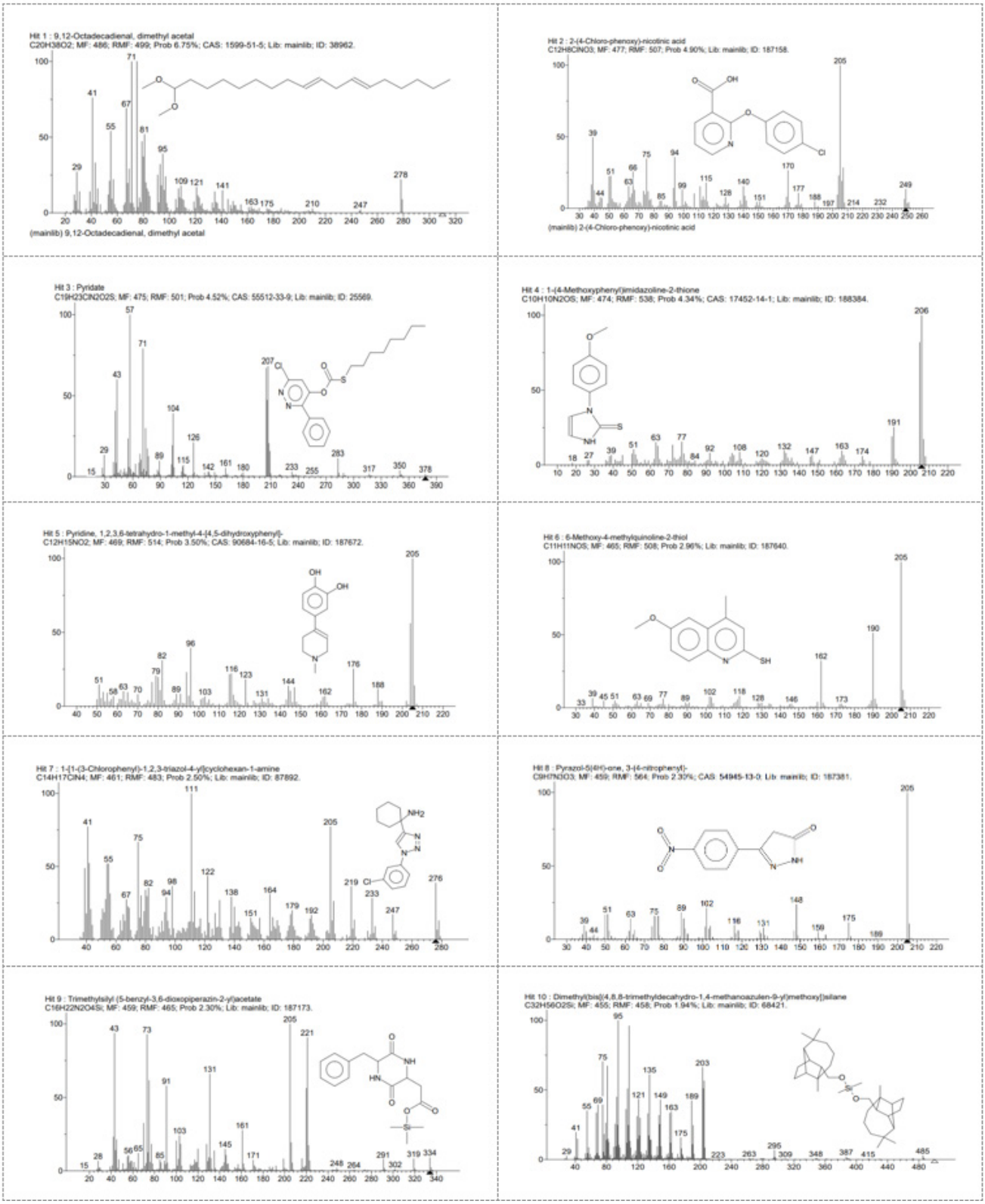
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Hit 3 : Pyridate
C19H23ClN2O2S; MF: 475; RMF: 501; Prob 4.52%; CAS: 55512-33-9; Lib: mainlib; ID: 25569.
