ACEMFS FUT Minna Bioinformatics Workshop

Introduction to Bioinformatics Training

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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.

https://bit.ly/ACE_IBT25_PreCourse

Pre Workshop Survey

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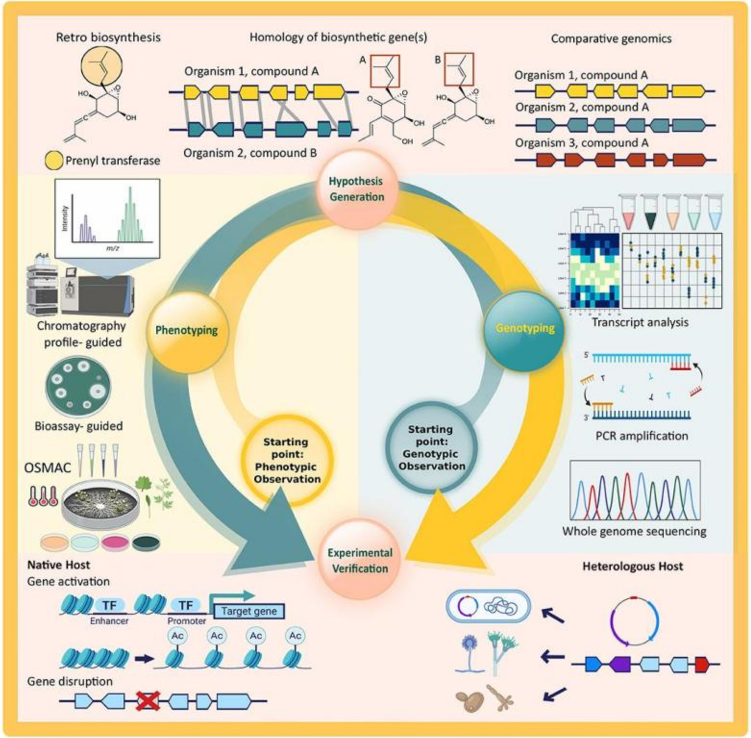
What is Bioinformatics?

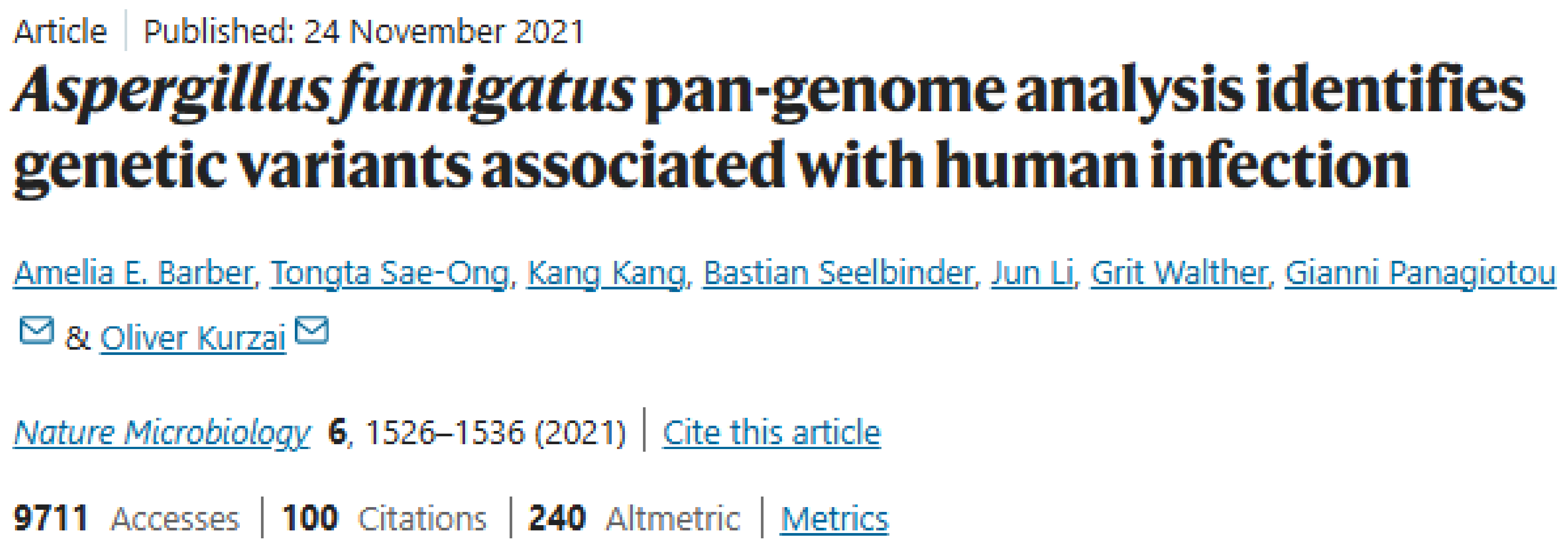
- **Definition:** Application of computational and statistical techniques to understand biological data.
- **Importance:** Handles large-scale genomic and molecular data.
- **Example:** Analyzing fungal genomes for mycotoxin biosynthesis genes.



