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Antibacterial and Molecular Docking Studies of Secondary Metabolites of *Claviceps purpurea* infected to Bajra *(Pennisetum glaucum)* Crop

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ABSTRACT: *Claviceps purpurea* a plant pathogenic fungus, this fungal extract contains number of therapeutic compounds, these compounds shows the significant pharmacological values. For evaluation of phytochemical analysis and antibacterial activity, first, to preparation of culture filtrate of *Claviceps purpur*ea on the potato dextrose broth. After collection of filtrate then add ethyl acetate solvent to the separating funnel for solvent extraction method. Dried ethyl acetate extract was subjected to HR-LCMS analysis, antibacterial screening was carried out against tested bacterial strains. Molecular docking study of HR-LCMS, identified compounds were performed by docking with bacterial enzyme DNA gyrase. HR-LCMS analysis of extract of *Claviceps purpurea* showed compounds are Aldicarb, Arecoline, Glimepiride, Gedunin and Pentobarbital are the major constituents. The antibacterial screening of ethyl acetate extract against bacterial strains showed significant bactericidal activity, *Pseudomonas aeruginosa* (16.80±0.15mm), As compared to the standard drug ciprofloxacin (39.4±0.2). The molecular docking of gedunin against the bacterial enzyme DNA gyrase exhibited decent inhibitor as compared to other 4 compounds. Finally, this study reveals that the ethyl acetate extract of *Claviceps purpurea* showed significant pharmacological activities.

Keywords*: Claviceps purpurea*, Antibacterial, ADMET, DNA Gyrase, Molecular docking.

INTRODUCTION

Ergot is a fungal disease caused by fungus of the genus *Claviceps*. Species in this genus are unique in that they only infect ovaries of the host plants, no other part of the plant is infected. There are approximately 40 species of *Claviceps* with *C. purpurea* (Fries) Tulasne being the species of greatest concern (Schumann and Uppala 2000).

Ergot alkaloids, named after the ergot fungus *Claviceps purpurea*, can infect grains and cause epidemics, especially during the Middle Ages (Gerhards *et al*., 2014).

Ergot *Claviceps purpurea* (Fries) Tulasne is of critical economic importance because it is a producer of many biologically active compounds (alkaloids) for the pharmaceutical industry, a unique model of the parasite-host system, and a mycotoxin-associated pathogen that causes significant economic damage to agriculture around the world (Volnin *et al*., 2024).

Ergot alkaloids show strong interactions with serotonin, dopamine and adrenergic receptors of the central nervous system and also with adrenergic receptors in blood vessels. Therefore, they can act as potent drugs. Examples with pharmaceutical applications are, methylergometrine used in gynecology to stop bleeding after childbirth, ergotamine used to treat vascular migraine headaches, Parkinson's disease (Paul and Schiff 2006).

Several studies point to the various activities of phytochemicals, antioxidant, cardioprotective, hepatoprotective, which are: antimicrobial, anti-inflammatory, analgesic, anti-hemorrhagic, antitussive, antitumor, immunostimulating, anticancer, antiviral, among other. Among these, some studies attribute considerable antimicrobial activity to phytochemicals commonly found in plants and microorganisms (Dantas *et al*., 2015).

Fungi provide a plentiful and diverse source of unique and often bioactive metabolites, and they have produced a number of medicinally important compounds, including penicillin, mevinolin, fingolimod, and caspofungin (VanderMolen *et al*., 2013).

Over the past decade, much attention has been placed on the study of phytochemicals for their antibacterial activity, especially against multidrug-resistant Gram-negative and Gram-positive bacteria. Antibiotic resistance, a major global health concern, is a result of the emergence of multidrug-resistant bacteria. This has led to the need for new, effective antibacterial agents to combat the problem. However, the process of

discovering new antibiotics is costly and time-consuming, taking approximately ten years to bring a new antibiotic to market (Borges *et al*., 2015).

The process of finding new antibiotic drugs heavily relies on the *in silico* prediction of ADMET characteristics. These days, molecules with poor absorption, distribution, metabolism, and elimination (ADME) characteristics are removed from the drug development pipeline early on in the process, which significantly reduces research and development expenditures. Many people employ Lipinski's "Rule of Five" as a filter for qualities similar to drugs (Lajiness *et al*., 2004). Molecular docking is a commonly used method for evaluating the complex formation of small ligands with large biomolecules (Rudnitskaya *et al*., 2010). Insight of the above, the present study was undertaken to isolate and characterize antibacterial compounds from the *in vitro* derived ethyl acetate extract of *Claviceps purpurea* fungus and to verify the antibacterial property against pathogenic bacterial isolates (Shiva *et al*., 2018).

