AG2PI
Agricultural Genome to Phenome Initiative

WORKSHOP

Water dynamics from molecular structure to phenotype

This workshop will introduce how to utilize protein structural information and sequencing data to predict the hydration phenotype of different organisms. First, participants will familiarize with the crystal structures of photosynthetic proteins and learn what a protein structure and its 3D folding can mean in terms of water dynamics. We will then walk the audience through the steps of a pipeline from sequences to phenotypic data. During the workshop, participants will also learn how to use the Multi-Conformation Continuum Electrostatics (MCCE) a biophysics simulation program developed at Gunner Lab at CUNY that combines continuum electrostatics and molecular mechanics.

For a full MCCE documentation and downloads: https://gunnerlab.github.io/Stable-MCCE/

*This workshop is a product of an AG2PI seed grant.

Presenters:

Benjamin Romanjenko is a first year Ph.D. student for the Botany Department at the University of Wyoming. Ben works to understand the effect of water limitations on photosynthetic proteins structure and activity which impacts whole plant physiology.

Jose Ortiz-Soto is a first year Ph.D. student at the City College of New York (CUNY) interested in computational simulations of electron and proton transfers in proteins using Monte Carlo sampling and network analysis.

Marilyn Gunner is a Physics Professor at CUNY and a Fellow of the American Physical Society. Her research interest is in molecular biophysics, particularly when and where electrostatic interactions are important in proteins structure.

Carmela Rosaria (Lina) Guadagno is an Associate Research Scientist at the University of Wyoming working on plant-environment interactions. She is particularly interested in characterizing cross-scale biophysical processes to enhance the mechanistic relevance of current phenotyping methods.

April 25, 2023

12:00 PM - 2:00 PM

(Central Time, UTC–5)

Purpose:
Describe how molecular dynamics can affect phenotypes and provide a pipeline for this type of analysis in plants.

Register for this Zoom virtual workshop:
https://tinyurl.com/AG2PI-w19

Upon registration, you will receive a confirmation email with information about joining the meeting.

A recording will be available at a later date at: **www.ag2pi.org.**

Registration is not required to view the recording.

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