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GC-MS METABOLITE PROFILING OF BIOACTIVE COMPOUNDS IN LEAF, FRUIT AND SEED EXTRACTS OF *SYZYGIUM CUMINI* (L.)

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ABSTRACT: The present study aimed to explore the primary metabolites present in leaf, fruit, and seed crude extracts of *Syzygium cumini* L by Gas chromatography - Mass spectrometry. The compounds in the leaf, seed, and fruit extracts resulted from the GC-MS analysis was relevant to the National Institute of Standards and Technology (NIST) library. The metabolite profiling of the extracts revealed the presence of carboxylic acid and fatty acid found to be common in leaf, fruit, and seed extracts. And metabolites 6-oxa-3-thiaoctanoic acid, bisoprolol, phenacetin, tropin, alizarin, gonodolic acid are present in seeds that are not found in leaves and fruit metabolite profile. In contrast, Tetra decanoic acid, Azelaic acid, Penicillamine and S (-)-Cathinone are found only in leaves. Leaf, fruit and seed extracts of *Syzygium cumini* L contains various bioactive compounds and consequently has a variety of medicinal properties for the treatment of different diseases like thyroid cancer, heart diseases, kidney stones and rheumatoid arthritis. Some metabolites found to be active as antidiabetic, anti-inflammatory, anti-cancerous, antioxidant, anti-bacterial and antifungal activities identified in leaf, fruit and seed extracts of *Syzygium cumini* L. This study may pave the way for the production of herbal medicines for various ailments using leaf, fruit, and seed extracts of *Syzygium cumini* L.

INTRODUCTION: In the olden days, people mostly used herbal medicines to treat all diseases. Treating diseases through natural medicine is the earlier method that is known to humankind. But currently proper biological study is needed to find novel drugs also discovery supplementary medicinal properties of the plants for medicinal care¹.

There are undefined medicinal properties of many medicinal plants yet to explore. In India, the medicinal plants using by Ayurveda, Siddha, Homeopathy, etc., for various ailments². 80% of the world's population (WHO) based on traditional plant-based medicines for primary healthcare needs. Recently much of the research was being carried out in medicinal plants^{3,4}.

Because the synthetic drugs which were used by human have many side effects that often lead to serious complications⁵. And the development of herbal medicine done by the primary screening of the compounds in the plant extracts^{6,7}. In modern or synthetic medicine, herbal medicine was the lifesaving drug^{8,9} due to its usual mystic powers as well as for medicinal merits and virtues and

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Around many plant drugs for which synthetic ones are quiet absent^{8, 9}. Only 6% of medicinal plant species studied for their biological activity and only a few have phytochemically investigated. So there is a need to study the metabolite profiling of medicinal plants¹⁰.

Syzygium cumini (Syn. *Eugenia jambolana*) belongs to the Myrtaceae family. Fruits and seeds of *Syzygium cumini* (Jamun) have hypoglycaemic, anti-inflammatory, antipyretic, hypolipidemic, and antioxidant activities¹¹.

Several phytochemicals identified in *Syzygium cumini* (Jamun) fruits, leaves, and seeds some of which include: alkaloids, saponins, flavonoids, tannins, glycosides, anthraquinones etc. and also phyto-chemicals of fruits, leaves, and seeds are non-nutritive chemicals of plants and possess disease preventive or protective properties. These include anticancer activity, antibacterial, antioxidant, hormonal action, enzyme stimulation, and many others¹².

GC-MS is a powerful technique used for the specific detection and potential identification of compounds based on the molecular mass in a complex mixture¹³. In a typical MS procedure, a sample is ionized and separated according to their mass-to-charge ratio. Ions of the same mass-to-charge ratio will undergo the same amount of deflection¹⁴.

The atoms or molecules in the sample can be identified by correlating known masses to the identified masses or through a characteristic fragmentation pattern¹⁵. In recent period GC-MS studies have been increasingly applied for the analysis of most of the medicinal plants¹⁶.

This technique has proved to be a valuable method for the analysis of non-polar components and volatile essential oils, fatty acids, and lipids present in plants as secondary metabolites^{17, 18}. All these medicinal properties of *Syzygium cumini* (Jamun) fruits, leaves, and seeds are due to the presence of its phytochemical constituents, which not yet explored thoroughly. So, in this study, the Gas Chromatogram Mass Spectrometric method (GCMS) was used to carry out metabolite profiling of the crude extracts of dried *Syzygium cumini* (Jamun) fruits, leaves, and seeds.