MATERIALS AND METHODS

Preparation of fungal Extract. Prepare potato dextrose broth, then autoclaved at 121 ℃ and 15lbs pressure. After sterilization, a loopful of fungal inoculum was inoculated into the broth and incubated in rotary shaker at 28ºC for 3-4 days. After incubation, using Whatmann filter paper 1 for separation of filtrate. Using separating funnel, the culture filtrate was exposed to solvent extraction with ethyl acetate. Three repetitions of the experiment were conducted again. In a desiccator, the compound was allowed to air dry.

Preliminary phytochemical screening. Using the conventional techniques outlined by (Harborne, 2005), a preliminary phytochemical study of the fungal extract of *Claviceps purpurea* was performed to see whether any desirable secondary metabolites were present.

HR-LCMS analysis of fungal extract. The bioactive components of ethyl acetate extract from *Claviceps purpurea* fungus were analyzed using a High-Resolution Liquid Chromatograph Mass Spectrometer (HR-LCMS) G6550A system. The method used was 30 mins ± ESI 10032014_MSMS.m, and the gas temperature was 250°C. The compounds were identified by comparing their retention time and mass with a stored metlin library from IIT, Bombay (Shivakumar *et al.,* 2018).

Antibacterial activity - Agar well diffusion assay. The study tested the antibacterial activity of aqueous and solvent extracts using an agar well diffusion method. The bacterial culture was spread on nutrient agar plates, and the extract was dissolved in DMSO at different concentrations. Wells were made on the plates, and 20 µl of each concentration of fungal extract was introduced. A positive control was ciprofloxacin (20 µg/ml). The plates were incubated for 24 hours at 37°C. The antibacterial activity was evaluated by measuring the growth inhibition zone for the test organisms compared to the control. The activity index was calculated to compare the zone of inhibition with the standard antibiotic (Pradeepa *et al*., 2014).

Minimum Inhibitory Concentration (MIC). The study confirmed antibacterial activity by determining the minimum inhibitory concentration (MIC) using microdilution method with resazurin. Bacterial suspensions were prepared using the direct colony method, with initial suspensions containing 10^6 CFU/ml. A twofold serial dilution of ethyl acetate fungal extract was made in Mueller-Hinton broth, and a final concentration of 5 x 10^6 CFU/ml was added to each well. Resazurin solution was added to each well to display microbial growth. The inoculated plates were incubated at 37°C for 24 hours. The MIC was defined as the lowest concentration that prevented resazurin color change from blue to pink. ANOVA was performed using ezANOVA software and Microsoft excels to determine the mean and standard error (Nikolic *et al*., 2014).

Molecular docking studies. The Lipinski "Rule of five" is used to filter drug-like properties, and *in silico* pharmacokinetic properties and ADME (absorption, distribution, metabolism, and elimination) and toxicity analysis were predicted using Data Warrior. The chemical structure of identified compounds, Aldicarb, Arecoline, Glimepiride, Gedunin, and Pentobarbital, and the standard Drug ciprofloxacin, were drawn using Chem Bio Draw tool. The energy of each molecule was minimized using ChemBio3D, and the energy minimized ligand molecules were input for AutoDock Vina for docking simulations. The protein data bank coordinate file was used as the receptor molecule, and the docking algorithm was used to search for the best-docked conformation between ligand and protein (Reece and Maxwell 1991; Bax *et al*., 2010; Trott and Olson 2010; Laskowski and Swindells 2011).

RESULTS AND DISCUSSIONS

Preparation of ethyl acetate extract. *Claviceps purpurea* filtrate was placed in separating funnel then add ethyl acetate solvent shake it for mixed thoroughly, then allowed for few minutes the secondary metabolites are settled in top layer, easily remove and collect the top layer and allowed for solidification (Fig. 1).

