



Original Research Paper

COMPOUNDS IDENTIFICATION THROUGH GC-MS, PHARMACOLOGICAL APPLICATIONS; IN-SILICO MOLECULAR DOCKING ANALYSIS AND ANTIMICROBIAL POTENTIAL OF ECLIPTA ALBA

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ABSTRACT

The *Eclipta alba* comes under Asteraceae family, is an yearly herbaceous plant, normally identified as false daisy, used a tonic, diuretic in hepatic, spleen expansion. Current study we focused identify bioactive compounds by GC-MS, pharmacological applications for *In-silico* molecular docking investigation and antimicrobial activity of various extract of *E. alba*. In results we done 6 extracts; aqueous (ARSB-01), ethanol (ARSB-02), acetonitrile (ARSB-03), ethyl acetate (ARSB-04), acetone (ARSB-05) and hexane (ARSB-06), in results the GC-MS analysis; 12 compounds were identified in ARSB-01 followed by 10 compounds in ARSB-06, 8 compounds in ARSB-03 and ARSB-05, 7 compounds from ARSB-02, 6 compounds in ARSB-04. propane, 1,2-dimethoxy- was predominant in ARSB-03 and ARSB-04 but was also detected at high (above 90%) levels in ethanol, acetone and hexane extracts, Among the tested organisms, *S. aureus* was the most susceptible to the acetonitrile and ethyl acetate extracts, both of which produced MIC values of 0.3125 mg/mL. It supports *E. alba* as a promising source of antimicrobial constituents and demonstrate that solvent selection substantially influences the resulting biological activity. Among the tested extracts, ARSB-03 and ARSB-04 were the most promising candidates. Comp 2 formed a hydrogen-bond interaction and π - π interactions involving TYR147 and TYR157, whereas Comp 1 was predominantly stabilized through π - π interactions with TYR147, TYR157 and PHE204. Hydrogen bonding can contribute to improved orientation and stabilization of a ligand within the active site, while aromatic and hydrophobic interactions, we concluded that from our research selected *E. alba* potential plant to kill human pathogens, also promising lead antimicrobial drug in future.

Keywords: Antibacterial Activity, Antifungal Activity, *Eclipta alba*, GC/MS profiling, *In-silico* studies

1. INTRODUCTION

The *Eclipta alba* (L.) comes under Asteraceae family, it's used in several parts of sub-tropical and tropical areas; Africa, South America, Asia (Timalsina and Devkota, 2021). This *E. alba* plant three kinds; yellow, white and black colours, all these are available all over India, is a medicinal herb, used traditionally in Siddha, Unani and Ayurveda systems of medicine, many herbal formulations it is an active ingredient in arranged for liver sicknesses and expressions effect on generation cells for liver; used as a diuretic and tonic in hepatic and spleen expansion (Sekar et al., 2023; Molligoda et al., 2023), used in skin diseases, catarrhal jaundice, antiviral activity against Ranikhet disease virus (Mukhopadhyay et al., 2018). It's used in all over India hair oil for healthy long hair and black, consuming leaf fresh juice used for appetite, refining digestion and minor intestine regulator,

viral hepatitis to help bile movement, defend the parenchyma, improve remembrance and knowledge (Timalsina and Devkota, 2021; Raffif et al., 2022). The *E. alba* phytochemicals exhibit the various pharmacological activities; immunomodulatory, Cerebro protective, hypocholesterolemic, diuretic, anti-diabetic, anti-pyretic, anticancer, antioxidant, neuroprotective (Prabhakar et al., 2023), hepatoprotective, bronchodilator, anti-inflammatory, anti-venom, anti-epileptic activity, antimicrobial and antiviral (Hou et al., 2024; Kora, 2023).

Medicinal plants performance vital role in the expansion of new antimicrobial agents to fight superbugs (Sivalingam and Pandian, 2024). Since long time the traditional medicinal plants are vital source for the traditional medicine includes Siddha, Unani, Ayurveda and in Traditional Chinese Medicine (Abdallah et al.,

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2023). It is assessed that 80% of the global population particularly from the emerging nations, regularly used herbal medicine as a foundation of rudimentary health care (Vimalraj and Saravanan, 2023; Sivalingam and Pandian, 2024). The natural products were very important source in the discovery of modern-day pharmaceuticals (Swami et al., 2022; Vimalraj and Saravanan, 2023). Due to alarming rise in the antibiotic resistance, the focus on the use of herbal plants as alternate foundations of antibacterial agents in enormously increases in recent year (Sivalingam and Pandian, 2024). Plants contain a widespread assortment of bioactive compounds which revelation important antibacterial properties, production them gifted applicants for novel drug expansion (El-Saadony et al., 2025).

The medicinal plants are expanded much consideration in contemporary medicine outstanding to their affordability, accessibility, extensive safety and acceptance, production of herbal remedies extremely esteemed worldwide (Krithika Shree et al., 2023; Izah et al., 2024). The World Health Organization (WHO) agrees several medicinal plants as replacements to treat different diseases. The development of herbal drugs from the medicinal plants experiences various preliminary stages, from pre-extraction to extraction steps, these will lead to obtained various bioactive components from these plants (Van Wyk and Wink, 2018).

Antimicrobial resistance (AMR) is emerging as an international health disaster and is connected by approximately 5 million deaths annually (Sivaraj et al., 2025). The recent 2025–2026 AMR data highlighting that India facing a critical AMR crisis, due to overuse of broad-spectrum drugs (Patra et al., 2025). It is reported that nearly 300,000 annual deaths are associated with the bacterial resistance. AMR mentions to the capability of microbes to fight the therapeutic properties of formerly effective antimicrobials (Murray et al., 2022; Sivalingam et al., 2024). It is predicted that by 2050, the AMR will cause 10 million mortalities globally. The COVID-19 pandemic significantly worsened the AMR globally, driven by widespread antibiotic over prescriptions, strained healthcare systems and deprioritized infection controls (Boccabella et al., 2024). The urgent need for the new antimicrobial's development after the COVID-19 pandemic is in uttermost need (Abdelsalam Elshenawy, 2025).

We targeted *Eclipta alba* plant, there are six different solvent extracts; aqueous, ethanol, acetonitrile, ethyl acetate, acetone and hexane extracts, besieged for compounds identification through GC-MS analysis and pharmacological applications; antibacterial activity against different human pathogenic bacteria and *in silico* molecular docking analysis for antibacterial activity targeted proteins.

2. EXPERIMENTAL SECTION

2.1 Chemicals and Reagents

All the chemicals, reagents and solvents are purchased from analytical reagent (AR) grade and were procured from Himedia, Merck, etc., all chemicals and solvents were used without further purification unless otherwise specified.

2.2 Collection and Extraction Preparation

The *E. alba* powder 10 g was extracted in a Soxhlet apparatus for 10 hours with 100 ml of Water (ARSB-01), Ethanol (ARSB-02), Acetonitrile (ARSB-03), Ethyl Acetate (ARSB-04), Acetone (ARSB-05) and Hexane (ARSB-06) tracked through air ventilation. In rotary evaporator preserved (40°C), the extract was condensed with abridged pressure to yield the solid products in 2-3 g quantity which were used for the GC-MS profiling and biological assays (Pandian et al., 2017).

2.3 Instrumentation and Sample Analysis in GC-MS

The phytochemical conformation of the extracts was analysed through a Shimadzu GC–MS–QP2010 system (Shimadzu, Japan) equipped with an SPL-1 injection port and an INJ-1 injector. The MS spectrometer was functioned in electron ionization (EI) mode at an ionization energy (70 eV), ion cause and border temperatures were preserved (230°C and 250°C), respectively. Separation was accomplished by a ZB-5 capillary column (30 m×0.32 mm i.d.; film thickness 0.25 µm). Helium (99.9% purity) was used as carrier gas at a flow rate of 1.71 mL/min. A sample 1 µL volume was injected at an injector temperature of 250°C under the specified split conditions. The linear velocity was maintained at 47.1 cm/s, with an elimination movement of 3 mL/min and an overall movement rate 90.0 mL/min. The oven temperature was initially preserved (40°C) for 1 min and subsequently amplified to 300°C at a rate of 10 °C/min. The entire run time 37 min. the acquired Mass spectra were over an m/z range of 0–1000. The obtained chromatographic peaks and mass spectra were used for the documentation of phytochemical constituent's current in the extracts (Saranya et al., 2025). GC–MS has been widely applied for the profiling and identification of bioactive phytoconstituents in medicinal plant extracts (Rangari and Margonwar, 2025).

