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EVALUATION OF THE PHARMACOPHORIC ACTIVITY OF DIFFERENT COMPOUNDS OBTAINED BY GC-MS IN AQUEOUS EXTRACT OF *LAWSONIA ALBA*

Simhadri V. S. D. N. A. Nagesh [*1], K. K. Bairagi [2] and Sudhir Modala [3]

Department of Pharmacology [1], Department of Forensic Medicine [2], Shri Ram Murti Smarak Institute of Medical Sciences, Bareilly - 243202, Uttar Pradesh, India.
Department of Physiology [3], Varun Arjun Medical College & Rohilkhand Hospital, Shahjahanpur - 242307, Uttar Pradesh, India.

Keywords:

Lawsonia alba, GC-MS, Pharmacokinetics, Pharmacodynamic, Secondary metabolites, SwissADME, Swiss target prediction

Correspondence to Author:
Simhadri V. S. D. N. A. Nagesh

Associate Professor,
Department of Pharmacology, Shri Ram Murti Smarak Institute of Medical Sciences, Bareilly - 243202, Uttar Pradesh, India.

E-mail: nageshsai117@gmail.com

ABSTRACT: Most of the medications currently in use are largely derived from the traditional plants and their products. *Lawsonia alba*, often known as henna, has a wide range of medicinal uses, from minor infections to cancer and is also used as a hair dye. All of these pharmacological actions and therapeutic uses are because of the presence of numerous secondary metabolites. These were isolated using the GC-MS technique from the aqueous extract of *L. alba* leaves. The compounds were then analyzed for pharmacokinetics and pharmacodynamics by using SwissADME, OPENBABEL, Swiss target prediction, *etc*., like software. In the aqueous extract of *L. alba*, we obtained 91 compounds; out of these 38 were significant, but only 09 compounds were in prominent concentration, and all of these 09 compounds were non-toxic, they are orally absorbable molecules with acceptable lipophilic and hydrophilic nature which were subjected to various software to obtain the target protein that can dock with specific properties of modulating various proteins/receptors/enzymes and these compounds or their derivatives can be considered as a "hit" or "lead" molecules and can be used further for pre-clinical studies.

INTRODUCTION: From the ancient days, early to the utilization of advanced medicine, men relied only on classical herbal medicine. Herbal plants have an important role in disease prevention and treatment, according to the World Health Organization (WHO); four thousand million people utilize herbal medicines as a primary healthcare product in some form.

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Also, it has been identified herbal medicine is a necessary component of primary health care, with plants accounting for around 11% of the 252 medications [1]. According to ethnobotanical literature, many medicinally prominent herbs are used to treat infections caused by microbes, especially in rural Algeria, where traditional medicine (folk medicine) is still a key source of treatment for minor ailments. There has been relatively little research on this historically therapeutic herb [2].

Lawsonia alba is also known as *Lawsonia inermis* Linn belongs to the family *Lythraceae* native to Arabia and Persia; presently planted primarily in Haryana and Gujarat, with a little expansion to

Madhya Pradesh, Tamil Nadu, and Rajasthan. In various vernacular languages, this plant is known as Henna; in Ayurvedic medicine, it is known as Madayanti, Madayantikaa, Mendika, Ranjaka; in Unani medicine, it is known as Hinaa, Mehndi, and in Siddha/Tamil medicine, it is known as Marithondi, Marudum. It has a myriad of therapeutic uses like leaves used as an astringent, anti-hemorrhagic, anti-spasmodic, oxytocic, antibacterial, antifungal and antifertility agent. Externally, it's used to cure *Tinea pedis* and as a hair conditioner. The leaves have been used in India's Ayurvedic Pharmacopoeia for dysuria, jaundice, bleeding problems, ulcers, prurigo and other persistent skin ailments. Leaf was also used for dizziness and vertigo.

The leaves are composed of naphthoquinones, especially lawsone; coumarins like laxanthone, I, II and III; flavones, luteolin and its 7-O-glucoside, acacetin-7-O-glucoside; beta – sitosterol – 3 – O - glucoside; all parts of the plant contain tannins. The antibacterial efficacy of chloroform and ethanol extracts of leaves against Shigella and *Vibrio cholera* appears promising [3]. Traditional medicine uses the plant's leaves as hematinic, expectorant, liver tonic, styptic, febrifuge, anti-inflammatory, and diuretic [4].

Leaf extract has antifungal properties against a variety of germs and fungi. Henna plant is a medicinal treatment for mycosis of the hands and feet. Lawsone, a naphthoquinone, is responsible for antimycotic action. Hepato-protective action has been found in an ethanol-water (1:1) preparation of the stem bark observed with carbon tetra chloride induced toxicity in the liver. The existence of isoplumbagin and lawsaritol in the stem, bark, and in research, root has been proven to have anti-inflammatory properties. In people with sickle cell anemia, the henna leaf may help reduce sickle cell production, which is also evident in many research publications [3]. *L. inermis*, with or without other plants, is used as an anti-corrosion agent and reported as a "green corrosion inhibitor" in some studies as it has 75% antibacterial activity [5]. All the activities observed in different studies are due to the secondary metabolites/phytoconstituents / bioactive ingredients [6]. This research aims to evaluate the phytoconstituents with their potential targets and safety.

Objectives: To evaluate the various compounds present in the aqueous extract of *L. alba* by GC-MS analytical method. To know the properties of Absorption, Distribution, Metabolism, Elimination, and Toxicology of the major compounds obtained by the analytical method**.** To obtain the pharmacodynamic properties for the major compounds obtained in GC-MS analysis.

MATERIALS AND METHODS: A botanist, Mr. M. J. Prasad, Retd. Lecturer in Government Arts and Science College, Rajamahendravaram, recognized and authenticated the *L. alba* leaves. Fresh leaves were picked in the Rathinamangalam neighborhood of Chennai, Tamil Nadu, India, cleaned with fresh running tap water, distilled water, and dried in shaded sunlight. After that, the dried leaves were finely pulverized and macerated to obtain an aqueous extract from the powdered leaves. The extracted material was subjected to quantitative chemical analysis using GC-MS to determine the chemicals contained, which were used to treat a variety of diseases. We looked at the characteristics of those substances as well as their pharmacodynamic action.

Gas Chromatography-Mass Spectrometry: The aqueous extract of *L. alba* was analyzed using GC-MS equipment. A TR 5MS capillary standard non-polar column with a diameter of 30 Mts, an ID of 0.25 mm, and a film thickness of 0.25 m was used in the GC-MS [7] system's experiments. The mobile phase flow rate was fixed at 1.0 mL/min. The temperature was elevated from 40°C to 250°C at a rate of 5°C/min in the gas chromatography division, and the injection volume was 1 microliter. At a range of 50650 m/z, the outcomes of the samples saturated in chloroform were assessed utilizing Wiley Spectral library finder.