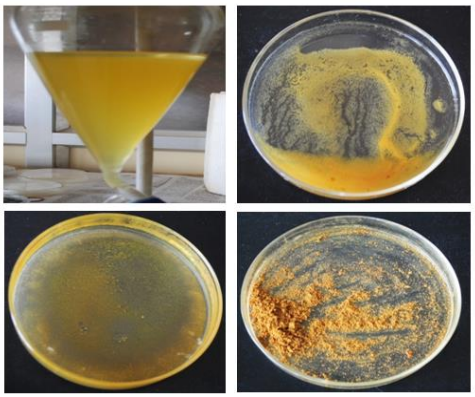

Fig. 1. Preparation of ethyl acetate extract of *Claviceps purpurea.*

Preliminary Phytochemical analysis. The preliminary phytochemical analysis of ethyl acetate extract of *Claviceps purpurea* showed a positive result for alkaloids, tannins, steroids, glycosides and terpenoids. The results are presented in Table 1 and Fig. 2.

Table 1: Preliminary phytochemical analysis of ethyl acetate extracts of *C. purpurea.*

Sr. No.	Phytochemical Test	Results
1.	Alkaloids	Present
2.	Tannins	Present
3.	Steroids	Present
4.	Glycosides	Present
5.	Terpenoids	Present

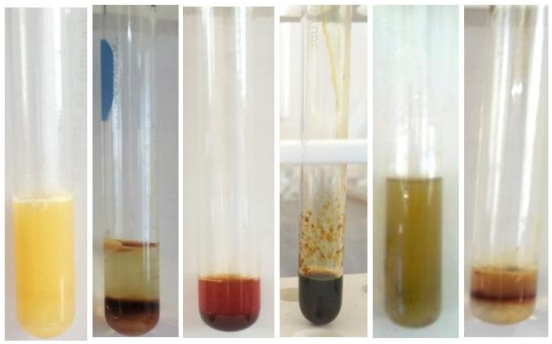

Fig. 2. Control Alkaloids Terpenoids Steroids Tannins Glycosides.

In earlier Nandan Patel and Krishnappa (2017), studied, the Preliminary biochemicals screening from crude extract of Xylaria. carpophila fungus showed presence of alkaloids, tannins, flavonoids, sterols, glycosides, terpinoids and phenols.

HR-LCMS analysis. The results of HR-LCMS analysis of *Claviceps purpurea* extract resulted in the presence of some of the compounds (Table 2) and the chromatogram of the phytoconstituents is shown in Fig. 3. Among them, the compounds Aldicarb, Arecoline, Glimepiride, Gedunin and Pentobarbital are known for antibacterial properties *Claviceps purpurea* fungal secondary metabolites are very useful to drugs and can be directly extracted from the liquid broth using ethyl acetate as a solvent. In the present study, HR-LCMS analysis showed the presence of various compounds. Among them the compounds Aldicarb, Arecoline, Glimepiride, Gedunin and Pentobarbital are reported as worthy antibacterial agents (Cheloufi *et al*., 2014).

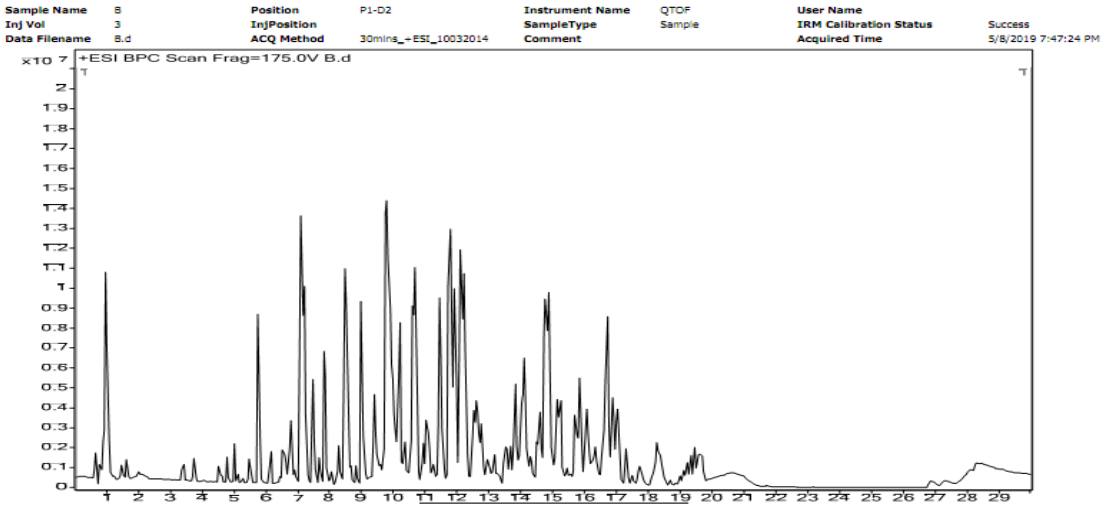

Fig. 3. HR-LCMS Chromatograph of Ethyl acetate extract of *Claviceps purpurea*.