2.4 Biological Evaluation

2.4.1 Minimum Inhibitory Concentrations (MIC)

The antibacterial activity by minimum inhibitory concentration (MIC) of the plant extracts (ARSB-01-06) was evaluated against two gram +ve bacterial strains are *S. aureus* (ATCC 25923) and *B. subtilis* (ATCC 6633) and two gram -ve bacterial strains, *P. aeruginosa* (ATCC 27853) and *E. coli* (ATCC 25922), using the broth microdilution method. Fresh bacterial cultures were grown overnight in Mueller-Hinton broth (MHB) at 37°C and accustomed to approximately 1×10^6 CFU mL⁻¹ before inoculation. The values of MIC were identified by the broth microdilution technique in sterile microplates

(96-well), serial dilutions 2 fold of separately compound were prepared in MHB, followed through inoculation with bacterial suspension to get a final inoculum density of roughly 1×10^6 CFU mL⁻¹. At 37°C plates were incubated for 24 h, MIC was clear as the lowermost concentration that entirely inhibited observable bacterial growth, each experiment was carried out in triplicate to ensure reproducibility (Nagarajan et al., 2010; Kaderabkova et al., 2024).

2.4.2 Minimum Fungicidal Concentrations

The determination of the antifungal activity by minimum Fungicidal concentration (MFC) of plant extracts (ARSB-01-06) was evaluated against *A. niger* and *C. albicans* using the broth microdilution method. *C. albicans* was cultured in Sabouraud dextrose broth (SDB) for 24 h at 28-30°C, whereas spores of *A. niger* were harvested from 5 to 7 d old cultures using sterile saline contains Tween 80 (0.05%). The inoculum density was adjusted to approximately 1×10^6 CFU mL⁻¹ for *C. albicans* and 1×10^5 - 10^6 spores mL⁻¹ for *A. niger*. The prepared derivatives were dissolved in DMSO to prepare stock solutions, followed by two-fold serial dilution in SDB. Equal volumes of fungal inoculum were added to individually well and the microplates were incubated at 28°C for 48 h. Growing and sterility controls were included in each experiment. The MIC was defined as the lowermost attention showing no observable fungal growth, all experiments were performed in triplicate (Nagarajan et al., 2012; Ward et al., 2025).

2.5 In silico studies

Ligand Preparation:

The 2D structure of **Comp 1 & 2** was sketched and converted to 3D using LigPrep, module of Schrödinger. H atoms were added and low-energy ionization and tautomeric states were generated at pH 7.4. The structures were then minimized using the OPLS-2005 force field. The crystal ligand (W32) was used as the reference standard for docking studies (Zhao et al., 2025).

Molecular Docking studies

The molecular docking studies for the arranged compounds were accomplished using the Glide module in Maestro Schrodinger Suite. 3D crystal co-ordinates of *S. aureus* enoyl-ACP reductase (PDB ID: 4FS3) was recovered from Protein Data Bank (Purakkel et al., 2024).

3. RESULTS AND DISCUSSION

The different plant extracts of *E. alba* obtained these are aqueous (ARSB-01), ethanol (ARSB-02), acetonitrile (ARSB-03), ethyl acetate (ARSB-04), acetone (ARSB-05) and hexane (ARSB-06) extracts, its targeted compounds identifications by GC-MS, antimicrobial activities (MIC), these results are discussed in detail. The selection of extraction solvent can substantially influence the phytochemical profile and resulting antimicrobial activity of plant extracts, as demonstrated in comparative studies of medicinal plants using different extraction solvents (Abhang et al., 2024)

Bioactive compounds identification through GC-MS analysis

Aqueous Extract (ARSB-01):

The GC-MS chromatograph of the aqueous extract (ARSB-01) showed that 19 compounds are presented in the **Table-1**. Among these compounds the highest % was observed that Propane, 1,2-dimethoxy- it showed 49.58%, followed by Cyclopentasiloxane, Deca methyl showed 4.85%, other compounds in trace level. Compounds are Benzeneethanamine, 2,5-difluoro-β,3,4-trihydroxy-N-methyl,1,3-Hexadien-5-yne, vinylcyclobutane, Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, N-(Trifluoroacetyl)-N,O,O',O"-tetrakis(trimethylsilyl) norepinephrine, Dodecanedioic acid, bis(tert-butyl dimethylsilyl) ester, Tetradecamethylcycloheptasiloxane, Diethyl Phthalate, Benzofuran-5,6-diol-3-one, 2-benzylidene-, 2-Pyrazinyl-4-methoxyphenylketone and Taurine (2-Aminoethanesulfonic acid). (**Fig. 1; Table 1**)

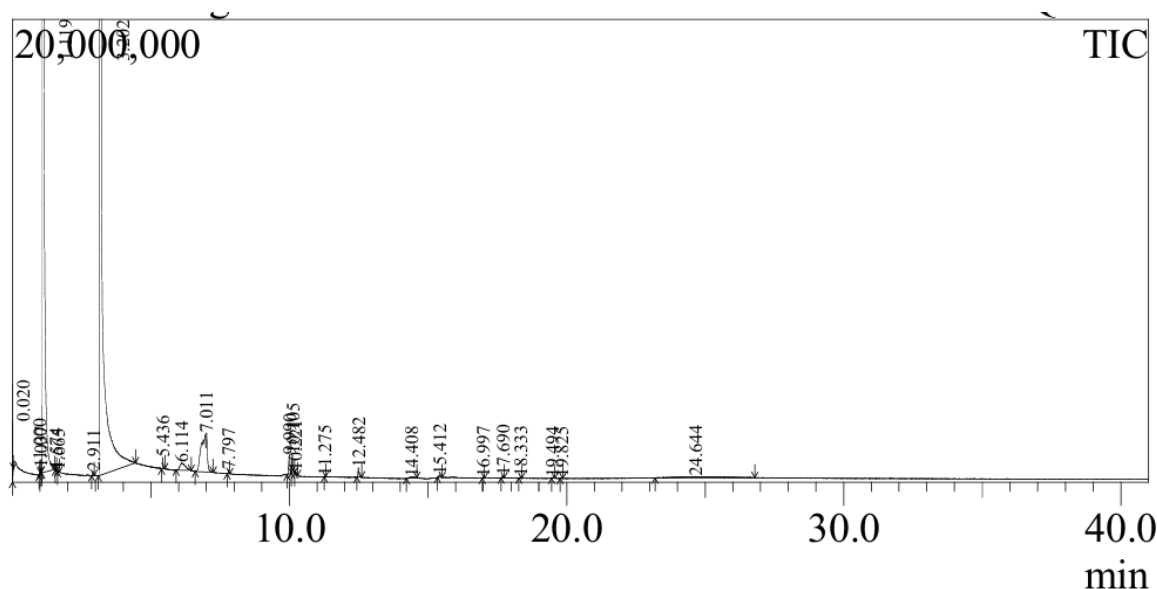


Figure 1. Compounds identification by GC/MS analysis of aqueous extract (ARSB-01) of *E. alba*

Table-1: List of compounds identified in GC-MS analysis in aqueous extract (ARSB-01) of *E. alba*