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

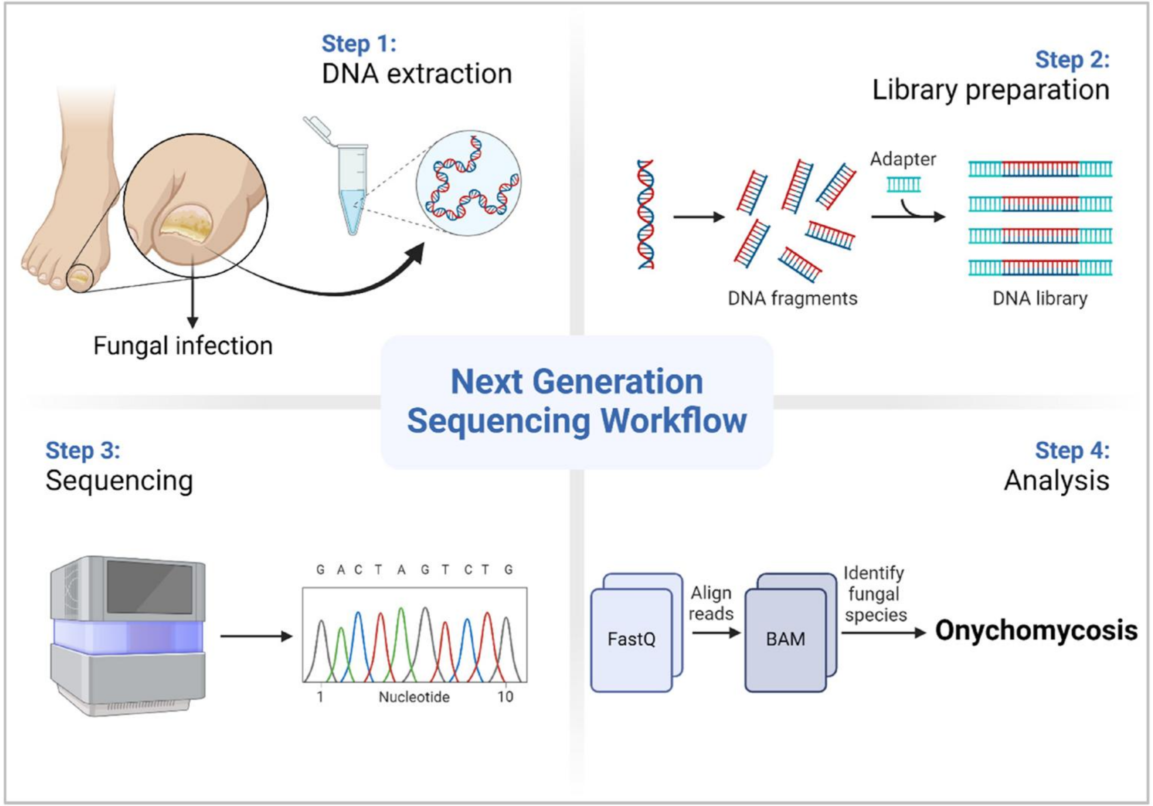
Amelia E. Barber, Tongta Sae-Ong, Kang Kang, Bastian Seelbinder, Jun Li, Grit Walther, Gianni Panagiotou ✉ & Oliver Kurzai ✉