Table 2: Molecular docking values of ethyl acetate extract of *Claviceps purpurea* fungal compounds obtained from LCMS analysis.

Compound Label	RT	Mass	Formula	DBDiff (ppm)	Hits
Cpd1:AREC0LINE	1.1	155.0974	C8H13N02	-17.98	3
Cpd2:6-Methylmercaptopurine	5.709	166.0335	C6H6N4S	-13.4	1
Cpd3:aldicarb	5.799	190.0766	C7H14N202S	5.09	1
Cpd4:5.811	5.811				
Cpd5:d-Camphorsulfonate	6.204	232.0767	C10H1604S	0.85	7
Cpd6:DIMETHYLCAFFEIC ACID	6.634	208.0761	C11H1204	-12.34	4
Cpd7:bisdeallyalmitrine	6.679	397.1819	C20H21F2N7	1.79	3
Cpd8:L-4-Hydroxy-3-methoxy-a-methylphenylalanine	6.832	225.1041	C11H15N04	-17.72	4
Cpd11:Digitoxigeninmonodigitoxoside	7.565	504.3031	C29H4407	11.17	1
Cpd13:8.387	8.387				
Cpd14:ANDR0STA-1,4-DIEN 3,17-DI0NE	8.388	284.1797	C19H2402	-7.15	2
Cpd16:GAMB0GICACID	8.501	628.2903	C38H4408	21.25	1
Cpd20:Ubiquinone	9.468	250.1237	C14H1804	-12.91	8

Cpd21:4-Ketoretinoicacid Glucuronide	9.617	488.2203	C26H3409	4096.45	2
Cpd22:8-HYDR0XYCARAPINICACID	9.773	470.2048	C26H3008	-22.9	2
Cpd23:9.808	9.808				
Cpd24:9.858	9.858				
Cpd25:MDL74156 Glucuronide	9.968	488.2154	C25H32N208	0.98	10
Cpd26:2-Hydroxyimipramine Glucuronide	9.99	472.221	C25H32N207	-0.21	7
Cpd27:4-Ketoretinoicacid Glucuronide	9.99	490.2315	C26H3409	-22.84	2
Cpd28:9.995	9.995				
Cpd29:Pentobarbital	10.125	226.1267	C11H18N203	22.15	3
Cpd31:Ubiquinone	10.22	250.1245	C14H1804	-16.1	6
Cpd32:C0NVALLAT0XIN	10.279	550.2706	C29H42010	13.12	1
Cpd33:2-Hydroxyimipramine Glucuronide	10.341	472.2202	C25H32N207	1.61	4
Cpd34:10.564	10.564				
Cpd35:10.565	10.565				
Cpd36:10.567	10.567				
Cpd37:10.638	10.638				
Cpd38:10.662	10.662				
Cpd39:10.907	10.907				
Cpd40:10.954	10.954				
Cpd41:11.000	11				
Cpd42:11.233	11.233				
Cpd43:11.328	11.328				
Cpd44:2- Hydroxydesmethylimipramine	11.335	458.2045	C24H30N207	1.75	1
Cpd45:11.378	11.378				
Cpd46:11.515	11.515				
Cpd47:11.605	11.605				
Cpd48:11.694	11.694				
Cpd49:Neu5Acalpha2-6Galbeta1-4Glcbeta-Sp	11.845	701.2414	C25H42N4019	1430.26	4
Cpd50:11.893	11.893				
Cpd51:11.909	11.909				
Cpd52:11.988	11.988				
Cpd53:11.988	11.988				
Cpd54:12.082	12.082				
Cpd55:12.139	12.139				
Cpd56:12.282	12.282				
Cpd57:12.384	12.384				
Cpd58:12.408	12.408				
Cpd59:12.479	12.479				
Cpd60:3beta,7beta-Dihydroxy-12-oxo-5beta-cholan-24-oicAcid	12.528	406.2802	C24H3805	-20.38	10
Cpd61:o-Hydroxyfinasteride	12.577	388.2691	C23H36N203	8.88	10