Peak	R.Time	Area	Area%	Height	A/H	Base m/z	Name
1	0.02	786560	0.12	22975	0.34	44.05	Benzeneethanamine, 2,5-difluoro-.beta.,3,4-trihydroxy-
2	1	344365	0.05	58346	0.59	44.05	Nitrous Oxide
3	1.037	171258	0.03	19063	0.9	44.05	o-Methylisourea hydrogen sulfate
4	1.119	329404543	49.58	10893	3.02	39.05	Propane, 1,2-dimethoxy-
5	1.574	33410	0.01	38332	0.87	78.1	1,3-Hexadien-5-yne
6	1.665	68379	0.01	71256	0.96	67.05	Cyclobutane, ethenyl-
7	2.911	248914	0.04	18875	1.32	207.15	Cyclotrisiloxane, hexamethyl-
9	5.436	707123	0.11	48841	1.45	281.25	Cyclotetrasiloxane, octamethyl-
10	6.114	4153272	0.63	32080	12.95	73.1	N-(Trifluoroacetyl)-N,O,O',O"-tetrakis(trimethylsilyl)no
11	7.011	23654294	3.56	16873	14.02	73.1	Cyclopentasiloxane, decamethyl-
12	7.797	266166	0.04	16917	1.57	73.1	N-(Trifluoroacetyl)-N,O,O',O"-tetrakis(trimethylsilyl)no
13	9.99	2866181	0.43	800720	3.58	73.15	Cyclohexasiloxane, dodecamethyl-
14	10.105	1681078	0.25	81069	2.07	73.15	Cyclohexasiloxane, dodecamethyl-
15	10.221	125207	0.02	12514	1	73.1	Cyclohexasiloxane, dodecamethyl-
16	11.275	35691	0.01	38688	0.92	73.1	Dodecanedioic acid, bis(tert-butyltrimethylsilyl) ester
17	12.482	1026437	0.15	39588	2.59	73.1	Cycloheptasiloxane, tetradecamethyl-
18	14.408	518356	0.08	45411	11.41	149.15	Diethyl Phthalate
19	15.412	355878	0.05	11071	3.21	73.15	Cyclooctasiloxane, hexadecamethyl-
20	16.997	94196	0.01	40225	2.34	253.2	Benzofuran-5,6-diol-3-one, 2-benzylidene-
21	17.69	235916	0.04	10069	2.34	73.15	1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetras
22	18.333	144314	0.02	69281	2.08	327.35	Borazine, 2,4,6-triphenyl-1,3,5-tripropyl-
23	19.494	112355	0.02	39590	2.84	73.1	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethyl
24	19.825	86026	0.01	43827	1.96	135.2	2-Pyrazinyl-4-methoxyphenylketone
25	24.644	5377198	0.81	62198	86.45	48.05	Taurine

Ethanol extract (ARSB-02):

In ethanol extract (ARSB-02) we identified 11 compounds, among that high level of compound Propane, 1,2-dimethoxy- found that contains 92.72%, followed by other compounds are in trace level, they are Diacetone Alcohol (4-hydroxy-4-methyl-2-pentanone),

Octamethylcyclotetrasiloxane, N-(Trifluoroacetyl)-N,O,O',O''-tetrakis(trimethylsilyl)norepinephrine, 6-Oxo-3-thiooctanoic acid, 2-(3-Bromo-but-3-enyl)-[1,3]dioxolane, and 2-Chloroaniline-5-sulfonic acid, Dodecamethyl cyclohexasiloxane (**Fig. 2, Table 2**)

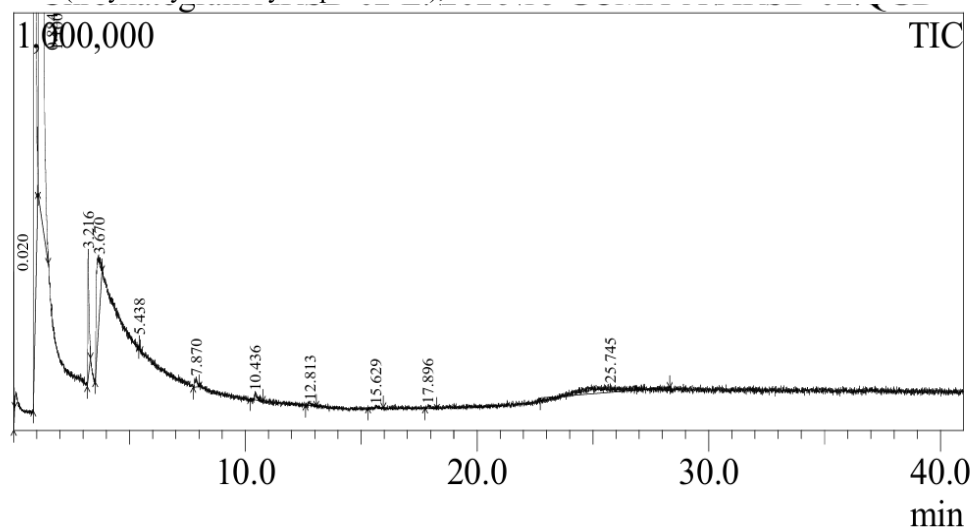


Figure 2. Compounds identification by GC/MS analysis of ethanol extract (ARSB-02) of *E. alba*

Table 2. List of compounds identified in GC-MS analysis in ethanol extract (ARSB-02) of *E. alba*

Peak	R.Time	Area	Area %	Height	A/H	Base m/z	Name
1	0.02	138026	0.04	358677	0.38	44.05	d-Alanine
2	1.1	302863165	92.72	103935124	2.91	39.05	Propane, 1,2-dimethoxy-
3	3.216	1043574	0.32	311266	3.35	43.05	2-Pentanone, 4-hydroxy-4-methyl-
4	3.67	2237478	0.69	172568	12.97	63.05	Dimethyl Sulfoxide
5	5.438	33038	0.01	32274	1.02	281.25	Cyclotetrasiloxane, octamethyl-
6	7.87	146895	0.04	24856	5.91	73.1	N-(Trifluoroacetyl)-N,O,O',O''-tetrakis(trimethylsilyl)no
7	10.436	108446	0.03	19947	5.44	73.1	Cyclohexasiloxane, dodecamethyl-
8	12.813	86954	0.03	11838	7.35	73.05	6-Oxo-3-thiooctanoic acid
9	15.629	-1835	0	7190	-0.25	73.1	N-(Trifluoroacetyl)-N,O,O',O''-tetrakis(trimethylsilyl)no
10	17.896	93365	0.03	9283	10.06	73.15	1,3-Dioxolane, 2-(3-bromo-3-buten-1-yl)-
11	25.745	1220471	0.37	21198	57.57	207.15	2-Chloroaniline-5-sulfonic acid

Acetonitrile Extract (ARSB-03):

In acetonitrile extract (ARSB-03) we identified 13 compounds, among that high level of compound Propane, 1,2-dimethoxy- found that contains 99.22%, followed by other compounds are in trace level, 2-Pentanone, 4-hydroxy-4-methyl-(diacetone alcohol), N-

(Trifluoroacetyl)-N,O,O',O''-tetrakis(trimethylsilyl)norepinephrine, Dodecamethylcyclohexasiloxane, 3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane, 1-Iodoundecane, 2-Heptyl-1,3-dioxolane, 1-Ethylpropyl methyl ether, 2-Phenyl-1-benzopyrylium, (**Fig. 3, Table 3**)

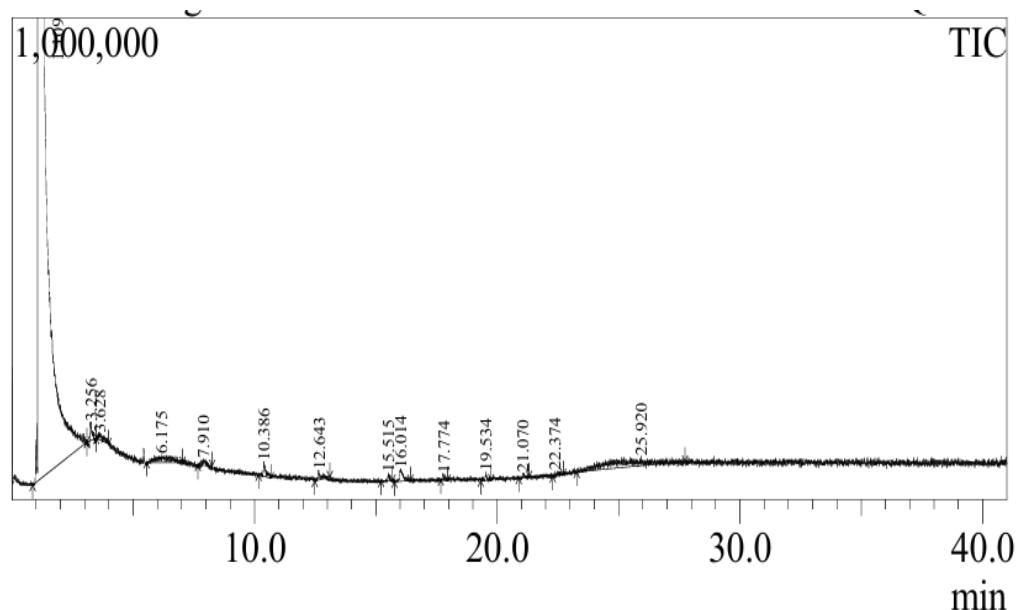


Figure 3. Compounds identification by GC/MS analysis of Acetonitrile extract (ARSB-03) of *E. alba*