Preparation of Ligand to Know the Pharmacological Properties: The chemicals identified by GC-MS analysis were investigated further to determine their IUPAC designations /names. We retrieved the SMILES from the Pubmed compound NCBI website. Using those SMILES, we obtained the various data on physicochemical characteristics, solubility, Pharmacokinetic parameters, drug likeliness, and medicinal properties using the same SMILES and the SwissADME [8, 9] web application.

We got the toxicity profile by utilizing admetSAR [10, 11], a user-friendly interface for searching the Absorption, Distribution, Metabolism, Excretion, and/or Toxicity (ADME/T) features of any chemical.

The pharmacodynamic parameters were obtained from the Swiss target prediction interface, which predicts the most ostensible macromolecular targets of a small molecule that is believed to be bioactive by combining 2D and 3D similarities with a set of known activites on over 3000 proteins from various species.

RESULTS: Table 1 depicts the availability of various compounds in the aqueous extract of *L. alba*, which may be important for the pharmacodynamic and pharmacokinetic potency and their general physicochemical properties. A total of 91 compounds were seen in the chromatogram, but only 38 compounds were predominantly observed; only 09 compounds are a maximum number of hits based on the area and peak obtained in the chromatogram and may be responsible for the pharmacological actions of aqueous extract of *L. alba*.

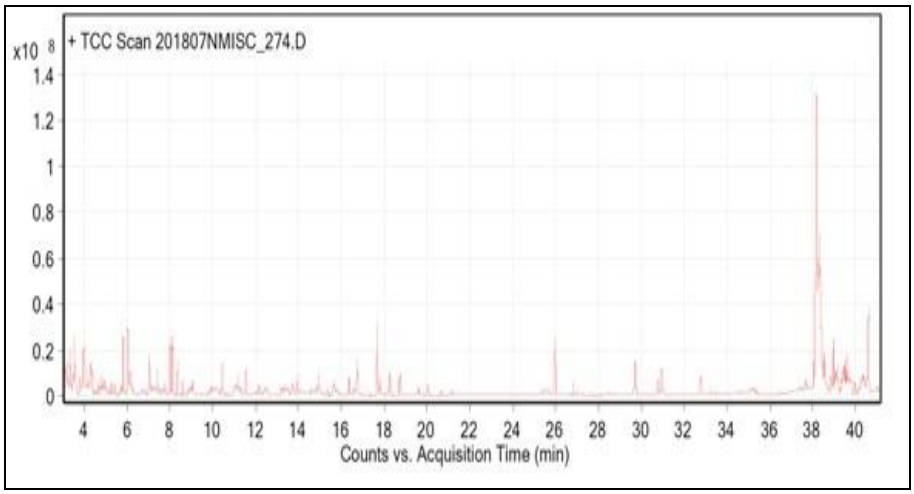
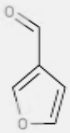
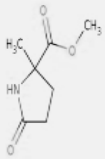
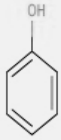
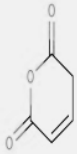
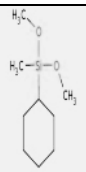
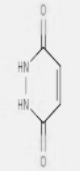
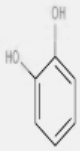
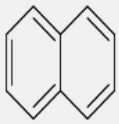
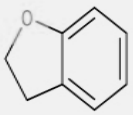
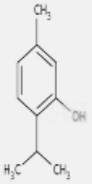
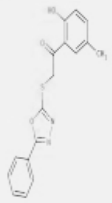
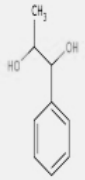
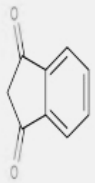
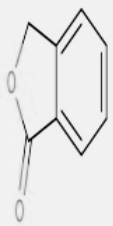
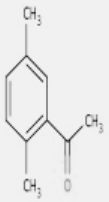
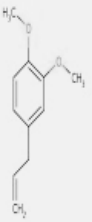
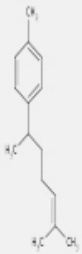
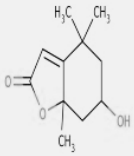
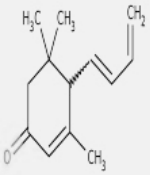
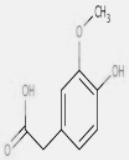
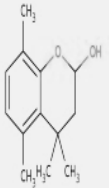


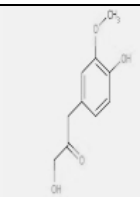
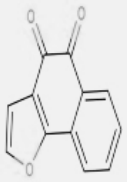
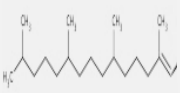
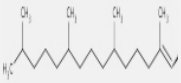
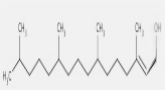
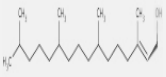
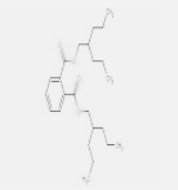
FIG. 1: CHROMATOGRAM OF THE COMPOUNDS PRESENT IN THE AQUEOUS EXTRACT IMAGE OF *L. ALBA* OBTAINED FROM GC-MS ANALYSIS

TABLE 1: GENERAL PROPERTIES OF THE COMPOUNDS RETRIEVED FROM GC-MS ANALYSIS OF AN AQUEOUS EXTRACT OF *L. ALBA*

Comp. No.	Name of the compound	Reaction Time (minutes)	Height (%)	Area (%)	Hits	Chemical formulae	Chemical structure	IUPAC Name	Smiles	Mol.Wt. (g/mol)
1	3-Furaldehyde	3.125	12.22	7.11	1	C5H4O2		furan-3-carbaldehyde	C1=COC=C1C=O	96.08
2	Proline, 2-methyl-5-oxo-, methyl ester	3.253	6.05	2.19	1	C7H11NO3		methyl 2-methyl-5-oxopyrrolidine-2-carboxylate	CC1(CCC(=O)N1)C(=O)OC	157.17
3	Phenol	3.798	15.65	9.23	1	C6H6O		phenol	C1=CC=C(C=C1)O	94.11
4	2H-Pyran-2,6(3H)-dione	3.942	9.05	12.74	1	C5H4O3		3H-pyran-2,6-dione	C1C=CC(=O)OC1=O	112.08