Antibacterial activity - Agar well diffusion assay. The antibacterial activity of *Claviceps purpurea* fungal extract was evaluated at the concentrations of 25, 50, 75 and 100 µg/m1 of DMSO and using different tested bacterial strains. In this test 100 µg/m1 concentrations showed significant antibacterial property against bacterial pathogenic strains like *Pseudomonas aeruginosa* (16.80±0.15), *Escherichia coli* (14.13±0.41), *Staphylococcus aureus* (13.37±0.27), *Salmonella typhi* (12.27±0.15), and *Xanthomonas compestris* (16.47±0.20), as compared to the standard drug ciprofloxacin.

In earlier studies *S. aureus* bacteremia is a significant cause of morbidity and mortality in neutropenic patients with cancer (Gonzalez *et al*., 2001). In our study, the metabolites of *Claviceps purpurea* exhibited significant inhibitory effect on both gram-positive *Staphylococcus aureus*, and gram-negative *Salmonella typhi*, *Escherichia coli*, *Xanthomonas compestris* and *Pseudomonas aeruginosa* strains which causes different disease symptoms. Previous studies of, The actinomycete isolate *Streptomyces* sp. VITBT7 was screened for antifungal and antibacterial activity on Sabaurauds Dextrose Agar (SDA) and Muller Hinton Agar (MHA) respectively. The cell free supernatant of the isolate exhibited antimicrobial activity against both Gram negative and Gram positive bacterial pathogens. The cell free supernatant also showed bactericidal activity with the inhibition zone of 37 mm against *P. aeruginosa*, 25 mm against *K. pneumonia* (Subashini and Kannabiran 2013).

Minimum Inhibitory Concentration (MIC). The MIC assay was performed by modified resazurin assay, the extract showed the highest inhibitory activity against *Escherichia coli* with a significant MIC value of $2.09\pm0.15\times10^{-2.}$ Inhibitions of bacterial strains are summarized in Table 3.

Table 3: Zone of inhibition and MIC values of ethyl acetate extract against tested bacterial strains.

Sr. No.	Inhibition zone diameter (mm) and MIC (mg/ml-1)					
	Microorganisms	ZI of Fungal extract (100 mg/well)	Activity index	MIC	ZI of Ciprofloxacin (20 µg/well)	MIC
1	*Escherichia coli*	14.13±0.41	0.443	$2.09\pm0.15\times10^{-2}$	31.83±0.33	$3.94\pm0.10\times10^{-3}$
2	*Pseudomonas aeruginosa*	16.80±0.15	0.431	$3.72\pm0.10\times10^{-2}$	38.93±0.18	$4.2\pm0.25\times10^{-3}$
3	*Salmonella typhi*	12.27±0.15	0.334	$2.63\pm0.10\times10^{-2}$	36.73±0.23	$5.13\pm0.10\times10^{-3}$
4	*Staphylococcus aureus*	13.37±0.27	0.333	$2.94\pm0.01\times10^{-2}$	40.10±0.06	$3.23\pm0.50\times10^{-3}$
5	*Xanthomonas compestris*	16.47±0.20	0.442	$5.30\pm0.15\times10^{-2}$	37.23±0.15	$3.08\pm0.30\times10^{-3}$

Molecular docking studies

Toxicity prediction. Aldicarb, Arecoline, Glimepiride, Gedunin and Pentobarbital these five compounds showed pharmacokinetic properties and toxicity analysis properties identified by HR-LCMS as shown in Table 4. All the 5 compounds obey the Lipinski's 'Rule of 5 limits better LogS values and were free from mutagenic tumorigenic, reproductive and irritant effect. In general, a poor solubility is associated with bad absorption and the aqueous solubility (Log S) of the compound which significantly affects its absorption and distribution characteristics. Based on the results from the Data Warrior, LogP, better LogS, and good drug score and less toxicity risk parameters are predicted as shown in the Table 4.

Table 4: *In silico* ADMET and drug-likeness prediction using data warrior.

