



## 2018 PlantSEED METABOLIC MODELING WORKSHOP BROCHURE

A two-day workshop on plant genome annotation, metabolic modeling and reconstruction comprising formal lectures and hands-on instruction, will be held at **Northwestern University, Evanston, IL from the 16<sup>th</sup> to the 17<sup>th</sup> of August 2018**. The workshop content is of interest to computational scientists associated to agriculture and biology departments as well as plant scientists interested in metabolic modeling including plant breeders, geneticists, physiologists and biochemists. **The workshop is free of charge.**

### PROGRAM

#### WORKSHOP AIMS

- Be familiar with the capabilities of the PlantSEED database and its suite of comparative genomics tools.
- Be equipped for use of the PlantSEED and related platforms like STRING to annotate genes and use subsystems to predict functions for genes.
- Be able to use advanced PlantSEED functions that increase the efficiency of GENE ANNOTATION and allow the user to focus on particular genes and genomes.
- Generate metabolic reconstruction models by mapping between annotations and reactions.
- Perform GAP FILLING and connect the curation of gapfilling results with existing external tools (e.g. KEGG, PlantCyc).
- Do FLUX BALANCE ANALYSIS and use modeling to analyze plants metabolism.
- Give examples of problem solutions in sandbox models

#### RELATED INFORMATION

- For more background please read the following manuscripts:

Orth JD, Thiele I, Palsson BØ (2010) What is flux balance analysis? *Nat Biotechnol.* 28(3):245-8.

doi: 10.1038/nbt.1614.

PMID:20212490

Oberhardt MA, Palsson BØ, Papin JA (2009) Applications of genome-scale metabolic reconstructions.

*Mol Syst Biol.* 5:320.

doi: 10.1038/msb.2009.77.

PMID:19888215

Seaver SM, Gerdes S, Frelin O, Lerma-Ortiz C, *et al* (2014) High-throughput comparison, functional annotation, and metabolic modeling of plant genomes using the PlantSEED resource. *Proc Natl Acad Sci U S A.* 111: 9645-50.

doi: 10.1073/pnas.1401329111.

PMID: 24927599

Seaver SM, Bradbury LM, Frelin O *et al* (2015) Improved evidence-based genome-scale metabolic models for maize leaf, embryo, and endosperm. *Front Plant Sci.* 6:142.

doi: 10.3389/fpls.2015.00142.

PMID: 25806041

#### TEAM OF EXPERT INSTRUCTORS

**Dr. Christopher Henry** and **Dr. Samuel Seaver** (Argonne National Laboratory and the Computation Institute of the University of Chicago)

**Dr. Donald McCarty** (Horticultural Sciences Department, University of Florida)

#### LOGISTICS

- The workshop takes two full days (9 am to 4 pm with an hour break for lunch). It will combine formal instruction and individual hands-on tuition. Participants should plan to attend for the whole two days. This

schedule is not final. We might alter it slightly, following the development of the workshop and the participants needs.

### **Day 1: Annotation and modeling of plant genomes in PlantSEED**

- A. Introduction to PlantSEED
  - a. What is PlantSEED?
  - b. What public genomes and datasets are available?
  - c. How was the data derived?
  - d. What tools are available?
  - e. How is user data managed and shared?
- B. Annotation of transcripts (Learn about signature k-mers and FIGFams)
  - a. Introduction and tour of PlantSEED subsystems and reference genomes
  - b. Overview of PlantSEED signature k-mers and FIGFams
  - c. Tools for submission of sequences for annotation and viewing results
- C. View and Comparison of PlantSEED annotations
  - a. Tour of PlantSEED genome viewer, including annotation overview and genome feature pages
  - b. Tools for comparison of PlantSEED annotation between two genomes/transcripts
  - c. Upload, annotation, and comparison of sequences from multiple fasta files
- D. Introduction to metabolic modeling
  - a. What is a metabolic model?
  - b. What is flux balance analysis?
  - c. How are models useful?
  - d. Overview of how annotation maps to reactions
- E. Interactive Walkthrough of PlantSEED using Sandbox Model
  - a. Users will construct own copy of a sandbox model
  - b. Users use the PlantSEED interface to explore the sandbox model
  - c. Users will run flux balance analysis on sandbox model
  - d. Users will run gapfilling on sandbox model
  - e. Users will edit the sandbox model and associated genome

