



# **ACEMFS FUT Minna Bioinformatics Workshop**

## **Introduction to Bioinformatics Training**

**Itunuoluwa Isewon PhD**  
Covenant University



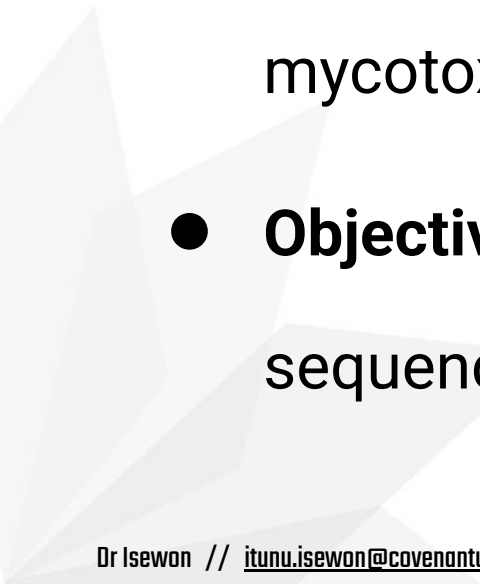
# CAPIC-ACE

- Covenant Applied Informatics and Communication Africa Centre of Excellence (CAPIC-ACE) domiciled at Covenant University
- Mission: dedicated to building indigenous capacity through training in Computer Science, Bioinformatics, Chemistry, Biology and ICT to reduce the disease burden in Africa.
- Role in this workshop: Providing support, guidance, and networking for participants.



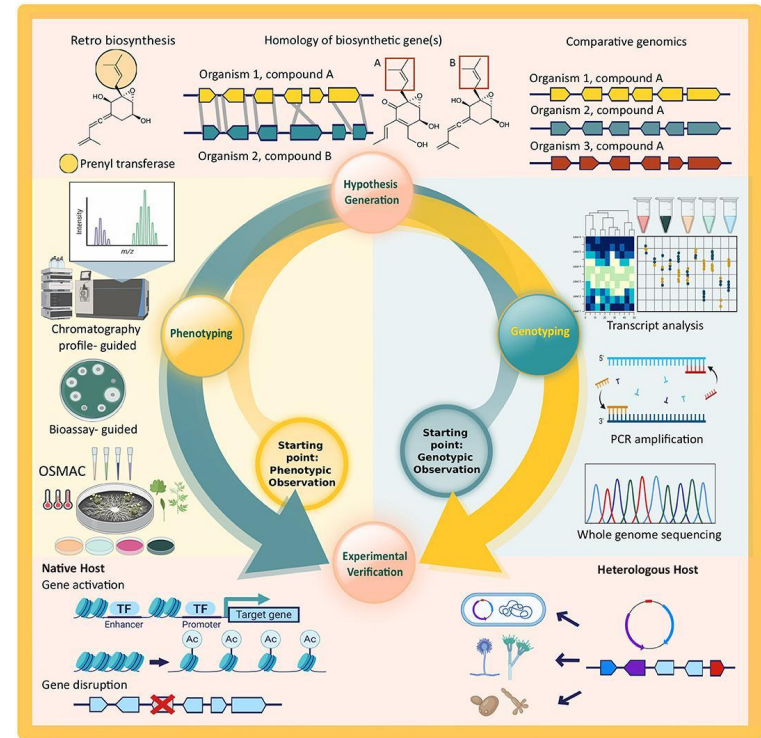
# Workshop Overview



- 3-day hands-on training
  - **Focus:** Bioinformatics for mycology and mycotoxicology research
  - **Objective:** Equip participants with foundational skills for sequence analysis and structural bioinformatics.
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# What is Bioinformatics?

- **Definition:** Application of computational and statistical techniques to understand biological data.
- **Importance:** Handles large-scale genomic and molecular data.
- **Example:** Analyzing fungal genomes for mycotoxin biosynthesis genes.