5	Silane, cyclohexyldimethoxymethyl	5.275	3.76	2.1	1	C9H20O2Si		cyclohexyl-dimethoxy-methylsilane	CO[Si](C)(C1CCCCC1)OC	188.34
6	Maleic hydrazide	5.418	2.59	1.66	1	C4H4N2O2		1,2-dihydropyridazine-3,6-dione	C1=CC(=O)NNC1=O	112.09
7	Catechol	5.803	2.12	1.2	3	C6H6O2		benzene-1,2-diol	C1=CC=C(C(=C1)O)O	110.11
8	Naphthalene	5.817	12.84	7.16	10	C10H8		naphthalene	C1=CC=C2C=CC=CC2=C1	128.17
9	Benzofuran, 2,3-dihydro-	6.029	25.72	15.92	10	C8H8O		2,3-dihydro-1-benzofuran	C1COC2=CC=CC=C21	120.15
10	Thymol	7.03	13.83	6.06	10	C10H14O		5-methyl-2-propan-2-ylphenol	CC1=CC(=C(C=C1)C(C)C)O	150.22
11	Ethanone, 1-(2-hydroxy-5-methyl phenyl	7.414	0.7	1.12	10	C17H14N2O3S		1-(2-hydroxy-5-methylphenyl)-2-[(5-phenyl-1,3,4-oxadiazol-2-yl)sulfanyl]ethanone	CC1=CC(=C(C=C1)O)C(=O)CSC2=NN=C(O2)C3=CC=CC=C3	326.4
12	dl-Erythro-1-phenyl-1,2-propanediol	7.745	8.36	4.46	10	C9H12O2		1-phenylpropane-1,2-diol	CC(C(C1=CC=CC=C1)O)O	152.19
13	1H-Indene-1,3(2H)-dione	7.996	16.74	10.11	4	C9H6O2		indene-1,3-dione	C1C(=O)C2=CC=CC=C2C1=O	146.14
14	1(3H)-Isobenzofuranone	8.116	18.26	10.93	10	C8H6O2		3H-2-benzofuran-1-one	C1C2=CC=CC=C2C(=O)O1	134.13

15	Ethanone, 1-(2,5-dimethyl phenyl)-	8.348	12.87	6.56	10	C10H12O		1-(2,5-dimethylphenyl)ethanone	CC1=CC(=C(C=C1)C)C(=O)C	148.20
16	Methyleugenol	8.827	5.36	2.6	6	C11H14O2		1,2-dimethoxy-4-prop-2-enylbenzene	COC1=C(C=C(C=C1)CC=C)OC	178.23
17	Phenol, 2-methoxy-4-(1-propenyl)-	9.811	1.84	1.06	10	C10H12O2		2-methoxy-4-[(E)-prop-1-enyl]phenol	CC=CC1=CC(=C(C=C1)O)OC	164.20
18	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl	10.438	1.43	3.31	6	C15H22		1-methyl-4-(6-methylhept-5-en-2-yl)benzene	CC1=CC=C(C=C1)C(C)CCC=C(C)C	202.33
19	1,4-Naphthalenediol	10.664	9.33	4.38	1	C10H8O2		naphthalene-1,4-diol	C1=CC=C2C(=C1)C(=CC=C2O)O	160.17
20	2(4H)-Benzofuranone, 5,6,7,7atetrahydro-4,4,7a-trimethyl-, (R)	11.54	3.53	6.31	3	C11H16O3		6-hydroxy-4,4,7a-trimethyl-6,7-dihydro-5H-1-benzofuran-2-one	CC1(CCCC2(C1=CC(=O)O2)C)O)C	196.24
21	Megastigmatrienone	13.35	3.15	1.8	4	C13H18O		4-[(1E)-buta-1,3-dienyl]-3,5,5-trimethylcyclohex-2-en-1-one	CC1=CC(=O)CC(C1C=CC=C)(C)C	190.28
22	Homovanillic acid	13.759	2.92	3.16	2	C9H10O4		2-(4-hydroxy-3-methoxyphenyl)acetic acid	COC1=C(C=CC(=C1)CC(=O)O)O	182.17
23	4,4,5,8-Tetramethylchroman-2-ol	13.968	7.59	4.68	1	C13H18O2		4,4,5,8-tetramethyl-2,3-dihydrochromen-2-ol	CC1=C2C(=C(C=C1)C)OC(CC2(C)C)O	206.28

24	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl	15.341	2.14	2.38	2	C10H12O4		1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)propan-2-one	COC1=C(C=CC(=C1)CC(=O)CO)O	196.20
25	Naphtho[1,2-b]furan-4,5-dione	17.37	10.3	8.02	2	C12H6O3		benzo[g][1]benzofuran-4,5-dione	C1=CC=C2C(=C1)C3=C(C=CO3)C(=O)C2=O	198.17
26	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	17.671	25.59	16.34	8	C20H40O		(E)-3,7,11,15-tetramethylhexadec-2-en-1-ol	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C	296.5
27	2-Pentadecanone, 6,10,14-trimethyl	17.794	6.47	4.15	2	C18H36O		6,10,14-trimethylpentadecan-2-one	CC(C)CCCC(C)CCCC(C)CCCC(=O)C	268.5
28	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	18.256	5.44	4.34	3	C20H40O		(E)-3,7,11,15-tetramethylhexadec-2-en-1-ol	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C	296.5
29	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	18.731	7.98	5.81	3	C20H40O		(E)-3,7,11,15-tetramethylhexadec-2-en-1-ol	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C	296.5
30	Hexadecanoic acid, methyl ester	20.032	4.4	3.73	4	C17H34O2		methyl hexadecanoate	CCCCCCCCCCCCCCCC(=O)OC	270.5
31	n-Hexadecanoic acid	21.176	1.23	1.13	1	C16H32O2		hexadecanoic acid	CCCCCCCCCCCCCCCC(=O)O	256.42
32	Phytol	25.979	21.12	22.54	2	C20H40O		(E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-ol	CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C	296.5
33	Phytol, acetate	29.72	12.42	12.36	2	C22H42O2		[(E)-3,7,11,15-tetramethylhexadec-2-enyl] acetate	CC(C)CCCC(C)CCCC(C)CCCC(=CCOC(=O)C)C	338.6
34	Phthalic acid, di(2-propylpentyl) ester	35.398	2.63	1.23	10	C24H38O4		bis(2-propylpentyl) benzene-1,2-dicarboxylate	CCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC	390.6

									C)CCC	
35	Squalene	37.719	3.99	1.44	3	C30H50		(6E,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene	CC(=CCCC(=CCCC(=CCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C	410.7
36	Squalene	38.979	15.39	4.87	2	C30H50		(6E,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracosa-12,6,10,14,18,22-hexaene	CC(=CCCC(=CCCC(=CCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C	410.7
37	Squalene	39.557	10.23	4.35	1	C30H50		(6E,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene	CC(=CCCC(=CCCC(=CCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C	410.7
38	Squalene	39.619	12.27	5.48	3	C30H50		(6E,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene	CC(=CCCC(=CCCC(=CCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C	410.7

TABLE 2: THE PHYSICOCHEMICAL PROPERTIES OF THE COMPOUNDS RETRIEVED FROM GC-MS ANALYSIS OF AN AQUEOUS EXTRACT OF *L. ALBA*