Table 3. List of compounds identified in GC-MS analysis in acetonitrile extract (ARSB-03) of *E. alba*

Peak	R.Time	Area	Area%	Height	A/H	Base m/z	Name
1	1.109	409691392	99.22	106874680	3.83	39.05	Propane, 1,2-dimethoxy-
2	3.256	136347	0.03	38195	3.57	43.1	2-Pentanone, 4-hydroxy-4-methyl-
3	3.628	162913	0.04	13587	11.99	43.05	Acetic acid, 1,1-dimethylethyl ester
4	6.175	472768	0.11	16443	28.75	78.1	Dimethyl Sulfoxide
5	7.91	47944	0.01	13699	3.5	73.15	N-(Trifluoroacetyl)-N,O,O',O"-tetrakis(trimethylsilyl)no
6	10.386	217429	0.05	30999	7.01	73.1	Cyclohexasiloxane, dodecamethyl-
7	12.643	124395	0.03	20738	6	73.15	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimeth
8	15.515	48159	0.01	16730	2.88	73.1	N-(Trifluoroacetyl)-N,O,O',O"-tetrakis(trimethylsilyl)no
9	16.014	268548	0.07	26691	10.06	57.15	1-Iodoundecane
10	17.774	55289	0.01	13343	4.14	73.15	1,3-Dioxolane, 2-heptyl-
11	19.534	86870	0.02	18163	4.78	73.15	1,3-Dioxolane
12	21.07	16666	0	8958	1.86	73.15	1,3-Dioxolane
13	22.374	61377	0.01	10652	5.76	73.1	Pentane, 3-methoxy-
14	25.92	1511569	0.37	19451	77.71	207.2	1-Benzopyrylium, 2-phenyl-

Ethyl Acetate Extract (ARSB-04):

In the ethyl acetate extract (ARSB-04) 8 compounds are identified, among that maximum level of compound Propane, 1,2-dimethoxy- found that contains 92.72%, followed by other compounds are in trace level,

chemicals i.e., 3-Hexen-2-one (1-Butenyl methyl ketone), Diacetone alcohol, Octamethylcyclotetrasiloxane, N-(Trifluoroacetyl)-N,O,O',O"-tetrakis(trimethylsilyl)norepinephrine, Propanamide and 2-Chloroaniline-5-sulfonic acid were identified. (Fig. 4, Table 4)

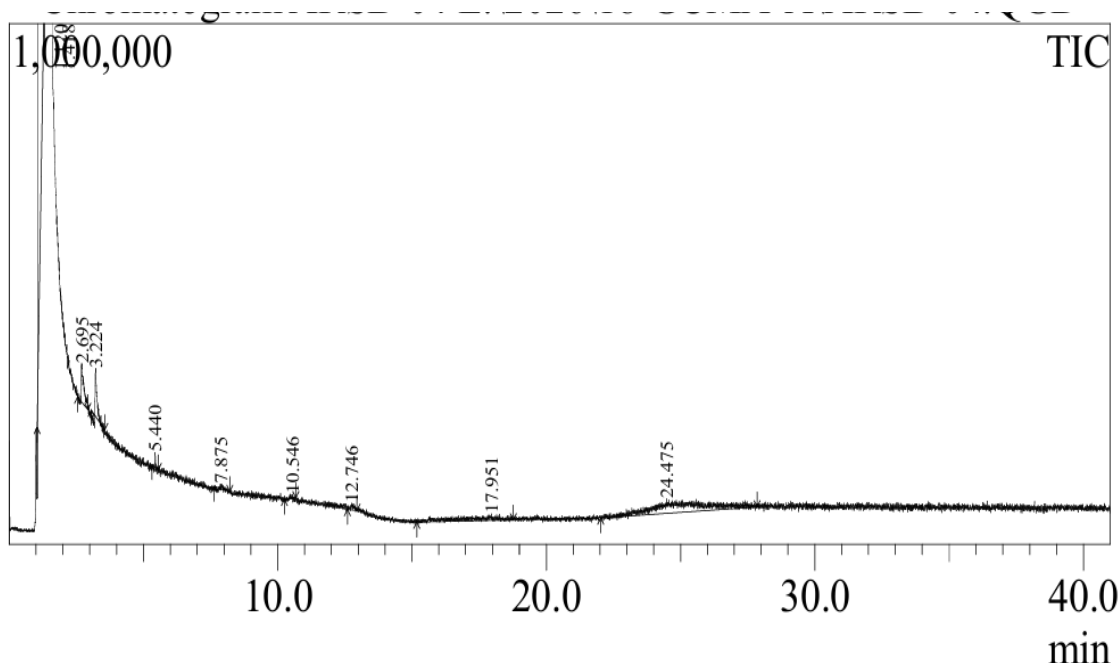


Figure 4. Compounds identification by GC/MS analysis of ethyl acetate extract (ARSB-04) of *E. alba*

Table 4. List of compounds identified in GC-MS analysis in ethyl acetate extract (ARSB-04) of *E. alba*

Pea	R.Time	Area	Area%	Height	A/H	Base m/z	Name
1	1.12	439441424	87.63	108656380	4.04	60.65	Propane, 1,2-dimethoxy-
2	2.695	471850	0.09	73085	6.46	55.1	3-Hexen-2-one
3	3.224	238953	0.05	92238	2.59	43.05	2-Pentanone, 4-hydroxy-4-methyl-
4	5.44	-5197	0	28718	-0.17	281.2	Cyclotetrasiloxane, octamethyl-
5	7.875	-14474	0	8897	-1.62	73.1	N-(Trifluoroacetyl)-N,O,O',O''-tetrakis(trimethylsilyl)no
6	10.546	-9471	0	8156	-1.15	341.3	1,3-Dioxolane
7	12.746	98445	0.02	12674	7.77	73.1	1,3-Dioxolane
8	17.951	751943	0.15	12731	59.06	44.05	Propanamide
9	24.475	2887869	0.58	28040	102.99	207.1	2-Chloroaniline-5-sulfonic acid

Acetone Extract (ARSB-05):

The acetone extract (ARSB-05) showed 15 compounds, among that chief level of compound Propane, 1,2-dimethoxy- found that contains 97.15%, followed by other compounds are in trace level, phytochemicals: 2-

Butynoic acid (tetrolic acid), 3-Penten-2-one, 4-methyl-(Isobutenyl methyl ketone), 2-Pentanone, Diacetone alcohol, 1-Pentene, 4,4-dimethyl-1,3-diphenyl-1-(trimethylsilyloxy)-, n-Propanesulphonylacetonitrile, 2,2'-Bi-1,3-dioxolane, Rs-2,3-hexanediol and 2-Chloroaniline-5-sulfonic acid. (**Fig. 5, Table 5**)