<https://doi.org/10.3389/fbioe.2021.649906>

# Bioinformatics in Mycology



- Bioinformatics as a tool to study fungi
- Applications in fungal identification and genome analysis
- Detecting pathogenic and industrially important fungi



Article | Published: 24 November 2021

# ***Aspergillus fumigatus* pan-genome analysis identifies genetic variants associated with human infection**

[Amelia E. Barber](#), [Tongta Sae-Ong](#), [Kang Kang](#), [Bastian Seelbinder](#), [Jun Li](#), [Grit Walther](#), [Gianni Panagiotou](#)

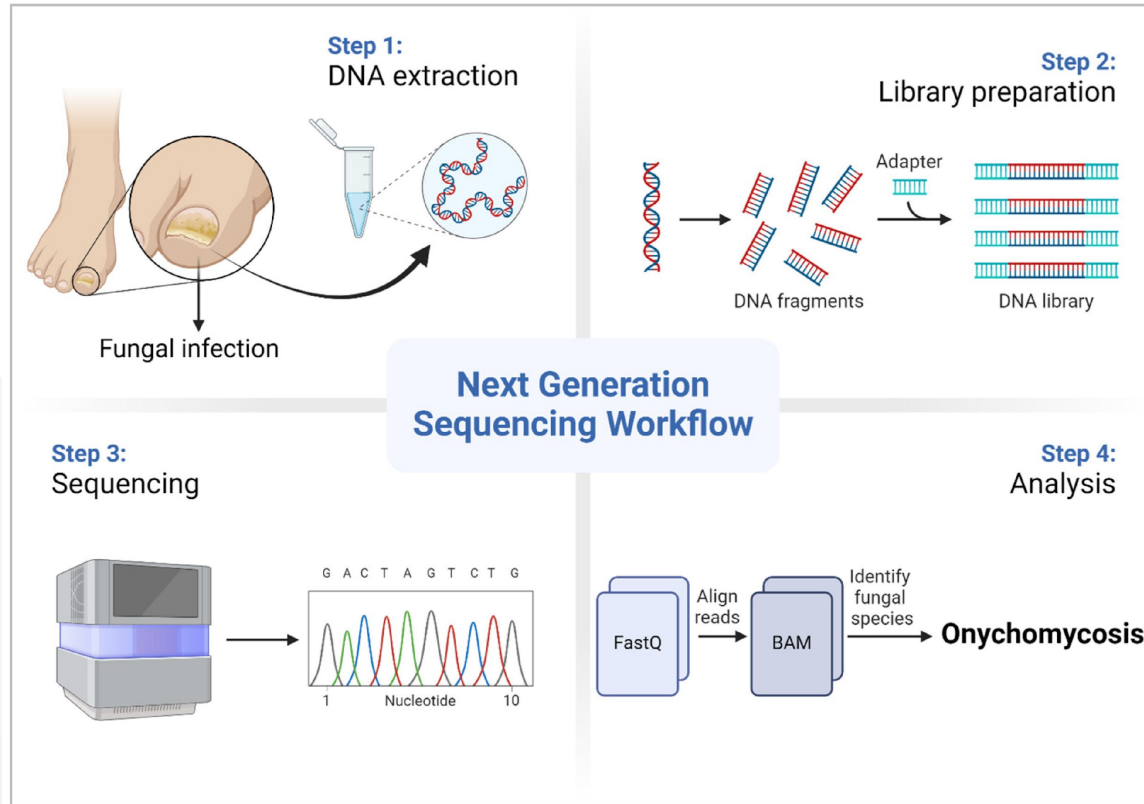
✉ & [Oliver Kurzai](#) ✉

[Nature Microbiology](#) **6**, 1526–1536 (2021) | [Cite this article](#)

