Program Profile		
Program	Program name	**GC-MS based metabolic profiling and *In-vitro-In-silico* evaluation of *Phyllanthus niruri* phytochemicals for antibacterial potential and novel drug discovery**
	Category	A3

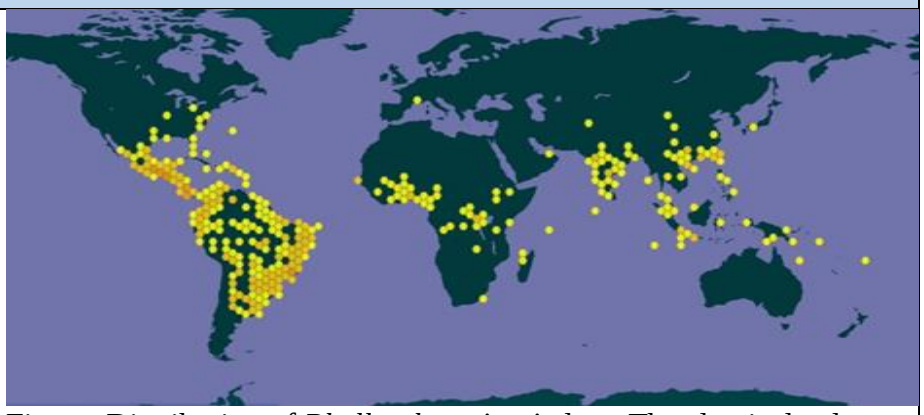
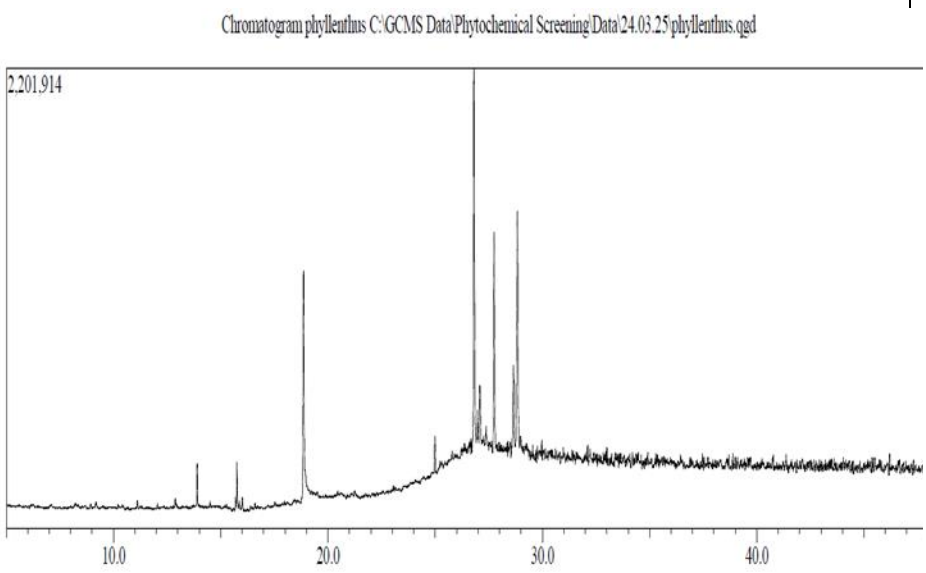
Summary of Program	
Program Name	**GC-MS based metabolic profiling and *In-vitro-In-silico* evaluation of *Phyllanthus niruri* phytochemicals for antibacterial potential and novel drug discovery**
Category	A3
Abstract of Program	The study aimed to explore the antibacterial potential of *Phyllanthus niruri* through both laboratory-based and computational analyses. Leaves of the plant were collected and extracted using methanol, then fractionated via the Kupchan method to separate compounds based on polarity. Preliminary phytochemical screening confirmed the presence of flavonoids and phenolics key bioactive groups known for their therapeutic potential. Gas chromatography–mass spectrometry (GC-MS) identified 75 chemical constituents in the methanol extract; many previously associated with antimicrobial effects. The antibacterial efficacy of the plant's various fractions was tested against nine bacterial strains using the disc diffusion method. The polar extracts, particularly methanol and ethyl acetate fractions, exhibited significant inhibitory activity against both Gram-positive and Gram-negative bacteria, most notably *Staphylococcus aureus* and *Escherichia coli*. In contrast, non-polar extracts showed negligible antibacterial action. To deepen the analysis, molecular docking simulations using PyRx were performed, revealing that certain phytochemicals demonstrated strong binding affinities with crucial bacterial enzymes like DNA gyrase and penicillin-binding proteins. These interactions suggest a potential mechanism of antibacterial action at the molecular level. Furthermore, pharmacokinetic and drug-likeness profiling using pkCSM and SwissADME tools indicated that the top-performing compounds have favorable absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties, along with good oral bioavailability. Overall, the study highlights *P. niruri*'s promise as a source of potent natural antibacterial agents, offering strong support for its traditional medicinal use and paving the way for future drug development initiatives targeting bacterial infections.