Hit 4 : 1-(4-Methoxyphenyl)imidazoline-2-thione
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Hit 5 : Pyridine, 1,2,3,6-tetrahydro-1-methyl-4-[4,5-dihydroxyphenyl]-
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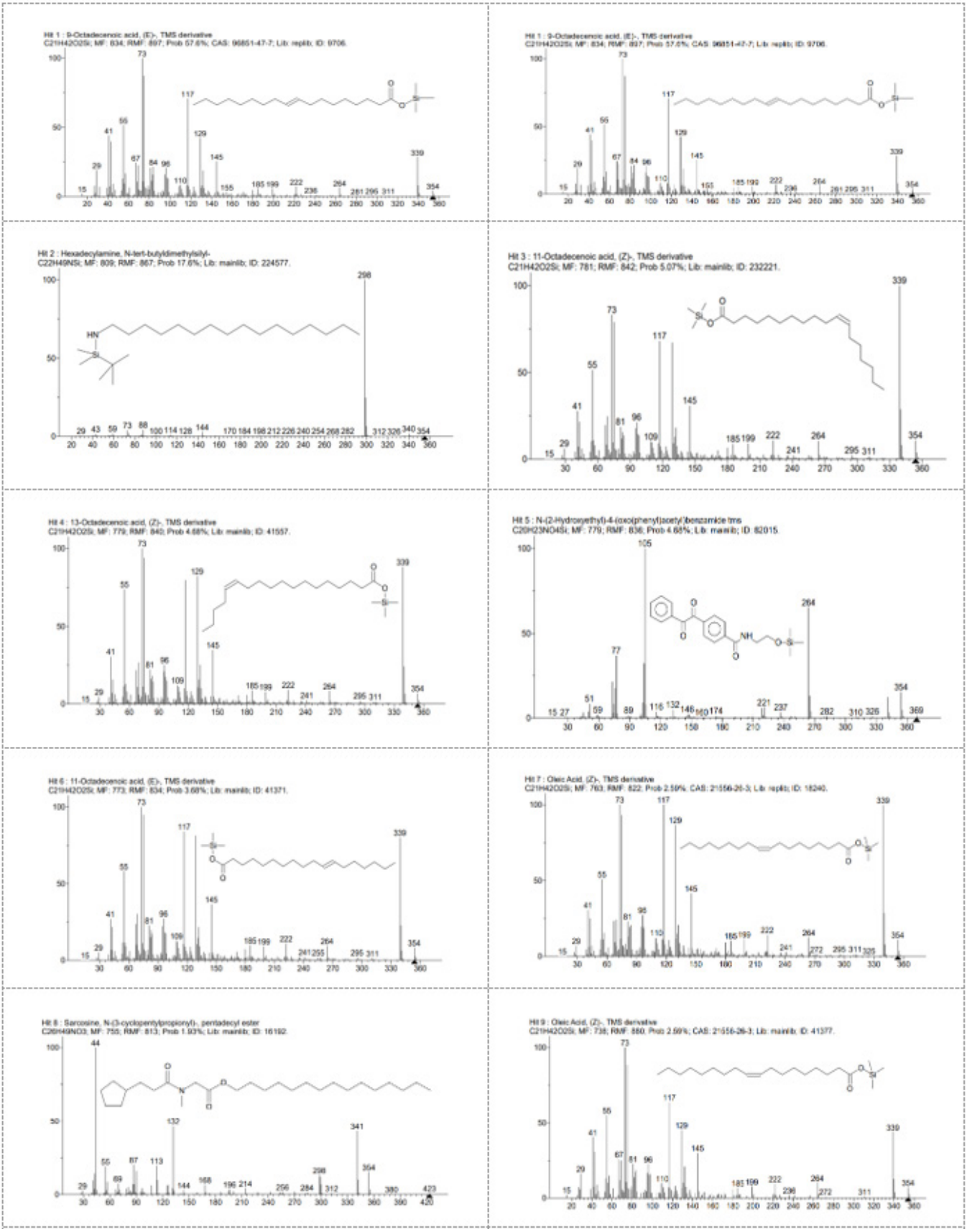
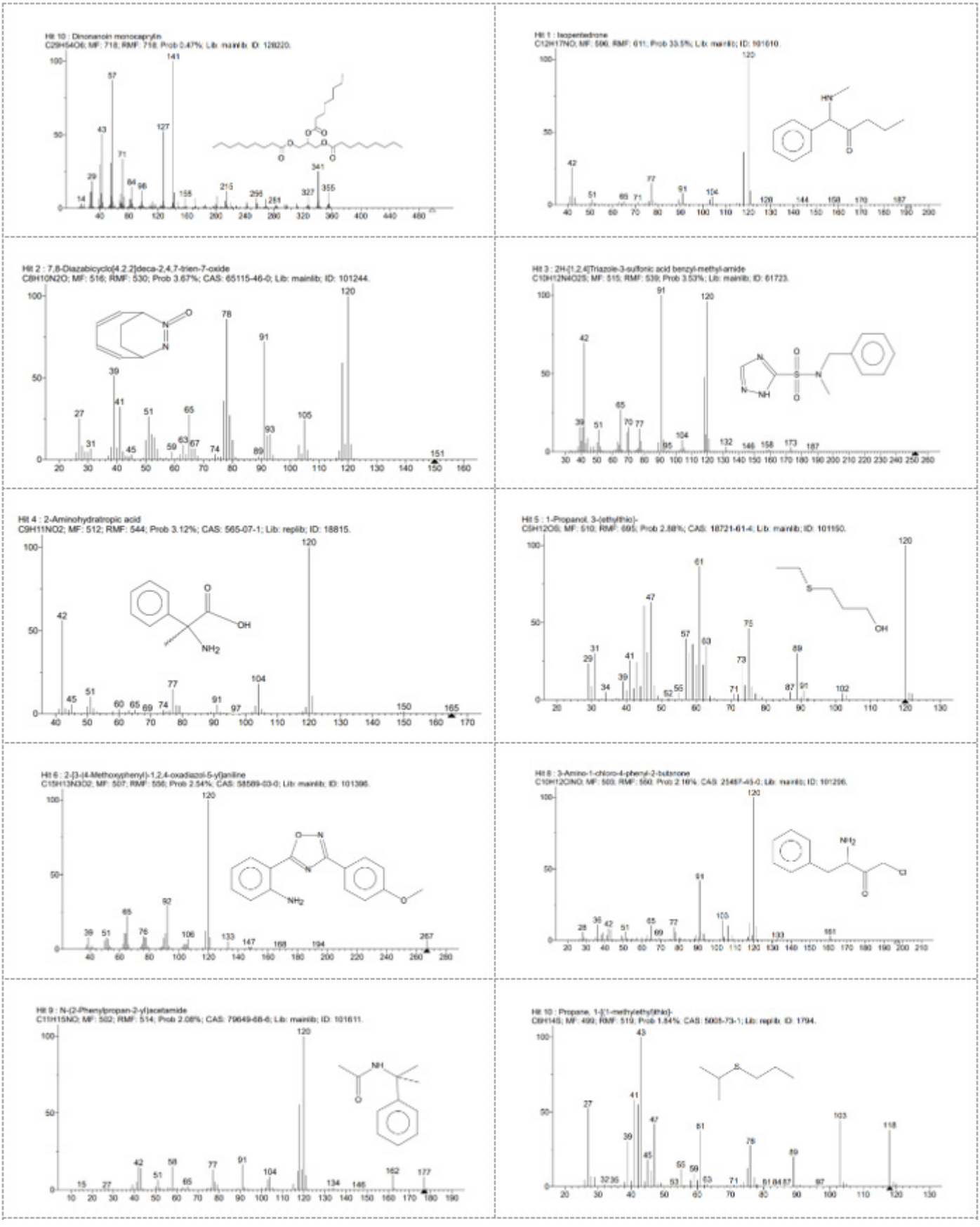
Hit 6 : 6-Methoxy-4-methylquinoline-2-thiol
C11H11NOS; MF: 465; RMF: 508; Prob 2.96%; Lib: mainlib; ID: 187640.
