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Application Deadline: 29th FEB, 2024. INT'L VIRTUAL RESEARCH FELLOWSHIP ON ADVANCED GENOMICS AND BIOINFORMATICS

<u>Dive into Advance Genomics and Bioinformatics Research, and Transform</u> <u>Your Findings into Publishable Papers within 3 - 5 Months</u>

We envision inspiring and empowering life scientists to leverage **GENOMICS** AND BIOINFORMATICS to tackle critical challenges, drive innovation, and promote sustainable progress globally.

Research Domain: Therapeutics R&D (Multi-Omics) Research Focus: Anti-Malaria R&D Research Topic: To be crafted by the participant Research Aim: To be crafted by the participant Research Objectives: To be crafted by the participant

LEARNING OBJECTIVES

- **Comprehensive Understanding of Microbial and Plant-Derived Peptides:** Acquire in-depth knowledge of the structural and functional characteristics of peptides derived from microbial and plant sources, including their mechanisms of action and potential interactions with the malaria parasite.
- **Proficiency in Multi-Omics Techniques:** Develop the skills to employ multi-omics approaches, including genomics, proteomics, and metabolomics, to systematically analyze the biological pathways and molecular interactions associated with the selected peptides, providing a holistic understanding of their potential as anti-malarial agents.
- Application of Machine Learning in Drug Development: Gain practical expertise in utilizing machine learning algorithms for the analysis of complex biological datasets, enabling the identification of patterns, correlations, and predictive models to guide the rational design and optimization of anti-malarial peptides.
- In Silico Analysis and Docking Techniques: Gain proficiency in silico analyses of designed peptides, including the prediction of phytochemical properties, structure, and function. Develop skills in molecular docking techniques, exploring various software tools for drug target identification, ligand selection, and evaluation of results.
- **Craft Research Papers for Publication:** Learn how to synthesize and present your findings coherently, culminating in preparing research papers suitable for publication, contributing to the broader understanding of the therapeutic research and development of anti-malaria peptides.

EXPECTATIONS WHILE UNDERTAKING THIS FELLOWSHIP PROGRAM:

- Knowledge of Genomics and Bioinformatics: Develop a solid foundation in genomics and bioinformatics, including an understanding of key concepts, methodologies, and technologies used in the program
- **Proficiency in Data Analysis:** Gain proficiency in analyzing genomic data using bioinformatics tools and software. This includes skills in data preprocessing, quality control, data visualization, and statistical analysis.
- **Research Skills:** Acquire research skills for conducting genomics and bioinformatics studies. This includes formulating research questions, designing experiments, collecting and analyzing data, and interpreting research findings.
- Critical Thinking and Problem-Solving: Develop critical thinking skills to analyze complex genomic and bioinformatics problems and propose creative solutions. You would be able to evaluate scientific literature, identify research gaps, and contribute to the advancement of knowledge in the field.
- **Computational Skills:** Gain proficiency in software and applications commonly used in bioinformatics, such as Geneious software, web servers, etc. to analyze genomics data and interpret results
- **Communication Skills:** You would be able to effectively communicate your research findings and scientific concepts to both technical and non-technical audiences. This includes writing scientific reports, presenting research orally, and participating in scientific discussions and collaborations.
- **Collaboration and Teamwork:** Develop skills in collaborating with peers and professionals in multidisciplinary research teams. This includes effective communication, teamwork, and the ability to contribute constructively to group projects.
- **Professional Development:** You would be able to develop a professional mindset, including skills in time management, organization, and project management. They should also be aware of current trends and advancements in genomics and bioinformatics, and actively seek opportunities for professional growth and development.
- **Publication and Dissemination:** Contribute to the scientific community by publishing their research findings in peer-reviewed journals

CLASSES	TOPICS/FOCUS	SCHEDULE & DELIVERABLES
General Classes	Overview of genomics, bioinformatics, and their applications in various fields Understanding the central dogma of molecular biology Introduction to genomics technologies and data generation Data formats in Genomics and Bioinformatics (Practical) Internet tools and Databases (Practical on data retrieval, Blast etc.) Introduction to software tools and their installation, web servers, and pipeline tools (Practical), Basic Linux Command Line Interface	WEEK 1

PROGRAM OUTLINE AND SCHEDULE

	 sequence data relevant to malaria targets Utilize genomics and a bioinformatics tool called Antismash for predictive analysis. Apply these tools to diverse datasets to identify potential bioactive compounds that may serve as targets for anti- malaria 	
	Prediction of Biosynthetic Genes/Secondary Metabolites Using Bagel4 or Antismash: Identify potential biosynthetic genes and secondary metabolites in microbial, plant, or animal assemble	Deliverable: (Results)
	PHASE TWO Prediction of Discumptatic Conce/Secondary Matchelites	
	Go assignments, PGfam, Cripsr, etc.	
	Table 2: Construction of Chromosomal Genome Properties:CDS, Genes, RNA, Hypothetical Protein, Functional Protein,	Deliverable: (Results)
	Write Up 3: Functional Genome Annotation/Protein Identification	Deliverable: (Materials and Methods)
Comprehensive Genome Analysis	Functional Genome Annotation: Gene prediction, Protein features, Specialty features, Chromosomal properties, and Circus-view, among others.	WEEK 3
	the diverse data samples recovered from different data sources. Write Up 1 and 2: Reads Processing and Genome Assembly	-
	filter out low-quality reads to ensure reliable results. Genome Assembly: Assemble the whole genome sequence of the diverse data samples recovered from different data sources	
	Quality Control: Assess data quality, perform trimming, and	Deliverable: (Results)
	Table 1: Construction of General Sequence Properties: viadata table based on genome information which includesaccession number, raw data size, sources, geographical regionsplatform, genome type, layout, file types, etc.	Deliverable: (Materials and Methods)
	bioinformatics analyses crucial for the discovery and optimization of anti-malaria peptides.	
	natural sources, to initiate comprehensive genomics and	
Data Collection and Preprocessing	Raw Data Retrieval: Gather diverse raw data samples, encompassing microbial metagenomics and other pertinent	
	PHASE ONE	_
GENOMICS AND E	BIOINFORMATICS ANALYSIS	
PRACTICAL SE	ESSIONS	WEEK 2
	hypothesis in solving identified problems	_
	healthcare, industrial, and other life science research space The use of critical thinking and problem-solving tools to design a	-
	study Problem identification relative to the above area in the	-
	The experimental application of each of these in your field of	-
Specialized Classes	(Practical DNA, RNA and Protein samples)Introduction to Therapeutic Peptide R&D (Anti-Malaria)	
	Genomics Data and its Analysis using cutting-edge tools	