S. No.	Name of the compound	No. heavy atoms	No. arom. heavy atoms	Fraction CSP3	No. rotatable bonds	No. H-bond acceptors	No. H-bond donors	Molar Refractivity	Topological Polar Surface Area (TPSA) $^{0}A^{2}$
1	Naphthalene	10	10	0	0	0	0	43.95	0
2	Benzofuran, 2,3-dihydro-	9	6	0.25	0	1	0	35.79	9.23
3	Thymol	11	6	0.4	1	1	1	48.01	20.23
4	Ethanone, 1-(2-hydroxy-5-methyl phenyl	23	17	0.12	5	5	1	88.16	101.52
5	dl-Erythro-1-phenyl-1,2-propanediol	11	6	0.33	2	2	2	43.35	40.46
6	1(3H)-Isobenzofuranone	10	6	0.12	0	2	0	35.77	26.3
7	Ethanone, 1-(2,5-dimethyl phenyl)-	11	6	0.3	1	1	0	46.57	17.07
8	Phenol, 2-methoxy-4-(1-propenyl)-	12	6	0.2	2	2	1	49.86	29.46
9	Phthalic acid, di(2-propylpentyl) ester	28	6	0.67	16	4	0	116.3	52.6

The molecular weight, number of heavy atoms and aromatic heavy atoms, molar refractivity, fraction CSP3, number of rotatable bonds and Topological Polar Surface Area (TPSA) [7] of the compounds

obtained from GC-MS analysis of *L. alba* aqueous extract are listed in **Table 2**, where the number of atoms is within the acceptable range, molar refractivity is maintaining the range 40-130 except "Benzofuran, 2,3-dihydro-"as 35.79 and "1(3H)-Isobenzofuranone" as 35.77; the topological polar surface area of all the compounds is also less than 140 A^o that indicates these compounds are lipid-soluble.

The Log*P* Octanol-Water partition coefficient [8, 9] values of the small molecules/compounds obtained are in the range of acceptable -0.4 to +5.6 range that signifies as a good lipophilic compound except "Phthalic acid, di(2-propylpentyl) ester and all the compounds show solubility in water except "Phthalic acid, di(2-propylpentyl) ester" and "Ethanone, 1-(2-hydroxy-5-methyl phenyl" which are poorly soluble according to their hydrophilicity.

The pharmacokinetic property of the compounds retrieved from GC-MS analysis shows high oral bioavailability [8] except "Naphthalene". All these compounds cross Blood-Brain Barrier [8] (BBB) except 2 compounds which are "Phthalic acid, di(2-propylpentyl) ester" and "Ethanone, 1-(2-hydroxy-5-methyl phenyl". These compounds are not a substrate or inhibitors for p-glycoprotein efflux pump but only "Phthalic acid, di(2-propylpentyl) ester" shows P-gp inhibition [10, 11].

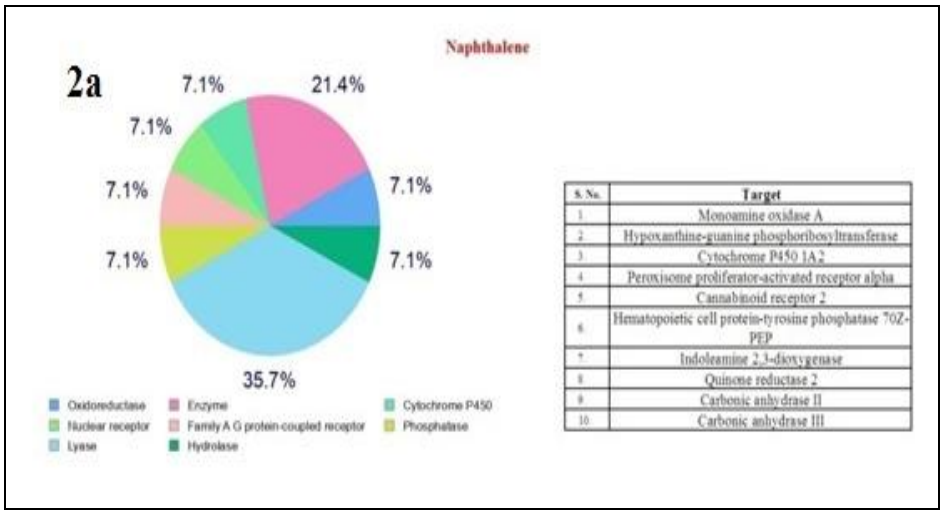
Caco-2 permeability [12] is a parameter that mimics the human intestinal epithelium to measure the human intestinal absorption of the compounds, all the molecules obtained are excellent Caco-2 except "Ethanone, 1-(2-hydroxy-5-methyl phenyl". The compounds obtained are located in the mitochondria as a site for subcellular localization [10, 11] except "Naphthalene" for which is lysosomes. All the compounds are CYP1A2 inhibitors [8, 11] except "dl-Erythro-1-phenyl-1,2-propanediol"and "1(3H)-Isobenzofuranone"; all are Not CYP2C19 and CYP2C9 inhibitors except "Ethanone, 1-(2-hydroxy-5-methyl phenyl";"Thymol" and "Phenol" are substrates of CYP2C9; none was inhibitor for CYP2D6 but "Naphthalene", "Benzofuran, 2,3-dihydro-", and "Thymol" are substrates, Ethanone, 1-(2-hydroxy-5-methyl phenyl and "Phthalic acid, di(2-propylpentyl) ester" are only CYP3A4 inhibitor but not all. None of the compounds were substrates for the CYP3A4 enzyme.

These compounds are not inhibitors of OATP2B1, MATE1, and OCT2 transporter but inhibitor to OATP1B1 and OATP1B3 transporter, and the compounds "Ethanone, 1-(2-hydroxy-5-methyl phenyl and Phthalic acid, di(2-propylpentyl) ester are BSEP inhibitors but not others.