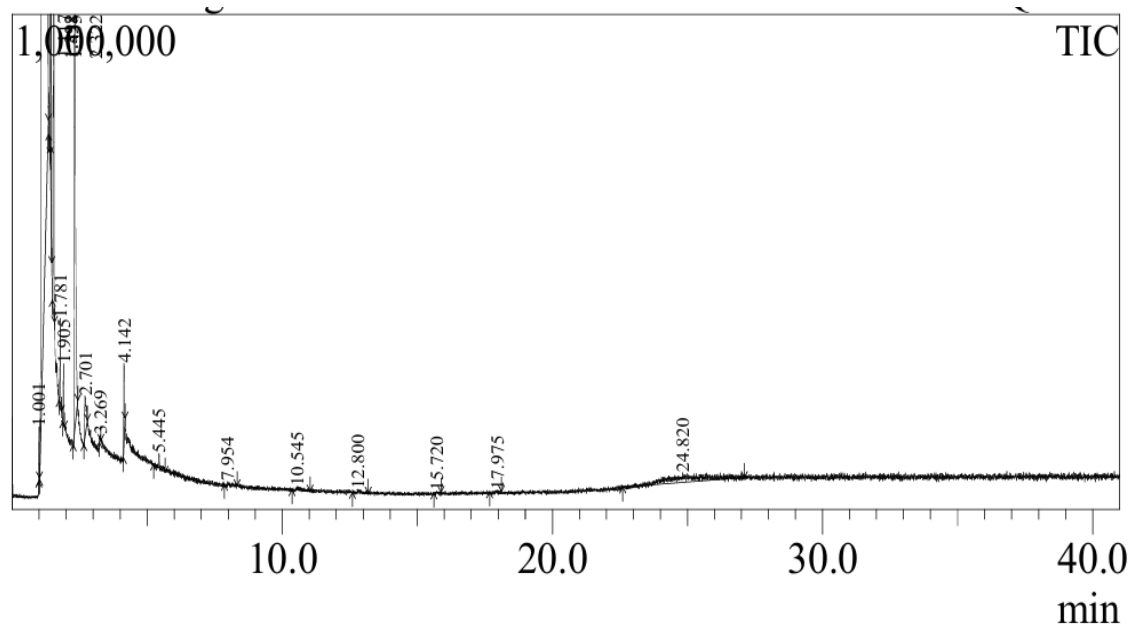


Figure 5. Compounds identification by GC/MS analysis of Acetone extract (ARSB-05) of *E. alba*

Table 5. List of compounds identified in GC-MS analysis in acetone extract (ARSB-05) of *E. alba*

Peak	R.Time	Area	Area%	Height	A/H	Base m/z	Name
1	1.001	65364	0.02	106413	0.61	44	2-Butynoic acid
2	1.117	3457543	97.15	104876496	3.3	59.7	Propane, 1,2-dimethoxy-
3	1.438	282989	0.08	373118	0.76	42.05	Furan, tetrahydro-
4	1.535	2063846	0.58	2083536	0.99	73.1	Propane, 2,2-dimethoxy-
5	1.781	246000	0.07	175597	1.4	63	Propane, 1,2-dichloro-
6	1.905	137893	0.04	122159	1.13	73.15	Silane, ethyltrimethyl-
7	2.322	496249	1.39	2670154	1.86	91.1	Toluene
8	2.701	277101	0.08	80377	3.45	55.1	3-Penten-2-one, 4-methyl-
9	3.269	26984	0.01	12603	2.14	43.05	2-Pentanone, 4-hydroxy-4-methyl-
10	4.142	313747	0.09	161880	1.94	43.05	2-Pentanone, 4-methoxy-4-methyl-
11	5.445	76679	0.02	29450	2.6	281.2	1-Pentene, 4,4-dimethyl-1,3-diphenyl-1-(trim
12	7.954	-3534	0	6589	-0.53	41.15	n-Propanesulphonylacetonitrile
13	10.545	51944	0.01	7592	6.84	73.05	2,2'-Bi-1,3-dioxolane
14	12.8	35681	0.01	7010	5.09	73.05	1,3-Dioxolane
15	17.975	-55036	-0.02	3116	-17.65	73.1	Rs-2,3-hexanediol
16	24.82	1246028	0.35	19831	62.83	207.1	2-Chloroaniline-5-sulfonic acid

Hexane Extract (ARSB-06):

In hexane extract (ARSB-06) 13 compounds identified, in that uppermost level of compound Propane, 1,2-dimethoxy- found that contains 99.26%, followed by other compounds are in trace level, phytochemicals identified: (+)-2-Aminoheptane, 2-Butynoic acid (Tetrolic acid), 1,2,4-Benzenetricarboxylic acid, 1,2-dimethyl ester, Dimethadione, 1-[2,4-

Bis(trimethylsiloxy)phenyl]-2-[(4-trimethylsiloxy)phenyl]propan-1-one, N-(Trifluoroacetyl)-N,O,O',O"-tetrakis(trimethylsilyl)norepinephrine, Dodecamethylcycl ohexasiloxane, Acetamide, N-methyl-(Methylacetamide), 3-Ethoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane and Arsenous acid, tris(trimethylsilyl) ester were identified. (Fig. 6, Table 6)

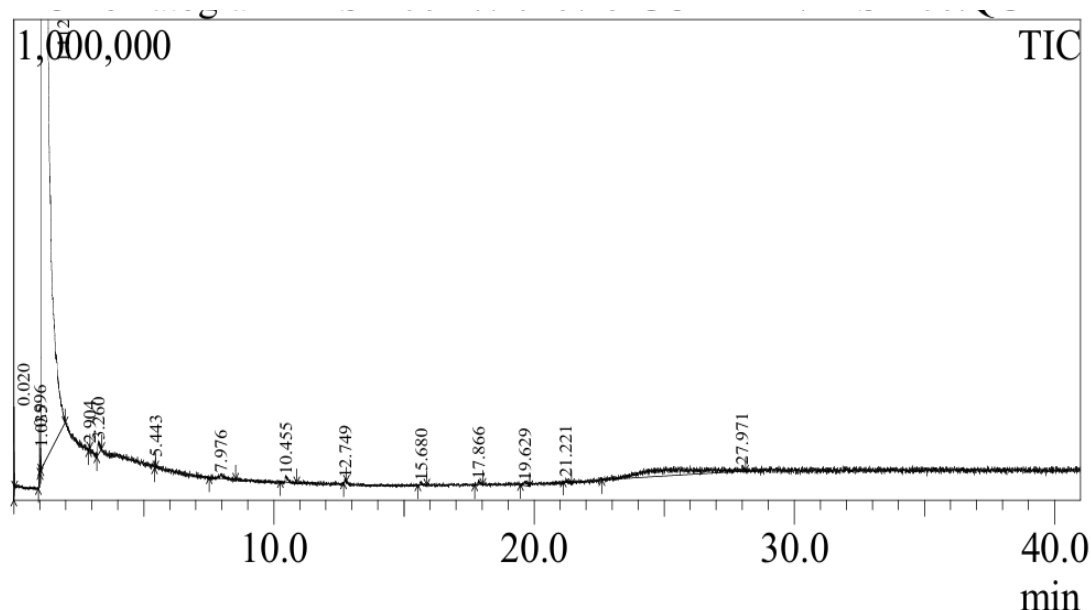


Figure 6. Compounds identification by GC/MS analysis of hexane extract (ARSB-06) of *E. alba*

Table 6. List of compounds identified in GC-MS analysis in hexane extract (ARSB-06) of *E. alba*

Peak	R.Time	Area	Area%	Height	A/H	Base m/z	Name
1	0.02	72324	0.02	185035	0.39	44	(+)-2-Aminoheptane
2	0.996	101774	0.03	102125	1	44	2-Butynoic acid
3	1.035	32200	0.01	48156	0.67	44.05	Acetaldehyde
4	1.112	3879019	99.26	1050832	3.69	57.75	Propane, 1,2-dimethoxy-
5	2.904	6542	0	11687	0.56	207.05	1,2,4-Benzenetricarboxylic acid, 1,2-dimethyl ester
6	3.26	132051	0.03	28423	4.65	43.05	Dimethadione
7	5.443	23269	0.01	18961	1.23	281.2	1-[2,4-Bis(trimethylsiloxy)phenyl]-2-[(4-trimethylsiloxy)phenyl]ethane
8	7.976	93847	0.02	10939	8.58	73.15	N-(Trifluoroacetyl)-N,O,O',O'-tetrakis(trimethylsilyl)no
9	10.455	65316	0.02	14744	4.43	73.05	Cyclohexasiloxane, dodecamethyl-
10	12.749	5601	0	7267	0.77	73.1	Acetamide, N-methyl-
11	15.68	19667	0.01	7020	2.8	73.1	1,3-Dioxolane
12	17.866	35280	0.01	9715	3.63	73.05	1,3-Dioxolane
13	19.629	89148	0.02	8988	9.92	73	1,3-Dioxolane
14	21.221	41513	0.01	9370	4.43	73.1	3-Ethoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsilyl)ethane
15	27.971	2192017	0.56	12002	182.64	207.1	Arsenous acid, tris(trimethylsilyl) ester

Antimicrobial Activity (MIC)

The antimicrobial activity of these extracts showed that these compounds are more active for their antibacterial activity (Table 7 & 8).

