

GC–MS Profiling of Essential Oils from Medicinal Plants and Their Pharmacological Correlations

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Abstract

Celastrus paniculatus Willd. (Celastraceae) is a woody liana. Its seeds are used to treat abdominal disorders, arthritis, asthma, body ache, leprosy, dysmenorrhea, gout, menorrhea, paralysis, rheumatism, ulcers and skin disease. All things considered, this thorough investigation of fruit extracts from *Mallotus philippensis* lays the groundwork for future research and development of this therapeutic plant. *Muell Mallotus philippinensis*. Arg (Euphorbiaceae) is a perennial shrub or small tree that grows abundantly in tropical and subtropical parts of the outer Himalayas at elevations below 1,000 meters. It is said to offer a variety of medicinal properties. In order to evaluate the ocular toxicity of *Calotropis gigantea* and *Calotropis procera*, an observational research was conducted. Plants are widely utilized to cure a variety of illnesses and serve an important role in the development of novel drugs. These days, researchers are looking for safe, therapeutically useful phytochemical components that have less adverse effects than other conventional medications.

1. Introduction

Use of botanical agents for immunomodulation is still at an early stage of development. Various herbal preparations found in the traditional system of medicines are known to possess the ability to modulate the immune system of the body. Numerous biologically active compounds such as polysaccharides, lectins, peptides, flavonoids, and tannins have shown modulation of the immune response. Traditional Indian medical systems such as Siddha and Ayurveda have recommended certain methods to enhance the immune response of the body against diseases. Many Indian medicinal plants along with a number of herbal preparations known as Rasayanas are known to possess immunomodulating abilities. The rasayana drugs have properties for enhancing overall health and longevity along with immunostimulation. As per the teachings of Ayurveda, these drugs help in strengthening all body tissues, prevent aging, boost intellect, and avoid diseases.[1][2][3][4][5]. The plant *Caesalpinia bonduc*, also known as *C. bonduc*, is classified under the “Fabaceae” family. It is a large straggling, very spiny bush. The stem is armed with hook and yellow, stiff spines. In the Indian traditional herbal medicines, the plant has been regarded as a valuable

drug against filarial infection, tumor, asthma, and diabetes.[6] *Mallotus philippinensis* Muell., known as Kamala, Kampillaka, Kapila, and Shendri locally, is an extremely common perennial shrub or small tree growing in outer Himalayas up to 1500 meters. The ripe fruits contain glandular hairs in the form of reddish-brown powder, which can be harvested by shaking and rubbing the fruits manually, collecting the material in cloth. The harvested powder is fine and granular, dull red or madder red in color, and is buoyant in water. *Mallotus philippinensis* Muell. is commonly used in traditional medicine for its antifilarial.[7] Diarrhea is caused by infections in the gastro intestinal tract, which may arise due to the presence of several types of bacteria, viruses, and parasites. Diarrhea may be spread by means of ingestion of contaminated food, drinking of water, as well as unsanitary surroundings. Apart from any other pathology that may exist, some of the physiological reasons why an individual develops diarrhea include water and electrolyte transport issues in the body which occur through four different methods: high osmotic pressure, increase in electrolyte secretion, decrease in electrolyte absorption, and rapid intestinal transit.[8] Because of the negative effects associated with NSAID drugs and opioid painkillers, a lot of research efforts have been aimed at trying to develop alternative drug types that lack such side effects. The current research trends have therefore focused on the use of herbal remedies because they are cheaper and easily accessible, among other benefits.[9] In the soil, plants are directly exposed to Cd contamination, and vegetables are the primary means for Cd exposure to humans via the food chain. Toxic effects of Cadmium on plant physiology are mostly represented by growth and physiological disorders.[10] Sorafenib is a drug that functions to inhibit the activities of Raf proto-oncogene serine/ threonine protein kinase, B-Raf proto-oncogene serine/ threonine kinase, and kinases of the RAS/ Raf/Mitogen activated Protein Kinase Kinase/ Extracellular Signal-Regulated Kinase pathway. This leads to reduced proliferation of tumor cells. Another mechanism of action of sorafenib is that it inhibits angiogenesis through the inhibition of HGF receptor, Fms-like tyrosine kinase, vascular endothelial growth factor receptor-2/-3, platelet-derived growth factor receptor, and other tyros. [11] Additionally, inflammatory responses may be immediate to skin injuries, resulting in the up-regulation of several pro-inflammatory cytokines, among them cyclooxygenase-2 (COX-2) and inducible nitric oxide synthase (iNOS), which plays an important role in inflammatory processes. Activation of enzymes to produce mediators of inflammation increases the expression of cytokines, including tumor necrosis factor-alpha (TNF- α) and interleukin-6 (IL-6). A number of herbal medicines and products have found applications in the healing of wounds for several years since some herbal products like alkaloids, tannins, flavonoids, and terpenes contribute in the process of wound healing. But traditional herbal medical products for the healing of wounds still need clarification regarding their molecular basis, which would provide useful information to facilitate the healing process and also fight against skin infections. Several experiments have shown the wound healing abilities of *H. integrifolia*. In one study, wound-healing activity of *H. integrifolia* extracts was evaluated in excision wounds in Wister rats where more than 90% wound healing was obtained at the 14th day post-surgery in the experimental groups while only 62.99% in control groups. Besides, in the incision model experiment, there was greater re-deposition of collagen in experimental groups as compared to the control group. Not only wound healing abilities, but also protected the wound area against any microbial infection.[12][13] Furthermore, infrared spectroscopy has served as an excellent technique for the investigation of the structure and behavior of molecules in biological tissues and cells and was also utilized in analyzing the structural variations of the primary, secondary and tertiary structures of nucleic acids in rats that were irradiated with gamma radiations using FT-IR spectroscopic studies. Macromolecules in biology are categorized into proteins, lipids, nucleic acids, and polysaccharides. Living things can be distinguished from one another by the number and importance of macromolecules that they use, as well as the important role played by macromolecules within their physiology. The functionality of biological

macromolecules always depends upon their structure. In addition, they serve as a good illustration of the relationship between molecular structure and chemical/physical properties of a substance.[14]

Methodology

Collection of materials:-

The plant seeds *Caesalpinia bonduc*, *Mallotus philippensis*, and *Holoptelea integrifolia*, flower *Calotropis gigantea*, and root *Hemidesmus indicus* that have been collected from the field of the Rama University of Agriculture and Technology at Kanpur are used for this research experiment. Seeds of the plant species of Solanaceae, *Caesalpinia bonduc*, *Mallotus philippensis*, *Calotropis gigantea*, *Holoptelea integrifolia*, and *Hemidesmus indicus* are expected to be available in the month of March 2024. These plants were identified and verified by the Department of the Faculty of Engineering at Rama University of Mndhana Kanpur,

Oil Extraction using Soxhlet:-

The seeds had an off-white appearance and their moisture content was 4%. Oil extraction is made easy when crushing is done on the seeds prior to extraction. This method involves breaking down the cell wall of the seeds, making it easy for oil to be extracted. Seeds were heated up to 105 degrees Celsius for two hours. Heating is helpful since it enables the oil to be easily extracted by eliminating the moisture content within the seeds. Pre-treatment and heat treatment were then followed by setting up the apparatus for solvent extraction. The solvents used for the extraction process were benzene, n-hexane, and a combination solvent mixture. The extraction process involved using the Soxhlet extractor for the process. The extraction process will involve using petroleum ether as the solvent for extracting the seed oil. After extraction, simple distillation will be used to remove the solvent. The resulting product will be placed inside a desiccator and allowed to cool before weighing. It will be stored inside a dark brown bottle with a tightly sealed cap. The objective is to determine the various qualities of the oil and yield percentage. The solvent that was used in the Soxhlet extraction to extract

Methanol Extraction Using a 1:2 ratio of feed to solvent

In order to remove any moisture, dry the following samples weighing 50 grams each: *Caesalpinia bonduc*, *Mallotus philippensis*, *Calotropis gigantea*, *Holoptelea integrifolia*, and *Hemidesmus indic*

- First, grind the date seeds to obtain their powder.
- The date seed powder will be used in a 1:1:2 ratio to 100 milliliters of methanol solvent.
- Then take a cloth or a filter paper and pack it with the date seed powder.
- Put the packed filter paper in the Soxhlet extraction apparatus thimble.
- Add methanol (solvent) to the Soxhlet flask containing 100 ml of methanol.
- Heat the reaction mixture for two to three hours at 60 to 65 degrees Celsius (solvent boiling point).
- At the end of the extraction process, detach the round-bottomed flask from the Soxhlet apparatus.
- Separate the date seed oil from the solvent through simple distillation.
- The process of simple distillation will be conducted at 60 to 65 degrees Celsius.
- As a result of the distillation process, the date seed oil forms at the bottom while the petroleum ether remains on top.

Gas chromatography mass spectrometry

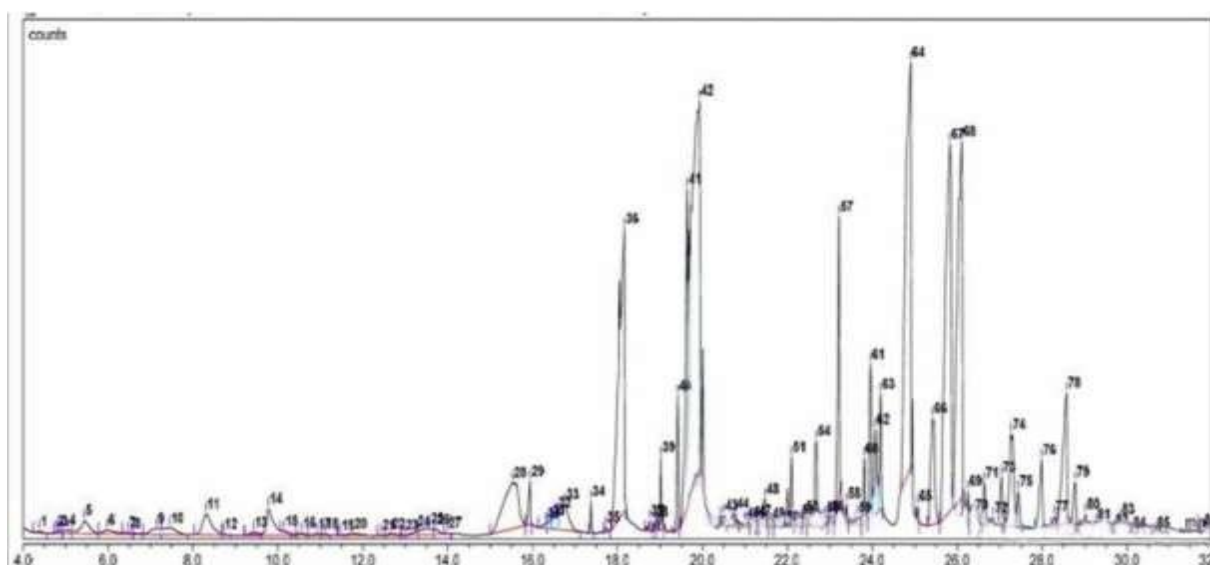
- GC-MS System: In the study under discussion, a GC-MS system named as GCMS-QP2010 has been employed. GC-MS technology involves a combination of gas chromatography (GC) and mass spectrometry (MS), enabling scientists to separate different compounds from a sample.