MATERIALS AND METHODS: One mg of the finely powdered leaf, fruit, and seeds powder is added to 60 ml ribitol in Milli-Q water along with 20 ml of methoxy pyridine solution in a separate test tubes. The mixture incubated for 90 min at 70 °C and supernatant was collected. Then the supernatant sample solution is added to 40 ml of N trimethylsilyl-N-methyl tri-fluoroacetamide. This sample mixture incubated at 70 °C for 30 min followed by centrifugation at 12000 rpm for 15 minutes.

These samples then analyzed by LECO-PEGATUS GCXGC-TOF-MS system (LECO Corporation, USA) equipped with a 30m Rxi-5ms column with 0.25 internal diameter and 0.25µm film thickness (Restek, USA). The injection temperature, interface, ion source set at 250 °C, 225 °C, 200 °C respectively for the samples.

For separation of metabolites according to their groups, the run program was set at isothermal heating at 70 °C program for 5 min, followed by 5 °C of minimum oven temperature and final heating at 290 °C for 5 min and results are observed. The separation of compounds results in more than one peak for a metabolite of interest. Due to partial silylation or isomerization of methoxy animated compounds such as sugars¹⁹.

Results: The metabolite profiling of the leaf, fruit, and seed were analyzed through gas chromatography and mass spectroscopy and presented in (Fig. 1-4 and Table 1- 4).

Metabolite Profiling of Leaf Extracts: GC-MS is the best technique to identify the constituents of volatile matter, long-chain, branched-chain hydrocarbons, alcohols acids, esters, etc. Peak area, retention time, and the molecular formula used for the confirmation of phytochemical compounds. The active principles with their Retention time (RT), Molecular formula, Molecular weight (MW) and peak area in percentage presented. GC/MS analysis of an ethanolic extract of leaf, fruit and seeds of *Syzygium cumini* revealed the existence of 105 compounds in the leaf extract. Of which carboxylic acid (19%), organic compound (11%), fatty acid (10%), carbohydrates (9%), sugars (7%), amino acid (6%), ester (6%), sugar alcohol (5%), alkane hydrocarbon (5%), heterocyclic compound (4%),

phenols (3), hydrocarbon (3%), alcohol (2%), amine (2%), steroid (2%), alkaloid (2%), amine (1%), shikimic acid (1%) and amide (1%) found to be present in leaf extract metabolite profile. Whereas metabolite profiling of fruit extract revealed the presence of a total of 75 compounds. Of which fatty acids (11%), carbohydrates (8%), carboxylic acid (8%), organic acid (7%), amino acids (6%), sugars (5%), hydrocarbons (3%), heterocyclic compounds (3%), amides (3%), alkanes (3%), alkenes (3%), phenols (3%), sugar alcohol (3%), alcohol (2%), amine (2%), ester (2%), anilid (1%), ether (1%) and steroids (1%)

were found to be present in fruit extract metabolite profile. And the metabolite profiling of seed extract revealed the presence of a total of 87 compounds. Of which carbohydrates (15%), fatty acids (13%), carboxylic acid (10%), dicarboxylic acid (9%), amino acids (8%), organic acids (6%), sugars (4%), alkane (3%), conjugated acid (3%), hydrocarbons (2%), organic compounds (2%), sugar alcohol (2%), heterocyclic compounds (2%), gondoic acid (1%), esters (1%), phenols (1%), amides (1%), amines (1%), phenacetin (1%), steroids (1%) and alkaloids (1%) were found to be present in seed extract metabolite profile.