Antibacterial Activity

The antibacterial activity very important against human pathogenic bacteria, the Minimum inhibitory

concentration of bacterial activity observed that, the highest amount of pathogenic bacteria *S. aureus* killed by **ARSB-03** **ARSB-04** showed that 0.31 mg/mL, followed by **ARSB-02** showed that 0.625 mg/mL against same organism. That same time **ARSB-01** not showed any MIC against *B. subtilis* and *E. coli* (Table 7).

Table 7. Antibacterial activity (MIC values in mg/mL) of the plant extracts (ARSB-01-06)

S. No	List of extract samples	MIC values in mg/mL			
		<i>S. aureus</i>	<i>B. subtilis</i>	<i>E. coli</i>	<i>P. aeruginosa</i>
1	ARSB-01	2.5	NIL	NIL	1.25
2	ARSB-02	0.625	1.25	1.25	2.5
3	ARSB-03	0.3125	1.25	1.25	1.25
4	ARSB-04	0.3125	0.625	0.625	1.25
5	ARSB-05	1.25	1.25	1.25	1.25
6	ARSB-06	1.25	1.25	1.25	0.625
7	Ciprofloxacin	5 µg/mL	5 µg/mL	5 µg/mL	5 µg/mL

Antifungal activity:

The antifungal activity very important against human pathogenic fungi, the Minimum inhibitory concentration of fungal activity observed that, the highest amount of

pathogenic Fungi *C. albicans*, *A. niger* killed by ARSB-03 sample showed that 1.25 mg/mL, followed by other samples not showed any activity against selected fungi (Table 8).

Table 8. Antifungal activity (MIC values in mg/mL) of the plant extracts (ARSB-01-06)

S. No	List of extract samples	MIC mg/mL	
		<i>Candida albicans</i>	<i>Aspergillus niger</i>
1	ARSB-01	NIL	NIL
2	ARSB-02	NIL	NIL
3	ARSB-03	1.25	1.25
4	ARSB-04	NIL	NIL
5	ARSB-05	NIL	NIL
6	ARSB-06	NIL	NIL
7	Flucanazole	5 µg/ml	5 µg/ml

In silico studies

After getting the promising antibacterial activity, the *In-silico* studies were performed to show the interactions,

the *In Silico* studies the targeted two compounds (Comp 1 and Comp2) (**Fig. 7**) are selected from active acetonitrile (ARSB-03) and ethyl acetate extract (ARSB-04)

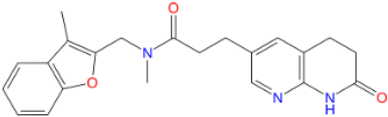
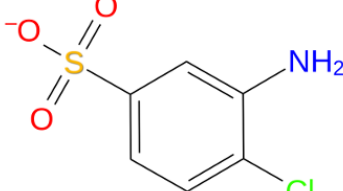
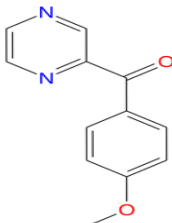
Crystal ligand	Comp 1 from Acetonitrile extract (ARSB-03)	Comp 2 from ethyl acetate Extract (ARSB-04)
		

Fig. 7. Structures of the active compound taken for *in silico* studies

The process of molecular docking included the following steps:

Preparation of Protein, Receptor grid generation, Ligand docking

Initially, the retrieved protein assembly was equipped through the Protein Preparation Wizard. The protein was imported and preprocessed by assigning appropriate bond orders and adding hydrogen atoms. Water molecules located more than 5 Å from the co-crystallized ligand were removed. The protein structure was subsequently optimized and minimized using the OPLS-2005 force field.

A receptor grid was then generated around the co-crystallized ligand using the Receptor Grid Generation tool to define the active binding site of the target protein. The centroid coordinates of the co-crystallized ligand (X = 110.57, Y = 68.04, and Z = 36.98) were used as the center of the grid, with an enclosing box size of 10 Å. Subsequently, the prepared compounds were docked into the defined vigorous site by the Glide Extra Precision (XP) flexible ligand docking protocol. The van der Waals radius grading factor was preserved at 0.8. The resulting docking scores and protein–ligand interactions were subsequently analysed to evaluate the obligatory empathy and interaction patterns of the selected compounds.

MM-GBSA

The binding free energies of the protein–ligand developments were projected by Prime MM-GBSA approach, this computational method is widely used to evaluate the binding affinity and stability of protein ligand developments through calculating the binding free energy (ΔG_{bind}). The Prime MM-GBSA module of the Schrödinger suite was employed for these calculations. The binding free energy was determined by considering three structural states: the free receptor, the free ligand, and the corresponding receptor–ligand complex. The resulting ΔG_{bind} values were subsequently used to measure the relative constancy and binding affinity of the docked protein–ligand complexes.

$$\Delta G(\text{bind}) = \Delta G(\text{solv}) + \Delta E(\text{MM}) + \Delta G(\text{SA})$$

where:

ΔG_{solv} (solvation free energy): This parameter represents the change in widespread born solvation energy based on the complex establishment and is considered as the transformation between the solvation energy of the protein ligand multifaceted and the combined solvation dynamisms of the unbound receptor and ligand. It includes contributions from both electrostatic and non-polar solvation components. ΔE_{MM} (molecular mechanics energy): This term represents the difference in molecular mechanics energy between the protein–ligand complex and the corresponding unbound receptor and ligand. It primarily includes van der Waals and electrostatic interaction energies. ΔG_{SA} (surface-area solvation energy): This component corresponds to the alteration in solvent-accessible surface area-dependent energy between the bound multifaceted and the separate unbound receptor and ligand. It primarily characterizes the non-polar involvement to the solvation free energy.

In addition, ligand strain energy was evaluated by comparing the energy of the ligand in its bound conformation with that of its corresponding unbound

state. This parameter accounts for the energetic penalty associated with conformational changes required for ligand binding. Incorporating ligand strain into the binding-energy analysis provides a more realistic estimation of the energetic contribution associated with complex formation and helps improve the interpretation of the calculated binding free energies.

Molecular Dynamics studies:

Molecular dynamics simulations were conducted by Desmond module of the Schrödinger Suite to assess the dynamic constancy and conformational behavior of the selected protein–ligand complexes. The best-scoring docked protein–ligand poses attained from the molecular docking analysis were used as the starting structures for the simulations. Individually complex was positioned in an orthorhombic simulation box with a 10 Å buffer and solvated using the TIP3P water model. Counterions were introduced to neutralize the system, followed by the addition of NaCl (0.15 M) to estimated functional ionic strength. Prior to the production run, the solvated systems were subjected to energy minimization to eliminate unfavorable steric contacts and subsequently equilibrated using the standard Desmond relaxation protocol. The systems were gradually heated to 300 K under the NVT ensemble and then equilibrated under NPT conditions at a pressure of 1 atm. Production simulations were performed for 100 ns under the NPT ensemble at 300 K and 1 atm using the Nosé–Hoover thermostat and Martyna–Tobias–Klein barostat. A 2 fs integration time step was employed, while long-range electrostatic interactions were treated using the Particle Mesh Ewald (PME) method with a 9.0 Å cutoff radius. Trajectory coordinates were recorded at regular intervals throughout the simulation for subsequent analysis. The stability and structural characteristics of the protein–ligand developments were estimated using root mean square deviation (RMSD), root mean square fluctuation (RMSF), hydrogen-bond analysis, and radius of gyration (R_g) calculations using the analysis tools implemented in the Schrödinger Suite.