- **GC Column:** As to the GC column, the Rxi-1MS one has been chosen for the current research project. The Rxi-1MS GC column possesses the length of 30 m, inner diameter of 0.25 mm and film thickness of 0.25 μm . The column consists solely of 100% dimethyl polysiloxane and produced in the USA by Restek. The Rxi-1MS column is known for being widely used in standard GC separation techniques.
- **Autosampler:** An autosampler named as AOC-20i by Shimadzu (Japan) was utilized for introducing test samples. The function of the autosampler is the automated introduction of samples into GC systems.
- **Mass Range and Maximum Temperature:** In the current study, the mass spectrometer could measure samples within 45-500 g. The maximum temperature, at which the oven of the GC system could work, is 330°C, which corresponds to the maximum temperature the GC column can tolerate.
- **Carrier Gas:** Helium (He) is used as the carrier gas in the current GC study. At

Results

4.3.1. GC-MS Gas chromatography–mass spectrometry *Caesalpinia bonduc*

In the ethanol extract of seed kernel, 87 bioactive phytochemical compounds were identified through this GC-MS analysis, while the number of bioactive phytochemical compounds was found to be 50 in the ethanol extract of seed coat. In the ethanol extract of seed coat, three phytochemical compounds acquired the highest relative peak area (>2%), and the one having the highest relative peak area is 9,12-Octadecadienoic acid (Z,Z)- with a retention time of 19.65 minutes. In the ethanol extract of seed kernel, seven phytochemical compounds acquired the highest relative peak area (>2%), and the one having the highest relative peak area is 6-Octadecenoic acid with a retention time of 19.93 minutes.



Graph4.1. of Gc-MS of *Caesalpinia bonduc*

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² ($\text{\AA}^2$)
1.	4.38	$\text{C}_4\text{H}_9\text{NO}_2$	Sec-Butyl nitrite	63.3
2.	4.78	$\text{C}_4\text{H}_7\text{NO}_3$	2-Nitro-1-buten-3-ol	66.4
3.	4.87	$\text{C}_7\text{H}_{11}\text{NO}_5$	Isoxazolidine-3,5-dicarboxylic acid, dimethyl ester	104

4.	5.05	$C_{10}H_{22}N_2O$	N-Isopentyl-N-nitroso-pentylamine	32.34
5.	5.43	$C_7H_{14}O_3$	Propanoic acid, 3-ethoxy-, ethyl ester	46.5
6.	5.98	$C_6H_{12}O_5$	Alpha-l-rhamnopyranose	98
7.	6.47	$C_7H_{14}O_7$	d-Glycero-d-ido-heptose	131
8.	6.59	$C_6H_{12}O_5$	2-Deoxy-D-galactose	98
9.	7.14	$C_6H_8N_2O_8$	Isosorbide Dinitrate	63.8
10.	7.45	$C_3H_8O_3$	Glycerin	92.09
11.	8.30	$C_6H_8O_4$	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	52.6
12.	8.71	$C_8H_{15}NO_6$	a-D-Galactopyranose, 2-(acetylamino)-2-deoxy-	119
13.	9.42	$C_6H_8N_2O_8$	Isosorbide Dinitrate	63.8
14.	9.77	$C_6H_6O_3$	5-Hydroxymethylfurfural	58.5
15.	10.15	$C_8H_{14}O_7$	6-Acetyl-B-d-mannose	116
16.	10.56	$C_{10}H_{16}O_3$	Ascaridole epoxide	54.37
17.	10.92	$C_8H_{14}O_8$	1-Gala-l-ido-octonic lactone	156
18.	11.10	$C_7H_{13}NO$ S_2	Dithiocarbamate, S-methyl-,N-(2-methyl-3-oxobutyl)-	80.7
19.	11.47	$C_{18}H_{32}O_{16}$	Melezitose	268.68
20.	11.77	$C_{18}H_{32}O_{16}$	Melezitose	268.68
21.	12.43	$C_{17}H_{36}O$	1-Hexadecanol, 2-methyl-	20.2
22.	12.66	$C_{18}H_{32}O_{16}$	Melezitose	268.68
23.	12.98	$C_{18}H_{32}O_{16}$	Melezitose	268.68
24.	13.25	$C_{10}H_{17}NO$ $_6S$	Desulphosinigrin	148
25.	13.56	$C_{12}H_{24}O_3$	Dodecanoic acid, 3-hydroxy-	57.5
26.	13.72	$C_{18}H_{32}O_{16}$	Melezitose	268.68
27.	13.99	$C_{25}H_{44}N_2$ O_5S	2-Myristynoyl pantetheine	116
28.	15.52	$C_8H_{16}O_6$	Ethyl a-d-glucopyranoside	99.4
29.	15.94	$C_{14}H_{28}O_2$	Tetradecanoic acid	37.3
30.	16.32	$C_7H_{14}O_6$	3-O-Methyl-d-glucose	99.4
31.	16.42	$C_7H_{14}O_6$	3-O-Methyl-d-glucose	99.4
32.	16.57	$C_7H_{14}O_6$	3-O-Methyl-d-glucose	99.4
33.	16.76	$C_7H_{14}O_6$	3-O-Methyl-d-glucose	99.4
34.	17.37	$C_{17}H_{34}O_2$	Hexadecanoic acid, methyl ester	26.3
35.	17.72	$C_{16}H_{30}O_2$	9-Hexadecenoic acid	37.3
36.	18.16	$C_{38}H_{68}O_8$	1-(+)-Ascorbic acid 2,6-dihexadecanoate	119
37.	18.75	$C_{20}H_{40}O_2$	Ethanol, 2-(9-octadecenylloxy)-, (Z)-	37.3
38.	18.86	$C_{16}H_{32}O_2$	n-Hexadecanoic acid	37.3

39.	19.02	C ₁₉ H ₃₄ O ₂	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	26.3
40.	19.41	C ₁₉ H ₂₆ O	Androsta-4,16-dien-3-one	17.1
41.	19.64	C ₂₀ H ₃₆ O ₂	9,12-Octadecadienoic acid, ethyl ester	26.3
42.	19.93	C ₁₈ H ₃₄ O ₂	6-Octadecenoic acid	37.3
43.	20.50	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
44.	20.77	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
45.	21.02	C ₂₅ H ₄₂ O ₂	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl] methyl]-, methyl ester	37.3
46.	21.16	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
47.	21.29	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
48.	21.47	C ₂₀ H ₃₄ O ₂	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-	37.3
49.	21.60	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
50.	21.94	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
51.	22.09	C ₂₀ H ₂₂	2-Phenyl-4-tret-butyl-7-methylindene	
52.	22.30	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
53.	22.40	C ₁₉ H ₂₂ N ₂	Curan, 16,17,19,20-tetradehydro-	12.89
54.	22.68	C ₁₈ H ₃₀ S	2,4,6-Tri-t-butylbenzenethiol	1
55.	22.89	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
56.	23.00	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
57.	23.21	C ₂₁ H ₃₂ O	Pregna-5,17(20)-dien-3-ol, (36,17E)-	17.07
58.	23.39	C ₃₅ H ₆₈ O ₅	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	72.83
59.	23.64	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
60.	23.81	C ₂₀ H ₂₆ O ₅	Gibbane-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1a,4aa,4bβ,108)-	61.80
61.	23.95	C ₂₃ H ₂₈ O ₅	1,4,9(11)-Pregnatriene-3,20-dione, 21-acetoxy-17-hydroxy-	72.83
62.	24.07	C ₃₇ H ₇₆ O	1-Heptatriacotanol	20.2
63.	24.19	C ₂₂ H ₃₀ O ₄	17Alpha-ethynyl-17beta-hydroxy-6beta-methoxy-3alpha, 5-cyclo-5alpha-androstan-19-oic acid	77.75
64.	24.90	C ₂₁ H ₃₂ O ₂	Pregnenolone	37.3
65.	25.06	C ₂₀ H ₂₈ O ₃	68-Hydroxymethandienone	49.69
66.	25.42	C ₂₂ H ₂₈ O ₃	Norethindrone Acetate	43.40
67.	25.82	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bβ,4aβ,5β,7aa,7ba,8a,9β,9aa)]-	20.23

68.	26.11	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bß,4aß,5ß,7aa,7ba,8a,9ß,9aa)]-	20.23
69.	26.25	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bß,4aß,5ß,7aa,7ba,8a,9ß,9aa)]-	20.23
70.	26.40	C ₂₅ H ₃₄ O ₄	5,16,20-Pregnatriene-3beta,20-diol diacetate	60.33
71.	26.63	C ₂₆ H ₃₆ O ₈	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bß,4aß,5ß,7aa,7ba,8a,9ß,9aa)]-	113.29
72.	26.84	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bß,4aß,5ß,7aa,7ba,8a,9ß,9aa)]	113.29
73.	27.04	C ₂₈ H ₃₈ O ₉	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3- [(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bß,4aß,5ß,7aa,7ba,8a,9ß,9aa)]-	20.23
74.	27.27	C ₂₆ H ₃₆ O ₈	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 1a,1b,4,4a,5,7a,8,9-octahydro-3-(hydroxymethyl)-1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bß,4aß,5ß,7aa,7ba,8a,9ß,9aa)]	113.29
75.	27.44	C ₂₅ H ₃₆ O ₇	4,13,20-Tri-O-methylphorbol 12-acetate	107.22
76.	27.99	C ₂₆ H ₃₄ O ₉	Phorbol 12,13,20-triacetate	154
77.	28.28	C ₂₅ H ₃₄ O ₅	Acetic acid, 17-(1-acetoxy-ethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	82.1
78.	28.57	C ₂₁ H ₃₀ O ₅	2-Cyclopenten-1-one, 3,4-dihydroxy-5-(3-methyl-2-butenyl)-2- (3-methyl-1-oxobutyl)-4-(4-methyl-1-oxo-3-pentenyl)-	94.8
79.	28.77	C ₃₂ H ₃₉ NO ₁₀	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	144.13

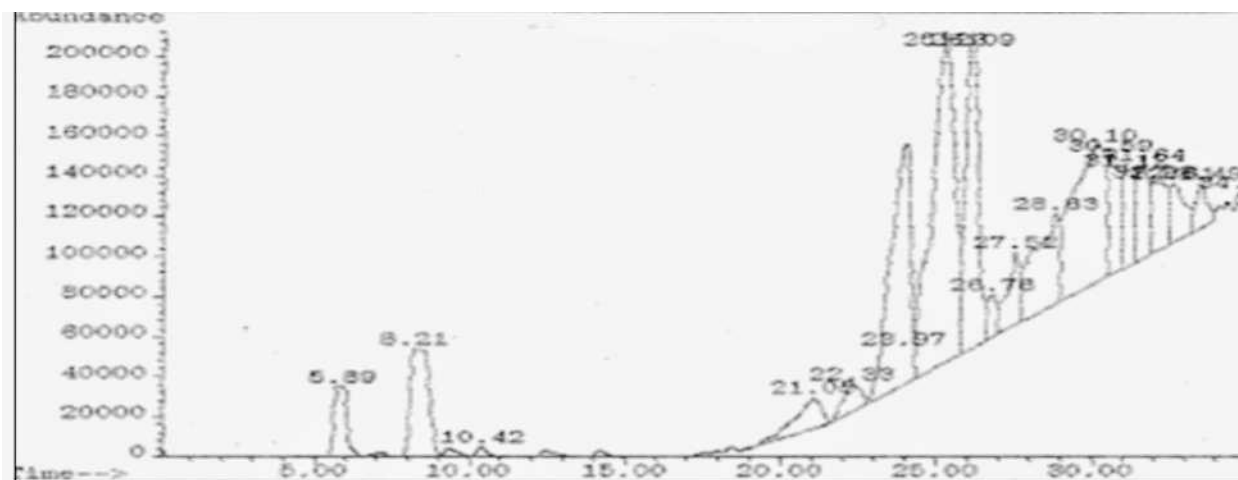
80.	29.02	C ₂₄ H ₃₄ O ₇	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	85.22
81.	29.27	C ₂₅ H ₃₄ O ₅	Acetic acid, 17-(1-acetoxy-ethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	82.10
82.	29.69	C ₂₆ H ₄₄ O ₅	Ethyl iso-allocholate	87.0
83.	29.84	C ₂₈ H ₄₄ O ₇	Pregn-5-ene-3,11,12,14,20-pentol, 11-acetate 12-(3-methylbutanoate), (3 β ,11a,12 β ,14 β)-	127
84.	30.11	C ₂₄ H ₃₄ O ₆	Butanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4- (hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,[1aR-(1aa,2a,5 β ,5a β ,6 β ,8aa,9a,10aa)]-	55.38
85.	30.67	C ₂₉ H ₄₈ O	Stigmasterol	20.23
86.	31.78	C ₂₉ H ₅₀ O	7-Sitosterol	40.46
87.	31.96	C ₂₈ H ₄₀ O ₄	9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester	60.33

Table 4.1. Chemical properties of GC-MS predicted compounds of *Caesalpinia*

GC-MS Gas chromatography–mass spectrometry of *Mallotus philippensis*

The methanolic extract of bark contains several chemical compounds with varying retention times based on the results obtained from the GC-MS spectrum. The structures and composition of the chemical compounds are determined from the analysis carried out using the mass spectrometry. The breakdown of complex organic compounds into smaller subunits produces mass spectra containing peaks with different m/z values. This mass spectrum serves as the fingerprinting technique for that specific compound. Analysis using the GC-MS method revealed that there are five different chemical compounds in the methanol bark extract of *M. philippensis*. They are presented in Table 2 with their molecular weight, molecular formula, and percentage of peak areas. The prevalent chemical compounds with high percentages of area include Amlexanox (8.08%), bis(2-ethylhexyl) ester (15.96%), sucrose (67.43%), and 1,3-benzene dicarboxylic acid. Others include 4-hydroxy-2',3,4',6'-tetramethoxy chalcone (5.74%) and isosorbide dinitrate (2.80%).