Sr. No.	Compound	CLogP	CLogS	H-Acceptor	H-Donors	TPSA	Ligand Efficiency	Drug likeness
1	Aldicarb	1.389	-2.285	4	1	75.99	0.230	-2.375
2	Pentobarbital	1.296	-2.587	5	2	75.27	0.456	8.277
3	Glimepiride	3.518	-4.409	9	3	133.06	0.220	9.657
4	Gedunin	2.883	-4.768	7	0	95.34	0.0752	-1.153
5	Arecoline	0.313	-0.262	3	0	29.54	0.704	3.097

In association with *in vitro* antimicrobial activity, it is useful to carry out *in silico* studies to predict the orientation and binding affinity at the active site of the receptor. The molecular docking of HR-LCMS identified ligand molecules are Aldicarb, Arecoline, Glimepiride, Gedunin and Pentobarbital. Among them, the compound gedunin exhibited better docking efficiency with DNA Gyrase. It forms three hydrogen bonds with amino acids His 1081, Gly 459 and Gly 458 in the active site of the target protein with bond length 2.94, 2.98 and 3.29 Å respectively, with the least binding affinity -6.3 and hence is considered as the best dock conformation (Table 5).

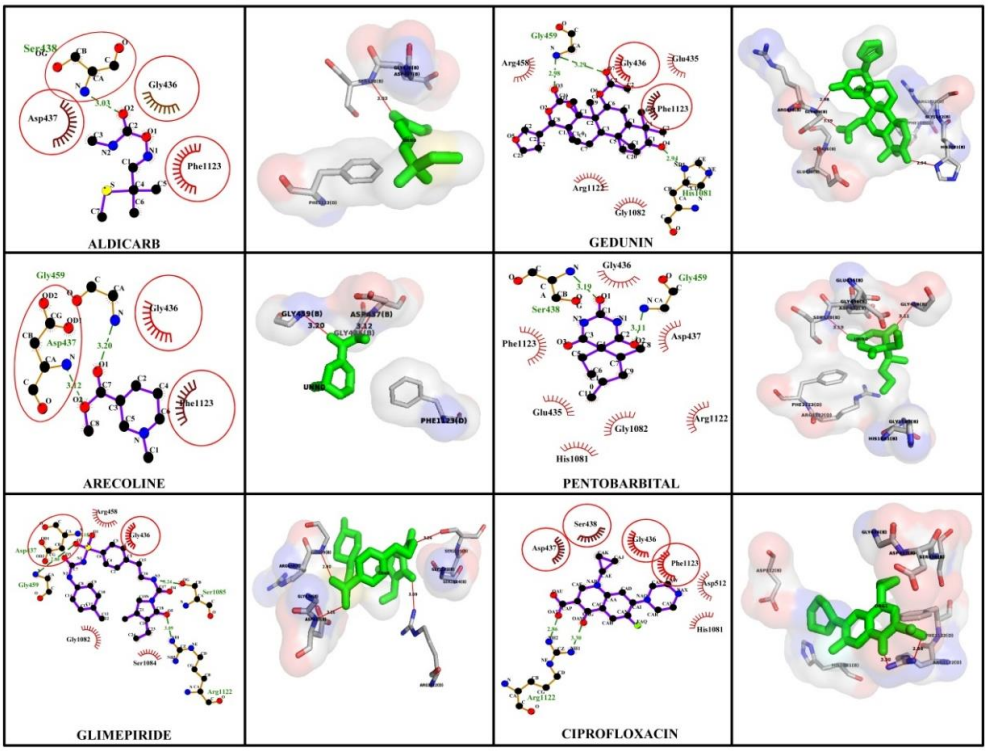

Fig. 4. 2D and 3D protein-ligand interaction DNA gyrase with the ligands aldicarb, gedunin, arecoline, pentobarbital and glimepiride.

Compound aldicarb forms one hydrogen bond with Ser438 amino acid with bond length of 3.03 Å. The compound arecoline forms two hydrogen bonds with the amino acids Asp437 with bond lengths 3.12 and 3.20Å and the compound Glimepiride forms three hydrogen bonding with Gly459, Arg1122 and: Ser1085 with bond length 2.80, 3.09 and3.24 Å respectively. The last compound pentobarbital forms two hydrogen bonds with amino acids Gly459 and Ser438 with bond length 3.11 and 3.19 Å respectively in this active pocket. However, all these docked molecules exhibited more hydrophobic interaction than the standard drug ciprofloxacin. The RMSD has often been used to measure the quality of reproduction of a known binding pose by molecules with ligands. All docked molecules have zero RMSD values as shown in the Table 5, Fig. 4.