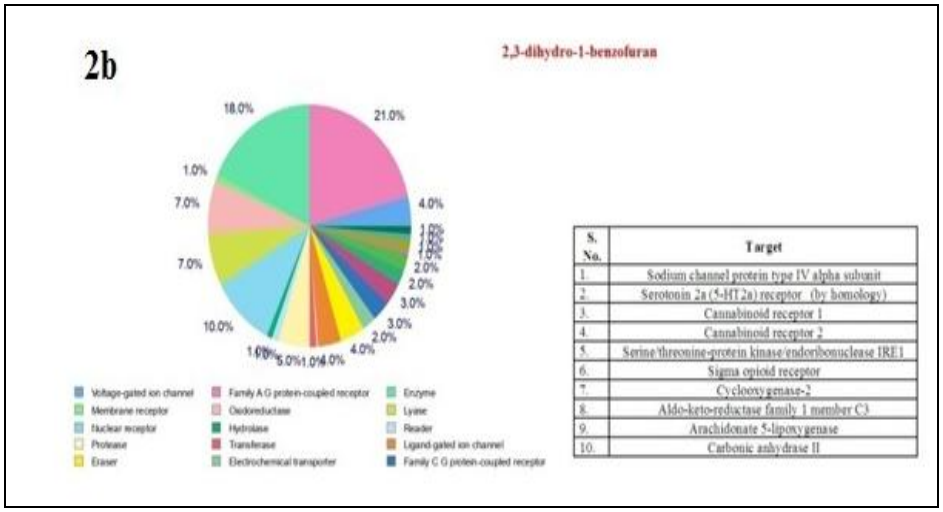
The drug likeliness [8, 13] and lead likeliness of the compounds retrieved from GC-MS analysis of an aqueous extract of *L. alba* are follow the Lipinski's rule [14–17] of 5 except Naphthalene and Phthalic acid, di(2-propylpentyl) ester" with one violation each; the Ghose rule [15, 17, 18] is not followed by the compounds "Naphthalene'' with two violations, "Benzofuran, 2,3-dihydro-" and "1(3H)-Isobenzofuranone" with three violations, "Thymol", "dl-Erythro-1-phenyl-1,2-propanediol", "Ethanone, 1-(2-hydroxy-5-methylphenyl" and "Phthalic acid, di(2-propylpentyl) ester" with one violation; Veber rule [15, 17, 19] and Egan rule [15, 17, 20] is not followed by only "Phthalic acid, di(2-propylpentyl) ester"; but only "Ethanone, 1-(2-hydroxy-5-methylphenyl" is following the Muegge's rule [17, 21] and the bioavailability score [8] for all the compounds is 0.55 and synthetic accessibility score is between 1.00 to 4.35 for all the compounds.

The toxicity profile of the compounds that retrieved from GC-MS analysis of aqueous extract of *L. alba,* by using admetSAR [10, 11] web server, the compounds "Ethanone, 1-(2-hydroxy-5-methyl-phenyl" and "1(3H)-Isobenzofuranone" are AMES mutagenic but not other compounds which is commonly used to screen to determine the mutagenic potential of new chemicals and drugs; all the compounds exhibit acute oral toxicity as category III which means LD_{50} value is greater than 500 mg kg^{-1} but less than 5000 mg kg^{-1} except & " Phthalic acid, di(2-propylpentyl) ester" which the LD_{50} value is greater than 5000 mg kg^{-1}; "Phthalic acid, di(2-propylpentyl) ester" shows hERG inhibition leads to Q-T prolongation; "Naphthalene", "Benzofuran, 2,3-dihydro-" and "Phthalic acid, di(2-propylpentyl) ester" shows carcinogenicity as warning sign means the TD_{50} is above 10 mg per kg body weight per day and others are non-carcinogenic; all the compounds except "Ethanone, 1-(2-hydroxy-5 -methylphenyl" shows eye irritation; fish aquatic toxicity is exhibiting with "Benzofuran, 2,3-dihydro-" and "dl-Erythro-1-

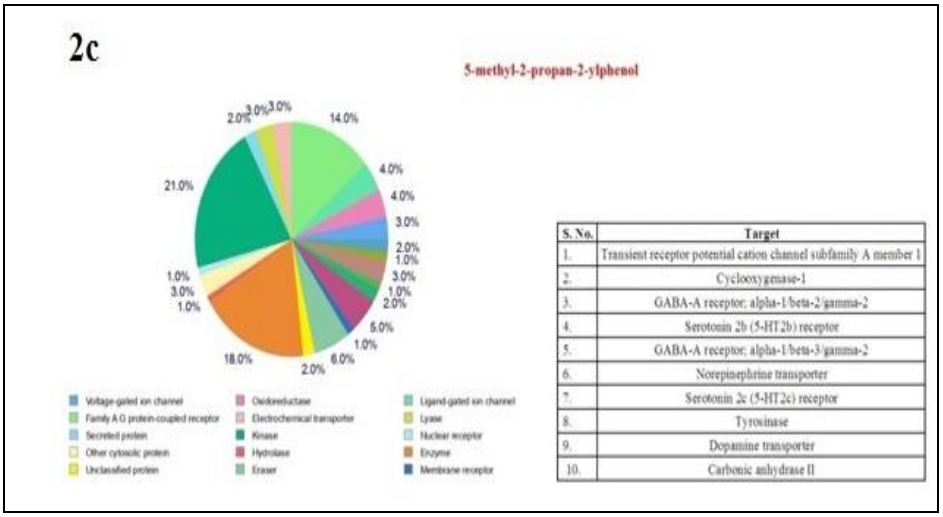
phenyl-1,2-propanediol; only Ethanone, 1-(2-hydroxy - 5-methylphenyl" exhibits hepatotoxicity; reproductive toxicity is showing by "Benzofuran, 2,3-dihydro-" "Ethanone, 1-(2-hydroxy-5-methylphenyl" and "Phenol, 2-methoxy-4-(1-propenyl)-"; no compound is showing honeybee toxicity.



S. No.	Target
1	Monoamine oxidase A
2	Hypoxanthine-guanine phosphoribosyltransferase
3	Cytochrome P450 1A2
4	Peroxisome proliferator-activated receptor alpha
5	Cannabinoid receptor 2
6	Hematopoietic cell protein-tyrosine phosphatase 70Z-PEP
7	Indoleamine 2,3-dioxygenase
8	Quinone reductase 2
9	Carbonic anhydrase II
10	Carbonic anhydrase III



S. No.	Target
1.	Sodium channel protein type IV alpha subunit
2.	Serotonin 2a (5-HT2a) receptor (by homology)
3.	Cannabinoid receptor 1
4.	Cannabinoid receptor 2
5.	Serine/threonine-protein kinase/endoribonuclease IRE1
6.	Sigma opioid receptor
7.	Cyclooxygenase-2
8.	Aldo-keto-reductase family 1 member C3
9.	Arachidonate 5-lipoxygenase
10.	Carbonic anhydrase II



S. No.	Target
1.	Transient receptor potential cation channel subfamily A member 1
2.	Cyclooxygenase-1
3.	GABA-A receptor; alpha-1/beta-2/gamma-2
4.	Serotonin 2b (5-HT2b) receptor
5.	GABA-A receptor; alpha-1/beta-3/gamma-2
6.	Norepinephrine transporter
7.	Serotonin 2c (5-HT2c) receptor
8.	Tyrosinase
9.	Dopamine transporter
10.	Carbonic anhydrase II

FIG. 2: A PICTURE SHOWING THE ACTIVITY AGAINST ALL THE PROTEINS / RECEPTORS/ TRANSPORTERS/ ENZYMES OF THE COMPOUNDS"NAPHTHALENE","2,3-DIHYDRO-1-BENZOFURAN", "5-METHYL-2-PROPAN-2-YLPHENOL"AND THE TOP 10 FROM THE LIST BASED ON HIGH PROBABILITY WHICH OBTAINED FROM THE AQUEOUS EXTRACT OF *L. ALBA* OBTAINED FROM GC-MS ANALYSIS