**9711** Accesses | **100** Citations | **240** Altmetric | [Metrics](#)

<https://doi.org/10.1038/s41564-021-00993-x>

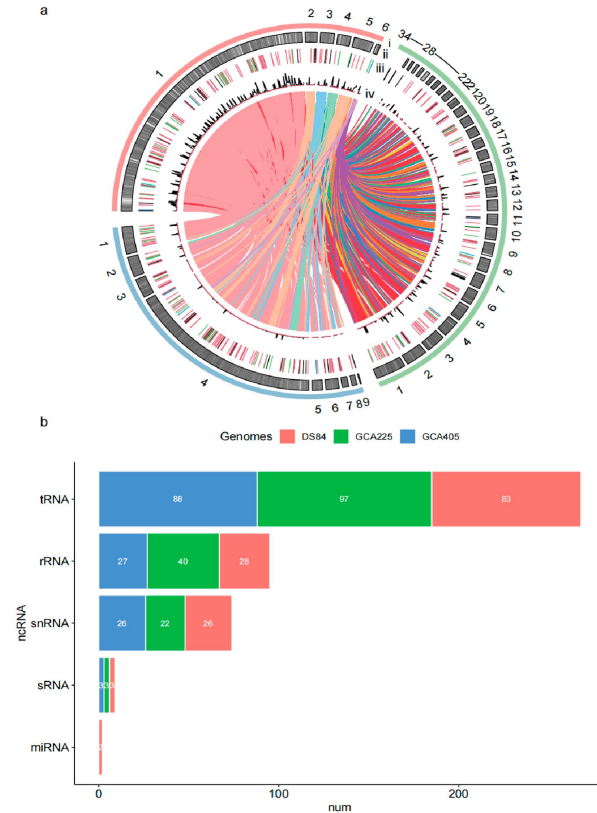
# Fungal Genome Sequencing



<https://doi.org/10.3390/diagnostics14151664>

# Comparative Genomics in Fungi

- Comparing genomes across strains/species
- Identification of conserved and variable regions
- Detecting genes involved in toxin biosynthesis
- Case study: *Aspergillus flavus* vs. *Aspergillus parasiticus*