Details of Program		
Planning		
Objectives	Long-term Goals	**long-term program** grows from **compound identification → mechanistic studies → preclinical validation → drug development → clinical translation**, while also strengthening traditional medicine

		knowledge and contributing to the fight against antimicrobial esistance.
	Short-term Targets	the program targets GC-MS profiling of *Phyllanthus niruri*, antibacterial screening, and computational analyses to identify and validate potential drug-like compounds. In the long term, it aims to optimize promising leads, advance them through preclinical studies, and translate findings into patentable, plant-based antibacterial therapies that address antimicrobial resistance
	Rationale	The program is designed to profile *Phyllanthus niruri* through GC-MS, antibacterial screening, and computational analyses to identify drug-like compounds. In the long term, it aims to optimize promising leads, establish a phytochemical repository, and develop affordable plant-based antibacterial therapies to help combat antimicrobial resistance
Subject (Leader)	Initiator(s)	LABU, Zubair Khalid
	Champion(s)	KARIM SAMIRA, LABU ZUBAIR
	Major team member(s)	Dr. Samira Karim
Environment	Nature/Society	The study is relevant to pharmaceutical and biomedical sciences, focusing on discovering plant-derived antibacterial agents through experimental and computational methods. It benefits society by contributing to the fight against antibiotic resistance and promoting natural, accessible drug development pathways.
	Industry/Market	The study is relevant to the pharmaceutical industry, focusing on the discovery of natural antibacterial compounds for potential drug development. It aligns with market needs by offering plant-based alternatives to address antibiotic resistance and expand therapeutic options
	Citizen/Government	To support public health and reduce reliance on synthetic antibiotics, effective plant-based antimicrobials must be identified and validated. To inform government health strategies, such research encourages the integration of traditional medicine into affordable and sustainable healthcare solutions.
Resources	Human resources	To support teaching and learning methodology of the university therefore teaching faculties and three students involved in the program for further smooth conduction of the work
	Financial resources	Funding would be necessary for research development, and computational resources.
	Technological resources	Gas Chromatography (GC), Mass Spectrometry (MS), UV spectrophotometer, FTIR, Rotary evaporator, Lyophilizer
Mechanism	Strategy (Weight/Sequence)	The long-term strategy is to advance from compound identification and antibacterial validation of *Phyllanthus niruri* towards building a phytochemical repository, optimizing promising leads through preclinical studies, and developing patentable plant-based antibacterial therapies. This approach aims to integrate traditional

		knowledge with modern drug discovery to address antimicrobial resistance.
	Organization	Certainly, the university's structure supports the program's strategies by providing research facilities, ethical oversight, and collaboration platforms. This enables both short-term experimental work and long-term goals like lead optimization and drug development, ensuring alignment between institutional resources and program objectives.
	Culture	The university's culture supports the program by promoting collaboration, training, and integration of traditional knowledge with modern research.
Doing		
Launch date		October,2024
Responsible organization		World University of Bangladesh.)
Program content and process		This study explores the antibacterial potential of Phyllanthus niruri by identifying bioactive phytochemicals through GC-MS and validating their efficacy using both in vitro and molecular docking methods. The integration of experimental and computational approaches offers a comprehensive platform for drug discovery, allowing rapid screening of compounds, prediction of drug-likeness, and assessment of pharmacokinetic properties. The findings highlight compounds with promising interactions against key bacterial targets, supporting their potential as natural antibacterial agents. This work emphasizes the value of ethnomedicinal plants in developing cost-effective and sustainable therapies, particularly in the face of rising antibiotic resistance. The study provides a scientific foundation for future pharmaceutical development based on nature-derived compounds.
Key highlights of the content/process		• *Phyllanthus niruri* • GC-MS analysis • Antibacterial activity • *In vitro* and *in silico* evaluation • Molecular docking • Novel drug discovery.
Differences from traditional approaches		Unlike traditional approaches that rely mainly on empirical use of *Phyllanthus niruri*, this program integrates GC-MS profiling, antibacterial screening, computational analyses, and drug-likeness evaluation to scientifically validate and optimize bioactive compounds for potential drug development.
Progress as of today		Almost finish
Problems in implementation		Potential problems in implementation include limited access to advanced analytical and computational facilities, challenges in correlating experimental and in-silico results, and the complexity of translating bioactive compounds into safe, effective drug candidates. Additionally, high costs, regulatory hurdles, and limited infrastructure in some regions can hinder practical application