Hit 7 : 1-[1-(3-Chlorophenyl)-1,2,3-triazol-4-yl]cyclohexan-1-amine
C14H17ClN4; MF: 461; RMF: 483; Prob 2.50%; Lib: mainlib; ID: 87892.
Hit 8 : Pyrazol-5(4H)-one, 3-(4-nitrophenyl)-
C9H7N3O3; MF: 459; RMF: 564; Prob 2.30%; CAS: 54945-13-0; Lib: mainlib; ID: 187381.
Hit 9 : Trimethylsilyl (5-benzyl-3,6-dioxopiperazin-2-yl)acetate
C16H22N2O4Si; MF: 459; RMF: 465; Prob 2.30%; Lib: mainlib; ID: 187173.
Hit 10 : Dimethyl(bis)(4,8,8-trimethyldecahydro-1,4-methanoazulen-9-yl)methoxy]silane
C32H56O2Si; MF: 455; RMF: 458; Prob 1.94%; Lib: mainlib; ID: 68421.


Hit 1 : 9-Octadecenoic acid, (E)-, TMS derivative
Hit 1 : 9-Octadecenoic acid, (E)-, TMS derivative
Hit 2 : Hexadecylamine, N-tert-butyldimethylsilyl-
Hit 3 : 11-Octadecenoic acid, (Z)-, TMS derivative
C21H42O2Si; MF: 781; RMF: 842; Prob 5.07%; Lib: mainlib; ID: 232221.
Hit 4 : 13-Octadecenoic acid, (Z)-, TMS derivative
Hit 5 : N-(2-Hydroxyethyl)-4-(oxo(phenyl)acetyl)benzamide tms
Hit 6 : 11-Octadecenoic acid, (E)-, TMS derivative
Hit 7 : Oleic Acid, (Z)-, TMS derivative
Hit 8 : Sarcosine, N-(3-cyclopentylpropionyl)-, pentadecyl ester
Hit 9 : Oleic Acid, (Z)-, TMS derivative


Hit 10 : Dinonanoin monocaprylin
C29H54O6; MF: 718; RMF: 718; Prob 0.47%; Lib: mainlib; ID: 128220.
Hit 1 : Isopentedrone
C12H17NO; MF: 596; RMF: 611; Prob 33.5%; Lib: mainlib; ID: 101610.
Hit 2 : 7,8-Diazabicyclo[4.2.2]deca-2,4,7-trien-7-oxide
C8H10N2O; MF: 516; RMF: 530; Prob 3.67%; CAS: 65115-46-0; Lib: mainlib; ID: 101244.
Hit 3 : 2H-[1,2,4]Triazole-3-sulfonic acid benzyl-methyl-amide
C10H12N4O2S; MF: 515; RMF: 539; Prob 3.53%; Lib: mainlib; ID: 61723.
Hit 4 : 2-Aminohydratropic acid
C9H11NO2; MF: 512; RMF: 544; Prob 3.12%; CAS: 565-07-1; Lib: replib; ID: 18815.
Hit 5 : 1-Propanol, 3-(ethylthio)-
C5H12OS; MF: 510; RMF: 695; Prob 2.88%; CAS: 18721-61-4; Lib: mainlib; ID: 101150.
Hit 6 : 2-[3-(4-Methoxyphenyl)-1,2,4-oxadiazol-5-yl]aniline
C15H13N3O2; MF: 507; RMF: 556; Prob 2.54%; CAS: 58569-03-0; Lib: mainlib; ID: 101396.
Hit 8 : 3-Amino-1-chloro-4-phenyl-2-butanone
C10H12ClNO; MF: 503; RMF: 590; Prob 2.16%; CAS: 25487-45-0; Lib: mainlib; ID: 101206.
Hit 9 : N-(2-Phenylpropan-2-yl)acetamide
C11H15NO; MF: 502; RMF: 514; Prob 2.08%; CAS: 79649-68-6; Lib: mainlib; ID: 101611.