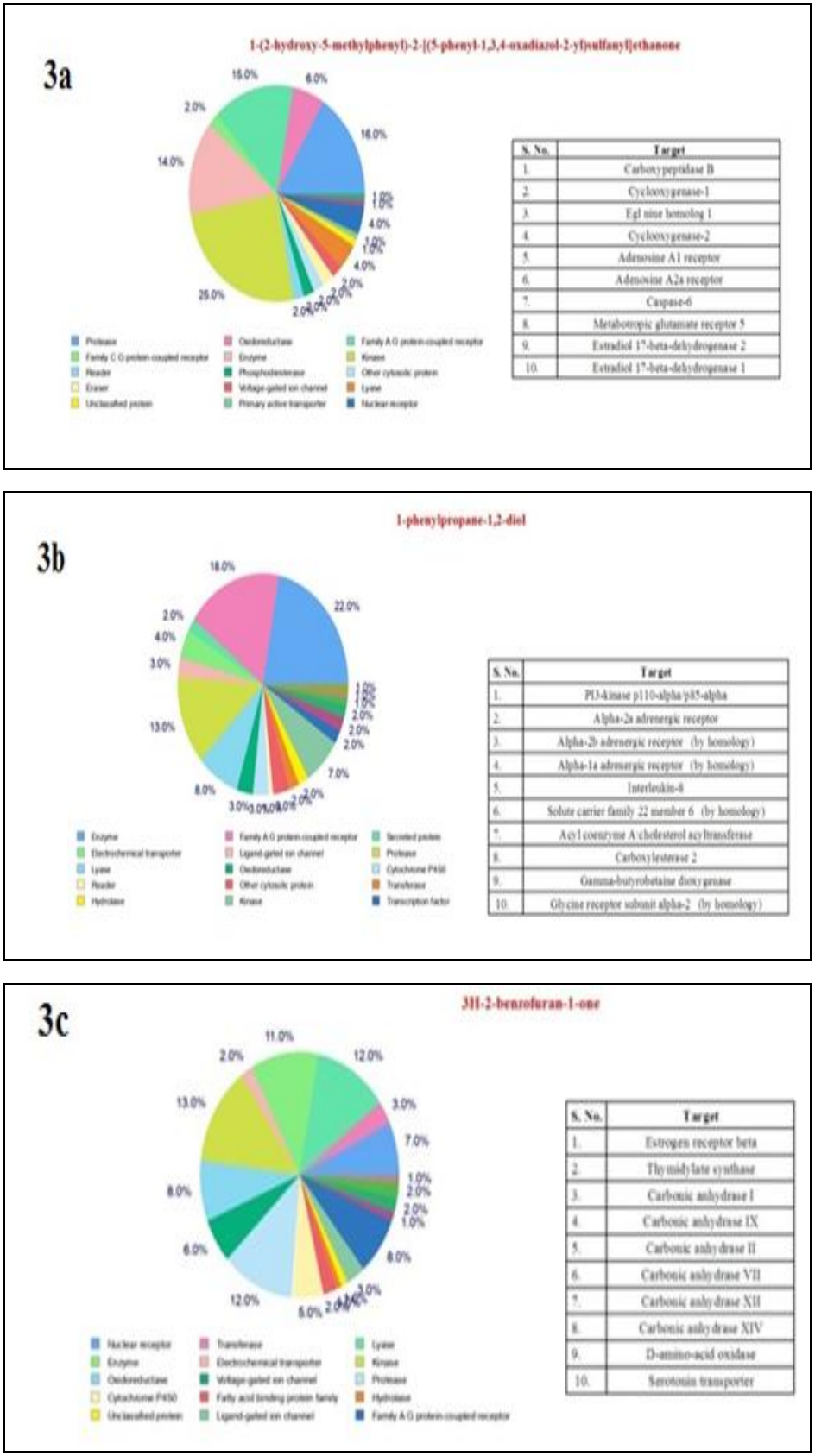


FIG 3: A PICTURE SHOWING THE ACTIVITY AGAINST ALL THE PROTEINS/RECEPTORS/TRANSPORTERS / ENZYMES OF THE COMPOUNDS "1-(2-HYDROXY-5-METHYL PHENYL)-2-[(5-PHENYL-1,3,4-OXADIAZOL-2-YL)SULFANYL]ETHANONE", "1-PHENYLPROPANE-1,2-DIOL", "3H-2-BENZOFURAN-1-ONE" AND THE TOP 10 FROM THE LIST BASED ON HIGH PROBABILITY WHICH OBTAINED FROM THE AQUEOUS EXTRACT OF *L. ALBA* OBTAINED FROM GC-MS ANALYSIS

The above **Fig. 2** shows the ligands' probability with various proteins/ receptors/ transporters/ enzymes with the help of the web tool Swiss Target Prediction [22] used to predict the protein/receptor that can be modulated after their ligand-receptor interaction.