Table 9. Docking scores and mMGBSA bind energy, interaction pattern of crystal ligand, comp1 and comp2

Compound code	Docking score	mMGBSA	Lig Strain energy	Interactions	
				Hydrogen Bond	Pi-Pi interaction
Crystal ligand	-12.59	-81.62	1.50	ALA97,Tyr157	TYR157
Comp 1	-6.031	-27.06	0.06		TYR147, TYR157, PHE204
Comp 2	-8.365	-55.10	0.47	TYR147	Tyr147, TYR157

The reference crystal ligand exhibited the strongest binding affinity, with a docking score of -12.590 and MM-GBSA value of -81.62 kcal/mol, stabilized by hydrogen bonding with ALA97 and π – π interactions with TYR157. **Comp 2** showed comparatively better binding among the test compounds, with a docking score of -8.365 and MM-GBSA energy of -55.10 kcal/mol,

forming both hydrogen bonding and π – π interactions with TYR147 and TYR157. **Comp 1** demonstrated weaker binding, with a docking score of -6.031 and MM-GBSA value of -27.06 kcal/mol, primarily stabilized through π – π interactions with TYR147, TYR157, and PHE204.

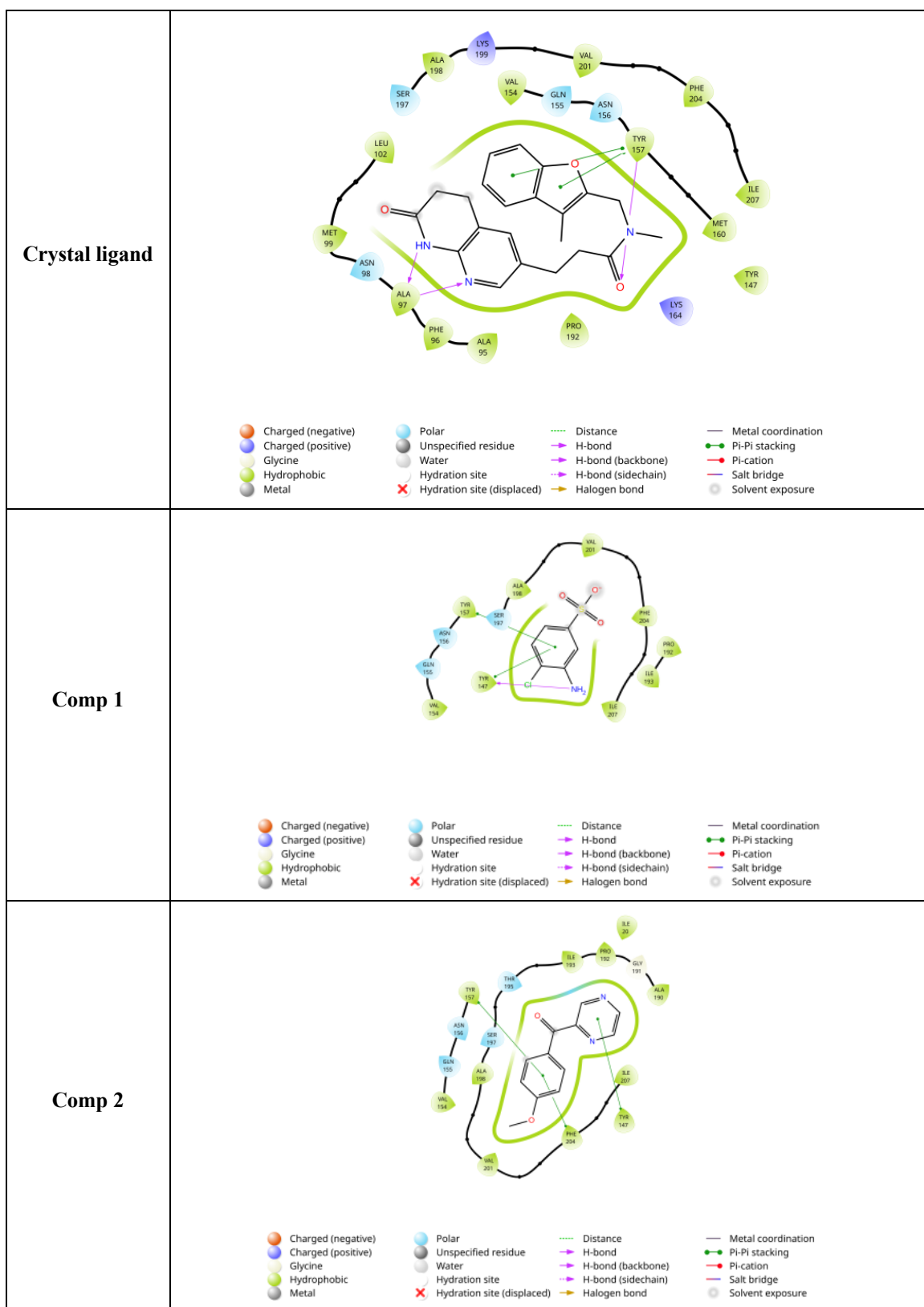


Fig. 8. 2D Ligand interaction diagram



Fig. 9. RMSD, Interaction profile of crystal ligand, comp1 and 2

The MD simulation results show that the crystal ligand maintains relatively stable binding throughout the trajectory, as indicated by consistent RMSD values and strong, persistent interactions, particularly with key residues such as TYR157. In comparison, Comp 2 exhibits comparable stability, with RMSD values stabilizing over time and maintaining meaningful interactions, including hydrogen bonding and hydrophobic contacts, suggesting a reasonably stable

complex. Comp1, however, shows greater fluctuations in RMSD, indicating comparatively lower structural stability during the simulation. The protein–ligand contact analysis further supports this observation, as the crystal ligand demonstrates a higher fraction of consistent interactions, especially hydrophobic and hydrogen bonds. Comp 2 shows moderate interaction persistence, while Comp 1 displays fewer and less stable contacts overall.

Table 10. ADME study results

Title	PSA	%Oral Absorption	QPP Caco	QPPM DCK	QPlog BB	QPlogH ERG	QPlogP o/w	SA SA	Accp tor	don or	MW
Crystal_1 igand	90.404	85.5	256.3	193.7	-1.18	-4.200	2.6	675	7	1	377.4
Comp 1	85.711	58.3	41.4	48.1	-0.96	-1.737	0.4	367	5	2	207.6
Comp 2	57.262	91.9	1683.2	868.5	-0.31	-4.764	1.2	445	5	0	214.2

PSA: Polar Surface Area
QPPCaco – Predicted Caco-2 cell permeability
QPPMDCK – Predicted MDCK cell permeability
QPlogBB – Predicted brain/blood partition coefficient (log BB)
QPlogHERG – Predicted HERG K⁺ channel inhibition (log IC₅₀)
QPlogPo/w – Predicted octanol/water partition coefficient (log P)
SASA – Solvent Accessible Surface Area
Acceptor – Number of hydrogen bond acceptors
Donor – Number of hydrogen bond donors
MW – Molecular Weight