The methanol bark extract of *Mallotus philippensis* has a wide variety of chemical compounds ranging from commonly occurring natural sugars to bioactive compounds, as well as environmental contaminants. This finding has shown the immense possibility for the use of plant extracts in the field of toxicology and pharmaceutical applications. It is intriguing to know that there was a considerable amount of

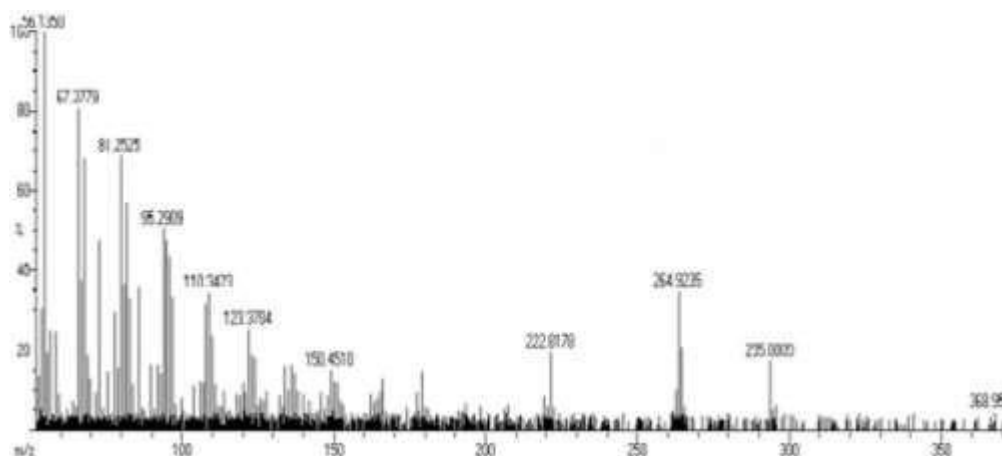
Graph4.2. oGc-Ms of *Mallotus philippensis*

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	21.03	C ₈ H ₆ O ₄	1, 2-benzenecarboxylic acid	74.6
2.	22.33	C ₂₄ H ₃₈ O ₄	Di-n-octyl phthalate	52.6
3.	25.23	C ₆ H ₄ (C ₈ H ₁₇ COO) ₂	Bis (2-ethyl hexyl) phthalate	52.6
4.	27.32	C ₆ H ₁₄ O ₆	d-mannitol, 1-0-heptyl	14.886
5.	28.83	C ₁₇ H ₃₂ O ₂	E-8-methyl-9-tetradecen-1-ol acetate	26.30
6.	30.10	C₅H₆O	3-methyl-2-(2-oxopropyl) furan	13.1
7.	30.59	C ₁₇ H ₃₄ O ₂	4-methyl-Z-4-hexadecen-1-ol	140
8.	31.12	C ₅₀ H ₁₀ O ₂	Tetrapentacontane, 1,34-dibromo	2.00
9.	31.63	C ₁₈ H ₃₆ O ₂	Octadecanoic acid, 2-oxo	37.3
10.	31.96	C ₁₁ H ₃₄ O	4-methyl-dodecec-3-en-1-ol	9.23
11.	32.61	C ₁₅ H ₂₆ O	Longiborneol	20.23
12.	33.49	C ₁₀ H ₈ O	p-menth-8(10)-en-9-ol, cis	20.23
13.	34.73	C ₁₂ H ₂₄ Br ₂	Dodecane, 1, 2-dibromo	0

Table 4.2. Chemical properties of GC-MS predicted compounds of *Mallotus philippensis*

4.3.3. GC-MS Gas chromatography–mass spectrometry of *Calotropis gigantea*

Through the application of gas chromatography coupled with mass spectrometry analysis, it was revealed that there are thirty phytochemical compounds present in *C. gigantea* (Figure 8 and Table 3). They include Cholesta-5-en-3-ol, 24-propylidene-, having a retention time of 54.01, 5H-3,5a-Epoxy-naphth[2,1-c]oxepin, a retention time of 57.34, Lup-20(29)-Ene-3,28-Diol, (3.β)-, with a retention time of 58.31, Veridiflorol with a retention time of 58..



Graph 4.3. of Gc-Ms of Calotropis gigantea

S.No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	22.78	C ₁₀ H ₂₂ O	1-Octanol-3,7-dimethyl	20.23
2.	53.21	C ₉ H ₁₀ O ₂	2- Methoxy 4-vinyl phenol ethenone	37.3
3.	4.34	C ₁₅ H ₁₃ N	Methyl-2-phenylindole	15.8
4.	33.40	C ₁₉ H ₃₈	5-Nonadecen-1-ol	0
5.	52.82	C ₁₉ H ₃₂ O ₂	9,12,15-Octadecatricenoic acid, methyl ester	26.30
6.	11.56	C ₁₀ H ₈	Azulene	0.0
7.	22.78	C ₂₀ H ₂₃ NO ₃	Benalaxyl	46.6
8.	50.19	BeH ₈ O ₈ S	Beryllium sulfate tetrahydrate	2
9.	3.44	C ₁₂ H ₁₀	Biphenyl	0.0
10.	6.66	C ₆ H ₁₄	Butane-2,2-dimethyl	0.0
11.	49.87	C ₂₈ H ₄₈ O	Campesterol	20.2
12.	41.79	C ₂₉ H ₄₈ O ₂	Cholest-5-en-3 ol, 24 Propylidene (3.beta.)	26.3
13.	22.78	C ₁₈ H ₃₄ O ₂	Cis-vaccenic acid	37.3
14.	3.46	C ₆ H ₁₂	Cyclohexane	0
15.	46.98	C ₁₀ H ₂₂	Decane	2
16.	6.66	C ₆ H ₁₃ O ₉ P	D-Mannose-1-phosphate sodium salt	157
17.	46.98	C ₂₀ H ₄₂	Eicosane	2
18.	53.21	C ₉ H ₂₂ O ₄ P ₂ S ₄	Ethion	152
19.	51.73	CH ₆ N ₄ O ₃	Guanidine nitrate	141
20.	49.87	C ₁₅ H ₂₆ O	Levomenol	20.23
21.	33.40	C ₂₅ H ₅₂	Pentacosane	0
22.	22.78	C ₁₁ H ₁₅ BrClO ₃ PS	Profenofos	60.8
23.	22.78	C ₂₈ H ₄₈ O ₂	B-Tocopherol	29.5
24.	46.98	C ₂₉ H ₅₀ O	B-Sitosterol	20.23

Table 4.3. Chemical properties of GC-MS predicted compounds of Calotropis gigantea

4.3.4. GC-MS Gas chromatography–mass spectrometry of *holoptelea integrifolia*

All of the isolates had some of the major constituents like n-hexadecanoic acid, phytol, and some more fatty acids and carboxylic acids, yet their proportions were different, indicating that they played a role in their anti-microbial activity. Because there was no availability of authentic samples and data from the library for similar GC-MS peaks, many of them could not be identified.



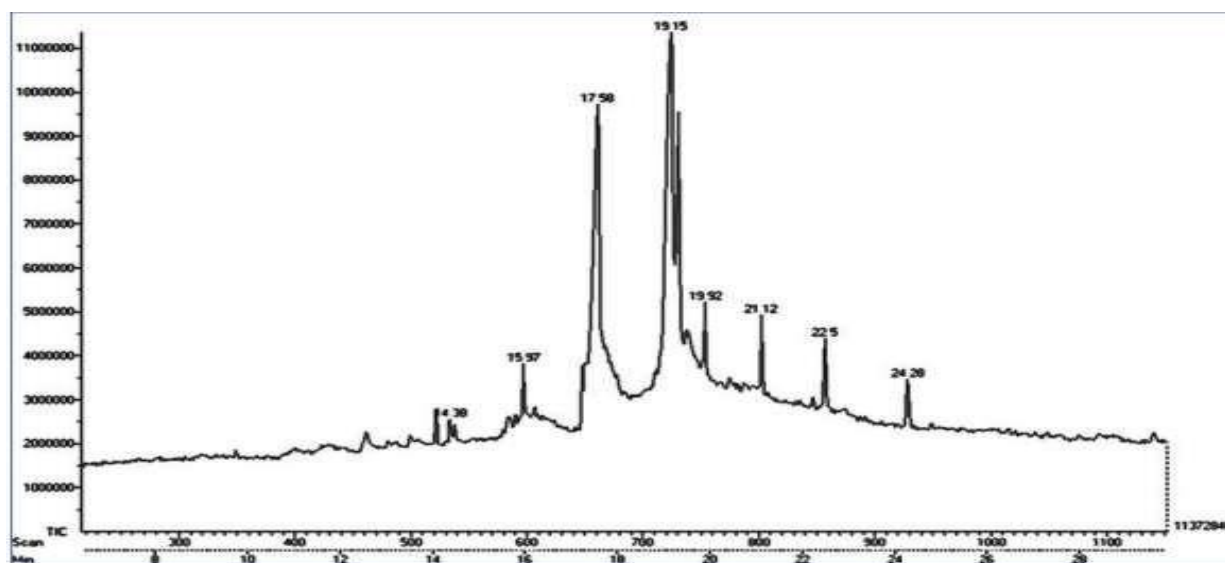
Graph 4.4. Gc-Ms of *Holoptelea integrifolia*