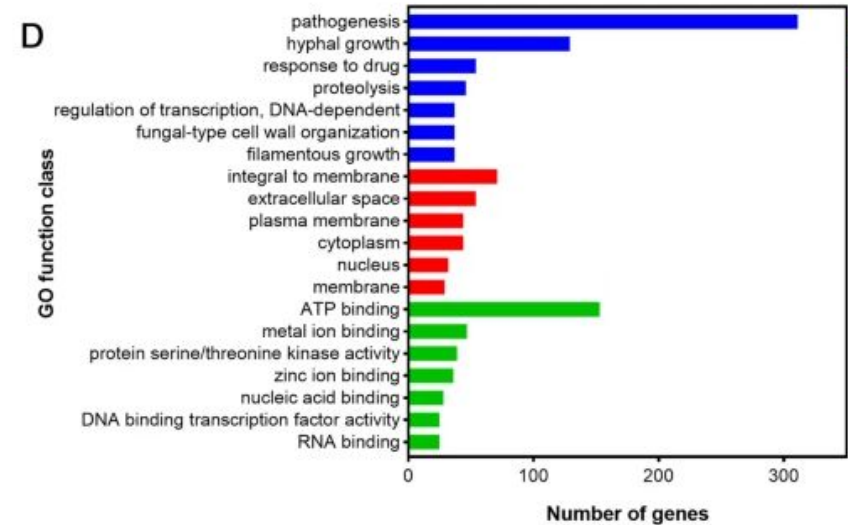


<https://doi.org/10.3390/jof9101022>



# Functional Annotation of Fungal Genes

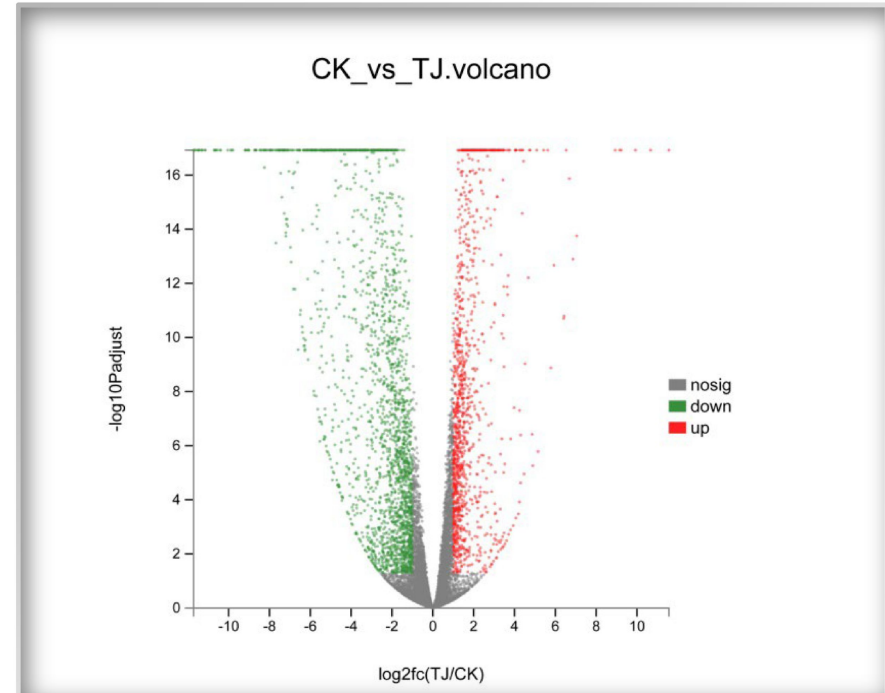
- Predicting gene function using bioinformatics
- Gene ontology and pathway mapping
- Tools: InterProScan, BLAST, KEGG
- Relevance to mycotoxin pathway discovery



<https://doi.org/10.1186/s40246-023-00512-5>

# Transcriptomics in Mycology

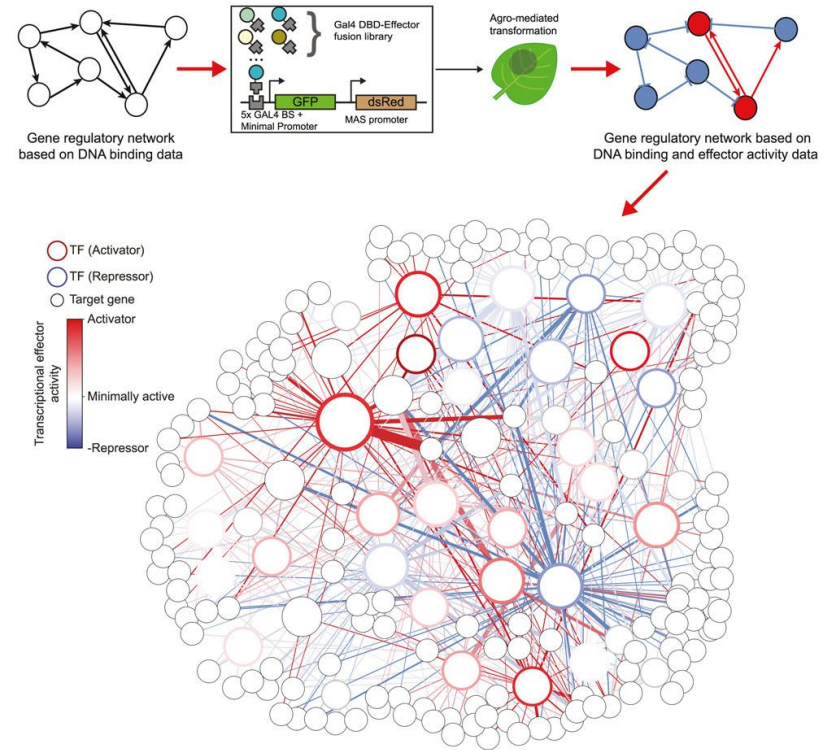
- RNA-seq for studying gene expression
- Detecting genes activated under stress or toxin-producing conditions
- Example: Upregulation of aflatoxin biosynthesis genes
- Tools: HISAT2, featureCounts, DESeq2