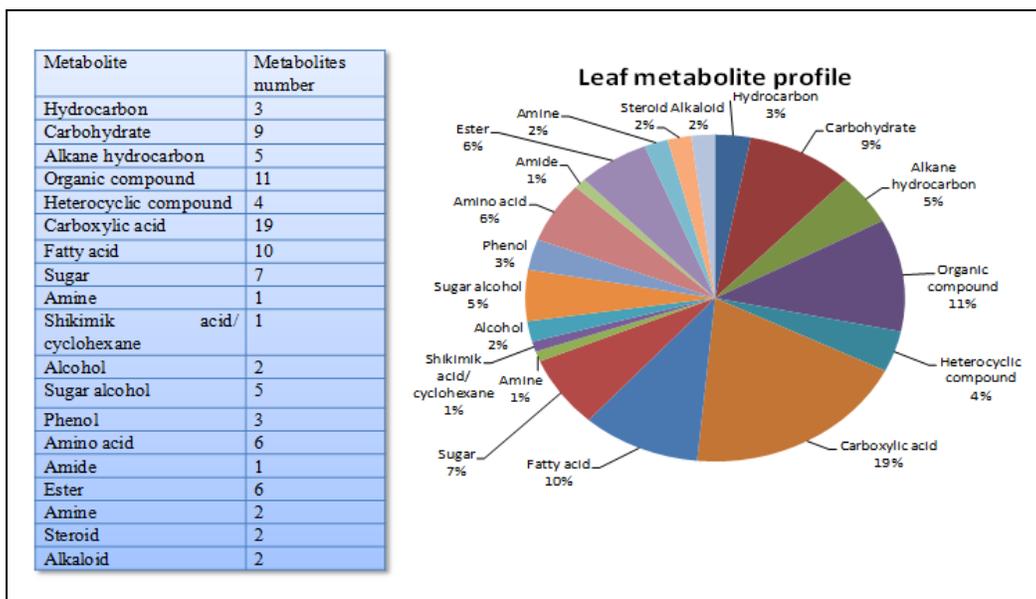


TABLE 1 AND FIG. 1: THE ABUNDANCE OF EACH PRIMARY AND SECONDARY METABOLITES OF LEAF EXTRACTS OF SYZYGIUM CUMINI (L.)

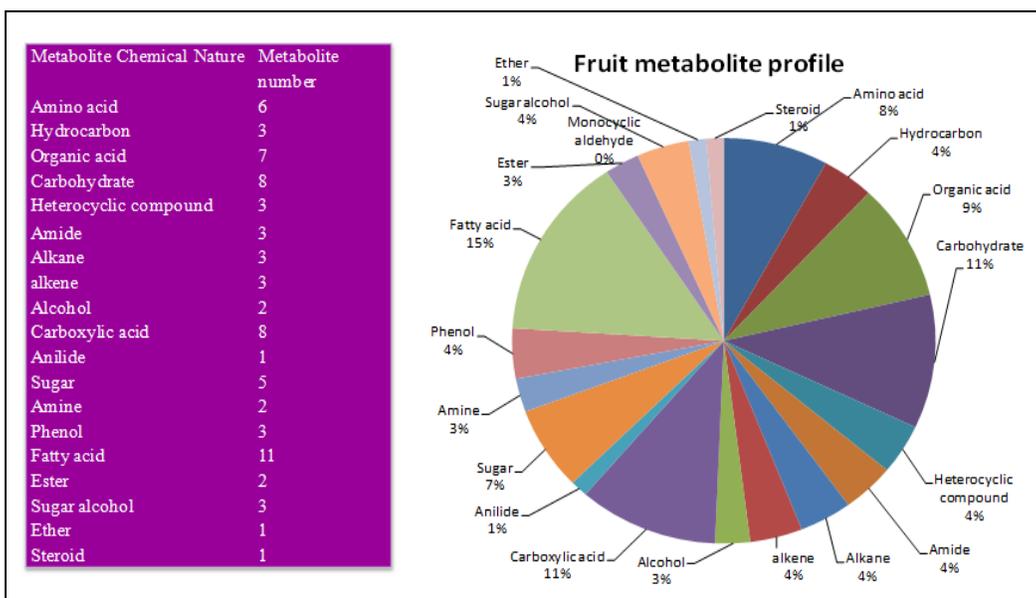


TABLE 2 AND FIG. 2: THE ABUNDANCE OF EACH PRIMARY AND SECONDARY METABOLITES OF FRUIT EXTRACTS OF SYZYGIUM CUMINI (L.)