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	6.309	C ₉ H ₁₅ NO ₂	Cyclohexenylalanine	49.3
2.	6.859	C ₂ HBrF ₂	1-bromo-1,2-difluoroethene	0
3.	8.3128	C ₃ H ₄ Cl ₂ O ₂	2,2-dichloropropanoic acid	37.3
4.	8.669	C ₁₃ H ₂₂ O ₂	3,7-dimethylocta-1,6-dien-3-yl propanoate	26.3
5.	47.52	C ₁₇ H ₂₄ O ₃	(4-methoxyphenyl)4-propylcyclohexane-1-carboxylate	46.5
6.	57.558	C ₁₄ H ₁₈ N ₂ O	2-methyl-1-(2-propan-2-ylpyrazolo[1,5 a]pyridin-3-yl)propan-1-one	23.6
7.	58.57	C ₁₉ H ₃₈ O ₂	2,6,10,14-Tetramethylpentadecanoic acid	26.3
8.	62.852	C ₁₈ H ₃₄ O ₄	Octadecane-1,18-dioic acid	52.6
9.	64.3	C ₁₄ H ₁₆ N ₂ O ₃	(3S,8aR)-3-benzyl-8a-hydroxy-3,6,7,8-tetrahydro-2H-pyrrolo(1,2-a)pyrazine-1,4-dione	73.4
10.	64.726	C ₂₁ H ₄₂ O ₂	18-Methyleicosanoic acid	37.3
11.	66.873	C ₂₀ H ₃₅ O ₂ ⁻	(8Z,11Z)-eicosa-8,11-dienoate	37.3
12.	67.499	C ₁₂ H ₂₄ O ₃	ethyl 5-hydroxy-4-keto-octadecanoate	57.5
13.	68.128	C ₂₀ H ₃₈ O ₂	cis-11-eicosenoic acid	37.3
14.	68.866	C ₂₃ H ₄₆ O ₂	n-Tricosanoic acid	37.3
15.	69.178	C ₂₄ H ₃₈ O ₄	di-N-Octyl Phthalate	37.3
16.	70.277	C ₁₆ H ₃₄ O	Hexadecan-1-ol	20.23
17.	70.605	C ₂₄ H ₄₈ O ₂	Tetracosanoic acid	37.3
18.	70.686	C ₂₆ H ₄₄ O ₅	ethyl 3,7,12-trihydroxy-5-cholan-24-oate.	86.7
19.	72.211	C ₂₅ H ₅₀ O ₂	Pentacosanoic acid	26.3

20.	72.95	C ₂₂ H ₄₃ NO	Erucic acid amide	43.1
21.	77.077	C ₂₇ H ₄₀ O ₃	(5Z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1 α ,3 β ,24-trio	43.37

Table 4.4. Chemical properties of GC-MS predicted compounds of *holoptelea integrifolia*4.3.5. GC-MS Gas chromatography–mass spectrometry of *Hemidesmus indicus*

Steam distillation of *H. indicus* roots yielded an average of $1.28 \pm 0.11\%$ essential oil. Nerolidol and camphor were the other significant chemicals found in the essential oil, with 2-hydroxy-4-methoxy benzaldehyde being the most prevalent ingredient in the plant (92.3%).

Graph 4.5. Gc-Ms of *Hemidesmus indicus*

S. No	R.T ¹	Molecular Formula	Compound	TPSA ² (Å ²)
1.	14.38	C ₁₀ H ₁₂ O	Trans-2-methyl-3-phenyl-2-propen-1-ol	9.23
2.	15.97	C ₁₄ H ₂₂ O	Dibutylphenol 2,3-dibutylphenol Phenol	20.23
3.	19.15	C ₁₆ H ₁₆ O ₃	Ethanone,1-[4-methoxy-3-(4-methylphenoxy)phenyl]-	38.69
4.	22.5	C ₁₈ H ₁₈ N ₂ O ₂	Piperazine-2,5-dione,1,4-(4-methylphenyl)-	12.03
5.	24.28	C ₂₁ H ₄₂ O ₂	Isopropyl stearate	37.3
6.	21.12	C ₁₉ H ₃₆ O	Z,E-2-Methyl-3,13-octadecadien-1-ol	17.07
7.	19.92	C ₁₁ H ₁₄ N ₄ O ₄	Butanal,3-methyl-[2,4-dinitrophenyl] hydrazone	76.9
8.	17.58	C ₁₅ H ₁₀ O ₂	Flavone	26.3

Table 4.5. Chemical properties of GC-MS predicted compounds of *Hemidesmus indicus*

PubChem:-

It allows a one-to-one correspondence between the chemical structure and its textual notation, which is critical in indexing and removing duplicate chemical compounds from large chemical databases such as PubChem and ChEMBL. It is commonly known as “canonical smiles” in some situations and represents the basic atom and bond information without stereochemistry or isotopic information.

S.No .	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	Sec-Butyl nitrite	119	103.12	C ₄ H ₉ NO ₂	CCC(C(=O)O)N
2.	2-Nitro-1-buten-3-ol	10972	117.10	C ₄ H ₇ NO ₃	NC(=O)CCC(=O)O
3.	Isoxazolidine-3,5-dicarboxylic acid, dimethyl ester	70914	189.17	C ₇ H ₁₁ NO ₅	CC(=O)NCCC(C(=O)O)C(=O)O
4.	N-Isopentyl-N-nitroso-pentylamine	252237	186.29	C ₁₀ H ₂₂ N ₂ O	NCCCCCCCCCNCO
5.	Propanoic acid, 3-ethoxy-, ethyl ester	11182677	146.18	C ₇ H ₁₄ O ₃	CCOC(=O)CCCCO
6.	Alpha-l-rhamnopyranose	108223	164.16	C ₆ H ₁₂ O ₅	CC1C(C(C(C(O1)O)O)O)O
7.	d-Glycero-d-ido-heptose	5459879	210.18	C ₇ H ₁₄ O ₇	OCC(O)C(O)C(O)C(=O)CO
8.	2-Deoxy-D-galactose	108223	164.16	C ₆ H ₁₂ O ₅	CC1C(C(C(C(O1)O)O)O)O
9.	Isosorbide Dinitrate	6883	236.14	C ₆ H ₈ N ₂ O ₈	O=N(=O)OC1COC2C(ON(=O)=O)COC12
10.	Glycerin	753	92.09	C ₃ H ₈ O ₃	OCC(O)CO
11.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	911525	144.12	C ₆ H ₈ O ₄	O=C(O)CCCCC(=O)O
12.	a-D-Galactopyranose, 2-(acetylamino)-2-deoxy-	1738118	221.21	C ₈ H ₁₅ NO ₆	CC(=O)NC1C(C(C(C(O1)CO)O)O)O
13.	Isosorbide Dinitrate	6883	236.14	C ₆ H ₈ N ₂ O ₈	O=N(=O)OC1COC2C(ON(=O)=O)COC12
14.	5-Hydroxymethylfurfural	8369	126.11	C ₆ H ₆ O ₃	C1=CC(=C(C(=C1)O)O)O
15.	6-Acetyl-B-d-mannose	18392195	222.19	C ₈ H ₁₄ O ₇	CC(=O)OC1C(C(C(C(O1)CO)O)O)OC(=O)C
16.	Ascaridole epoxide	138243	184.23	C ₁₀ H ₁₆ O ₃	COC(=O)C1CCC(=O)C(C1)(C)C.
17.	1-Gala-l-ido-octonic lactone	119228	238.19	C ₈ H ₁₄ O ₈	O=C(O)C(O)C(O)C(O)C(O)C(=O)O
18.	Dithiocarbamate, S-methyl-,N-(2-methyl-3-oxobutyl)-	206035	191.3	C ₇ H ₁₃ NOS ₂	CC(C)SSC(C(=O)N)CC

19.	Melezitose	92817	504.4	C ₁₈ H ₃₂ O ₁₆	OCC1OC(OC2C(OC3OC(CO)C(O)C(O)C3O)OC(CO)C(O)C2O)(CO)C(O)C1O
20.	1-Hexadecanol, 2-methyl-	17218	256.5	C ₁₇ H ₃₆ O	CCCCCCCCCCCCCCCCC(O)
21.	Desulphosinigrin	9601716	279.31	C ₁₀ H ₁₇ NO ₆ S	O=C(O)CNC(=O)C(NC(=O)CCC(N)C(=O)O)CS
22.	Dodecanoic acid, 3-hydroxy-	94216	216.32	C ₁₂ H ₂₄ O ₃	OCCCCCCCCCCCCC(=O)O
23.	2-Myristynoyl pantetheine	535560	484.7	C ₂₅ H ₄₄ N ₂ O 5S	CCCCCCCCCCCCC#CC(=O)SCCNC(=O)CCNC(=O)C(C(C)(C)CO)O
24.	Ethyl α-d-glucopyranoside	121667	208.21	C ₈ H ₁₆ O ₆	CCOC1C(C(C(C(O1)CO)O)O)O
25.	Tetradecanoic acid	11005	228.37	C ₁₄ H ₂₈ O ₂	CCCCCCCCCCCCCCC(=O)O
26.	3-O-Methyl-d-glucose	64947	194.18	C ₇ H ₁₄ O ₆	OCC(O)C(O)C(O)C(O)CO
27.	Hexadecanoic acid, methyl ester	8181	270.5	C ₁₇ H ₃₄ O ₂	CCCCCCCCCCCCCCCCC(=O)O
28.	9-Hexadecenoic acid	4668	254.41	C ₁₆ H ₃₀ O ₂	CCCCCCCC=CCCCCCC(=O)O
29.	1-(+)-Ascorbic acid 2,6-dihexadecanoate	54686917	652.9	C ₃₈ H ₆₈ O ₈	CCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCC)O
30.	Ethanol,2-(9-octadecenyl)-, (Z)-	5364713	312.5	C ₂₀ H ₄₀ O ₂	CCCCCCCCCCCCCCCCCCCCC(=O)O
31.	n-Hexadecanoic acid	985	256.42	C ₁₆ H ₃₂ O ₂	CCCCCCCCCCCCCCCCC(=O)O
32.	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	5284421	294.5	C ₁₉ H ₃₄ O ₂	CCCCCCCC=CCCCCCCCC(=O)O
33.	Androsta-4,16-dien-3-one	71306304	270.4	C ₁₉ H ₂₆ O	O=C1C=C2CCC3C4CC=CC4(C)CCC3C2(C)CC1
34.	9,12-Octadecadienoic acid, ethyl ester	73114	308.5	C ₂₀ H ₃₆ O ₂	O=C(OCC)CCCCCCCC=CCC=CCCCC
35.	6-Octadecenoic acid	11634	282.5	C ₁₈ H ₃₄ O ₂	CCCCCCC/C=C\CCCCCCCC(=O)O
36.	1-Heptatriacotanol	537071	537.0	C ₃₇ H ₇₆ O	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
37.	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	554084	374.6	C ₂₅ H ₄₂ O ₂	CCCCC1CC1CC2CC2CC3CC3CC4CC4CCCC(=O)OC

38.	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-	6436665	306.5	C ₂₀ H ₃₄ O ₂	CC1=CC(O)CC(C)(O)C=CC(C(C)C)CCC(C)=CCC1
39.	2-Phenyl-4-tret-butyl-7-methylindene	6425788	262.4	C ₂₀ H ₂₂	CC1=CC=C(C2=C1CC(=C2)C3=CC=CC=C3)C(C)(C)C
40.	Curan,16,17,19,20-tetradehydro-	5378056	278.4	C ₁₉ H ₂₂ N ₂	CC=C1CN2CCCC34C2CC1=CC3NC5=CC=CC=C45
41.	2,4,6-Tri-t-butylbenzenethiol	621824	278.5	C ₁₈ H ₃₀ S	CC(C)(C)c1cc(C(C)(C)C)c(S)c(C(C)(C)C)c1
42.	Pregna-5,17(20)-dien-3-ol, (36,17E)-	235905	300.5	C ₂₁ H ₃₂ O	CC=C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
43.	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	99931	568.9	C ₃₅ H ₆₈ O ₅	CCCCCCCCCCCCCCCCC(=O)OC C(CO)OC(=O)CCCCCCCCCCCC CCC
44.	Gibbane-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1a,4aa,4bß,108)-	11725176	346.4	C ₂₀ H ₂₆ O ₅	CC12C(CCC34C1CC(C(=C)C3)O)C5(CCC(C5(C4)C(=O)OC)C2)O C(=O)
45.	1,4,9(11)-Pregnatriene-3,20-dione, 21-acetoxy-17-hydroxy-	11876453	384.5	C ₂₃ H ₂₈ O ₅	CC(=O)OCC(=O)C1(CCC2C1(CC C3=C2C=CC4=CC(=O)C=CC43C)C)O
46.	17Alpha-ethynyl-17beta-hydroxy-6beta-methoxy-3alpha, 5-cyclo-5alpha-androstan-19-oic acid	624715	358.5	C ₂₂ H ₃₀ O ₄	CCC(C)CC(C)OC(=O)c1ccc(cc1) C(=O)OCC(C)CC
47.	Pregnenolone	92810	316.5	C ₂₁ H ₃₂ O ₂	CC(=O)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
48.	68-Hydroxymethandienone	8955	316.4	C ₂₀ H ₂₈ O ₃	CC12CCC3=C(C1CCC45C2CCC(C4)C5(CO)O)C=CO3
49.	Norethindrone Acetate	5832	340.5	C ₂₂ H ₂₈ O ₃	CC12CCC(=O)C=C1C=CC3C2CC C4(C3CCC45CCC(=O)O5)C