<https://doi.org/10.3390/jof9121193>

# Regulatory Networks in Fungi

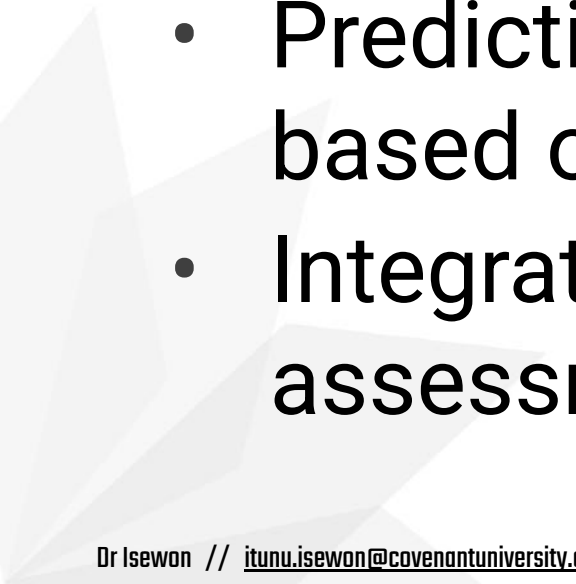
- Gene regulatory networks controlling toxin production
- Transcription factors and secondary metabolite clusters
- Visualizing networks: Cytoscape and co-expression analysis



<https://doi.org/10.1016/j.cels.2023.05.002>

# Bioinformatics in Mycotoxicology: Overview



- Linking fungal genomics to toxin production
  - Predicting mycotoxin potential based on gene content
  - Integrating omics data for risk assessment
- 

# Detection of Mycotoxin-Producing Fungi

- Using genome and transcriptome data to identify toxin producers
- Marker genes for aflatoxins, fumonisins, ochratoxins
- Case study: *Aspergillus flavus* detection in stored grains

## Machine Learning for Predicting Mycotoxin Occurrence in Maize



Marco Camardo Leggieri



Marco Mazzoni



Paola Battilani\*

Department of Sustainable Crop Production, Università Cattolica del Sacro Cuore, Piacenza, Italy

<https://doi.org/10.3389/fmicb.2021.661132>

# Predicting Toxin Production

- Correlating gene presence with observed toxin levels
- Using bioinformatics pipelines for secondary metabolite prediction
- Tools: antiSMASH, SMURF, PRISM

Use of predictive modelling as tool for prevention of fungal spoilage at different points of the food chain

[sonia Marín<sup>1</sup>](#) , [Luísa Freire<sup>2</sup>](#), [Antoni Femenias<sup>1</sup>](#), [Anderson S Sant'Ana<sup>2</sup>](#)

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<https://doi.org/10.1016/j.cofs.2021.02.006>

## Bioinformatic Analysis of Secondary Metabolite Biosynthetic Potential in Pathogenic *Fusarium*

by [Chao Lin<sup>1</sup>](#), [Xi-long Feng<sup>1</sup>](#) , [Yu Liu<sup>1</sup>](#), [Zhao-chen Li<sup>1</sup>](#), [Xiu-Zhang Li<sup>2</sup>](#) and [Jianzhao Qi<sup>1,\\*</sup>](#) 

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<sup>2</sup> State Key Laboratory of Plateau Ecology and Agriculture, Qinghai Academy of Animal and Veterinary Sciences, Qinghai University, Xining 810016, China







\* Author to whom correspondence should be addressed.