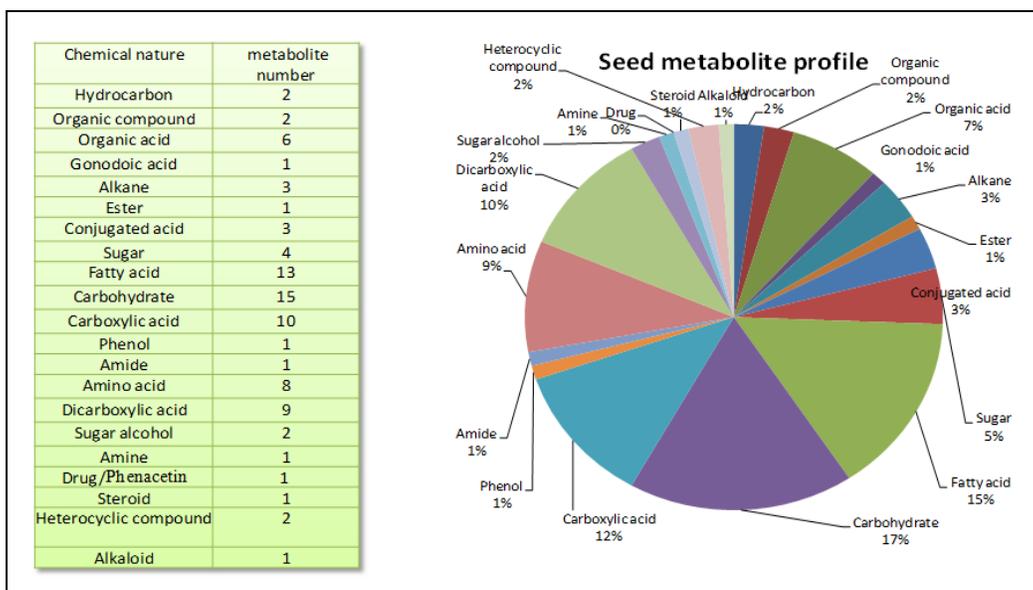


TABLE 3 AND FIG. 3: THE ABUNDANCE OF EACH PRIMARY AND SECONDARY METABOLITES OF SEED EXTRACTS OF SYZYGIUM CUMINI (L.)