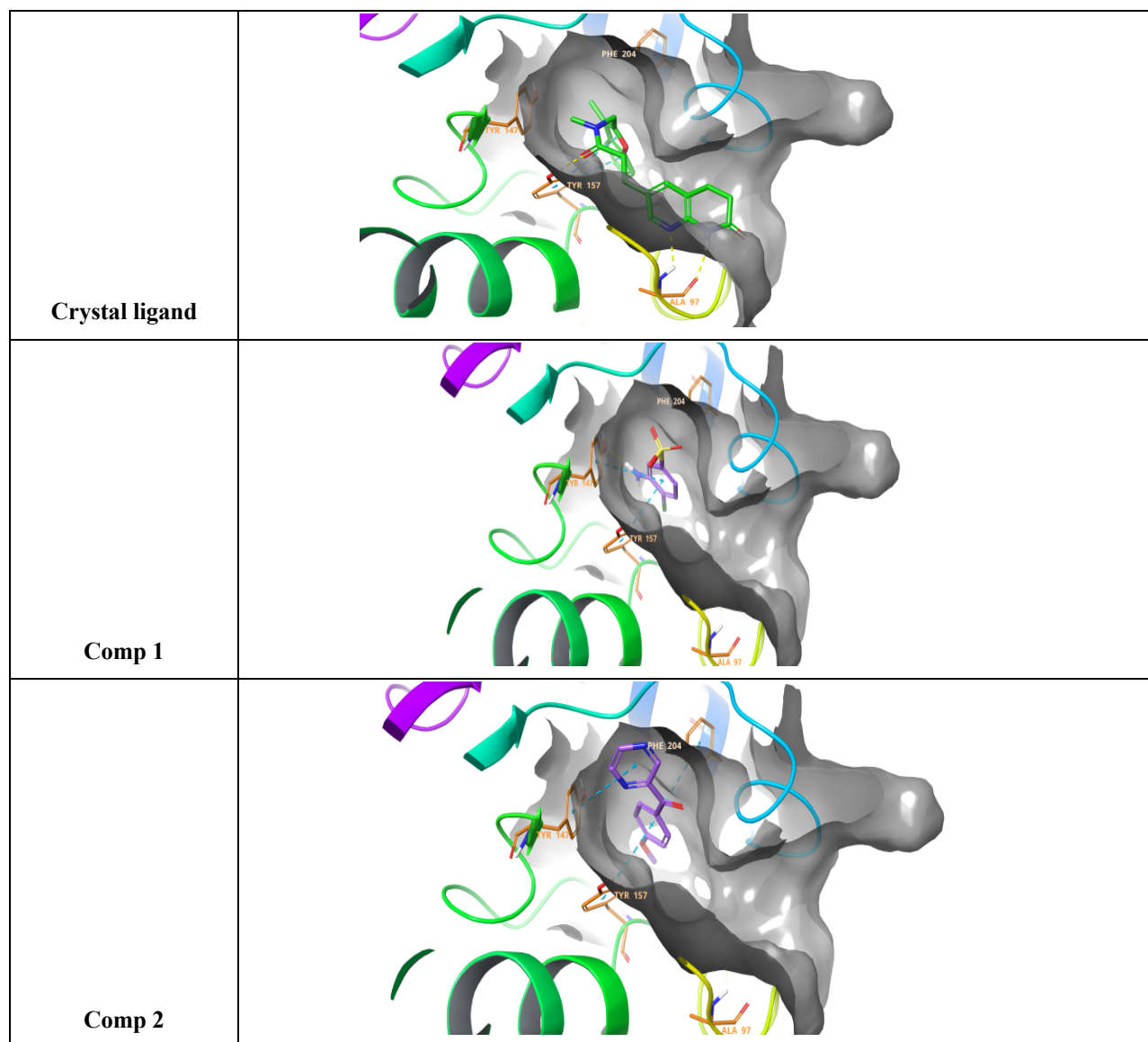


Fig. 10. 3D Surface diagram of the crystal ligand, comp1 and 2

DISCUSSION

The results of the GC–MS analysis showed that all six extracts differed significantly from each other by the number of identified peaks and their relative abundance. At the same time, interpreting the obtained data is complicated by the fact that in most cases, the largest peak corresponded to propane, 1,2-dimethoxy. For instance, this substance content varied from 49.58% in

the aqueous extract to over 99% in some other extracts. Additionally, cyclic siloxanes such as hexamethylcyclotrisiloxane, octamethylcyclotetrasiloxane and dodecamethylcyclohexasiloxane were detected in most of the analyzed samples. This finding can explain why similar major peaks were detected in different extracts since they are known to possess very high relative

abundances. Therefore, it is possible that propane, 1,2-dimethoxy- and other silicon-containing hydrocarbons did not come from *E. alba* but instead resulted from the GC-MS analysis, septa, solvents and other sources. The GC-MS Profiling of Leaves extract of *E. alba* Revealed the Existence of 17 Major Phytoconstituents are n-Undecane, Cyclohexasiloxane-Dodecamethyl, Methyl Ester, Nonahexacontanoic Acid, Phthalic Acid-Butyl Nonyl Ester, Palmitic acid, 2,4-Ditertbutylphenol, 1,2-Benzenedicarboxylic Acid-Butyl Octyl Ester, 2-Myristynoyl Pantetheine, Isobutyl Octadecyl Ester, Phthalic Acid (Sharma et al., 2022),

The antimicrobial potential of several phytoconstituents identified in *E. alba* has been well documented in previous studies. Bioactive compounds belonging to classes such as coumarins, flavonoids, phenolic compounds, alkaloids, terpenoids, tannins, and polyacetylenes have demonstrated broad-spectrum antimicrobial properties, exhibiting bacteriostatic, bactericidal, and fungicidal activities against diverse human pathogenic microorganisms (Thomas and Anandan, 2013). These findings suggest that the antimicrobial activity of *E. alba* may be attributed, at least in part, to the synergistic or individual effects of these phytochemical constituents (Motaleb et al., 2011). Although *E. alba* has demonstrated considerable therapeutic potential through traditional applications and empirical studies, further investigations using advanced molecular approaches and comprehensive physicochemical and analytical techniques are necessary. Such studies would provide deeper insights into its bioactive constituents, molecular mechanisms, and pharmacological properties, thereby strengthening the scientific evidence supporting its traditional and therapeutic applications (Gangil et al., 2025).

The antibacterial activity of the methanolic extract of *E. alba* was evaluated against a range of clinically relevant bacterial and fungal pathogens. The extract demonstrated concentration-dependent antibacterial activity against selected bacterial strains. Notably, *Pseudomonas aeruginosa* (sensitive) exhibited inhibition zones of 26 and 27 mm at 100 and 200 mg/mL, respectively, while *Staphylococcus aureus* (MRSA) showed inhibition zones of 23 and 24 mm at the corresponding concentrations (Sharma et al., 2022). Another sensitive strain of *P. aeruginosa* showed comparatively higher inhibition, with zones of 29 and 32 mm at 100 and 200 mg/mL, respectively. In contrast, the methanolic extract showed no detectable inhibitory effect against sensitive and ESBL-producing *Escherichia coli*, *Klebsiella pneumoniae*, resistant *P. aeruginosa*, *Candida albicans*, *Aspergillus fumigatus*. Overall, these findings indicate that the antibacterial efficacy of *E. alba* methanolic extract is pathogen-specific and may vary according to the susceptibility profile of the tested microorganisms (Sharma et al., 2022).

the observed biological activity of the methanolic leaf extract of *E. alba*, molecular docking analysis demonstrated that its phytoconstituents could interact strongly with the NOX and NOS enzymes of *Oreochromis mossambicus*. For comparison, levamisole exhibited binding affinities corresponding to dissociation constants (K_i) of 11.11 μ M for NOX and 37.8 μ M for NOS. In the present study, the K_i values predicted for the *E. alba* phytoconstituents were within the nanomolar-to-micromolar range, indicating favorable and relatively strong ligand-target interactions at low concentrations. These computational findings provide additional support for the observed in vivo responses and suggest that the identified phytoconstituents may contribute to the enhancement of the reactive nitrogen intermediate (RNI)-mediated response in *O. mossambicus* (Christyapita et al., 2025). The molecular docking results provide further insight into the potential molecular mechanisms underlying the biological activity of *E. alba*. Wedelolactone exhibited favorable interactions with both β -catenin and the VEGF receptor, with binding energies of -8.1 and -7.9 kcal/mol, respectively (Gangil et al., 2025).

CONCLUSION

The present study we carried out the GC-MS profiling, *in vitro* antimicrobial activity in different human pathogenic microbes and *In silico* (protein interaction, RMSD), we selected the 6 extracts i.e., aqueous (ARSB-01), ethanol (ARSB-02), acetonitrile (ARSB-03), ethyl acetate (ARSB-04), acetone (ARSB-05) and hexane (ARSB-06) were obtained and subjected for GCMS profiling. GCMS results showed that Propane, 1,2-dimethoxy- all extracts in high level. Acetonitrile extract (ARSB-03) and Ethyl Acetate Extract (ARSB-04) were taken on for further details, crystal ligand, comp 1 and 2, antibacterial studies, we concluded that further next level of research will emerge as potential herbal medicine to fight against the bacterial infections will give a solution for the Antimicrobial Resistant (AMR).

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Conflict of Interest:

The authors declare that don't have any conflict of interest.

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