



POLITÉCNICA



E.T.S. DE INGENIERÍA AGRONÓMICA,
ALIMENTARIA Y DE BIOSISTEMAS

Título de las prácticas:

Development of a computational pipeline for protein-ligand docking and virtual drug screening

Descripción de las funciones del alumno

The student will participate in the EU-ERANET Suscrop project FruitFlow (<https://www.suscrop.eu/projects-second-call/fruitflow>). The main objective of FruitFlow is the development of climate-smart technologies to predict and promote flowering and fruit production and attenuate the negative impact of global warming on EU agricultural sustainability and food security, with a special focus on two highly economically important fruit crops in north-eastern (apple) and southern EU countries (peach).

Biostimulant chemicals that promote budbreak and flowering have been widely used in fruit tree management; however, the first generation of chemicals has been reported to show high risk for human health and new generation of bio-stimulants (plant metabolites) would be extremely useful for maintaining and enhancing fruit crop productions in Mediterranean and mild winter areas, while reducing chemicals. Furthermore, the identification of protein target of this bio-stimulants will result in the identification of novel genetic variants and genes that will be available for breeding programs to better adapt apple and peach cultivars to future climatic scenarios.

The student will contribute to develop activities for the work package 3 of FruitFlow:

To identify metabolites and their putative target proteins involved in dormancy cycle control in apple and peach. A metabolomics approach will determine metabolites differentially accumulated during dormancy-cycle and between two apple and peach cultivars displaying contrasted bud break dates. In parallel, a proteomics approach will isolate potential target proteins of these metabolites. Combining metabolomics, proteomics, computational virtual screening and protein-ligand docking, we will define metabolite (ligand)-protein interactions that could be involved in dormancy-cycle regulation. These identified metabolites and proteins, named Dormancy Associated Metabolites (DAMEs) and Target Proteins of DAME (TP-DAME).

Requisitos: *(indicar titulación y curso); otros requisitos adicionales (idiomas, informática, otros conocimientos, etc).*

Computational Biology Master Student
Experience in Structural Bioinformatics
Skills with programming languages



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Proyecto formativo

Módulo PRACTICAS EXTERNAS. El objetivo fundamental de las Prácticas Externas es guiar al alumno para que aplique en el mundo real los conocimientos que ha adquirido previamente en un entorno de trabajo en grupo que reproduzca de una manera realista las condiciones que se puede encontrar en su futuro lugar de trabajo. El estudiante podrá familiarizarse con el mundo laboral (horarios, responsabilidad, actitud, organización, etc), y con la metodología de trabajo adecuada a la realidad profesional, contrastando y aplicando los conocimientos académicos adquiridos.

Actividades a desarrollar en la práctica académica:

- To design and apply a computational pipeline for the identification of potential bio-stimulants and their protein target from metabolomic and proteomic data previously obtained from apple and peach flower buds.
- To perform protein modeling, computational protein-ligand docking calculation of selected targets. Identification of interaction key features.
- Pull down assays to test *in vitro* interaction of selected protein-ligand candidates
- Testing biostimulant potential of discovered metabolites using *in vitro* plants.

Nº de plazas:	1
¿El alumno tendrá trato habitual con menores?	NO
Fecha de inicio:	Febrero 2022
Fecha de fin:	Junio 2022
Horas semanales:	20 h
Horario jornada laboral:	A convenir con el estudiante



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Importe Ayuda/Bolsa de estudio:	€/mes
Tutor académico:	Dra Maria Garrido Arandia email: maria.garrido@upm.es
Email:	Dr. Mariano Perales email: mariano.perales@upm.es
Departamento tutor académico:	Biotecnología y Biología Celular
Tutor empresa:	
Email tutor empresa:	
Departamento tutor empresa:	
Ubicación de la estancia de las practicas	Centro de Biotecnología y Genómica de Plantas UPM – INIA Parque Científico y Tecnológico de la U.P.M. Campus de Montegancedo Autopista M-40, Km 38 - 28223 Pozuelo de Alarcón (Madrid)
ENTIDAD COLABORADORA:	
A cumplimentar por Oficina Prácticas ETSIAAB:	
Créditos a reconocer (Nº ECTS):	

Enviar por email a: OFICINA DE PRÁCTICAS ACADEMICAS EXTERNAS – ETSIAAB
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