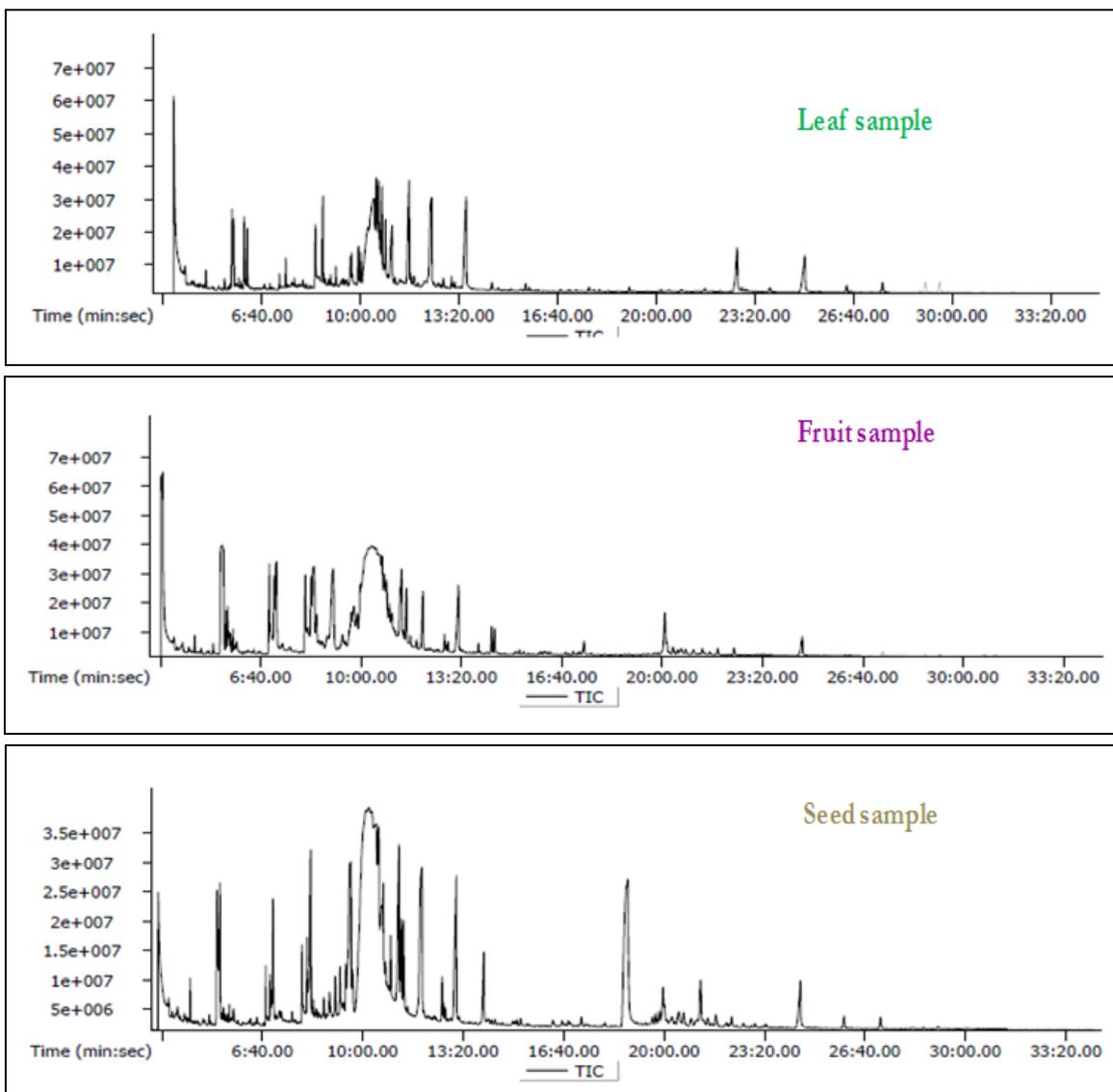


FIG. 4: GC-MS ANALYSIS OF LEAF, FRUIT AND SEED EXTRACTS OF SYZYGIUM CUMINI L.

TABLE 4: APPLICATIONS OF METABOLITES OBSERVED IN LEAF, FRUIT, AND SEED OF *S. CUMINI* BY GC-MS ANALYSIS

S. no.	Metabolite	Uses	Present in
1	6-Oxa-3-thiaoctanoic acid	Potential Inhibitor against Thyroid Cancer	Seed
2	Bisoprolol	Medicine for heart diseases specifically includes high blood pressure, chest pain from not enough blood flow to the heart, and heart failure.	Seed
3	Phenacetin	Phenacetin is a pain-relieving and fever-reducing drug	Seed
4	Tropine	Anticholinergic medicine is used to decrease the production of saliva and other fluid secretions during surgery. It is also used to treat spasms or cramps in the stomach, intestines, and other organs of the body	Seed
5	Nicotinaldehydethiosemicarbazone	Used in the treatment of pulmonary tuberculosis in adults	Leaf and seed
6	Alizarin / 1,2-Dihydroxyanthraquinone,	Used in carbon dating to identify carbonates	Seed
7	Pregnenolone	Pregnenolone is a precursor to many hormones. It relieves from blues or depression	Leaf, fruit, and seed
8	Gondoic acid/ 1,1-Eicosenoic acid,	Omega fatty acid	Seed
9	2-Butenedioic acid	Multiple sclerosis, psoriasis and to cure the autoimmune disorder	Leaf, fruit, and seed
10	Hexadecenoic acid	Antidiabetic, Anti-inflammatory, Antioxidant, hypocholesterolemia, nematocide, pesticide, and potent mosquito larvicide.	Leaf and seed
12	Octadecadienoic acid	Antidiabetic, Anti-cancer, Anti-inflammatory, antiandrogenic, cancer preventive, spermatogenic, hypo cholesterol emic and antidiabetic activity,	Seed and fruit
13	Tetra decanoic acid, trimethylsilyl ester	Antidiabetic, Larvicidal and repellent activity	Leaf
14	Benzoic acid trimethylsilyl ester	Intermediate in the biosynthesis of many secondary metabolites, anticancer and antimicrobial activity	Leaf, Fruit, and seed
15	Eicosane	Anti-androgenic and antimicrobial activity.	Fruit and seed
16	Heptadecanoic acid	antifungal and trypanocidal activity	Fruit and seed
17	Hexadecanoic acid	Antioxidant and antimicrobial activity	Fruit and seed
18	1,2,5,6-Hexanetetrol, tetrakis-O-(trimethylsilyl)-	Antifungal, antioxidant, antiallergic, antitumoral and antiparasitic activity	Fruit and leaf
19	Azelaic acid, bis(trimethylsilyl) ester	Acts as a "distress flare" involved in defense responses after infection. An important component of the plant's defensive response. Anti-inflammatory, anticancer and tyrosine inhibitor	Leaf
20	Penicillamine, tri-TMS	Treatment of Wilson's disease. Treatment for kidney stones which have high urine cystine levels, rheumatoid arthritis, and various heavy metal poisonings	Leaf
21	S (-)-Cathinone	Antidepressant	Leaf
22	Octadecanoic acid	anti-inflammatory, antiviral and antiasthmatic	Leaf, fruit, and seed
23	Tetracosane	Antimicrobial, Antidiabetic, and antioxidant	Leaf, fruit, and seed
24	Tridecane, 5-propyl-	Antimicrobial agent	Leaf, fruit, and seed