<https://doi.org/10.3390/jof9080850>




# Transcriptomic Analysis for Toxin Regulation

- RNA-seq to monitor expression of toxin biosynthesis genes
- Differential expression under different environmental conditions
- Visualizing results: heatmaps, volcano plots, PCA

Transcriptome analysis reveals the mechanism of tolerance to copper toxicity in the white rot fungus *Trametes hirsuta* AH28-2

Chenkai Wang <sup>a b c</sup>, Kun Wu <sup>a b c</sup>, Na Pang <sup>a b c</sup>, Huifang Zhao <sup>a b c</sup>, Shenglong Liu <sup>a b c</sup>,  
Xinlei Zhang <sup>a b c</sup>, Yazhong Xiao <sup>a b c</sup>  , Zemin Fang <sup>a b c</sup>  ,  
Juanjuan Liu <sup>a b c</sup>  

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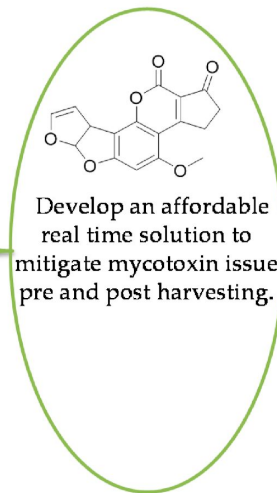
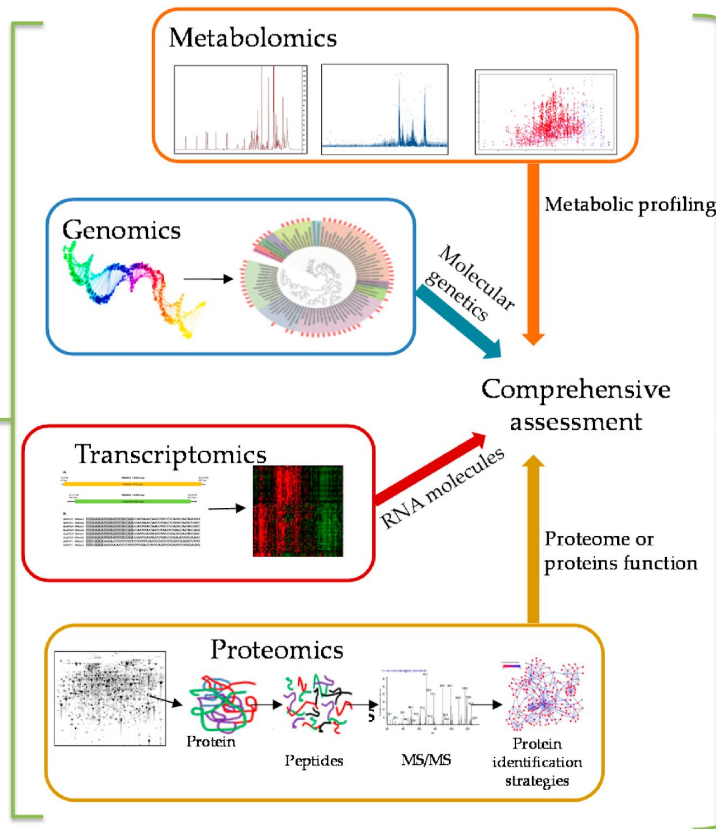
<https://doi.org/10.1016/j.ecoenv.2025.118194>



# Integrating Multi-Omics Data



Mycotoxin contamination



<https://doi.org/10.3390/toxins10110433>



# Key Benefits of Bioinformatics in Mycotoxin Research



- Rapid identification of fungal strains and toxin potential
- Predicting secondary metabolite production pathways
- Understanding regulatory networks for toxin biosynthesis
- Designing targeted interventions or detection assays