50.	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8-tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bβ,4aβ,5β,7aa,7ba,8a,9β,9aa)]-	12443279	518.6	C ₂₈ H ₃₈ O ₉	<chem>CC(=CCC/C(=C/C(C/C(=C\CC(/C(=C/OC(=O)C)/C=C/OC(=O)C)OC(=O)C)/C=O)OC(=O)C)/C)C</chem>
51.	5,16,20-Pregnatriene-3beta,20-diol diacetate	222820	398.5	C ₂₅ H ₃₄ O ₄	<chem>CC(=O)O[C@@H]1CC[C@H]2[C@@H]3CCC4=CC=CC(=O)C4(C)C3CCC12OC(=O)C</chem>
52.	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8-tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1bβ,4aβ,5β,7aa,7ba,8a,9β,9aa)]-	5281877	476.6	C ₂₆ H ₃₆ O ₈	<chem>CC1=C(C(CCC1)(C)C)C=CC(=C)C=CC(=CC(=O)OC2C(C(C(C(O2)C(=O)O)O)O)O)C)C</chem>
53.	4,13,20-Tri-O-methylphorbol 12-acetate	10547963	448.5	C ₂₅ H ₃₆ O ₇	<chem>CC(=O)OCC1=CC2C(C(=O)C=C(C)C2(C)O)C3C(C(C1)O)C4(C)C(C)C43OC</chem>
54.	Phorbol 12,13,20-triacetate	499954	490.5	C ₂₆ H ₃₄ O ₉	<chem>CC(=O)OC1CC(CC2(C13C4C(CC2)C5(CCC(C5(CC4OC3O)C)C6=COC(=O)C=C6)O)O)O</chem>
55.	Acetic acid, 17-(1-acetoxyethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	77389706	414.5	C ₂₅ H ₃₄ O ₅	<chem>CC(=O)OC(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C(C)C(=O)O</chem>
56.	2-Cyclopenten-1-one, 3,4-dihydroxy-5-(3-methyl-2-butenyl)-2-(3-methyl-1-oxobutyl)-4-(4-methyl-1-oxo-3-pentenyl)-	58473839	362.5	C ₂₁ H ₃₀ O ₅	<chem>CC(C)=CCC1C(=O)C(=C(C1(C(=O)CC=C(C)C)O)O)C(=O)CC(C)C</chem>

57.	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	5363175	597.7	C ₃₂ H ₃₉ NO ₁₀	CCC(=O)OCC1(C(CCC2(C1CC(C3(C2C(C4=C(O3)C=C(OC4=O)C5=CN=CC=C5)O)C)OC(=O)C)C)OC(=O)C)C
58.	Ethyl iso-allocholate	6452096	436.6	C ₂₆ H ₄₄ O ₅	CCOC(=O)C1CCC2C3C(CC=C4C3(CCC5C4(CCC(C5)O)C)C)C2(C1)O
59.	Pregn-5-ene-3,11,12,14,20-pentol, 11-acetate 12-(3-methylbutanoate), (3β,11a,12β,14β)-			C ₂₈ H ₄₄ O ₇	CC(C)CC(=O)OC1C(C2(C(CC3C2(CCC4C3(CC(CC4)O)C)C)OC(=O)C)C)C(C)O
60.	Butanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,[1aR-(1aa,2a,5β,5aβ,6β,8aa,9a,10aa)]-	539279	418.5	C ₂₄ H ₃₄ O ₆	CCCC(=O)OC1C(C)C2(O)C(C=C(CO)CC3(O)C2C=C(C)C3=O)C4C1(C)C4(C)C
61.	Stigmasterol	5280794	412.7	C ₂₉ H ₄₈ O	CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
62.	7-Sitosterol	5283634	412.7	C ₂₉ H ₅₀ O	OC1CC2=CC=C3C(CCC4(C)C3CCC4(C)CCC(CC)C(C)C)C2(C)CC1
63.	9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester	5367498	440.6	C ₂₈ H ₄₀ O ₄	CCC=CCC=CCC=CCCCCCCCC(=O)OC1COC(C2=CC=CC=C2)OC1

Table:- Pubchem CID M.W.g/mol M.F. Canonical smile *Caesalpinia bonduc*

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	1, 2-benzenecarboxylic acid	181977	164.11	C ₈ H ₆ O ₄	<chem>C1=CC=C(C(=C1)C(=O)O)C(=O)O</chem>
2.	Di-n-octyl phthalate	8346	390.6	C ₂₄ H ₃₈ O ₄	<chem>CCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCC</chem>
3.	Bis (2-ethyl hexyl) phthalate	16213881	394.6	C ₆ H ₄ (C ₈ H ₁₇ COO) ₂	<chem>CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC</chem>
4.	E-8-methyl-9-tetradecen-1-ol acetate	5363273	268.4	C ₁₇ H ₃₂ O ₂	<chem>CCCC/C=C/C(C)CCCCCCCCOC(=O)C</chem>
5.	3-methyl-2-(2-oxopropyl) furan	545772	138.16	C ₅ H ₆ O ₂	<chem>CC1=C(OC(=O)C)CC(=O)C</chem>
6.	4-methyl-Z-4-hexadecen-1-ol	5367910	254.5	C ₁₇ H ₃₄ O	<chem>CCCCCCCCCCCC/C=C/C(C)\CCCCO</chem>
7.	Octadecanoic acid, 2-oxo	5281	284.5	C ₁₈ H ₃₆ O ₂	<chem>CCCCCCCCCCCCCCCCCCCC(=O)O</chem>
8.	4-methyl-dodecec-3-en-1-ol	5364665	198.34	C ₁₁ H ₂₄ O	<chem>CCCCCCCC/C(=C/CCO)/C</chem>
9.	Longiborneol	11447401	222.37	C ₁₅ H ₂₆ O	<chem>CC1(CCCC2(C3C1C(C2(CC3)C)O)C)C</chem>
10.	p-menth-8(10)-en-9-ol, cis	543946	154.25	C ₁₀ H ₁₈ O	<chem>CC1CCC(CC1)C(=C)CO</chem>
11.	Dodecane, 1, 2-dibromo	18766	328.13	C ₁₂ H ₂₄ Br ₂	<chem>BrCCCCCCCCCCCCBr</chem>

Table:- Pubchem CID M.W.g/mol M.F. Canonical smile *Mallotus philippensis*

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	1-Octanol-3,7-dimethyl	7792	158.28	C ₁₀ H ₂₂ O	<chem>CC(C)CCCC(C)CCO</chem>
2.	2- Methoxy 4-vinyl phenol ethenone	332	150.17	C ₉ H ₁₀ O ₂	<chem>COC1CC(CCC1O)C=C</chem>
3.	Methyl-2-phenylindole	77095	207.27	C ₁₅ H ₁₃ N	<chem>CN1C2=CC=CC=C2C=C1C3=CC=CC=C3</chem>
4.	5-Nonadecen-1-ol	5367600	282.5	C ₁₉ H ₃₈	<chem>CCCCCCCCCCCCCCCC/C=C/CCCCO</chem>
5.	9,12,15-Octadecatrienoic acid, methyl ester	5319706	292.5	C ₁₉ H ₃₂ O ₂	<chem>CCC=CCC=CCC=CCCCCCCCC(=O)OC</chem>
6.	Azulene	9231	128.17	C ₁₀ H ₈	<chem>C1=CC=C2C=CC=CC2=C1</chem>
7.	Benalaxyl	51369	325.4	C ₂₀ H ₂₃ NO ₃	<chem>CC1=C(C(=CC=C1)C)N(C(C)C(=O)OC)C(=O)CC2=CC=CC=C2</chem>
8.	Beryllium sulfate tetrahydrate	62672	177.14	BeH ₈ O ₈ S	<chem>O.O.O.O.[Be+2].[O-]S(=O)(=O)[O-]</chem>

9.	Biphenyl	7095	154.21	C ₁₂ H ₁₀	<chem>C1CCC(CC1)-C2CCCCC2</chem>
10.	Butane-2,2-dimethyl	6403	86.18	C ₆ H ₁₄	<chem>CCC(C)(C)C</chem>
11.	Campesterol	173183	400.7	C ₂₈ H ₄₈ O	<chem>CC(C)C(C)CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C</chem>
12.	Cholest-5-en-3 ol, 24 Propylidene (3.beta.)	222529	428.7	C ₂₉ H ₄₈ O ₂	<chem>CC(C)CCCC(C)C1CCC2C3CC=C4CC(CCC4(C)C3CCC12C)OC(=O)C</chem>
13.	Cis-vaccenic acid	5282761	282.5	C ₁₈ H ₃₄ O ₂	<chem>CCCCCCC/C=C\CCCCCCCCC C(=O)O</chem>
14.	Cyclohexane	8078	84.16	C ₆ H ₁₂	<chem>C1CCCCC1</chem>
15.	Decane	15600	142.28	C ₁₀ H ₂₂	<chem>CCCCCCCCC</chem>
16.	Eicosane	8222	282.5	C ₂₀ H ₄₂	<chem>CCCCCCCCCCCCCCCCCCCC</chem>
17.	Ethion	3286	384.5	C ₉ H ₂₂ O ₄ P ₂ S ₄	<chem>CCOP(=S)(OCC)SCSP(=S)(OCC)OCC</chem>
18.	Guanidine nitrate	10481	122.08	CH ₆ N ₄ O ₃	<chem>NC(N)=N.O[N+](=[O-])=O</chem>
19.	Levomenol	442343	222.37	C ₁₅ H ₂₆ O	<chem>CC1=CCC(CC1)C(C)(CCC=C(C)C)O</chem>
20.	Pentacosane	12406	352.7	C ₂₅ H ₅₂	<chem>CCCCCCCCCCCCCCCCCCCC CCCCC</chem>
21.	Profenofos	38779	373.63	C ₁₁ H ₁₅ BrC IO ₃ PS	<chem>CCCSP(=O)(OCC)OC1=C(C=C(C=C1)Br)Cl</chem>
22.	B-Tocopherol	6857447	416.7	C ₂₈ H ₄₈ O ₂	<chem>Cc1cc(O)c(C)c2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2</chem>
23.	B-Sitosterol	57347730	421.7	C ₂₉ H ₅₀ O	<chem>CCC(CCC(C)C1CCC2C3CCC4=CC(O)CCC4(C)C3CCC12C)C(C)C</chem>