DISCUSSION AND CONCLUSION: 6-oxa-3-thiaoctanoic acid compound found in the seed is a potential inhibitor against thyroid cancer. Bisoprolol metabolites found in the seed used as medicine for heart diseases like high blood

pressure, chest pain due to less blood flow to the heart and heart failure. Phenacetin compound found in the seed is a pain-relieving and fever-reducing drug. Tropine metabolite found in the seed is used as anticholinergic medicine to decrease the

production of saliva and other fluid secretions during surgery. It also used to treat spasms or cramps in the stomach, intestine, and other organs of the body²⁰.

Nicotinaldehydethiosemicarbazone found in leaf and seed is used in the treatment of pulmonary tuberculosis in adults. Alizarin / 1, 2. Dihydroxy-anthraquinone found in the seed is used in carbon dating to identify carbonates. Pregnenolone compound found in leaf, fruit, and seed is a precursor of many hormones and also relieves depression. Gondoic acid metabolite found in the seed is an omega fatty acid. 2-butenedioic acid found in leaf, fruit and seed used for multiple sclerosis, psoriasis and to cure the autoimmune disorder. Hexadecenoic acid compound found in leaf and seed is used as antidiabetic, anti-inflammatory, antioxidant, nematicide and pesticide and potent mosquito larvicide²¹.

Octadecadienoic acid found in seed and fruit used as antidiabetic, anti-inflammatory, antiandrogenic and cancer preventive. Tetra decanoic acid trimethylsilyl ester - found in the leaf used as an antidiabetic, anti larvicidal and anti-repellent activity. Benzoic acid trimethylsilyl ester metabolite found in leaf, fruit and seed is used for biosynthesis of many secondary metabolites, anticancer antimicrobial activity. Heptadecanoic acid compound found in fruit and seed is used as an antifungal and for trypanocide activity. Hexadecanoic acid found in fruit and seed is used for antioxidant and antimicrobial activity. 1,2,5,6-Hexanetetrol a compound found in fruit and leaf is used as an antifungal, anti-oxidant, anti-allergic, antitumoral and anti-parasitic activity. Azelaic acid bis (trimethylsilyl) ester found in leaf acts as a distress flare after infection, defensive response, anti-inflammatory, anti-cancer, and tyrosine inhibitor. Penicillamine, tri-TMS metabolite found in the leaf used to treat Wilson's disease treatment for kidney stones and rheumatoid arthritis. S (-)-Cathinone found in leaf used as an antidepressant. Octadecanoic acid compound found in leaf, fruit, and seed used to cure asthma, anti-inflammatory, and antiviral. Tetracosane metabolite found in leaf, fruit and seed is used as anti-microbial, antidiabetic and antioxidant and tridecane, 5-propyl compound found in leaf, fruit and seed as an antimicrobial agent²². GC-MS technique is one of the effective

technique for the studies related to medicinal properties and antibacterial properties of herbal extracts²³. There are studies conducted to deal with the downstream processing of anthocyanins from black plum (*S. cumini*) to obtain anthocyanins in a purified form²⁴ this study includes adsorption employing six different adsorbents. Among these, Amberlite XAD7HP showed the highest adsorption capacity (1.07 mg/mL of adsorbent) and desorption ratio (87.62%). Characterization and evaluation of anthocyanin pigments from *Syzygium cumini* fruit peels for their antioxidant efficacy and stability²⁵. Furthermore identified and reported by high-performance liquid chromatography (HPLC) three anthocyanins compounds as glucosides are delphinidin, petunidin, and malvidin. It can be concluded that the compounds present in leaf, fruit and seeds of *Syzygium cumini* is extensively used traditional ailment for the treatment of various diseases especially diabetes and their associated complications²⁶. The plant has many important compounds that confer the main characteristics of the plant. Further investigations needed with HPLC data to support with specifically identifiable fractions of compounds, with the intention that this plant could be exploited as an antioxidant agent, natural medicine, or a nutritional supplement. It also makes a potential medicinal plant and the plant parts studied can be used as a traditional medicine to cure various ailments.

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CONFLICTS OF INTEREST: Nil

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