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

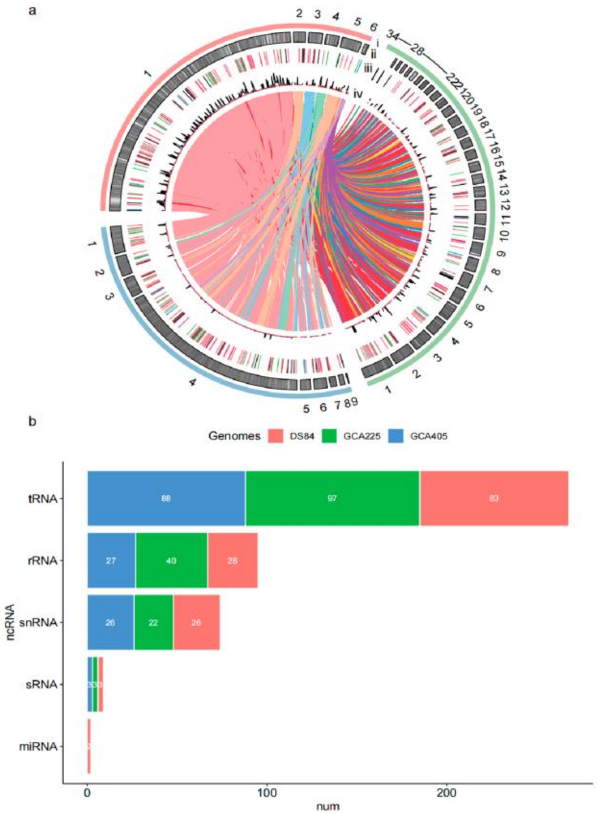
Fungal Genome Sequencing



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

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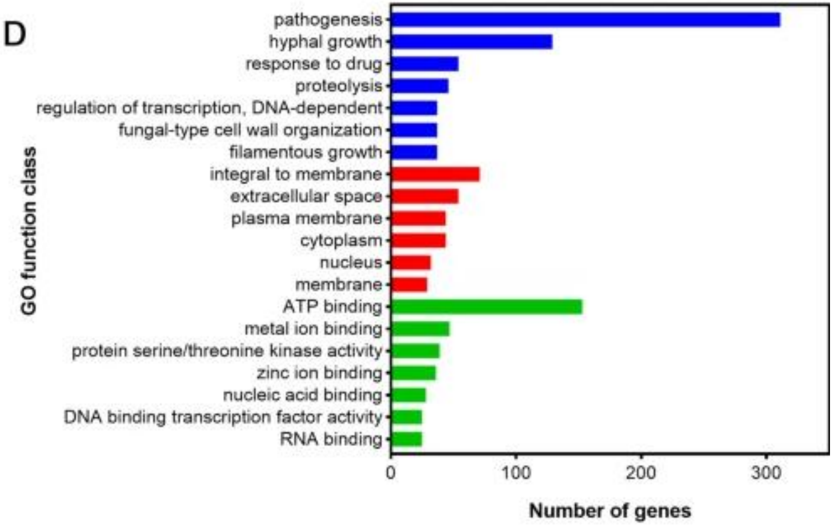
Functional Annotation of Fungal Genes