# Training Objectives



Understand  
bioinformatics concepts  
and databases



Perform sequence  
quality control and  
alignment



Conduct differential gene  
expression analysis



Visualize genomic and  
structural data



Apply computational  
tools to mycotoxin  
research

# Day 1 Plan: Genomics & Sequence Analysis



Time	Session	Details
9:00 – 9:30	<b>Welcome &amp; Overview</b>	Workshop objectives, introduction to bioinformatics, relevance to mycotoxin research
9:30 – 10:30	<b>Introduction to Biological Databases</b>	NCBI, ENA, UniProt, PDB, Ensembl, KEGG – how to search, download, and interpret
10:30 – 11:00	Break	
11:00 – 12:30	<b>Sequence Retrieval &amp; Quality Control (Galaxy)</b>	Tool: FastQC; Dataset: Mycotoxin-related fungal genome from ENA
12:30 – 1:30	Lunch	
1:30 – 3:00	<b>Sequence Alignment &amp; BLAST</b>	Tool: BLAST (via Galaxy); Task: Homology search for mycotoxin biosynthesis genes
3:00 – 4:30	<b>Primer Design for Gene Targeting</b>	Tool: Primer3 (via Galaxy or Primer-BLAST); Task: Design primers for a conserved gene

# Day 2 Plan: Phylogeny, Biostatistics & Transcriptomics



Time	Session	Details
9:00 – 10:30	<b>Phylogenetic Tree Construction</b>	Tool: Clustal Omega , MEGA
10:30 – 11:00	Break	
11:00 – 12:30	<b>Biostatistics in R for Omics Data</b>	Tool: RStudio (cloud or local); Task: Volcano plots, boxplots, PCA
12:30 – 1:30	Lunch	
1:30 – 3:00	<b>Transcriptomic Data Analysis: RNA-Seq</b>	Tools: Galaxy RNA-seq workflow – HISAT2, featureCounts
3:00 – 4:30	<b>Differential Expression Analysis in Galaxy</b>	Tools: DESeq2; Task: Fold change and volcano plots using example dataset (e.g., stress response in <i>Aspergillus</i> )

# Day 3 Plan: Structural Bioinformatics



Time	Session	Details
9:00 – 10:30	Recap of Day 1 and Day 2 Activities	-----
10:30 – 11:00	Break	
11:00 – 12:30	<b>Introduction to Protein Structure &amp; Databases</b>	Tools: RCSB PDB, UniProt, AlphaFold; Visualizers: PyMOL or ChimeraX
12:30 – 1:30	Lunch	
1:30 – 3:00	<b>Ligand Preparation and Protein-Ligand Binding</b>	Tools: AutoDock Vina, Chimera; Dataset: Mycotoxin + fungal enzyme PDB structure
3:00 – 4:00	<b>Wrap-up: Tools Integration &amp; Project Ideas</b>	Group discussion: Apply tools to participants' own datasets or design mini-projects
4:00 – 4:30	<b>Certificates &amp; Feedback</b>	Evaluation, group photo

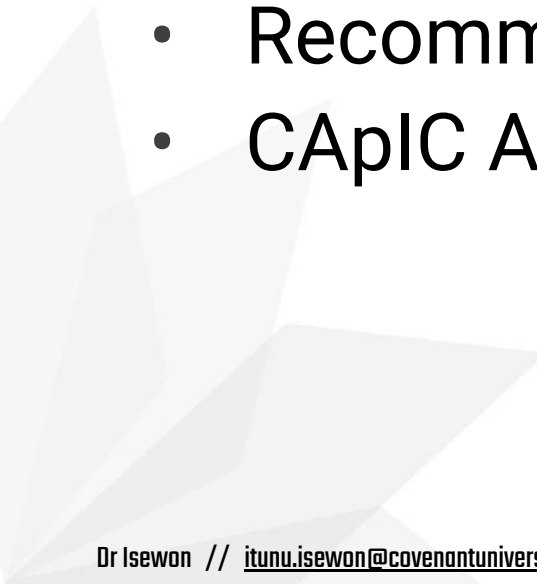
# Expected Outcomes for Participants



- Practical skills in sequence and transcriptomic analysis
- Ability to use Galaxy , MEGA and R for mycotoxin research
- Understanding structural bioinformatics basics
- Confidence to start independent projects

# Post-Training Resources



- Access to Galaxy workflows and R scripts
  - Recommended readings and databases
  - CApIC ACE support and networking
- 

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# **Closing & Questions**

## **Recap of Objectives and Day Plans**