### **Day 2: Application of models to understand and discover plant biology**

- A. Demonstration of model applications with sandbox model
  - a. Predicting essential genes and reactions
  - b. Finding a missing or erroneous annotation
  - c. Identifying the pathways responsible for producing a particular compound
  - d. Simulating transcriptome data to predict flux
  - e. Integrating plant and microbial models
- B. Question and answer session
- C. Application of full genomes, transcriptomes, and models to answer biological questions
  - a. Users apply PlantSEED tools to aid their own research

### **CLASSROOM**

The workshop will be held in room

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which has the necessary technical support (projectors, extensions, power outlets near desks).

**Participants need to bring their personal computers** (either OS X or Windows 10 operating systems with Firefox or Chrome installed).

## REQUIREMENTS

To benefit from the course, applicants need:

- To have some familiarity with the NCBI, detecting sequence homology via alignment phylogenetic analysis.
- To be acquainted with the biochemistry available in KEGG and Plant Metabolic Networks and phylogenetic gene trees in Gramene/ Ensembl and Phytozome.
- Participants will be required to choose a plant from the Phytozome platform:  
<https://phytozome.jgi.doe.gov/pz/portal.html>

and load their own set of gene or transcript sequences in the workshop registration webpage, three weeks before the workshop. If the participant has a special set of plant gene or transcript sequences, which the participant wants to use for the workshop, he/she may consult with Dr. Henry ([chrishenry@gmail.com](mailto:chrishenry@gmail.com)) about this possibility, at least a month before the workshop.

-Some lectures may be recorded and later posted to our website.

## APPLICATION PROCEDURE, DEADLINES AND PARTICIPANTS SELECTION

- The workshop can only accommodate up to 20 participants coming from Northwestern and Chicago Universities as well as other colleges and universities. Faculty as well as postdocs and graduate students may participate.

-Candidates wishing to participate in our workshop should fill the “PlantSEED Workshop Application Form” (PSWA form) found at:

<https://www.dropbox.com/s/p2hfm3de0p9ctoij/Application%202018Plant%20workshop.docx?dl=0>

no later than the 1<sup>st</sup> of June and send it with to [clerma@ufl.edu](mailto:clerma@ufl.edu)

-Applicants will be selected in a first-arrive, first-served basis as well as their qualifications descriptions in order not to exceed 20 subscriptions. Accepted participants will receive an acceptance email and a detailed workshop/travel general guide. Later a set of instructions about registration, choosing a plant genome and loading it in PlantSEED will be supplied.

**-It is very important to apply as soon as possible, so you can make your hotel and airplane reservations in a timely manner, that is, as soon as you are approved to register.**

Remember the workshop is free of charge.

## TRAVEL EXPENSES REFUNDS

- Up to **\$1,000** for travel, food and lodging expenses will be awarded only to **three faculty members** who work at a minority serving institution and are chosen by the panel. To qualify for funding, applicants need to fulfill the following requirements:

1) To be an American citizen or Permanent Resident of the USA.

2) To be a **faculty** member of a US College or University that is registered as **Minority Serving Institution**. If you are unsure about your college being this kind of institution go to:

<https://www2.ed.gov/about/offices/list/ocr/edlite-minorityinst.html>

-These refunds will be paid through the University of Florida and since it takes some time to process the paperwork, the later ought to be completed at least **a month before the workshop starts**. Hence the applications need to be processed with a great deal of anticipation.

- The information included in the PSWA form will allow our coordination panel to screen the applications to ensure that the selected participants have the background needed to benefit most from the workshop. This information will also be used to fill up the statistics report required by the NSF.

If you have other questions regarding our workshop syllabus, please contact Dr. Sam Seaver at:

[samseaver@gmail.com](mailto:samseaver@gmail.com). If you have questions about the application process, please contact Dr Claudia Lerma-Ortiz at: [clerma@ufl.edu](mailto:clerma@ufl.edu).