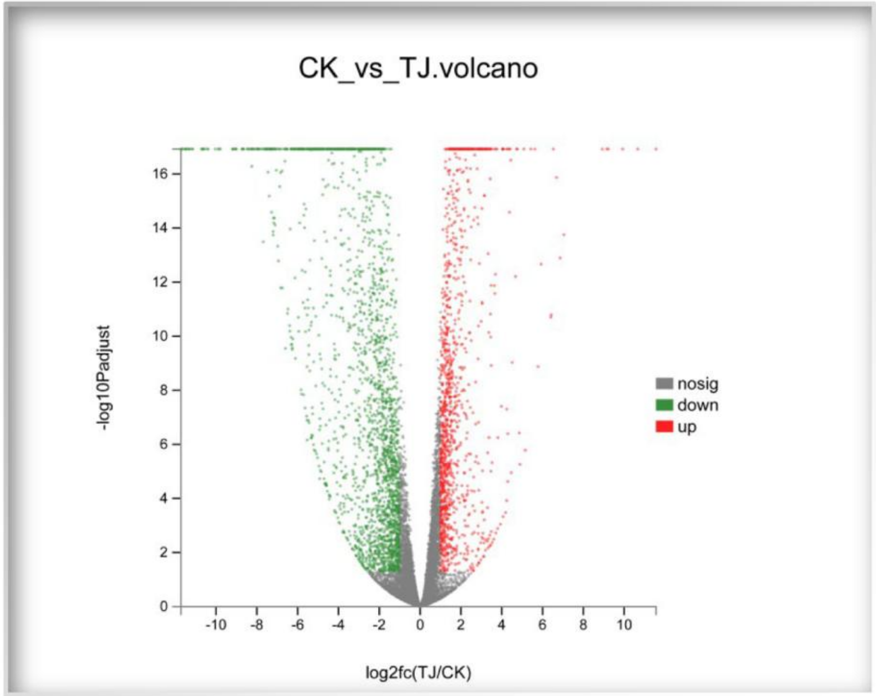
- Predicting gene function using bioinformatics
- Gene ontology and pathway mapping
- Tools: InterProScan, BLAST, KEGG
- Relevance to mycotoxin pathway discovery



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

Transcriptomics in Mycology

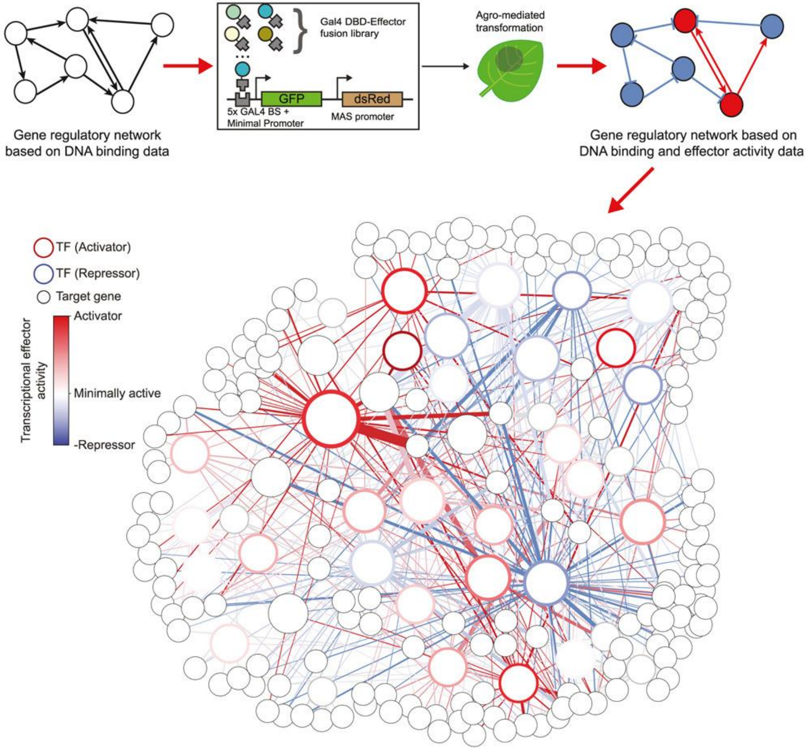
- RNA-seq for studying gene expression
- Detecting genes activated under stress or toxin-producing conditions
- Example: Upregulation of aflatoxin biosynthesis genes
- Tools: HISAT2, featureCounts, DESeq2



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[1] ✉, Luísa Freire[2], Antoni Femenias[1], Anderson S Sant'Ana[2]

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

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

by Chao Lin[1], Xi-long Feng[1], Yu Liu[1], Zhao-chen Li[1], Xiu-Zhang Li[2] and Jianzhao Qi[1,*] ✉

