

## MASTER THESIS OFFER OF CEPLAS

*(FOR COMPUTATIONAL MASTER STUDENTS FROM TECHNICAL UNIVERSITY OF MADRID, UPM)*

### Title of Master Thesis

Kinetic modelling of terpene synthase in specialised cells of tomato

### Description of student's tasks

The goal of this project is to understand the developmental patterns of terpenes accumulation in tomato by building kinetic model of terpene synthesis.

**Why?** Because terpenes are considered high valuable compounds as they play essential role in the survival strategies of plants against biotic attacks, in defense against pathogens and herbivores, and in attracting pollinators. There are two major pathways leading to their production and a large family of structurally related enzymes involved in the synthesis. We would like to understand the interplay between these pathways and the dynamics better.

**How?** For this you will develop a kinetic computational model of terpene biosynthesis inside specialized cells of a tomato, called glandular trichomes. Because of the specialized function of terpenes, their biosynthesis in plants is usually restricted to specific tissues, including trichomes, a diverse epidermal structures covering the surface of a large number of plant species. All glandular trichomes are characterized by the ability to produce, secrete and store large quantities of specialized metabolites. You will learn i) how to extract essential information for a model construction from experimental omics data, e.g. gene expression analysis of terpene metabolism-related genes and ii) how to construct an ordinary differential equations based mathematical model of plant metabolism. Ideally, using the model you will accurately simulate the difference in the accumulated terpenes between young and mature leaf trichomes. The experimental data necessary for such work has been recently published [1] and the modeling environment is provided by the modelbase, an in-house developed modeling software fully integrated with Python programming language [2].

References:

[1] Zhou and Pitchersky (2020) *New Phytologist* 226: 1341–1360, doi: 10.1111/nph.16431

[2] van Aalst, Ebenhöh and Matuszyńska (2020) BioRxiv, doi: <https://doi.org/10.1101/2020.09.30.321380>

**Prerequisites** (*languages, informatics skills, bioinformatic skills, other knowledge, etc*)

Programming skills required, preferentially in Python  
Strong understanding of calculus (in particular solving systems of ordinary differential equations)  
Genuine interest in plant biology and biochemistry is advantageous  
Working language: English

**Training Project**

The integration of mathematical modeling and experimental techniques continues to emerge as a powerful approach for improving our understanding of the regulation of metabolic pathways. Through this project you will get acquainted with a set of tools, methods and theories necessary for a construction of a computational model capable of simulating the dynamics of biochemical pathways. Suggested project will cover topics that will prepare you both for an academic career as well as improve/provide skills highly valuable in the industry such as data analysis and programming.

Through this project you will get familiar with the working environment at German research institution, and you will have an opportunity to work with an international group of scientists. You will have a chance to apply your academic knowledge to a real, biological problem and further train your analytical and computational skills.

A successful implementation of the proposed mathematical model will be the prerequisite to share this work in a form of a scientific publication of the first generation kinetic model of terpene synthesis in glandular trichomes of tomato. Hence, for students already considering further academic career, it may be a strategic project to embark on.

**Activities that will be performed in the academic internship/Master Thesis:**

You will learn how to develop kinetic model of a biochemical pathway and will be trained in different types of kinetic modeling analysis, namely time-course simulation, steady-state analysis, and Metabolic Control Analysis (MCA).



You will work according to the Good Scientific Practice, keeping track of your computational work using gitlab, a version control software. We will learn together how to construct mathematical models in compliance with the Minimal Information Requested in the Annotation of Biochemical Models (MIRIAM) guidelines for annotating biochemical models.

As the member of the Institute you will have a chance to attend weekly group seminar and also deliver two presentations during their (virtual) stay: an introductory one and a final, summarizing the project.

Support in preparing the master thesis in Latex, a high-quality typesetting system designed for the production of technical and scientific documentation, will be offered.

<b>Nº of positions offered:</b>	<b>1</b>
<b>Has the student dealings with underage persons?</b>	<b>NO</b>
<b>Starting date:</b>	<b>Feb 2021</b>
<b>End date:</b>	<b>Jul 2021 (possible extension till Sep 2021)</b>
<b>Weekly hours</b> ( <i>only for internship in CEPLAS lab</i> ):	
<b>Working hours</b> ( <i>only for internship in CEPLAS lab</i> ):	
<b>Fellowships</b> ( <i>if any, NOT REQUIRED</i> ): <b>Remuneration</b> (€/month):	
<b>Academic tutor</b> (UPM/CBGP): <i>(you need a Tutor from UPM Master, not involved in the research activity)</i> <b>Email:</b>	
<b>Department/Research Group of UPM/CBGP</b> <b>Academic tutor:</b>	
<b>CEPLAS Internship/Master Thesis Tutor/Director:</b>	<b>Dr. Anna Matuszyńska</b>
<b>Email CEPLAS tutor:</b>	<b>Anna.matuszynska@hhu.de</b>
<b>Department CEPLAS tutor:</b>	<b>Institute for Quantitative and Theoretical Biology</b>
<b>Location of the internship (telecommuting?):</b>	<b>Heinrich Heine University Düsseldorf possible telecommuting</b>



<b>CEPLAS Institution:</b>	<b>Heinrich Heine University Düsseldorf</b>
<i>To be completed by Internship Office ETSIAAB-UPM:</i> <b>Number of ECTS (Nº ECTS):</b>	

Send by email to: [international.cbgp@upm.es](mailto:international.cbgp@upm.es) (Pablo Gómez)