Table:- Pubchem CID M.W.g/mol M.F. Canonical smile Calotropis gigantea

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	Cyclohexenylalanine	95475	171.24	C ₉ H ₁₅ NO ₂	<chem>C1CCC(CC1)CC(C(=O)O)N</chem>
2.	1-bromo-1,2-difluoroethene	588440	142.93	C ₂ HBrF ₂	<chem>C(=CF)(F)Br</chem>
3.	2,2-dichloropropanoic acid	6418	142.97	C ₃ H ₄ Cl ₂ O ₂	<chem>CC(C(=O)O)(Cl)Cl</chem>
4.	3,7-dimethylocta-1,6-dien-3-yl propanoate	61098	210.31	C ₁₃ H ₂₂ O ₂	<chem>CCC(=O)OC(C)(C=C)CCC=C(C)C</chem>
5.	(4-methoxyphenyl)4-propylcyclohexane-1-carboxylate	106715	276.4	C ₁₇ H ₂₄ O ₃	<chem>CCCC1CCC(CC1)C(=O)OC2=CC=C(C=C2)OC</chem>

6.	2-methyl-1-(2-propan-2-ylpyrazolo[1,5-a]pyridin-3-yl)propan-1-one	3671	230.31	C ₁₄ H ₁₈ N ₂ O	CC(C)C(=O)C1=C2C=CC=CN2N=C1C(C)C
7.	2,6,10,14-Tetramethylpentadecanoic acid	123929	298.50	C ₁₉ H ₃₈ O ₂	CCCCCCCC(C)CCCC(C)CCCC(C)CC(=O)O
8.	Octadecane-1,18-dioic acid	70095	314.5	C ₁₈ H ₃₄ O ₄	C(CCCCCCCC(=O)O)CCCCCCCC(=O)O
9.	(3S,8aR)-3-benzyl-8a-hydroxy-3,6,7,8-tetrahydro-2H-pyrrolo(1,2-a)pyrazine-1,4-dione	11673336	260.29	C ₁₄ H ₁₆ N ₂ O ₃	C1CC2C(=O)NC(C(=O)N2C1O)CC3=CC=CC=C3
10.	18-Methyleicosanoic acid	5282602	326.6	C ₂₁ H ₄₂ O ₂	CCC(C)CCCCCCCCCCCCCCCCC(C(=O)O)
11.	(8Z,11Z)-eicosa-8,11-dienoate	86289633	307.5	C ₂₀ H ₃₅ O ₂ ⁻	CCCCCCCC=CCC=CCCCCCC(C(=O)O)
12.	ethyl 5-hydroxy-4-keto-octadecanoate	94216	216.32	C ₁₂ H ₂₄ O ₃	OCCCCCCCCCCCC(O)=O
13.	cis-11-eicosenoic acid	5282768	310.5	C ₂₀ H ₃₈ O ₂	CCCCCCCC=CCCCCCCCCCC(=O)O
14.	n-Tricosanoic acid	17085	354.6	C ₂₃ H ₄₆ O ₂	CCCCCCCCCCCCCCCCCCCCCCC(CC(=O)O)
15.	di-N-Octyl Phthalate	8346	390.6	C ₂₄ H ₃₈ O ₄	CCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCC
16.	Hexadecan-1-ol	2682	242.44	C ₁₆ H ₃₄ O	CCCCCCCCCCCCCCCCCO
17.	Tetracosanoic acid	11197	368.6	C ₂₄ H ₄₈ O ₂	CCCCCCCCCCCCCCCCCCCCCCC(CC(=O)O)
18.	ethyl 3,7,12-trihydroxy-5-cholan-24-oate.	24853674	436.6	C ₂₆ H ₄₄ O ₅	CCOC(=O)CCC(C)C1CCC2C1(C(CC3C2C(CC4C3(CCC(C4)O)C)O)O)C
19.	Pentacosanoic acid	10468	382.7	C ₂₅ H ₅₀ O ₂	CCCCCCCCCCCCCCCCCCCCCCC(CC(=O)O)
20.	Erucic acid amide	5365371	337.6	C ₂₂ H ₄₃ NO	CCCCCCCC=CCCCCCCCCCC(C(=O)N)
21.	(5Z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1 α ,3 β ,24-trio	6012	412.6	C ₂₇ H ₄₀ O ₃	CC12CCC(=O)C=C1CCC1C2CCC2(C)C(OC(=O)CCC3CCCC3)CCC12

Table;- Pubchem CID M.W.g/mol M.F. Canonical smile holoptelea integrifolia

S.No.	Compounds name	Pubchem CID	M.W. g/mol	M.F.	Canonical smile
1.	Trans-2-methyl-3-phenyl-2-propen-1-ol	6393846	148.2	C ₁₀ H ₁₂ O	<chem>CC(C)C(=O)C1=CC=CC=C1</chem>
2.	Dibutylphenol 2,3-dibutylphenol Phenol	3015343	206.32	C ₁₄ H ₂₂ O	<chem>C1=CC=C(C=C1)O</chem>
3.	Ethanone,1-[4-methoxy-3-(4-methylphenoxy)phenyl]-	617872	256.3	C ₁₆ H ₁₆ O ₃	<chem>CC1=CC=C(C=C1)OC2=C(C=CC(=C2)C(=O)C)OC</chem>
4.	Piperazine-2,5-dione,1,4-(4-methylphenyl)-	576878	294.3	C ₁₈ H ₁₈ N ₂ O ₂	<chem>CC1=CC=C(C=C1)N2CC(=O)N(C2=O)C3=CC=C(C=C3)C</chem>
5.	Isopropyl stearate	8162	326.6	C ₂₁ H ₄₂ O ₂	<chem>CCCCCCCCCCCCCCCCCCCC(=O)OC(C)C</chem>
6.	Z,E-2-Methyl-3,13-octadecadien-1-ol	5364521	280.5	C ₁₉ H ₃₆ O	<chem>CCCC=CCCCCCCCC=CC(C)CO</chem>
7.	Butanal,3-methyl-[2,4-dinitrophenyl] hydrazone	9569524	266.25	C ₁₁ H ₁₄ N ₄ O ₄	<chem>CC(C)CC=NNC1CCC(CC1[N+](=O)[O-])[N+](=O)[O-]</chem>
8.	Flavone	10680	222.24	C ₁₅ H ₁₀ O ₂	<chem>O=C1C=C(OC2=CC=CC=C12)C3=CC=CC=C3</chem>

Table;- Pubchem CID M.W.g/mol M.F. Canonical smile Hemidesmus indicus

SwissADME:-

SwissADME is an online software application which is used for the determination of physicochemical properties, pharmacokinetic properties, and drug-likeness of a small molecule using algorithms. The SwissADME tool utilizes a model known as BOILED-Egg for the prediction of whether a compound will get absorbed into the gastrointestinal tract or pass through the blood brain barrier. Furthermore, there are five other models that calculate the lipophilicity of a compound, these models include; iLOGP, XLOGP3, WLOGP, MLOGP, SILICOS-IT. On the other hand, SVM, which stands for support vector machine, is the algorithm used to predict if a compound can act as a substrate or an inhibitor. In order to get results using this program you will need the canonical smile of your compounds; therefore, the first step involves visiting the drug bank website at <https://go.drugbank.com/>.

S.No.	Phytocompounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
1.	Sec-Butyl nitrite	0	3	0	0	3	0.55
2.	2-Nitro-1-buten-3-ol	0	4	0	0	2	0.56
3.	Isoxazolidine-3,5-dicarboxylic acid, dimethyl ester	0	1	0	0	1	0.56
4.	N-Isopentyl-N-nitroso-pentylamine	0	0	0	0	1	0.56

5.	Propanoic acid, 3-ethoxy-, ethyl ester	0	2	0	0	1	0.55
6.	Alpha-l-rhamnopyranose	0	2	0	0	2	0.55
7.	d-Glycero-d-ido-heptose	1	1	0	1	2	0.55
8.	2-Deoxy-D-galactose	0	2	0	0	2	0.55
9.	Isosorbide Dinitrate	0	0	0	0	0	0.55
10.	Glycerin	0	0	0	0	0	0.55
11.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	0	2	0	0	1	0.85
12.	a-D-Galactopyranose, 2-(acetylamino)-2-deoxy-	0	1	0	0	0	0.55
13.	Isosorbide Dinitrate	0	0	0	0	0	0.55
14.	5-Hydroxymethylfurfural	0	3	0	0	1	0.55
15.	6-Acetyl-B-d-mannose	0	1	0	0	0	0.55
16.	Ascaridole epoxide	0	0	0	0	1	0.55
17.	1-Gala-l-ido-octonic lactone	1	2	1	1	3	0.11
18.	Dithiocarbamate, S-methyl-,N-(2-methyl-3-oxobutyl)-	0	0	0	0	1	0.55
19.	Melezitose	3	2	1	1	4	0.17
20.	1-Hexadecanol, 2-methyl-	1	1	1	0	2	0.55
21.	Desulphosinigrin	0	1	2	1	2	0.11
22.	Dodecanoic acid, 3-hydroxy-	0	0	1	0	0	0.85

23.	2-Myristynoyl pantetheine	0	3	2	1	2	0.55
24.	Ethyl α-d- glucopyranoside	0	1	0	0	1	0.55
25.	Tetradecanoic acid	0	0	1	0	1	0.85
26.	3-O-Methyl-d- glucose	1	2	0	0	3	0.55
27.	Hexadecanoic acid, methyl ester	1	1	1	1	1	0.85
28.	9-Hexadecenoic acid	0	0	1	0	1	0.85
29.	1-(+)-Ascorbic acid 2,6-dihexadecanoate	2	4	1	1	2	0.17
30.	Ethanol,2-(9- octadecenylloxy)-, (Z)-	1	1	1	1	2	0.85
31.	n-Hexadecanoic acid	1	0	1	0	1	0.85
32.	9,12- Octadecadienoic acid (Z,Z)-, methyl ester	1	1	1	1	1	0.85
33.	Androsta-4,16-dien- 3-one	1	0	0	0	1	0.55
34.	9,12- Octadecadienoic acid, ethyl ester	1	1	1	1	2	0.55
35.	6-Octadecenoic acid	1	1	1	0	1	0.85
36.	1-Heptatriacotanol	2	4	1	1	3	0.17
37.	Cyclopropanebutano ic acid, 2-[[2-[[2- [[2- pentylcyclopropyl) methyl]cyclopropyl] methyl]cyclopropyl] methyl]-, methyl ester	1	1	1	1	1	0.55

	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-	0	0	0	0	0	0.55
38.	2-Phenyl-4-tret-butyl-7-methylindene	1	0	0	0	2	0.55
39.	Curan,16,17,19,20-tetradehydro-	0	0	0	0	0	0.55
40.	Pregna-5,17(20)-dien-3-ol, (36,17E)-	1	0	0	0	1	0.55
41.	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	2	4	1	1	2	0.17
42.	Gibbane-1,10-dicarboxylic acid, 4a,7-dihydroxy-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1a,4aa,4bβ,108)-	0	0	0	0	0	0.55
43.	1,4,9(11)-Pregnatriene-3,20-dione, 21-acetoxy-17-hydroxy-	0	0	0	0	0	0.55
44.	17Alpha-ethynyl-17beta-hydroxy-6beta-methoxy-3alpha, 5-cyclo-5alpha-androstan-19-oic acid	1	0	1	0	1	0.55
45.	Pregnenolone	0	0	0	0	0	0.55
46.	68-Hydroxymethandienone	0	0	0	0	0	0.55
47.	Norethindrone Acetate	0	0	0	0	0	0.55

48.	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8-tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1b β ,4a β ,5 β ,7aa,7ba,8a,9 β ,9aa)]-	1	3	1	0	1	0.55
49.	5,16,20-Pregnatriene-3beta,20-diol diacetate	0	0	0	0	0	0.55
50.	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8-tetramethyl-, 5,9,9a-triacetate, [1aR-(1aa,1b β ,4a β ,5 β ,7aa,7ba,8a,9 β ,9aa)]-	0	0	0	1	0	0.56
51.	4,13,20-Tri-O-methylphorbol 12-acetate	0	0	0	0	0	0.55
52.	Phorbol 12,13,20-triacetate	0	1	1	1	0	0.55
53.	Acetic acid, 17-(1-acetoxy-ethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	0	0	0	0	0	0.55