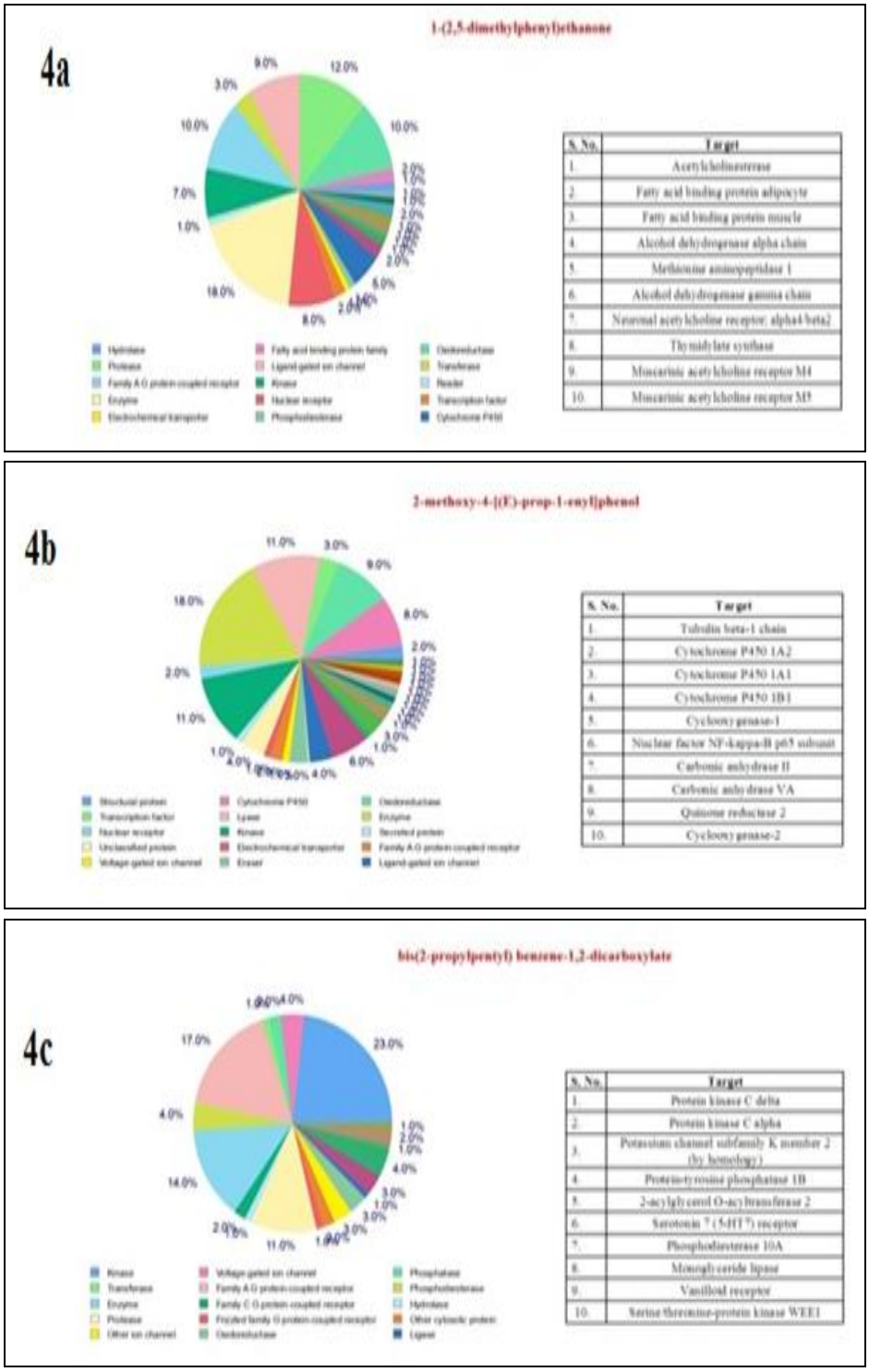


FIG. 4: A PICTURE SHOWING THE ACTIVITY AGAINST ALL THE PROTEINS/RECEPTORS/TRANSPORTERS / ENZYMES OF THE COMPOUNDS "1-(2,5-DIMETHYL PHENYL)ETHANONE", "2-METHOXY-4-[(E)-PROP-1-ENYL]PHENOL", "BIS(2-PROPYLPENTYL) BENZENE-1,2-DICARBOXYLATE" AND THE TOP 10 FROM THE LIST BASED ON HIGH PROBABILITY WHICH OBTAINED FROM THE AQUEOUS EXTRACT OF *L. ALBA* OBTAINED FROM GC-MS ANALYSIS

The compounds "Naphthalene (2a), "2,3-dihydro-1-benzofuran"(2b) and "5-methyl-2-propan-2-ylphenol"(2c)act as a ligand and show their activity on 14, 100, 100 proteins/targets respectively. The

above **Fig. 3** shows the ligands' probability with various proteins/ receptors/ transporters/ enzymes with the help of the web tool, swiss target prediction [22], used to predict the protein/receptor that can be modulated after their ligand-receptor interaction. The compounds "1-(2-hydroxy-5-methyl phenyl)-2-[(5 – phenyl - 1, 3, 4 – oxadiazol - 2-yl) sulfanyl] ethanone (3a), "1-phenylpropane-1,2-diol"(3b), "3H-2-benzofuran-1-one"(3c) which acts as a ligand and shows its activity on 100, 100, 100 proteins/targets respectively. The above **Fig. 4** shows the ligands' probability with various proteins/ receptors/ transporters/ enzymes with the help of the web tool, swiss target prediction [22], used to predict the protein/receptor that can be modulated after their ligand-receptor interaction. The compounds "1-(2,5-dimethyl phenyl) ethanone (4a), "2-methoxy-4-[(E)-prop-1-enyl]phenol (4b), bis(2-propylpentyl) benzene-1, 2-dicarboxylate (4c) which acts as a ligand and shows its activity on 100, 100, 100 proteins/targets respectively.

DISCUSSION: For many years, *Lawsonia alba* has been recognized for a wide range of therapeutic characteristics. This research aimed to find the active chemicals in the extract that have pharmacological effects. The aqueous extract yielded 38 distinct active chemicals in this analysis. According to Swami Narsingh Chandra Dev [23] *et. al.,* there are 51 compounds with various peaks in methanolic extract of *L. inermis* leaves, the most prominent of which is Squalene (19.77%) 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-(14.90%); 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-(11.52%); Pentadecanoic acid (10.54%); Vitamin E (6.82); Hexadecanoic acid, methyl ester (5.85%); 9,12-Octadecadienoicc acid (Z,Z)-, Methyl ester (4.98%); Stigmast-5-En-3- Ol, (3.Beta.)- (5.67), Phytol (1.77%).

In another study by Ritesh Kumar Sharma, Anjana Goel [24] hexane fraction showed 56 peaks, out of it, 13 phytochemical constituents were identified by GC-MS software library and most of them showed biological activity, 5 chemical compounds were present in high concentration, out of which 2 were identified viz. Hexadecanoic acid (9.47%), Vit. E (7.41%) while 3 peaks which were not identified having % area *i.e*. 1.43%, 1.22%, and 1.01% with RT- 55.07, 75.342, and 76.506 respectively. In GC-MS of ethyl acetate fraction 108 peaks were observed, and 17 phytochemical compounds were identified. Out of which 1, 4 Napthalenedione was identified as a major constituent; aqueous methanol fraction had 19 peaks, and 7 compounds were identified.

The other study by Asma Elaguel [25] *et al.*, states the essential oil contains a total of 30 components, with Monoterpene hydrocarbons, being the main class of constituents with 81.40% including the α-limonene (55.06%), β–limonene (24.06%) and β–myrcene (2.28%), followed by the linalool (2.41%). In another study by Hosam O. Elansary [26], high amounts of apigetrin, at 1180.9 mg/100 g DW; apigenin 5-glucoside, at 596.3 mg Plants 2020 /100 g DW and gallic acid, at 81.0 mg/100 g DW. But-LI fraction contains high amounts of catechin, chlorogenic acid, ellagic acid, and kaempferol, according to Manish Kumar [4, 27] *et al.,* while phytochemicals such as gallic acid, epicatechin, and quercetin are present in moderate amounts.