Table 5: Molecular docking values of ethyl acetate extract of *Claviceps purpurea* fungal compounds obtained from LCMS analysis.

LIGAND	AFFINITY (kcal/mol)	H-BONDS	H-BOND LENGTH (Å)	H-BOND WITH	HYDROPHOBIC INTERACTIONS
Aldicarb	-3.6	1	3.03	2XCT:Ser438::1:O2	Gly436, Asp437, phe1223
Arecoline	-3.2	2	3.12	2XCT:Asp437::2:O2	Gly436, Phe1123
			3.20	2XCT:Asp437::2:O1	
Glimepiride	-5.2	3	2.80	2XCT:Gly459::3:O2	Gly436, Asp437, Arg458, Gly1082, Ser1084
			3.09	2XCT:Arg1122::3:O5	
			3.24	2XCT:Ser1085::3:N3	
Gedunin	-6.3	3	2.94	2XCT:His1081::4:O4	Glu435, Gly436, Arg458, Gly1082, Arg1122, Phe1123
			2.98	2XCT:Gly459::4:O3	
			3.29	2XCT:Gly458::4:O7	
Pentobarbital	-4.3	2	3.11	2XCT:Gly459::5:O2	Gly436, Glu435, Asp437, His1081, Gly1082, Arg1122, Phe1123
			3.19	2XCT:Ser438::5:O1	
Ciprofloxacin	-6.0	2	2.86	2XCT:Arg1122::CIP:OAT	Gly436, Asp437, Ser438, Asp512, His1081, Phe1123
			3.30	2XCT:Arg1122::CIP:OAM	

Aldicarb, Arecoline, Glimepiride, Gedunin and Pentobarbital compounds were present in *Claviceps purpurea* which acts as antibacterial agents and it was supported by molecular docking studies. The *in silico* docking of gedunin with the DNA Gyrase showed the highest binding affinity and hydrophobic interaction with the amino acids of the active pocket. DNA gyrase is an essential bacterial enzyme that catalyzes the introduction of negative (−) supercoils into chromosomal and plasmid DNA. Gyrase was discovered soon after it was clear that *in vitro* recombination of bacteriophage λ required a negatively supercoiled DNA substrate. DNA Gyrase cleaves and transfers DNA to regulate DNA topology and are a major class of antibacterial and anticancer drug targets (Reece and Maxwell 1991). The 5 ligand molecules exhibited the antibacterial activity by hindering the function of DNA Gyrase. In earlier studies of Ravikumar and Thangaraj (2024), identification of phytochemicals in *Bougainvillea glabra* to assess their suitability for drug development. In this pursuit, they employed predictive models and computational tools to evaluate crucial pharmacokinetic parameters, bioavailability, and drug-likeness of the 36 phytochemicals

CONCLUSIONS

Ethyl acetate extract of *Claviceps purpurea* contains number of therapeutic antibacterial compounds like Aldicarb, Arecoline, Glimepiride, Gedunin and Pentobarbital. The antibacterial activity of result was in more in *Pseudomonas aeruginosa* (16.80±0.15mm). *In silico* docking studies also supported the inhibition of DNA Gyrase with the highest bonding efficiency and hydrophobic interaction. Due to unscientific overexploitation, many of the medicinal are becoming endangered. The harvesting of antibacterial compounds from the *in vitro* grown-up fungus *Claviceps purpurea* ethyl acetate extract is a better method to fight infectious microbial diseases. This extract is further use for *in vivo* studies of animals.

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Conflict of Interest. None.

ABBREVIATIONS

ADMET: Absorption, Distribution, Metabolism, Excretion and Toxicity; **AI:** Activity Index; **ANOVA:** Analysis of variance; **DMSO:** Dimethyl sulfoxide; **HR-LCMS:** High Resolution Liquid Chromatograph Mass Spectrometer; **MIC:** Minimum Inhibitory Concentration; **MS:** Murashige and Skoog; **RMSD:** Root Mean Square Deviation; **ZI:** Zone of inhibition.

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