54.	2-Cyclopenten-1-one, 3,4-dihydroxy-5-(3-methyl-2-butenyl)-2- (3-methyl-1-oxobutyl)-4-(4-methyl-1-oxo-3-pentenyl)-	0	0	0	0	0	0.56
55.	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropana[f]cycloundecen-11-yl ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	2	3	1	1	2	0.17
56.	Ethyl iso-allocholate	0	0	0	0	0	0.55
57.	Pregn-5-ene-3,11,12,14,20-pentol, 11-acetate 12-(3-methylbutanoate), (3R,11a,12R,14R)-	0	0	0	0	0	0.55
58.	Butanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropana[e]cyclodecen-6-yl ester,[1aR-	0	0	0	0	0	0.55

	(1a,2a,5 β ,5a β ,6 β ,8a,9a,10aa)]-						
59.	Stigmasterol	1	3	0	1	2	0.55
60.	7-Sitosterol	1	3	0	1	2	0.55
61.	9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester	1	3	1	1	2	0.55

Table:-Phytocompounds Lipinski Ghose Veber Egan Muegge Bioavailability Score *Caesalpinia bonduc* phytoconstituents using swissadme

S.No.	Phytocompounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
1.	1, 2-benzenecarboxylic acid	0	1	0	0	1	0.85
2.	Di-n-octyl phthalate	1	1	1	1	2	0.55
3.	Bis (2-ethyl hexyl) phthalate	1	1	1	1	2	0.55
4.	E-8-methyl-9-tetradecen-1-ol acetate	1	0	1	0	1	0.55
5.	3-methyl-2-(2-oxopropyl) furan	0	2	0	0	1	0.55
6.	4-methyl-Z-4-hexadecen-1-ol	1	1	1	0	2	0.55
7.	Octadecanoic acid, 2-oxo	1	1	1	1	2	0.85
8.	4-methyl-dodecec-3-en-1-ol	0	0	0	0	3	0.55
9.	0Longiborneol	0	0	0	0	1	0.55
10.	p-menth-8(10)-en-9-ol, cis	0	1	0	0	2	0.55
11.	Dodecane, 1, 2-dibromo	1	1	1	0	2	0.55

Table:- Phytocompounds Lipinski Ghose Veber Egan Muegge Bioavailability Score *Mallotus philippensis*
phytoconstituents using swissadme

S.No.	Phytocompounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
1.	1-Octanol-3,7-dimethyl	0	1	0	0	2	0.55
2.	2- Methoxy 4-vinyl phenol ethenone	0	1	0	0	1	0.55
3.	Methyl-2-phenylindole	0	0	0	0	1	0.55
4.	5-Nonadecen-1-ol	1	1	1	1	3	0.55
5.	9,12,15-Octadecatricenoic acid, methyl ester	1	1	1	0	1	0.55
6.	Azulene	1	2	0	0	2	0.55
7.	Benalaxyl	0	0	0	0	0	0.55
8.	Biphenyl	1	0	0	0	3	0.55
9.	Butane-2,2-dimethyl	0	2	0	0	2	0.55
10.	Campesterol	1	2	0	1	2	0.55
11.	Cholest-5-en-3 ol, 24 Propylidene (3.beta.)	1	3	0	1	1	0.55
12.	Cis-vaccenic acid	1	1	1	1	2	0.85
13.	Cyclohexane	0	3	0	0	2	0.55
14.	Decane	1	1	0	0	3	0.55
15.	Eicosane	1	1	1	1	3	0.55
16.	thion	0	1	2	2	2	0.55
17.	Guanidine nitriate	0	4	1	1	2	0.55
18.	Levomenol	0	0	0	0	1	0.55
19.	Pentacosane	1	2	1	1	3	0.55
20.	Profenofos	0	1	0	0	0	0.55
21.	B-Tocopherol	1	3	1	1	1	0.55
22.	B-Sitosterol	1	3	0	1	2	0.55

Table:- Phytocompounds Lipinski Ghose Veber Egan Muegge Bioavailability Score , *Calotropis gigantea* phytoconstituents using swissadme

S.No.	Phytocompounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
1.	Cyclohexenylalanine	0	0	0	0	1	0.55
2.	1-bromo-1,2-difluoroethene	0	3	0	0	3	0.55
3.	2,2-dichloropropanoic acid	0	3	0	0	2	0.85
4.	3,7-dimethylocta-1,6-dien-3-yl propanoate	0	0	0	0	0	0.55
5.	(4-methoxyphenyl)4-propylcyclohexane-1-carboxylate	0	0	0	0	1	0.55
6.	2-methyl-1-(2-propan-2-ylpyrazolo[1,5-a]pyridin-3-yl)propan-1-one	0	0	0	0	0	0.55
7.	2,6,10,14-Tetramethylpentadecanoic acid	0	0	0	0	0	0.55
8.	Octadecane-1,18-dioic acid	0	0	1	0	1	0.85
9.	(3S,8aR)-3-benzyl-8a-hydroxy-3,6,7,8-tetrahydro-2H-pyrrolo(1,2-a)pyrazine-1,4-dione	0	1	0	0	0	0.55
10.	18-Methyleicosanoic acid	1	1	1	1	2	0.85
11.	(8Z,11Z)-eicosa-8,11-dienoate	1	1	1	1	2	0.85

12.	ethyl 5-hydroxy-4-keto-octadecanoate	0	0	1	0	0	0.85
13.	cis-11-eicosenoic acid	1	1	1	1	2	0.85
14.	n-Tricosanoic acid	1	2	1	1	2	0.85
15.	di-N-Octyl Phthalate	1	1	1	1	2	0.55
16.	Hexadecan-1-ol	1	0	1	0	2	0.55
17.	Tetracosanoic acid	1	2	1	1	2	0.85
18.	ethyl 3,7,12-trihydroxy-5-cholan-24-oate.	0	1	0	0	0	0.55
19.	Pentacosanoic acid	1	2	1	1	2	0.85
20.	Erucic acid amide	1	1	1	1	2	0.55
21.	(5Z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1 α ,3 β ,24-trio	1	1	0	1	1	0.55

Table:- Phytocompounds Lipinski Ghose Veber Egan Muegge Bioavailability Score *Holoptelea integrifolia* phytoconstituents using swissadme

S.No.	Phytocompounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
1.	Trans-2-methyl-3-phenyl-2-propen-1-ol	0	1	0	0	2	0.55
2.	Dibutylphenol 2,3-dibutylphenol Phenol	0	3	0	0	2	0.55
3.	Ethanone,1-[4-methoxy-3-(4-methylphenoxy)phenyl]-	0	0	0	0	0	0.55
4.	Piperazine-2,5-dione,1,4-(4-methylphenyl)-	0	0	0	0	0	0.55
5.	Isopropyl stearate	1	1	1	1	2	0.55
6.	Z,E-2-Methyl-3,13-octadecadien-1-ol	1	1	1	1	2	0.55

7.	Butanal,3-methyl-[2,4-dinitrophenyl]hydrazone	0	0	0	0	0	0.55
8.	Flavone	0	0	0	0	0	0.55

Table:- Phytocompounds Lipinski Ghose Veber Egan Muegge Bioavailability Score *Hemidesmus indicus* phytoconstituents using swissadme

Protox||:-

As we said in our last paper, the acute toxicity models are based on the fact that chemicals that are known to be toxic have similar chemical structures and toxic fragments.

S.No.	Phytocompounds	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
1.	Sec-Butyl nitrite	Inactive	Inactive	Inactive	Inactive	Inactive
2.	2-Nitro-1-buten-3-ol	Inactive	Inactive	Inactive	Inactive	Inactive
3.	Isoxazolidine-3,5-dicarboxylic acid, dimethyl ester	Inactive	Inactive	Inactive	Inactive	Inactive
4.	N-Isopentyl-N-nitroso-pentylamine	Inactive	active	Inactive	Inactive	Inactive
5.	Propanoic acid, 3-ethoxy-, ethyl ester	Inactive	active	Inactive	Inactive	Inactive
6.	Alpha-l-rhamnopyranose	Inactive	Inactive	Inactive	Inactive	Inactive
7.	d-Glycero-d-ido-heptose	Inactive	Inactive	Inactive	Inactive	Inactive
8.	2-Deoxy-D-galactose	Inactive	Inactive	Inactive	Inactive	Inactive
9.	Isosorbide Dinitrate	Inactive	active	Inactive	Inactive	Inactive
10.	Glycerin	Inactive	Inactive	Inactive	Inactive	Inactive
11.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	Inactive	Inactive	Inactive	Inactive	Inactive
12.	a-D-Galactopyranose	Inactive	Inactive	Inactive	Inactive	Inactive

	, 2- (acetylamino)-2- deoxy-					
13.	Isosorbide Dinitrate	Inactive	active	Inactive	Inactive	Inactive
14.	5- Hydroxymethylf urfural	Inactive	active	Inactive	active	Inactive
15.	6-Acetyl-B-d- mannose	Inactive	Inactive	Inactive	Inactive	Inactive
16.	Ascaridole epoxide	Inactive	Inactive	Inactive	Inactive	Inactive
17.	1-Gala-l-ido- octonic lactone	Inactive	Inactive	Inactive	Inactive	Inactive
18.	Dithiocarbamate , S-methyl-,N- (2-methyl-3- oxobutyl)-	Inactive	active	Inactive	Inactive	Inactive
19.	Melezitose	Inactive	Inactive	active	Inactive	Inactive
20.	1-Hexadecanol, 2- methyl-	Inactive	Inactive	Inactive	Inactive	Inactive
21.	Desulphosinigri n	Inactive	Inactive	Inactive	active	Inactive
22.	Dodecanoic acid, 3-hydroxy-	Inactive	Inactive	Inactive	Inactive	Inactive
23.	2-Myristynoyl pantetheine	Inactive	Inactive	Inactive	Inactive	Inactive
24.	Ethyl a-d- glucopyranoside	Inactive	Inactive	Inactive	Inactive	Inactive
25.	Tetradecanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive
26.	3-O-Methyl-d- glucose	Inactive	Inactive	Inactive	Inactive	Inactive
27.	Hexadecanoic acid, methyl ester	Inactive	Inactive	Inactive	Inactive	Inactive
28.	9-Hexadecenoic acid	Inactive	Inactive	Inactive	Inactive	Inactive

29.	1-(+)-Ascorbic acid 2,6-dihexadecanoate	Inactive	Inactive	Inactive	Inactive	active
30.	Ethanol,2-(9-octadecenyloxy)-, (Z)-	Inactive	Inactive	Inactive	Inactive	Inactive
31.	n-Hexadecanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive
32.	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	Inactive	Inactive	Inactive	Inactive	Inactive
33.	Androsta-4,16-dien-3-one	Inactive	Inactive	active	Inactive	Inactive
34.	9,12-Octadecadienoic acid, ethyl ester	Inactive	active	Inactive	Inactive	Inactive
35.	6-Octadecenoic acid	Inactive	Inactive	Inactive	Inactive	Inactive
36.	1-Heptatriacotanol	Inactive	Inactive	Inactive	Inactive	Inactive
37.	Cyclopropanebutanolic acid, 2-[[2-[[2-(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	Inactive	Inactive	Inactive	Inactive	Inactive
38.	4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-	Inactive	Inactive	active	Inactive	Inactive
39.	2-Phenyl-4-tert-butyl-7-methylindene	Inactive	Inactive	Inactive	Inactive	Inactive