[1] Shaanxi Key Laboratory of Natural Products & Chemical Biology, College of Chemistry & Pharmacy, Northwest A&F University, Yangling, Xianyang 712100, China

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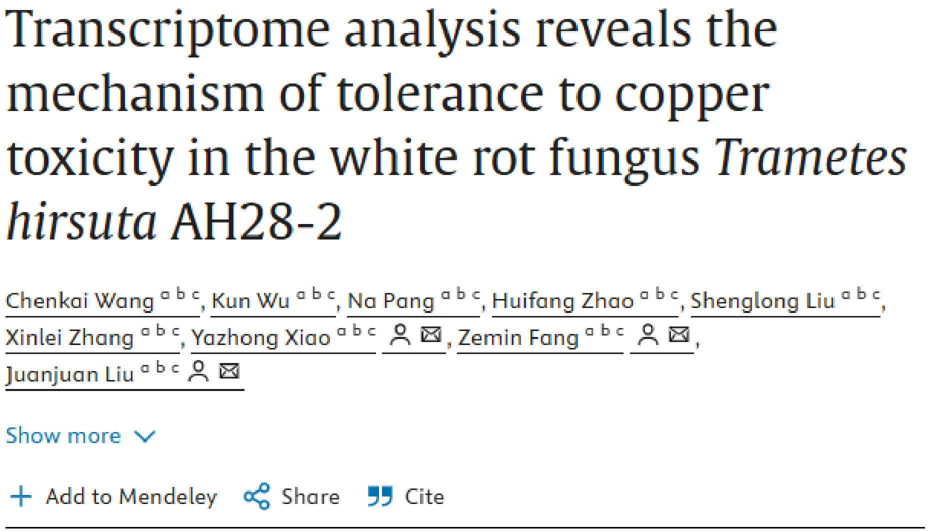
https://doi.org/10.3390/jof9080850