	Conduct functional analysis to understand the potential roles and	
	functions of the identified genes and metabolites in the context of	
	anti-malaria therapeutic peptide discovery	
	Write Up 4: Biosynthetic Gene Prediction or Prediction of Secondary Metabolites	Deliverable: (Materials and Methods)
Genomics and	Post-Prediction Result Analysis and Documentation	WEEK 4
Predictive Metabolite	Table 4: Table Construction for Predicted Biosynthetic	
Analysis	Genes/Secondary Metabolites that includes the following	
(Identification of	• Relevant features such as gene names, associated	
Biomarkers)	pathways, predicted metabolite structures, and any	
Diomai KCi Sj	relevant scores or probabilities	
	• Metadata details in the table, such as the source organism,	
	sample type (microbial, plant, or animal), and specific	
	datasets used	
	• Figure 1: Figure showing predicted biosynthetic genes/secondary metabolites with relevant figures.	
		WEEK 5
	PHASE THREE	
	Machine Learning-Based Therapeutic Peptide Prediction and Design: Each step in the machine learning-based therapeutic peptide prediction and design process contributes to the specificity, diversity, and customization of the designed peptides, fostering a more efficient and targeted drug development approach.	
	STAGE 1: AMP PREDICTION	
	CAMPR3 for AMP Collection: CAMPR3 serves as a specialized	
	machine-learning model for collecting of AMPs from biosynthetic genes, enhancing the specificity of peptide selection for further analysis	Deliverable: (Materials and Methods)
	 Prediction of One 99-Length AMP: Predict a single 99-length AMP with the highest probability across all models Breakdown to Twenty 20-length AMPs: Break down the prediction to identify twenty 20-length AMPs with the highest probability across the majority of models. 	
	NOTE: Predicting one 99-length AMP offers insights into the	
	characteristics of longer peptides while breaking down twenty 20-	
	length AMPs ensures diversity and practicality for experimental validation.	
	Write Up 5: Machine Learning-Based Therapeutic Peptide	
	Prediction and Design	
	Table 5: Containing the predicted AMPs for each category (99 and20)	
	STAGE 2: ACTIVITY-BASED PEPTIDE	
	RECONSTRUCTION AND FUNCTIONAL PREDICTION	
	Reconstructed predicted AMPs from CAMPR3, emphasizing	WEEK 6
PREDICTION AND	antimalarial activity, to generate novel peptides with	
DESIGNING OF	enhanced therapeutic potential	
THERAPEUTIC PEPTIDES WITH	 Prioritized parameters such as SVM scores, N & C terminus preferences, and other details during the redesign process. 	
MACHINE LEARNING	Write Up 6: Activity-based Peptide Reconstruction and	Deliverable: (Materials
	Functional Prediction	and Methods)

	Table 6: Contained the reconstructed peptides and parameters of the activities of each peptide	Deliverable: (Results)
	PHASE FOUR	WEEK 7
In Silico Characterization of Designed Therapeutic Peptides	 Phytochemical properties of designed therapeutic Peptides, in silico prediction of structure & function of the peptide. Hydrophobicity (numbers or ratio) Number of G and p Negative or Positive Net charge Molecular formula Boman Index Experimental Verification of peptide using BLAST Estimated half-life Predicted peptide toxicity Cell penetration and others Instability Index, Aliphatic index, Grand average of hydropathicity (GRAVY) 	Deliverable: (Results)
	Write Up: Phytochemical Properties and In Silico Prediction of Peptide Structure and FunctionalVisualization of all Peptide/Phytochemical Results (Tables and Figures for All or Most of the Phytochemical Properties)	Deliverable: (Materials and Methods) Deliverable: (Results)
	PHASE FIVE	
Computational Drug Design/Molecular Docking	 The Application of drug design and discovering therapeutic peptide Molecular Docking: Drug target identification and retrieval Ligand selection of leads hits, and retrieval Pharmacokinetics analysis and Lipinski rule of 5 Exploring software used for docking, their peculiarities, similarities, and differences Protein preparation and ligand preparation process Exploring docking types based on protein structure: rigid-rigid, rigid-flexible, protein-ligand, protein-protein, protein-DNA Docking analysis using different software like Pymol, Ds visualizer, etc. 	WEEK 8 & 9
	Write Up: Drug Design and Molecular Docking Evaluation and Visualization of Results	Deliverable: (Materials and Methods) Deliverable: (Results)

RESEARCH PROJECT OUTLINE FOR PUBLICATION

Introduction	BTW WEEK 6 -7
Materials and Methods	WEEK 9
Results	WEEK 10 and 11
Discussion	WEEK 12
Conclusion	WEEK 12

References	
Certification and Recommendation Letter	WEEK 13
Follow up and Publication	