According to Tamara Mengoni [28] *et. al.,* aliphatic compounds (9.0-64.7 %), terpenoids (5.8-45.5 %), and aromatics (7.9-45.2 %), with alkanes (0.9-18.5 %), aldehydes (2.1-18.8 %) and carboxylic acids (3.1 n-hexadecane (0.5-4.7 %), (2E)-hexenal (0.5-11.7 %) and acetic acid (2.8-24.5 %), limonene (0.8-14.7 %), carvol (3.8-7.1 %), geranyl acetone (1.4-7.9%) and (E)-caryophyllene (3.3-8.4 %) and (E)-anethole (0.6-35.0 %) respectively were the major representatives of these groups. Hatil Hashim EL-Kamali [29] *et. al.,* found that the D-allose (17.61%), lawsone (12.87%), beta-D-glucopyranoside, methyl (12.74%), phytol (10.78%), 1-isobutoxy-1-methoxypropane (9.18%), n-hexadecanoicacidin (6.33%), 9,12,15-octadecatrienoic acid (Z, Z, Z) (4.44%), squalene (4.06%) and vitamin E (3.60%) as the major biomolecules in ethanol extract of leaves of *L. inermis* (AL-Fetaehab sample), whereas in the ethanol extract of leaves of *L. inermis* (Ed-Damer sample) observed the compounds like beta-D-glucopyranoside, methyl (36.10%), phytol (10.85%), 9,12,15-Octadecatrienoic acid, Z,Z,Z (7.31%), squalene (7.20%), vitamin E (6.82%) and lawsone (6.79%) as the major bioactive constituents. In a study by Snehal N. Bhangale and Moitreyee Saha [30] both leaf and callus powders of *L. inermis* L., the preliminary phytochemical analysis revealed the presence of alkaloids,

anthraquinone, carbohydrates, glycosides, phenols, flavonoids, tannins, saponins and essential oils, which were then confirmed by the presence of alkaloids, anthraquinone, carbohydrates, glycosides, phenols, flavonoids, tannins, saponins, and essential oils which confirmed with the assistance of TLC.

Tansukh Barupal [31] *et. al.;* reported the inhibitory effects of leaf extract of *L. inermis* against *Curvularia lunata* in their study due to the availability of 6 constituents which are hexacosane, octadecane, docosane, heptacosane methyl, octacosane, and tetracosane. In a study by Dhananjay Kumar Singh [32] *et al.,* phytochemical studies of the roots and leaves of the henna plant revealed the presence of bioactive chemicals like isoplumpagin, lupeol, 30-norlupan-3-ol-20-one, betuhennan, betuhennanic acid and n-tridecanoatephenolic glycosides, lawsoniaside, β-sitosterol and stigmasterol.

The crimson orange color found in henna leaf paste is due to lawsone (2-hydroxy-1,4-naphthoquinone) and is employed in modern pharmacopeia as a starting chemical for the manufacture of therapeutically relevant anti-cancer medications including lapachol, atovaquone, and dichloroallyllawsone. According to Ruchi Badoni Semwal [33] *et. al.,* nearly 70 phenolic chemicals have been extracted from the plant's various sections. Many pharmacological effects have been attributed to naphthoquinones, which include the dying principle lawsone. The strong odor of the essential oil derived from the petals is mostly attributable to the presence of terpene β-ionone. Non-volatile terpenoids, asinglesterol, two alkaloids, and two dioxin by-products have also been identified from the plant, in addition to various volatile terpenes. Numra Tariq Mir [34] *et. al.,* reported the presence of twelve components in the phytochemical observation of *L. inermis* chloroform extract, and the largest quantities were found in phytol, pseudoephedrine, aspidofractinine-3-methanol, phenol, 2,6-bis(1,1-dimethyl ethyl)-4-methyl-, and methylcarbamate, the highest concentration of phenol was found in 2,6-bis (1,1-dimethyl ethyl)-4-methyl-, a phenolic methyl-carbamate molecule that may be involved in the extract's antioxidant and nootropic properties. Phytol was the component with the abundant concentration in both extracts. Sixteen substances were found in the phytochemical analysis of *L. inermis* ethanolic extract, among them, the most common molecules were 3,7,11,15-tetramethyl-2-hexadecen-1, E-2-tetradecen-1-ol, 2-tridecen-1-ol, phytol, 1-eicosanol, Z,Z-2, 5-pentadecadien-1-ol, 3-hexadecyloxy-carbonyl-5- (2-hydroxyethyl)-4-methyl imidazolium.

Kashif Iqbal, Javeid Iqbal, Dan Staerk, and Kenneth T. Kongstad [35], identified six known compounds 2,4,6-trihydroxyacetophenone-2-O-b-D-glucopyranoside (1), lalioside (2), luteolin-40-O-b-Dglucopyranoside (3), apigenin-40-O-b-D-glucopyranoside (4), luteolin (5) and apigenin (6). In another research by Mohamed A. A. Orabi [36] *et. al.,* from *L. inermis* leaves, isolated two new C-glycosidic ellagitannins (1 and 2), as well as seven recognized ellagitannins (3–9) and a related polyphenolic ingredient with anticancer activities.Chang-Syun Yang [37] *et. al.,* observed the presence of diphenol, (Z)-4,40 -(prop-1-ene-1,3-diyl) diphenol (1), two new isocoumarin carbonates, inermiscarbonates A (2) and B (3) and six known compounds, 4 0 -hydroxyflavanone (4), apigenine (5), kampferol (6), luteolin (7), quercetin (8) and (-)-catechin (9) in ethyl acetate (EtOAc)-soluble fractions from methanol extract.

In this research, we observed a total of 91 compounds and 09 compounds were of high concentration on basis of height, peak and area covered such as “naphthalene”, “2,3-dihydro-1-benzofuran”, “5-methyl-2-propan-2-ylphenol”, “1-(2-hydroxy-5-methyl phenyl)-2-[(5-phenyl-1,3,4-oxadiazol-2-yl)sulfanyl] ethanone”, “1-phenylpropane-1,2-diol”, “3H-2-benzofuran-1-one”, “1-(2,5-dimethyl phenyl)ethanone”, “2-methoxy-4-[(E)-prop-1-enyl]phenol”, “bis(2-propylpentyl) benzene-1,2-dicarboxylate”and also we were successful to retrieve the potent drug targets/ receptors/ enzymes/ transporters which can be modified and show the variation in the pharmacological actions by these above mentioned major compounds. The research findings observed in this research have few similarities and are far different from other researchers’ findings which may be due to the variation in the ethnicity of plants or maybe a variation in the GC-MS analytical methodology.

CONCLUSION: The medicinal plant *L. alba* has been of top-notch importance since ancient days as it has shown helpful in the treatment of a myriad of diseases, but the real active principle, which is the basis of its pharmacological actions, is not yet known comprehensively. An attempt was made, using the GC-MS analytical technique, a total of 90 compounds were isolated, out of which 09 compounds in the highest concentration were observed in the aqueous extract of *L. alba* that may be helpful after pre-clinical and clinical trials by using these as a "Hit" molecule or "Lead" molecule or their derivatives.

Limitations: In this research, we were able to retrieve the compounds by GC-MS and know the pharmacokinetic and pharmacodynamic properties, but it is required to evaluate these compounds for pre-clinical studies and clinical trials.

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