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

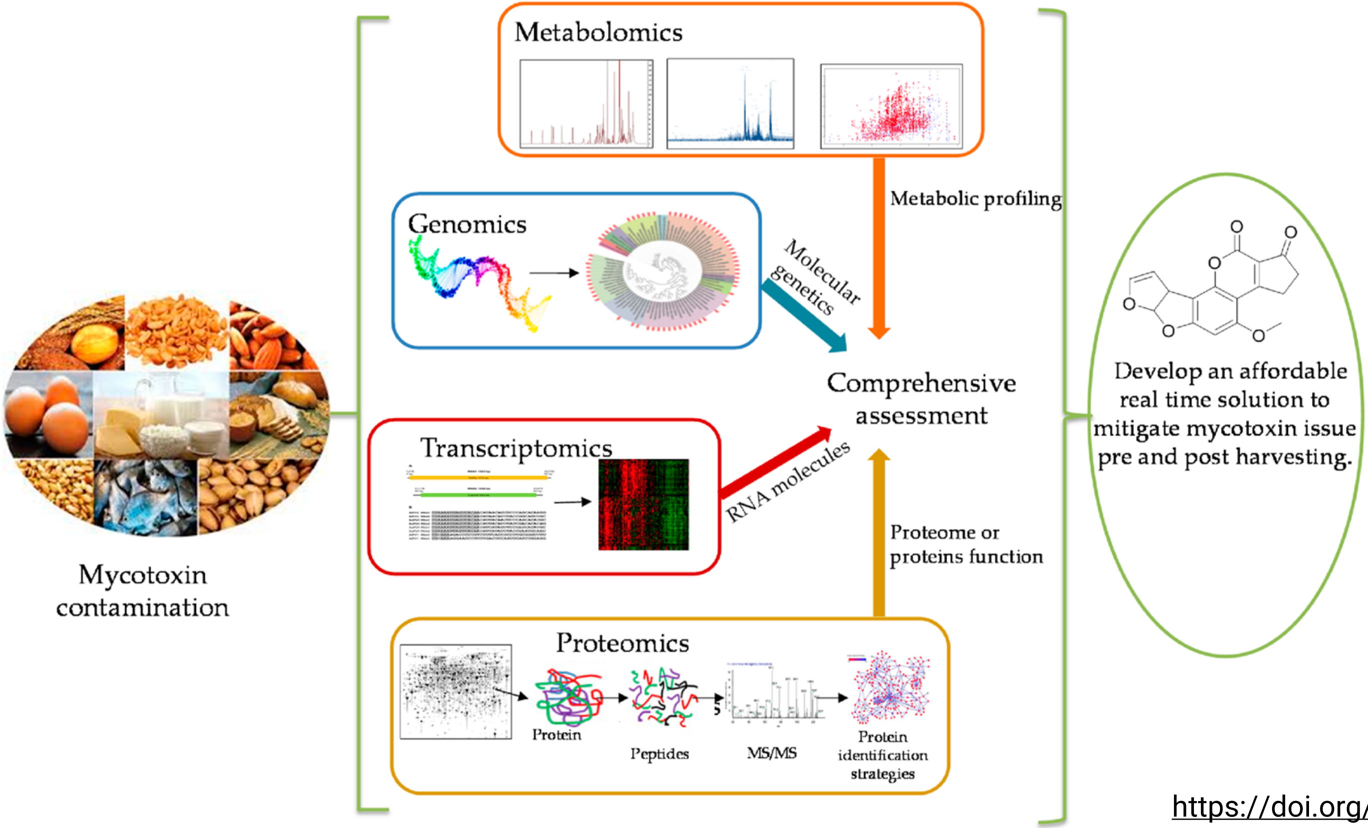


Transcriptome analysis reveals the mechanism of tolerance to copper toxicity in the white rot fungus *Trametes hirsuta* AH28-2

Chenkai Wang [a b c], Kun Wu [a b c], Na Pang [a b c], Huifang Zhao [a b c], Shenglong Liu [a b c], Xinlei Zhang [a b c], Yazhong Xiao [a b c], Zemin Fang [a b c], Juanjuan Liu [a b c]

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

Integrating Multi-Omics Data



Develop an affordable real time solution to mitigate mycotoxin issue pre and post harvesting.

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

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Facilitators

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Day 1 Plan: Genomics & Sequence Analysis

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

Day 2 Plan: Phylogenetics, Biostatistics & Transcriptomics

Time	Session	Details
9:00 – 09:30	Recap of Day 1 Activities	
9:30 – 10:30	**Phylogenetic Tree Construction**	Tool: Clustal Omega , MEGA
10:30 – 11:00	Break	
11:00 – 12:30	**Biostatistics in R for Omics Data**	Tool: RStudio ; Task: Statistical tests and Visualizations
12:30 – 1:30	Lunch	
1:30 – 3:00	**Transcriptomic Data Analysis: RNA-Seq**	Tools: Galaxy RNA-seq workflow – HISAT2, featureCounts
3:00 – 4:30	**Differential Expression Analysis in Galaxy**	Tools: DESeq2; Task: Fold change and volcano plots using example dataset

Day 3 Plan: Structural Bioinformatics

Time	Session	Details
9:00 – 10:30	Recap of Day 1 and Day 2 Activities	
9:30 – 10:30	**Introduction to Protein Structure & Databases**	Tools: RCSB PDB, UniProt, AlphaFold; Visualizers: PyMOL or ChimeraX
10:30 – 12:00	**Ligand Preparation and Protein-Ligand Binding**	Tools: AutoDock Vina, Chimera; Dataset: Mycotoxin + fungal enzyme PDB structure
12:00 – 1:00	Lunch	
1:00 – 2:50	**Mini - Project Implementation**	
2:50 – 3:30	**Presentation of Mini-Projects**	
3:30 – 4:00	**Wrap-up: Tools Integration & Project Ideas**	Group discussion: Apply tools to participants' own datasets or design mini-projects
4:00 – 4:30	**Certificates & Feedback**	Evaluation, group photo

Group Mini Projects

- Genomics
- Phylogenetics
- Transcriptomics

https://bit.ly/ACE_IBT25

Course Page

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

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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