Hit 10 : Propane, 1-[(1-methylethyl)thio]-
C6H14S; MF: 499; RMF: 519; Prob 1.84%; CAS: 5008-73-1; Lib: replib; ID: 1794.

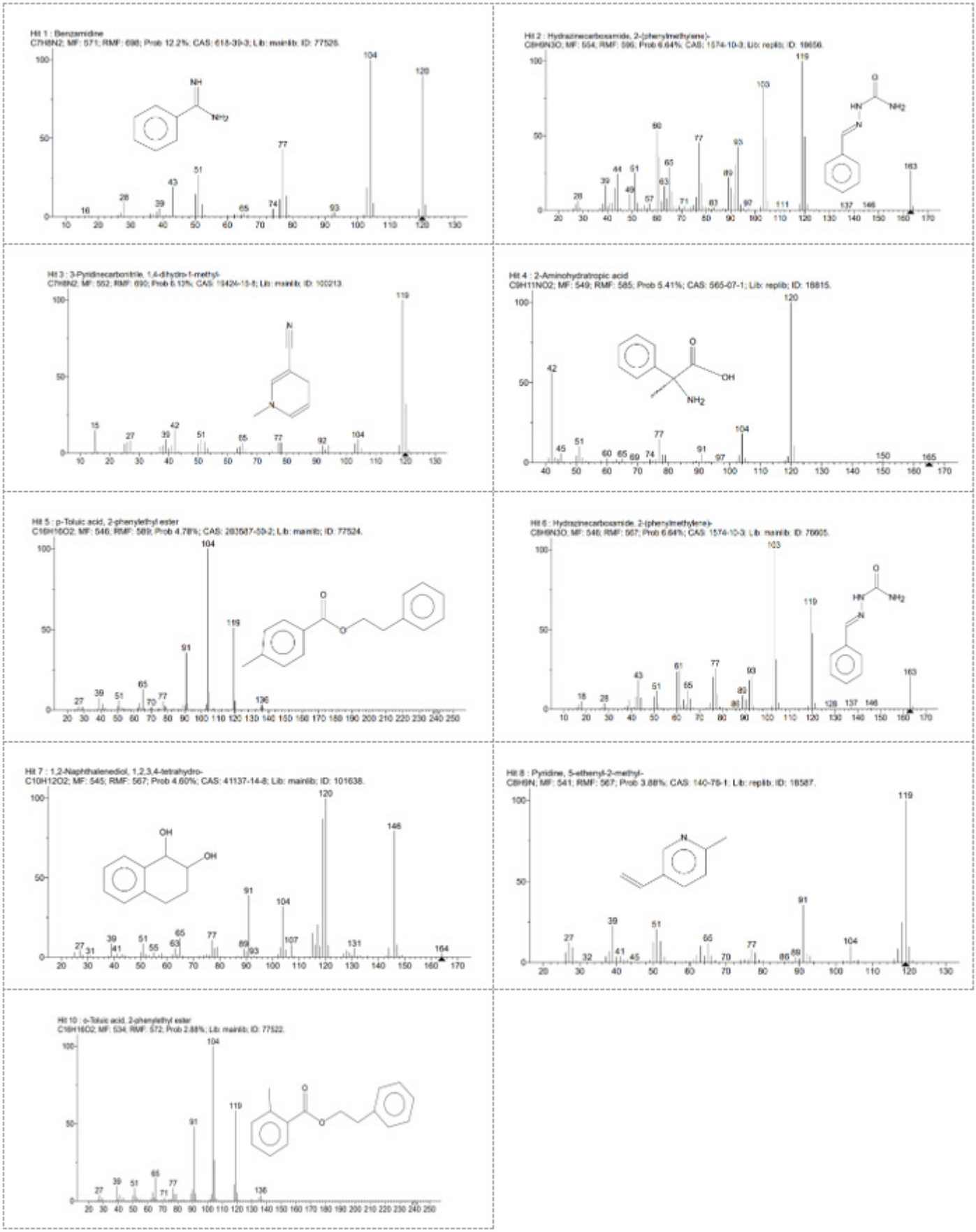


Figure S1: Bioactive molecule of hydroethanolic extract CS.