Approaches to solve the problems	These problems can be addressed by strengthening laboratory and computational infrastructure, fostering collaborations with specialized research centers, providing targeted training for researchers, and adopting a stepwise approach from experimental validation to preclinical optimization.
Completion date, if completed	Last of December, 2025
Seeing	
Impacts on students	The program will enhance students' skills in experimental techniques, computational analysis, and drug discovery, while fostering critical thinking, research collaboration, and exposure to translational science.
Impacts on professors	The program will enable professors to advance their research expertise, mentor students in cutting-edge experimental and computational methods, and contribute to translational drug discovery and publications.
Impacts on university administration	The program strengthens the university's research profile, promotes collaborations, and attracts funding through high-impact interdisciplinary studies.
Responses from industry/market	Not yet introduced with any industry for response
Responses from citizen/government	It has not yet been determined whether local citizens and the government are involved.
Measurable output (revenues)	• GC-MS based metabolic profiling (Identification of bioactive phytochemicals, molecular weight and chemical structure data) • *In vitro* antibacterial evaluation (Zone of inhibition in mm against bacterial strains, minimum inhibitory concentration and Comparative results with standard antibiotics • *In silico* Analysis (Docking scores, interaction details, and ADMET predictions).
Measurable input (expenses)	Measurable inputs include costs for GC-MS and laboratory consumables, bacterial culture materials, computational software licenses, training programs, and personnel support for research activities.
Cost-benefit analysis for effectiveness	The program's costs, including laboratory equipment, computational resources, and personnel, are justified by the potential benefits of discovering novel antibacterial compounds, enhancing student and faculty skills, increasing publications, and contributing to affordable plant-based therapies against antimicrobial resistance. **Costs:** • High investment in GC-MS, NMR, and computational tools • Skilled personnel required for data interpretation • Time-consuming validation through *in vitro and in silico* stages. **Benefits:** • Precise identification of active compounds, reducing trial-and-error • Early prediction of drug-likeness and toxicity via *in silico* tools

	• Reduced animal testing through computational modeling • Faster lead optimization compared to traditional ethnobotanical screening.
Future Planning	
Where does the project go from here?	In industry-based pilot projects.
Addendum	
Exhibits, pictures, diagrams, etc.	 Figure: Distribution of *Phyllanthus niruri* plant. The classical color (yellow and orange) hexagonal symbol indicates the distribution of PN on the world  Figure: Chromatogram of GC-MS analysis of *Phyllanthus niruri* leaf extract