40.	Curan,16,17,19, 20-tetradehydro-	Inactive	Inactive	Inactive	Inactive	Inactive
41.	2,4,6-Tri-t- butylbenzenethi ol	Inactive	Inactive	Inactive	Inactive	Inactive
42.	Pregna- 5,17(20)-dien-3- ol, (36,17E)-	Inactive	Inactive	active	Inactive	Inactive
43.	Hexadecanoic acid, 1- (hydroxymethyl) -1,2-ethanediyl ester	Inactive	Inactive	Inactive	Inactive	active
44.	Gibbane-1,10- dicarboxylic acid, 4a,7- dihydroxy-1- methyl-8- methylene-, 1,4a-lactone, 10- methyl ester, (1a,4aa,4bß,108) -	Inactive	Inactive	active	Inactive	Inactive
45.	1,4,9(11)- Pregnatriene- 3,20-dione, 21- acetoxy-17- hydroxy-	Inactive	active	active	Inactive	Inactive
46.	17Alpha- ethynyl-17beta- hydroxy-6beta- methoxy-3alpha, 5-cyclo-5alpha- androstan-19-oic acid	Inactive	active	Inactive	Inactive	Inactive
47.	Pregnenolone	active	Inactive	active	Inactive	Inactive
48.	68- Hydroxymethan dienone	Inactive	Inactive	Inactive	Inactive	Inactive

49.	Norethindrone Acetate	Inactive	active	active	Inactive	Inactive
50.	1H- Cyclopropa[3,4] benz[1,2- e]azulene- 5,7b,9,9a-tetrol, 3- [(acetyloxy)met hyl]- 1a,1b,4,4a,5,7a, 8,9-octahydro- 1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bβ,4aβ,5β, 7aa,7ba,8a,9β,9a a)]-	Inactive	Inactive	Inactive	Inactive	Inactive
51.	5,16,20- Pregnatriene- 3beta,20-diol diacetate	Inactive	active	active	Inactive	Inactive
52.	1H- Cyclopropa[3,4] benz[1,2- e]azulene- 5,7b,9,9a-tetrol, 3- [(acetyloxy)met hyl]- 1a,1b,4,4a,5,7a, 8,9-octahydro- 1,1,6,8- tetramethyl-, 5,9,9a-triacetate, [1aR- (1aa,1bβ,4aβ,5β, 7aa,7ba,8a,9β,9a a)]-	Inactive	active	active	Inactive	Inactive

53.	4,13,20-Tri-O-methylphorbol 12-acetate	Inactive	Inactive	active	active	Inactive
54.	Phorbol 12,13,20-triacetate	Inactive	Inactive	active	Inactive	active
55.	Acetic acid, 17-(1-acetoxyethyl)-10,13-dimethyl-3-oxo2,3,8,9,10,11,12,13,14,15,16,17-dodecahydro-1Hcyclopenta[a]phenanthren-11-yl (ester)	Inactive	active	active	Inactive	Inactive
56.	2-Cyclopenten-1-one, 3,4-dihydroxy-5-(3-methyl-2-butenyl)-2-(3-methyl-1-oxobutyl)-4-(4-methyl-1-oxo-3-pentenyl)-	Inactive	Inactive	active	Inactive	Inactive
57.	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cyclo undecen-11-yl	Inactive	Inactive	active	Inactive	Inactive

	ester,[1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-					
58.	Ethyl iso-allocholate	Inactive	Inactive	Inactive	Inactive	Inactive
59.	Butanoic acid, 1a,2,5,5a,6,9,10, 10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropana[e]cyclodec-6-en-6-yl ester,[1aR-(1aa,2a,5β,5aβ,6β,8aa,9a,10aa)]-	Inactive	Inactive	active	Inactive	Inactive
60.	Stigmasterol	Inactive	Inactive	active	Inactive	Inactive
61.	7-Sitosterol	Inactive	Inactive	active	Inactive	Inactive
62.	9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester	Inactive	Inactive	active	Inactive	Inactive

Table: Using Protox II to test the toxicity of *Caesalpinia bonduc* phytoconstituents

S.No.	Phytocompounds	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
1.	1, 2-benzenecarboxylic acid	Inactive	Inactive	Inactive	Inactive	Inactive
2.	Di-n-octyl phthalate	Inactive	active	Inactive	Inactive	Inactive
3.	Bis (2-ethyl hexyl) phthalate	Inactive	active	Inactive	Inactive	Inactive
4.	E-8-methyl-9-tetradecen-1-ol acetate	Inactive	active	Inactive	Inactive	Inactive
5.	3-methyl-2-(2-oxopropyl) furan	Inactive	active	Inactive	Inactive	Inactive
6.	4-methyl-Z-4-hexadecen-1-ol	Inactive	Inactive	Inactive	Inactive	Inactive
7.	Octadecanoic acid, 2-oxo	Inactive	Inactive	Inactive	Inactive	Inactive
8.	4-methyl-dodecec-3-en-1-ol	Inactive	Inactive	Inactive	Inactive	Inactive
9.	Longiborneol	Inactive	Inactive	Inactive	Inactive	Inactive
10.	p-menth-8(10)-en-9-ol, cis	Inactive	Inactive	Inactive	Inactive	Inactive
11.	Dodecane, 1, 2-dibromo	Inactive	active	Inactive	active	Inactive

Table: Using Protox II to test the toxicity of *Mallotus philippensis* phytoconstituents

S.No.	Phytocompounds	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
1	1-Octanol-3,7-dimethyl	Inactive	Inactive	Inactive	Inactive	Inactive
2	2- Methoxy 4-vinyl phenol ethenone	Inactive	Inactive	Inactive	Inactive	Inactive

3	Methyl-2-phenylindole	Inactive	active	Inactive	active	Inactive
4	5-Nonadecen-1-ol	Inactive	Inactive	Inactive	Inactive	Inactive
5	9,12,15-Octadecatricoic acid, methyl ester	Inactive	Inactive	Inactive	Inactive	Inactive
6	Azulene	Inactive	active	Inactive	active	Inactive
7	Benalaxyl	Inactive	Inactive	Inactive	Inactive	Inactive
8	Beryllium sulfate tetrahydrate	Inactive	Inactive	Inactive	Inactive	Inactive
9	Biphenyl	Inactive	Inactive	Inactive	Inactive	Inactive
10	Butane-2,2-dimethyl	Inactive	active	Inactive	Inactive	Inactive
11	Campesterol	Inactive	Inactive	active	Inactive	Inactive
12	Cholest-5-en-3 ol, 24 Propylidene (3.beta.)	Inactive	active	active	Inactive	Inactive
13	Cis-vaccenic acid	Inactive	Inactive	Inactive	Inactive	Inactive
14	Cyclohexane	Inactive	active	Inactive	Inactive	Inactive
15	Decane	Inactive	Inactive	Inactive	Inactive	Inactive
16	Eicosane	Inactive	Inactive	Inactive	Inactive	Inactive
17	Ethion	Inactive	Inactive	Inactive	Inactive	Inactive
18	Guanidine nitrate	Inactive	active	Inactive	active	Inactive
19	Levomenol	Inactive	Inactive	Inactive	Inactive	Inactive
20	Pentacosane	Inactive	Inactive	Inactive	Inactive	Inactive
21	Profenofos	Inactive	Inactive	Inactive	Inactive	Inactive

22	B-Tocopherol	Inactive	Inactive	Inactive	Inactive	Inactive
23	B-Sitosterol	Inactive	Inactive	active	Inactive	Inactive

Table: Using Prottox II to test the toxicity of *Calotropis gigantea* phytoconstituents

S.No.	Phytocompounds	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
1.	Cyclohexenyl alanine	Inactive	Inactive	Inactive	Inactive	Inactive
2.	1-bromo-1,2-difluoroethene	Inactive	active	Inactive	active	active
3.	2,2-dichloropropionic acid	Inactive	active	Inactive	Inactive	Inactive
4.	3,7-dimethylocta-1,6-dien-3-yl propanoate	Inactive	Inactive	Inactive	Inactive	Inactive
5.	(4-methoxyphenyl)4-propylcyclohexane-1-carboxylate	Inactive	Inactive	Inactive	Inactive	Inactive
6.	2-methyl-1-(2-propan-2-ylpyrazolo[1,5-a]pyridin-3-yl)propan-1-one	Inactive	Inactive	Inactive	Inactive	Inactive
7.	2,6,10,14-Tetramethylpentadecanoic acid	active	Inactive	Inactive	Inactive	Inactive
8.	Octadecane-1,18-dioic acid	Inactive	Inactive	Inactive	Inactive	Inactive
9.	(3S,8aR)-3-benzyl-8a-hydroxy-	Inactive	Inactive	Inactive	Inactive	Inactive

	3,6,7,8-tetrahydro-2H-pyrrolo(1,2-a)pyrazine-1,4-dione					
10.	18-Methyleicosa noic acid	active	Inactive	Inactive	Inactive	Inactive
11.	(8Z,11Z)-eicosa-8,11-dienoate	Inactive	Inactive	Inactive	Inactive	Inactive
12.	ethyl 5-hydroxy-4-keto-octadecanoate	Inactive	Inactive	Inactive	Inactive	Inactive
13.	cis-11-eicosenoic acid	Inactive	Inactive	Inactive	Inactive	Inactive
14.	n-Tricosanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive
15.	di-N-Octyl Phthalate	Inactive	active	Inactive	Inactive	Inactive
16.	Hexadecan-1-ol	Inactive	Inactive	Inactive	Inactive	Inactive
17.	Tetracosanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive
18.	ethyl 3,7,12-trihydroxy-5-cholan-24-oate.	Inactive	Inactive	active	Inactive	Inactive
19.	Pentacosanoic acid	Inactive	Inactive	Inactive	Inactive	Inactive
20.	Erucic acid amide	Inactive	Inactive	Inactive	Inactive	Inactive
21.	(5Z,7E,22E,24S)-24-cyclopropyl-9,10-	Inactive	active	active	Inactive	Inactive

Table: Using Protox II to test the toxicity of *Holoptelea integrifolia* phytoconstituents

S.No.	Phytochemicals	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
1.	Trans-2-methyl-3-phenyl-2-propen-1-ol	Inactive	Inactive	Inactive	Inactive	Inactive
2.	Dibutylphenol 2,3-dibutylphenol Phenol	Inactive	Inactive	Inactive	Inactive	Inactive
3.	Ethanone,1-[4-methoxy-3-(4-methylphenoxy)phenyl)-	Inactive	Inactive	Inactive	Inactive	Inactive
4.	Piperazine-2,5-dione,1,4-(4-methylphenyl)-	Inactive	Inactive	Inactive	Inactive	Inactive
5.	Isopropyl stearate	Inactive	Inactive	Inactive	Inactive	Inactive
6.	Z,E-2-Methyl-3,13-octadecadien-1-ol	Inactive	Inactive	Inactive	Inactive	Inactive
7.	Butanal,3-methyl-[2,4-dinitrophenyl] hydrazone	Inactive	active	Inactive	active	Inactive
8.	Flavone	Inactive	active	Inactive	Inactive	active

Table: Using Protox II to test the toxicity of *Hemidesmus indicus* phytoconstituents

Conclusion

The present study on *G. procumbens* using rat models gives additional information about the hepatoprotective effect of this plant. The reduction of SGPT, SGOT, ALP, creatinine, TC, LDL, TG, SOD, MDA, DNA fragmentation range, γ -GT, and an increase in HDL levels in CCl₄-induced rats by both drugs, namely, silymarin and *G. procumbens* leaves' extract, indicated the potential hepatoprotective effect of this plant extract. Additionally, from the histopathological examination, it is evident that *G. procumbens* leaves' extract can revert the pathological condition when the rats were induced by CCl₄. In the molecular docking investigation, a number of bioactive compounds exhibited promising binding energy towards the receptors, while the ADMET study revealed the drug-like properties of those compounds. The findings from both in vivo and in silico analyses provide optimism in considering *G. procumbens* leaves' extract as a promising source of hepatoprotective drugs for future use as an alternative treatment of liver toxicity. However, further researches are required to identify the exact active components of this plant extract and their mechanism of action.

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