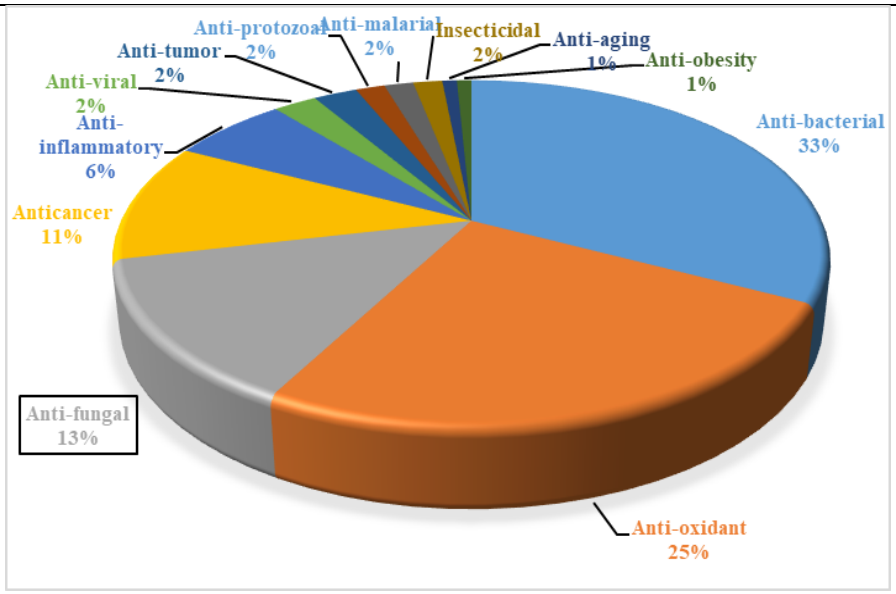


Figure: Distribution of Identified Compounds Based on Major Biological Activities

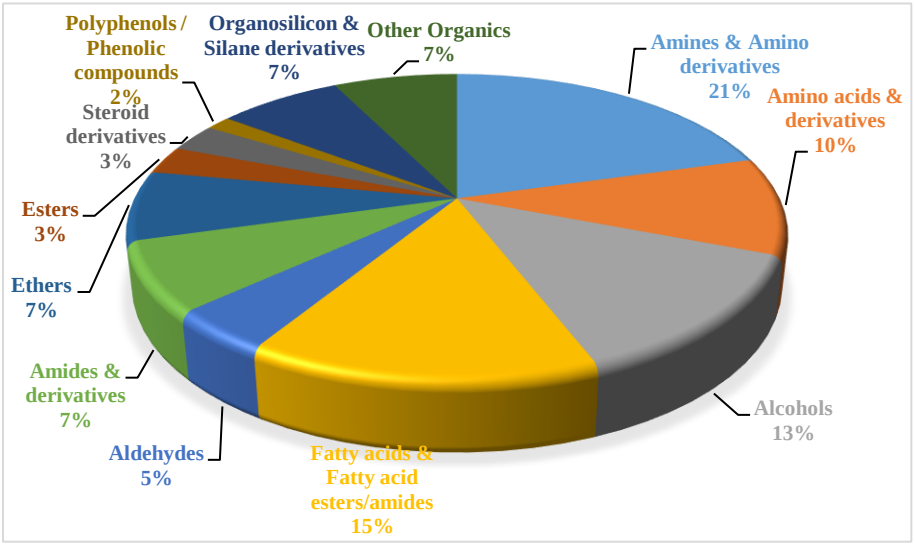
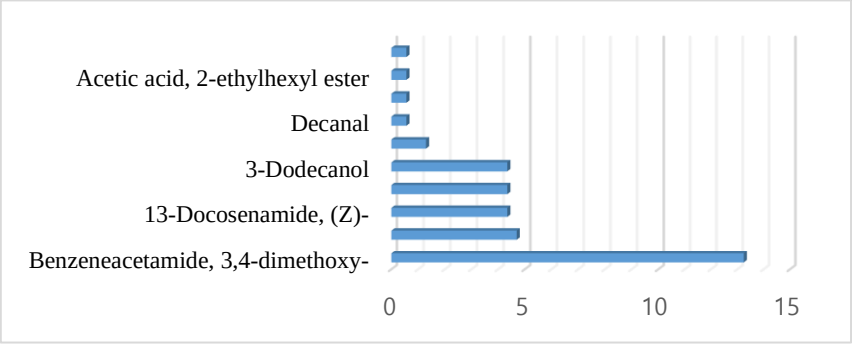


Figure: Chemical Classification of the identified compounds

	 Figure: Abundance of chosen compounds
Reports, mimeos, monographs, books, etc.	Expected outputs include research reports, mimeos, monographs, peer-reviewed journal articles, and reference books documenting the phytochemical and antibacterial studies of *Phyllanthus niruri*.
Others which may help explain the program (including website links)	Additional elements include workshops, seminars, collaborative projects, databases of phytochemicals, and digital resources to support research, training, and knowledge dissemination.